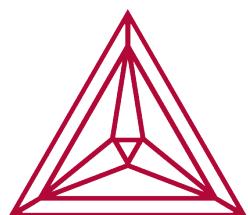


Thermo-Calc Console Mode Example Macros

Thermo-Calc Version 2023b



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Calculation of the Fe-C binary phase diagram.

[tce02](#)

Plotting thermodynamic functions

[tce03](#)

Calculating an isothermal section using the Ternary module

[tce04](#)

Calculating the miscibility gap in the Fe-Cr system.

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Calculating a vertical section in the Al-Cu-Si system

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The As-Ga phase diagram: Plotting the partial pressures of a gas species

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Note the following examples are deprecated:

- tce45, tce46, tce47, and tce50 are deprecated as of Thermo-Calc version 2019b

- tce25 and tce40d are deprecated as of Thermo-Calc version 2022a

Pitting Resistance Equivalence (PRE) for a duplex stainless steel.

tce_x29

Calculating the speciation of a gas

tce_x30A

Scheil calculation for an Al-4Mg-2Si-2Cu alloy

tce_x30B

Scheil calculation for an Al-4Mg-2Si-2Cu alloy

tce_x31

Using the GES module to calculate CVM

tce_x32

Calculating oxide layers on steel

tce_x33

Benchmark calculation for Fe-Cr-C isopleth

tce_x34

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tce_x35

Calculating a potential diagram using the POTENTIAL module.

tce_x36a

Assessment. The use of the PARROT module

tce_x37

Calculating an Isothermal Section

tce_x38

Calculating the Morral *rose*

tce_x39

Calculating reversible Carnot cycles of a heat engine

tce_x40

Working with the POURBAIX module.

tce_x41

Calculation of a solubility product

tce_x42

Paraequilibrium calculation - Formation of Para-pearlite - Isopleth

tce_x43

Paraequilibrium calculation - Formation of Para-pearlite - Isothermal

tce_x44

Exploring variables and functions.

tce_x48

Scheil solidification with C "back diffusion"

tce_x49

Quasichemical model using the GES module

tce_x51

Calculation of molar volume, thermal expansivity, and density.

tce_x52

Changing the excess models for interaction parameters in a solution phase

tce_x53

Some Pourbaix diagrams

tce_x54

Simulating the solidification of a Al-2.1Cu-1Si alloy with a Scheil calculation including back diffusion

tce_x55

Plotting viscosity of Cr-Ni at 1873 K

tce_x56

Plotting Surface Tension of Cu-Zr at 1373 K

tce_x57

Calculating a Scheil with Solute Trapping Solidification in a Al-Si-Cu system

tce_x58

Calculate volumetric thermal expansion coefficients of the L12-type Al₃Sc.

tce59

Calculate volumetric thermal expansion coefficients of the L12-type Al3Zr.

tce60

Calculate the electrical resistivity (ELRS) and thermal conductivity (THCD) from FCC_A1 to liquid.

Results

tce01

SYS:About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

```
SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce01\tce01.TCM"
SYS: set-echo
SYS:
SYS: @@ Calculation of the Fe-C binary phase diagram.
SYS:
SYS: @@ This example calculates the binary Fe-C phase
SYS: @@ diagram using the Binary module.
SYS:
SYS: set-log ex01,,
SYS:
SYS: @@ The log file is set to get command echo.
SYS: @@ The menu is shown by typing a question mark "?"
SYS: ?
... the command in full is HELP
ABOUT          HP_CALCULATOR      SET_INTERACTIVE_MODE
BACK           INFORMATION        SET_LOG_FILE
CLOSE_FILE     MACRO_FILE_OPEN   SET_PLOT_ENVIRONMENT
DISPLAY_LICENSE_INFO OPEN_FILE      SET_TC_OPTIONS
EXIT            SET_COMMAND_UNITS SET_TERMINAL
GOTO_MODULE    SET_ECHO          STOP_ON_ERROR
HELP            SET_GES_VERSION

SYS: @@ When you give a command the program may ask questions.
SYS: @@ You may obtain help for each question by typing a ? .
SYS: @@ If you accept the default answer suggested /within slashes/
SYS: @@ just press "return"
SYS: info
... the command in full is INFORMATION
FILE SYSTEM ERROR          37
*** ERROR 1717 IN MOPEN: FILE DOES NOT EXIST: c:\jenkins\workspace\generate_console_examples\unite\distribution\help\sysmon.hlp
ERROR          1717  RESET
SYS: ?
... the command in full is HELP
ABOUT          HP_CALCULATOR      SET_INTERACTIVE_MODE
BACK           INFORMATION        SET_LOG_FILE
CLOSE_FILE     MACRO_FILE_OPEN   SET_PLOT_ENVIRONMENT
DISPLAY_LICENSE_INFO OPEN_FILE      SET_TC_OPTIONS
EXIT            SET_COMMAND_UNITS SET_TERMINAL
GOTO_MODULE    SET_ECHO          STOP_ON_ERROR
HELP            SET_GES_VERSION

SYS:
SYS:
SYS:Hit RETURN to continue
SYS: @@ For a binary phase diagram calculation we use the binary module
SYS: go
... the command in full is GOTO_MODULE
MODULE NAME: ?
NO SUCH MODULE, USE ANY OF THESE:
SYSTEM_UTILITIES
GIBBS_ENERGY_SYSTEM
TABULATIONREACTION
POLY_3
DICTRA_MONITOR
BINARY_DIAGRAM_EASY
DATABASE_RETRIEVAL
DIC_PARROT
REACTOR_SIMULATOR_3
PARROT
POTENTIAL_DIAGRAM
SCHEIL_SIMULATION
OLD_SCHEIL_SIM
POURBAIX_DIAGRAM
TERNARY_DIAGRAM
MODULE NAME: BIN
THERMODYNAMIC DATABASE module
Database folder: C:\jenkins\workspace\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA                  /- DEFINED
DICTRA_FCC_A1      REJECTED

Simple binary phase diagram calculation module

Database: /TCBIN/: TCBIN
Current database: TC Binary Solutions v1.1

VA                  /- DEFINED
BCC_B2              FCC_L12
D021_HCP            REJECTED
FCC_L102

First element: fe
Second element: c
Phase Diagram, Phase fraction (F), G- or A-curves (G/A): /Phase_Diagram/: Phase-Diagram
```

```

... the command in full is REJECT
VA                      /- DEFINED
BCC_B2                  FCC_L12          FCC_L102
D021_HCP REJECTED
REINITIATING GES .....
... the command in full is DEFINE_ELEMENTS
C                      FE DEFINED
LIQUID:L              IONIC_LIQUID:Y    FCC_A1
BCC_A2                 A2_BCC          HCP_A3
HCP_ZN                 DIAMOND_A4      GRAPHITE_A9
CBCC_A12               CUB_A13         B2_FEPD
C14_LAVES              C15_LAVES       D011_CEMENTITE
D82_FEZN_GAMMA          L12_FEPD3      ALSFE4
FE3AS2                 FEZN4           FEZN_DELTA
FEZN_ZETA REJECTED
LIQUID:L RESTORED
FCC_A1 RESTORED
BCC_A2 RESTORED
D011_CEMENTITE RESTORED
GRAPHITE_A9 RESTORED
DIAMOND_A4 RESTORED
... the command in full is GET_DATA
15:19:38,035 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS .....
FUNCTIONS .....

List of references for assessed data

'A T Dinsdale, SGTE Data for Pure Elements, Calphad 15(1991)4 p 317-425; '
'P Gustafson, Scan J Metall 14(1985) p 259-267; C-Fe'
-OK-
... the command in full is SET_CONDITION
... the command in full is SET_AXIS_VARIABLE
The condition X(FE)=.1234 created
... the command in full is SET_AXIS_VARIABLE
The condition T=1319.08 created
... the command in full is SET_REFERENCE_STATE
... the command in full is SET_REFERENCE_STATE
... the command in full is SAVE_WORKSPACES
... the command in full is SET_CONDITION
... the command in full is SET_ALL_START_VALUES
Forcing automatic start values
Automatic start values will be set
... the command in full is COMPUTE_EQUILIBRIUM
... the command in full is COMPUTE_EQUILIBRIUM
Start points provided by database
... the command in full is SAVE_WORKSPACES
Version S mapping is selected

Organizing start points

Generating start point 1
Generating start point 2

Phase region boundary 1 at: 9.944E-01 1.100E+03
  BCC_A2
  ** FCC_A1
Calculated.          5 equilibria

Phase region boundary 2 at: 9.838E-01 1.011E+03
  BCC_A2
  ** FCC_A1
  ** GRAPHITE_A9

Phase region boundary 3 at: 4.996E-01 1.011E+03
  BCC_A2
  ** GRAPHITE_A9
Calculated..        30 equilibria
Terminating at axis limit.

Phase region boundary 4 at: 4.845E-01 1.011E+03
  FCC_A1
  ** GRAPHITE_A9
Calculated.          18 equilibria

Phase region boundary 5 at: 4.561E-01 1.427E+03
  ** LIQUID
  FCC_A1
  ** GRAPHITE_A9

Phase region boundary 6 at: 8.690E-01 1.427E+03
  ** LIQUID
  FCC_A1
Calculated.          15 equilibria

Phase region boundary 7 at: 9.840E-01 1.768E+03
  ** LIQUID
  ** BCC_A2
  FCC_A1

Phase region boundary 8 at: 9.939E-01 1.768E+03
  ** BCC_A2
  FCC_A1
Calculated.          25 equilibria

Phase region boundary 9 at: 9.858E-01 1.768E+03
  LIQUID
  ** BCC_A2
Calculated.          20 equilibria

Phase region boundary 10 at: 4.129E-01 1.427E+03
  ** LIQUID
  GRAPHITE_A9
Calculated..        44 equilibria
Terminating at axis limit.

Phase region boundary 11 at: 9.841E-01 1.011E+03
  BCC_A2
  ** FCC_A1
Calculated.          25 equilibria

```

```

Phase region boundary 12 at: 9.944E-01 1.100E+03
  BCC_A2
  ** FCC_A1
Calculated           16 equilibria
*** BUFFER SAVED ON FILE: C:\Users\azureuser\AppData\Local\Temp\BINARY_002.POLY3
CPU time for mapping      4 seconds
POSTPROCESSOR VERSION 3.2

```

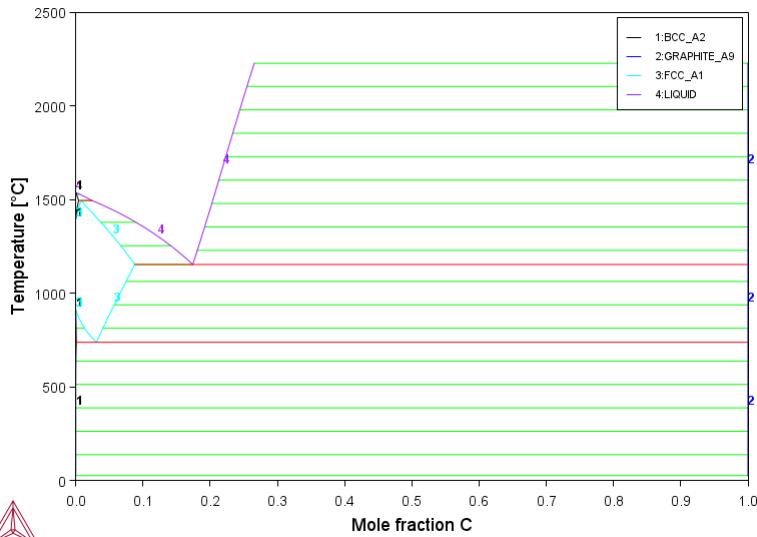
Setting automatic diagram axes

POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

... the command in full is SET_TIELINE_STATUS
... the command in full is SET_LABEL_CURVE_OPTION
... the command in full is PLOT_DIAGRAM

C FE

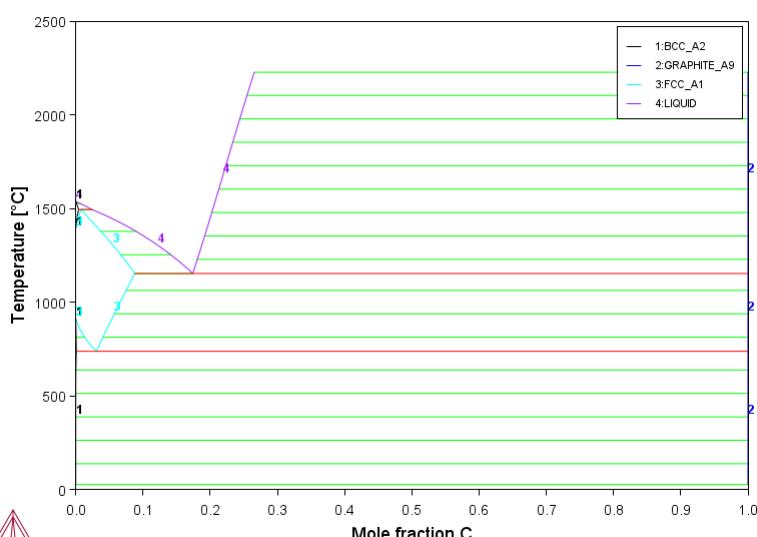


POST:
POST:Hit RETURN to continue
POST:

POST: set-title example 1a
POST: plot

... the command in full is PLOT_DIAGRAM

example 1a



POST:
POST:Hit RETURN to continue
POST: @@ By default labels is given for phase boundaries lines.
POST: @@ If you want to label areas the user must supply a coordinate for the
POST: @@ label, for example

POST: ADD

... the command in full is ADD_LABEL_TEXT

Give X coordinate in axis units: .1

Give Y coordinate in axis units: 2000

Automatic phase labels? /Y/: Y

Automatic labelling not always possible

Using global minimization procedure

Calculated 630 grid points in 0 s

Found the set of lowest grid points in 0 s

Calculated POLY solution 0 s, total time 0 s

Stable phases are: LIQUID

Text size: /.36/:

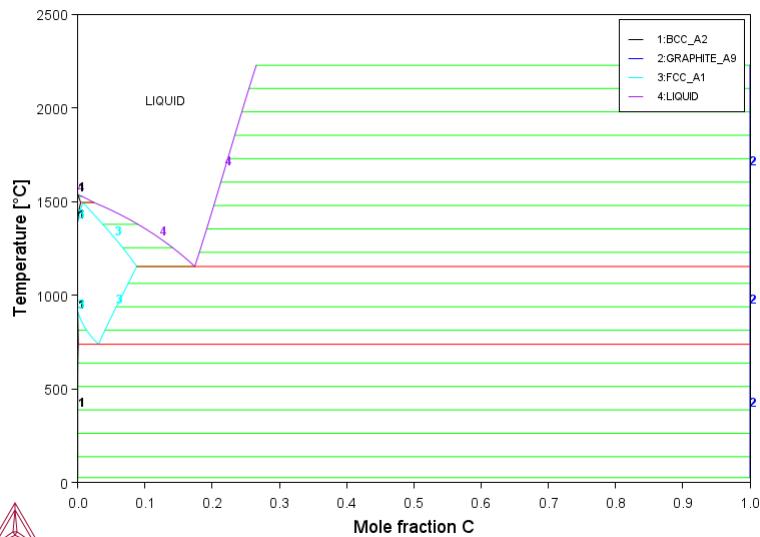
POST: set-title example 1b

POST:

POST: plot

... the command in full is PLOT_DIAGRAM

example 1b

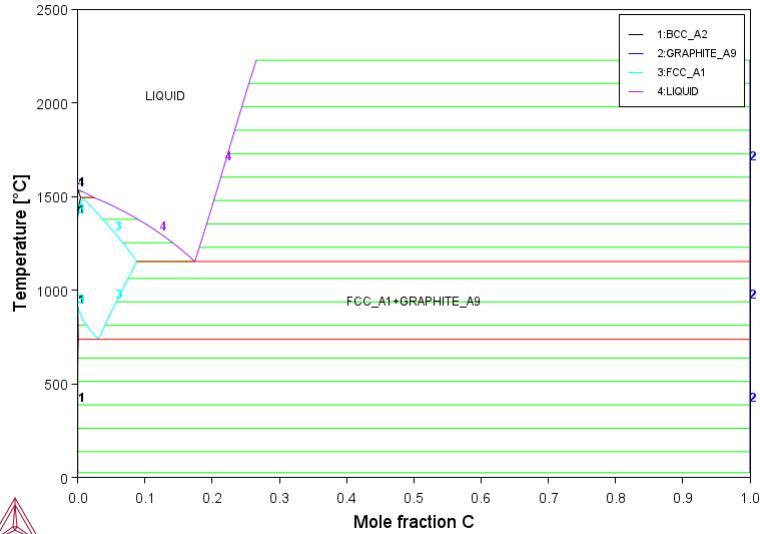


```

POST:
POST:
POST:Hit RETURN to continue
POST: add .4 900
... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/: Y
Automatic labelling not always possible
Using global minimization procedure
Calculated          630 grid points in      0 s
Found the set of lowest grid points in      0 s
Calculated POLY solution    0 s, total time   0 s
Stable phases are: FCC_A1+GRAPHITE_A9
Text size: /.36/:
POST: set-title example 1c
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 1c



```

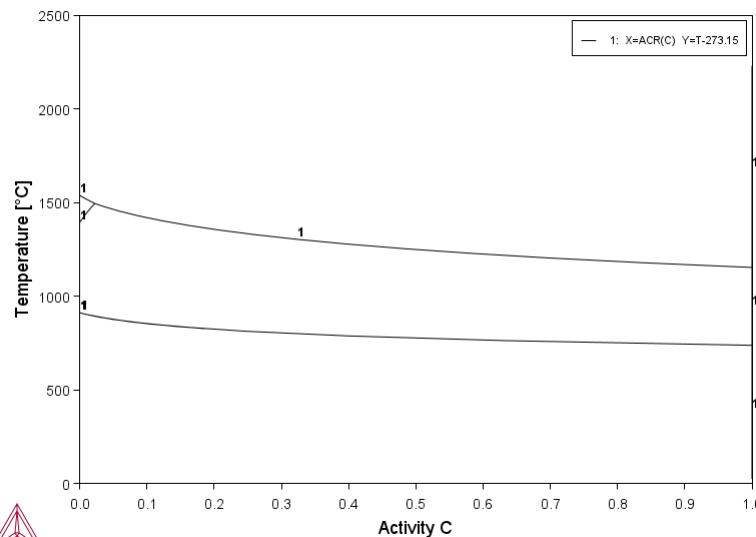
POST:
POST:
POST:
POST: @@ This is the stable phase diagram with graphite and no cementite.
POST: @@ In Thermo-Calc all relevant data from the calculation of the diagram is saved
POST: @@ and it is possible to plot the same diagram using other thermodynamic
POST: @@ quantities, for example replace the carbon composition with its activity
POST: @@ Find out the commands in the post processor by entering ?
POST:Hit RETURN to continue
POST: ?
... the command in full is HELP
ADD_LABEL_TEXT      PLOT_DIAGRAM      SET_INTERACTIVE_MODE
APPEND_EXPERIMENTAL_DATA PRINT_DIAGRAM  SET_LABEL_CURVE_OPTION
BACK                QUICK_EXPERIMENTAL_PLOT SET_PLOT_FORMAT
CHANGE_LEGEND       REINITIATE_PLOT_SETTINGS SET_PLOT_OPTIONS
CREATE_3D_PLOTFILE RESTORE_PHASE_IN_PLOT SET_PLOT_SIZE
DUMP_DIAGRAM        SELECT_PLOT        SET_PREFIX_SCALING
ENTER_SYMBOL        SET_AXIS_LENGTH    SET_RASTER_STATUS
EXIT                SET_AXIS_PLOT_STATUS SET_REFERENCE_STATE
FIND_LINE           SET_AXIS_TEXT_STATUS SET_SCALING_STATUS
HELP                SET_AXIS_TYPE     SET_TIC_TYPE
LIST_DATA_TABLE    SET_COLOR         SET_TIELINE_STATUS
LIST_PLOT_SETTINGS SET_CORNER_TEXT   SET_TITLE
LIST_SYMBOLS        SET_DIAGRAM_AXIS  SET_TRUE_MANUAL_SCALING
MAKE_EXPERIMENTAL_DATAFI SET_DIAGRAM_TYPE SUSPEND_PHASE_IN_PLOT
MODIFY_LABEL_TEXT   SET_FONT         TABULATE
POST: @@ The command to set axis for the diagram is SET_DIAGRAM-AXIS
POST: s-d-a x
... the command in full is SET_DIAGRAM_AXIS
VARIABLE : ?
FILE SYSTEM ERROR IN FILHLP

```

```

ERROR 1717 READING HELP FILE
VARIABLE : ac
FOR COMPONENT : c
POST: set-title example 1d
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
example 1d

```



```

POST:
POST:
POST:
POST: @@ The diagram stops at unit activity which represent graphite.
POST: @@ The area labels disappear when one sets a new diagram axis because they
POST: @@ are relative to the axis values, not the axis quantities.
POST: @@
POST:Hit RETURN to continue
POST:
POST: @@ The metastable diagram, with cementite, can also be calculated but then
POST: @@ one must do some manipulations in POLY. We can use the data
POST: @@ we already retrieved from the database.
POST: back
Current database: Steels/Fe-Alloys v11.0

VA           /- DEFINED
DICTRA_FCC_A1 REJECTED
SYS: go p-3
... the command in full is GOTO_MODULE
POLY:
POLY: @@ The BIN module has used the poly-3 workspace to calculate the
POLY: @@ diagram. We have all data available here. The workspace has been
POLY: @@ saved on a file and we can read this back with the command READ.
POLY:
POLY: read,,
... the command in full is READ_WORKSPACES
POLY:
POLY: @@ There are many commands in the POLY module. This enables you
POLY: @@ to calculate almost any kind of equilibrium and diagram.
POLY: @@ With the ? you can list all commands
POLY:Hit RETURN to continue
POLY: ?
... the command in full is HELP
ADD_INITIAL_EQUILIBRIUM GOTO_MODULE      REINITIATE_MODULE
ADVANCED_OPTIONS        HELP_              SAVE_WORKSPACES
AMEND_STORED_EQUILIBRIA INFORMATION         SELECT_EQUILIBRIUM
BACK                   LIST_AXIS_VARIABLE SET_ALL_START_VALUES
CHANGE_STATUS          LIST_CONDITIONS   SET_AXIS_VARIABLE
COMPUTE_EQUILIBRIUM    LIST_EQUILIBRIUM  SET_CONDITION
COMPUTE_TRANSITION     LIST_INITIAL_EQUILIBRIA SET_INPUT_AMOUNTS
CREATE_NEW_EQUILIBRIUM LIST_STATUS        SET_INTERACTIVE
DEFINE_COMPONENTS      LIST_SYMBOLS      SET_NUMERICAL_LIMITS
DEFINE_DIAGRAM         LOAD_INITIAL_EQUILIBRIUM SET_REFERENCE_STATE
DEFINE_MATERIAL        MACRO_FILE_OPEN  SET_START_CONSTITUION
DELETE_INITIAL_EQUILIB MAKE_COMPONENT_ENTERED SET_START_VALUE
DELETE_SYMBOL          MAKE_COMPONENT_SUSPENDED SHOW_VALUE
ENTER_SYMBOL          MAP               STEP_WITH_OPTIONS
EVALUATE_FUNCTIONS    POST             TABULATE
EXIT                  READ_WORKSPACES
POLY:
POLY:Hit RETURN to continue
POLY: @@ Get more command information with the HELP command
POLY: help
COMMAND: list-status
*** ERROR 37 IN FILDOC: FILE SYSTEM ERROR
POLY:Hit RETURN to continue
POLY: @@ General information can be obtained using the INFORMATION command
POLY: INFO
... the command in full is INFORMATION
FILE SYSTEM ERROR          37
POLY:
POLY: ?
... the command in full is HELP
ADD_INITIAL_EQUILIBRIUM GOTO_MODULE      REINITIATE_MODULE
ADVANCED_OPTIONS        HELP_              SAVE_WORKSPACES
AMEND_STORED_EQUILIBRIA INFORMATION         SELECT_EQUILIBRIUM
BACK                   LIST_AXIS_VARIABLE SET_ALL_START_VALUES
CHANGE_STATUS          LIST_CONDITIONS   SET_AXIS_VARIABLE
COMPUTE_EQUILIBRIUM    LIST_EQUILIBRIUM  SET_CONDITION
COMPUTE_TRANSITION     LIST_INITIAL_EQUILIBRIA SET_INPUT_AMOUNTS
CREATE_NEW_EQUILIBRIUM LIST_STATUS        SET_INTERACTIVE
DEFINE_COMPONENTS      LIST_SYMBOLS      SET_NUMERICAL_LIMITS
DEFINE_DIAGRAM         LOAD_INITIAL_EQUILIBRIUM SET_REFERENCE_STATE

```

```

DEFINE_MATERIAL      MACRO_FILE_OPEN      SET_START_CONSTITUITION
DELETE_INITIAL_EQUILIB  MAKE_COMPONENT_ENTERED  SET_START_VALUE
DELETE_SYMBOL        MAKE_COMPONENT_SUSPENDED SHOW_VALUE
ENTER_SYMBOL         MAP                  STEP_WITH_OPTIONS
EVALUATE_FUNCTIONS   POST                 TABULATE
EXIT                READ_WORKSPACES

POLY: state
No such command: state. Use ? for list of available commands
POLY:
POLY:Hit RETURN to continue
POLY: @@ List the current equilibrium by
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: ?
FILE SYSTEM ERROR IN FILHLP
Options /VWCS/:
Output from POLY-3, equilibrium = 1, label A0 , database: TCBIN

Conditions:
N=1, P=100000, X(FE)=0.99, T=1100
DEGREES OF FREEDOM 0

Temperature 1100.00 K ( 826.85 C), Pressure 1.000000E+05
Number of moles of components 1.000000E+00, Mass in grams 5.54086E+01
Total Gibbs energy -4.90502E+04, Enthalpy 3.18534E+04, Volume 0.000000E+00

Component      Moles      W-Fraction Activity Potential Ref.stat
C             1.0000E-02  2.1677E-03 1.8555E-01 -1.5406E+04 GRAPHITE
FE            9.9000E-01  9.9783E-01 9.9957E-01 -3.9762E+00 BCC_A2

FCC_A1          Status ENTERED     Driving force 0.0000E+00
Moles 9.2463E-01, Mass 5.1201E+01, Volume fraction 0.0000E+00 Mass fractions:
FE 9.97662E-01 C 2.33819E-03

BCC_A2          Status ENTERED     Driving force 0.0000E+00
Moles 7.5373E-02, Mass 4.2079E+00, Volume fraction 0.0000E+00 Mass fractions:
FE 9.99907E-01 C 9.33835E-05

POLY:Hit RETURN to continue
POLY: @@ The actual conditions are listed by the list-equil command but
POLY: @@ can be obtained also by
POLY: l-c
... the command in full is LIST_CONDITIONS
N=1, P=100000, X(FE)=0.99, T=1100
DEGREES OF FREEDOM 0
POLY:
POLY:Hit RETURN to continue
POLY: @@ The meaning of the state variables T, P, X, N and many others
POLY: @@ are explained by the INFO command
POLY: INFO
... the command in full is INFORMATION
FILE SYSTEM ERROR           37
POLY: state
No such command: state. Use ? for list of available commands
POLY:
POLY:Hit RETURN to continue
POLY: @@ The use of state variables as conditions is the key to the
POLY: @@ flexibility of Thermo-Calc. Each condition is set independently and
POLY: @@ any condition can be set as an axis variable.
POLY: @@
POLY: @@ Now we just want to take away the graphite in order to calculate the
POLY: @@ metastable Fe-C diagram with cementite. We can list all phases with the
POLY: @@ LIST_STATUS command
POLY: l-st
... the command in full is LIST_STATUS
Option /CPS/:
*** STATUS FOR ALL COMPONENTS
COMPONENT      STATUS      REF. STATE      T(K)      P(Pa)
VA             ENTERED    SER
C              ENTERED    GRAPHITE_A9   *          100000
FE             ENTERED    BCC_A2       *          100000
*** STATUS FOR ALL PHASES
PHASE          STATUS      DRIVING FORCE MOLES
FCC_A1         ENTERED    0.000000E+00 9.246266E-01
BCC_A2         ENTERED    0.000000E+00 7.537335E-02
D011_CEMENTITE ENTERED   -4.153716E-01 0.000000E+00
LIQUID         ENTERED   -4.668963E-01 0.000000E+00
GRAPHITE_A9    ENTERED   -1.684424E+00 0.000000E+00
DIAMOND_A4     ENTERED   -2.386932E+00 0.000000E+00
*** STATUS FOR ALL SPECIES
C   ENTERED   C3  ENTERED   FE  ENTERED   VA  ENTERED
C1  ENTERED   C4  ENTERED   FE+2 ENTERED  VA-2 ENTERED
C2  ENTERED   C5  ENTERED   FE+3 ENTERED  VA-4 ENTERED

POLY:Hit RETURN to continue
POLY: @@ The status is changed with the CHANGE_STATUS command
POLY: ch-st
... the command in full is CHANGE_STATUS
For phases, species or components? /PHASES/:
Phase name(s): ?
FILE SYSTEM ERROR IN FILHLP
Phase name(s): gra
Status: /ENTERED/: sus
POLY: l-st
... the command in full is LIST_STATUS
Option /CPS/:
*** STATUS FOR ALL COMPONENTS
COMPONENT      STATUS      REF. STATE      T(K)      P(Pa)
VA             ENTERED    SER
C              ENTERED    GRAPHITE_A9   *          100000
FE             ENTERED    BCC_A2       *          100000
*** STATUS FOR ALL PHASES
PHASE          STATUS      DRIVING FORCE MOLES
FCC_A1         ENTERED    0.000000E+00 9.246266E-01
BCC_A2         ENTERED    0.000000E+00 7.537335E-02
D011_CEMENTITE ENTERED   -4.153716E-01 0.000000E+00
LIQUID         ENTERED   -4.668963E-01 0.000000E+00
DIAMOND_A4     ENTERED   -2.386932E+00 0.000000E+00
SUSPENDED PHASES:
GRAPHITE_A9
*** STATUS FOR ALL SPECIES
C   ENTERED   C3  ENTERED   FE  ENTERED   VA  ENTERED
C1  ENTERED   C4  ENTERED   FE+2 ENTERED  VA-2 ENTERED
C2  ENTERED   C5  ENTERED   FE+3 ENTERED  VA-4 ENTERED

POLY:Hit RETURN to continue

```

```

POLY: @@ Note that the graphite is listed as suspended this time.
POLY: @@ Now try to calculate the equilibrium without graphite.
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 629 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY: @@ A number of,,, after a command means to accept default values.
POLY: l-e,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: TCBIN

Conditions:
N=1, P=100000, X(FE)=0.99, T=1100
DEGREES OF FREEDOM 0

Temperature 1100.00 K ( 826.85 C), Pressure 1.000000E+05
Number of moles of components 1.000000E+00, Mass in grams 5.54086E+01
Total Gibbs energy -4.90502E+04, Enthalpy 3.18534E+04, Volume 0.00000E+00

Component Moles W-Fraction Activity Potential Ref.stat
C 1.0000E-02 2.1677E-03 1.8555E-01 -1.5406E+04 GRAPHITE
FE 9.9000E-01 9.9783E-01 9.9957E-01 -3.9762E+00 BCC_A2

FCC_A1 Status ENTERED Driving force 0.0000E+00
Moles 9.2463E-01, Mass 5.1201E+01, Volume fraction 0.0000E+00 Mass fractions:
FE 9.97662E-01 C 2.33819E-03

BCC_A2 Status ENTERED Driving force 0.0000E+00
Moles 7.5373E-02, Mass 4.2079E+00, Volume fraction 0.0000E+00 Mass fractions:
FE 9.99907E-01 C 9.33835E-05
POLY:Hit RETURN to continue
POLY: @@ It may seem surprising that diamond is stable but the total mole fraction
POLY: @@ of iron is less than 0.5, so we are on the carbon rich side
POLY: @@ of cementite, and it is reasonable.
POLY:
POLY: @@ Now try to map the metastable diagram
POLY: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Generating start point 27
Generating start point 28
Generating start point 29
Generating start point 30
Working hard
Generating start point 31
Generating start point 32

Phase region boundary 1 at: 5.000E-01 3.100E+02
  BCC_A2
  ** DIAMOND_A4
Calculated.. 2 equilibria
Terminating at axis limit.

Phase region boundary 2 at: 5.000E-01 3.000E+02
  BCC_A2
  ** DIAMOND_A4
Calculated.. 24 equilibria

Phase region boundary 3 at: 4.999E-01 8.605E+02
  BCC_A2
  ** D011_CEMENTITE
  ** DIAMOND_A4

Phase region boundary 4 at: 8.749E-01 8.605E+02
  BCC_A2
  ** D011_CEMENTITE
Calculated.. 7 equilibria

Phase region boundary 5 at: 8.746E-01 9.998E+02

```

```

      BCC_A2
** D011_CEMENTITE
** FCC_A1
Phase region boundary  6 at:  9.823E-01  9.998E+02
      BCC_A2
** FCC_A1
Calculated.          23 equilibria

Phase region boundary  7 at:  8.578E-01  9.998E+02
      D011_CEMENTITE
** FCC_A1
Calculated.          18 equilibria

Phase region boundary  8 at:  8.354E-01  1.422E+03
** LIQUID
      D011_CEMENTITE
** FCC_A1
Calculated.          5 equilibria

Phase region boundary  9 at:  7.872E-01  1.422E+03
** LIQUID
      D011_CEMENTITE
Calculated.          26 equilibria
Terminating at known equilibrium

Phase region boundary 10 at:  7.657E-01  1.484E+03
** LIQUID
      D011_CEMENTITE
** DIAMOND_A4
Calculated.          42 equilibria
Terminating at axis limit.

Phase region boundary 11 at:  3.750E-01  1.484E+03
** DIAMOND_A4
Calculated..         26 equilibria
Terminating at axis limit.

Phase region boundary 12 at:  3.907E-01  1.484E+03
      LIQUID
** DIAMOND_A4
Calculated..         42 equilibria
Terminating at axis limit.

Phase region boundary 13 at:  8.678E-01  1.422E+03
** LIQUID
** FCC_A1
Calculated.          15 equilibria

Phase region boundary 14 at:  9.840E-01  1.768E+03
** LIQUID
** BCC_A2
      FCC_A1
Calculated.          25 equilibria

Phase region boundary 15 at:  9.939E-01  1.768E+03
** BCC_A2
      FCC_A1
Calculated.          25 equilibria

Phase region boundary 16 at:  9.858E-01  1.768E+03
      LIQUID
** BCC_A2
Calculated.          20 equilibria
Terminating at known equilibrium

Phase region boundary 17 at:  5.000E-01  3.100E+02
      BCC_A2
** DIAMOND_A4
Calculated.          24 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 18 at:  5.000E-01  3.100E+02
      BCC_A2
** DIAMOND_A4
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 19 at:  5.000E-01  3.100E+02
      BCC_A2
** DIAMOND_A4
Calculated..         24 equilibria
Terminating at known equilibrium
Terminating at known equilibrium

Phase region boundary 20 at:  5.000E-01  3.100E+02
      BCC_A2
** DIAMOND_A4
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 21 at:  5.000E-01  3.100E+02
      BCC_A2
** DIAMOND_A4
Calculated..         24 equilibria
Terminating at known equilibrium
Terminating at known equilibrium

Phase region boundary 22 at:  5.000E-01  3.100E+02
      BCC_A2
** DIAMOND_A4
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 23 at:  5.000E-01  3.100E+02
      BCC_A2
** DIAMOND_A4
Calculated..         24 equilibria
Terminating at known equilibrium
Terminating at known equilibrium

Phase region boundary 24 at:  5.000E-01  3.100E+02
      BCC_A2
** DIAMOND_A4
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 25 at:  5.000E-01  3.100E+02
      BCC_A2
** DIAMOND_A4

```

Calculated. 24 equilibria
 Terminating at known equilibrium
 Phase region boundary 26 at: 5.000E-01 3.100E+02
 BCC_A2
 ** DIAMOND_A4
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.
 Phase region boundary 27 at: 5.000E-01 3.100E+02
 BCC_A2
 ** DIAMOND_A4
 Calculated. 24 equilibria
 Terminating at known equilibrium
 Phase region boundary 28 at: 3.750E-01 1.037E+03
 ** D011_CEMENTITE
 DIAMOND_A4
 Calculated. 9 equilibria
 Terminating at known equilibrium
 Phase region boundary 29 at: 3.750E-01 1.037E+03
 ** D011_CEMENTITE
 DIAMOND_A4
 Calculated. 19 equilibria
 Terminating at known equilibrium
 Phase region boundary 30 at: 9.877E-01 1.037E+03
 BCC_A2
 ** FCC_A1
 Calculated. 3 equilibria
 Terminating at known equilibrium
 Phase region boundary 31 at: 9.877E-01 1.037E+03
 BCC_A2
 ** FCC_A1
 Calculated. 23 equilibria
 Phase region boundary 32 at: 3.754E-01 1.763E+03
 LIQUID
 ** DIAMOND_A4
 Calculated. 13 equilibria
 Terminating at known equilibrium
 Phase region boundary 33 at: 3.754E-01 1.763E+03
 LIQUID
 ** DIAMOND_A4
 Calculated.. 31 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.
 Phase region boundary 34 at: 9.820E-01 1.763E+03
 LIQUID
 ** FCC_A1
 Calculated. 15 equilibria
 Terminating at known equilibrium
 Phase region boundary 35 at: 9.820E-01 1.763E+03
 LIQUID
 ** FCC_A1
 Calculated. 2 equilibria
 Terminating at known equilibrium
 Phase region boundary 36 at: 3.306E-01 2.490E+03
 LIQUID
 ** DIAMOND_A4
 Calculated. 42 equilibria
 Terminating at known equilibrium
 Phase region boundary 37 at: 3.306E-01 2.490E+03
 LIQUID
 ** DIAMOND_A4
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.
 Phase region boundary 38 at: 3.306E-01 2.490E+03
 LIQUID
 ** DIAMOND_A4
 Calculated. 42 equilibria
 Terminating at known equilibrium
 Phase region boundary 39 at: 3.306E-01 2.490E+03
 LIQUID
 ** DIAMOND_A4
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.
 Phase region boundary 40 at: 3.306E-01 2.490E+03
 LIQUID
 ** DIAMOND_A4
 Calculated. 42 equilibria
 Terminating at known equilibrium
 Phase region boundary 41 at: 3.306E-01 2.490E+03
 LIQUID
 ** DIAMOND_A4
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.
 Phase region boundary 42 at: 3.317E-01 2.475E+03
 LIQUID
 ** DIAMOND_A4
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.
 Phase region boundary 43 at: 3.317E-01 2.475E+03
 LIQUID
 ** DIAMOND_A4
 Calculated. 41 equilibria
 Terminating at known equilibrium

```

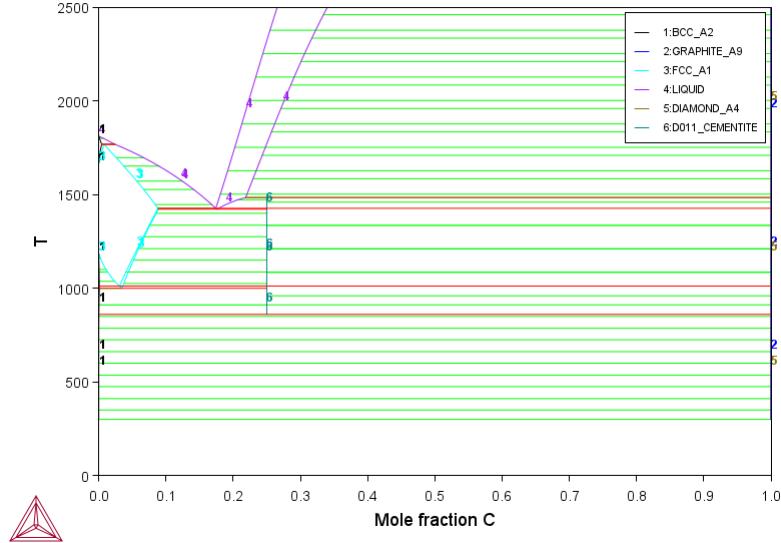
Phase region boundary 44 at: 3.306E-01 2.490E+03
    LIQUID
    ** DIAMOND_A4
Calculated.          42 equilibria
Terminating at known equilibrium

Phase region boundary 45 at: 3.306E-01 2.490E+03
    LIQUID
    ** DIAMOND_A4
Calculated..          2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 46 at: 9.941E-01 1.794E+03
    LIQUID
    ** BCC_A2
Calculated.          2 equilibria
Terminating at known equilibrium

Phase region boundary 47 at: 9.941E-01 1.794E+03
    LIQUID
    ** BCC_A2
Calculated.          12 equilibria
*** BUFFER SAVED ON FILE: C:\Users\azureuser\AppData\Local\Temp\BINARY_002.POLY3
CPU time for mapping   3 seconds
POLY:
POLY: post
POST: s-d-a y t
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a x m-f C
... the command in full is SET_DIAGRAM_AXIS
POST: set-tieline
... the command in full is SET_TIELINE_STATUS
PLOTTING EVERY TIE-LINE NO /5/: 5
POST:
POST: set-title example 1e
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
example 1e

```



POST:

POST:

POST:Hit RETURN to continue

POST: @@ The previous stable diagram is also plotted. The reason is that
POST: @@ we never removed it from the workspace. (It can be done with a **SAVE**
POST: @@ command. Search the online help to read more about this command).

POST:

POST: @@ It may be surprising to find that diamond is more stable than
POST: @@ cementite at low temperatures. However, diamonds are never
POST: @@ found in steel as graphite forms first.

POST:

POST: @@ Now change the axis to composition, use weight-percent of carbon

POST: s-d-a x

... the command in full is SET_DIAGRAM_AXIS

VARIABLE : ?

FILE SYSTEM ERROR IN FILHLP
 ERROR 1717 READING HELP FILE

VARIABLE : w-p

FOR COMPONENT : c

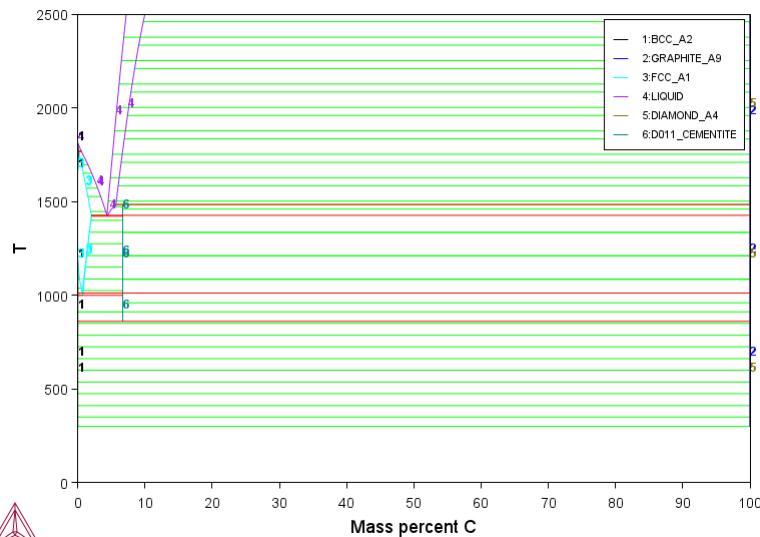
POST: set-title example 1f

POST:

POST: plot

... the command in full is PLOT_DIAGRAM

example 1f

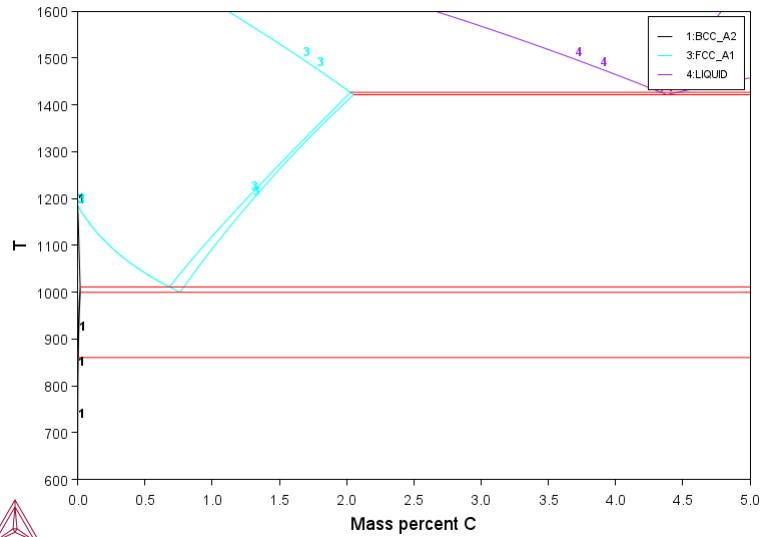


```

POST:
POST:
POST:Hit RETURN to continue
POST: @@ The tie-lines now obscure the diagram. Remove these and
POST: @@ also change the scale of the x and y axis
POST: s-t-s 0
... the command in full is SET_TIELINE_STATUS
POST: s-s x n 0 5
... the command in full is SET_SCALING_STATUS
POST: s-s y n 600 1600
... the command in full is SET_SCALING_STATUS
POST: set-title example 1g
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 1g

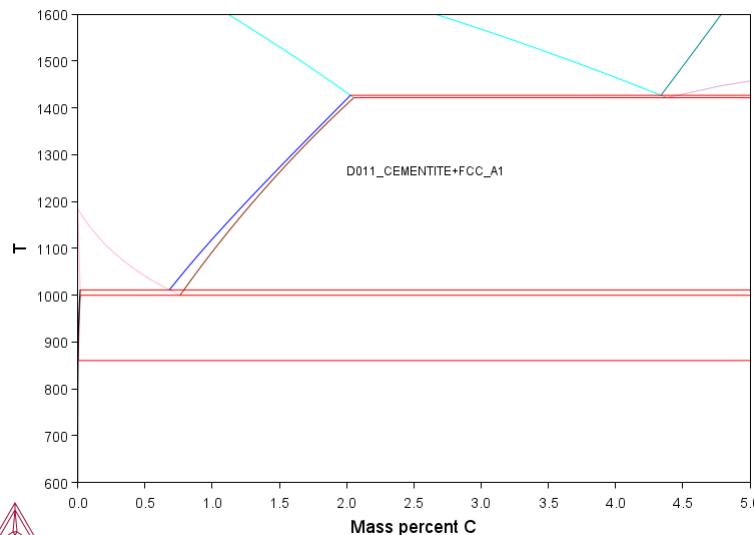


```

POST:
POST:
POST:Hit RETURN to continue
POST: @@ Finally add some labels
POST: set-lab n
... the command in full is SET_LABEL_CURVE_OPTION
POST: add 2 1250
... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
Automatic labelling not always possible
Using global minimization procedure
Calculated 629 grid points in      0 s
Found the set of lowest grid points in      0 s
Calculated POLY solution      0 s, total time      0 s
Stable phases are: D011_CEMENTITE+FCC_A1
Text size: /.36/:
POST: set-title example 1h
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 1h

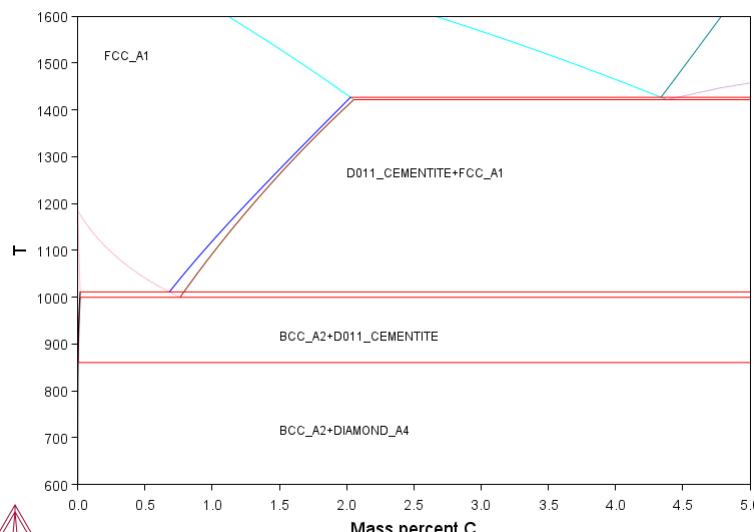


```

POST:
POST:
POST:Hit RETURN to continue
POST: add 1.5 900
... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
Automatic labelling not always possible
Using global minimization procedure
Calculated      629 grid points in      0 s
Found the set of lowest grid points in      0 s
Calculated POLY solution 0 s, total time 0 s
Stable phases are: BCC_A2+D011_CEMENTITE
Text size: /.36/:
POST: add 1.5 700
... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
Automatic labelling not always possible
Using global minimization procedure
Calculated      629 grid points in      0 s
Found the set of lowest grid points in      0 s
Calculated POLY solution 0 s, total time 0 s
Stable phases are: BCC_A2+DIAMOND_A4
Text size: /.36/:
POST: add 1.2 1500
... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
Automatic labelling not always possible
Using global minimization procedure
Calculated      629 grid points in      0 s
Found the set of lowest grid points in      0 s
Calculated POLY solution 0 s, total time 0 s
Stable phases are: FCC_A1
Text size: /.36/:
POST: set-title example 1i
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 1i



```

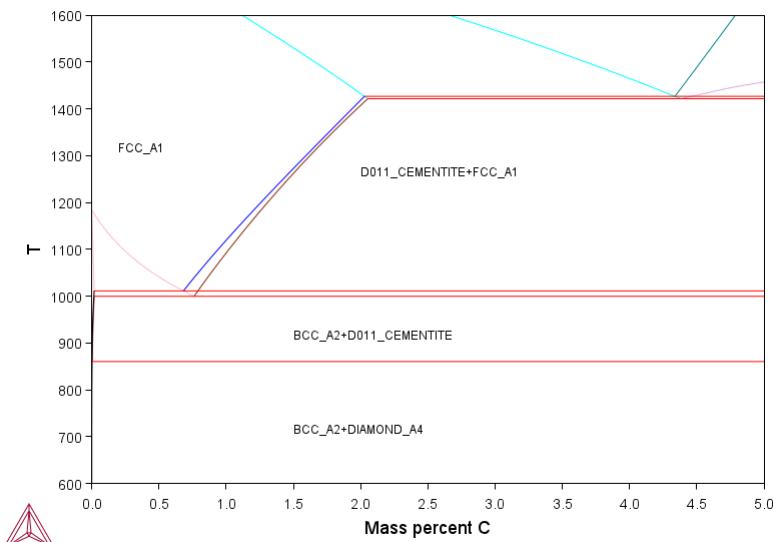
POST:
POST:
POST:Hit RETURN to continue
POST: @@ As graphite is suspended, cementite is the stable carbide
POST: @@ so that is the phase that is listed in the two-phase regions.
POST: @@ The label for the FCC region is a bit too high, move it down
POST: modify
... the command in full is MODIFY_LABEL_TEXT
These labels are defined
No 1 at 2.00000E+00 1.25000E+03 : D011_CEMENTITE+FCC_A1
No 2 at 1.50000E+00 9.00000E+02 : BCC_A2+D011_CEMENTITE

```

```

No 3 at 1.50000E+00 7.00000E+02 : BCC_A2+DIAMOND_A4
No 4 at 2.00000E-01 1.50000E+03 : FCC_A1
Which label to modify? /4/:
New X coordinate /.2/: .2
New Y coordinate /1500/: 1300
New text /FCC_A1/:
POST: set-title example 1j
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
example 1j

```



```

POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:

```



tce02

SYS:About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

```
SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce02\tce02.TCM.test"
SYS: set-echo
SYS: @@
SYS: @@ Plotting thermodynamic functions
SYS:
SYS: @@ This example shows how to plot thermodynamic
SYS: @@ functions in unary, binary and ternary systems.
SYS: @@ It also involves working with partial derivatives
SYS: @@ and partial quantities.
SYS:
SYS: set-log ex02.,
SYS:
SYS: go da
... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module
Database folder: C:\jenkins\workspace\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA           /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE11: sw ssol6
... the command in full is SWITCH_DATABASE
Current database: SGTE Alloy Solutions v6.0

VA   DEFINED
BCC_B2          FCC_L12          FCC_COV
FCC_AUCU        HCP_ORD  REJECTED
GAS:G  REJECTED
TDB_SSOL6: @@ Pure Fe is selected as a unary system
TDB_SSOL6: d-sys fe
... the command in full is DEFINE_SYSTEM
FE   DEFINED
TDB_SSOL6: get
... the command in full is GET_DATA
15:21:10,280 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS .....
FUNCTIONS .....

List of references for assessed data
'Benyan Pei, B Bjorkman, B Sundman, and B Jansson: Calphad, 1995, 19(1), 1
-15. "A thermodynamic assessment of the Iron-Antimony system". >> Fe
-Sb '
-OK-
TDB_SSOL6:
TDB_SSOL6: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY: @@ In POLY-3 first define a single equilibrium

POLY: s-c t=300,p=1e5,n=1
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated      21 grid points in       6 s
POLY: l-e,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium =    1, label A0 , database: SSOL6

Conditions:
T=300, P=100000, N=1
DEGREES OF FREEDOM 0

Temperature 300.00 K ( 26.85 C), Pressure 1.000000E+05
Number of moles of components 1.000000E+00, Mass in grams 5.58470E+01
Total Gibbs energy -8.18407E+03, Enthalpy 4.59751E+01, Volume 0.00000E+00

Component      Moles      W-Fraction Activity Potential Ref.stat
FE            1.0000E+00 1.0000E+00 3.7589E-02 -8.1841E+03 SER

BCC_A2          Status ENTERED      Driving force 0.0000E+00
Moles 1.0000E+00, Mass 5.5847E+01, Volume fraction 0.0000E+00 Mass fractions:
FE 1.0000E+00

POLY:
POLY:Hit RETURN to continue
POLY: @@ Set T as an axis variable
POLY: s-a-v
... the command in full is SET_AXIS_VARIABLE
Axis number: /1/: 1
Condition /NONE/: t
Min value /0/: 300
Max value /1/: 2000
Increment /42.5/: 42.5
POLY: @@ Save the macro to be able to come back to this point
```

```

POLY: save tcex02a y
... the command in full is SAVE_WORKSPACES
POLY: @@ Step along the axis
POLY: step
... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/: NORMAL
No initial equilibrium, using default
Step will start from axis value 300.000
...OK

Phase Region from 300.000 for:
  BCC_A2
Global test at 3.80000E+02 .... OK
Global test at 4.80000E+02 .... OK
Global test at 5.80000E+02 .... OK
Global test at 6.80000E+02 .... OK
Global test at 7.80000E+02 .... OK
Global test at 8.80000E+02 .... OK
Global test at 9.80000E+02 .... OK
Global test at 1.08000E+03 .... OK
Global test at 1.18000E+03 .... OK
Global check of adding phase at 1.18481E+03
Calculated 91 equilibria

Phase Region from 1184.81 for:
  BCC_A2
  FCC_A1
Calculated 2 equilibria

Phase Region from 1184.81 for:
  FCC_A1
Global test at 1.26000E+03 .... OK
Global test at 1.36000E+03 .... OK
Global test at 1.46000E+03 .... OK
Global test at 1.56000E+03 .... OK
Global test at 1.66000E+03 .... OK
Global check of adding phase at 1.66747E+03
Calculated 51 equilibria

Phase Region from 1667.47 for:
  BCC_A2
  FCC_A1
Calculated 2 equilibria

Phase Region from 1667.47 for:
  BCC_A2
Global test at 1.74000E+03 .... OK
Global check of adding phase at 1.81095E+03
Calculated 18 equilibria

Phase Region from 1810.95 for:
  LIQUID
  BCC_A2
Calculated 2 equilibria

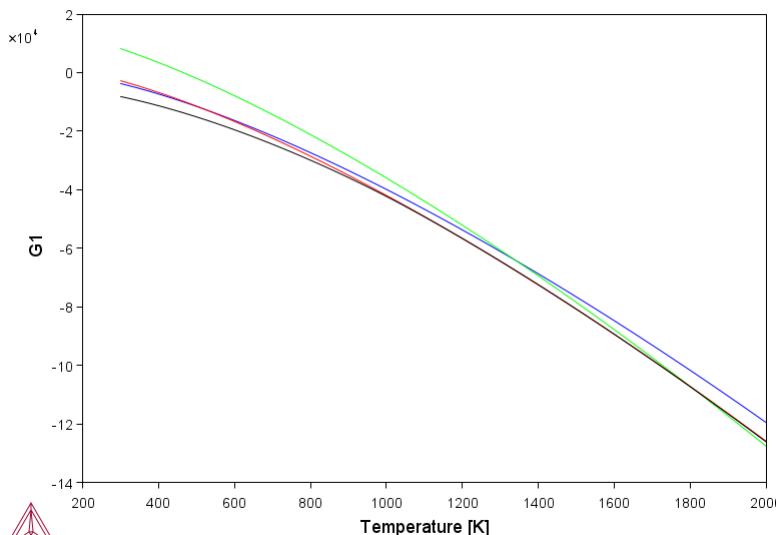
Phase Region from 1810.95 for:
  LIQUID
Global test at 1.89000E+03 .... OK
Global test at 1.99000E+03 .... OK
Terminating at 2000.00
Calculated 22 equilibria
*** Buffer saved on file: c:\jenkins\workspace\generate_console_examples\examples\tcex02\tcex02a.POLY3
POLY: @@ Post processing (plotting) is the essential part of this example
POLY: @@ We will plot Gm, Hm and Cp for some phases
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST:
POST:
POST: @@ The x-axis is the temperature in Kelvin
POST: s-d-a x
... the command in full is SET_DIAGRAM_AXIS
VARIABLE : ?
FILE SYSTEM ERROR IN FILHLP
ERROR 1717 READING HELP FILE
VARIABLE : t-k
POST: @@ The phases for which Gm shall be plotted must be defined
POST: @@ in a table
POST: ent tab
... the command in full is ENTER_SYMBOL
Name: g1
Variable(s): gm(bcc_a2) gm(fcc_a1) gm(liq) gm(hcp_a3)
&
POST:
POST: @@ The table is set as the y-axis and all columns are included
POST: @@ by using *
POST: s-d-a y g1
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*:/ *
POST: set-title example 2a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

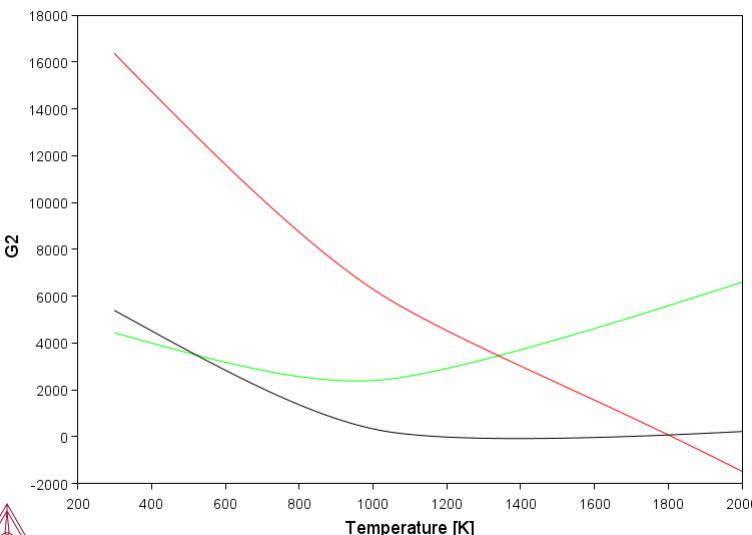
```

example 2a



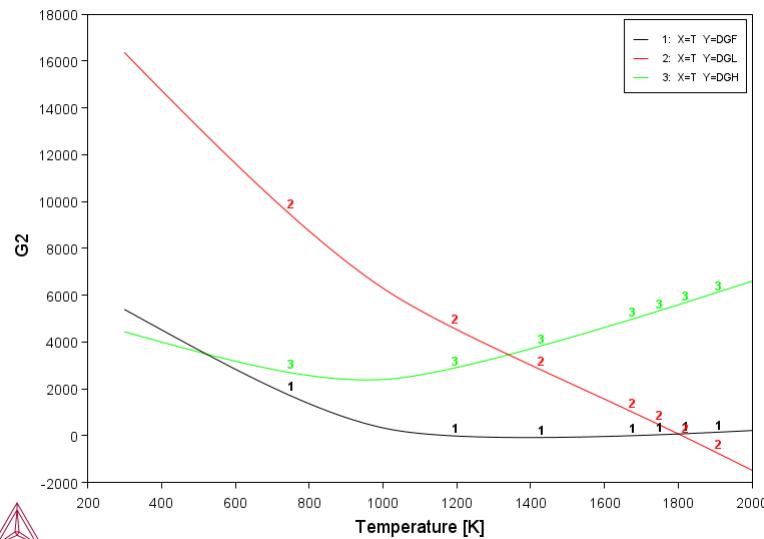
```
POST:  
POST:Hit RETURN to continue  
POST: @@  
POST:  
POST:  
POST: @@ The magnitude makes it difficult to see anything. Enter  
POST: @@ functions for the differences with respect to bcc  
POST: ent fun dgf=gm(fcc_a1)-gm(bcc_a2);  
... the command in full is ENTER_SYMBOL  
POST: ent fun dgl=gm(lig)-gm(bcc_a2);  
... the command in full is ENTER_SYMBOL  
POST: ent fun dgh=gm(hcp_a3)-gm(bcc_a2);  
... the command in full is ENTER_SYMBOL  
POST: @@ and enter a new table and set it as the y-axis  
POST: ent tab g2  
... the command in full is ENTER_SYMBOL  
Variable(s): dgf dgl dgh;  
POST: s-d-a y g2  
... the command in full is SET_DIAGRAM_AXIS  
COLUMN NUMBER /*/: *  
POST: set-title example 2b  
POST:  
POST:  
POST: SET_EXP_FILE_FORMAT 5  
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y  
... the command in full is MAKE_EXPERIMENTAL_DATAFI  
POST: SET_EXP_FILE_FORMAT 10  
POST:  
POST: plot  
... the command in full is PLOT_DIAGRAM
```

example 2b



```
POST:  
POST:Hit RETURN to continue  
POST: @@ In order to have some identification on the lines  
POST: @@ use the command Set_Label  
POST: s-lab  
... the command in full is SET_LABEL_CURVE_OPTION  
CURVE LABEL OPTION (A, B, C, D, E, F OR N) /N/: D  
POST: set-title example 2c  
POST:  
POST:  
POST: SET_EXP_FILE_FORMAT 5  
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y  
... the command in full is MAKE_EXPERIMENTAL_DATAFI  
POST: SET_EXP_FILE_FORMAT 10  
POST:  
POST: plot  
... the command in full is PLOT_DIAGRAM
```

example 2c

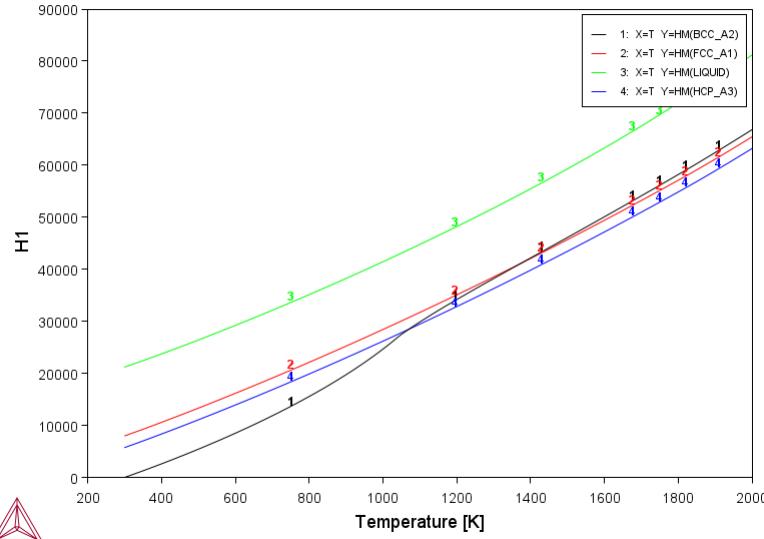


```

POST:
POST:Hit RETURN to continue
POST: @@ Now plot enthalpies
POST: ent tab h1
... the command in full is ENTER_SYMBOL
Variable(s): hm(bcc_a2) hm(fcc_a1) hm(liq) hm(hcp_a3);
POST: s-d-a y h1
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*: *
POST: set-title example 2d
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 2d

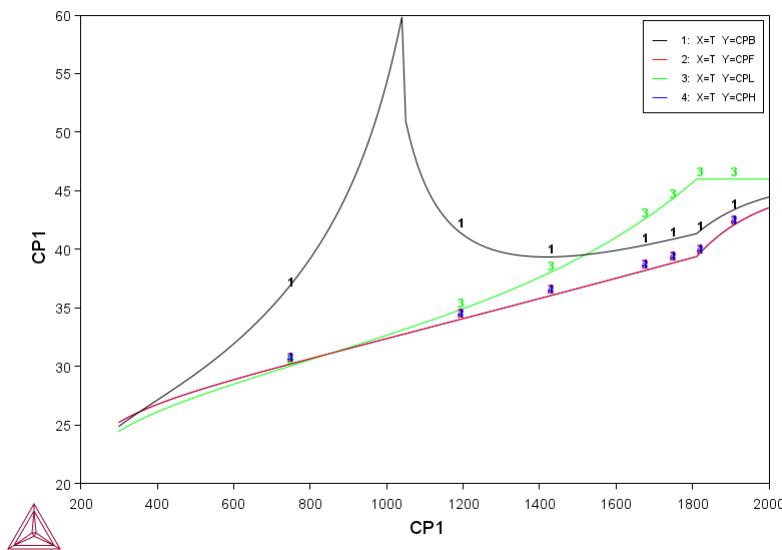


```

POST:
POST:Hit RETURN to continue
POST: @@ And finally plot heat capacities
POST: ent fun cpb=hm(bcc_a2).t;
... the command in full is ENTER_SYMBOL
POST: ent fun cpf=hm(fcc_a1).t;
... the command in full is ENTER_SYMBOL
POST: ent fun cpl=hm(liq).t;
... the command in full is ENTER_SYMBOL
POST: ent fun cph=hm(hcp_a3).t;
... the command in full is ENTER_SYMBOL
POST: ent tab cpl
... the command in full is ENTER_SYMBOL
Variable(s): t cpb cpf cpl cph;
POST: s-d-a y
... the command in full is SET_DIAGRAM_AXIS
VARIABLE : cpl
COLUMN NUMBER /*: 2-5
POST: s-d-a x cpl 1
... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 2e
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:

```

POST: plot
... the command in full is PLOT_DIAGRAM
example 2e



POST:

POST: Hit RETURN to continue

POST:

POST: @@ The next example plots functions for a binary system

POST:

POST: ba

... the command in full is BACK

POLY: go da

... the command in full is GOTO_MODULE

TDB_SSOL6: rej sys

... the command in full is REJECT

VA DEFINED

BCC_B2 FCC_L12 FCC_COV

FCC_AUCU HCP_ORD REJECTED

GAS:G REJECTED

REINITIATING GES

TDB_SSOL6: @@ Select the Cu-Fe system and only

TDB_SSOL6: @@ the fcc, bcc, liquid and hcp phases

TDB_SSOL6: d-sys fe cu

... the command in full is DEFINE_SYSTEM

FE CU DEFINED

TDB_SSOL6: rej ph /all

... the command in full is REJECT

LIQUID:L FCC_A1

HCP_A3 HCP_ZN

Cbcc_A12 CUB_A13

Laves_C14 Laves_C15

M4n Alcu_eta

Alcuzn_gamma_H Al5fe4

Cuti Cu4ti

Cuzn_gamma D_gamma

Fepd3 Fesb

Fe2u Feuzr_delta

Fezr3 REJECTED

TDB_SSOL6: rest ph fcc_a1 bcc_a2 liq hcp_a3

... the command in full is RESTORE

FCC_A1 BCC_A2 LIQUID:L

HCP_A3 RESTORED

TDB_SSOL6: l-sys

... the command in full is LIST_SYSTEM

ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/: CONSTITUENT

LIQUID:L :CU FE:

FCC_A1 :CU FE:VA:

BCC_A2 :CU FE:VA:

HCP_A3 :CU FE:VA:

TDB_SSOL6: get

... the command in full is GET_DATA

REINITIATING GES

ELEMENTS

SPECIES

PHASES

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

PARAMETERS ...

FUNCTIONS

List of references for assessed data

'Data for the Cu-Fe system are from an unpublished assessment of I Ansara and A Jansson published in the COST507 final report: COST507 Thermochemical Database for Light Metal Alloys, Vol 2, eds by I Ansara, AT Dinsdale and MH Rand, July 1998, EUR18499. The data were also reported by A Jansson in the KTH report TRITA-MAC-533, 1993. >> Cu-Fe '

-OK-

TDB_SSOL6: go p-3

... the command in full is GOTO_MODULE

POLY version 3.32

POLY: @@ Set conditions for a single equilibrium

POLY: s-c t=1000,p=1e5,n=1,w(cu)=.01

... the command in full is SET_CONDITION

POLY: c-e

... the command in full is COMPUTE_EQUILIBRIUM

Using global minimization procedure

Calculated 836 grid points in 0 s

Found the set of lowest grid points in 0 s

Calculated POLY solution 0 s, total time 0 s

POLY: @@ Select the fraction of Cu as the axis variable

```

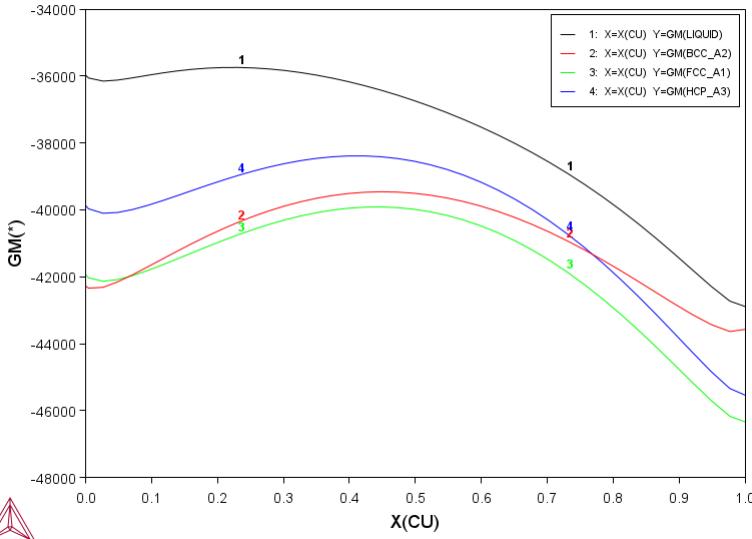
POLY: s-a-v 1
... the command in full is SET_AXIS_VARIABLE
Condition /NONE/: w(cu)
Min value /0/: 0
Max value /1/: 1
Increment /.025/: .025
POLY: @@ Remember to Save
POLY: save tcex02b y
... the command in full is SAVE_WORKSPACES
POLY: @@ Now a special STEP option is selected because the NORMAL
POLY: @@ option only calculates the stable phases. The option
POLY: @@ SEPARATE means that all entered phases are calculated
POLY: @@ separately.
POLY: step
... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/: ?
The following options are available:
NORMAL Stepping with given conditions
INITIAL_EQUILIBRIA An initial equilibrium stored at every step
EVALUATE Specified variables evaluated after each step
SEPARATE_PHASES Each phase calculated separately
T-ZERO T0 line calculation
PARAEQUILIBRIUM Paraequilibrium diagram
MIXED_SCHEIL Scheil with fast diffusing elements
ONE_PHASE_AT_TIME One phase at a time
Option? /NORMAL/: sep

Phase Region from 0.529789 for:
LIQUID
BCC_A2
FCC_A1
HCP_A3

Phase Region from 0.529789 for:
LIQUID
BCC_A2
FCC_A1
HCP_A3
*** Buffer saved on file *** c:\jenkins\workspace\generate_console_examples\examples\tcex02\tcex02b.POLY3
POLY: @@ Now plot the results in various ways
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2
POST: @@ Set the Gm of all phases on the y-axis
POST: s-d-a y gm(*)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*: *
POST: @@ and the mole percent of Cu on the x-axis
POST: s-d-a x x(cu)
... the command in full is SET_DIAGRAM_AXIS
POST: set-lab d
... the command in full is SET_LABEL_CURVE_OPTION
POST:
POST: set-title example 2f
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 2f

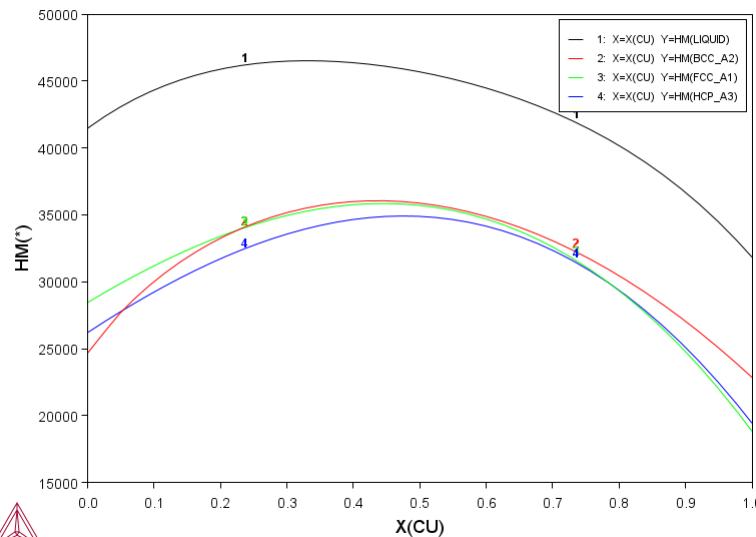


```

POST:
POST:Hit RETURN to continue
POST: @@ Now plot the enthalpy
POST: s-d-a y hm(*)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*: *
POST: set-title example 2g
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

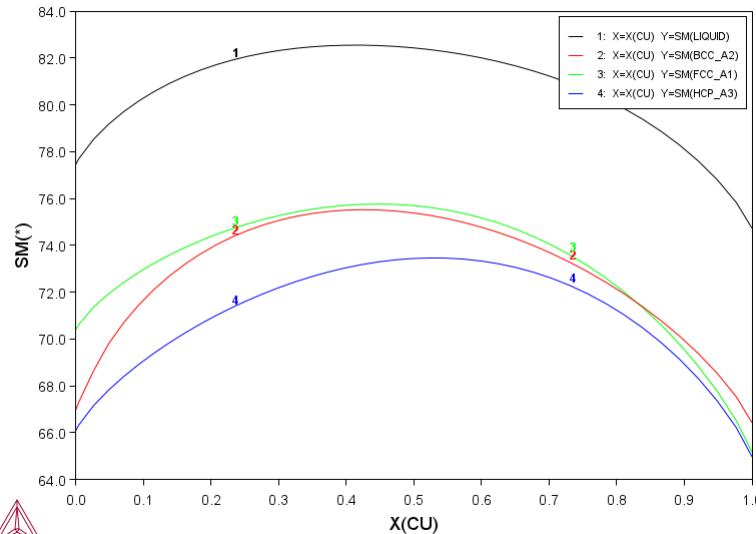
example 2g



```

POST:
POST:Hit RETURN to continue
POST: @@ and finally the entropy
POST: s-d-a y sm(*)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*: *
POST: set-title example 2h
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
example 2h

```



```

POST:
POST:Hit RETURN to continue
POST: @@ The last example plots the Fe-V-C ternary system.
POST: @@ Calculate and plot Gm from the iron corner to VC
POST: ba
... the command in full is BACK
POLY: go da
... the command in full is GOTO_MODULE
TDB_SSOL6: rej sys
... the command in full is REJECT
VA DEFINED
BCC_B2          FCC_L12          FCC_COV
FCC_AUCU        HCP_ORD        REJECTED
GAS:G REJECTED
REINITIATING GES .....
TDB_SSOL6: d-sys fe v c
... the command in full is DEFINE_SYSTEM
FE                  V                  C
DEFINED
TDB_SSOL6: rej ph / all
... the command in full is REJECT
LIQUID:L          FCC_A1          BCC_A2
HCP_A3          HCP_ZN          DIAMOND_A4
TETRAGONAL_U    CBCC_A12        CUB_A13
ORTORHOMBIC_A20 SIGMA           GRAPHITE
LAVES_C14        LAVES_C15        LAVES_C36
CEMENTITE        KSI_CARBIDE      M23C6
M7C3            M3C2            V3C2
M5C2            MC_ETA          M4N
FECN_CHI         ALM_D019        AL5FE4
ALTA_SIGMA       ALTI            FEPD
FEPD3           FESB            FEU6

```

```

FE2U           FEUZR_DELTA          FEZR2
FEZR3           VSSI _REJECTED
TDB_SSOL6: rest ph fcc_a1 bcc_a2 hcp_a3 liq
... the command in full is RESTORE
FCC_A1          BCC_A2            HCP_A3
LIQUID:L RESTORED
TDB_SSOL6: get
... the command in full is GET_DATA
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
Creating a new composition set FCC_A1#2
... the command in full is AMEND_PHASE DESCRIPTION
... the command in full is AMEND_PHASE DESCRIPTION
... the command in full is AMEND_PHASE DESCRIPTION
Creating a new composition set HCP_A3#2
PARAMETERS .....
FUNCTIONS .....

List of references for assessed data

'Data for the C-Fe system are taken from the assessment of P Gustafson,
Report TRITA-MAC-0237, October 1984, Scand. J. Metall., 1985, 14, 259
-267. "A Thermodynamic Evaluation of the Fe-C system". Data for other
phases not stable in the binary system are from: WM Huang: Report
TRITA-MAC 411 (Rev 1989); Metall. Trans. A, 1990, 21A, 2115-2123. "A
Thermodynamic Assessment of the Fe-Mn-C system", WM Huang: Report
TRITA-MAC 441 (1990), Metall. Trans. A, 1991, 22A(9), 1911-1920. "
Thermodynamic Properties of the Fe-Mn-V-C System", BJ Lee (1991),
unpublished revision of data for the C-Cr-Fe-Ni system. H Du and M
Hillert: Z. Metallkde, 1991, 82(4), 310-316. "An Assessment of the Fe
-C-N System". H Du: J. Phase Equil., 1993, 14(6), 682-693. "A
Reevaluation of the Fe-N and Fe-C-N systems". Note: Data for the V3C2
phase were modified to be 10 J/mol more positive than those for the
M3C2 phase. The data for the liquid data were modified by Tatjana
Buhler to prevent bcc phase from becoming stable at high temperatures.
>> C-Fe '
'P. Franke, unpublished revisions, Aachen, 2006-2008'
'Data for the C-Fe-V system are taken the assessments of WM Huang: Report
TRITA-MAC 432 (1990), Z. Metallkde, 1991, 82(5), 391-401. "A
thermodynamic evaluation of the Fe-V-C system". BJ Lee and DN Lee:
Report TRITA-MAC 474 (1991), Calphad, 1991, 15(3), 293-306. "A
thermodynamic study on the Fe-V-C system". >> C-Fe-V '
'Data for the C-V system are taken from the assessment of WM Huang: Z.
Metallkde, 1991, 82, (3), 174-181. "An Assessment of the V-C System".
Additional data are from further work by WM Huang: Report TRITA-MAC
441 (1990), BJ Lee: Report TRITA-MAC 475 (1991). >> C-V '
'Data for the Fe-V system are from the assessments of WM Huang: TRITA-MAC
432 (Rev 1989,1990), Z. Metallkde, 1991, 82(5), 391-401. "A
thermodynamic evaluation of the Fe-V-C system", WM Huang: Met. Trans.
A, 1991, 22(9), 1911-1920. "Thermodynamic properties of the Fe-Mn-V-C
system". >> Fe-V '
-OK-
TDB_SSOL6: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY: @@ Set conditions for a single equilibrium
POLY: s-c t=1000,p=1e5,n=1,w(v)=.0015,x(c)=.001
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated      7821 grid points in          0 s
Found the set of lowest grid points in          0 s
Calculated POLY solution          0 s, total time    0 s
POLY: l-e,..
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium =      1, label A0 , database: SSOL6

Conditions:
T=1000, P=100000, N=1, W(V)=1.5E-3, X(C)=1E-3
DEGREES OF FREEDOM 0

Temperature 1000.00 K ( 726.85 C), Pressure 1.000000E+05
Number of moles of components 1.000000E+00, Mass in grams 5.57951E+01
Total Gibbs energy -4.23963E+04, Enthalpy 2.45646E+04, Volume 0.000000E+00

Component      Moles      W-Fraction   Activity   Potential Ref.stat
C             1.0000E-03  2.1527E-04  3.4515E-02 -2.7990E+04 SER
FE            9.9736E-01  9.9828E-01  6.1891E-03 -4.2279E+04 SER
V              1.6429E-03  1.5000E-03  4.0605E-07 -1.2236E+05 SER

BCC_A2          Status ENTERED     Driving force 0.0000E+00
Moles 9.9814E-01, Mass 5.5735E+01, Volume fraction 0.0000E+00 Mass fractions:
FE 9.99368E-01 V 6.07213E-04 C 2.49276E-05

FCC_A1#2        Status ENTERED     Driving force 0.0000E+00
Moles 1.8638E-03, Mass 6.0520E-02, Volume fraction 0.0000E+00 Mass fractions:
V 8.23694E-01 C 1.75507E-01 FE 7.99487E-04

POLY:Hit RETURN to continue
POLY: l-st p
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES
PHASE          STATUS      DRIVING FORCE    MOLES
FCC_A1#2       ENTERED    0.000000E+00  1.863776E-03
BCC_A2         ENTERED    0.000000E+00  9.981362E-01
FCC_A1#1       ENTERED   -3.462152E-02  0.000000E+00
HCP_A3#2       ENTERED   -2.875358E-01  0.000000E+00
HCP_A3#1       ENTERED   -2.875358E-01  0.000000E+00
LIQUID         ENTERED   -6.510578E-01  0.000000E+00

POLY:Hit RETURN to continue
POLY: @@ Note we have several composition sets because fcc
POLY: @@ (and possibly hcp) can exist both as metallic and
POLY: @@ as carbide. However, in this case it is unnecessary
POLY: @@ as we are only interested in the value of the
POLY: @@ thermodynamic functions, not the equilibrium, and therefore
POLY: @@ we suspend them
POLY:
POLY: c-s p hcp_a3#
... the command in full is CHANGE_STATUS
Status: /ENTERED/: sus

```

```

POLY: l-c
... the command in full is LIST CONDITIONS
T=1000, P=100000, N=1, W(V)=1.5E-3, X(C)=1E-3
DEGREES OF FREEDOM 0
POLY: @@ We would like to calculate the Gibbs energy from
POLY: @@ pure Fe to the corner VC. Select a line with equal
POLY: @@ fraction of V and C
POLY: s=x(v)-x(c)=0
... the command in full is SET_CONDITION
POLY: s=c w(v)=none
... the command in full is SET_CONDITION
POLY: l-c
... the command in full is LIST_CONDITIONS
T=1000, P=100000, N=1, X(C)=1E-3, X(V)-X(C)=0
DEGREES OF FREEDOM 0
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
10 ITS, CPU TIME USED 0 SECONDS
POLY: l-e,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: SSOL6

Conditions:
T=1000, P=100000, N=1, X(C)=1E-3, X(V)-X(C)=0
DEGREES OF FREEDOM 0

Temperature 1000.00 K ( 726.85 C), Pressure 1.000000E+05
Number of moles of components 1.000000E+00, Mass in grams 5.57983E+01
Total Gibbs energy -4.23424E+04, Enthalpy 2.46245E+04, Volume 0.000000E+00

Component Moles W-Fraction Activity Potential Ref.stat
C 1.0000E-03 2.1526E-04 9.5381E-02 -1.9538E+04 SER
FE 9.9800E-01 9.9887E-01 6.1904E-03 -4.2277E+04 SER
V 1.0000E-03 9.1295E-04 1.6021E-07 -1.3010E+05 SER

BCC_A2 Status ENTERED Driving force 0.0000E+00
Moles 9.9858E-01, Mass 5.5752E+01, Volume fraction 0.0000E+00 Mass fractions:
FE 9.99691E-01 V 2.40126E-04 C 6.83917E-05

FCC_A1#2 Status ENTERED Driving force 0.0000E+00
Moles 1.4208E-03, Mass 4.5810E-02, Volume fraction 0.0000E+00 Mass fractions:
V 8.19759E-01 C 1.78955E-01 FE 1.28625E-03
POLY: Hit RETURN to continue
POLY: @@ Set the fraction of C as the axis
POLY: @@ The fraction of V will be the same
POLY: s-a-v
... the command in full is SET_AXIS_VARIABLE
Axis number: /1/: 1
Condition /NONE/: x(c)
Min value /0/: 0
Max value /1/: .5
Increment /.0125/: .0125
POLY: save tcex02c y
... the command in full is SAVE_WORKSPACES
POLY: @@ step along the axis
POLY: step
... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/: sep

Phase Region from 0.330065 for:
LIQUID
BCC_A2
FCC_A1#1
FCC_A1#2

Phase Region from 0.330065 for:
LIQUID
BCC_A2
FCC_A1#1
FCC_A1#2

Phase Region from 0.480604E-02 for:
HCP_A3#1

Phase Region from 0.480604E-02 for:
HCP_A3#1
*** Buffer saved on file *** c:\jenkins\workspace\generate_console_examples\examples\tcex02\tcex02c.POLY3
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2
POST: @@ plot the Gm versus carbon content
POST: l-p-s
... the command in full is LIST_PLOT_SETTINGS
GRAPHIC DEVICE: TC-UNITE Driver (#22) PLOTFILE: SCREEN
FONT: (# 1) Arial Bold
AXIS PLOT : YES
RASTER PLOT : NO
TRIANGULAR PLOT : NO

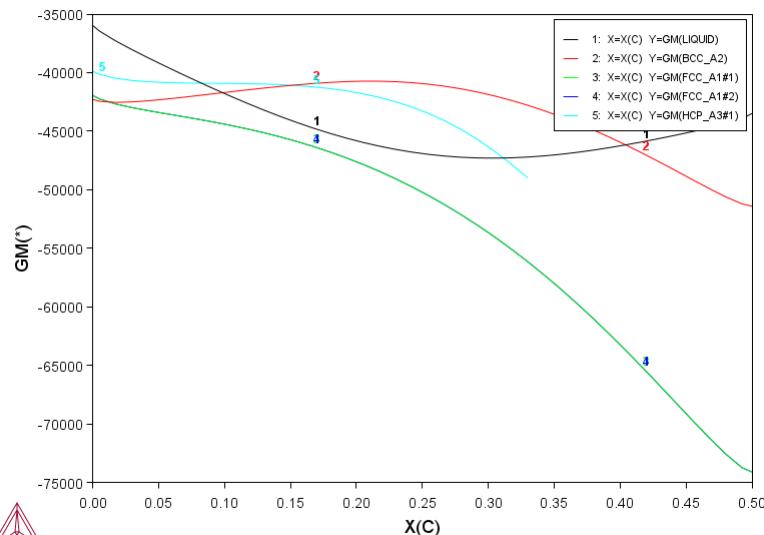
AUTOMATIC SCALING

AUTOMATIC AXIS TEXT

AXIS VARIABLES
POST: s-d-a x x(c)
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y gm(*)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST:
POST: set-lab d
... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 2i
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 2i



POST:

POST:Hit RETURN to continue

POST: @@ This example is about more partial derivatives

POST: back

POLY: go da

... the command in full is GOTO_MODULE

TDB_SSOL6: rej sys

... the command in full is REJECT

VA_DEFINED

BCC_B2 FCC_L12 FCC_COV
FCC_AUCU HCP_ORD REJECTED

GAS:G REJECTED

REINITIATING GES

TDB_SSOL6: def-sys al cu

... the command in full is DEFINE_SYSTEM

AL CU DEFINED

TDB_SSOL6: get

... the command in full is GET_DATA

REINITIATING GES

ELEMENTS

SPECIES

PHASES

... the command in full is AMEND_PHASE_DESCRIPTION

PARAMETERS ...

FUNCTIONS

List of references for assessed data

'Taken from ACMSZ-1, based on unpublished assessment of N Saunders published in the COST507 final report COST507 Thermochemical database for light metal alloys, Volume 2 eds I Ansara, A T Dinsdale and M H Rand, July 1998, EUR18499 Updates from V.T. Witusiewicz, U. Hecht, S.G. Fries, S. Rex, JALCOM 385 (2004) 133-143 (Al-Cu) and H.Liang, Y.A.Chang, JPE 19 (1998) 25-37 (Al-Cu-Zn). >> Al-Cu '
'C Servant and I Ansara: J. Chim. Phys. 1997, 94, 869-888. "Thermodynamic assessment of the Al-Nb system". >> Al-Nb '
' F. Yin, X. Su, Z. Li, P. Zhang, Z. Metallkde, 92, 5 (2001) 447-450. Data from ThermoData - supplied to SGTE December 2007 >> Al-Pr '
'SG Fries, HL Lukas, R Konetzki, and R Schmid-Fetzer: J. Phase Equil., 1994, 15(6), 606-614. "Experimental investigation and thermodynamic optimization of the Y-Cu binary system". Note: The data for the CuY phase have been modified slightly to correct the calculated invariant temperatures. >> Cu-Y '
'M Kowalski and PJ Spencer: J. Phase Equil., 1993, 14(4), 432-438. "Thermodynamic reevaluation of the Cu-Zn system". Some v. minor differences in gamma-brass data wrt SOLDERS >> Cu-Zn '
'Liang Y, Guo C, Li C, Du Z, Journal of Alloys and Compounds, 2008, 460, 314-319 "Thermodynamic modeling of the Al-Cr system." >> Al-Cr '
'Data for the Al-Li system are from an unpublished assessment of N Saunders published in the COST507 final report: COST507 Thermochemical Database for Light Metal Alloys, Vol 2, eds by I Ansara, AT Dinsdale and MH Rand, July 1998, EUR18499. >> Al-Li '
' Data supplied by ThermoData to SGTE - December 2007 A. Saccone, G. Cacciamani, D. Macchio, G. Borzone, R. Ferro, Intermetallics, 6 (1998) 201-215. >> Al-Sm '
'W. Huang, S.M. Opalka, D. Wang, T.B. Flanagan, Calphad, 31, 315-29(2007) > Cu-Pd '

-OK-

TDB_SSOL6: go p-3

... the command in full is GOTO_MODULE

POLY version 3.32

POLY: s-c t=1400 p=1e5 n=1 x(al)=.1

... the command in full is SET_CONDITION

POLY: c-e

... the command in full is COMPUTE_EQUILIBRIUM

Using global minimization procedure

Calculated 11669 grid points in 4 s

Found the set of lowest grid points in 0 s

Calculated POLY solution 0 s, total time 4 s

POLY: l-e,,,

... the command in full is LIST_EQUILIBRIUM

Output from POLY-3, equilibrium = 1, label A0 , database: SSOL6

Conditions:

T=1400, P=100000, N=1, X(AL)=0.1

DEGREES OF FREEDOM 0

```

Temperature 1400.00 K ( 1126.85 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 5.98896E+01
Total Gibbs energy -8.53069E+04, Enthalpy 3.62263E+04, Volume 0.00000E+00

Component Moles W-Fraction Activity Potential Ref.stat
AL 1.0000E-01 4.5053E-02 1.3593E-06 -1.5724E+05 SER
CU 9.0000E-01 9.5495E-01 1.3045E-03 -7.7314E+04 SER

LIQUID Status ENTERED Driving force 0.0000E+00
Moles 1.0000E+00, Mass 5.9890E+01, Volume fraction 0.0000E+00 Mass fractions:
CU 9.54947E-01 AL 4.50529E-02
POLY:Hit RETURN to continue
POLY: @@ Check the activity of aluminum
POLY: show acr(al)
... the command in full is SHOW_VALUE
ACR(AL)=1.359263E-6
POLY: @@ This activity value is referred to fcc Al at 298.15 K.
POLY: @@ Set the proper reference state for activities
POLY: set-ref-state al
... the command in full is SET_REFERENCE_STATE
Reference phase: liq
Temperature */*:
Pressure /1E5/:
POLY:
POLY: set-ref-state cu
... the command in full is SET_REFERENCE_STATE
Reference phase: liq
Temperature */*:
Pressure /1E5/:
POLY:
POLY: show acr(al)
... the command in full is SHOW_VALUE
ACR(AL)=8.0990275E-4
POLY: @@ This value is better. The corresponding chemical potential is
POLY: show mur(al)
... the command in full is SHOW_VALUE
MUR(AL)=-82862.697
POLY: @@ The relation is simply that acr(al)=exp(mur(al)/RT). Check that
POLY: enter fun test
... the command in full is ENTER_SYMBOL
Function: exp(mur(al)/8.31451/T);
POLY: show test
... the command in full is SHOW_VALUE
TEST=8.0990275E-4
POLY:Hit RETURN to continue
POLY: @@ POLY allows the calculation of partial derivatives of thermodynamic
POLY: @@ quantities of original reference state with respect to fractions
POLY: @@ that are conditions. For example
POLY: show gm.x(al)
... the command in full is SHOW_VALUE
GM.X(AL)=-79930.097
POLY: @@ This is not the same as the chemical potential. It actually
POLY: @@ is equal to the so-called diffusion potential: mu(al)-mu(cu).
POLY:
POLY: ent fun diffmu=mu(al)-mu(cu);
... the command in full is ENTER_SYMBOL
POLY: show diffmu
... the command in full is SHOW_VALUE
DIFFMU=-79930.097
POLY: @@ The relation between the chemical potential and the partial derivative is
POLY: @@ mu(al) = gm + gm.x(al) - x(al)*gm.x(al)
POLY:
POLY: @@ We can also enter this as a function.
POLY: enter fun dgdx=gm+gm.x(al)-x(al)*gm.x(al);
... the command in full is ENTER_SYMBOL
POLY: sh dgdx
... the command in full is SHOW_VALUE
DGDX=-157243.97
POLY: sh mu(al)
... the command in full is SHOW_VALUE
MU(AL)=-157243.97
POLY: @@ Partial entropy is the negative of mu(al).t;
POLY: ent fun ps=-mu(al).t;
... the command in full is ENTER_SYMBOL
POLY: sh ps
... the command in full is SHOW_VALUE
PS=95.218667
POLY: @@ Partial enthalpy is h = g + s*t
POLY: enter fun ph=mu(al)+ps*t;
... the command in full is ENTER_SYMBOL
POLY: sh ph
... the command in full is SHOW_VALUE
PH=-23937.838
POLY: @@ Partial enthalpy can also be calculated in a similar way as chemical
POLY: @@ potential
POLY: @@ partial enthalpy = hm + hm.x(al) - x(al)*hm.x(al)
POLY: ent fun ph1=hm+hm.x(al)-x(al)*hm.x(al);
... the command in full is ENTER_SYMBOL
POLY: sh ph1
... the command in full is SHOW_VALUE
PH1=-23937.838
POLY: @@ As can be seen, ph1 = ph.
POLY: @@ Another useful quantity is mu(al).x(al). That is related to
POLY: @@ the thermodynamic factor and part of the diffusion coefficient.
POLY: show mu(al).x(al)
... the command in full is SHOW_VALUE
MU(AL).X(AL)=324789.82
POLY:
POLY: set-inter
... the command in full is SET_INTERACTIVE
POLY:

```

tce03**SYS:About**

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

```
SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce03\tce03.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Calculating an isothermal section using the Ternary module
SYS:
SYS: set-log ex03.,
SYS:
SYS: go tern
... the command in full is GOTO_MODULE

Quick ternary phase diagram calculation module

THERMODYNAMIC DATABASE module
Database folder: C:\jenkins\workspace\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA           /- DEFINED
DICTRA_FCC_A1 REJECTED
Current database: Iron Demo Database v4.0

VA           /- DEFINED
Database: /FEDEMO/: FEDEMO
First element: ?
No list of assessed systems in this database
First element: fe
Second element: c
Third element: cr
Phase Diagram, Monovariants, or Liquidus Surface: /Phase_Diagram/: Phase_Diagram
Temperature (C) /1000/: 1200
Global minimization on: /Y/: Y
VA           /- DEFINED
REINITIATING GES .....
C           CR           FE
      DEFINED

*****
* WARNING: This database has no list of assessed systems *
*   The diagram may be wrong. *
*****


Quit? /Y/: N
15:22:45,606 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
Creating a new composition set FCC_A1#2
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS .....
FUNCTIONS .....

List of references for assessed data

'A.T. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121 -127; Molar
    volumes'
'M. Ghasemi, Thermo-Calc Software AB, Sweden, 2019; Viscosity of metallic
    liquid'
'M Ghasemi, Thermo-Calc Software AB: assessing the surface tension of
    metallic liquid'
'M. Ghasemi, Thermo-Calc Software AB, Sweden, 2020; Unifying liquid volume
    database'
'Y. Tang, in TCCU2, Thermo-Calc Software AB, Stockholm, Sweden'
'M. J. Assael, J. Phys. Chem. Ref. Data 35 (2006) 285; Fe, Al'
'A.V. Khvan, B. Hallstedt, K. Chang, CALPHAD, 39, 54-61(2012); C -Cr-Nb'
'A.V. Khvan, B. Hallstedt, C. Broeckmann, CALPHAD, 46, 24 -33(2014); Cr-Fe
    -C'
'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
'B.J. Lee, CALPHAD, 17 (1993) 251-268; revision of Fe-Cr and Fe -Ni liquid'
'J-O. Andersson, CALPHAD, 11 (1987) 271-276; TRITA 0314; C-CR'
'X.G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
'X.G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
    volumes'
'J-O. Andersson, Metall. Trans. A, 19A (1988) 627-636 TRITA 0207 (1986); C
    -CR-FE'
'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270
    (1986); CR-FE'
'N. Saunders, COST 507 Report (1998); Cr-Ti'
'B.J. Lee, unpublished work at KTH (1999); update of steel database'
'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equilib., 19
    (1998) 441-448; Fe-Ti'
'R. Naraghi, Thermo-Calc Software AB, Sweden, 2019; Cr-Fe-Nb'
'B.J. Lee, Metall. Trans. A, 24A (1993) 1017-1025; Fe-Cr-Mn-C'
'R. Naraghi, Thermo-Calc Software AB, Sweden, Volume data updated for
    TCFE9 database (TCFE v9.0, Jan, 2017).'
'W. Huang, Metall. Trans. A, 21A (1990) 2115-2123; TRITA-MAC 411 (Rev
    1989); C-FE-MN'
'B.J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
'P. Villars, L.D. Calvert. Pearson's handbook of crystallographic data for
    intermetallic phases, Metals park, Ohio 1985: American society for
    metals'
'B. Hallstedt, D. Djurovic, J. von Appen, R. Dronskowski, A. Dick, F.
    Koermann, T. Hickel, J. Neugebauer, CALPHAD, 34, 129 -33(2010); Fe-C'
'P. Gustafson, TRITA-MAC 354 (1987); C-Cr-Fe-Mo-W'
```

'J-O. Andersson, Metall. Trans. A, 19A (1988) 1385-1394; TRITA 0322 (1986);
 CR-FE-MO'
 'J. Bratberg, Z. Metallkd., 96 (2005) 335-344; Fe-Cr-Mo-C'
 'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2016; FCC Fe-Cr-C and C-Cr-Ni'
 'C. Qui, ISIJ International, 32 (1992), 1117-1127; Trita-MAC 482 (1992)
 Revision; C-Cr-Fe-Mo'
 'J-O. Andersson, CALPHAD, 12 (1988) 9-23; TRITA 0321 (1986); C -FE-MO'
 'P. Gustafson, Metall. Trans. A, 19A (1988) 2547-2554; TRITA-MAC 348,
 (1987); C-CR-FE-W'
 'H. Gohring, O. Fabrichnaya, A. Leineweber, E.J. Mittemeijer, Metall.
 Mater. Trans. A, 47A, 6173-86(2016); FE-N, and Fe-C-N'
 'K. Frisk, Metall. Trans. A, 21A (1990) 2477-2488; TRITA 0409 (1989); CR
 -FE-N'
 'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, Calphad 35.4
 (2011) 479-491; Fe-Mn-C'
 'B. Sundman et al., Report EUR 20315, Contract No 7210-PR/050, 2002; New
 Sigma model'

-OK-

The condition X(CR)=.1234 created

The condition X(FE)=.1234 created

Version S mapping is selected

Generating start equilibrium 1
 Generating start equilibrium 2
 Generating start equilibrium 3
 Generating start equilibrium 4
 Generating start equilibrium 5
 Generating start equilibrium 6
 Generating start equilibrium 7
 Generating start equilibrium 8
 Generating start equilibrium 9
 Generating start equilibrium 10

Organizing start points

Using ADDED start equilibria

Generating start point 1
 Generating start point 2
 Generating start point 3
 Generating start point 4
 Generating start point 5
 Generating start point 6
 Generating start point 7
 Generating start point 8
 Generating start point 9
 Generating start point 10
 Working hard
 Generating start point 11
 Generating start point 12
 Generating start point 13
 Generating start point 14
 Generating start point 15
 Generating start point 16
 Generating start point 17
 Generating start point 18
 Generating start point 19
 Generating start point 20
 Generating start point 21

Phase region boundary 1 at: 1.750E-01 1.750E-01
 ** GRAPHITE
 M7C3

Calculated. 11 equilibria

Phase region boundary 2 at: 2.652E-01 8.482E-02
 ** GRAPHITE
 ** M3C2
 M7C3

Calculated. 20 equilibria

Phase region boundary 3 at: 5.652E-01 8.482E-02
 ** M3C2
 M7C3

Calculated. 18 equilibria

Phase region boundary 4 at: 3.000E-01 0.000E+00
 GRAPHITE
 ** M3C2

Phase region boundary 5 at: 2.652E-01 8.482E-02
 ** GRAPHITE
 M7C3

Calculated. 18 equilibria

Phase region boundary 6 at: 9.822E-02 2.518E-01
 ** CEMENTITE
 ** GRAPHITE
 M7C3

Phase region boundary 7 at: 1.457E-01 5.793E-01
 ** CEMENTITE
 M7C3

Calculated. 3 equilibria

Phase region boundary 8 at: 1.610E-01 5.640E-01
 ** LIQUID
 ** CEMENTITE
 M7C3

Calculated. 7 equilibria

Phase region boundary 9 at: 1.414E-01 6.131E-01
 ** LIQUID
 M7C3

Calculated. 7 equilibria

Phase region boundary 10 at: 1.820E-01 5.842E-01
 ** LIQUID
 ** FCC_A1#2
 M7C3

Calculated. 28 equilibria

Phase region boundary 11 at: 1.646E-01 6.458E-01
 ** FCC_A1#1
 M7C3

Calculated. 28 equilibria

Phase region boundary 12 at: 3.658E-01 4.629E-01
 ** FCC_A1#1

** M23C6

M7C3

Phase region boundary 13 at: 5.141E-01 2.324E-01

** M23C6

M7C3

Calculated 33 equilibria

Phase region boundary 14 at: 3.369E-01 5.455E-01

** FCC_A1#1

** M23C6

Calculated. 2 equilibria

Phase region boundary 15 at: 3.450E-01 5.382E-01

** BCC_A2

** FCC_A1#1

** M23C6

Phase region boundary 16 at: 2.028E-01 7.787E-01

** BCC_A2

** FCC_A1#1

Calculated 21 equilibria

Phase region boundary 17 at: 3.620E-01 5.294E-01

** BCC_A2

M23C6

Calculated 65 equilibria

Phase region boundary 18 at: 6.933E-02 8.073E-01

LIQUID

** FCC_A1#1

Calculated 26 equilibria

Phase region boundary 19 at: 8.694E-02 6.926E-01

** LIQUID

CEMENTITE

Calculated. 5 equilibria

Phase region boundary 20 at: 6.004E-02 7.169E-01

** LIQUID

CEMENTITE

** GRAPHITE

Phase region boundary 21 at: 3.674E-02 3.383E-01

CEMENTITE

** GRAPHITE

Calculated. 3 equilibria

Terminating at known equilibrium

Phase region boundary 22 at: 2.330E-02 3.787E-01

LIQUID

** GRAPHITE

Calculated. 19 equilibria

Phase region boundary 23 at: 1.750E-01 1.750E-01

** GRAPHITE

M7C3

Calculated. 9 equilibria

Terminating at known equilibrium

Phase region boundary 24 at: 1.750E-01 1.750E-01

** GRAPHITE

M7C3

Calculated. 11 equilibria

Terminating at known equilibrium

Phase region boundary 25 at: 1.750E-01 1.750E-01

** GRAPHITE

M7C3

Calculated. 9 equilibria

Terminating at known equilibrium

Phase region boundary 26 at: 3.000E-01 0.000E+00

GRAPHITE

** M3C2

Calculated. 31 equilibria

Phase region boundary 27 at: 2.652E-01 8.482E-02

** GRAPHITE

M7C3

Calculated. 1 equilibria

Terminating at known equilibrium

Phase region boundary 28 at: 5.652E-01 8.482E-02

** M3C2

M7C3

Calculated. 31 equilibria

Phase region boundary 29 at: 6.432E-01 6.818E-03

** M3C2

M7C3

Calculated. 15 equilibria

Phase region boundary 30 at: 6.432E-01 6.818E-03

** M3C2

M7C3

Calculated. 9 equilibria

Terminating at known equilibrium

Phase region boundary 31 at: 8.930E-01 3.418E-03

BCC_A2

** M23C6

Calculated. 12 equilibria

Phase region boundary 32 at: 8.930E-01 3.418E-03

BCC_A2

** M23C6

Calculated. 54 equilibria

Terminating at known equilibrium

Phase region boundary 33 at: 1.172E-02 3.947E-01

LIQUID

** GRAPHITE

Calculated. 3 equilibria

Terminating at known equilibrium

Phase region boundary 34 at: 1.172E-02 3.947E-01

LIQUID

```

** GRAPHITE
Calculated           22 equilibria
Phase region boundary 35 at:   6.068E-03  4.025E-01
    LIQUID
** GRAPHITE
Calculated           4 equilibria
Terminating at known equilibrium

Phase region boundary 36 at:   6.068E-03  4.025E-01
    LIQUID
** GRAPHITE
Calculated           9 equilibria
Phase region boundary 37 at:   1.262E-02  8.673E-01
    ** LIQUID
    FCC_A1#1
Calculated           10 equilibria
Phase region boundary 38 at:   1.262E-02  8.673E-01
    ** LIQUID
    FCC_A1#1
Calculated           7 equilibria
Terminating at known equilibrium

Phase region boundary 39 at:   4.578E-01  4.348E-01
    BCC_A2
    ** M23C6
Calculated           57 equilibria
Phase region boundary 40 at:   4.578E-01  4.348E-01
    BCC_A2
    ** M23C6
Calculated           11 equilibria
Terminating at known equilibrium

Phase region boundary 41 at:   6.789E-01  2.163E-01
    BCC_A2
    ** M23C6
Calculated           30 equilibria
Phase region boundary 42 at:   6.789E-01  2.163E-01
    BCC_A2
    ** M23C6
Calculated           33 equilibria
Terminating at known equilibrium
*** BUFFER SAVED ON FILE: C:\Users\azureuser\AppData\Local\Temp\ISOTHER_002.POLY3
CPU time for mapping      7 seconds
POSTPROCESSOR VERSION 3.2

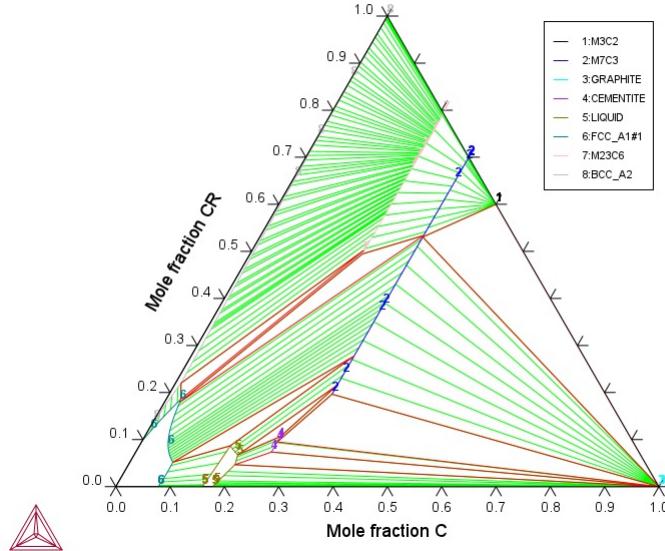
```

Setting automatic diagram axes

POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

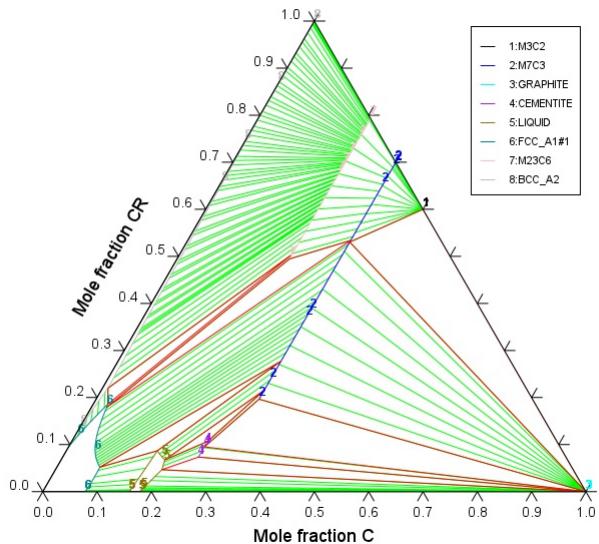
FE-C-CR at T=1473.15 K



```

POST:
POST: set-title example 3a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFILE
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

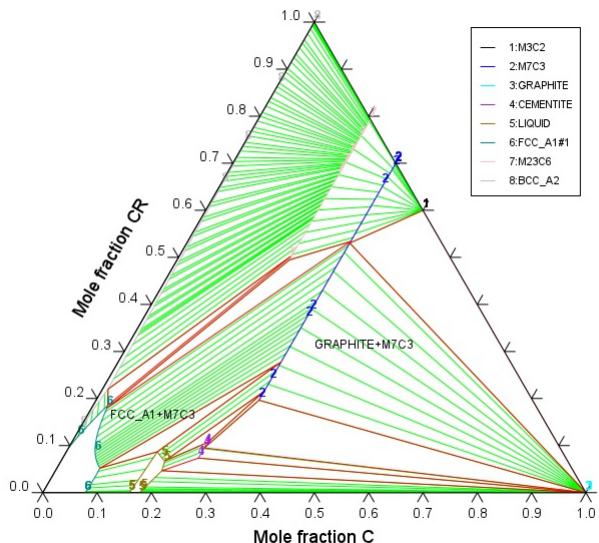
```

example 3a

```

POST:
POST:Hit RETURN to continue
POST: @@ Add some labels
POST: add .35 .3
... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
Automatic labelling not always possible
Using global minimization procedure
Using already calculated grid
Found the set of lowest grid points in          0 s
Calculated POLY solution   0 s, total time    0 s
Stable phases are: GRAPHITE+M7C3
Text size: /.36/:
POST: add .05 .15
... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
Automatic labelling not always possible
Using global minimization procedure
Using already calculated grid
Found the set of lowest grid points in          0 s
Calculated POLY solution   0 s, total time    0 s
Stable phases are: FCC_A1+M7C3
Text size: /.36/:
POST: set-title example 3b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 3b

```

POST:
POST:Hit RETURN to continue
POST: add .3 .01
... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
Automatic labelling not always possible
Using global minimization procedure
Using already calculated grid
Found the set of lowest grid points in          0 s
Calculated POLY solution   0 s, total time    0 s
Stable phases are: LIQUID+GRAPHITE
Text size: /.36/:
POST: add .35 .1
... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:

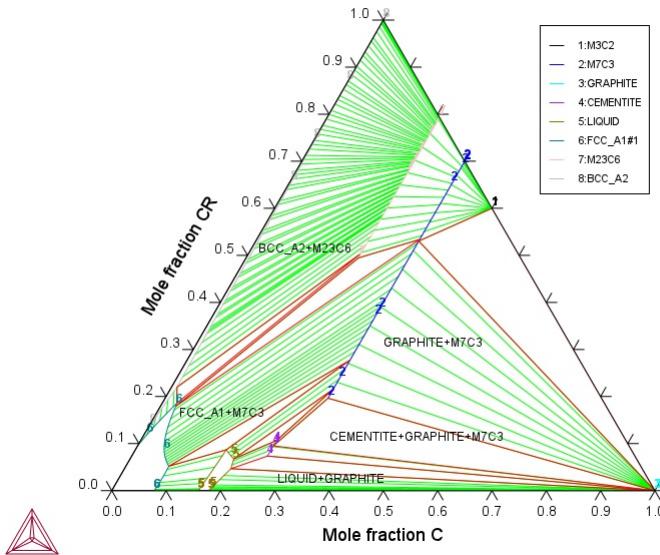
```

```

Automatic labelling not always possible
Using global minimization procedure
Using already calculated grid
Found the set of lowest grid points in          0 s
Calculated POLY solution      0 s, total time    0 s
Stable phases are: CEMENTITE+GRAPHITE+M7C3
Text size: / .36/:
POST: add .02 .5
... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
Automatic labelling not always possible
Using global minimization procedure
Using already calculated grid
Found the set of lowest grid points in          0 s
Calculated POLY solution      0 s, total time    0 s
Stable phases are: BCC_A2+M23C6
Text size: / .36/:
POST: set-title example 3c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 3c

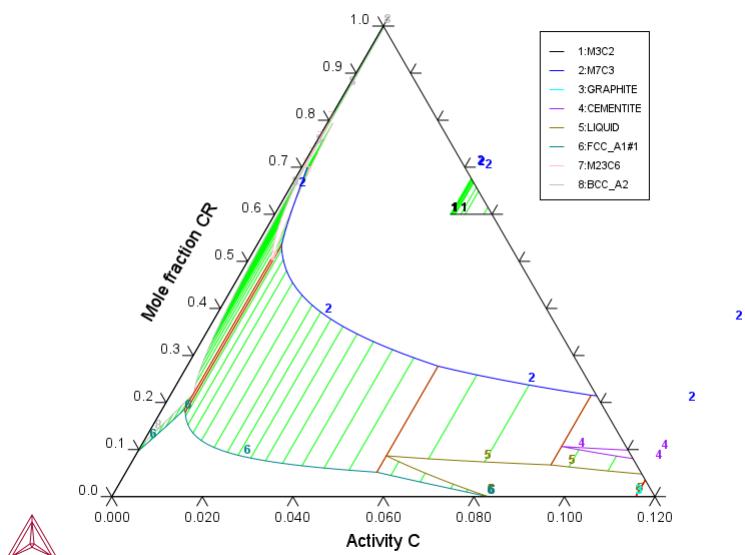


```

POST:
POST:Hit RETURN to continue
POST: @@ We can try the same exercise as in TCEX_01 which uses
POST: @@ carbon activity on one axis
POST: s-d-a x ac c
... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 3d
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 3d



```

POST:
POST:Hit RETURN to continue
POST: @@ With these axes it is better to have a square diagram.
POST: s-dia-type
... the command in full is SET_DIAGRAM_TYPE

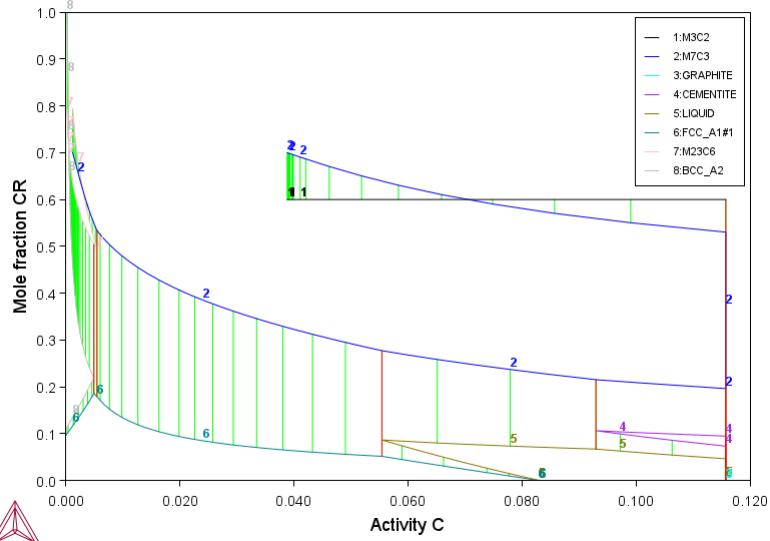
```

```

TRIANGULAR DIAGRAM (Y OR N) /N/: N
CREATE TETRAHEDRON WRML FILE (Y OR N) /N/:
POST:
POST: set-title example 3e
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 3e

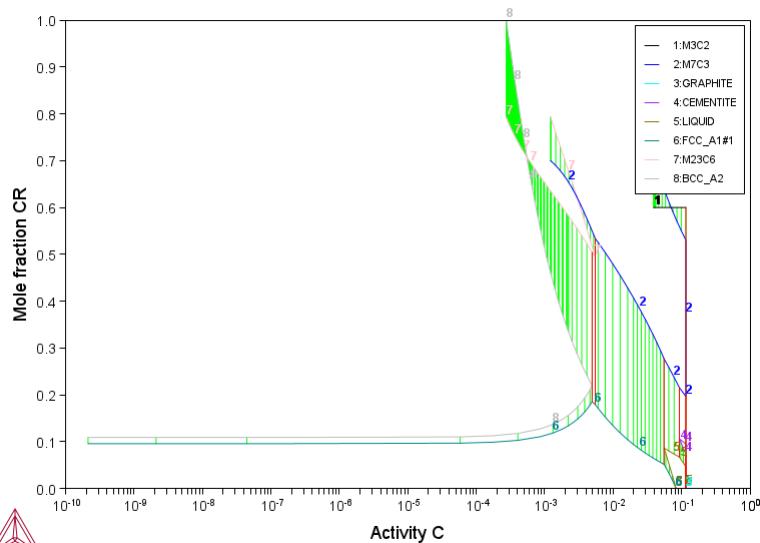


```

POST:
POST:Hit RETURN to continue
POST: @@ The activity axis is probably better as logarithmic
POST: s-a-ty x
... the command in full is SET_AXIS_TYPE
AXIS TYPE /LINEAR/: log
POST: set-title example 3f
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 3f



```

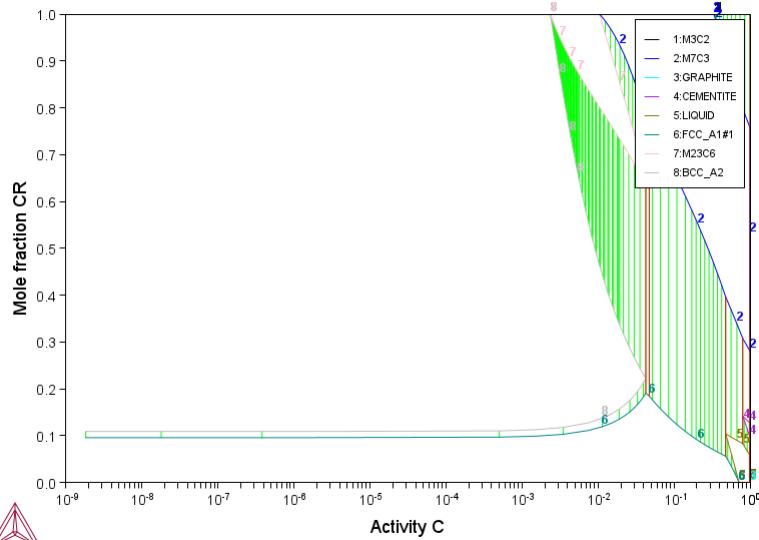
POST:
POST:Hit RETURN to continue
POST: @@ In order for pure graphite to have activity one, the reference
POST: @@ state of C should be set to graphite. In addition,
POST: @@ the solubility lines now cross. Is the diagram wrong?
POST: @@ No, in this case one should not use the mole fraction of Cr
POST: @@ but the metallic fraction. This can be fixed by setting
POST: @@ the status of C to "special". All species set as special
POST: @@ are excluded from the summation of fractions.
POST: @@ The special status is set in the POLY module
POST: ba
... the command in full is BACK
SYS: go p-3
... the command in full is GOTO_MODULE
POLY:
POLY: s-r-s
... the command in full is SET_REFERENCE_STATE
Component: c

```

```

Reference phase: gra
Temperature /*/:
Pressure /1E5/:
POLY: ch-st
... the command in full is CHANGE_STATUS
For phases, species or components? /PHASES/: c
Name(s): c
Status: /ENTERED/: ?
FILE SYSTEM ERROR IN FILHLP
ERROR          1717   READING HELP FILE
Status: /ENTERED/: special
POLY:
POLY: post
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
example 3g

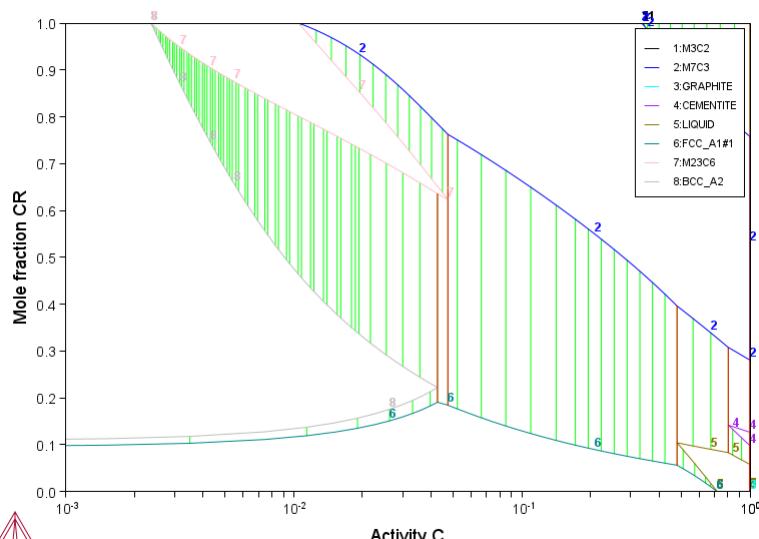
```



```

POST:
POST:Hit RETURN to continue
POST: @@ Finally scale
POST: s-s x n .001 1
... the command in full is SET_SCALING_STATUS
POST: set-title example 3h
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
example 3h

```



```

POST:
POST:Hit RETURN to continue
POST: @@ This kind of diagram is useful to understand diffusion paths.
POST:
POST: @@ The phase labels were lost when we changed axis
POST: @@ To add them back
POST: add .05 .3
... the command in full is ADD_LABEL_TEXT

```

Automatic phase labels? /Y/:

Automatic labelling not always possible
Testing POLY result by global minimization procedure

Stable phases are: FCC_A1+M7C3

Text size: / .36 /:

POST: set-title example 3i

POST:

POST: SET_EXP_FILE_FORMAT 5

POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y

... the command in full is MAKE_EXPERIMENTAL_DATAFI

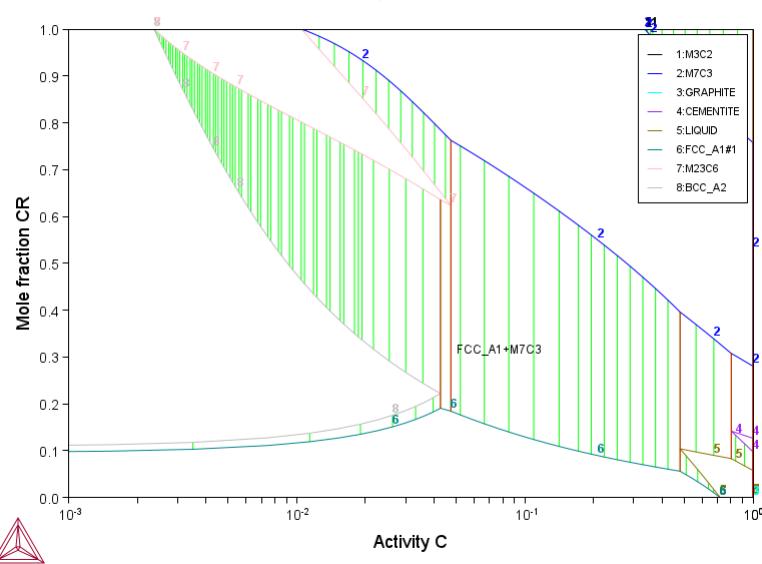
POST: SET_EXP_FILE_FORMAT 10

POST:

POST: plot

... the command in full is PLOT_DIAGRAM

example 3i



POST:

POST: set-inter

... the command in full is SET_INTERACTIVE_MODE

POST:

tce04

SYS:About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

```
SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce04\tce04.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Calculating the miscibility gap in the Fe-Cr system.
SYS:
SYS: set-log ex04,,
SYS:
SYS: go data
... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module
Database folder: C:\jenkins\workspace\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA           /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE11: SW FEDEMO
... the command in full is SWITCH_DATABASE
Current database: Iron Demo Database v4.0

VA           /- DEFINED
TDB_FEDEMO: def-sys
... the command in full is DEFINE_SYSTEM
ELEMENTS: fe cr
FE          CR DEFINED
TDB_FEDEMO: l-sys
... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/:
LIQUID:L :CR FE:
BCC_A2   :CR FE:VA:
LAVES_PHASE_C14 :CR FE:CR FE:
CBCC_A12 :CR FE:VA:
CHI_A12   :CR FE:CR:CR FE:
CUB_A13   :CR FE:VA:
FCC_A1    :CR FE:VA:
HCP_A3    :CR FE:VA:
SIGMA     :CR FE:CR:CR FE:
TDB_FEDEMO: rej ph /all
... the command in full is REJECT
LIQUID:L      BCC_A2      LAVES_PHASE_C14
CBCC_A12     CHI_A12      CUB_A13
FCC_A1       HCP_A3      SIGMA
REJECTED
TDB_FEDEMO: rest ph liquid fcc_a1 bcc_a2 sigma
... the command in full is RESTORE
LIQUID:L      FCC_A1      BCC_A2
SIGMA RESTORED
TDB_FEDEMO: get
... the command in full is GET_DATA
15:24:38,517 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES ....
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ...

List of references for assessed data

'A.T. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
'M. Ghasemi, Thermo-Calc Software AB, Sweden, 2020; Unifying liquid volume
database'
'M. Ghasemi, Thermo-Calc Software AB, Sweden, 2019; Viscosity of metallic
liquid'
'M. Ghasemi, Thermo-Calc Software AB: assessing the surface tension of
metallic liquid'
'Y. Tang, in TCCU2, Thermo-Calc Software AB, Stockholm, Sweden'
'M. J. Assael, J. Phys. Chem. Ref. Data 35 (2006) 285; Fe, Al'
'B.J. Lee, CALPHAD, 17 (1993) 251-268; revision of Fe-Cr and Fe -Ni liquid'
'X.G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
volumes'
'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270
(1986); CR-FE'
'X.G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
'B. Sundman et al., Report EUR 20315, Contract No 7210-PR/050, 2002; New
Sigma model'
OK
TDB_FEDEMO: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY: l-st
... the command in full is LIST_STATUS
Option /CPS/:
*** STATUS FOR ALL COMPONENTS
COMPONENT      STATUS      REF. STATE      T (K)      P (Pa)
VA             ENTERED    SER
CR             ENTERED    SER
FE             ENTERED    SER
*** STATUS FOR ALL PHASES
PHASE          STATUS      DRIVING FORCE    MOLES
SIGMA          ENTERED    0.000000E+00  0.000000E+00
FCC_A1          ENTERED    0.000000E+00  0.000000E+00
BCC_A2          ENTERED    0.000000E+00  0.000000E+00
LIQUID          ENTERED    0.000000E+00  0.000000E+00
*** STATUS FOR ALL SPECIES
CR ENTERED     FE ENTERED    VA ENTERED
```

```

POLY:Hit RETURN to continue
POLY: @@ There is a miscibility gap in BCC Fe-Cr.

POLY: @@ Let us first calculate the low temperature region.
POLY: s-c x(cr)=.6 t=700 p=101325 n=1
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 2579 grid points in 1 s
Found the set of lowest grid points in 0 s
Creating a new composition set BCC_A2#2
Calculated POLY solution 1 s, total time 2 s
Creating a new composition set BCC_A2#3
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
Output from POLY-3, equilibrium = 1, label A0 , database: FEDEMO

Conditions:
X(CR)=0.6, T=700, P=101325, N=1
DEGREES OF FREEDOM 0

Temperature 700.00 K ( 426.85 C), Pressure 1.013250E+05
Number of moles of components 1.00000E+00, Mass in grams 5.35364E+01
Total Gibbs energy -2.30658E+04, Enthalpy 1.31801E+04, Volume 7.26548E-06

Component Moles W-Fraction Activity Potential Ref.stat
CR 6.0000E-01 5.8274E-01 2.3703E-02 -2.1780E+04 SER
FE 4.0000E-01 4.1726E-01 1.3643E-02 -2.4995E+04 SER

BCC_A2#3 Status ENTERED Driving force 0.0000E+00
Moles 6.0116E-01, Mass 3.1437E+01, Volume fraction 6.0322E-01 Mass fractions:
CR 9.17514E-01 FE 8.24857E-02

BCC_A2#1 Status ENTERED Driving force 0.0000E+00
Moles 3.9884E-01, Mass 2.2100E+01, Volume fraction 3.9678E-01 Mass fractions:
FE 8.93487E-01 CR 1.06513E-01
POLY:Hit RETURN to continue
POLY: @@ Now make a calculation at a higher temperature
POLY: s-c t=900
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 2579 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
Output from POLY-3, equilibrium = 1, label A0 , database: FEDEMO

Conditions:
X(CR)=0.6, T=900, P=101325, N=1
DEGREES OF FREEDOM 0

Temperature 900.00 K ( 626.85 C), Pressure 1.013250E+05
Number of moles of components 1.00000E+00, Mass in grams 5.35364E+01
Total Gibbs energy -3.49346E+04, Enthalpy 2.36851E+04, Volume 7.26372E-06

Component Moles W-Fraction Activity Potential Ref.stat
CR 6.0000E-01 5.8274E-01 1.2779E-02 -3.2626E+04 SER
FE 4.0000E-01 4.1726E-01 5.9087E-03 -3.8398E+04 SER

SIGMA Status ENTERED Driving force 0.0000E+00
Moles 6.4237E-01, Mass 3.4605E+01, Volume fraction 6.3941E-01 Mass fractions:
FE 5.04665E-01 CR 4.95335E-01

BCC_A2#3 Status ENTERED Driving force 0.0000E+00
Moles 3.5763E-01, Mass 1.8932E+01, Volume fraction 3.6059E-01 Mass fractions:
CR 7.42495E-01 FE 2.57505E-01
POLY:Hit RETURN to continue
POLY: @@ The Fe-Cr phase diagram has three non-connected two-phase regions.
POLY:
POLY: s-a-v 1 x(cr)
... the command in full is SET_AXIS_VARIABLE
Min value /0/: 0
Max value /1/: 1
Increment /.025/:
POLY: s-a-v 2
... the command in full is SET_AXIS_VARIABLE
Condition /NONE/: t
Min value /0/: 600
Max value /1/: 2200
Increment /40/:
POLY: @@ Always use a SAVE command before MAP (or STEP) otherwise unless
POLY: @@ you want to overlay this calculation with an earlier one
POLY: save tceex04 y
... the command in full is SAVE_WORKSPACES
POLY: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2
Generating start point 3

```

```

Generating start point  4
Generating start point  5
Generating start point  6
Generating start point  7
Generating start point  8
Generating start point  9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Working hard

Phase region boundary  1 at:  1.067E-02  1.169E+03
   ** BCC_A2#1
   ** FCC_A1
Calculated              12 equilibria

Phase region boundary  2 at:  1.067E-02  1.169E+03
   ** BCC_A2#1
   ** FCC_A1
Calculated              42 equilibria

Phase region boundary  3 at:  5.119E-01  6.100E+02
   ** BCC_A2#1
   ** BCC_A2#2
Calculated..            2 equilibria
Terminating at axis limit.

Phase region boundary  4 at:  5.112E-01  6.000E+02
   ** BCC_A2#1
   ** BCC_A2#2
Calculated..            10 equilibria

Phase region boundary  5 at:  5.192E-01  7.875E+02
   ** BCC_A2#1
   ** BCC_A2#2
   ** SIGMA
Calculated..            54 equilibria
Calculated..            54 equilibria

Phase region boundary  6 at:  6.762E-01  7.875E+02
   ** BCC_A2#1
   ** SIGMA
Calculated..            54 equilibria
Calculated..            54 equilibria

Phase region boundary  7 at:  6.762E-01  7.875E+02
   ** BCC_A2#1
   ** SIGMA
Calculated..            109 equilibria
Terminating at known equilibrium

Phase region boundary  8 at:  5.119E-01  6.100E+02
   ** BCC_A2#1
   ** BCC_A2#2
Calculated..            9 equilibria
Terminating at known equilibrium

Phase region boundary  9 at:  5.119E-01  6.100E+02
   ** BCC_A2#1
   ** BCC_A2#2
Calculated..            2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 10 at:  5.119E-01  6.100E+02
   ** BCC_A2#1
   ** BCC_A2#2
Calculated..            9 equilibria
Terminating at known equilibrium

Phase region boundary 11 at:  4.325E-02  1.137E+03
   ** BCC_A2#1
   ** FCC_A1
Calculated..            49 equilibria

Phase region boundary 12 at:  4.325E-02  1.137E+03
   ** BCC_A2#1
   ** FCC_A1
Calculated..            14 equilibria

Phase region boundary 13 at:  1.006E-01  1.137E+03
   ** BCC_A2#1
   ** FCC_A1
Calculated..            25 equilibria

Phase region boundary 14 at:  1.006E-01  1.137E+03
   ** BCC_A2#1
   ** FCC_A1
Calculated..            34 equilibria

Phase region boundary 15 at:  1.224E-02  1.663E+03
   ** BCC_A2#1
   ** FCC_A1
Calculated..            43 equilibria

Phase region boundary 16 at:  1.224E-02  1.663E+03
   ** BCC_A2#1
   ** FCC_A1
Calculated..            12 equilibria

Phase region boundary 17 at:  9.640E-03  1.809E+03
   LIQUID
   ** BCC_A2#1
Calculated..            11 equilibria

Phase region boundary 18 at:  9.640E-03  1.809E+03
   LIQUID
   ** BCC_A2#1

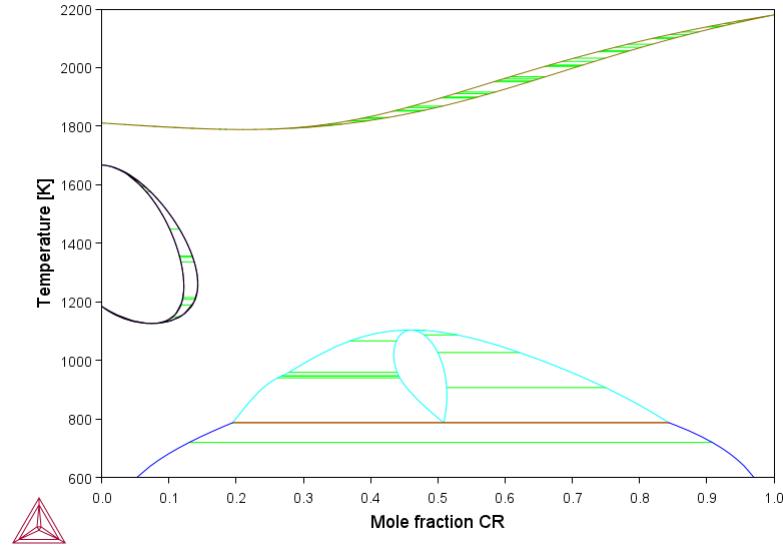
```

```

Calculated          93 equilibria
Phase region boundary 19 at: 3.471E-01 1.807E+03
    LIQUID
** BCC_A2#1
Calculated          38 equilibria
Phase region boundary 20 at: 3.471E-01 1.807E+03
    LIQUID
** BCC_A2#1
Calculated          64 equilibria
Phase region boundary 21 at: 6.881E-01 2.007E+03
    LIQUID
** BCC_A2#1
Calculated          68 equilibria
Phase region boundary 22 at: 6.881E-01 2.007E+03
    LIQUID
** BCC_A2#1
Calculated          39 equilibria
Phase region boundary 23 at: 9.910E-01 2.176E+03
    LIQUID
** BCC_A2#1
Calculated          90 equilibria
Phase region boundary 24 at: 9.910E-01 2.176E+03
    LIQUID
** BCC_A2#1
Calculated          12 equilibria
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\generate_console_examples\examples\tcex04\tcex04.POLY3
CPU time for mapping      5 seconds
POLY:
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST:
POST: s-t-s 6
... the command in full is SET_TIELINE_STATUS
POST: set_title example 4a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
example 4a
```



```

POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:
```

tce05

SYS:About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

```
SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce05\tce05.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Calculating a vertical section in the Al-Cu-Si system
SYS:
SYS: @@ This example calculates a vertical section in the Al-Cu-Si
SYS: @@ system and of a vertical section from Al to 10% Cu2Si.
SYS:
SYS: set-log ex05.,
SYS: go da
... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module
Database folder: C:\jenkins\workspace\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA           /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE11: sw ALDEMO
... the command in full is SWITCH_DATABASE
Current database: Aluminum Demo Database v4.1

VA           /- DEFINED
TDB_ALDEMO: def-sys al Cu si
... the command in full is DEFINE_SYSTEM
AL          CU          SI
DEFINED
TDB_ALDEMO: get
... the command in full is GET_DATA
15:25:59,255 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ...

List of references for assessed data

'A. Dinsdale, Calphad,15 317-425 (1991)'
'Volume data from TCFE4, 2006'
'H-L Chen, in TCAL7.0, Evaluation and modeling of electrical resistivity
    thermal conductivity'
'M J Assael, High Temp High Press 41 (2012); Sb, Pb, Bi, Ni, Ag'
'M Ghasemi, Thermo-Calc Software AB (2020)'
'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
    Molar volumes'
'M J Assael, J Phys Chem Ref Data 39 (2010) 033105; Cu, Sn'
'M J Assael, J Phys Chem Ref Data 41 (2012) 033101; Cd, Co, Ga, In, Hg, Si,
    Ti, Zn'
'I. Ansara (Editor), COST 507, (1998)'
'M Ghasemi, Thermo-Calc Software AB (2019)'
'C.-Y. He,Calphad, 33,200-210 (2009),Al-Cu-Si'
'J. Groebner,Calphad,20(2)247-254(1996),Al-C-Si'
'X.Y. Yan,J. Alloy and Compd. 308, 221-229 (2000),CU-Si'
'L. Kjellqvist, Thermo-Calc Software AB, Stockholm, 2010; Unassessed
    parameter, linear combination of unary volume data'
'H-L Chen, in TCAL3.0, Assessment, extrapolation and assumption'
'Hai-Lin Chen, electrical resistivity
    thermal conductivity (2020)'
'L. Kjellqvist, Thermo-Calc Software AB, Sweden 2012; Molar volumes'
'H-L Chen, Evaluation of molar volume'
'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
'N. Dupin, Calphad, 25(2)279-298(2001),Al-Cr-Ni'
'Nathalie Dupin, in TCNI6.0, Refinement of Al-Ni'
'Volume data, N. Dupin 2008'
'H-L Chen, in TCAL2.0, Assessment, extrapolation and assumption'
'J.R.Zhao, Y.Du, to be submitted, 2010,Sn-Sr,Cu-Mg-Si'
'W.H. Sun, unpublished (2010),Cu-Si-Zn,Cu-Ni-Zn'
'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
'H-L Chen, in TCAL1.2, assessment of Al-Cu-Mg-Si'
-OK-
TDB_ALDEMO: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY: s-c t=1000,p=1e5,n=1
... the command in full is SET_CONDITION
POLY: @@ We shall calculate along a line where the Cu content is twice

POLY: @@ that of the Si content. This can be used as a condition.
POLY: @@ Note that the whole equation must be given before the equal sign.
POLY: @@ It is wrong to write s-c x(cu)=2*x(si).
POLY: s-c x(cu)-2*x(si)=0
... the command in full is SET_CONDITION
POLY: l-c
... the command in full is LIST_CONDITIONS
T=1000, P=100000, N=1, X(CU)-2*X(SI)=0
DEGREES OF FREEDOM 1
POLY: s-c w(si)=0.05
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
```

Testing POLY result by global minimization procedure
Calculated 17676 grid points in 1 s
38 ITS, CPU TIME USED 4 SECONDS
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /WCS: WCS
Output from POLY-3, equilibrium = 1, label A0 , database: ALDEMO

Conditions:
T=1000, P=100000, N=1, X(CU)-2*X(SI)=0, W(SI)=5E-2
DEGREES OF FREEDOM 0

Temperature 1000.00 K (726.85 C), Pressure 1.00000E+05
Number of moles of components 1.00000E+00, Mass in grams 3.10908E+01
Total Gibbs energy -5.01533E+04, Enthalpy 2.90243E+04, Volume 1.09629E-05

| Component | Moles | W-Fraction | Activity | Potential | Ref.stat |
|-----------|------------|------------|------------|-------------|----------|
| AL | 8.3395E-01 | 7.2374E-01 | 4.7926E-03 | -4.4405E+04 | SER |
| CU | 1.1070E-01 | 2.2626E-01 | 9.6970E-06 | -9.5980E+04 | SER |
| SI | 5.5351E-02 | 5.0000E-02 | 4.4065E-03 | -4.5103E+04 | SER |

LIQUID Status ENTERED Driving force 0.0000E+00
Moles 1.0000E+00, Mass 3.1091E+01, Volume fraction 1.0000E+00 Mass fractions:
AL 7.23737E-01 CU 2.26263E-01 SI 5.00000E-02

POLY:@?<Hit_return_to_continue>

POLY: ?
... the command in full is HELP

| ADD_INITIAL_EQUILIBRIUM | GOTO_MODULE | REINITIATE_MODULE |
|-------------------------|--------------------------|------------------------|
| ADVANCED_OPTIONS | HELP | SAVE_WORKSPACES |
| AMEND_STORED_EQUILIBRIA | INFORMATION | SELECT_EQUILIBRIUM |
| BACK | LIST_AXIS_VARIABLE | SET_ALL_START_VALUES |
| CHANGE_STATUS | LIST_CONDITIONS | SET_AXIS_VARIABLE |
| COMPUTE_EQUILIBRIUM | LIST_EQUILIBRIUM | SET_CONDITION |
| COMPUTE_TRANSITION | LIST_INITIAL_EQUILIBRIA | SET_INPUT_AMOUNTS |
| CREATE_NEW_EQUILIBRIUM | LIST_STATUS | SET_INTERACTIVE |
| DEFINE_COMPONENTS | LIST_SYMBOLS | SET_NUMERICAL_LIMITS |
| DEFINE_DIAGRAM | LOAD_INITIAL_EQUILIBRIUM | SET_REFERENCE_STATE |
| DEFINE_MATERIAL | MACRO_FILE_OPEN | SET_START_CONSTITUTION |
| DELETE_INITIAL_EQUILIB | MAKE_COMPONENT_ENTERED | SET_START_VALUE |
| DELETE_SYMBOL | MAKE_COMPONENT_SUSPENDED | SHOW_VALUE |
| ENTER_SYMBOL | MAP | STEP_WITH_OPTIONS |
| EVALUATE_FUNCTIONS | POST | TABULATE |
| EXIT | READ_WORKSPACES | |

POLY: s-a-v 1
... the command in full is SET_AXIS_VARIABLE

Condition /NONE: w(si)
Min value /0/: 0
Max value /1/: .1
Increment /.0025/: .0025

POLY: s-a-v 2
... the command in full is SET_AXIS_VARIABLE

Condition /NONE: t
Min value /0/: 500
Max value /1/: 1300
Increment /20/: 10

POLY: l-a-v
... the command in full is LIST_AXIS_VARIABLE

| Axis No 1: W(SI) | Min: 0 | Max: 0.1 | Inc: 2.5E-3 |
|------------------|----------|-----------|-------------|
| Axis No 2: T | Min: 500 | Max: 1300 | Inc: 10 |

POLY:@?<Hit_return_to_continue>

POLY: save tceox05 y
... the command in full is SAVE_WORKSPACES

POLY: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Tie-lines not in the plane of calculation
Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Working hard

Phase region boundary 1 at: 2.500E-03 6.461E+02
** AL2CU_C16
DIAMOND_A4
FCC_A1
Calculated.. 16 equilibria
Terminating at axis limit.

Phase region boundary 2 at: 3.656E-04 5.000E+02

```

** AL2CU_C16
  DIAMOND_A4
  FCC_A1
Calculated.          31 equilibria

Phase region boundary  3 at:  1.067E-02  7.948E+02
  ** LIQUID
  ** AL2CU_C16
  ** DIAMOND_A4
  FCC_A1

Phase region boundary  4 at:  5.846E-02  7.948E+02
  LIQUID
  AL2CU_C16
  ** DIAMOND_A4
Calculated.          2 equilibria

Phase region boundary  5 at:  6.069E-02  8.026E+02
  LIQUID
  ** AL2CU_C16
  ** DIAMOND_A4

Phase region boundary  6 at:  6.069E-02  8.026E+02
  LIQUID
  ** DIAMOND_A4
Calculated..          18 equilibria
Terminating at axis limit.

Phase region boundary  7 at:  6.069E-02  8.026E+02
  LIQUID
  ** AL2CU_C16
Calculated.          3 equilibria

Phase region boundary  8 at:  5.704E-02  7.964E+02
  LIQUID
  ** AL2CU_C16
  ** FCC_A1
Calculated.          17 equilibria
Terminating at known equilibrium

Phase region boundary 10 at:  5.704E-02  7.964E+02
  LIQUID
  ** FCC_A1
Calculated.          41 equilibria

Phase region boundary 11 at:  5.704E-02  7.964E+02
  LIQUID
  AL2CU_C16
  ** FCC_A1
Calculated.          2 equilibria
Terminating at known equilibrium

Phase region boundary 12 at:  6.069E-02  8.026E+02
  LIQUID
  ** AL2CU_C16
  DIAMOND_A4
Calculated.          22 equilibria

Phase region boundary 13 at:  9.890E-02  8.509E+02
  LIQUID
  ** AL2CU_C16
  ** ALCU_ETA
  DIAMOND_A4

Phase region boundary 14 at:  1.058E-01  8.509E+02
  LIQUID
  AL2CU_C16
  DIAMOND_A4

Phase region boundary 15 at:  9.890E-02  8.509E+02
  LIQUID
  ** ALCU_ETA
  DIAMOND_A4
Calculated..          2 equilibria
Terminating at axis limit.

Phase region boundary 16 at:  1.350E-01  8.509E+02
  LIQUID
  ALCU_ETA
  DIAMOND_A4

Phase region boundary 17 at:  1.058E-01  8.509E+02
  AL2CU_C16
  ** ALCU_ETA
  DIAMOND_A4

Phase region boundary 18 at:  1.350E-01  8.509E+02
  ** AL2CU_C16
  ALCU_ETA
  DIAMOND_A4

Phase region boundary 19 at:  1.036E-01  7.948E+02
  ** LIQUID
  AL2CU_C16
  DIAMOND_A4

Phase region boundary 20 at:  1.669E-02  7.948E+02
  LIQUID
  ** DIAMOND_A4
  FCC_A1
Calculated.          4 equilibria

Phase region boundary 21 at:  1.013E-02  7.966E+02
  ** LIQUID
  ** DIAMOND_A4
  FCC_A1

Phase region boundary 22 at:  1.013E-02  7.966E+02
  ** DIAMOND_A4
  FCC_A1
Calculated..          31 equilibria

```

Terminating at axis limit.

Phase region boundary 23 at: 1.013E-02 7.966E+02
 ** LIQUID
 FCC_A1
 Calculated 26 equilibria

Phase region boundary 24 at: 1.013E-02 7.966E+02
 ** LIQUID
 DIAMOND_A4
 FCC_A1
 Calculated. 2 equilibria
 Terminating at known equilibrium

Phase region boundary 25 at: 1.036E-01 7.948E+02
 AL2CU_C16
 DIAMOND_A4
 ** FCC_A1
 Calculated. 16 equilibria
 Terminating at known equilibrium

Phase region boundary 27 at: 3.417E-02 7.948E+02
 ** LIQUID
 AL2CU_C16
 DIAMOND_A4
 FCC_A1
 Calculated. 11 equilibria
 Terminating at known equilibrium

Phase region boundary 28 at: 3.417E-02 7.948E+02
 ** LIQUID
 AL2CU_C16
 DIAMOND_A4
 FCC_A1
 Calculated.. 28 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 29 at: 6.583E-02 7.948E+02
 ** LIQUID
 AL2CU_C16
 DIAMOND_A4
 FCC_A1
 Calculated. 24 equilibria
 Terminating at known equilibrium

Phase region boundary 30 at: 6.583E-02 7.948E+02
 ** LIQUID
 AL2CU_C16
 DIAMOND_A4
 FCC_A1
 Calculated.. 15 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 31 at: 9.750E-02 7.948E+02
 ** LIQUID
 AL2CU_C16
 DIAMOND_A4
 FCC_A1
 Calculated. 36 equilibria
 Terminating at known equilibrium

Phase region boundary 32 at: 9.750E-02 7.948E+02
 ** LIQUID
 AL2CU_C16
 DIAMOND_A4
 FCC_A1
 Calculated.. 3 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 33 at: 7.899E-03 7.700E+02
 ** DIAMOND_A4
 FCC_A1
 Calculated.. 29 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 34 at: 7.899E-03 7.700E+02
 ** DIAMOND_A4
 FCC_A1
 Calculated. 4 equilibria
 Terminating at known equilibrium

Phase region boundary 35 at: 8.449E-03 7.700E+02
 ** AL2CU_C16
 DIAMOND_A4
 FCC_A1
 Calculated.. 29 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 36 at: 8.449E-03 7.700E+02
 ** AL2CU_C16
 DIAMOND_A4
 FCC_A1
 Calculated. 4 equilibria
 Terminating at known equilibrium

Phase region boundary 37 at: 2.500E-03 9.291E+02
 LIQUID
 ** FCC_A1
 Calculated. 18 equilibria

Phase region boundary 38 at: 2.500E-03 9.291E+02
 LIQUID
 ** FCC_A1
 Calculated. 23 equilibria
 Terminating at known equilibrium

```

Phase region boundary 39 at: 3.417E-02 8.648E+02
    LIQUID
    ** FCC_A1
Calculated.          26 equilibria

Phase region boundary 40 at: 3.417E-02 8.648E+02
    LIQUID
    ** FCC_A1
Calculated.          11 equilibria
Terminating at known equilibrium

Phase region boundary 41 at: 6.583E-02 8.227E+02
    LIQUID
    ** DIAMOND_A4
Calculated.          4 equilibria
Terminating at known equilibrium

Phase region boundary 42 at: 6.583E-02 8.227E+02
    LIQUID
    ** DIAMOND_A4
Calculated..          20 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 43 at: 9.750E-02 9.579E+02
    LIQUID
    ** DIAMOND_A4
Calculated.          20 equilibria
Terminating at known equilibrium

Phase region boundary 44 at: 9.750E-02 9.579E+02
    LIQUID
    ** DIAMOND_A4
Calculated..          4 equilibria
Terminating at known equilibrium
Terminating at axis limit.

*** BUFFER SAVED ON FILE: c:\jenkins\workspace\generate_console_examples\examples\tcex05\tcex05.POLY3
CPU time for mapping      12 seconds

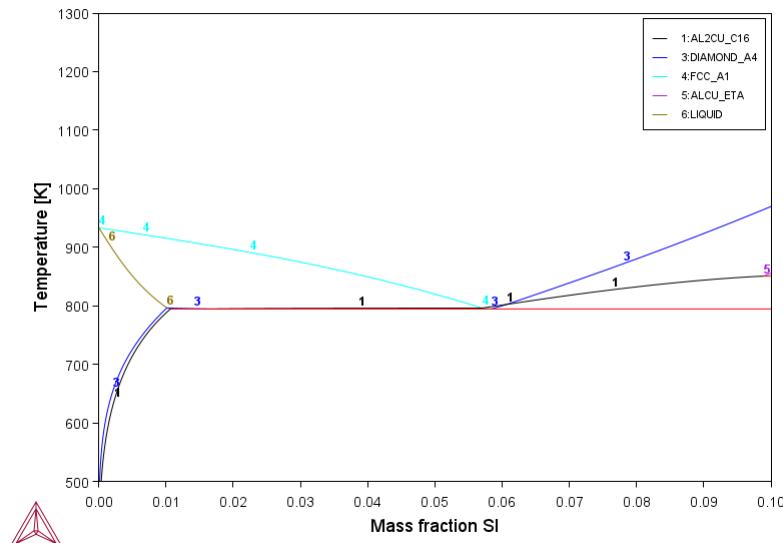
POLY:
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: s-lab
... the command in full is SET_LABEL_CURVE_OPTION
CURVE LABEL OPTION (A, B, C, D, E, F OR N) /N/: b
POST:
POST:
POST: set-title example 5a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 5a



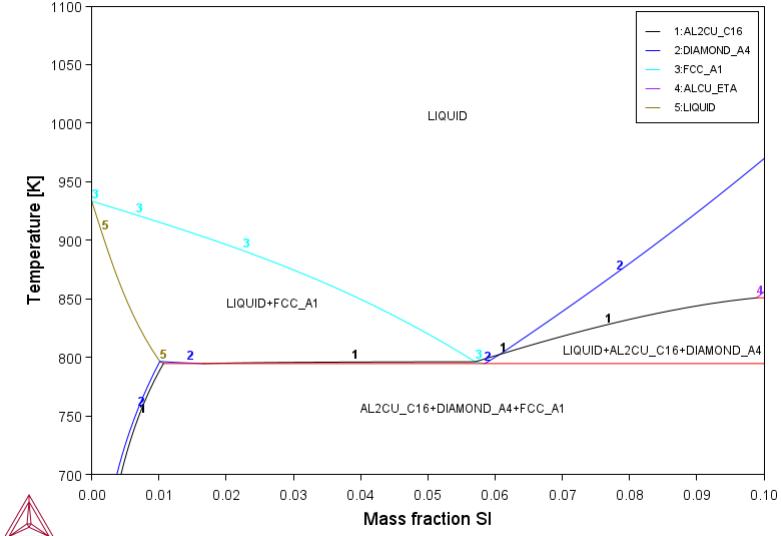
POST:
POST:?<Hit return to continue>
POST: s-s y n 700 1100
... the command in full is SET_SCALING_STATUS
POST: @@ Note that the three-phase region LIQ-Si-Al2Cu is an area and not
POST: @@ a single line as in a binary system. This is called a pseudo-binary section
POST: add .05 1000
... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
Automatic labelling not always possible
Stable phases are: LIQUID
Text size: /.36/:
POST: add .02 840
... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
Automatic labelling not always possible
Testing POLY result by global minimization procedure
Calculated 17676 grid points in 0 s
Stable phases are: LIQUID+FCC_A1
Text size: /.36/:
POST: add .04 750
... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:

```

Automatic labelling not always possible
Testing POLY result by global minimization procedure
Calculated      17676 grid points in          0 s
Stable phases are: AL2CU_C16+DIAMOND_A4+FCC_A1
Text size: /.36/:
POST: add .07 800
... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
Automatic labelling not always possible
Testing POLY result by global minimization procedure
Calculated      17676 grid points in          0 s
Stable phases are: LIQUID+AL2CU_C16+DIAMOND_A4
Text size: /.36/:
POST:
POST: set-title example 5b
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 5b



```

POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:

```

tce06**SYS:About**

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce06\tce06.TCM.test"

SYS:

SYS: @@ Calculation of an isopleth in low alloyed
SYS: @@ Fe-Mn-Si-Cr-Ni-C steel.

SYS:

SYS: @@ This example calculates a multicomponent phase diagram using

SYS: @@ the Define_Material command in POLY and the TCFE steel

SYS: @@ database. Note that TCFE database license is required to run the

SYS: @@ example.

SYS:Hit RETURN to continue

SYS: set-log ex06,,

SYS: go p-3

... the command in full is GOTO_MODULE

POLY version 3.32

POLY:

POLY: @@ The material contains 1.5 %Cr + 0.4 %Mn + 3.5 %Ni + 0.3 %Si and 1 %C

POLY: @@ (by weight). These conditions are set by the command and in

POLY: @@ addition the temperature. Hidden commands set the pressure to 1 bar

POLY: @@ and that iron is "the rest".

POLY: @@ After calculating the first equilibrium we calculate a phase diagram

POLY: @@ with one axis variable as temperature and the other as the

POLY: @@ carbon content

POLY:

POLY: def-mat

... the command in full is DEFINE_MATERIAL

THERMODYNAMIC DATABASE module

Database folder: C:\jenkins\workspace\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

Database /TCFE11/: tcfe11

Major element or alloy: ?

FILE SYSTEM ERROR IN FILHLP

ERROR 1717 READING HELP FILE

Major element or alloy: fe

Composition input in mass (weight) percent? /Y/: y

1st alloying element: c

Mass (weight) percent /1/: 1

2nd alloying element: si .3

Next alloying element: mn .4

Next alloying element: ni 3.5

Next alloying element: cr 1.5

Next alloying element:

Temperature (C) /1000/: 1000

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

REINITIATING GES

... the command in full is DEFINE_ELEMENTS

FE DEFINED

... the command in full is DEFINE_ELEMENTS

C DEFINED

... the command in full is DEFINE_ELEMENTS

SI DEFINED

... the command in full is DEFINE_ELEMENTS

MN DEFINED

... the command in full is DEFINE_ELEMENTS

NI DEFINED

... the command in full is DEFINE_ELEMENTS

CR DEFINED

This database has following phases for the defined system

| | | |
|-------------|----------------|---------------|
| GAS:G | LIQUID:L | BCC_A2 |
| A2_BCC | BCC_B2 | FCC_A1 |
| A1_FCC | FCC_L12 | HCP_A3 |
| CBCC_A12 | CUB_A13 | DIAMOND_A4 |
| GRAPHITE_A9 | CEMENTITE_D011 | M23C6_D84 |
| M7C3_D101 | M5C2 | M3C2_D510 |
| KSI_CARBIDE | FE4N_LP1 | SIGMA_D8B |
| HIGH_SIGMA | CHI_A12 | C14_LAVES |
| C15_LAVES | M3SI | MN9SI2 |
| MN11SI19 | MN6SI | G_PHASE |
| CR3SI_A15 | FESI2_H | FEST2_L |
| MSI_B20 | M5SI3_D88 | NBNI3_D0A |
| NI3Ti_D024 | NB5Si3_D8L | MSI2_C40 |
| M11Si18 | M6Si5 | AL4C3_D71 |
| FE8Si12C | SIC_B3 | MN5SiC |
| CRZN17 | CUZN_EPSILON | NIZN_B2 |
| NIZN_L10 | NI2ZN11_D82 | AL5FE4 |
| MNP_B31 | M2P_C22 | FLUORITE_C1:I |
| ZRO2_TETR:I | M2O3C_D53:I | M2O3H_D52:I |
| M4Si1_G3 | NI3Si12 | CO2Si_C37 |
| M2Si_TETA | NIST_B31 | NI3Si2 |
| CR5Si3_D8M | | |

Reject phase(s) /NONE/: NONE

Restore phase(s): /NONE/: NONE

The following phases are retained in this system:

GAS:G LIQUID:L BCC_A2

| | | |
|-------------|----------------|---------------|
| A2_BCC | BCC_B2 | FCC_A1 |
| A1_FCC | FCC_L12 | HCP_A3 |
| CBCC_A12 | CUB_A13 | DIAMOND_A4 |
| GRAPHITE_A9 | CEMENTITE_D011 | M23C6_D84 |
| M7C3_D101 | M5C2 | M3C2_D510 |
| KSI_CARBIDE | FE4N_LP1 | SIGMA_D8B |
| HIGH_SIGMA | CHI_A12 | C14_LAVES |
| C15_LAVES | M3SI | MN9Si2 |
| MN11Si19 | MN6Si | G_PHASE |
| CR3Si_A15 | FESI2_H | FESI2_L |
| MSI_B20 | M5Si3_D88 | NBNi3_D0A |
| NI3Ti_D024 | NB5Si3_D8L | MSi2_C40 |
| M11Si8 | M6Si5 | AL4C3_D71 |
| FE8Si2C | SIC_B3 | MN5SiC |
| CRZN17 | CUZN_EPSILON | NiZN_B2 |
| NIZN_L10 | NI2ZN11_D82 | AL5Fe4 |
| MNP_B31 | M2P_C22 | FLUORITE_C1:I |
| ZRO2_TETR:I | M2O3C_D53:I | M2O3H_D52:I |
| M4Si1_G3 | NI31Si12 | CO2Si_C37 |
| M2Si_TETA | NiSi_B31 | NI3Si2 |
| CR5Si3_DBM | | |

OK? /Y/: Y
15:27:29,167 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
ELEMENTS
SPECIES
PHASES
... the command in full is AMEND_PHASE_DESCRIPTION
Creating a new composition set FCC_A1#2
... the command in full is AMEND_PHASE_DESCRIPTION
Creating a new composition set HCP_A3#2
... the command in full is AMEND_PHASE_DESCRIPTION
Suspending FLUORITE_C1 as it has net charge
Suspending M2O3C_D53 as it has net charge
Suspending M2O3H_D52 as it has net charge
Suspending ZRO2_TETR as it has net charge
PARAMETERS ...
FUNCTIONS

List of references for assessed data

'A.T. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121-127; Molar volumes'
'X.G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
'M. Ghasemi, Thermo-Calc Software AB, Sweden, 2020; Unifying liquid volume database'
'X.G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar volumes'
'B. Sundman et al., Report EUR 20315, Contract No 7210-PR/050, 2002; New Sigma model'
'P. Gustafson, TRITA-MAC 354 (1987); C-Cr-Fe-Mo-W'
'N. Saunders, COST 507 Report (1998); Cr-Ti'
'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; C15_LAVES'
'N. Dupin, Private communication, (2008); Volume data'
'B.J. Lee, KRISS, unpublished research, during 1993-1995'
'R. Naraghi, Thermo-Calc Software AB, Sweden, Volume data updated for TCFE9 database (TCFE v9.0, Jan, 2017).'
'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; FE4N'
'Unassessed parameter; Linear combination of unary data'
'Y. Tang, in TCCU2, Thermo-Calc Software AB, Stockholm, Sweden'
'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equilib., 19 (1998) 441-448; Fe-Ti'
'N. Dupin, introduction of Nb to NI15VA-4SL'
'H. Gohring, O. Fabrichnaya, A. Leineweber, E.J. Mittemeijer, Metall. Mater. Trans. A, 47A, 6173-86(2016); Fe-N, and Fe-C-N'
'N. Saunders, COST 507 Report (1998); Mn-Ti'
'W. Zheng, J. Alloys Compd., 632 (2015) 661-675'
'L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2012; Molar volumes'
'A.F. Guillermet, Z. Metallkd., 79 (1988) 524-536, TRITA-MAC 362 (1988); C -CO-NI AND C-CO-FE-NI'
'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; C14_LAVES'
'J. De Keyzer, G. Cacciamani, N. Dupin, P. Wollants, Calphad, 33, 109 -23(2009).'
'Thermo-Calc Software, Sweden, 2008; Volume data updated for \$TCFE6 database (TCFE v6, April, 2008).'
'A. Bolcavage and U.R. Kattner, J. Phase Equilib., 2, (1996); Nb-Ni'
'W. Xiong, Y. Du, X. Lu, J.C. Schuster, H. Chen, Intermetallics. 15 (2007) 1401-1408.'
'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
'I. Ansara, unpublished work (1991); Cr-Si'
'M. Seiersten, Unpublished work (1989); Al-Fe'
'A.V. Khvan, B. Hallstedt, K. Chang, CALPHAD, 39, 54-61(2012); C-Cr-Nb'
'J-O. Andersson, CALPHAD, 11 (1987) 271-276; TRITA 0314; C-CR'
'J. Bratberg, Z. Metallkd., 96 (2005) 335-344; Fe-Cr-Mo-C'
'B.J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
'C. Qui, ISIJ International, 32 (1992), 1117-1127; Trita-MAC 482 (1992) Revision; C-Cr-Fe-Mo'
'P. Gustafson, Metall. Trans. A, 19A (1988) 2547-2554; TRITA-MAC 348, (1987); C-CR-FE-W'
'P. Villars, L.D. Calvert. Pearson's handbook of crystallographic data for intermetallic phases, Metals park, Ohio 1985: American society for metals'
'B.J. Lee, Metall. Trans. A, 24A (1993) 1017-1025; Fe-Cr-Mn-C'
'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
'J-O. Andersson, CALPHAD, 12 (1988) 9-23; TRITA 0321 (1986); C-FE-MO'
'B. Hallstedt, D. Djurovic, J. von Appen, R. Dronskowsk, A. Dick, F. Koermann, T. Hickel, J. Neugebauer, CALPHAD, 34, 129-33(2010); Fe-C'
'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowsk, Calphad 35.4 (2011) 479-491; Fe-Mn-C'
'W. Huang, Metall. Trans. A, 21A (1990) 2115-2123; TRITA-MAC 411 (Rev 1989); C-FE-MN'
'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowsk, CALPHAD, 34, 279

-85(2010); Mn-C'
 'A. Gabriel, C. Chatillon, and I. Ansara, published in High Temp. Sci.
 (Parameters listed in CALPHAD, 11 (1987) 203-218); C-NI'
 'A. Gabriel, P. Gustafson, and I. Ansara, CALPHAD, 11 (1987) 203-218;
 TRITA-MAC 285 (1986); C-FE-NI'
 'A.F. Guillermet and G. Grimvall, J. Phys. Chem. Solids, 1992, 53, 105-125;
 Molar volumes'
 'J. Grobner, H.L. Lukas, F. AlDinger, Calphad, 1996, 20 (2), 247-254; Al-C,
 Si-C, Al-Si-C'
 'P. Franke; revision of C-Si, Fe-Si and C-Fe-Si'
 'J. Lacaze and B. Sundman, Metall. Mater. Trans. A, 22A (1991) 2211-2223;
 Fe-Si and Fe-Si-C'
 'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; Cementite'
 'R. Naraghi, Thermo-Calc Software AB, Volume data updated for TCFE9
 database (TCFE v9.1, June, 2019).'
 'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; SIGMA and M7C3'
 'NPL, Unpublished work (1989); C-Mn-Si'
 'B.J. Lee, CALPHAD, 17 (1993) 251-268; revision of Fe-Cr and Fe-Ni liquid'
 'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270
 (1986); CR-FE'
 'K. Frisk, Metall. Trans. A, 21A (1990) 2477-2488; TRITA 0409 (1989); CR
 -FE-N'
 'J-O. Andersson, Metall. Trans. A, 19A (1988) 1385-1394; TRITA 0322 (1986);
 CR-FE-MO'
 'B.J. Lee, unpublished work at KTH (1999); update of steel database'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2019; Cr-Fe-Nb'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2014; Cr-Fe-Zn'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, Volume data updated for
 TCFE8 database (TCFE v8, May, 2015).'
 'B.J. Lee, Metall. Trans. A, 24A (1993) 1919-1933; Cr-Mn, Fe-Cr-Mn'
 'K. Frisk, CALPHAD, 17 (1993) 335-349; Cr-Mn-N'
 'SGTE (2008): SSOL4-SGTE Substance Database V4.1, provided by Thermo-Calc
 Software'
 'A.T. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); CR-NI'
 'N. Dupin, I. Ansara, B. Sundman, CALPHAD, 25 (2), 279-298 (2001); Al-Cr-Ni'
 'L.L. Zhu, H.Y. Qi, L. Jiang, Z.P. Jin, J.C. Zhao, Intermetallics. 64
 (2015) 86-95; Cr-Ru and Cr-Ni-Ru'
 'L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2010; Molar volumes'
 'L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2013; Reassessed
 solubility of Al, Cr, Fe, Ni in Mn2O3. When Mn2O3 is modelled as the
 same phase as cubic Y2O3 (M2O3).'
 'Y.Du and J.C.Schuster, J. Phase Equilibria, 21(3) 281-86(2000); Cr-Si'
 'N. Dupin, Private communication; Si systems'
 'L. Kjellqvist, Thermo-Calc Software AB, Stockholm, 2010; Unassessed
 parameter, linear combination of unary volume data'
 'A. Jacob, E. Povoden-Karadeniz, E. Kozeschnik, Calphad, 56 (2017) 80-91.'
 'W. Huang, CALPHAD, 13 (1989) 243-252; TRITA-MAC 388 (rev 1989); FE-MN'
 'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
 'S. Liu, B. Hallstedt, D. Music, Y. Du, CALPHAD, 38 (2012) 43-58; Mn-Nb
 and Fe-Mn-Nb'
 'A. Markstrom, Thermo-Calc software AB, Sweden, 2011'
 'A.T. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); FE-NI'
 'L. Zhang, J. Wang, Y. Du, R. Hu, P. Nash, X.G. Lu, et al., Acta Mater. 57
 (2009) 5324-5341; Al-Fe-Ni'
 'L.J. Zhang, Int.J. Mater. Res., 100(2) 160-175 (2009), Fe-Mn-Ni'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; Molar volume Fe-Mn-Si
 and Al-Fe-Mn'
 'S. Cotes, A.F. Guillermet, M. Sade, J. Alloys Compd., 208(1998) 168-177'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2019; Cr-Fe-Nb-Si'
 'A. Forsberg and J. Agren, J. Phase Equilb., 14 (1993) 354-363; Fe-Mn-Si'
 'R. Naraghi, Thermo-Calc Software AB, Sweden (2019); Fe-Ni-Si'
 'J. Miettinen, G. Vassilev, J. Phase Equilb. Diffus, 37(5) 2016, 283-290;
 Fe-P-Si'
 'Shuhong Liu, unpublished work (2010), Mn-Ni, Al-Mn-Ni, Mn-Ni-Zn, Al-Cu-Fe-Mg
 -Mn-Si'
 'C.P. Guo, Intermetallics, 13(5), 525-534, (2005), Mn-Ni'
 'M. Chen, B. Hallstedt, L. J. Gauckler, J. Alloys Compd., 393 (2005) 114
 -21; Mn-Y-O'
 'M. Chen, B. Hallstedt, L.J. Gauckler, Solid State Ionics, 176 (2005) 1457
 -64; Mn-Zr-O, Mn-Y-Zr-O'
 'J. Miettinen, CALPHAD, 28 (2004) 313-320; Mn-Zn'
 'L. Kjellqvist, Thermo-Calc Software AB (2013) estimated parameter; Ni-Zr-O'
 'T. Tokunaga, K. Nishio, H. Ohtani, M. Hasebe, Calphad, 27 (2003), 161-168;
 Ni-Si'
 'N. Dupin; L12 general relations, equivalence of 2 sublattice formalism
 with four sublattice formalism'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; Checking ternary P
 systems'
 'Same or similar interaction as in the corresponding stable phase'
 'B. Sundman, Private communication (2003-4); Refitted Fe-Ni-Si'
 'W.W. Zhang, unpublished (2010), Fe-Ni-Si'
 'R. Naraghi, Thermo-Calc Software AB, Sweden (2019); M4Si1_G3'
 'J. Miettinen, CALPHAD, 27 (2003) 263-274; Cu-Ni-Zn'
 'H. Liang, Y.A.Chang, J. Phase Equilb. 19 (1998) 25-37'
 'A.V. Khvan, B. Hallstedt, C. Broeckmann, CALPHAD, 46, 24-33(2014); Cr-Fe-C'
 'J-O. Andersson, Metall. Trans. A, 19A (1988) 627-636 TRITA 0207 (1986); C
 -CR-FE'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2016; FCC Fe-Cr-C and C-Cr-Ni'
 'NPL, unpublished work (1989); C-Cr-Ni'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; C-Cr-Si'
 'Y.Du, J.C.Schuster, J.Am.Ceram.Soc., 83 (8) 2067-73 (2000); C-Cr-Si'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; Adjusting hcp'
 'J. Miettinen and B. Hallstedt, CALPHAD, 22 (1998) 231-256; Fe-Si and Fe
 -Si-C'
 'W. Zheng et al., J. Iron Steel Res. Int. 24(2) (2017) 190-197'
 'R. Naraghi, Thermo-Calc Software AB, Sweden (2015); FROST project'
 'C. Qiu, Metall. Trans. A, 24A (1993) 2393-2409; Cr-Fe-Mn-N'
 'A. Markstrom, Thermo-Calc Software AB (2013), Extrapolations, assumptions
 adjustment'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; Cr-Fe-Si'
 'M. Lindholm, J. Phase Equilb., 18.5 (1997) 432; Cr-Fe-Si'
 'B.J. Lee, Private communication, (2000); Estimated parameter'
 'J.C. Schuster and Y.Du, Metall. Mater. Trans.A, 31A(7) 1795-803(2000); Cr
 -Ni-Si.'
 'R. Naraghi, Thermo-Calc Software AB, Sweden (2019); Cr-Ni-Si'
 'B. Hu, Unpublished (2010); Mn-Ni-Si, Al-Cu-Fe-Ni'
 'R. Naraghi, Thermo-Calc Software AB, Sweden (2019); Cheking the binaries.'
 'M. Ghasemi, Thermo-Calc Software AB, Sweden, 2019; Viscosity of metallic
 liquid'
 'M. J. Assael, J. Phys. Chem. Ref. Data 35 (2006) 285; Fe, Al'
 'M. J. Assael, High Temp. High Press., 41 (2012); Sb, Pb, Bi, Ni, Ag'
 'M. J. Assael, J. Phys. Chem. Ref. Data 41 (2012) 033101; Cd, Co, Ga, In,
 Hg, Si, Ti, Zn'
 'Q. Chen, Thermo-Calc Software AB (2014), L12 constraints'
 'M. Ghasemi, Thermo-Calc Software AB: assessing the surface tension of
 metallic liquid'

-OK-

Should any phase have a miscibility gap check? /N/: N

Using global minimization procedure
Calculated 45065 grid points in 18 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 3 s, total time 21 s

POLY:

POLY: l-e

... the command in full is LIST_EQUILIBRIUM

OUTPUT TO SCREEN OR FILE /SCREEN/:

Options /VWCS/: VWCS

Output from POLY-3, equilibrium = 1, label A0 , database: TCFE11

Conditions:

T=1273.15, W(C)=1E-2, W(SI)=3E-3, W(MN)=4E-3, W(NI)=3.5E-2, W(CR)=1.5E-2,
P=100000, N=1

DEGREES OF FREEDOM 0

Temperature 1273.15 K (1000.00 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 5.37536E+01
Total Gibbs energy -6.46661E+04, Enthalpy 3.76396E+04, Volume 7.13974E-06

| Component | Moles | W-Fraction | Activity | Potential | Ref.stat |
|-----------|------------|------------|------------|-------------|----------|
| C | 4.4754E-02 | 1.0000E-02 | 8.5166E-02 | -2.6074E+04 | SER |
| CR | 1.5507E-02 | 1.5000E-02 | 1.3307E-04 | -9.4473E+04 | SER |
| FE | 8.9803E-01 | 9.3300E-01 | 2.4799E-03 | -6.3509E+04 | SER |
| MN | 3.9138E-03 | 4.0000E-03 | 3.3252E-06 | -1.3353E+05 | SER |
| NI | 3.2056E-02 | 3.5000E-02 | 5.8057E-05 | -1.0325E+05 | SER |
| SI | 5.7419E-03 | 3.0000E-03 | 4.4487E-09 | -2.0357E+05 | SER |

FCC_A1#1 Status ENTERED Driving force 0.0000E+00
Moles 1.0000E+00, Mass 5.3754E+01, Volume fraction 1.0000E+00 Mass fractions:
FE 9.33000E-01 CR 1.50000E-02 MN 4.00000E-03
NI 3.50000E-02 C 1.00000E-02 SI 3.00000E-03

POLY:Hit RETURN to continue

POLY: @@ Note that values now must be set in fractions and Kelvin.

POLY: s-a-v 1 w(c)

... the command in full is SET_AXIS_VARIABLE

Min value /0/: 0

Max value /1/: .01

Increment /2.5E-04/: 1E-4

POLY: s-a-v 2 t

... the command in full is SET_AXIS_VARIABLE

Min value /0/: 700

Max value /1/: 1300

Increment /15/:

POLY: save tce06 y

... the command in full is SAVE_WORKSPACES

POLY: map

Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Tie-lines not in the plane of calculation

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Generating start point 27
Generating start point 28

Phase region boundary 1 at: 1.348E-03 7.100E+02

BCC_A2

FCC_A1#1

** M3C2_D510

M7C3_D101

Calculated..

2 equilibria

Terminating at axis limit.

Phase region boundary 2 at: 1.356E-03 7.000E+02

BCC_A2

FCC_A1#1

** M3C2_D510

M7C3_D101

Calculated..

22 equilibria

Phase region boundary 3 at: 2.413E-03 7.877E+02

```

BCC_A2
FCC_A1#1
** GRAPHITE_A9
** M3C2_D510
M7C3_D101

Phase region boundary  4 at:  2.413E-03  7.877E+02
BCC_A2
FCC_A1#1
GRAPHITE_A9
** M3C2_D510
M7C3_D101
Calculated..          78 equilibria
Terminating at axis limit.

Phase region boundary  5 at:  2.413E-03  7.877E+02
BCC_A2
FCC_A1#1
** GRAPHITE_A9
M7C3_D101
Calculated.           7 equilibria

Phase region boundary  6 at:  2.693E-03  8.693E+02
BCC_A2
CEMENTITE_D011
FCC_A1#1
** GRAPHITE_A9
M7C3_D101
Calculated.           22 equilibria

Phase region boundary  7 at:  2.693E-03  8.693E+02
BCC_A2
CEMENTITE_D011
FCC_A1#1
** GRAPHITE_A9
M7C3_D101
Calculated.           22 equilibria

Phase region boundary  8 at:  4.767E-03  8.798E+02
BCC_A2
CEMENTITE_D011
FCC_A1#1
** GRAPHITE_A9
** M7C3_D101
Calculated..          55 equilibria
Terminating at axis limit.

Phase region boundary  9 at:  4.767E-03  8.798E+02
BCC_A2
CEMENTITE_D011
FCC_A1#1
** GRAPHITE_A9
Calculated..          55 equilibria
Terminating at axis limit.

Phase region boundary 10 at:  4.767E-03  8.798E+02
BCC_A2
CEMENTITE_D011
FCC_A1#1
** M7C3_D101
Calculated.           27 equilibria

Phase region boundary 11 at:  5.567E-03  9.868E+02
** BCC_A2
CEMENTITE_D011
FCC_A1#1
** M7C3_D101
Calculated.           7 equilibria

Phase region boundary 12 at:  5.567E-03  9.868E+02
CEMENTITE_D011
FCC_A1#1
** M7C3_D101
Calculated.           7 equilibria

Phase region boundary 13 at:  5.692E-03  1.066E+03
** CEMENTITE_D011
FCC_A1#1
** M7C3_D101
Calculated.           27 equilibria

Phase region boundary 14 at:  5.692E-03  1.066E+03
FCC_A1#1
** M7C3_D101
Calculated.           27 equilibria

Phase region boundary 15 at:  3.176E-03  9.980E+02
** BCC_A2
FCC_A1#1
** M7C3_D101
Calculated..          51 equilibria
Terminating at axis limit.

Phase region boundary 16 at:  3.176E-03  9.980E+02
BCC_A2
FCC_A1#1
** M7C3_D101
Calculated..          51 equilibria
Terminating at axis limit.

Phase region boundary 17 at:  3.176E-03  9.980E+02
** BCC_A2
FCC_A1#1
Calculated.           38 equilibria

Phase region boundary 18 at:  3.176E-03  9.980E+02
** BCC_A2
FCC_A1#1
M7C3_D101
Calculated.           19 equilibria

Phase region boundary 19 at:  4.977E-03  9.872E+02
** BCC_A2
** CEMENTITE_D011
FCC_A1#1
M7C3_D101
Calculated..          19 equilibria

Phase region boundary 20 at:  4.977E-03  9.872E+02
** BCC_A2
CEMENTITE_D011
FCC_A1#1
M7C3_D101
Calculated..          7 equilibria

```

Terminating at known equilibrium

Phase region boundary 21 at: 4.977E-03 9.872E+02
 ** CEMENTITE_D011
 FCC_A1#1
 M7C3_D101
 Calculated. 12 equilibria
 Terminating at known equilibrium

Phase region boundary 22 at: 4.977E-03 9.872E+02
 BCC_A2
 ** CEMENTITE_D011
 FCC_A1#1
 M7C3_D101
 Calculated. 37 equilibria
 Terminating at known equilibrium

Phase region boundary 23 at: 5.692E-03 1.066E+03
 ** CEMENTITE_D011
 FCC_A1#1
 Calculated.. 46 equilibria
 Terminating at axis limit.

Phase region boundary 24 at: 5.567E-03 9.868E+02
 ** BCC_A2
 CEMENTITE_D011
 FCC_A1#1
 Calculated.. 47 equilibria
 Terminating at axis limit.

Phase region boundary 25 at: 4.767E-03 8.798E+02
 BCC_A2
 CEMENTITE_D011
 FCC_A1#1
 GRAPHITE_A9
 ** M7C3_D101
 Calculated.. 55 equilibria
 Terminating at axis limit.

Phase region boundary 26 at: 2.693E-03 8.693E+02
 BCC_A2
 ** CEMENTITE_D011
 FCC_A1#1
 GRAPHITE_A9
 M7C3_D101
 Calculated.. 76 equilibria
 Terminating at axis limit.

Phase region boundary 27 at: 2.413E-03 7.877E+02
 BCC_A2
 FCC_A1#1
 ** GRAPHITE_A9
 M3C2_D510
 M7C3_D101
 Calculated. 5 equilibria

Phase region boundary 28 at: 2.078E-03 7.585E+02
 BCC_A2
 FCC_A1#1
 ** GRAPHITE_A9
 M3C2_D510
 ** M7C3_D101
 Calculated.. 5 equilibria
 Terminating at axis limit.

Phase region boundary 29 at: 2.078E-03 7.585E+02
 BCC_A2
 FCC_A1#1
 ** GRAPHITE_A9
 M3C2_D510
 Calculated.. 5 equilibria
 Terminating at axis limit.

Phase region boundary 30 at: 2.078E-03 7.585E+02
 BCC_A2
 FCC_A1#1
 M3C2_D510
 ** M7C3_D101
 Calculated.. 29 equilibria
 Terminating at axis limit.

Phase region boundary 31 at: 2.078E-03 7.585E+02
 BCC_A2
 FCC_A1#1
 GRAPHITE_A9
 M3C2_D510
 ** M7C3_D101
 Calculated.. 82 equilibria
 Terminating at axis limit.

Phase region boundary 32 at: 1.348E-03 7.100E+02
 BCC_A2
 FCC_A1#1
 ** M3C2_D510
 M7C3_D101
 Calculated. 23 equilibria
 Terminating at known equilibrium

Phase region boundary 33 at: 1.000E-04 9.392E+02
 BCC_A2
 FCC_A1#1
 ** M7C3_D101
 Calculated.. 18 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 34 at: 1.000E-04 9.392E+02
 BCC_A2
 FCC_A1#1
 ** M7C3_D101
 Calculated. 32 equilibria
 Terminating at known equilibrium

Phase region boundary 35 at: 3.367E-03 7.586E+02
 BCC_A2
 FCC_A1#1
 GRAPHITE_A9
 M3C2_D510

```

** M7C3_D101
Calculated.          14 equilibria
Terminating at known equilibrium

Phase region boundary 36 at:  3.367E-03  7.586E+02
  BCC_A2
  FCC_A1#1
  GRAPHITE_A9
  M3C2_D510
** M7C3_D101
Calculated..        69 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 37 at:  6.633E-03  7.586E+02
  BCC_A2
  FCC_A1#1
  GRAPHITE_A9
  M3C2_D510
** M7C3_D101
Calculated..        47 equilibria
Terminating at known equilibrium

Phase region boundary 38 at:  6.633E-03  7.586E+02
  BCC_A2
  FCC_A1#1
  GRAPHITE_A9
  M3C2_D510
** M7C3_D101
Calculated..        36 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 39 at:  2.166E-03  7.100E+02
  BCC_A2
  FCC_A1#1
** GRAPHITE_A9
  M3C2_D510
Calculated..        2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 40 at:  2.166E-03  7.100E+02
  BCC_A2
  FCC_A1#1
** GRAPHITE_A9
  M3C2_D510
Calculated..        5 equilibria
Terminating at known equilibrium

Phase region boundary 41 at:  9.900E-03  7.586E+02
  BCC_A2
  FCC_A1#1
  GRAPHITE_A9
  M3C2_D510
** M7C3_D101
Calculated..        80 equilibria
Terminating at known equilibrium

Phase region boundary 42 at:  9.900E-03  7.586E+02
  BCC_A2
  FCC_A1#1
  GRAPHITE_A9
  M3C2_D510
** M7C3_D101
Calculated..        4 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 43 at:  2.556E-03  9.033E+02
  BCC_A2
** CEMENTITE_D011
  FCC_A1#1
  M7C3_D101
Calculated..        6 equilibria
Terminating at known equilibrium

Phase region boundary 44 at:  2.556E-03  9.033E+02
  BCC_A2
** CEMENTITE_D011
  FCC_A1#1
  M7C3_D101
Calculated..        31 equilibria
Terminating at known equilibrium

Phase region boundary 45 at:  5.545E-03  9.033E+02
  BCC_A2
  CEMENTITE_D011
  FCC_A1#1
** GRAPHITE_A9
Calculated..        9 equilibria
Terminating at known equilibrium

Phase region boundary 46 at:  5.545E-03  9.033E+02
  BCC_A2
  CEMENTITE_D011
  FCC_A1#1
** GRAPHITE_A9
Calculated..        47 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 47 at:  6.691E-03  1.097E+03
  ** CEMENTITE_D011
  FCC_A1#1
Calculated..        11 equilibria
Terminating at known equilibrium

Phase region boundary 48 at:  6.691E-03  1.097E+03
  ** CEMENTITE_D011
  FCC_A1#1
Calculated..        36 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 49 at:  6.691E-03  1.097E+03

```

```

** CEMENTITE_D011
FCC_A1#1
Calculated.          11 equilibria
Terminating at known equilibrium

Phase region boundary 50 at: 6.691E-03 1.097E+03
** CEMENTITE_D011
FCC_A1#1
Calculated..         36 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 51 at: 1.000E-04 1.050E+03
** BCC_A2
FCC_A1#1
Calculated.          4 equilibria

Phase region boundary 52 at: 1.000E-04 1.050E+03
** BCC_A2
FCC_A1#1
Calculated.          32 equilibria
Terminating at known equilibrium

Phase region boundary 53 at: 3.367E-03 1.004E+03
FCC_A1#1
** M7C3_D101
Calculated.          3 equilibria
Terminating at known equilibrium

Phase region boundary 54 at: 3.367E-03 1.004E+03
FCC_A1#1
** M7C3_D101
Calculated.          25 equilibria
Terminating at known equilibrium

Phase region boundary 55 at: 6.633E-03 1.095E+03
** CEMENTITE_D011
FCC_A1#1
Calculated.          11 equilibria
Terminating at known equilibrium

Phase region boundary 56 at: 6.633E-03 1.095E+03
** CEMENTITE_D011
FCC_A1#1
Calculated..         36 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 57 at: 9.900E-03 1.189E+03
** CEMENTITE_D011
FCC_A1#1
Calculated.          44 equilibria
Terminating at known equilibrium

Phase region boundary 58 at: 9.900E-03 1.189E+03
** CEMENTITE_D011
FCC_A1#1
Calculated..         4 equilibria
Terminating at known equilibrium
Terminating at axis limit.

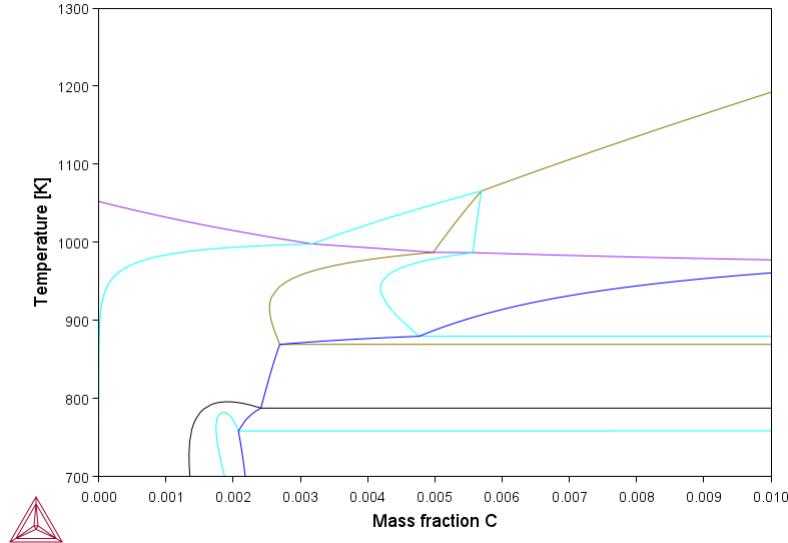
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\generate_console_examples\examples\tcex06\tcex06.POLY3
CPU time for mapping      59 seconds
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST:
POST:
POST: set-title example 6a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 6a



```

POST:
POST: Hit RETURN to continue
POST: @@ Use more practical quantities in the plot and
POST: @@ label the curves

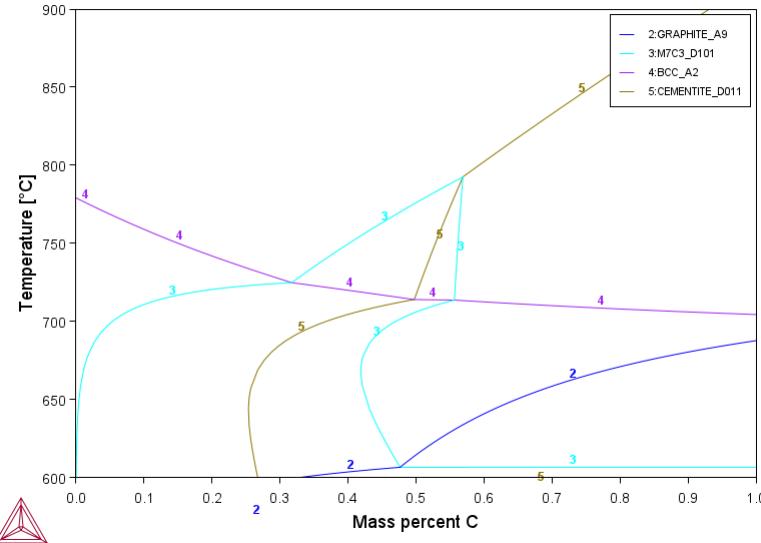
```

```

POST: s-d-a x w-p c
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t-c
... the command in full is SET_DIAGRAM_AXIS
POST: s-s x n 0 1
... the command in full is SET_SCALING_STATUS
POST:
POST: s-s y n 600 900
... the command in full is SET_SCALING_STATUS
POST:
POST: s-lab b
... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 6b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAIFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 6b

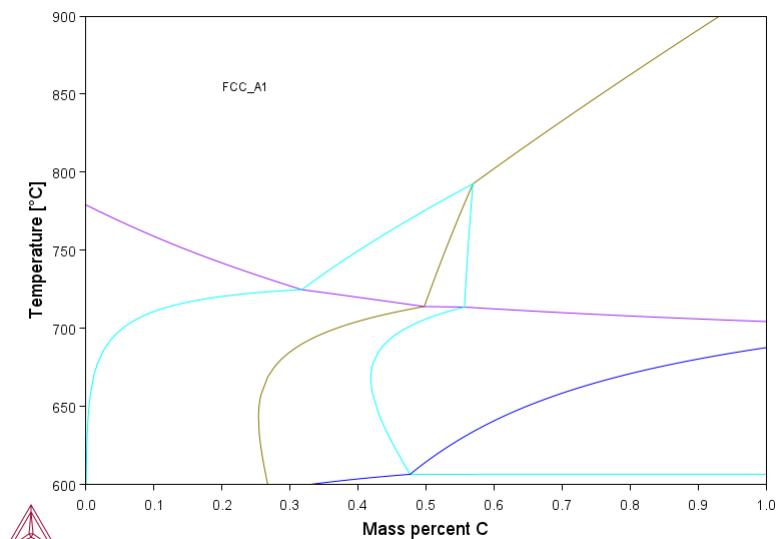


```

POST:
POST:Hit RETURN to continue
POST: @@ Determine the phase region at the iron rich side
POST: add .2 850
... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
Automatic labelling not always possible
Using global minimization procedure
Calculated 45065 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 1 s, total time 1 s
Stable phases are: FCC_A1
Text size: /.36/:
POST: @@ Knowing that only FCC (or austenite) is stable in that region and
POST: @@ which phase is stable along each line, one can determine the phases
POST: @@ in each region. For example at 0.3 % C and 630 degree C one should
POST: @@ have FCC+BCC+M7C3+CEMENTITE.
POST: @@ Check by adding a label
POST:
POST: add .3 630
... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
Automatic labelling not always possible
Using global minimization procedure
Calculated 45065 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
Stable phases are: BCC_A2+CEMENTITE_D011+FCC_A1+M7C3_D101
Text size: /.36/: @@ We remove the labels again.
*** ERROR 1034 IN GETREL: NO DIGIT
POST:
POST: s-lab n
... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 6c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAIFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 6c



POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:

tce07

SYS:About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

```
SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce07\tce07.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Calculating single equilibria in low alloyed
SYS: @@ Fe-Mn-Si-Cr-Ni-C steel
SYS:
SYS: @@ There are 2 common ways to perform a single equilibrium
SYS: @@ calculation.
SYS:
SYS: @@ 1) Get data from database, then in POLY use SET_CONDITION
SYS: @@ and COMPUTE_EQUILIBRIUM.
SYS: @@ 2) Go directly to POLY and use DEFINE_MATERIAL.
SYS:
SYS: @@ The COMPUTE_TRANSITION command is also used to determine the
SYS: @@ temperature or composition where one phase forms or
SYS: @@ disappears. It is the same as the CHANGE_STATUS -->
SYS: @@ SET_CONDITION --> COMPUTE_EQUILIBRIUM sequence of commands.
SYS: @@ Note that a TCFE database license is required to run the
SYS: @@ example.
SYS:Hit RETURN to continue
SYS:
SYS: set-log ex07.,
SYS: @@ The alloy composition is 1 wt% Cr, 0.3 wt% Si, 0.3wt% Mn,
SYS: @@ 2.8 wt% Ni and 0.55 wt% C
SYS: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY: def-mat
... the command in full is DEFINE_MATERIAL
THERMODYNAMIC DATABASE module
Database folder: C:\jenkins\workspace\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA                               /- DEFINED
DICTRA_FCC_A1 REJECTED
Database /TCFE11/: tcfe11
Major element or alloy: fe
Composition input in mass (weight) percent? /Y/:
1st alloying element: c .55
2nd alloying element: cr 1
Next alloying element: mn .3 ni 2.8 si .3
Next alloying element:
Temperature (C) /1000/: 600
VA                               /- DEFINED
DICTRA_FCC_A1 REJECTED
REINITIATING GES .....
... the command in full is DEFINE_ELEMENTS
FE DEFINED
... the command in full is DEFINE_ELEMENTS
C DEFINED
... the command in full is DEFINE_ELEMENTS
CR DEFINED
... the command in full is DEFINE_ELEMENTS
MN DEFINED
... the command in full is DEFINE_ELEMENTS
NI DEFINED
... the command in full is DEFINE_ELEMENTS
SI DEFINED

This database has following phases for the defined system

GAS:G                  LIQUID:L                  BCC_A2
A2_BCC                 BCC_B2                  FCC_A1
A1_FCC                 FCC_L12                 HCP_A3
CBCC_A12                CUB_A13                 DIAMOND_A4
GRAPHITE_A9              CEMENTITE_D011      M23C6_D84
M7C3_D101               M5C2                   M3C2_D510
KSI_CARBIDE             FE4N_LP1                SIGMA_D8B
HIGH_SIGMA              CHI_A12                C14_LAVES
C15_LAVES              M3SI                   MN9Si2
MN11Si19                MN6Si                 G_PHASE
CR3Si_A15                FESI2_H                FESI2_L
MSi_B20                 M5Si3_D88              NBNi3_D0A
Ni3Ti_D024               NB5Si3_D8L              MSi2_C40
M11Si8                 M6Si5                 AL4C3_D71
FE8Si12C                SIC_B3                 MN5SiC
CRZN17                  CUZN_EPSILON          NIZN_B2
NiZN_L10                 NI2ZN11_D82              AL5Fe4
MNP_B31                  M2P_C22                FLUORITE_C1:I
ZRO2_TETR:I              M2O3C_D53:I            M2O3H_D52:I
M4Si1_G3                 NI31Si12              CO2Si_C37
M2Si_TETA                NISI_B31              NI3Si2
CR5Si3_D8M

Reject phase(s) : /NONE/:
Restore phase(s): /NONE/:

.....
```

The following phases are retained in this system:

| | | |
|-------------|----------------|------------|
| GAS:G | LIQUID:L | BCC_A2 |
| A2_BCC | BCC_B2 | FCC_A1 |
| A1_FCC | FCC_L12 | HCP_A3 |
| CBCC_A12 | CUB_A13 | DIAMOND_A4 |
| GRAPHITE_A9 | CEMENTITE_D011 | M23C6_D84 |

| | | |
|-------------|--------------|---------------|
| M7C3_D101 | M5C2 | M3C2_D510 |
| KSI_CARBIDE | FE4N_LP1 | SIGMA_D8B |
| HIGH_SIGMA | CHI_A12 | C14_LAVES |
| C15_LAVES | M3SI | MN9SI2 |
| MN11SI19 | MN6SI | G_PHASE |
| CR3SI_A15 | FESI2_H | FESI2_L |
| MSI_B20 | M5SI3_D88 | NBN13_D0A |
| NI3TI_D024 | NB5SI3_D8L | MSI2_C40 |
| M11SI8 | M6SI5 | AL4C3_D71 |
| FE8SI2C | SIC_B3 | MN5SIC |
| CRZN17 | CUZN_EPSILON | NIZN_B2 |
| NIZN_L10 | NI2ZN11_D82 | AL5FE4 |
| MNP_B31 | M2P_C22 | FLUORITE_C1:I |
| ZRO2_TETR:I | M2O3C_D53:I | M2O3H_D52:I |
| M4S1I_G3 | NI31SI12 | CO2SI_C37 |
| M2SI_TETA | NIST_B31 | NI3SI2 |
| CR5SI3_D8M | | |

OK? /X/: Y
15:29:55,336 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
ELEMENTS
SPECIES
PHASES
... the command in full is AMEND_PHASE_DESCRIPTION
Creating a new composition set FCC_A1#2
... the command in full is AMEND_PHASE_DESCRIPTION
Creating a new composition set HCP_A3#2
... the command in full is AMEND_PHASE_DESCRIPTION
Suspending FLUORITE_C1 as it has net charge
Suspending M2O3C_D53 as it has net charge
Suspending M2O3H_D52 as it has net charge
Suspending ZRO2_TETR as it has net charge
PARAMETERS ...
FUNCTIONS ...

List of references for assessed data

'A.T. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121-127; Molar volumes'
'X.G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
'M. Ghasemi, Thermo-Calc Software AB, Sweden, 2020; Unifying liquid volume database'
'X.G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar volumes'
'B. Sundman et al., Report EUR 20315, Contract No 7210-PR/050, 2002; New Sigma model'
'P. Gustafson, TRITA-MAC 354 (1987); C-Cr-Fe-Mo-W'
'N. Saunders, COST 507 Report (1998); Cr-Ti'
'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; C15_LAVES'
'N. Dupin, Private communication, (2008); Volume data'
'B.J. Lee, KRISS, unpublished research, during 1993-1995'
'R. Naraghi, Thermo-Calc Software AB, Sweden, Volume data updated for TCFE9 database (TCFE v9.0, Jan, 2017).'
'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; FE4N'
'Unassessed parameter; Linear combination of unary data'
'Y. Tang, in TCCU2, Thermo-Calc Software AB, Stockholm, Sweden'
'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equilib., 19 (1998) 441-448; Fe-Ti'
'N. Dupin, introduction of Nb to NI15VA-4SI'
'H. Gohring, O. Fabrichnaya, A. Leineweber, E.J. Mittemeijer, Metall. Mater. Trans. A, 47A, 6173-86(2016); Fe-N, and Fe-C-N'
'N. Saunders, COST 507 Report (1998); Mn-Ti'
'W. Zheng, J. Alloys Compd., 632 (2015) 661-675'
'L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2012; Molar volumes'
'A.F. Guillermet, Z. Metallkd., 79 (1988) 524-536, TRITA-MAC 362 (1988); C -CO-NI AND C-CO-Fe-NI'
'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; C14_LAVES'
'J. De Keyzer, G. Cacciamani, N. Dupin, P. Wollants, Calphad, 33, 109 -23(2009).'
'Thermo-Calc Software, Sweden, 2008: Volume data updated for \$TCFE6 database (TCFE v6, April, 2008).'
'A. Bolcavage and U.R. Kattner, J. Phase Equilib., 2, (1996); Nb-Ni'
'W. Xiong, Y. Du, X. Lu, J.C. Schuster, H. Chen, Intermetallics. 15 (2007) 1401-1408.'
'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
'I. Ansara, unpublished work (1991); Cr-Si'
'M. Seiersten, Unpublished work (1989); Al-Fe'
'A.V. Khvan, B. Hallstedt, K. Chang, CALPHAD, 39, 54-61(2012); C-Cr-Nb'
'J-O. Andersson, CALPHAD, 11 (1987) 271-276; TRITA 0314; C-CR'
'J. Bratberg, Z. Metallkd., 96 (2005) 335-344; Fe-Cr-Mo-C'
'B.J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
'C. Qui, ISIJ International, 32 (1992), 1117-1127; TRITA-MAC 482 (1992) Revision; C-Cr-Fe-Mo'
'P. Gustafson, Metall. Trans. A, 19A (1988) 2547-2554; TRITA-MAC 348, (1987); C-CR-Fe-W'
'P. Villars, L.D. Calvert. Pearson's handbook of crystallographic data for intermetallic phases, Metals park, Ohio 1985: American society for metals'
'B.J. Lee, Metall. Trans. A, 24A (1993) 1017-1025; Fe-Cr-Mn-C'
'P. Gustafson, Scan. J. Metall.. 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
'J-O. Andersson, CALPHAD, 12 (1988) 9-23; TRITA 0321 (1986); C-Fe-MO'
'B. Hallstedt, D. Djurovic, J. von Appen, R. Dronskowsk, A. Dick, F. Koermann, T. Hickel, J. Neugebauer, CALPHAD, 34, 129-33(2010); Fe-C'
'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowsk, Calphad 35.4 (2011) 479-491; Fe-Mn-C'
'W. Huang, Metall. Trans. A, 21A (1990) 2115-2123; TRITA-MAC 411 (Rev 1989); C-FE-MN'
'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowsk, CALPHAD, 34, 279 -85(2010); Mn-C'
'A. Gabriel, C. Chatillon, and I. Ansara, published in High Temp. Sci. (Parameters listed in CALPHAD, 11 (1987) 203-218); C-NI'
'A. Gabriel, P. Gustafson, and I. Ansara, CALPHAD, 11 (1987) 203-218;

TRITA-MAC 285 (1986); C-FE-NI'
 'A.F. Guillermet and G. Grimvall, J. Phys. Chem. Solids, 1992, 53, 105-125;
 Molar volumes'
 'J. Grobner, H.L. Lukas, F. AlDinger, Calphad, 1996, 20 (2), 247-254; Al-C,
 Si-C, Al-Si-C'
 'P. Franke; revision of C-Si, Fe-Si and C-Fe-Si'
 'J. Lacaze and B. Sundman, Metall. Mater. Trans. A, 22A (1991) 2211-2223;
 Fe-Si and Fe-Si-C'
 'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; Cementite'
 'R. Naraghi, Thermo-Calc Software AB, Volume data updated for TCFE9
 database (TCFE v9.1, June, 2019).'
 'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; SIGMA and M7C3'
 'NPL, Unpublished work (1989); C-Mn-Si'
 'B.J. Lee, CALPHAD, 17 (1993) 251-268; revision of Fe-Cr and Fe-Ni liquid'
 'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270
 (1986); CR-FE'
 'K. Frisk, Metall. Trans. A, 21A (1990) 2477-2488; TRITA 0409 (1989); CR
 -FE-N'
 'J-O. Andersson, Metall. Trans. A, 19A (1988) 1385-1394; TRITA 0322 (1986);
 CR-FE-MO'
 'B.J. Lee, unpublished work at KTH (1999); update of steel database'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2019; Cr-Fe-Nb'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2014; Cr-Fe-Zn'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, Volume data updated for
 TCFE8 database (TCFE v8, May, 2015).'
 'B.J. Lee, Metall. Trans. A, 24A (1993) 1919-1933; Cr-Mn, Fe-Cr-Mn'
 'K. Frisk, CALPHAD, 17 (1993) 335-349; Cr-Mn-N'
 'SGTE (2008): SSOL4-SGTE Substance Database V4.1, provided by Thermo-Calc
 Software'
 'A.T. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); CR-NI'
 'N. Dupin, I. Ansara, B. Sundman, CALPHAD, 25 (2), 279-298 (2001); Al-Cr-Ni'
 'L.L. Zhu, H.Y. Qi, L. Jiang, Z.P. Jin, J.C. Zhao, Intermetallics. 64
 (2015) 86-95; Cr-Ru and Cr-Ni-Ru'
 'L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2010; Molar volumes'
 'L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2013; Reassessed
 solubility of Al, Cr, Fe, Ni in Mn2O3. When Mn2O3 is modelled as the
 same phase as cubic Y2O3 (M2O3C).'
 'Y. Du and J.C. Schuster, J. Phase Equilibria, 21(3) 281-86(2000); Cr-Si'
 'N. Dupin, Private communication; Si systems'
 'L. Kjellqvist, Thermo-Calc Software AB, Stockholm, 2010; Unassessed
 parameter, linear combination of unary volume data'
 'A. Jacob, E. Povoden-Karadeniz, E. Kozeschnik, Calphad, 56 (2017) 80-91.'
 'W. Huang, CALPHAD, 13 (1989) 243-252; TRITA-MAC 388 (rev 1989); FE-MN'
 'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
 'S. Liu, B. Hallstedt, D. Music, Y. Du, CALPHAD, 38 (2012) 43-58; Mn-Nb
 and Fe-Mn-Nb'
 'A. Markstrom, Thermo-Calc software AB, Sweden, 2011'
 'A.T. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); FE-NI'
 'L. Zhang, J. Wang, Y. Du, R. Hu, P. Nash, X.G. Lu, et al., Acta Mater. 57
 (2009) 5324-5341; Al-Fe-Ni'
 'L.J. Zhang, Int. J. Mater. Res., 100(2) 160-175 (2009), Fe-Mn-Ni'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; Molar volume Fe-Mn-Si
 and Al-Fe-Mn'
 'S. Cotes, A.F. Guillermet, M. Sade, J. Alloys Compd., 208(1998) 168-177'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2019; Cr-Fe-Nb-Si'
 'A. Forsberg and J. Agren, J. Phase Equilib., 14 (1993) 354-363; Fe-Mn-Si'
 'R. Naraghi, Thermo-Calc Software AB, Sweden (2019); Fe-Ni-Si'
 'J. Miettinen, G. Vassilev, J. Phase Equilib. Diffus, 37(5) 2016, 283-290;
 Fe-P-Si'
 'Shuhong Liu, unpublished work (2010), Mn-Ni, Al-Mn-Ni, Mn-Ni-Zn, Al-Cu-Fe-Mg
 -Mn-Si'
 'C.P. Guo, Intermetallics, 13(5), 525-534, (2005), Mn-Ni'
 'M. Chen, B. Hallstedt, L.J. Gauckler, J. Alloys Compd., 393 (2005) 114
 -21; Mn-Y-O'
 'M. Chen, B. Hallstedt, L.J. Gauckler, Solid State Ionics, 176 (2005) 1457
 -64; Mn-Zr-O, Mn-Y-Zr-O'
 'J. Miettinen, CALPHAD, 28 (2004) 313-320; Mn-Zn'
 'L. Kjellqvist, Thermo-Calc Software AB (2013) estimated parameter; Ni-Zr-O'
 'T. Tokunaga, K. Nishio, H. Ohtani, M. Hasebe, Calphad, 27 (2003), 161-168;
 Ni-Si'
 'N. Dupin; L12 general relations, equivalence of 2 sublattice formalism
 with four sublattice formalism'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; Checking ternary P
 systems'
 'Same or similar interaction as in the corresponding stable phase'
 'B. Sundman, Private communication (2003-4); Refitted Fe-Ni-Si'
 'W.W. Zhang, unpublished (2010), Fe-Ni-Si'
 'R. Naraghi, Thermo-Calc Software AB, Sweden (2019); M4Si1_G3'
 'J. Miettinen, CALPHAD, 27 (2003) 263-274; Cu-Ni-Zn'
 'H. Liang, Y.A.Chang, J. Phase Equilib. 19 (1998) 25-37'
 'A.V. Khvan, B. Hallstedt, C. Broeckmann, CALPHAD, 46, 24-33(2014); Cr-Fe-C'
 'J-O. Andersson, Metall. Trans. A, 19A (1988) 627-636 TRITA 0207 (1986); C
 -CR-FE'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2016; FCC Fe-Cr-C and C-Cr-Ni'
 'NPL, unpublished work (1989); C-Cr-Ni'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; C-Cr-Si'
 'Y.Du, J.C.Schuster, J.Am.Ceram.Soc., 83 (8) 2067-73 (2000); C-Cr-Si'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; Adjusting hcp'
 'J. Miettinen and B. Hallstedt, CALPHAD, 22 (1998) 231-256; Fe-Si and Fe
 -Si-C'
 'W. Zheng et al., J. Iron Steel Res. Int. 24(2) (2017) 190-197'
 'R. Naraghi, Thermo-Calc Software AB, Sweden (2015); FROST project'
 'C. Qiu, Metall. Trans. A, 24A (1993) 2393-2409; Cr-Fe-Mn-N'
 'A. Markstrom, Thermo-Calc Software AB (2013), Extrapolations, assumptions
 adjustment'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; Cr-Fe-Si'
 'M. Lindholm, J. Phase Equilib., 18.5 (1997) 432; Cr-Fe-Si'
 'B.J. Lee, Private communication, (2000); Estimated parameter'
 'J.C. Schuster and Y.Du, Metall. Mater. Trans.A, 31A(7) 1795-803(2000); Cr
 -Ni-Si.'
 'R. Naraghi, Thermo-Calc Software AB, Sweden (2019); Cr-Ni-Si'
 'B. Hu, Unpublished (2010); Mn-Ni-Si, Al-Cu-Fe-Ni'
 'R. Naraghi, Thermo-Calc Software AB, Sweden (2019); Cheking the binaries.'
 'M. Ghasemi, Thermo-Calc Software AB, Sweden, 2019; Viscosity of metallic
 liquid'
 'M. J. Assael, J. Phys. Chem. Ref. Data 35 (2006) 285; Fe, Al'
 'M. J. Assael, High Temp. High Press., 41 (2012); Sb, Pb, Bi, Ni, Ag'
 'M. J. Assael, J. Phys. Chem. Ref. Data 41 (2012) 033101; Cd, Co, Ga, In,
 Hg, Si, Ti, Zn'
 'Q. Chen, Thermo-Calc Software AB (2014), L12 constraints'
 'M. Ghasemi, Thermo-Calc Software AB: assessing the surface tension of
 metallic liquid'
 -OK-

Should any phase have a miscibility gap check? /N/: N
 Using global minimization procedure
 Calculated 45065 grid points in

```

Found the set of lowest grid points in          0 s
Calculated POLY solution      2 s, total time   16 s
POLY:

POLY: @@ The first equilibrium is calculated automatically
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS: VWCS
Output from POLY-3, equilibrium =      1, label A0 , database: TCFE11

Conditions:
T=873.15, W(C)=5.5E-3, W(CR)=1E-2, W(MN)=3E-3, W(NI)=2.8E-2, W(SI)=3E-3,
P=100000, N=1
DEGREES OF FREEDOM 0

Temperature     873.15 K (   600.00 C), Pressure 1.000000E+05
Number of moles of components 1.000000E+00, Mass in grams 5.46196E+01
Total Gibbs energy -3.56755E+04, Enthalpy 1.80441E+04, Volume 7.19873E-06

Component      Moles      W-Fraction Activity Potential Ref.stat
C              2.5011E-02  5.0000E-03  2.6153E-01 -9.7369E+03 SER
CR             1.0505E-02  1.0000E-02  3.0144E-04 -5.8855E+04 SER
FE              9.2961E-01  9.5050E-01  8.6912E-03 -3.4451E+04 SER
MN              2.9826E-03  3.0000E-03  2.7817E-05 -7.6155E+04 SER
NI              2.6058E-02  2.8000E-02  3.2474E-04 -5.8314E+04 SER
SI              5.8344E-03  3.0000E-03  2.1186E-11 -1.7843E+05 SER

BCC_A2           Status ENTERED     Driving force 0.0000E+00
Moles 9.4807E-01, Mass 5.2841E+01, Volume fraction 9.5831E-01 Mass fractions:
FE 9.63018E-01 SI 3.10097E-03 MN 2.01890E-03
NI 2.88252E-02 CR 3.01634E-03 C 2.00700E-05

CEMENTITE_D011    Status ENTERED     Driving force 0.0000E+00
Moles 2.4898E-02, Mass 1.1032E+00, Volume fraction 2.0766E-02 Mass fractions:
FE 7.19940E-01 C 6.77718E-02 NI 4.39878E-03
CR 1.71965E-01 MN 3.59240E-02 SI 4.75407E-13

M7C3_D101         Status ENTERED     Driving force 0.0000E+00
Moles 1.1910E-02, Mass 4.9370E-01, Volume fraction 9.6222E-03 Mass fractions:
FE 4.75579E-01 C 8.69279E-02 NI 2.71291E-03
CR 3.99236E-01 MN 3.55437E-02 SI 2.83764E-12

GRAPHITE_A9        Status ENTERED     Driving force 0.0000E+00
Moles 1.5125E-02, Mass 1.8167E-01, Volume fraction 1.1300E-02 Mass fractions:
C 1.00000E+00 NI 0.00000E+00 FE 0.00000E+00
SI 0.00000E+00 MN 0.00000E+00 CR 0.00000E+00

POLY: ?
... the command in full is HELP
ADD_INITIAL_EQUILIBRIUM GOTO_MODULE      REINITIATE_MODULE
ADVANCED_OPTIONS        HELP_              SAVE_WORKSPACES
AMEND_STORED_EQUILIBRIA INFORMATION        SELECT_EQUILIBRIUM
BACK                   LIST_AXIS_VARIABLE SET_ALL_START_VALUES
CHANGE_STATUS          LIST_CONDITIONS   SET_AXIS_VARIABLE
COMPUTE_EQUILIBRIUM    LIST_EQUILIBRIUM  SET_CONDITION
COMPUTE_TRANSITION     LIST_INITIAL_EQUILIBRIA SET_INPUT_AMOUNTS
CREATE_NEW_EQUILIBRIUM LIST_STATUS       SET_INTERACTIVE
DEFINE_COMPONENTS      LIST_SYMBOLS     SET_NUMERICAL_LIMITS
DEFINE_DIAGRAM         LOAD_INITIAL_EQUILIBRIUM SET_REFERENCE_STATE
DEFINE_MATERIAL        MACRO_FILE_OPEN  SET_START_CONSTITUTION
DELETE_INITIAL_EQUILIB MAKE_COMPONENT_ENTERED SET_START_VALUE
DELETE_SYMBOL          MAKE_COMPONENT_SUSPENDED SHOW_VALUE
ENTER_SYMBOL          MAP             STEP_WITH_OPTIONS
EVALUATE_FUNCTIONS    POST            TABULATE
EXIT                  READ_WORKSPACES

POLY:Hit RETURN to continue
POLY: @@ Increase Cr until all Graphite disappears. Calculate this
POLY: @@ directly using the COMPUTE-TRANSITION command. You
POLY: @@ must release the Cr content
POLY: c-t
... the command in full is COMPUTE_TRANSITION
This command is a combination of CHANGE_STATUS and SET_CONDITION
to calculate directly when a phase may form by releasing one condition.
Phase to form: grap
You must release one of these conditions
T=873.15, W(C)=5.5E-3, W(CR)=1E-2, W(MN)=3E-3, W(NI)=2.8E-2,
P=100000, N=1 DEGREES OF FREEDOM 0
Give the state variable to be removed /T/: w(cr)
Testing POLY result by global minimization procedure
Using already calculated grid
To form GRAP the condition is set to W(CR)=.0287719523467
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS: VWCS
Output from POLY-3, equilibrium =      1, label A0 , database: TCFE11

Conditions:
T=873.15, W(C)=5.5E-3, W(CR)=2.877195235E-2, W(MN)=3E-3, W(NI)=2.8E-2,
W(SI)=3E-3, P=100000, N=1
DEGREES OF FREEDOM 0

Temperature     873.15 K (   600.00 C), Pressure 1.000000E+05
Number of moles of components 1.000000E+00, Mass in grams 5.45454E+01
Total Gibbs energy -3.61530E+04, Enthalpy 1.78811E+04, Volume 7.15509E-06

Component      Moles      W-Fraction Activity Potential Ref.stat
C              2.4977E-02  5.0000E-03  2.6153E-01 -9.7369E+03 SER
CR             3.0183E-02  2.8772E-02  3.0842E-04 -5.8689E+04 SER
FE              9.1001E-01  9.3173E-01  8.6876E-03 -3.4454E+04 SER
MN              2.9786E-03  3.0000E-03  2.0228E-05 -7.8467E+04 SER
NI              2.6023E-02  2.8000E-02  3.3357E-04 -5.8119E+04 SER
SI              5.8265E-03  3.0000E-03  2.1648E-11 -1.7827E+05 SER

BCC_A2           Status ENTERED     Driving force 0.0000E+00
Moles 9.1702E-01, Mass 5.1108E+01, Volume fraction 9.3254E-01 Mass fractions:
FE 9.62515E-01 SI 3.20176E-03 MN 1.47289E-03
NI 2.96997E-02 CR 3.09060E-03 C 1.98381E-05

M7C3_D101         Status ENTERED     Driving force 0.0000E+00
Moles 8.2976E-02, Mass 3.4372E+00, Volume fraction 6.7456E-02 Mass fractions:
FE 4.73949E-01 C 8.69853E-02 NI 2.72688E-03
CR 4.10632E-01 MN 2.57069E-02 SI 2.90090E-12

GRAPHITE_A9        Status ENTERED     Driving force 0.0000E+00

```

```

Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mass fractions:
C 1.00000E+00 NI 0.00000E+00 FE 0.00000E+00
SI 0.00000E+00 MN 0.00000E+00 CR 0.00000E+00
POLY:Hit RETURN to continue
POLY: @@ Graphite disappears when we have this chromium content 2.89 w/o
POLY: @@ The amount of Cr can be obtained directly with a Show command
POLY: show w(cr)
... the command in full is SHOW_VALUE
W(CR)=2.8771952E-2
POLY: @@ This is automatically set as a new condition by the C-T command
POLY: @@ and the amount of graphite is zero.
POLY: l-st ph
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES
PHASE STATUS DRIVING FORCE MOLES
M7C3_D101 ENTERED 0.000000E+00 8.297554E-02
GRAPHITE_A9 ENTERED 0.000000E+00 0.000000E+00
BCC_A2 ENTERED 0.000000E+00 9.170245E-01
BCC_B2 ENTERED -1.377319E-04 0.000000E+00
CEMENTITE_D011 ENTERED -4.665913E-03 0.000000E+00
FCC_A1#2 ENTERED -1.129409E-02 0.000000E+00
FCC_A1#1 ENTERED -1.129409E-02 0.000000E+00
FCC_L12 ENTERED -1.143122E-02 0.000000E+00
M23C6_D84 ENTERED -8.127100E-02 0.000000E+00
M3C2_D510 ENTERED -1.346313E-01 0.000000E+00
HCP_A3#2 ENTERED -2.666922E-01 0.000000E+00
HCP_A3#1 ENTERED -2.666922E-01 0.000000E+00
M5C2 ENTERED -2.780639E-01 0.000000E+00
ENTERED PHASES WITH DRIVING FORCE LESS THAN -5.489230E-01
CUB_A13 M4S11_G3 FE4N_LP1 LIQUID BNBN13_DOA CHI_A12 SIGMA_D8B DIAMOND_A4
CBCC_A12 C14_LAVES C15_LAVES AL5FE4 KS1_CARBIDE NI3TI_D024 CRZN17 FE8SI2C
NI3SI12 G_PHASE M3SI_C02SI_C37 M2SI_TETA M2P_C22 CR3SI_A15 NI2ZN11_D82
NI3SI2 M5SI3 D88 NIZN_L10 NIZN_B2 MNSSIC HIGH_SIGMA CR5SI3 D8M_MN6SI MSI_B20
CUZN_EPSILON_MN9SI2_NISI_B31 MNP_B31 SIC_B3 M6SIS FESI2_L_AL4C3_D71 MN11SI19
MSI2_C40 FESI2_H_M11SI8 NB5SI3_D8L GAS
POLY: @@ Now determine the maximum temperature with no Austenite (FCC_A1),
POLY: @@ i.e. A1 temperature.
POLY: @@ Use the command COMPUTE-TRANSITION again
POLY: c-t
... the command in full is COMPUTE_TRANSITION
This command is a combination of CHANGE_STATUS and SET_CONDITION
to calculate directly when a phase may form by releasing one condition.
Phase to form: fcc_a1
You must release one of these conditions
T=873.15, W(C)=5.5E-3, W(CR)=2.877195235E-2, W(MN)=3E-3, W(NI)=2.8E-2,
W(SI)=3E-3, P=100000, N=1 DEGREES OF FREEDOM 0
Give the state variable to be removed /T/: t
Testing POLY result by global minimization procedure
Calculated 45065 grid points in 0 s
To form FCC_A1 the condition is set to T=910.926169574
POLY: l-c
... the command in full is LIST_CONDITIONS
T=910.9261696, W(C)=5.5E-3, W(CR)=2.877195235E-2, W(MN)=3E-3, W(NI)=2.8E-2,
W(SI)=3E-3, P=100000, N=1
DEGREES OF FREEDOM 0
POLY: @@ This command does the same as Change_Status/Set_Cond/Compute_Equil sequence.
POLY: @@ Notice that the temperature is set back as condition with the new value.
POLY: @@ If we want temperatures in Celsius enter a function.
POLY: ent fun tc=t-273;
... the command in full is ENTER_SYMBOL
POLY: sh tc
... the command in full is SHOW_VALUE
TC=637.92617
POLY:Hit RETURN to continue
POLY:
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWC5/: VWC5
Output from POLY-3, equilibrium = 1, label A0 , database: TCFE11

Conditions:
T=910.9261696, W(C)=5.5E-3, W(CR)=2.877195235E-2, W(MN)=3E-3, W(NI)=2.8E-2,
W(SI)=3E-3, P=100000, N=1
DEGREES OF FREEDOM 0

Temperature 910.93 K ( 637.78 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 5.45454E+01
Total Gibbs energy -3.85270E+04, Enthalpy 1.95997E+04, Volume 7.16809E-06

Component Moles W-Fraction Activity Potential Ref.stat
C 2.4977E-02 5.5000E-03 2.1677E-01 -1.1580E+04 SER
CR 3.0183E-02 2.8772E-02 3.1863E-04 -6.0981E+04 SER
FE 9.1001E-01 9.3173E-01 7.7657E-03 -3.6794E+04 SER
MN 2.9786E-03 3.0000E-03 1.7785E-05 -8.2837E+04 SER
NI 2.6023E-02 2.8000E-02 2.7915E-04 -6.1983E+04 SER
SI 5.8265E-03 3.0000E-03 4.2177E-11 -1.8093E+05 SER

BCC_A2 Status ENTERED Driving force 0.0000E+00
Moles 9.1675E-01, Mass 5.1087E+01, Volume fraction 9.3232E-01 Mass fractions:
FE 9.61370E-01 CR 3.99660E-03 MN 1.69140E-03
NI 2.97053E-02 SI 3.20309E-03 C 3.31203E-05

M7C3_D101 Status ENTERED Driving force 0.0000E+00
Moles 8.0497E-02, Mass 3.3366E+00, Volume fraction 6.5375E-02 Mass fractions:
FE 4.85354E-01 C 8.69306E-02 NI 2.74957E-03
CR 4.02641E-01 MN 2.23247E-02 SI 6.70624E-12

CEMENTITE_D011 Status ENTERED Driving force 0.0000E+00
Moles 2.7483E-03, Mass 1.2174E-01, Volume fraction 2.3072E-03 Mass fractions:
FE 7.26713E-01 C 6.77895E-02 NI 4.43780E-03
CR 1.78567E-01 MN 2.24927E-02 SI 4.75531E-13

FCC_A1#1 Status ENTERED Driving force 0.0000E+00
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mass fractions:
FE 8.44258E-01 MN 1.10217E-02 CR 5.80937E-03
NI 1.27409E-01 SI 9.744943E-03 C 1.75747E-03
POLY: l-st
... the command in full is LIST_STATUS
Option /CPS/: CPS
*** STATUS FOR ALL COMPONENTS
COMPONENT STATUS REF. STATE T(K) P(Pa)
VA ENTERED SER
C ENTERED SER
CR ENTERED SER

```

```

FE          ENTERED   SER
MN          ENTERED   SER
NI          ENTERED   SER
SI          ENTERED   SER
*** STATUS FOR ALL PHASES
PHASE      STATUS     DRIVING FORCE    MOLES
M7C3_D101  ENTERED   0.000000E+00  8.049708E-02
FCC_A1#2   ENTERED   0.000000E+00  0.000000E+00
FCC_A1#1   ENTERED   0.000000E+00  0.000000E+00
CEMENTITE_D011 ENTERED   0.000000E+00  2.748313E-03
BCC_A2     ENTERED   0.000000E+00  9.167546E-01
FCC_L12    ENTERED   -1.309646E-04  0.000000E+00
BCC_B2     ENTERED   -1.320120E-04  0.000000E+00
M23C6_D84  ENTERED   -6.812021E-02  0.000000E+00
GRAPHITE_A9 ENTERED   -1.334968E-01  0.000000E+00
M3C2_D510  ENTERED   -1.866450E-01  0.000000E+00
HCP_A3#2   ENTERED   -2.563175E-01  0.000000E+00
HCP_A3#1   ENTERED   -2.563175E-01  0.000000E+00
M5C2       ENTERED   -2.766353E-01  0.000000E+00
CUB_A13    ENTERED   -5.142755E-01  0.000000E+00
FE4N_LP1   ENTERED   -5.394909E-01  0.000000E+00
ENTERED PHASES WITH DRIVING FORCE LESS THAN -5.870182E-01
M4S11_G3 LIQUID_CHT_A12_NBNI3_D04 SIGMA_D8B_Cbcc_A12_C14_LAVES C15_LAVES
DIAMOND_A4 AL5FE4 KSI_CARBIDE CRZN17 NI3TI_D024 FE8SI2C NI3SI12 G_PHASE M3SI
CO2SI_C37 M2SI_TETA M2P_C22 CR3SI_A15 NI2ZN11_D82 M5SI3_D88 NI3SI2_NIZN_L10
NIZN_B2 MN5SIC HIGH_SIGMA CR5SI3_D8M MSI_B20 MN6SI CUZN_EPSILON MN9SI2
NISI_B31 MNP_B31 SIC_B3 M6SI5 FESI2_L AL4C3_D71 MN11SI19 MSI2_C40 FESI2_H
M11SI8 NB5SI3_D8L GAS
*** STATUS FOR ALL SPECIES
C  ENTERED   C60  ENTERED   FE+2 ENTERED   MN+3 ENTERED   SI  ENTERED
C2 ENTERED   CR   ENTERED   FE+3 ENTERED   MN+4 ENTERED   SI+4 ENTERED
C3 ENTERED   CR+2 ENTERED   FE+4 ENTERED   NI   ENTERED   VA   ENTERED
C4 ENTERED   CR+3 ENTERED   MN   ENTERED   NI+2 ENTERED
C5 ENTERED   FE   ENTERED   MN+2 ENTERED   NI+3 ENTERED
POLY: @@ Now determine maximum temperature where no Ferrite (BCC_A2) exists
POLY: @@ Use
POLY: c-t
... the command in full is COMPUTE_TRANSITION
This command is a combination of CHANGE_STATUS and SET_CONDITION
to calculate directly when a phase may form by releasing one condition.
Phase to form: bcc_a2
You want to find when the current major phase is formed, please give
New major phase: fcc_a1
You must release one of these conditions
T=910.9261696, W(C)=5.5E-3, W(CR)=2.877195235E-2, W(MN)=3E-3, W(NI)=2.8E-2,
W(SI)=3E-3, P=100000, N=1 DEGREES OF FREEDOM 0
Give the state variable to be removed /T/: t
Testing POLY result by global minimization procedure
Calculated 45065 grid points in 1 s
To form BCC_A2 the condition is set to T=1008.10465885
POLY:
POLY: show tc
... the command in full is SHOW_VALUE
TC=735.10466
POLY:Hit RETURN to continue
POLY: @@ Check how this varies with the carbon content
POLY: ch-st phase fcc_a1
... the command in full is CHANGE_STATUS
Status: /ENTERED/: ent
Start value, number of mole formula units /0/: 1
POLY: ch-st phase bcc_a2
... the command in full is CHANGE_STATUS
Status: /ENTERED/: fix
Number of mole formula units /0/: 0
POLY:
POLY: s-c t=none
... the command in full is SET_CONDITION
POLY:
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
7 ITS, CPU TIME USED 0 SECONDS
POLY: l-e,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: TCFE11

Conditions:
W(C)=5.5E-3, W(CR)=2.877195235E-2, W(MN)=3E-3, W(NI)=2.8E-2, W(SI)=3E-3,
P=100000, N=1
FIXED PHASES
BCC_A2=0
DEGREES OF FREEDOM 0

Temperature 1008.10 K ( 734.95 C), Pressure 1.000000E+05
Number of moles of components 1.000000E+00, Mass in grams 5.45454E+01
Total Gibbs energy -4.50693E+04, Enthalpy 2.77195E+04, Volume 7.08502E-06

Component      Moles      W-Fraction Activity Potential Ref.stat
C              2.4977E-02  5.5000E-03 8.7621E-02 -2.0408E+04 SER
CR             3.0183E-02  2.8772E-02  5.0980E-04 -6.3547E+04 SER
FE             9.1001E-01  9.3173E-01  5.8696E-03 -4.3066E+04 SER
MN             2.9786E-03  3.0000E-03  5.0117E-06 -1.0229E+05 SER
NI             2.6023E-02  2.8000E-02  7.6292E-05 -7.9468E+04 SER
SI              5.8265E-03  3.0000E-03  2.5738E-10 -1.8508E+05 SER

FCC_A1#1      Status ENTERED   Driving force 0.0000E+00
Moles 9.6475E-01, Mass 5.3092E+01, Volume fraction 9.7078E-01 Mass fractions:
FE 9.45651E-01 CR 1.63193E-02 SI 3.08210E-03
NI 2.87421E-02 C 3.25815E-03 MN 2.94707E-03

M7C3_D101      Status ENTERED   Driving force 0.0000E+00
Moles 3.5250E-02, Mass 1.4529E+00, Volume fraction 2.9128E-02 Mass fractions:
CR 4.83816E-01 C 8.74213E-02 NI 8.82838E-04
FE 4.22946E-01 MN 4.93402E-03 SI 4.97830E-11

BCC_A2         Status FIXED     Driving force 0.0000E+00
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mass fractions:
FE 9.71935E-01 CR 1.08640E-02 MN 9.22867E-04
NI 1.29484E-02 SI 3.24854E-03 C 8.13589E-05

POLY: show tc
... the command in full is SHOW_VALUE
TC=735.10466
POLY:
POLY:Hit RETURN to continue

```

```

POLY:
POLY: s-a-v 1 w(c) 0 .08 0.001,,,
... the command in full is SET_AXIS_VARIABLE
POLY: save tce07 y
... the command in full is SAVE_WORKSPACES
POLY: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 0.550000E-02
...OK

Phase Region from 0.550000E-02 for:
BCC_A2
FCC_A1#1
M7C3_D101
Global check of adding phase at 7.92117E-03
Calculated 5 equilibria

Phase Region from 0.792117E-02 for:
BCC_A2
CEMENTITE_D011
FCC_A1#1
M7C3_D101
Global check of removing phase at 1.03956E-02
Calculated 5 equilibria

Phase Region from 0.103956E-01 for:
BCC_A2
CEMENTITE_D011
FCC_A1#1
Global test at 1.75000E-02 .... OK
Global check of adding phase at 2.24931E-02
Calculated 15 equilibria

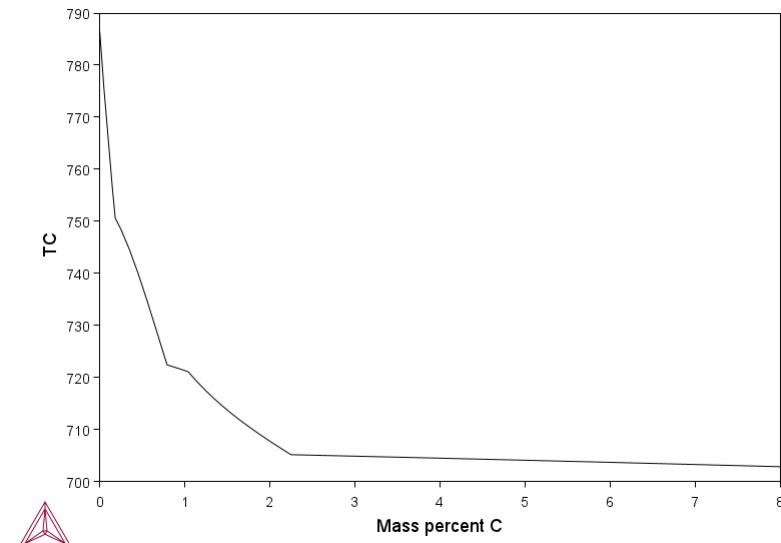
Phase Region from 0.224931E-01 for:
BCC_A2
CEMENTITE_D011
FCC_A1#1
GRAPHITE_A9
Global test at 3.05000E-02 .... OK
Global test at 4.05000E-02 .... OK
Global test at 5.05000E-02 .... OK
Global test at 6.05000E-02 .... OK
Global test at 7.05000E-02 .... OK
Global test at 8.00000E-02 .... OK
Terminating at 0.800000E-01
Calculated 61 equilibria

Phase Region from 0.550000E-02 for:
BCC_A2
FCC_A1#1
M7C3_D101
Global check of removing phase at 1.81940E-03
Calculated 6 equilibria

Phase Region from 0.181940E-02 for:
BCC_A2
FCC_A1#1
Global test at 9.98984E-16 .... OK
Terminating at 0.215885E-12
Calculated 6 equilibria
*** Buffer saved on file: c:\jenkins\workspace\generate_console_examples\examples\tce07\tce07.POLY3
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2
POST: s-d-a x w-p c
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y tc
... the command in full is SET_DIAGRAM_AXIS
POST:
POST: set-title example 7a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 7a



```

POST:
POST: Hit RETURN to continue
POST: s-s y n 700 800
... the command in full is SET_SCALING_STATUS

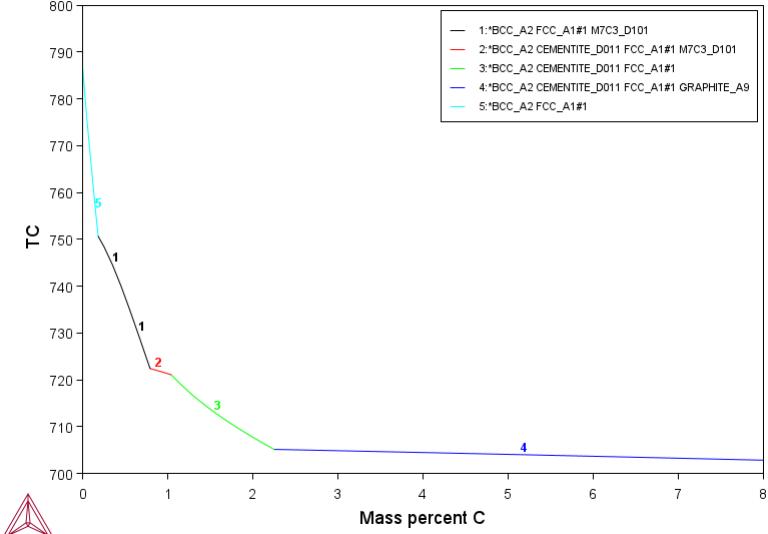
```

```

POST: s-lab b
... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 7b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAIFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 7b



```

POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:

```

tce08

SYS:About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce08\tce08.TCM.test"

SYS: set-echo

SYS:
SYS: @@ Calculation of a property diagram for a high speed steel
SYS:
SYS: @@ This example shows how to calculate property diagrams
SYS: @@ for a high speed steel i.e. phase fraction plots,
SYS: @@ activity vs temperature, and so forth.
SYS: @@ Note that a TCFE database license is required to run
SYS: @@ the example.
SYS:
SYS: set-log ex08,,
SYS: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32

POLY: def-dia

... the command in full is DEFINE_DIAGRAM
For binary or ternary diagrams you may prefer the special modules

You must specify a value for all compositions and the temperature even if you want to use it as axis.

THERMODYNAMIC DATABASE module

Database folder: C:\jenkins\workspace\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED
DICTRA_FCC_A1 REJECTED
Database /TCFE11/: tcfe11
Major element or alloy: fe
Composition input in mass (weight) percent? /Y/:
1st alloying element: c .9 cr 4 mn .3 si .3 w 8 mo 5 v 2
Next alloying element:

Temperature (C) /1000/: 1300

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

REINITIATING GES

... the command in full is DEFINE_ELEMENTS

FE DEFINED

... the command in full is DEFINE_ELEMENTS

C DEFINED

... the command in full is DEFINE_ELEMENTS

CR DEFINED

... the command in full is DEFINE_ELEMENTS

MN DEFINED

... the command in full is DEFINE_ELEMENTS

SI DEFINED

... the command in full is DEFINE_ELEMENTS

W DEFINED

... the command in full is DEFINE_ELEMENTS

MO DEFINED

... the command in full is DEFINE_ELEMENTS

V DEFINED

This database has following phases for the defined system

| | | |
|-------------|----------------|---------------|
| GAS:G | LIQUID:L | BCC_A2 |
| A2_BCC | BCC_B2 | FCC_A1 |
| A1_FCC | FCC_L12 | HCP_A3 |
| CBCC_A12 | CUB_A13 | DIAMOND_A4 |
| GRAPHITE_A9 | CEMENTITE_D011 | M23C6_D84 |
| M7C3_D101 | M6C_E93 | M5C2 |
| M3C2_D510 | MC_ETA | MC_SHP |
| KSI_CARBIDE | Z_PHASE | FE4N_LP1 |
| SIGMA_D8B | HIGH_SIGMA | MU_D85 |
| P_PHASE | R_PHASE | CHI_A12 |
| C14_LAVES | C15_LAVES | M3SI |
| MN9Si2 | MN11Si19 | MN6Si |
| G_PHASE | CR3Si_A15 | FESI2_H |
| FESI2_L | MSI_B20 | M5Si3_D88 |
| NBNi3_D0A | CO3V | MOSi2_C11B |
| Mo5Si3_D8M | NB5Si3_D8L | MSi2_C40 |
| M11Si18 | M6Si5 | AL4C3_D71 |
| Fe8Si2C | SIC_B3 | MN5SiC |
| CRZN17 | CUZn_EPSILON | AL5Fe4 |
| MnP_B31 | M2P_C22 | FLUORITE_C1:I |
| ZrO2_TETR:I | M2O3C_D53:I | M2O3H_D52:I |
| NI31Si12 | CO2Si_C37 | M2Si_TETA |
| NiSi_B31 | NI3Si2 | CR5Si3_D8M |
| DELTA_TIH2 | DIS_BETA | BETA_PHASE |

Reject phase(s) /NONE/: NONE

Restore phase(s) : /NONE/: NONE

The following phases are retained in this system:

| | | |
|-------------|----------------|------------|
| GAS:G | LIQUID:L | BCC_A2 |
| A2_BCC | BCC_B2 | FCC_A1 |
| A1_FCC | FCC_L12 | HCP_A3 |
| CBCC_A12 | CUB_A13 | DIAMOND_A4 |
| GRAPHITE_A9 | CEMENTITE_D011 | M23C6_D84 |
| M7C3_D101 | M6C_E93 | M5C2 |
| M3C2_D510 | MC_ETA | MC_SHP |
| KSI_CARBIDE | Z_PHASE | FE4N_LP1 |
| SIGMA_D8B | HIGH_SIGMA | MU_D85 |

| | | |
|-------------|--------------|---------------|
| P_PHASE | R_PHASE | CHI_A12 |
| C14_LAVES | C15_LAVES | M3SI |
| MN9SI12 | MN11SI19 | MN6SI |
| G_PHASE | CR3SI_A15 | FESI2_H |
| FESI2_L | MSI_B20 | M5SI3_D88 |
| NBNi3_D0A | CO3V | MOSI2_C11B |
| MO5Si3_D8M | NB5Si3_D8L | MSI2_C40 |
| M11Si8 | M6Si5 | AL4C3_D71 |
| FE8Si2C | SIC_B3 | MN5SiC |
| CRZN17 | CUZN_EPSILON | AL5FE4 |
| MNP_B31 | M2P_C22 | FLUORITE_C1:I |
| ZRO2_TETR:I | M2O3C_D53:I | M2O3H_D52:I |
| NI3Si12 | CO2Si_C37 | M2Si_TETA |
| NiSi_B31 | NI3Si2 | CR5Si3_D8M |
| DELTA_TIH2 | DIS_BETA | BETA_PHASE |

OK? /Y/: Y
15:31:31,846 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
ELEMENTS
SPECIES
PHASES
... the command in full is AMEND_PHASE_DESCRIPTION
Creating a new composition set FCC_A1#2
... the command in full is AMEND_PHASE_DESCRIPTION
Creating a new composition set HCP_A3#2
... the command in full is AMEND_PHASE_DESCRIPTION
Suspending FLUORITE_C1 as it has net charge
Suspending M2O3C_D53 as it has net charge
Suspending M2O3H_D52 as it has net charge
Suspending ZRO2_TETR as it has net charge
PARAMETERS
FUNCTIONS

List of references for assessed data

'A.T. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121-127; Molar volumes'
'X.G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
'M. Ghasemi, Thermo-Calc Software AB, Sweden, 2020; Unifying liquid volume database'
'X.G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar volumes'
'B. Sundman et al., Report EUR 20315, Contract No 7210-PR/050, 2002; New Sigma model'
'P. Gustafson, TRITA-MAC 354 (1987); C-Cr-Fe-Mo-W'
'N. Saunders, COST 507 Report (1998); Cr-Ti'
'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; C15_LAVES'
'N. Dupin, Private communication, (2008); Volume data'
'B.J. Lee, KRISS, unpublished research, during 1993-1995'
'R. Naraghi, Thermo-Calc Software AB, Sweden, Volume data updated for TCFE9 database (TCFE v9.0, Jan, 2017).'
'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; FE4N'
'Unassessed parameter; Linear combination of unary data'
'Y. Tang, in TCCU2, Thermo-Calc Software AB, Stockholm, Sweden'
'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equilib., 19 (1998) 441-448; Fe-Ti'
'N. Dupin, introduction of Nb to Ni15VA-4SL'
'H. Gohring, O. Fabrichnaya, A. Leineweber, E.J. Mittemeijer, Metall. Mater. Trans. A, 47A, 6173-86(2016); Fe-N, and Fe-C-N'
'N. Saunders, COST 507 Report (1998); Mn-Ti'
'W. Zheng, J. Alloys Compd., 632 (2015) 661-675'
'L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2012; Molar volumes'
'J-O. Andersson, CALPHAD, 12 (1988) 9-23; TRITA 0321 (1986); C-FE-MO'
'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; C14_LAVES'
'I. Ansara, unpublished work (1991); Cr-Si'
'J. Bratberg and B. Sundman, J. Phase Equilib., 24, No. 6, 2003, 495-503; Co-V'
'J. Bratberg and Karin Frisk, CALPHAD, 26, No. 3, 459-476, 2002; Mo-V-C'
'R. Naraghi, Thermo-Calc Software AB, Sweden, 2015; C14_LAVES'
'B.J. Lee, unpublished work at KTH (1999); update of steel database'
'P. Gustafson, Z. Metallkd., 79 (1988) 397-402; TRITA-MAC 330 (1987); C-MO -W'
'M. Seiersten, Unpublished work (1989); Al-Fe'
'A.V. Khvan, B. Hallstedt, K. Chang, CALPHAD, 39, 54-61(2012); C-Cr-Nb'
'J-O. Andersson, CALPHAD, 11 (1987) 271-276; TRITA 0314; C-CR'
'J. Bratberg, Z. Metallkd., 96 (2005) 335-344; Fe-Cr-Mo-C'
'B.J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
'C. Qui, ISIJ International, 32 (1992), 1117-1127; TRITA-MAC 482 (1992) Revision; C-Cr-Fe-Mo'
'P. Gustafson, Metall. Trans. A, 19A (1988) 2547-2554; TRITA-MAC 348, (1987); C-CR-FE-W'
'P. Villars, L.D. Calvert. Pearson's handbook of crystallographic data for intermetallic phases, Metals park, Ohio 1985: American society for metals'
'B.J. Lee, Metall. Trans. A, 24A (1993) 1017-1025; Fe-Cr-Mn-C'
'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
'B. Hallstedt, D. Djurovic, J. von Appen, R. Drönkowsk, A. Dick, F. Koermann, T. Hickel, J. Neugebauer, CALPHAD, 34, 129-33(2010); Fe-C'
'D. Djurovic, B. Hallstedt, J. von Appen, R. Drönkowsk, Calphad 35.4 (2011) 479-491; Fe-Mn-C'
'W. Huang, Metall. Trans. A, 21A (1990) 2115-2123; TRITA-MAC 411 (Rev 1989); C-FE-MN'
'D. Djurovic, B. Hallstedt, J. von Appen, R. Drönkowsk, CALPHAD, 34, 279 -85(2010); Mn-C'
'J.H. Shim, C.S. Oh, D.N. Lee, Metall. Mater. Trans. B, 27 (1996) 955-966; Ti-Mo-C'
'R. Naraghi, Thermo-Calc Software AB, Volume data updated for TCFE9 database (TCFE v9.1, June, 2019).'
'J. Grobner, H.L. Lukas, F. Aldinger, Calphad, 1996, 20 (2), 247-254; Al-C, Si-C, Al-Si-C'

'P. Franke; revision of C-Si, Fe-Si and C-Fe-Si'
 'J. Lacaze and B. Sundman, Metall. Mater. Trans. A, 22A (1991) 2211-2223;
 'Fe-Si and Fe-Si-C'
 'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; Cementite'
 'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; SIGMA and M7C3'
 'Thermo-Calc Software, Sweden, 2008; Volume data updated for \$TCFE6
 database (TCFE v6, April, 2008).'
 'NPL, Unpublished work (1989); C-Mn-Si'
 'W. Huang, TRITA-MAC 432 (1990); C-Fe-V'
 'A.F. Guillermet and W. Huang, TRITA-MAC 440 (1990); Mn-V-C'
 'A.F. Guillermet and G. Grimvall, J. Phys. Chem. Solids, 1992, 53, 105-125;
 'Molar volumes'
 'B.J. Lee, TRITA-MAC 475 (1991); C-Cr-Fe-V'
 'A.F. Guillermet, Z Metallkd. 82(1991)6 p 478-487; Nb-Zr'
 'S. Jonsson, PhD Thesis; TRITA-MAC 519 (1993); W-C and Ti-W-C'
 'P. Gustafson, Mat. Sci. Tech., 2 (1986) 653-658; TRITA 0212 (1985); C-W'
 'P. Gustafson, Metall. Trans. A, 18A (1987) 175-188; TRITA 0257 (1985); C
 -FE-W'
 'P. Gustafson, Z. Metallkd., 79 (1988) 421-425; TRITA-MAC 331 (1987); C
 -FE-MO-W'
 'N. Dupin, Private communication; Introduction of V'
 'B.J. Lee, CALPHAD, 17 (1993) 251-268; revision of Fe-Cr and Fe-Ni liquid'
 'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270
 (1986); CR-FE'
 'K. Frisk, Metall. Trans. A, 21A (1990) 2477-2488; TRITA 0409 (1989); CR
 -FE-N'
 'J-O. Andersson, Metall. Trans. A, 19A (1988) 1385-1394; TRITA 0322 (1986);
 CR-FE-MO'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2019; Cr-Fe-Nb'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2014; Cr-Fe-Zn'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, Volume data updated for
 TCFE8 database (TCFE v8, May, 2015).'
 'B.J. Lee, Metall. Trans. A, 24A (1993) 1919-1933; Cr-Mn, Fe-Cr-Mn'
 'K. Frisk, CALPHAD, 17 (1993) 335-349; Cr-Mn-N'
 'SGTE (2008): SSOL4-SGTE Substance Database V4.1, provided by Thermo-Calc
 Software'
 'K. Frisk, KTH Report D 60 (1984); CR-MO'
 'B. Sundman, Private communication; FCC parameter same as BCC; Cr-Mo'
 'J-O. Andersson, TRITA-MAC 323 (1986); C-CR-FE-MO'
 'K. Frisk, TRITA-MAC 429 (1990); CR-MO-NI'
 'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; Z_PHASE'
 'L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2013; Reassessed
 solubility of Al, Cr, Fe, Ni in Mn2O3. When Mn2O3 is modelled as the
 same phase as cubic Y2O3 (M2O3C).'
 'Y. Du and J.C. Schuster, J. Phase Equilibria, 21(3) 281-86(2000); Cr-Si'
 'N. Dupin, Private communication; Si systems'
 'L. Kjellqvist, Thermo-Calc Software AB, Stockholm, 2010; Unassessed
 parameter, linear combination of unary volume data'
 'A. Jacob, E. Povoden-Karadeniz, E. Kozeschnik, Calphad, 56 (2017) 80-91.'
 'B.J. Lee, TRITA-MAC 474 (1991); Cr-Fe-V'
 'H.K. Danielsen and J. Hald, CALPHAD, 31 (2007) 505-514; Z-PHASE'
 'P. Gustafson, CALPHAD, 11 (1987) 277-292; TRITA-MAC 320 (1986); CR-NI-W'
 'W. Huang, CALPHAD, 13 (1989) 243-252; TRITA-MAC 388 (rev 1989); FE-MN'
 'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
 'S. Liu, B. Hallstedt, D. Music, Y. Du, CALPHAD, 38 (2012) 43-58; Mn-Nb
 and Fe-Mn-Nb'
 'A. Markstrom, Thermo-Calc software AB, Sweden, 2011'
 'A.F. Guillermet, CALPHAD, 6 (1982) 127-140; (sigma phase revised 1986);
 TRITA-MAC 200 (1982); FE-MO'
 'K. Frisk, TRITA-MAC 428 (1990); FE-MO-NI'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; Molar volume Fe-Mn-Si
 and Al-Fe-Mn'
 'S. Cotes, A.F. Guillermet, M. Sade, J. Alloys Compd., 208(1998) 168-177'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2019; Cr-Fe-Nb-Si'
 'A. Forsberg and J. Agren, J. Phase Equilib., 14 (1993) 354-363; Fe-Mn-Si'
 'R. Naraghi, Thermo-Calc Software AB, Sweden (2019); Fe-Ni-Si'
 'J. Miettinen, G. Vassilev, J. Phase Equilib. Diffus., 37(5) 2016, 283-290;
 Fe-P-Si'
 'J-O. Andersson, CALPHAD, 7 (1983) 305-315 (Parameters revised 1986 due to
 new description of V) TRITA 0201 (1982); FE-V'
 'A.V. Khvan, K. Chang, B. Hallstedt, CALPHAD, 43, 143-48(2013); Fe-Nb-V'
 'W. Huang, TRITA-MAC 439 (1990) also in W. Huang, CALPHAD, 15, 195
 -208(1991); Mn-V, Fe-Mn-V'
 'R. Naraghi, Thermo-Calc Software AB, Sweden (2015); FROST project'
 'P. Gustafson, Z. Metallkd., 79 (1988) 388-396; TRITA-MAC 329 (1987); MO-W,
 FE-MO-W'
 'Y. Yang, Testing for TCTI2.0, Thermo-Calc Software AB, Sweden, Oct-Nov.
 2018; C-H, Ti-Y, H-V, Hf-Y, Nb-Y, V-Y, Y-Zr'
 'Y. Yang, Thermo-Calc Software AB, Sweden, 2019; Volume data updated for
 TCTI3.0 database (TCTI v3.0, Aug-Oct 2019).'
 'S. Ukita, H. Ohtani, M. Hasebe, Materials Transactions, 49 (2008) 2528
 -2533.'
 'M. Chen, B. Hallstedt, L. J. Gauckler, J. Alloys Compd., 393 (2005) 114
 -21; Mn-Y-O'
 'M. Chen, B. Hallstedt, L.J. Gauckler, Solid State Ionics, 176 (2005) 1457
 -64; Mn-Zr-O, Mn-Y-Zr-O'
 'W. Huang, TRITA-MAC 441 (1990) also in W. Huang, Metall. Trans. A, 22A,
 1911-20 (1991); Fe-Mn-V-C'
 'P. Franke, unpublished revisions, Aachen, 2006-2008; Mn-W'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2017; Estimated parameter'
 'COST2 database 1997'
 'J. Miettinen, CALPHAD, 28 (2004) 313-320; Mn-Zn'
 'Y. Liu, G. Shao, P. Tsakirooulos, Intermatallics 8 (2000) 953-962; Mo-Si,
 Al-Mo-Si'
 'M.H. Rand and N. Saunders, COST 507 Report (1998); Si-V'
 'C. Vahlas, P-Y. Chevalier and E. Blanquet, CALPHAD, 13 (1989) 273-292'
 'S. Huang, J. Vleugels, L. Li, O. Van Der Biest, J. Alloys Compd., 395
 (2005) 68-74; V-W-C'
 'A.V. Khvan, B. Hallstedt, C. Broeckmann, CALPHAD, 46, 24-33(2014); Cr-Fe-C'
 'J-O. Andersson, Metall. Trans. A, 19A (1988) 627-636 TRITA 0207 (1986); C
 -CR-FE'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2016; FCC Fe-Cr-C and C-Cr-Ni'
 'J. Bratberg, Thermo-Calc Software AB, Sweden, 2008; Fe-Cr-Mo-V-W-C'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; C-Cr-Si'
 'Y. Du, J.C. Schuster, J. Am. Ceram. Soc., 83 (8) 2067-73 (2000); C-Cr-Si'
 'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; Carbonitrides and
 M23C6'
 'J. Bratberg, Thermo-Calc Software AB, Sweden, 2008; Fe-Cr-V-C'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; Adjusting hcp'
 'S. Nagakura, Transactions of the Iron and Steel Institute of Japan, 8
 (1968) 265-294; Molar volumes'
 'I.K. Kupalova, V.I. Pavlova, High Speed Steels: Physical Properties,
 Prop. Data Updat. 2 (1988) 67-78; Molar volumes'
 'J. Miettinen and B. Hallstedt, CALPHAD, 22 (1998) 231-256; Fe-Si and Fe
 -Si-C'
 'W. Zheng et al., J. Iron Steel Res. Int. 24(2) (2017) 190-197'

'C. Qiu, Metall. Trans. A, 24A (1993) 2393-2409; Cr-Fe-Mn-N'
 'A. Markstrom, Thermo-Calc Software AB (2013), Extrapolations, assumptions
 adjustment'
 'B. Sundman, estimated parameter (2000); Cr-Ni-Mo'
 'B.J. Lee, Private communication, (2000); Estimated parameter'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; Cr-Fe-Si'
 'M. Lindholm, J. Phase Equilib., 18.5 (1997) 432; Cr-Fe-Si'
 'A. Markstrom, Thermo-calc Software AB, Sweden, 2011; SIGMA phase in Cr-Fe
 -W'
 'J. Miettinen, CALPHAD, 22 (1998) 275-300; Fe-Mo-Si'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2016; C-Cr-Fe-V'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2016; C-Cr-Fe-W'
 'J. Bratberg, Thermo-Calc Software AB, Sweden, 2008; Solubilities in M6C'
 'P. Gustafson, Inst. Met. Res. (Sweden) (1990); Estimations of C-CR-FE-V,
 C-CR-FE-MO-V-W, FE-N-W, FE-MN-N, FE-N-SI, CR-N-V, C-CR-N, FE-MO-N, CR
 -N-W, CR-TI-N'
 'M. Ghasemi, Thermo-Calc Software AB, Sweden, 2019; Viscosity of metallic
 liquid'
 'M. J. Assael, J. Phys. Chem. Ref. Data 35 (2006) 285; Fe, Al'
 'M. J. Assael, J. Phys. Chem. Ref. Data 41 (2012) 033101; Cd, Co, Ga, In,
 Hg, Si, Ti, Zn'
 'J. T. Okada, J. Chem. Thermodynamics 42 (2010) 856; V'
 'T. Ishikawa, J. Chem. Thermodynamics 65 (2013) 1; Mo, Os, Re, Ta, W'
 'Q. Chen, Thermo-Calc Software AB (2014), L12 constraints'
 'M Ghasemi, Thermo-Calc Software AB: assessing the surface tension of
 metallic liquid'

-OK-

Should any phase have a miscibility gap check? /N/: N

Using global minimization procedure
 Calculated 48087 grid points in 20 s
 Found the set of lowest grid points in 0 s
 Calculated POLY solution 4 s, total time 24 s
 You must now set an independent axis for your diagram
 as one of the following conditions:
 Condition 1 is temperature (Celsius)
 Condition 2 is mass percent of C
 Condition 3 is mass percent of CR
 Condition 4 is mass percent of MN
 Condition 5 is mass percent of SI
 Condition 6 is mass percent of W
 Condition 7 is mass percent of MO
 Condition 8 is mass percent of V

Give the number of the condition to vary /1/: 1

Minimum value (C) /800/: 600

Maximum value (C) /1800/: 1600

The second axis can be another of the conditions above and you will then
 calculate a phase diagram.
 Or you may want to plot how some other quantities depend on the selected
 condition and you will then calculate a "property" diagram.

In addition to the conditions above you may use these selected
 dependent quantities on the vertical axis:

Dependent 9 is mass fraction of all phases
 Dependent 10 is composition of a phase
 Dependent 11 is the fraction of a component in all phases
 (In the post processor you may select many other quantities)

Give the number of the quantity on second axis /9/: 9 tcex08 y

No initial equilibrium, using default
 Step will start from axis value 1573.15

...OK

Phase Region from 1573.15 for:
 LIQUID

BCC_A2
 FCC_A1#1
 M6C_E93

Global check of removing phase at 1.57870E+03
 Calculated 3 equilibria

Phase Region from 1578.70 for:
 LIQUID

BCC_A2
 FCC_A1#1

Global check of removing phase at 1.59784E+03
 Calculated 5 equilibria

Phase Region from 1597.84 for:
 LIQUID

BCC_A2

Global test at 1.67315E+03 OK

Global check of removing phase at 1.69235E+03

Calculated 12 equilibria

Phase Region from 1692.35 for:

LIQUID

Global test at 1.76315E+03 OK

Global test at 1.86315E+03 OK

Terminating at 1873.15

Calculated 22 equilibria

Phase Region from 1573.15 for:

LIQUID

BCC_A2

FCC_A1#1

M6C_E93

Global check of removing phase at 1.57109E+03

Calculated 3 equilibria

Phase Region from 1571.09 for:

LIQUID

FCC_A1#1

M6C_E93

Global check of adding phase at 1.52095E+03

Calculated 8 equilibria

Phase Region from 1520.95 for:

LIQUID

FCC_A1#1

FCC_A1#2

M6C_E93

Global check of removing phase at 1.52080E+03

Calculated 3 equilibria

Phase Region from 1520.80 for:

FCC_A1#1

```

FCC_A1#2
M6C_E93
Global test at 1.44315E+03 .... OK
Global test at 1.34315E+03 .... OK
Global test at 1.24315E+03 .... OK
Global test at 1.14315E+03 .... OK
Global check of adding phase at 1.12062E+03
Calculated 43 equilibria

Phase Region from 1120.62 for:
FCC_A1#1
FCC_A1#2
M23C6_D84
M6C_E93
Global check of adding phase at 1.11212E+03
Calculated 4 equilibria

Phase Region from 1112.12 for:
BCC_A2
FCC_A1#1
FCC_A1#2
M23C6_D84
M6C_E93
Global check of removing phase at 1.09550E+03
Calculated 4 equilibria

Phase Region from 1095.50 for:
BCC_A2
FCC_A1#2
M23C6_D84
M6C_E93
Global test at 1.02315E+03 .... OK
Global test at 9.23150E+02 .... OK
Terminating at 873.150
Calculated 26 equilibria
*** Buffer saved on file: c:\jenkins\workspace\generate_console_examples\examples\tcex08\tcex08.POLY3
POSTPROCESSOR VERSION 3.2

```

Setting automatic diagram axes

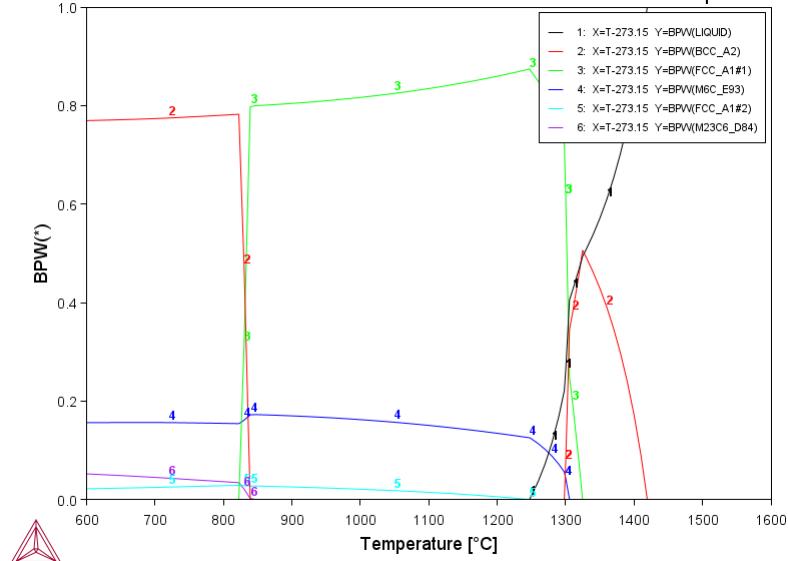
... the command in full is REINITIATE_PLOT_SETTINGS
POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

... the command in full is SET_AUTOMATIC_DIAGRAM_A

Setting automatic diagram axes

... the command in full is PLOT_DIAGRAM

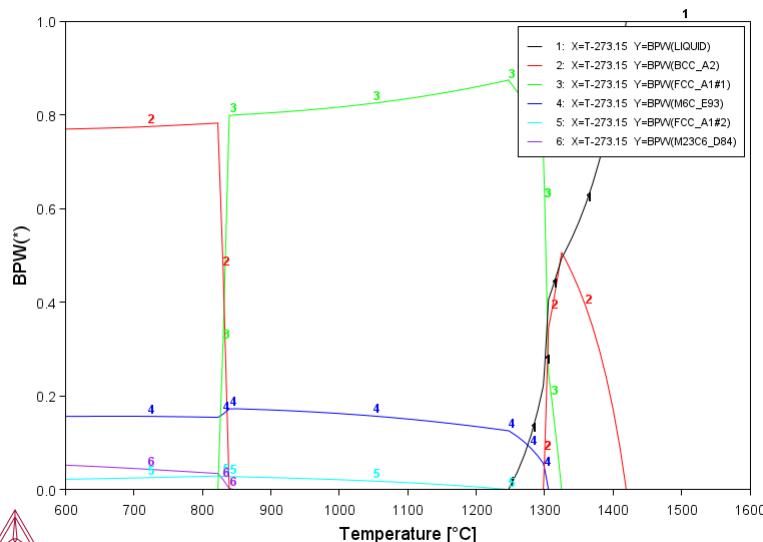


```

POST:
POST:Hit RETURN to continue
POST: set-title example 8a
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 8a

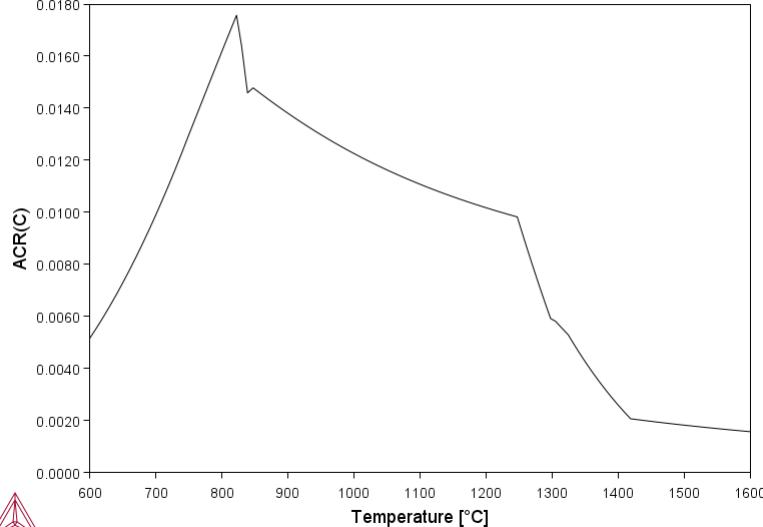


```

POST:
POST:Hit RETURN to continue
POST: s-d-a y acr(c)
... the command in full is SET_DIAGRAM_AXIS
POST: set_lab
... the command in full is SET_LABEL_CURVE_OPTION
CURVE LABEL OPTION (A, B, C, D, E, F OR N) /D/: n
POST: set-title example 8b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 8b

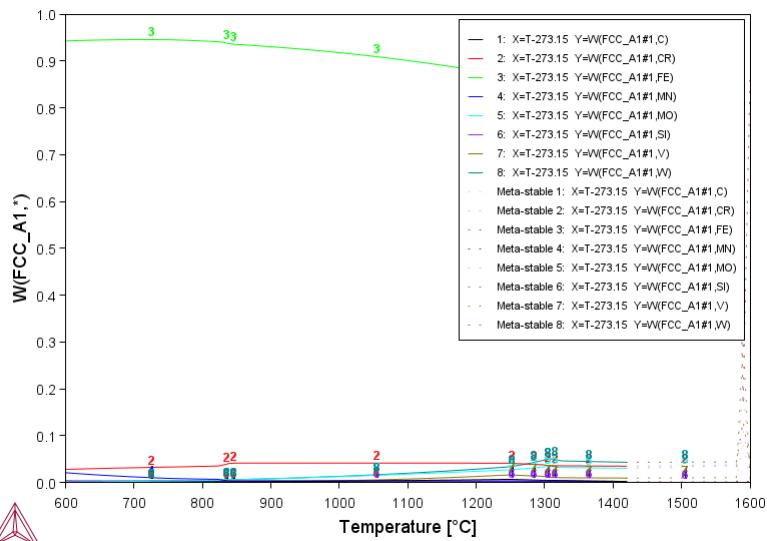


```

POST:
POST:Hit RETURN to continue
POST: @@ Plot how the composition of the austenite (called fcc) varies
POST: @@ Note this is plotted also where the austenite is not stable.
POST: s-d-a y w(fcc_a1,*)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*:
POST: set_lab d
... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 8c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

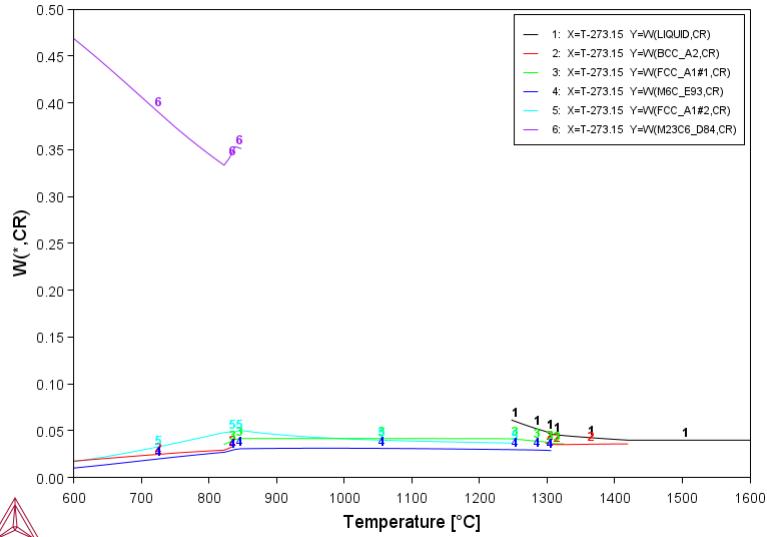
example 8c



```

POST:
POST:Hit RETURN to continue
POST: @@ Plot the fraction of Cr in all phases
POST: s-d-a y w(*,cr)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*:
POST: set-title example 8d
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
      
```

example 8d



```

POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:
      
```

tce09

SYS:About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce09\tce09.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Calculating a dew point with the POLY3 module
SYS:
SYS: go data
THERMODYNAMIC DATABASE module
Database folder: C:\jenkins\workspace\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE11: sw subdemo
Current database: Substance Demo Database v1.0

VA /- DEFINED
TDB_SUBDEMO: def-sp h2 h2o1
H2 H2O1 DEFINED
TDB_SUBDEMO: get
15:33:36,700 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES
ELEMENTS
SPECIES
PHASES
PARAMETERS ...
FUNCTIONS

List of references for assessed data

'H2<G> JANAF THERMOCHEMICAL TABLES SGTE ** H2<G> H2<G> HYDROGEN<G>
 STANDARD STATE FROM CODATA KEY VALUES. CP FROM JANAF PUB. 3/61'
'H2O1<G> T.C.R.A.S. Class: 1 H2O1<G> H2O<G> WATER <GAS>, STEAM'
'H2O1<L> T.C.R.A.S. Class: 4 H2O1_Liquid H2O_Liquid Pure_Water WATER
 T.C.R.A.S. Class: 4 cp modified by atd 12/9/94 and 5/7/2002'
-OK-
TDB_SUBDEMO: go p-3

POLY version 3.32
POLY: s-c n=1 p=1e5 t=233
POLY: ch-st ph h2o1=f 0
POLY: c-e
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated 210 grid points in 0 s
 22 ITS, CPU TIME USED 2 SECONDS
POLY: l-e,,
Output from POLY-3, equilibrium = 1, label A0 , database: SUBDEMO

Conditions:
N=1, P=100000, T=233
FIXED PHASES
H2O1 L=0
DEGREES OF FREEDOM 0

Temperature 233.00 K (-40.15 C), Pressure 1.000000E+05
Number of moles of components 1.000000E+00, Mass in grams 1.00931E+00
Total Gibbs energy -1.53589E+04, Enthalpy -9.53654E+02, Volume 9.68549E-03

Component Moles W-Fraction Activity Potential Ref.stat
H 9.9991E-01 9.9851E-01 3.6499E-04 -1.5335E+04 SER
O 9.3929E-05 1.4889E-03 1.0377E-61 -2.7203E+05 SER

GAS Status ENTERED Driving force 0.0000E+00
Moles 1.000000E+00, Mass 1.00931E+00, Volume fraction 1.0000E+00 Mass fractions:
H 9.98511E-01 O 1.48890E-03
Constitution:
H2 9.99812E-01 H2O1 1.87875E-04

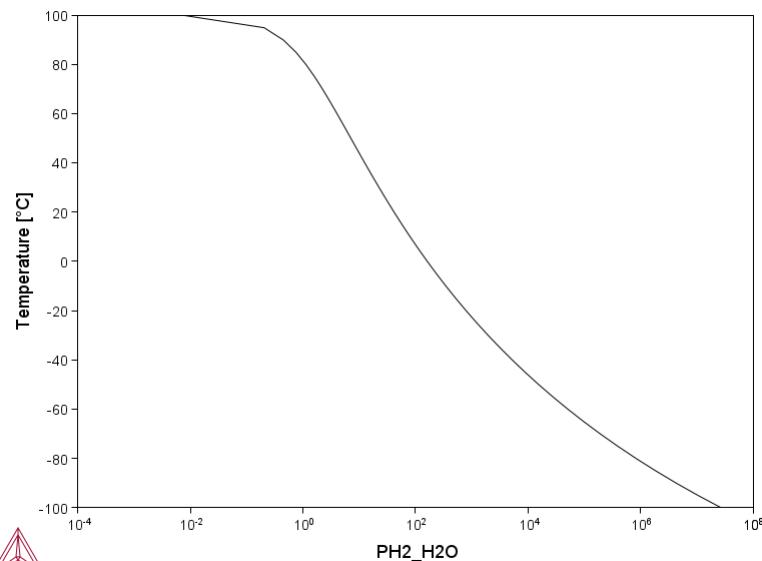
H2O1_L Status FIXED Driving force 0.0000E+00
Moles 0.000000E+00, Mass 0.000000E+00, Volume fraction 0.0000E+00 Mass fractions:
O 8.88103E-01 H 1.11897E-01
POLY: ent fun ph2_h2o=acr(h2,gas)/acr(h2o,gas);
POLY: s-a-v 1 t 173.15 373.15 ,
POLY: save dew y
POLY: step normal
No initial equilibrium, using default
Step will start from axis value 233.000
...OK

Phase Region from 233.000 for:
 GAS
 H2O1_L
Global test at 2.73000E+02 OK
Global test at 3.23000E+02 OK
Global test at 3.73000E+02 OK
Terminating at 373.150
Calculated 32 equilibria

Phase Region from 233.000 for:
 GAS
 H2O1_L
Global test at 1.93000E+02 OK
Terminating at 173.150
Calculated 15 equilibria
*** Buffer saved on file: c:\jenkins\workspace\generate_console_examples\examples\tce09\dew.POLY3
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

```
Setting automatic diagram axes
```

```
POST: s-d-a x ph2_h2o
POST: s-a-ty x log
POST: s-d-a y t-c
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
```



```
POST:
POST:
POST: set-inter
POST:
```

tce10

SYS:About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

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Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

```
SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce10\tce10.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Preventing Cr3O4 clogging in a continuous casting process
SYS:
SYS: @@ This example calculates an equilibrium with suspended or
SYS: @@ dormant phases and shows how to avoid Cr-oxide clogging in
SYS: @@ a continuous casting process.
SYS: @@ Note that a license for the TCOX11 database is required to
SYS: @@ run the example.
SYS:
SYS: @@ The background to this example is that a manufacturer
SYS: @@ wanted to increase the Cr content of a material from 18
SYS: @@ to 25 weight percent. He then had trouble in the continuous
SYS: @@ casting of this material because solid Cr3O4 was formed.
SYS: @@ By calculating the equilibria in the steel/slag system a
SYS: @@ simple correction could be found: modify the Mn or Si
SYS: @@ content, thus decrease the oxygen potential.
SYS:
SYS: @@ In Thermo-Calc, you can FIX a phase with zero amount to
SYS: @@ simulate how to avoid forming this phase. You can then
SYS: @@ release one of the conditions, usually one of the
SYS: @@ compositions, and this composition is determined by the
SYS: @@ equilibrium calculation.
SYS:
SYS: set-log ex10,,
SYS: @@ Go to the database module to obtain data
SYS: go da
... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module
Database folder: C:\jenkins\workspace\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA          /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE11: @@ Switch to the database with slag data
TDB_TCFE11: sw TCOX11
... the command in full is SWITCH_DATABASE
Current database: Metal Oxide Solutions v11.1

VA          /- DEFINED
TDB_TCOX11: @@ Some information about the database is given by this command
TDB_TCOX11: d-i
... the command in full is DATABASE_INFORMATION
Current database: Metal Oxide Solutions v11.1

TCOX: TCS Metal Oxide Solutions Database
*****Version 11.1, Dec 2021*****
Copyright @ 1992-2021: Thermo-Calc Software, Stockholm, Sweden.
The TCOX, Metal Oxide Solutions Database - Version 11.1, contains
critically assessed data for many multicomponent oxides, fluorides and
sulfides, as well as all alloy phases needed to calculate the Me-O, Me-F
and Me-S binary phase diagrams. The intended application is for solid and
liquid ionized materials, such as development of ceramics, metallurgical
processing, materials corrosion, solid oxide fuel cell materials, ESR
slags, sulfide formation, dephosphorization, desulfurization and Thermal
Barrier Coatings (TBC) but the database is of course not limited to this.
TCOX has been developed in a CALPHAD spirit with all of the oxygen (and
sulfur and fluor) containing binary systems assessed for their full range
of composition including all phases, plus the majority of the ternary
oxide/fluoride/sulfide systems, and many quaternary oxide/fluoride/sulfide
systems, including also oxy-fluoride and oxy-sulfide systems as well, in
order to give an accurate thermodynamic description of the multicomponent
systems of interest.
Since version 11, carbides and nitrides are included in TCOX. However,
other intermetallic compounds (Me1-Me2) and order-disorder transformations
are not included in the database. For those phases, the TCOX database is
compatible with TCFE Steels/Fe-Alloys Database, TCNI Ni-based Superalloys
Database and SSOL Solutions Database. Thus, if needed, more solid metallic
phases can be obtained by appending from TCFE, TCNI, SSOL and/or other
appropriate databases. However, one must keep in mind that the LIQUID
phase from other databases and the IONIC_LIQ phase from TCOX should never
be simultaneously considered in the same defined system/calculation, as
they both represent the liquid phase using two different models.
Viscosity and surface tension of the ionic liquid phase are incorporated
in TCOX. Now it is able to calculate the viscosity and surface tension
for the system Al2O3-CaF2-CaO-CrO-Cr2O3-Cu2O-CuO-FeO-Fe2O3-Gd2O3-K2O-La2O3
-MgO-MnO-MoO2-MoO3-Na2O-Nb2O5-NiO-P2O5-SiO2-TiO2-V2O5-Y2O3-ZrO2
and its sub-systems relevant to slags for various industrial applications.
The calculated viscosity and surface tension of the ionic liquid phase
are connected to the distribution and connectivity of species in the oxide
melts in the whole composition and a broad range of temperatures.
Molar volumes are described, both for liquid and solid oxides.
The primary thermodynamic models applied for various solution phases are:
- Compound Energy Formalism with several sublattices and neutral or ionic
constituents (Hillert, 2001) for various solid solution phases.
- Ionic Two-Sublattice Liquid Model (Hillert et al., 1985) for the ionic
liquid solution phase (IONIC_LIQ). The same model is used both for
metallic and ionized melts. At low levels of ionization, the model becomes
equivalent to a substitutional solution model between metallic atoms.
Different composition sets of IONIC_LIQ designated by #1, #2 etc. (e.g.
IONIC_LIQ#1) may be observed which often represent the metallic and
ionized liquid phases. Different composition sets also describe
miscibility gaps frequently found in e.g. Silicate systems. The #n suffix
(where n is an integer) is generated dynamically by Thermo-Calc when using
global minimization and therefore the identification of the phases should
```

be determined from their compositions.

- Ideal Gas Model (GAS). A reduced gaseous mixture is used in the TCOX database. If a complete gas is needed, it should be appended from the SGTE substance database.

ALLOY ELEMENTS (29): Al Ar C Ca Co Cr Cu F Fe
Gd H K La Mg Mn Mo N Na Nb
Ni O P S Si Ti V W Y Zr

Ar and H is only included in the gas phase. There are 550 different phases included in the database. Many of the solid oxide and sulfide phases are modelled as solution phases.

The assessed systems in TCOX are given in the extended information, found on the Thermo-Calc website.

The TCOX database was called ION prior to version 4.0.

Release History of the TCOX database:

Version 1.0: Aug. 1992 (initial release)
Version 1.1: Nov. 1994 (with some modifications)
Version 1.2: Nov. 2001 (with some modifications)
Version 2.0: Aug. 2002 (with major updates and improvements)
Version 2.1: Apr. 2004 (with major improvements)
Version 2.2: Jun. 2005 (with minor improvements)
Version 2.3: Mar. 2006 (with minor improvements)
Version 3.0: May 2009 (with major updates and improvements)
Version 4.0: Mar. 2011 (with major updates and improvements)
Version 4.1: Aug. 2012 (with minor improvements)
Version 5.0: Oct. 2012 (with major improvements)
Version 5.1: Jan. 2013 (with major improvements)
Version 5.2: Sep. 2014 (with major improvements)
Version 6.0: Jan. 2015 (with major improvements)
Version 7.0: Mar. 2017 (with major improvements)
Version 8.0: May 2018 (with major improvements)
Version 9.0: May 2019 (with major improvements)
Version 9.0.1: Aug. 2019 (with minor modifications)
Version 9.0.2: Dec. 2019 (with minor modifications)
Version 10.0: Apr. 2020 (with major improvements)
Version 10.1: Dec. 2020 (with minor improvements)
Version 10.2: Dec. 2021 (bugfix)
Version 11.0: May 2021 (with major improvements)
Version 11.1: Dec. 2021 (bugfix)

Edited by: Lina Kjellqvist, Thermo-Calc Software AB, Stockholm, Sweden.

Revision info: \$Rev: 12822 \$

TDE_TCOX11: Hit RETURN to continue

TDB_TCOX11: @@ Define the system by giving the elements.

TDE_TCOX11:

TDB_TCOX11: d-sys Fe o mn si cr al

... the command in full is DEFINE_SYSTEM

FE O MN
SI CR AL

DEFINED

TDB_TCOX11: @@ 'GET' reads thermodynamic data from the database files to the

TDE_TCOX11: @@ program

TDB_TCOX11: get

... the command in full is GET_DATA

15:34:56,834 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

REINITIATING GES

ELEMENTS

SPECIES

PHASES

... the command in full is AMEND_PHASE_DESCRIPTION

Creating a new composition set IONIC_LIQ#2

... the command in full is AMEND_PHASE_DESCRIPTION

Creating a new composition set IONIC_LIQ#3

... the command in full is AMEND_PHASE_DESCRIPTION

MN+4 IN NIMNO3:I SUBLATTICE 1 REJECTED

AL+3 IN QUARTZ:I SUBLATTICE 1 REJECTED

AL+3 IN TRIDYMITE:I SUBLATTICE 1 REJECTED

AL+3 IN CRYSTOBALITE:I SUBLATTICE 1 REJECTED

FE+2 IN CORUNDUM:I SUBLATTICE 1 REJECTED

MN+2 IN CORUNDUM:I SUBLATTICE 1 REJECTED

VA IN CORUNDUM:I SUBLATTICE 1 REJECTED

... the command in full is AMEND_PHASE_DESCRIPTION

AL+3 IN ALPO4_S1:I SUBLATTICE 1 REJECTED

AL+3 IN ALPO4_S2:I SUBLATTICE 1 REJECTED

AL+3 IN ALPO4_S3:I SUBLATTICE 1 REJECTED

Suspending CA2SiO4_ALPHA_A as it has net charge

Suspending CA2SiO4_ALPHA_PRIME as it has net charge

Suspending HATRURITE as it has net charge

Suspending K4Al22O35 as it has net charge

Suspending KAl11O17 as it has net charge

Suspending NBO2 as it has net charge

Suspending PSEUDO_BROOKITE as it has net charge

PARAMETERS ...

FUNCTIONS

List of references for assessed data

'SGTE Substances Database v6.0 (2017)'
'A.N. Grundy et al., JPED 26 (2005) 131-51; La-Mn-O'
'L. Kjellqvist, Thermo-Calc Software AB (2018), based on Sundman (2008);
Ti-O'
'A. Dinsdale, SGTE Data for Pure Elements, Calphad 15 (1991) 317-425'
'L. Kjellqvist, Thermo-Calc Software AB (2020), tentative vacancy fraction
in pure FCC metals and its carbides.'
'SGTE Unary (Pure Elements) Database V5.1 (2010)'
'M.H.G. Jacob and P.J. Spencer, Calphad 20 (1996) 307-320; Si-Zn and Al-Si
-Zn'
'S. Lakiza et al., J. Eur. Ceram. Soc. 26 (2006) 233-246; ZrO2-Gd2O3-Al2O3'
'O. Fabrichnaya et al., JPED 27 (2006) 343-352; ZrO2-Gd2O3-Y2O3-Al2O3'
'L. Kjellqvist, Thermo-Calc Software AB (2013); Reassessed solubility of
Al, Cr, Fe, Ni in Mn2O3. Mn2O3 is now modelled as the same phase as
cubic Y2O3 (M2O3C).'
'TCS, TCMP2 - TCS Materials Processing Database v2 (2004)'
'L. Kjellqvist, Thermo-Calc Software AB (2013); Cr-Zr-O'
'E. Povoden et al., JPED 30 (2009) 12-27; Cr-La-O'
'L. Kjellqvist, Thermo-Calc Software AB (2016); Cr-La-O'
'L. Kjellqvist, Thermo-Calc Software AB (2016); Cr-Nb-O'
'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; FE4N'
'L. Kjellqvist, Thermo-Calc Software AB (2013); Fe-Zr-O'
'E. Povoden et al., JPED 30 (2009) 351-366; Fe-La-O'
'H. Mao, Thermo-Calc Software AB (2015); Fe-Nb-O'
'H. Gohring, O. Fabrichnaya, A. Leineweber, E.J. Mittemeijer, Metall.

- Mater. Trans. A 47A (2016) 6173-86; FE-N, and Fe-C-N'
- 'W. Zheng, J. Alloys Compd., 632 (2015) 661-675; Mn-Si, Fe-Mn-Si'
- 'M. Chen, B. Hallstedt and L. J. Gauckler, J. Alloys Compd. 393 (2005) 114-21; Mn-Y-O'
- 'M. Chen, B. Hallstedt and L.J. Gauckler, Solid State Ionics 176 (2005) 1457-64; Mn-Zr-O, Mn-Y-Zr-O'
- 'N. Subasic, licentiate thesis 2000, KTH, Sweden; Al-Cr-Fe'
- 'I. Ansara (Editor), COST 507 report (1998); Al-Cr, Cr-Cu, Cr-Mg, Cu-Zr, Mg-Zr, Mn-Zr'
- 'M. Seiersten, Unpublished work (1989); Al-Fe'
- 'D. Conneta et al., Calphad 32 (2008) 361-370; Al-C-Fe'
- 'B. Sundman, I. Ohnuma, N. Dupin, U.R. Kattner, S.G. Fries, Acta Mater. 57 (2009) 2896-2908; Al-Fe'
- 'B. Lindahl and M. Selleby, Calphad 43 (2013) 86-93; Al-Fe-Mn'
- 'K.G. Chin, H.J. Lee, J.H. Kwak, J.Y. Kang, B.J. Lee, J. Alloys Compd. 505 (2010) 217-23; Al-Mn-C, Al-Fe-Mn-C'
- 'Y. Du, J. Wang, J. Zhao, J.C. Schuster, F. Weitzer, R. Schmid-Fetzer, M. Ohno, H. Xu, Z.K. Liu, S. Shang, W. Zhang, Int. J. Mater. Res. 98 (2007) 855-71; Al-Mn'
- 'H. Mao, M. Selleby and O. Fabrichnaya, Calphad 32 (2008) 399-412; Al2O3-SiO2-Y2O3'
- 'H. Mao and M. Selleby, Calphad 31 (2007) 269-280; Si3N4-AlN-Al2O3-SiO2'
- 'M. Selleby and H. Mao, Preliminary work (2007); Al-O, Al-Fe-O'
- 'B-J. Lee and N. Saunders, Z. Metallkd. 88 (1997) 152-161; Al-O-Ti'
- 'L. Kjellqvist, Thermo-Calc Software AB, Sweden, estimations, 2016'
- 'L. Kjellqvist, Thermo-Calc Software AB (2012); Si-O DIAMOND_A4'
- 'A. Dinsdale, Private Communication; liquid and solid Al2O3, CaO, MgO'
- 'B. Hallstedt, J. Am. Ceram. Soc. 75 (1992) 1497-1507; Al2O3-MgO'
- 'L. Kjellqvist, Thermo-Calc Software AB (2016); Revised Gd2O3 and La2O3 systems; Al2O3-Gd2O3, CaO-Gd2O3, Gd2O3-ZrO2'
- 'T. Godecke, F. Sommer and H.-L. Lukas, unpublished work (1996); Al-Si parameters available from J. Grobner et al. Calphad 20 (1996) 247; Al-Si, C-Si'
- 'N. Dupin, Unpublished work'
- 'M.H.G. Jacobs, P.J. Spencer, Calphad 20 (1996) 307-320; Al-Si-Zn'
- 'A. Gabriel, P. Gustafson and I. Ansara, Calphad 11 (1987) 203-218; C-Fe-Ni'
- 'J-O. Andersson and B. Sundman, Calphad 11 (1987) 83-92; CR-FE'
- 'K. Frisk, Metall. Trans. A 21 (1990) 2477-2488; Cr-Fe-N'
- 'B-J. Lee, Metall. Trans. A 24 (1993) 1919-1933; Cr-Mn, Fe-Cr-Mn'
- 'K. Frisk, Calphad, 17 (1993) 335-349; Cr-Mn-N'
- 'SSOL4 - SGTE Alloy Solutions Database v4 (2008)'
- 'L. Kjellqvist, Unpublished revision of liquid phase (2010); Cr-Fe-Mn-Ni-O'
- 'J.R. Taylor and A.T. Dinsdale, Z. Metallkd. 81 (1990) 354-366; Ni-O, Cr-O and Cr-Ni-O'
- 'L. Kjellqvist, Thermo-Calc Software AB (2019), reassessment; Cr-O'
- 'M. Kowalski and P.J. Spencer, Calphad 19 (1995) 229-243; Cr-O, Fe-O and Ni-O'
- 'J.R. Taylor and A.T. Dinsdale, Z. Metallkd. 84 (1993) 335-345; Cr-Fe-O'
- 'L. Kjellqvist, M. Selleby and B. sundman, Calphad 32 (2008) 577-592; Cr-Fe-Ni-O'
- 'Y. Du and J.C. Schuster, J. Phase Equilib. 21 (2000) 281-86; Cr-Si'
- 'W. Huang, Calphad 13 (1989) 243-252; Fe-Mn'
- 'B. Hallstedt, unpublised work (2016); C-Fe-Mn Epsilon martensite.'
- 'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, Calphad 35 (2011) 479-491; Fe-Mn-C'
- 'L. Kjellqvist, Thermo-Calc Software AB (2016); Columbite, (Ca,Fe,Mg, Mn)Nb2O6'
- 'B. Sundman, J. Phase Equilib. 12 (1991) 127-140; Fe-O'
- 'P. Franke, estimated parameter within SGTE (2008); Fe-Mn-C'
- 'J. Lacaze and B. Sundman, Metall. Trans. A 22 (1991) 2211-2223; C-Fe-Si'
- 'A. Forsberg and J. Agren, J. Phase Equilib. 14 (1993) 354-363; Fe-Mn-Si'
- 'A.N. Grundy, B. Hallstedt and L.J. Gauckler, J. Phase Equilib. 24 (2003) 21-39; Mn-O'
- 'B-J. Lee, KRISS, unpublished research, during 1993-1995'
- 'L. Kjellqvist and M. Selleby, JPED 31 (2010) 113-134; Fe-Mn-O'
- 'M. Chen, PhD thesis, ETH Zurich (2005); La-Zr-O, Mn-Zr-O, Mn-Y-Zr-O'
- 'L. Kjellqvist and M. Selleby, Int. J. Mater. Res. (formerly Z. Metallkd.) 101 (2010) 1222-1231; Mn-Ni-O'
- 'T.I. Barry, NPL, Unpublished work (1987); liquid and solid SiO2'
- 'B. Hallstedt, J. Phase Equilib. 14 (1993) 662-675; Al-Ca-Mg-Si-O'
- 'B. Hallstedt, Calphad 16 (1992) 53-61; Si-O'
- 'B-J. Lee, estimated parameter (1999)'
- 'L. Kjellqvist, Thermo-Calc Software AB (2016); Revised CaO-SiO2-Y2O3'
- 'L. Kjellqvist, Thermo-Calc Software AB (2018); Al2O3-P2O5-SiO2'
- 'L. Kjellqvist, Thermo-Calc Software AB (2020), estimated; Fe-O-Na2O-SiO2'
- 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2016; Fe-Al-Cr-Ni'
- 'L. Kjellqvist, Thermo-Calc Software AB (2012); Al-Cr-O'
- 'Unassessed Linear combination of parameters'
- 'P. Saltykov et al., J. Alloys Compd. 381 (2004) 99-113; Al-Cr-Ni-O'
- 'L. Kjellqvist, Thermo-Calc Software, AB, Sweden (2010); Spinel's'
- 'I.-H. Jung, S. Deckerov and A.D. Pelton, J. Am. Ceram. Soc. 88 (2005) 1921-1928; MgO-Al2O3-Cr2O3'
- 'L. Kjellqvist, Thermo-Calc Software AB (2019); Making the LAAP, YAP, V3O5 HT and CaSiO4 phases less stable in higher order systems.'
- 'L. Kjellqvist, Thermo-Calc Software AB (2016), added Fe solubility in Mullite; Al2O3-FeO-SiO2'
- 'L. Kjellqvist and M. Selleby, Unpublished research (2013); Al-Fe-Si-O'
- 'D.-G. Kim, E. Moosavi-Khoonsari, I.-H. Jung, J. Eur. Ceram. Soc. 38 (2018) 3188-3200; Al2O3-K2O, Al2O3-K2O-MgO'
- 'L. Kjellqvist, Thermo-Calc Software AB, Sweden (2010); Al-Mn-O'
- 'L. Kjellqvist, reassessed ALPHA-SPINEL, Thermo-Calc Software AB (2012); Al-Mn-O'
- 'L. Kjellqvist, Thermo-Calc Software AB (2019), estimated; Al2O3-MnO-TiO2'
- 'H-L. Chen, Thermo-Calc Software AB (2013); Al-Mn-Si, Al-Fe-Mn-Si'
- 'H. Mao, estimated parameter (2010); Al-Si-O'
- 'L. Kjellqvist, Thermo-Calc Software AB (2014), Fix to remove ternary miscibility gap close to the SiO2 corner; Al-SiO2'
- 'M. Hillert, B. Sundman and X. Wang, TRITA-MAC 402 (1989); Al2O3-SiO2'
- 'H. Mao, Recalculated from ION2 (2010); Al2O3-MgO, Al2O3-SiO2'
- 'H. Mao, M. Selleby and B. Sundman, J. Am. Ceram. Soc. 88 (2005) 2544-2551; Al2O3-SiO2'
- 'L. Kjellqvist, Thermo-Calc Software AB (2018); Al-Ti-O'
- 'L. Kjellqvist, Thermo-Calc Software AB (2020); Reassessment of Al, Mg solubility in V407 and V305.'
- 'R. Naraghi, Thermo-Calc Software AB, Sweden (2015); FROST project'
- 'C. Qiu, Metall. Trans. A 24 (1993) 2393-2409; Cr-Fe-Mn-N'
- 'A. Markstrom, Thermo-Calc Software AB (2013), CBCC_A12; Cr-Fe-Mn'
- 'L. Kjellqvist, Thermo-Calc Software AB (2019), introducing low-temp miscibility gap; Cr-Fe-O Corundum'
- 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; Cr-Fe-Si'
- 'M. Lindholm, J. Phase Equilib. 18 (1997) 432; Cr-Fe-Si'
- 'L. Kjellqvist, M. Selleby, J. Alloys Compd. 507 (2010) 84-92; Cr-Mn-O'
- 'L. Kjellqvist, Thermo-Calc Software AB (2019), reassessment; Cr-O-Si'
- 'L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2013; Cr-Si-O'
- 'L. Kjellqvist, Thermo-Calc Software AB (2017); estimated solubility between metals and oxide liquids.'

'S. Arnout et al., J. Am. Ceram. Soc. 92 (2009) 1831-1839; Cr-O-MgO-SiO₂'
' L. Kjellqvist, Thermo-Calc Software AB (2019), reassessment of solubility
in M4O7 and V3O5, due to change of model.'
' L. Kjellqvist, Thermo-Calc Software AB (2020); Fe-O-K2O'
' W. Zheng et al., J. Iron Steel Res. Int. 24 (2017) 190-197; C-Mn-Si, Fe
-Mn-Si'
' M. Selleby, Metall. Mater. Trans. B 28 (1997) 563-576; Fe-O-Si'
' L. Kjellqvist, Thermo-Calc Software AB (2016); Fe-Mn-O-SiO₂'
' M. Selleby, Metall. Mater. Trans. B 28 (1997) 577-596; Ca-Fe-O-Si'
' L. Kjellqvist, Thermo-Calc Software AB (2020), reassessment metastable
FeSiO₃ ortho-pyroxene; FeO-SiO₂, FeO-MgO-SiO₂'
' L. Kjellqvist, Thermo-Calc Software AB (2014); Fe-O-MgO-SiO₂'
' L. Kjellqvist, Thermo-Calc Software AB (2018); Fe-Ti-O'
' L. Kjellqvist, reassessment, Thermo-Calc Software AB (2018); Mn-Si-O, Al
-Mn-Si-O, Ca-Mn-Si-O, Al2O3-FeO-MnO-SiO₂'
' L. Kjellqvist, Thermo-Calc Software AB, Sweden (2011); Mn-Si-O'
' L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2014; Reassess liquid
phase; Mn-Si-O'
' G. Eriksson et al., Can. Metall. Q. 33 (1994) 13-21; MnO-SiO₂'
' Y. Kang et al., ISIJ Int. 44 (2004) 965-974; CaO-MnO-SiO₂, CaO-MnO-Al2O3'
' L. Kjellqvist, Thermo-Calc Software AB (2019) estimated parameter; Al-Cr
-Fe-O'
' L. Kjellqvist, Thermo-Calc Software AB, Sweden (2010); Al-Cr-O'
' L. Kjellqvist, Thermo-Calc Software AB (2021); Al2O3-Fe-O-K2O'
' L. Kjellqvist, Thermo-Calc Software AB (2016); Al2O3-FeO-MnO'
' L. Kjellqvist, Thermo-Calc Software AB (2018); Al-Fe-Ti-O'
' L. Kjellqvist, Thermo-Calc Software AB (2014); Al2O3-MnO-SiO₂'
' G. Lambotte, P. Chartrand, J. Chem. Thermodynamics 57 (2013) 306-334;
Al2O3-Na2O-SiO₂'
' L. Kjellqvist, Thermo-Calc Software AB (2018); TiO₂-ZrO₂'
' L. Kjellqvist, Thermo-Calc Software AB (2018), Reassessed solubility of
Fe, Ga, Mg, Mn and Y in CA2SiO₄_ALPHA and CA2SiO₄_PRIME due to
change of model'
' L. Kjellqvist, Thermo-Calc Software AB (2017), Garnet; estimated
solubility between Spessartine and Grossular.'
' L. Kjellqvist, Thermo-Calc Software AB (2017), estimated cation
distribution in Olivine (M1,M2)2SiO₄ systems.'
' L. Kjellqvist, Thermo-Calc Software AB (2019); Fe-Mn-O-TiO₂'
'D.-G. Kim, B. Konar, I.-H. Jung, Metall. Mater. Trans. B 48B (2017) 2788
-2803; K2O-MgO-SiO₂'
' Y.Tang, in TCCU2, Thermo-Calc Software AB, Stockholm, Sweden'
' X.G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
volumes'
' Volume data for TCFE4, 2006'
' Estimated values, 2019'
' X.G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
' L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2012; Molar volumes'
' M. Ghasemi, Thermo-Calc Software: Unifying liquid volume database, 2020'
' N. Dupin, Private communication, (2008); Volume data'
' H. Mao, Thermo-Calc Software AB, Sweden, 2013; Molar volumes'
' R. Zhang, Molar volumes for oxide liquid in TCOX, Thermo-Calc Software AB,
Sweden, 2018-2020'
' A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
' R. Naraghi, Thermo-Calc Software AB, Sweden, Volume data updated for
TCFE9 database (TCFE v9.0, Jan, 2017).'
' H. Mao, Thermo-Calc Software AB, Sweden, 2011; Molar volumes'
' L. Kjellqvist, Thermo-Calc Software AB, Stockholm, 2013; Unassessed PARAM,
linear combination of unary volume data'
' H. Mao, B. Sundman, Z. Wang and S.K. Saxena, J. Alloys Compd., 327, 2001,
253-262'
' H. Mao, M. Selleby and B. Sundman, J. Am. Cera. Soc., 88 (2005) 2544-2551;
Al2O3-SiO₂'
' R. Zhang, Viscosity of liquid oxides, Thermo-Calc Software AB, 2018-2020'
' M. Ghasemi, Viscosity of liquid metals, Thermo-Calc Software AB, 2019'
' R. Zhang, Surface tensions for oxide liquid in TCOX, Thermo-Calc Software
AB, Sweden, 2020'

-OK-

TDB_TCOX11: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32

POLY: @@ There are many commands in the POLY-3 module

POLY: ?

| | | |
|---------------------------------|--------------------------|-------------------------|
| ... the command in full is HELP | | |
| ADD_INITIAL_EQUILIBRIUM | GOTO_MODULE | REINITIATE_MODULE |
| ADVANCED_OPTIONS | HELP | SAVE_WORKSPACES |
| AMEND_STORED_EQUILIBRIA | INFORMATION | SELECT_EQUILIBRIUM |
| BACK | LIST_AXIS_VARIABLE | SET_ALL_START_VALUES |
| CHANGE_STATUS | LIST_CONDITIONS | SET_AXIS_VARIABLE |
| COMPUTE_EQUILIBRIUM | LIST_EQUILIBRIUM | SET_CONDITION |
| COMPUTE_TRANSITION | LIST_INITIAL_EQUILIBRIA | SET_INPUT_AMOUNTS |
| CREATE_NEW_EQUILIBRIUM | LIST_STATUS | SET_INTERACTIVE |
| DEFINE_COMPONENTS | LIST_SYMBOLS | SET_NUMERICAL_LIMITS |
| DEFINE_DIAGRAM | LOAD_INITIAL_EQUILIBRIUM | SET_REFERENCE_STATE |
| DEFINE_MATERIAL | MACRO_FILE_OPEN | SET_START_CONSTITUITION |
| DELETE_INITIAL_EQUILIB | MAKE_COMPONENT_ENTERED | SET_START_VALUE |
| DELETE_SYMBOL | MAKE_COMPONENT_SUSPENDED | SHOW_VALUE |
| ENTER_SYMBOL | MAP | STEP_WITH_OPTIONS |
| EVALUATE_FUNCTIONS | POST | TABULATE |
| EXIT | | READ_WORKSPACES |

POLY: Hit RETURN to continue

POLY: @@ Some basic information is given by the INFORMATION command

POLY: @@ Look at TCEX-01 for more details.

POLY: info

... the command in full is INFORMATION

FILE SYSTEM ERROR 37

*** ERROR 1717 IN MOPEN: FILE DOES NOT EXIST: c:\jenkins\workspace\generate_console_examples\unite\distribution\help\poly3.hlp

POLY: ?

| | | |
|---------------------------------|--------------------------|-------------------------|
| ... the command in full is HELP | | |
| ADD_INITIAL_EQUILIBRIUM | GOTO_MODULE | REINITIATE_MODULE |
| ADVANCED_OPTIONS | HELP | SAVE_WORKSPACES |
| AMEND_STORED_EQUILIBRIA | INFORMATION | SELECT_EQUILIBRIUM |
| BACK | LIST_AXIS_VARIABLE | SET_ALL_START_VALUES |
| CHANGE_STATUS | LIST_CONDITIONS | SET_AXIS_VARIABLE |
| COMPUTE_EQUILIBRIUM | LIST_EQUILIBRIUM | SET_CONDITION |
| COMPUTE_TRANSITION | LIST_INITIAL_EQUILIBRIA | SET_INPUT_AMOUNTS |
| CREATE_NEW_EQUILIBRIUM | LIST_STATUS | SET_INTERACTIVE |
| DEFINE_COMPONENTS | LIST_SYMBOLS | SET_NUMERICAL_LIMITS |
| DEFINE_DIAGRAM | LOAD_INITIAL_EQUILIBRIUM | SET_REFERENCE_STATE |
| DEFINE_MATERIAL | MACRO_FILE_OPEN | SET_START_CONSTITUITION |
| DELETE_INITIAL_EQUILIB | MAKE_COMPONENT_ENTERED | SET_START_VALUE |
| DELETE_SYMBOL | MAKE_COMPONENT_SUSPENDED | SHOW_VALUE |
| ENTER_SYMBOL | MAP | STEP_WITH_OPTIONS |
| EVALUATE_FUNCTIONS | POST | TABULATE |

```

EXIT                                READ_WORKSPACES
POLY:
POLY:Hit RETURN to continue
POLY: @@ Now set the conditions i.e. the temperature, pressure and
POLY: @@ composition. We are interested in the situation at the
POLY: @@ outflow of steel
POLY:
POLY: s-c t=1800,p=101325,n=
    ... the command in full is SET_CONDITION
POLY: @@ As conditions you can specify that the steel should have
POLY: @@ 18 weight percent of Cr, 0.4 w/o Mn and 0.4 w/o Si
POLY: @@ (Note that the overall amount of Cr and Mn is not specified).
POLY:
POLY: s-c w(mn)=.004,w(cr)=.18,w(si)=.004
    ... the command in full is SET_CONDITION
POLY: @@ The amount of Al is very small, assume 8 ppm
POLY: s-c w(al)=8e-6
    ... the command in full is SET_CONDITION
POLY: @@ We will later assume that the oxygen potential is determined
POLY: @@ by the equilibrium with liquid slag but initially we assume
POLY: @@ there is 50 ppm O
POLY:
POLY: s-c w(o)=5e-5
    ... the command in full is SET_CONDITION
POLY: l-c
    ... the command in full is LIST_CONDITIONS
T=1800, P=101325, N=1, W(MN)=4E-3, W(CR)=0.18, W(SI)=4E-3, W(AL)=8E-6,
W(O)=5E-5
DEGREES OF FREEDOM 0
POLY:Hit RETURN to continue
POLY: @@ Check what phases there are
POLY: l-st p
    ... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES
PHASE          STATUS      DRIVING FORCE     MOLES
ZRTIO4_BETA   ENTERED    0.000000E+00  0.000000E+00
ZRO2_TETR     ENTERED    0.000000E+00  0.000000E+00
ZRO2_MONO    ENTERED    0.000000E+00  0.000000E+00
WOLLASTONITE ENTERED    0.000000E+00  0.000000E+00
V305_HT       ENTERED    0.000000E+00  0.000000E+00
TRIDYMITE    ENTERED    0.000000E+00  0.000000E+00
SPINEL        ENTERED    0.000000E+00  0.000000E+00
SILLIMANITE  ENTERED    0.000000E+00  0.000000E+00
RUTILE        ENTERED    0.000000E+00  0.000000E+00
RHODONITE    ENTERED    0.000000E+00  0.000000E+00
QUARTZ        ENTERED    0.000000E+00  0.000000E+00
PROTO_PYROXENE ENTERED   0.000000E+00  0.000000E+00
PEROVSKITE   ENTERED    0.000000E+00  0.000000E+00
ORTHO_PYROXENE ENTERED   0.000000E+00  0.000000E+00
OLIVINE       ENTERED    0.000000E+00  0.000000E+00
NIMNO3        ENTERED    0.000000E+00  0.000000E+00
NAFE02_G      ENTERED    0.000000E+00  0.000000E+00
NAFE02_B      ENTERED    0.000000E+00  0.000000E+00
NAAL02_D      ENTERED    0.000000E+00  0.000000E+00
MULLITE       ENTERED    0.000000E+00  0.000000E+00
M407          ENTERED    0.000000E+00  0.000000E+00
M203H         ENTERED    0.000000E+00  0.000000E+00
M203C         ENTERED    0.000000E+00  0.000000E+00
M203B         ENTERED    0.000000E+00  0.000000E+00
KYANITE       ENTERED    0.000000E+00  0.000000E+00
KAPPA_E21     ENTERED    0.000000E+00  0.000000E+00
K2MGSIO4_LT   ENTERED    0.000000E+00  0.000000E+00
K2MGSIO4HT   ENTERED    0.000000E+00  0.000000E+00
HCP_A3        ENTERED    0.000000E+00  0.000000E+00
HALITE        ENTERED    0.000000E+00  0.000000E+00
GARNET        ENTERED    0.000000E+00  0.000000E+00
FLUORITE     ENTERED    0.000000E+00  0.000000E+00
FE4N_LP1     ENTERED    0.000000E+00  0.000000E+00
FCC_A1        ENTERED    0.000000E+00  0.000000E+00
DIAMOND_FCC_A4 ENTERED   0.000000E+00  0.000000E+00
DHCPC         ENTERED    0.000000E+00  0.000000E+00
CUB_A13       ENTERED    0.000000E+00  0.000000E+00
CRNB04        ENTERED    0.000000E+00  0.000000E+00
CRISTOBALITE ENTERED    0.000000E+00  0.000000E+00
CORUNDUM     ENTERED    0.000000E+00  0.000000E+00
CORDIERITE   ENTERED    0.000000E+00  0.000000E+00
COLUMBITE    ENTERED    0.000000E+00  0.000000E+00
CLINO_PYROXENE ENTERED   0.000000E+00  0.000000E+00
CBCC_A12      ENTERED    0.000000E+00  0.000000E+00
CARNEGIEITE_B ENTERED    0.000000E+00  0.000000E+00
CARNEGIEITE_A ENTERED    0.000000E+00  0.000000E+00
BCC_A2        ENTERED    0.000000E+00  0.000000E+00
ANDALUSITE   ENTERED    0.000000E+00  0.000000E+00
ALPO4_S3      ENTERED    0.000000E+00  0.000000E+00
ALPO4_S2      ENTERED    0.000000E+00  0.000000E+00
ALPO4_S1      ENTERED    0.000000E+00  0.000000E+00
ALPHA_SPINEL  ENTERED    0.000000E+00  0.000000E+00
AF             ENTERED    0.000000E+00  0.000000E+00
IONIC_LIQ#3   ENTERED    0.000000E+00  0.000000E+00
IONIC_LIQ#2   ENTERED    0.000000E+00  0.000000E+00
IONIC_LIQ#1   ENTERED    0.000000E+00  0.000000E+00
GAS            ENTERED    0.000000E+00  0.000000E+00

POLY: @@ Start by assuming all other phases except Metallic liquid are suspended
POLY: @@ In TCOX10 the liquid metal and Liquid slag(s) are modelled as the same phase
POLY: @@ IONIC_LIQ, were miscibility gap(s) are separating the Liquid Metal
POLY: @@ and Liquid slag(s). By default IONIC_LIQ#1 is Liquid metals and
POLY: @@ IONIC_LIQ#2... are liquid slag(s).
POLY: @@ In order to secure that only Liquid metal is stable in the calculation
POLY: @@ we first need to turn Global minimization off.
POLY: advance glob n
    ... the command in full is ADVANCED_OPTIONS
Settings for global minimization:
POLY:
POLY: ch-st p *=sus
    ... the command in full is CHANGE_STATUS
POLY: ch-st p Ionic_Liq#1=ent 0
    ... the command in full is CHANGE_STATUS
POLY: l-c
    ... the command in full is LIST_CONDITIONS
T=1800, P=101325, N=1, W(MN)=4E-3, W(CR)=0.18, W(SI)=4E-3, W(AL)=8E-6,
W(O)=5E-5
DEGREES OF FREEDOM 0
POLY:Hit RETURN to continue
POLY: @@ The degree of freedom is zero and we can make a calculation.

```

```

POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Global equilibrium calculation turned off, you can turn it on with
ADVANCED_OPTIONS GLOBAL_MINIMIZATION Y,,,
*** ERROR 1611 IN QTHISS: TOO MANY ITERATIONS
Give the command INFO TROUBLE for help
POLY:
POLY: @@ The calculation failed and
POLY: @@ we need to change the start values for the phase in order
POLY: @@ to find equilibrium.
POLY: @@ The metallic elements can be set as the alloy composition and the
POLY: @@ Oxide constituents should be low (Log amount of slag formers).
POLY: s-a-s n
... the command in full is SET_ALL_START_VALUES
Should IONIC_LIQ#1 be stable? /N/: y
Major constituent(s) /*/: Fe
No such constituent
Y(IONIC_LIQ#1,AL+3) /1/: 8e-6
Y(IONIC_LIQ#1,CR+2) /1/: .18
Y(IONIC_LIQ#1,FE+2) /1/: .8
Y(IONIC_LIQ#1,MN+2) /1/: 4e-3
Y(IONIC_LIQ#1,SI+4) /1/: 4e-3
Y(IONIC_LIQ#1,ALO2-1#2) /1/: 1e-8
Y(IONIC_LIQ#1,O-2#2) /1/: 5e-5
Y(IONIC_LIQ#1,SIO4-4#2) /1/: 1e-8
Y(IONIC_LIQ#1,VAl#2) /1/: .99
Y(IONIC_LIQ#1,CRO3/2#2) /1/: 1e-8
Y(IONIC_LIQ#1,FEO3/2#2) /1/: 1e-8
Y(IONIC_LIQ#1,MNO3/2#2) /1/: 1e-8
Y(IONIC_LIQ#1,SIO2#2) /1/: 1e-8
POLY:
POLY: @@ Now we can calculate equilibrium again
POLY:
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
16 ITS, CPU TIME USED 0 SECONDS
POLY:
POLY: @@ Now set the suspended phases as dormant and keep Metalic liquid entered.
POLY:
POLY: c-st p *s=d
... the command in full is CHANGE_STATUS
POLY:
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
18 ITS, CPU TIME USED 7 SECONDS
POLY: l-st p
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES
PHASE STATUS DRIVING FORCE MOLES
IONIC_LIQ#1 ENTERED 0.000000E+00 1.000000E+00
MULLITE DORMANT 2.961770E+00
SPINEL DORMANT 2.115262E-01
M2O3C DORMANT -1.536179E-01
CORUNDUM DORMANT -1.645427E-01
SILLIMANITE DORMANT -2.007987E-01
ANDALUSITE DORMANT -2.189914E-01
KYANITE DORMANT -3.022632E-01
M2O3B DORMANT -3.340336E-01
CORDIERITE DORMANT -3.488419E-01
IONIC_LIQ#3 DORMANT -3.560059E-01
IONIC_LIQ#2 DORMANT -3.560059E-01
FE4N_LP1 DORMANT -4.269682E-01
DORMANT PHASES WITH DRIVING FORCE LESS THAN -4.570081E-01
CUB_A13_ALPHA_SPINEL GARNET CRISTOBALITE TRIDYMITE HALITE CBCC_A12 QUARTZ
CARNEGIEITE_B CARNEGIEITE_A K2MGSIO4_LT RHODONITE K2MGSIO4 HT WOLLASTONITE
OLIVINE PROTO_PYROXENE NAALO2_D CRNBO4 NAFE02_G NAFE02_B ZRTIO4_BETA FLUORITE
HCP_A3 ALPO4_S3 ALPO4_S2 ALPO4_S1 ZRO2_TETR ORTHO_PYROXENE CLINO_PYROXENE
V3O5 HT FCC_A1 ZRO2_MONO AF RUTILE KAPPA_E21 M407 BCC_A2 COLUMBITE PEROVSKITE
NIMNO3 M2O3H GAS DIAMOND_FCC_A4 DHCP P
POLY: Hit RETURN to continue
POLY: @@ If the stable phases do not change in 12 iterations the program
POLY: @@ terminates even if the program has not calculated the correct
POLY: @@ driving forces for the metastable phases.
POLY: @@ You can change this with the command SET-NUMERICAL-LIMITS
POLY: @@ Use this command to change the lowest value of a fraction variable.
POLY:
POLY: s-n-1 500 1E-6 1E-12 n
... the command in full is SET_NUMERICALLIMITS
LIMITATIONS of the present version of Thermo-Calc
Max number of elements : 80
Max number of species : 5000
Max number of sublattices in a phase : 10
Max number of constituents in a phase: : 200
Max number of constituents in an ideal phase : 5000
POLY: Hit RETURN to continue
POLY: @@ Calculate again
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
45 ITS, CPU TIME USED 0 SECONDS
POLY: l-st p
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES
PHASE STATUS DRIVING FORCE MOLES
IONIC_LIQ#1 ENTERED 0.000000E+00 1.000000E+00
CORUNDUM DORMANT 7.138767E-02
BCC_A2 DORMANT -5.908357E-03
SPINEL DORMANT -1.875540E-02
FCC_A1 DORMANT -3.309774E-02
MULLITE DORMANT -3.683035E-02
IONIC_LIQ#3 DORMANT -7.786479E-02
IONIC_LIQ#2 DORMANT -7.786479E-02
SILLIMANITE DORMANT -2.007987E-01
ANDALUSITE DORMANT -2.189914E-01
KYANITE DORMANT -3.022632E-01
HCP_A3 DORMANT -3.046852E-01
DORMANT PHASES WITH DRIVING FORCE LESS THAN -3.454070E-01
M2O3C CORDIERITE_CUB_A13_M2O3B_ALPHA_SPINEL CBCC_A12_FE4N_LP1 GARNET
CRISTOBALITE TRIDYMITE HALITE QUARTZ CARNEGIEITE_B CARNEGIEITE_A K2MGSIO4_LT
RHODONITE K2MGSIO4 HT WOLLASTONITE OLIVINE PROTO_PYROXENE NAALO2_D CRNBO4
NAFE02_G NAFE02_B ZRTIO4_BETA FLUORITE ZRO2_TETR ALPO4_S3 ALPO4_S2 ALPO4_S1
ORTHO_PYROXENE CLINO_PYROXENE V3O5 HT RUTILE ZRO2_MONO_AF KAPPA_E21 M407
PEROVSKITE COLUMBITE GAS NIMNO3 M2O3H DIAMOND_FCC_A4 DHCP K

```

```

POLY:Hit RETURN to continue
POLY: @@ The driving forces are quite stable.
POLY: @@ Now set the slag phase to stable and let the program
POLY: @@ adjust the amount of oxygen to make it stable
POLY:
POLY: c-st p Ionic_Liq#2=fix 0
... the command in full is CHANGE_STATUS
POLY: s-c w(o)
... the command in full is SET_CONDITION
Value /5.00000246E-05/: none
POLY: l-c
... the command in full is LIST_CONDITIONS
T=1800, P=101325, N=1, W(MN)=4E-3, W(CR)=0.18, W(SI)=4E-3, W(AL)=8E-6
FIXED PHASES
IONIC_LIQ#2=0
DEGREES OF FREEDOM 0
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
10 ITS, CPU TIME USED 0 SECONDS
POLY: l-e
... the command in full is LIST_EQUIlibrium
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
Output from POLY-3, equilibrium = 1, label A0 , database: TCOX11

Conditions:
T=1800, P=101325, N=1, W(MN)=4E-3, W(CR)=0.18, W(SI)=4E-3, W(AL)=8E-6
FIXED PHASES
IONIC_LIQ#2=0
DEGREES OF FREEDOM 0

Temperature 1800.00 K ( 1526.85 C), Pressure 1.013250E+05
Number of moles of components 1.00000E+00, Mass in grams 5.48863E+01
Total Gibbs energy -1.12673E+05, Enthalpy 6.87577E+04, Volume 8.02004E-06

Component Moles W-Fraction Activity Potential Ref.stat
AL 1.6273E-05 8.0000E-06 3.8647E-10 -3.2437E+05 SER
CR 1.9001E-01 1.8000E-01 4.9780E-04 -1.1382E+05 SER
FE 7.9797E-01 8.1193E-01 6.2151E-04 -1.1050E+05 SER
MN 3.9962E-03 4.0000E-03 1.3493E-06 -2.0228E+05 SER
O 1.9707E-04 5.7443E-05 2.8780E-13 -4.3217E+05 SER
SI 7.8172E-03 4.0000E-03 4.7775E-08 -2.5228E+05 SER

IONIC_LIQ#1 Status ENTERED Driving force 0.0000E+00
Moles 1.0000E+00, Mass 5.4886E+01, Volume fraction 1.0000E+00 Mass fractions:
FE 8.11935E-01 SI 4.00000E-03 O 5.74434E-05
CR 1.8000E-01 MN 4.00000E-03 AL 8.00000E-06

IONIC_LIQ#2 Status FIXED Driving force 0.0000E+00
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mass fractions:
O 4.14521E-01 MN 1.39216E-01 CR 4.83542E-02
AL 2.63816E-01 SI 9.91993E-02 FE 3.48940E-02

IONIC_LIQ#3 Status DORMANT Driving force 5.9075E-15
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mass fractions:
O 4.14521E-01 MN 1.39216E-01 CR 4.83542E-02
AL 2.63816E-01 SI 9.91993E-02 FE 3.48940E-02

CORUNDUM Status DORMANT Driving force 1.4847E-01
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mass fractions:
AL 5.00058E-01 CR 3.77458E-02 MN 2.92521E-06
O 4.62189E-01 FE 3.55083E-06 SI 0.00000E+00

MULLITE Status DORMANT Driving force 4.2348E-02
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mass fractions:
O 4.85409E-01 SI 1.10919E-01 MN 0.00000E+00
AL 4.03672E-01 FE 6.95088E-08 CR 0.00000E+00

SPINEL Status DORMANT Driving force 5.7990E-02
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mass fractions:
AL 4.73508E-01 CR 4.20692E-02 FE 8.10378E-03
O 4.50374E-01 MN 2.59453E-02 SI 0.00000E+00
POLY:Hit RETURN to continue
POLY: @@ List the status of the phases.
POLY: l-st p
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES
PHASE STATUS DRIVING FORCE MOLES
IONIC_LIQ#2 FIXED 0.000000E+00 0.000000E+00
IONIC_LIQ#1 ENTERED 0.000000E+00 1.000000E+00
CORUNDUM DORMANT 1.484719E-01
SPINEL DORMANT 5.798977E-02
MULLITE DORMANT 4.234826E-02
IONIC_LIQ#3 DORMANT 5.907521E-15
BCC_A2 DORMANT -5.931197E-03
FCC_A1 DORMANT -3.311745E-02
SILLIMANITE DORMANT -1.204373E-01
ANDALUSITE DORMANT -1.386300E-01
KYANITE DORMANT -2.219018E-01
M2O3C DORMANT -2.683147E-01
CORDIERITE DORMANT -2.689991E-01
HCP_A3 DORMANT -3.047151E-01
M2O3B DORMANT -3.241464E-01
ALPHA_SPINEL DORMANT -3.327446E-01

DORMANT PHASES WITH DRIVING FORCE LESS THAN -3.606493E-01
CUB_A13 GARNET CBCC_A12 FE4N LP1 CRYSTOBALITE TRIDYMITE HALITE QUARTZ
CARNEGIEITE_B CARNEGIEITE_A K2MGSIO4_LT K2MGSIO4_HT RHODONITE WOLLASTONITE
OLIVINE NAALO2_D PROTO_PYROXENE CRNB04_NAFeO2_G NAFeO2_B ZRTIO4_BETA FLUORITE
ZRO2_TETR ALPO4_S3 ALPO4_S2 ALPO4_S1 ORTHO_PYROXENE CLINO_PYROXENE V305 HT
RUTILE ZRO2_MONO_AF M407 KAPPA_E21 PEROVSKITE COLUMBITE GAS NIMNO3 M2O3H
DIAMOND FCC_A4 DHCE_M
POLY:Hit RETURN to continue
POLY: @@ Note that mullite, corundum and spinel are stable.
POLY: @@ All Al-rich oxides.
POLY: @@ The amount of Al is probably too high, set it
POLY: @@ to 1/4 of the initial value
POLY:
POLY: s-c w(al)=2e-6
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
28 ITS, CPU TIME USED 1 SECONDS
POLY: l-st p
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES

```

PHASE STATUS DRIVING FORCE MOLES
 IONIC_LIQ#2 FIXED 0.000000E+00 0.000000E+00
 IONIC_LIQ#1 ENTERED 0.000000E+00 1.000000E+00
 IONIC_LIQ#3 DORMANT 7.893069E-15
 BCC_A2 DORMANT -6.028231E-03
 SPINEL DORMANT -2.523278E-02
 FCC_A1 DORMANT -3.320249E-02
 CORUNDUM DORMANT -1.074144E-01
 MULLITE DORMANT -1.212736E-01
 CORDIERITE DORMANT -2.109429E-01
 SILLIMANITE DORMANT -2.161782E-01
 ANDALUSITE DORMANT -2.343709E-01
 CRISTOBALITE DORMANT -2.428439E-01
 TRIDYMITE DORMANT -2.432419E-01
 DORMANT PHASES WITH DRIVING FORCE LESS THAN -2.660646E-01
 QUARTZ GARNET HCP_A3 KYANITE CARNEGIEITE_B CARNEGIEITE_A K2MGSIO4_LT CUB_A13
 ALPHASPINEL K2MGSIO4 HT RHODONITE CBCC_A12 WOLLASTONITE FE4N_LPI M203C
 OLIVINE HALITE NAALO2_D PROTO_PYROXENE CRNBO4 M203B NAFEO2_G NAFEO2_B
 ALPO4_S3 ALPO4_S2 ALPO4_S1 ORTHO_PYROXENE CLINO_PYROXENE FLUORITE ZR02_TETR
 V305_HT ZRTIO4_BETA_ZR02_MONO_AF RUTILE PEROVSKITE M4O7 KAPPA_E21 COLUMBITE
 GAS NIMNO3 M203H DIAMOND_FCC_A4 DHCP L
POLY: @@ Now the Al-oxide phases are not stable.
POLY: l-e,,
 ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium = 1, label A0 , database: TCOX11
 Conditions:
 T=1800, P=101325, N=1, W(MN)=4E-3, W(CR)=0.18, W(SI)=4E-3, W(AL)=2E-6
 FIXED PHASES
 IONIC_LIQ#2=0
 DEGREES OF FREEDOM 0
 Temperature 1800.00 K (1526.85 C), Pressure 1.013250E+05
 Number of moles of components 1.000000E+00, Mass in grams 5.48824E+01
 Total Gibbs energy -1.12705E+05, Enthalpy 6.87354E+04, Volume 8.01986E-06
 Component Moles W-Fraction Activity Potential Ref.stat
 AL 4.0681E-06 2.0000E-06 9.6461E-11 -3.4515E+05 SER
 CR 1.8999E-01 1.8000E-01 4.9755E-04 -1.1383E+05 SER
 FE 7.9789E-01 8.1191E-01 6.2152E-04 -1.1050E+05 SER
 MN 3.9960E-03 4.0000E-03 1.3487E-06 -2.0229E+05 SER
 O 3.0507E-04 8.8932E-05 4.3018E-13 -4.2615E+05 SER
 SI 7.8166E-03 4.0000E-03 4.7790E-08 -2.5228E+05 SER
 IONIC_LIQ#1 Status ENTERED Driving force 0.0000E+00
 Moles 1.0000E+00, Mass 5.4882E+01, Volume fraction 1.0000E+00 Mass fractions:
 FE 8.11909E-01 SI 4.00000E-03 O 8.89318E-05
 CR 1.80000E-01 MN 4.00000E-03 AL 2.00000E-06
 IONIC_LIQ#2 Status FIXED Driving force 0.0000E+00
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mass fractions:
 O 4.01491E-01 SI 1.68497E-01 CR 9.83335E-02
 MN 1.70218E-01 AL 1.35365E-01 FE 2.60951E-02
POLY: Hit RETURN to continue
POLY: @@ We assume that this describes the situation at 18 w/o Cr. Some
POLY: @@ liquid slag that later will form mainly SiO₂-Al₂O₃-MnO is present.
POLY: @@ Now increase the Cr-content to 25 w/o
POLY:
POLY: s-c w(cr)=.25
 ... the command in full is SET_CONDITION
POLY: c-e
 ... the command in full is COMPUTE_EQUILIBRIUM
 12 ITS, CPU TIME USED 0 SECONDS
POLY: l-e,,,
 ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium = 1, label A0 , database: TCOX11
 Conditions:
 T=1800, P=101325, N=1, W(MN)=4E-3, W(CR)=0.25, W(SI)=4E-3, W(AL)=2E-6
 FIXED PHASES
 IONIC_LIQ#2=0
 DEGREES OF FREEDOM 0
 Temperature 1800.00 K (1526.85 C), Pressure 1.013250E+05
 Number of moles of components 1.000000E+00, Mass in grams 5.45993E+01
 Total Gibbs energy -1.12735E+05, Enthalpy 6.82146E+04, Volume 8.03918E-06
 Component Moles W-Fraction Activity Potential Ref.stat
 AL 4.0471E-06 2.0000E-06 1.0339E-10 -3.4411E+05 SER
 CR 2.6252E-01 2.5000E-01 6.9514E-04 -1.0882E+05 SER
 FE 7.2530E-01 7.4187E-01 5.6333E-04 -1.1197E+05 SER
 MN 3.9753E-03 4.0000E-03 1.4649E-06 -2.0105E+05 SER
 O 4.2871E-04 1.25622E-04 4.1318E-13 -4.2676E+05 SER
 SI 7.7763E-03 4.0000E-03 4.4507E-08 -2.5334E+05 SER
 IONIC_LIQ#1 Status ENTERED Driving force 0.0000E+00
 Moles 1.0000E+00, Mass 5.4599E+01, Volume fraction 1.0000E+00 Mass fractions:
 FE 7.41872E-01 SI 4.00000E-03 O 1.25622E-04
 CR 2.50000E-01 MN 4.00000E-03 AL 2.00000E-06
 IONIC_LIQ#2 Status FIXED Driving force 0.0000E+00
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mass fractions:
 O 3.82050E-01 MN 1.58249E-01 AL 1.16335E-01
 CR 1.75603E-01 SI 1.49110E-01 FE 1.86519E-02
 SPINEL Status DORMANT Driving force 3.0996E-02
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mass fractions:
 CR 3.62302E-01 MN 2.12647E-01 FE 3.05878E-02
 O 3.10358E-01 AL 8.41044E-02 SI 0.00000E+00
POLY: Hit RETURN to continue
POLY: @@ Now Cr3O4 (SPINEL) would like to be stable. The simplest correction is to modify
POLY: @@ the composition of the steel in order to decrease the oxygen potential.
POLY: @@ For example the Mn or Si content could be changed.
POLY: @@ In order to determine which of these has the largest influence
POLY: @@ on the oxygen potential, calculate this by the partial derivative
POLY: @@ of the oxygen activity w.r.t. the Mn and Si content.
POLY:
POLY: s-ref-s o gas
 ... the command in full is SET_REFERENCE_STATE
 Temperature /*/:

```

Pressure /1E5/:
POLY: show acr(o)
... the command in full is SHOW_VALUE
ACR(O)=6.0547514E-7
POLY: show acr(o).w(mn)
... the command in full is SHOW_VALUE
ACR(O).W(MN)=-1.7572407E-5
POLY: show acr(o).w(si)
... the command in full is SHOW_VALUE
ACR(O).W(SI)=-3.7854829E-5
POLY:
POLY: @@ The value is largest for Si and thus the smallest change is necessary
POLY: @@ for that. Instead of modifying this content in steps one may
POLY: @@ specify that the Cr3O4 phase should be on its limit of stability, i.e.
POLY: @@ use the command FIX with zero amount and calculate the change
POLY: @@ in composition.
POLY:Hit RETURN to continue
POLY:
POLY: c-s p SPINEL=fix 0
... the command in full is CHANGE_STATUS
POLY: l-c
... the command in full is LIST_CONDITIONS
T=1800, P=101325, N=1, W(MN)=4E-3, W(CR)=0.25, W(SI)=4E-3, W(AL)=2E-6
FIXED PHASES
IONIC_LIQ#2=0 SPINEL=0
DEGREES OF FREEDOM -1
POLY: s-c w(si)=none
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
10 ITS, CPU TIME USED 0 SECONDS
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
Output from POLY-3, equilibrium = 1, label A0 , database: TCOX11

Conditions:
T=1800, P=101325, N=1, W(MN)=4E-3, W(CR)=0.25, W(AL)=2E-6
FIXED PHASES
IONIC_LIQ#2=0 SPINEL=0
DEGREES OF FREEDOM 0

Temperature 1800.00 K ( 1526.85 C), Pressure 1.013250E+05
Number of moles of components 1.00000E+00, Mass in grams 5.45524E+01
Total Gibbs energy -1.12972E+05, Enthalpy 6.80054E+04, Volume 8.04490E-06

Component Moles W-Fraction Activity Potential Ref.stat
AL 4.0436E-06 2.0000E-06 1.0504E-10 -3.4387E+05 SER
CR 2.6229E-01 2.5000E-01 6.9387E-04 -1.0885E+05 SER
FE 7.2379E-01 7.4097E-01 5.6222E-04 -1.1200E+05 SER
MN 3.9719E-03 4.0000E-03 1.4460E-06 -2.0125E+05 SER
O 4.0114E-04 1.1764E-04 5.7398E-07 -2.1507E+05 GAS
SI 9.5369E-03 4.9098E-03 5.5948E-08 -2.4992E+05 SER

IONIC_LIQ#1 Status ENTERED Driving force 0.0000E+00
Moles 1.00000E+00, Mass 5.4552E+01, Volume fraction 1.00000E+00 Mass fractions:
FE 7.40971E-01 SI 4.90983E-03 O 1.17644E-04
CR 2.50000E-01 MN 4.00000E-03 AL 2.00000E-06

IONIC_LIQ#2 Status FIXED Driving force 0.0000E+00
Moles 0.00000E+00, Mass 0.00000E+00, Volume fraction 0.00000E+00 Mass fractions:
O 3.86795E-01 SI 1.60487E-01 AL 1.11691E-01
CR 1.65678E-01 MN 1.57072E-01 FE 1.82772E-02

IONIC_LIQ#3 Status DORMANT Driving force 1.9388E-14
Moles 0.00000E+00, Mass 0.00000E+00, Volume fraction 0.00000E+00 Mass fractions:
O 3.86795E-01 SI 1.60487E-01 AL 1.11691E-01
CR 1.65678E-01 MN 1.57072E-01 FE 1.82772E-02

SPINEL Status FIXED Driving force 0.0000E+00
Moles 0.00000E+00, Mass 0.00000E+00, Volume fraction 0.00000E+00 Mass fractions:
CR 3.60476E-01 MN 2.12357E-01 FE 3.09181E-02
O 3.10766E-01 AL 8.54830E-02 SI 0.00000E+00
POLY:Hit RETURN to continue
POLY: @@ We can read the new Si content from this list but also
POLY: @@ directly show the value of a variable
POLY: sh w(si)
... the command in full is SHOW_VALUE
W(SI)=4.9098278E-3
POLY: @@ Increase the Si content to 0.6 w/o to avoid forming Cr3O4.
POLY: @@ Calculate also how much the Mn content must be changed
POLY: s-c w(si)=.006
... the command in full is SET_CONDITION
POLY: s-c w(mn)=none
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
13 ITS, CPU TIME USED 0 SECONDS
POLY: sh w(mn)
... the command in full is SHOW_VALUE
W(MN)=8.1885922E-3
POLY: @@ Check with Si content equal to .4. It should be consistent with
POLY: @@ the plot below, i.e. Mn content decreases with decreasing Si content.
POLY: s-c w(si)=.004
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
15 ITS, CPU TIME USED 1 SECONDS
POLY: sh w(mn)
... the command in full is SHOW_VALUE
W(MN)=2.2055904E-3
POLY:Hit RETURN to continue
POLY: @@ Plot how the Mn content varies when the Si content
POLY: @@ varies between 0.2 and 1 w/o.
POLY: s-a-v 1 w(si) 0.002 .01 0.0002
... the command in full is SET_AXIS_VARIABLE
POLY: save tcoex10 y
... the command in full is SAVE_WORKSPACES
POLY: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 0.400000E-02
POLY has calculated initial equilibrium

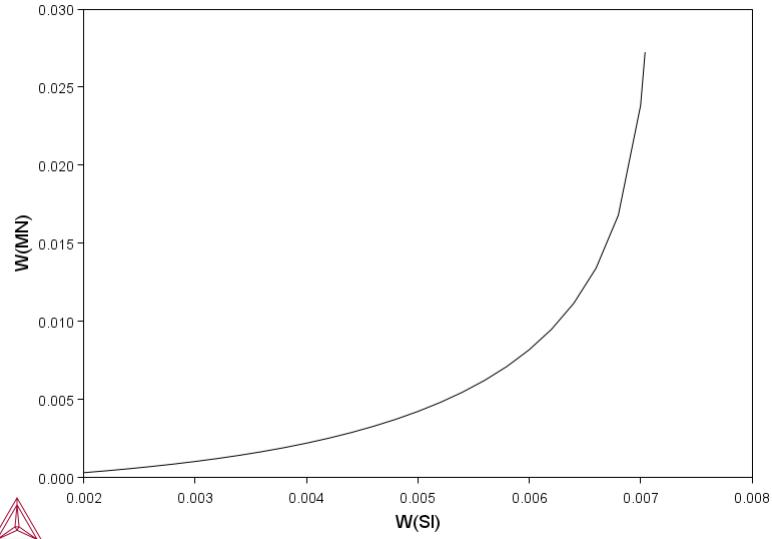
```

```

Phase Region from 0.400000E-02 for:
  IONIC_LIQ#1
  IONIC_LIQ#2
  SPINEL
QBSMER trying to find equilibrium at 7.0800000E-03
QBSMER: Second global calculation
Calculated 19 equilibria
Sorry cannot continue 1717 55 1 7.0400000E-03

Phase Region from 0.400000E-02 for:
  IONIC_LIQ#1
  IONIC_LIQ#2
  SPINEL
Terminating at 0.200000E-02
Calculated 13 equilibria
*** Buffer saved on file: c:\jenkins\workspace\generate_console_examples\examples\tcex10\tcex10.POLY3
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2
POST: s-d-a x w(si)
  ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y w(mn)
  ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 10a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
  ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
  ... the command in full is PLOT_DIAGRAM
example 10a

```

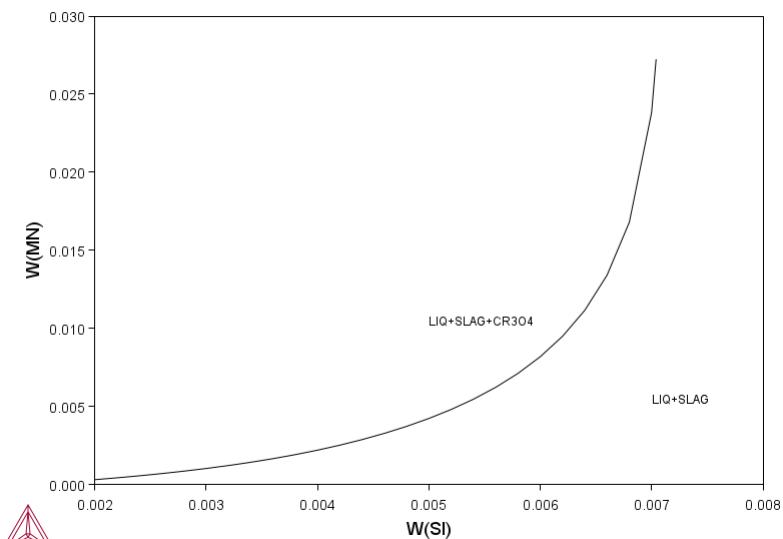


```

POST: Hit RETURN to continue
POST: add .005 .01 n
  ... the command in full is ADD_LABEL_TEXT
Text: LIQ+SLAG+CR3O4
Text size: /.36/:
POST: add .007 .005 n
  ... the command in full is ADD_LABEL_TEXT
Text: LIQ+SLAG
Text size: /.36/:
POST: set-title example 10b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
  ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
  ... the command in full is PLOT_DIAGRAM

```

example 10b



```
POST:  
POST:  
POST:  
POST: set-inter  
... the command in full is SET_INTERACTIVE_MODE  
POST:
```

tce11

SYS:About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce11\tce11.TCM.test"

SYS: set-echo

SYS:

SYS: @@ Oxidation of Cu2S with an H2O/O2 gas mixture

SYS:

SYS: @@ This example demonstrates the oxidation of Cu2S
SYS: @@ with an H2O/O2 gas mixture. Thermo-Calc is used to find
SYS: @@ the optimum O/H ratio (i.e. oxygen potential) as certain
SYS: @@ oxygen potential values can desulphurize Cu2S without
SYS: @@ forming copper oxides.

SYS:

SYS: @@ In Thermo-Calc, the problem reduces to perform equilibria
SYS: @@ calculations in a Cu-S-H-O system. The amounts of the
SYS: @@ components should be kept to correct ratio corresponding
SYS: @@ to Cu2S and H2O using a command SET_INPUT_AMOUNTS in POLY3.

SYS:

SYS: @@ Initially, O/H = 0.5 is given. Optimum O/H ratio is
SYS: @@ calculated with the desired calculation conditions. For
SYS: @@ example, to simulate one phase disappearing, you can FIX
SYS: @@ the phase with zero amount.

SYS:

SYS: set-log ex11,,,

SYS: go da

... the command in full is GOTO_MODULE

THERMODYNAMIC DATABASE module

Database folder: C:\jenkins\workspace\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

TDB_TCFE11: sw

... the command in full is SWITCH_DATABASE

Use one of these databases

TCFE11 = Steels/Fe-Alloys v11.0
TCFE9 = Steels/Fe-Alloys v9.3
SSOL7 = SGTE Alloy Solutions v7.0
SSOL6 = SGTE Alloy Solutions v6.0
SSUB6 = SGTE Substances v6.0
TOOX11 = Metal Oxide Solutions v11.1
FEDEMO = Iron Demo Database v4.0
ALDEMO = Aluminum Demo Database v4.1
OXDEMO = Oxide Demo Database v4.0
SUBDEMO = Substance Demo Database v1.0
PAQ2 = Public Aqueous Solution (SIT) v2.5
PG35 = PG35 Binary Semi-Conductors v1.3
MALDEMO = Al-Alloys Mobility demo database v2.0.1
USER = User defined Database

DATABASE NAME /TCFE11/: user tce11.tdb

Current database: User defined Database

This database does not support the DATABASE_INFORMATION command

VA /- DEFINED

15:36:29,106 [Thread-0] INFO TDBfileParser: USER_1434537374_14, number of lines read: 547
15:36:29,341 [Thread-0] INFO DatabaseUtils: Parsing of USER_1434537374_14 completed in 283 ms

TDB_USER: def-sys cu s o h

... the command in full is DEFINE_SYSTEM

CU S O H DEFINED

TDB_USER: l-sys

... the command in full is LIST_SYSTEM

ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/:

GAS:G :CU CU1H1 CU1H1O1 CU1O1 CU1S1 CU2 CU2S1 H H1O1 H1O1S1_HSO
H1O1S1_SOH H1O2 H1S1 H2 H2O1 H2O1S1_H2SO H2O1S1_HSOH H2O2 H2O4S1_H2S1 H2S2
O O1S1 O1S2 O2 O2S1 O3 O3S1 S S2 S3 S4 S5 S6 S7 S8:
CU_S :CU:
CU2O_S :CU2O1:
CU2O_L :CU2O1:
CU2S_S1 :CU2S1:
CU2S04 :CU2O4S1:
CU2S05 :CU2O5S1:
CU2S_L :CU2S1:
CU2S_S2 :CU2S1:
CU2S_S3 :CU2S1:
CUO :CU1O1:
CUS_S :CU1S1:
CUSO4 :CU1O4S1:
CU_L :CU:
H2O2_L :H2O2:
H2O_L :H2O1:
H2SO4_L :H2O4S1:
SS :S:
S_L :S:
S_S2 :S:
TDB_USER:Hit RETURN to continue

TDB_USER: get

... the command in full is GET_DATA

15:36:29,487 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

FUNCTIONS

List of references for assessed data

```

'TCS public data set for gaseous species, stoichiometric solids and
liquids in the Cu-Fe-H-N-O-S system.'
-OK-
TDB_USER: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY: ?
... the command in full is HELP
ADD_INITIAL_EQUILIBRIUM GOTO_MODULE      REINITIATE_MODULE
ADVANCED_OPTIONS HELP                   SAVE_WORKSPACES
AMEND_STORED_EQUILIBRIA INFORMATION        SELECT_EQUILIBRIUM
BACK LIST_AXIS_VARIABLE   SET_ALL_START_VALUES
CHANGE_STATUS LIST_CONDITIONS    SET_AXIS_VARIABLE
COMPUTE_EQUILIBRIUM LIST_EQUILIBRIUM   SET_CONDITION
COMPUTE_TRANSITION LIST_INITIAL_EQUILIBRIA SET_INPUT_AMOUNTS
CREATE_NEW_EQUILIBRIUM LIST_STATUS        SET_INTERACTIVE
DEFINE_COMPONENTS LIST_SYMBOLS          SET_NUMERICAL_LIMITS
DEFINE_DIAGRAM LOAD_INITIAL_EQUILIBRIUM SET_REFERENCE_STATE
DEFINE_MATERIAL MACRO_FILE_OPEN        SET_START_CONSTITUTION
DELETE_INITIAL_EQUILIB MAKE_COMPONENT_ENTERED SET_START_VALUE
DELETE_SYMBOL MAKE_COMPONENT_SUSPENDED SHOW_VALUE
ENTER_SYMBOL MAP                  STEP_WITH_OPTIONS
EVALUATE_FUNCTIONS POST             TABULATE
EXIT READ_WORKSPACES

POLY: li-st
... the command in full is LIST_STATUS
Option /CPS/:
*** STATUS FOR ALL COMPONENTS
COMPONENT STATUS REF. STATE T (K) P (Pa)
VA ENTERED SER
CU ENTERED SER
H ENTERED SER
O ENTERED SER
S ENTERED SER
*** STATUS FOR ALL PHASES
PHASE STATUS DRIVING FORCE MOLES
S_S2 ENTERED 0.000000E+00 0.000000E+00
S_L ENTERED 0.000000E+00 0.000000E+00
SS ENTERED 0.000000E+00 0.000000E+00
H2SO4_L ENTERED 0.000000E+00 0.000000E+00
H2O_L ENTERED 0.000000E+00 0.000000E+00
H2O2_L ENTERED 0.000000E+00 0.000000E+00
CU_S ENTERED 0.000000E+00 0.000000E+00
CU_L ENTERED 0.000000E+00 0.000000E+00
CUS_S ENTERED 0.000000E+00 0.000000E+00
CUSO4 ENTERED 0.000000E+00 0.000000E+00
CUO ENTERED 0.000000E+00 0.000000E+00
CU2S_S3 ENTERED 0.000000E+00 0.000000E+00
CU2S_S2 ENTERED 0.000000E+00 0.000000E+00
CU2S_S1 ENTERED 0.000000E+00 0.000000E+00
CU2S_L ENTERED 0.000000E+00 0.000000E+00
CU2S05 ENTERED 0.000000E+00 0.000000E+00
CU2S04 ENTERED 0.000000E+00 0.000000E+00
CU2O_S ENTERED 0.000000E+00 0.000000E+00
CU2O_L ENTERED 0.000000E+00 0.000000E+00
GAS ENTERED 0.000000E+00 0.000000E+00
*** STATUS FOR ALL SPECIES
CU ENTERED H15010.5S1 ENTERED O ENTERED
CU1H1 ENTERED H1O1 ENTERED O1S1 ENTERED
CU1H1009S1 ENTERED H1O1S1_HSO ENTERED O1S2 ENTERED
CU1H1O1 ENTERED H1O1S1_SOH ENTERED O2 ENTERED
CU1H202 ENTERED H1O2 ENTERED O2S1 ENTERED
CU1H205S1 ENTERED H1S1 ENTERED O3 ENTERED
CU1H607S1 ENTERED H2 ENTERED O3S1 ENTERED
CU1O1 ENTERED H2O1 ENTERED S ENTERED
CU1O4S1 ENTERED H2O1S1_H2SO ENTERED S2 ENTERED
CU1S1 ENTERED H2O1S1_HSOH ENTERED S3 ENTERED
CU2 ENTERED H2O2 ENTERED S4 ENTERED
CU2O1 ENTERED H2O4S1 ENTERED S5 ENTERED
CU2O4S1 ENTERED H2S1 ENTERED S6 ENTERED
CU2OSS1 ENTERED H2S2 ENTERED S7 ENTERED
CU2S1 ENTERED H4O5S1 ENTERED S8 ENTERED
H ENTERED H6O6S1 ENTERED VA ENTERED
H1O08S1 ENTERED H8O7S1 ENTERED
POLY:
POLY:Hit RETURN to continue
POLY: @@ Assume initially that we have one mole of Cu2S and 50 moles water vapor
POLY: s-i-a n(cu2s1)=1,n(h2o1)=50
... the command in full is SET_INPUT_AMOUNTS
POLY: set-cond t=1400,p=101325
... the command in full is SET_CONDITION
POLY: l-c
... the command in full is LIST_CONDITIONS
N(CU)=2, N(S)=1, N(H)=100, N(O)=50, T=1400, P=101325
DEGREES OF FREEDOM 0
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
15:36:30,033 [Thread-0] INFO Database: Preparing system for use: USER_1434537374_14
15:36:31,201 [Thread-0] INFO Phase: Preparing phase for use: GAS
Using global minimization procedure
15:36:31,742 [Thread-0] INFO Phase: Preparing phase for use: CU2O_L
15:36:32,153 [Thread-0] INFO Phase: Preparing phase for use: CU2O_S
15:36:32,500 [Thread-0] INFO Phase: Preparing phase for use: CU2S04
15:36:32,844 [Thread-0] INFO Phase: Preparing phase for use: CU2S05
15:36:33,236 [Thread-0] INFO Phase: Preparing phase for use: CU2S_L
15:36:33,577 [Thread-0] INFO Phase: Preparing phase for use: CU2S_S1
15:36:33,915 [Thread-0] INFO Phase: Preparing phase for use: CU2S_S2
15:36:34,260 [Thread-0] INFO Phase: Preparing phase for use: CU2S_S3
15:36:34,592 [Thread-0] INFO Phase: Preparing phase for use: CUO
15:36:34,926 [Thread-0] INFO Phase: Preparing phase for use: CUSO4
15:36:35,257 [Thread-0] INFO Phase: Preparing phase for use: CUS_S
15:36:35,590 [Thread-0] INFO Phase: Preparing phase for use: CU_L
15:36:35,922 [Thread-0] INFO Phase: Preparing phase for use: CU_S
15:36:36,253 [Thread-0] INFO Phase: Preparing phase for use: H2O2_L
15:36:36,585 [Thread-0] INFO Phase: Preparing phase for use: H2O_L
15:36:36,917 [Thread-0] INFO Phase: Preparing phase for use: H2SO4_L
15:36:37,248 [Thread-0] INFO Phase: Preparing phase for use: SS
15:36:37,576 [Thread-0] INFO Phase: Preparing phase for use: S_L
15:36:37,911 [Thread-0] INFO Phase: Preparing phase for use: S_S2
Calculated 685 grid points in 9 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 9 s
POLY: l-e

```

... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
Output from POLY-3, equilibrium = 1, label A0 , database: USER

Conditions:
N(CU)=2, N(S)=1, N(H)=100, N(O)=50, T=1400, P=101325
DEGREES OF FREEDOM 0

Temperature 1400.00 K (1126.85 C), Pressure 1.013250E+05
Number of moles of components 1.53000E+02, Mass in grams 1.05989E+03
Total Gibbs energy -2.75931E+07, Enthalpy -9.82382E+06, Volume 5.76972E+00

| Component | Moles | W-Fraction | Activity | Potential | Ref.stat |
|-----------|------------|------------|------------|-------------|----------|
| CU | 2.0000E+00 | 1.1991E-01 | 1.6098E-03 | -7.4867E+04 | SER |
| H | 1.0000E+02 | 9.5095E-02 | 9.5714E-06 | -1.3452E+05 | SER |
| O | 5.0000E+01 | 7.5475E-01 | 5.1729E-11 | -2.7570E+05 | SER |
| S | 1.0000E+00 | 3.0248E-02 | 2.0746E-08 | -2.0593E+05 | SER |

GAS Status ENTERED Driving force 0.0000E+00
Moles 1.5022E+02, Mass 9.0794E+02, Volume fraction 1.0000E+00 Mass fractions:
O 8.81060E-01 H 1.11009E-01 S 7.92556E-03 CU 5.01241E-06

Constitution:
H2O1 9.86660E-01 CU1H1O1 1.96753E-08 CU1O1 8.58177E-12
H2 8.86811E-03 O3S1 1.43507E-08 H2O2 5.46461E-12
O2S1 4.44169E-03 H2O1S1_HSOH 7.52014E-09 H2O1S1_H2SO 3.12748E-12
H2S1 2.10471E-05 S 4.30477E-09 H2O4S1 3.10120E-12
O1S1 5.63051E-06 O2 2.46248E-09 S3 1.29650E-12
CU 1.32327E-06 H1O1S1_SOH 1.77241E-09 H1O2 4.13438E-13
H1O1 1.00104E-06 CU1S1 1.23642E-09 S4 3.25596E-18
H 4.55656E-07 CU2 4.47851E-10 S5 1.21560E-21
H1S1 3.40802E-07 CU2S1 2.11636E-10 O3 1.70006E-22
S2 1.38936E-07 H2S2 1.77731E-10 S6 5.54892E-27
CU1H1 8.04525E-08 O 4.66615E-11 S8 1.00000E-30
O1S2 2.49875E-08 H1O1S1_HSO 3.35706E-11 S7 1.00000E-30

CU_S3 Status ENTERED Driving force 0.0000E+00
Moles 2.3266E+00, Mass 1.2343E+02, Volume fraction 0.0000E+00 Mass fractions:
CU 7.98557E-01 S 2.01443E-01 O 0.00000E+00 H 0.00000E+00

CU_L Status ENTERED Driving force 0.0000E+00
Moles 4.4883E-01, Mass 2.8522E+01, Volume fraction 0.0000E+00 Mass fractions:
CU 1.00000E+00 S 0.00000E+00 O 0.00000E+00 H 0.00000E+00

POLY:Hit RETURN to continue
POLY: @@ Now set the status of the digitine (CU2S_S3) to be fixed with
POLY: @@ zero amount. This means that this is reduced completely
POLY: c-s
... the command in full is CHANGE_STATUS
For phases, species or components? /PHASES/:
Phase name(s): cu2s_s3
Status: /ENTERED/: fix
Number of mole formula units /0/: 0
POLY: @@ There are now too many conditions. The gas must be allowed to vary
POLY: @@ in composition to find the correct oxygen potential
POLY: l-c
... the command in full is LIST_CONDITIONS
N(CU)=2, N(S)=1, N(H)=100, N(O)=50, T=1400, P=101325
FIXED PHASES
CU2S_S3=0
DEGREES OF FREEDOM -1
POLY:Hit RETURN to continue
POLY: set-c n(o)=none
... the command in full is SET_CONDITION
POLY: l-c
... the command in full is LIST_CONDITIONS
N(CU)=2, N(S)=1, N(H)=100, T=1400, P=101325
FIXED PHASES
CU2S_S3=0
DEGREES OF FREEDOM 0
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
10 ITS, CPU TIME USED 0 SECONDS
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
Output from POLY-3, equilibrium = 1, label A0 , database: USER

Conditions:
N(CU)=2, N(S)=1, N(H)=100, T=1400, P=101325
FIXED PHASES
CU2S_S3=0
DEGREES OF FREEDOM 0

Temperature 1400.00 K (1126.85 C), Pressure 1.013250E+05
Number of moles of components 1.54785E+02, Mass in grams 1.08845E+03
Total Gibbs energy -2.80759E+07, Enthalpy -1.00131E+07, Volume 5.85888E+00

| Component | Moles | W-Fraction | Activity | Potential | Ref.stat |
|-----------|------------|------------|------------|-------------|----------|
| CU | 2.0000E+00 | 1.1676E-01 | 1.6098E-03 | -7.4867E+04 | SER |
| H | 1.0000E+02 | 9.2600E-02 | 6.5700E-06 | -1.3890E+05 | SER |
| O | 5.1785E+01 | 7.6118E-01 | 1.0863E-10 | -2.6707E+05 | SER |
| S | 1.0000E+00 | 2.9455E-02 | 2.0746E-08 | -2.0593E+05 | SER |

GAS Status ENTERED Driving force 0.0000E+00
Moles 1.5278E+02, Mass 9.6136E+02, Volume fraction 1.0000E+00 Mass fractions:
O 8.61805E-01 H 1.04841E-01 S 3.33486E-02 CU 4.75131E-06

Constitution:
H2O1 9.76211E-01 O1S2 5.24705E-08 H2O4S1 2.84109E-11
O2S1 1.95855E-02 CU1H1O1 2.83599E-08 CU1O1 1.80206E-11
H2 4.17844E-03 O2 1.08582E-08 H2O2 1.13535E-11
O1S1 1.18234E-05 H2O1S1_HSOH 7.44050E-09 H2O1S1_H2SO 3.09435E-12
H2S1 9.91688E-06 S 4.30477E-09 S3 1.29650E-12
H1O1 1.44290E-06 H1O1S1_SOH 2.55475E-09 H1O2 1.25138E-12
CU 1.32327E-06 CU1S1 1.23642E-09 S4 3.25596E-18
H 3.12773E-07 CU2 4.47851E-10 O3 1.57414E-21
H1S1 2.33934E-07 CU2S1 2.11636E-10 S5 1.21560E-21
S2 1.38936E-07 O 9.79832E-11 S6 5.54892E-27
O3S1 1.32878E-07 H2S2 8.37427E-11 S8 1.00000E-30
CU1H1 5.52244E-08 H1O1S1_HSO 4.83886E-11 S7 1.00000E-30

CU_L Status ENTERED Driving force 0.0000E+00
Moles 1.9999E+00, Mass 1.2709E+02, Volume fraction 0.0000E+00 Mass fractions:

```

CU 1.00000E+00 S 0.00000E+00 O 0.00000E+00 H 0.00000E+00
CU2S_S3 Status FIXED Driving force 0.0000E+00
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mass fractions:
CU 7.98557E-01 S 2.01443E-01 O 0.00000E+00 H 0.00000E+00
POLY: sh n(*)
... the command in full is SHOW VALUE
N(CU)=2, N(H)=100., N(O)=51.784749, N(S)=1.
POLY:Hit RETURN to continue
POLY: @@ If we have too much oxygen we may get some copper oxides,
POLY: @@ check which one is the closest to be stable
POLY: l-st p
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES
PHASE STATUS DRIVING FORCE MOLES
CU2S_S3 FIXED 0.000000E+00 0.000000E+00
CU_L ENTERED 0.000000E+00 1.999928E+00
GAS ENTERED 0.000000E+00 1.527848E+02
CU2S_L ENTERED -3.931114E-04 0.000000E+00
CU2S_S2 ENTERED -3.309936E-02 0.000000E+00
CU_S ENTERED -3.549960E-02 0.000000E+00
CU2S_S1 ENTERED -3.332974E-01 0.000000E+00
CU2O_S ENTERED -1.086153E+00 0.000000E+00
CU2O_L ENTERED -1.231036E+00 0.000000E+00
H2O_L ENTERED -1.738865E+00 0.000000E+00
CUS_S ENTERED -3.173417E+00 0.000000E+00
CUO ENTERED -3.229722E+00 0.000000E+00
CU2SO4 ENTERED -3.322206E+00 0.000000E+00
ENTERED PHASES WITH DRIVING FORCE LESS THAN -3.797595E+00
CU2S05 CUSO4_H2SO4_L H2O2_L S_L S_S2 SS
POLY: @@ Set Cu2O to fix with zero amount and remove the fix status of CU2S_S3
POLY: c-s p cu2o_s=fix 0
... the command in full is CHANGE_STATUS
POLY: c-s p cu2s_s3
... the command in full is CHANGE_STATUS
Status: /ENTERED/:
Start value, number of mole formula units /0/:
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
 39 ITS, CPU TIME USED 0 SECONDS
POLY: l-e,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: USER

Conditions:
N(CU)=2, N(S)=1, N(H)=100, T=1400, P=101325
FIXED PHASES
CU2O_S=0
DEGREES OF FREEDOM 0

Temperature 1400.00 K ( 1126.85 C), Pressure 1.013250E+05
Number of moles of components 1.54993E+02, Mass in grams 1.09178E+03
Total Gibbs energy -2.81294E+07, Enthalpy -1.00609E+07, Volume 5.85900E+00

Component Moles W-Fraction Activity Potential Ref.stat
CU 2.0000E+00 1.1641E-01 1.6098E-03 -7.4867E+04 SER
H 1.0000E+02 9.2317E-02 1.2909E-06 -1.5784E+05 SER
O 5.1993E+01 7.6191E-01 2.8253E-09 -2.2914E+05 SER
S 1.0000E+00 2.9365E-02 3.0696E-11 -2.8178E+05 SER

GAS Status ENTERED Driving force 0.0000E+00
Moles 1.5299E+02, Mass 9.6469E+02, Volume fraction 1.0000E+00 Mass fractions:
O 8.62282E-01 H 1.04479E-01 S 3.32335E-02 CU 4.97350E-06
Constitution:
H2O1 9.80215E-01 H2O4S1 7.42671E-10 H1O1S1_HSO 3.65881E-13
O2S1 1.96037E-02 H2S1 5.66454E-10 CU2S1 3.13135E-13
H2 1.61310E-04 CU1O1 4.68706E-10 S2 3.04157E-13
H1O1 7.37378E-06 CU2 4.47851E-10 H2O1S1_H2SO 4.59716E-15
O2 7.34547E-06 H2O2 2.96508E-10 O3 2.76971E-17
O3S1 3.45929E-06 H1O2 1.66331E-10 H2S2 7.07748E-18
CU 1.32327E-06 H1S1 6.80080E-11 S3 4.19951E-21
O1S1 4.55002E-07 H1O1S1_SOH 1.93172E-11 S4 1.56044E-29
CU1H1O1 1.44930E-07 H2O1S1_HSOH 1.10541E-11 S7 1.00000E-30
H 6.14543E-08 S 6.36932E-12 S5 1.00000E-30
CU1H1 1.08506E-08 O1S2 2.98765E-12 S6 1.00000E-30
O 2.54848E-09 CU1S1 1.82939E-12 S8 1.00000E-30

CU_L Status ENTERED Driving force 0.0000E+00
Moles 1.9999E+00, Mass 1.2709E+02, Volume fraction 0.0000E+00 Mass fractions:
CU 1.00000E+00 S 0.00000E+00 O 0.00000E+00 H 0.00000E+00

CU2O_S Status FIXED Driving force 0.0000E+00
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mass fractions:
CU 8.88190E-01 O 1.11810E-01 S 0.00000E+00 H 0.00000E+00
POLY: show n(*)
... the command in full is SHOW VALUE
N(CU)=2, N(H)=100., N(O)=51.992866, N(S)=1.
POLY:Hit RETURN to continue
POLY: @@ The ratio N(O) to N(H) should thus be between 0.5178 and 0.52
POLY: @@ in order to reduce all Cu2S and not forming any Cu2O
POLY: @@ Make a diagram showing this amount of phases
POLY: c-st p cu2o_s
... the command in full is CHANGE_STATUS
Status: /ENTERED/:
Start value, number of mole formula units /0/:
POLY: s-a-v 1 n(o)
... the command in full is SET_AXIS_VARIABLE
Min value /0/: 45
Max value /1/: 55
Increment /.25/:
POLY: s-c n(o)
... the command in full is SET_CONDITION
Value /51.99286556/:
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY: save tce11 y
... the command in full is SAVE_WORKSPACES
POLY: step normal
... the command in full is STEP_WITH_OPTIONS

```

```

No initial equilibrium, using default
Step will start from axis value      51.9929
...OK

Phase Region from    51.9929      for:
  GAS
  CU_L
Global check of adding phase at  5.19929E+01
Calculated      2 equilibria

Phase Region from    51.9929      for:
  GAS
  CU2O_S
  CU_L
Global check of removing phase at  5.29928E+01
Calculated      6 equilibria

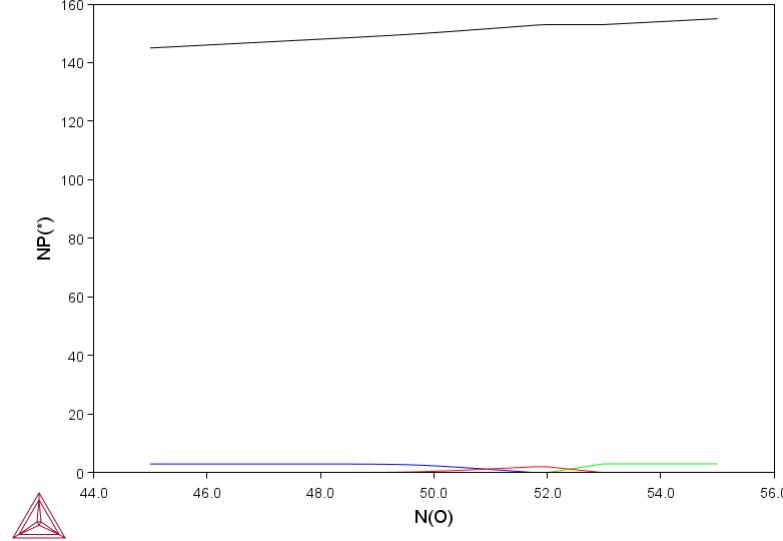
Phase Region from    52.9928      for:
  GAS
  CU2O_S
Global test at  5.49929E+01 .... OK
Terminating at    55.0000
Calculated      12 equilibria

Phase Region from    51.9929      for:
  GAS
  CU_L
Global check of adding phase at  5.17847E+01
Calculated      3 equilibria

Phase Region from    51.7847      for:
  GAS
  CU2S_S3
  CU_L
Global test at  4.99929E+01 .... OK
Global test at  4.74929E+01 .... OK
Global test at  4.50000E+01 .... OK
Terminating at    45.0000
Calculated      31 equilibria
*** Buffer saved on file: c:\jenkins\workspace\generate_console_examples\examples\tcex11\tcex11.POLY3
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2
POST: s-d-a x n(o)
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y np(*)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*:
POST: set-title example 11a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

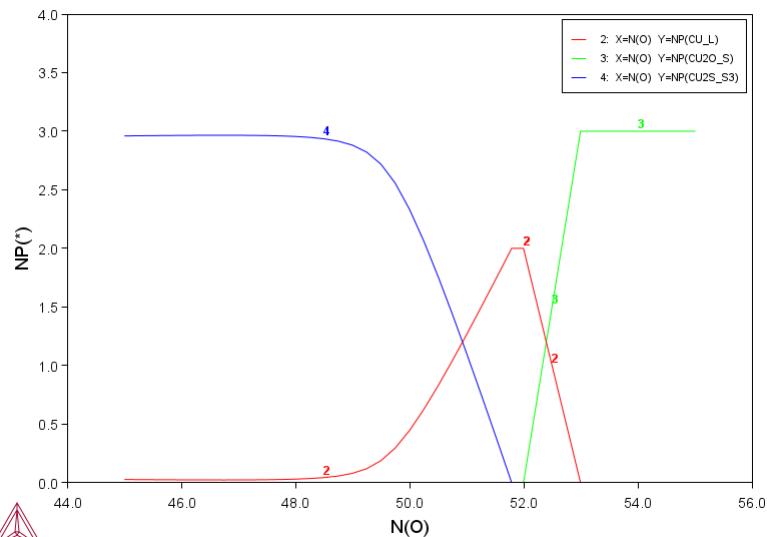
```

example 11a



POST:
POST:Hit RETURN to continue
POST: s-lab d
... the command in full is SET_LABEL_CURVE_OPTION
POST: s-s y n 0 4
... the command in full is SET_SCALING_STATUS
POST: set-title example 11b
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

example 11b



POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:

tce12

SYS:About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce12\tce12.TCM.test"

SYS: set-echo

SYS:

SYS: @@ Tabulation of thermodynamic data for reactions

SYS:

SYS: @@ This example shows a number of independent cases using
SYS: @@ the TABULATEREACTION (TAB) module to tabulate thermodynamic
SYS: @@ data for reactions.

SYS:

SYS: @@ Note that a SSUB database license is required to run
SYS: @@ the example.

SYS:

SYS: @@ Each case is separated by a line such as this
SYS: =====

SYS: set-log ex12,,

SYS: go tab

... the command in full is GOTO_MODULE

TAB: ?

... the command in full is HELP

| | | |
|----------------|-----------------|----------------------|
| BACK | LIST_SUBSTANCES | SWITCH_DATABASE |
| ENTER_FUNCTION | MACRO_FILE_OPEN | TABULATE_DERIVATIVES |
| ENTERREACTION | PATCH | TABULATEREACTION |
| EXIT | SET_ENERGY_UNIT | TABULATE_SUBSTANCE |
| GOTO_MODULE | SET_INTERACTIVE | |
| HELP | SET_PLOT_FORMAT | |

TAB: @@ Tabulate data for a reaction

TAB: tab-reac 3H2+N2=2N1H3;

... the command in full is TABULATEREACTION

THERMODYNAMIC DATABASE module

Database folder: C:\jenkins\workspace\generate_console_examples\databases\data

Current database: SGTE Substances v6.0

VA DEFINED

... the command in full is REJECT

VA DEFINED

REINITIATING GES

... the command in full is DEFINE_SPECIES

H2 N2 H3N1

DEFINED

... the command in full is GET DATA

15:37:55,453 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

FUNCTIONS

List of references for assessed data

H2<G> JANAF THERMOCHEMICAL TABLES SGTE **

H2<G> H2<G>

HYDROGEN<G>

STANDARD STATE FROM CODATA KEY VALUES. CP FROM JANAF PUB. 3/61

H3N1<G> T.C.R.A.S. Class: 2

H3N1<G> NH3<G>

AMMONIA <GAS>

N2<G> JANAF THERMOCHEMICAL TABLES SGTE **

N2<G> N2<G>

NITROGEN <DIATOMIC GAS>

PUBLISHED BY JANAF AT 09/65

-OK-

Pressure /100000/: SSUB6

Graphical output? /Y/: 100000

*** ERROR 1034 IN TBMOUF: FILE SYSTEM ERROR

Reaction: 3H2<G>+N2<G>=2H3N1<G>

ATTEMPT TO SET NEGATIVE, T = 0.00000000000000E+000

*** ERROR 1114 IN GSSPB : NO SPECIES WITH THIS INDEX

ERROR 1114 RESET

TAB: 298.15

NO SUCH COMMAND, USE HELP *

TAB: 2000

NO SUCH COMMAND, USE HELP *

TAB: 100

NO SUCH COMMAND, USE HELP *

TAB:

TAB: Hit RETURN to continue

TAB: @@ Add a final column with a function. In this function

TAB: @@ you may use G, S, H, V, CP, T and R with the obvious

TAB: @@ meaning. You may also use H298 and ALPHA (thermal expansivity)

TAB: @@ and KAPPA (isothermal compressibility). In most databases

TAB: @@ there are no pressure dependence and thus V, ALPHA and KAPPA

TAB: @@ will not be correct.

TAB:

TAB: e-fun

... the command in full is ENTER_FUNCTION

Name: fef

Function: (g-h298)/t

&

TAB: t-r

... the command in full is TABULATEREACTION

Same reaction? /Y/: y

Pressure /100000/: 100000

Low temperature limit /0/: 298.15

High temperature limit /9.733463994-313/: 2000

Step in temperature /6.953149686-310/: 100

Output file /SCREEN/:

O U T P U T F R O M T H E R M O - C A L C
2023. 4.27 15.38. 0

Column 6: fef (G-H298)/T
Reaction: 3H2<G>+N2<G>=2H3N1<G>
H2<GAS>
N2<GAS>
H3N1<GAS>

| T | Delta-Cp | Delta-H | Delta-S | Delta-G | fef |
|---------|--------------|--------------|--------------|--------------|-------------|
| (K) | (Joule/K) | (Joule) | (Joule/K) | (Joule) | |
| 298.15 | -4.44006E+01 | -9.18800E+04 | -1.98115E+02 | -3.28120E+04 | 1.98115E+02 |
| 300.00 | -4.43267E+01 | -9.19621E+04 | -1.98389E+02 | -3.24452E+04 | 1.98116E+02 |
| 400.00 | -3.92294E+01 | -9.61533E+04 | -2.10482E+02 | -1.19604E+04 | 1.99799E+02 |
| 500.00 | -3.34122E+01 | -9.97861E+04 | -2.18613E+02 | 9.52022E+03 | 2.02800E+02 |
| 600.00 | -2.77768E+01 | -1.02842E+05 | -2.24200E+02 | 3.16779E+04 | 2.05930E+02 |
| 700.00 | -2.26324E+01 | -1.05358E+05 | -2.28088E+02 | 5.43040E+04 | 2.08834E+02 |
| 800.00 | -1.81080E+01 | -1.07390E+05 | -2.30808E+02 | 7.72568E+04 | 2.11421E+02 |
| 900.00 | -1.41889E+01 | -1.09000E+05 | -2.32710E+02 | 1.00438E+05 | 2.13687E+02 |
| 1000.00 | -1.08095E+01 | -1.10245E+05 | -2.34025E+02 | 1.23779E+05 | 2.15659E+02 |
| 1100.00 | -7.77802E+00 | -1.11169E+05 | -2.34908E+02 | 1.47229E+05 | 2.17372E+02 |
| 1200.00 | -5.07556E+00 | -1.11807E+05 | -2.35464E+02 | 1.70750E+05 | 2.18858E+02 |
| 1300.00 | -2.93467E+00 | -1.12203E+05 | -2.35782E+02 | 1.94314E+05 | 2.20149E+02 |
| 1400.00 | -1.19414E+00 | -1.12407E+05 | -2.35934E+02 | 2.17901E+05 | 2.21272E+02 |
| 1500.00 | 2.55400E-01 | -1.12452E+05 | -2.35966E+02 | 2.41497E+05 | 2.22251E+02 |
| 1600.00 | 1.49022E+00 | -1.12363E+05 | -2.35909E+02 | 2.65091E+05 | 2.23107E+02 |
| 1700.00 | 2.56484E+00 | -1.12159E+05 | -2.35785E+02 | 2.88676E+05 | 2.23857E+02 |
| 1800.00 | 3.51909E+00 | -1.11854E+05 | -2.35611E+02 | 3.12246E+05 | 2.24515E+02 |
| 1900.00 | 4.38259E+00 | -1.11458E+05 | -2.35397E+02 | 3.35797E+05 | 2.25093E+02 |
| 2000.00 | 5.17775E+00 | -1.10980E+05 | -2.35152E+02 | 3.59325E+05 | 2.25602E+02 |

TAB: Hit RETURN to continue

TAB: t-r

... the command in full is TABULATEREACTION

Same reaction? /Y/: y

Pressure /100000/: 100000

Low temperature limit /298.15/: 298.15

High temperature limit /2000/: 2000

Step in temperature /100/: 100

Output file /SCREEN/: tcex12a

Graphical output? /Y/: y

Plot column? /2/: 6

O U T P U T F R O M T H E R M O - C A L C
2023. 4.27 15.38. 0

Column 6: fef (G-H298)/T
Reaction: 3H2<G>+N2<G>=2H3N1<G>
H2<GAS>
N2<GAS>
H3N1<GAS>

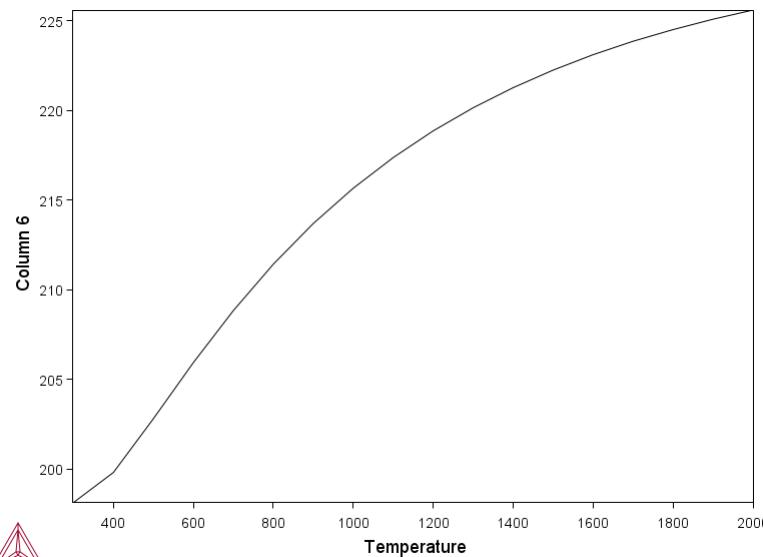
| T | Delta-Cp | Delta-H | Delta-S | Delta-G | fef |
|---------|--------------|--------------|--------------|--------------|-------------|
| (K) | (Joule/K) | (Joule) | (Joule/K) | (Joule) | |
| 298.15 | -4.44006E+01 | -9.18800E+04 | -1.98115E+02 | -3.28120E+04 | 1.98115E+02 |
| 300.00 | -4.43267E+01 | -9.19621E+04 | -1.98389E+02 | -3.24452E+04 | 1.98116E+02 |
| 400.00 | -3.92294E+01 | -9.61533E+04 | -2.10482E+02 | -1.19604E+04 | 1.99799E+02 |
| 500.00 | -3.34122E+01 | -9.97861E+04 | -2.18613E+02 | 9.52022E+03 | 2.02800E+02 |
| 600.00 | -2.77768E+01 | -1.02842E+05 | -2.24200E+02 | 3.16779E+04 | 2.05930E+02 |
| 700.00 | -2.26324E+01 | -1.05358E+05 | -2.28088E+02 | 5.43040E+04 | 2.08834E+02 |
| 800.00 | -1.81080E+01 | -1.07390E+05 | -2.30808E+02 | 7.72568E+04 | 2.11421E+02 |
| 900.00 | -1.41889E+01 | -1.09000E+05 | -2.32710E+02 | 1.00438E+05 | 2.13687E+02 |
| 1000.00 | -1.08095E+01 | -1.10245E+05 | -2.34025E+02 | 1.23779E+05 | 2.15659E+02 |
| 1100.00 | -7.77802E+00 | -1.11169E+05 | -2.34908E+02 | 1.47229E+05 | 2.17372E+02 |
| 1200.00 | -5.07556E+00 | -1.11807E+05 | -2.35464E+02 | 1.70750E+05 | 2.18858E+02 |
| 1300.00 | -2.93467E+00 | -1.12203E+05 | -2.35782E+02 | 1.94314E+05 | 2.20149E+02 |
| 1400.00 | -1.19414E+00 | -1.12407E+05 | -2.35934E+02 | 2.17901E+05 | 2.21272E+02 |
| 1500.00 | 2.55400E-01 | -1.12452E+05 | -2.35966E+02 | 2.41497E+05 | 2.22251E+02 |
| 1600.00 | 1.49022E+00 | -1.12363E+05 | -2.35909E+02 | 2.65091E+05 | 2.23107E+02 |
| 1700.00 | 2.56484E+00 | -1.12159E+05 | -2.35785E+02 | 2.88676E+05 | 2.23857E+02 |
| 1800.00 | 3.51909E+00 | -1.11854E+05 | -2.35611E+02 | 3.12246E+05 | 2.24515E+02 |
| 1900.00 | 4.38259E+00 | -1.11458E+05 | -2.35397E+02 | 3.35797E+05 | 2.25093E+02 |
| 2000.00 | 5.17775E+00 | -1.10980E+05 | -2.35152E+02 | 3.59325E+05 | 2.25602E+02 |

POSTPROCESSOR VERSION 3.2

... the command in full is QUICK_EXPERIMENTAL_PLOT

... the command in full is SET_SCALING_STATUS

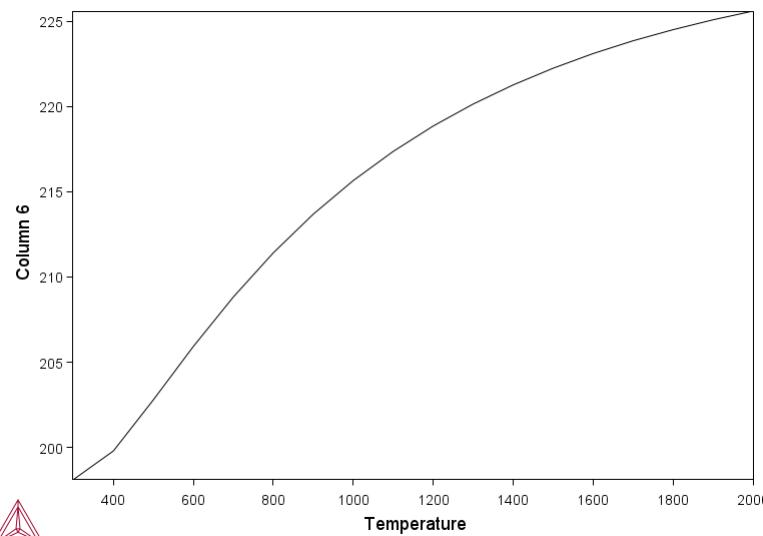
... the command in full is PLOT_DIAGRAM



```

POST:
POST: set-title example 12a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFILE
*** ERROR 3004 IN LPOSTP: NO AXIS DEFINED
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
example 12a

```



```

POST:
POST:Hit RETURN to continue
POST: back
TAB:
TAB:
TAB: @@ In the Gibbs-Energy-System list the data using
TAB: go g
... the command in full is GOTO_MODULE
GIBBS ENERGY SYSTEM
GES6: l-d
... the command in full is LIST_DATA
OUTPUT TO SCREEN OR FILE /SCREEN/:
OPTIONS?: ?
FILE SYSTEM ERROR IN FILHLP
ERROR 1717 READING HELP FILE
OPTIONS?: rs

```

1OUTPUT FROM GIBBS ENERGY SYSTEM ON PC/WINDOWS NT DATE 2023- 4-27
FROM DATABASE: SSUB6

ALL DATA IN SI UNITS
FUNCTIONS VALID FOR 298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED

| ELEMENT | STABLE ELEMENT | REFERENCE | MASS | H298-H0 | S298 |
|---------|------------------|-----------|------------|------------|------------|
| 0 VA | VACUUM | | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 1 H | 1/2_MOLE_H2(GAS) | | 1.0079E+00 | 4.2340E+03 | 6.5285E+01 |
| 2 N | 1/2_MOLE_N2(GAS) | | 1.4007E+01 | 4.3350E+03 | 9.5751E+01 |

| SPECIES | STOICHIOMETRY |
|---------|---------------|
| 1 H | H |
| 2 H2 | H2 |
| 3 H3N1 | H3N1 |
| 4 N | N |
| 5 N2 | N2 |
| 6 VA | VA |

```

Property type /ALL/: ALL
GAS:G      (H2,H3N1,N2)1.0

===== [H] =====
G(GAS,H2;0)          298.15 F11937T#+R#*T*LN(1.0E-5*P);      6000 N

===== [N] =====
G(GAS,N2;0)          298.15 F14172T#+R#*T*LN(1.0E-5*P);      6000 N

===== [H, N] =====
G(GAS,H3N1;0)        298.15 F12196T#+R#*T*LN(1.0E-5*P);      6000 N

GES6:Hit RETURN to continue
GES6: back
TAB:
TAB: @@ Tabulate another reaction
TAB: @@ =====
TAB: t-r
... the command in full is TABULATEREACTION
Same reaction? /Y/: n
Reaction: INP+GA=GAP+IN;
... the command in full is REJECT
VA DEFINED
REINITIATING GES .....
... the command in full is DEFINE_SPECIES
GA1P1           IN1P1           IN
GA1P1 DEFINED
... the command in full is GET_DATA
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS .....

List of references for assessed data

GA1<G> T.C.R.A.S. Class: 1
GA1<G> Ga<G>
GALLIUM <GAS>
GA1P1<G> S.G.T.E.
GA1P1<G> GaP<G>
GALLIUM PHOSPHIDE <GAS>
ASSESSED DATA BY C. CHATILLON MARCH 1994. Ga(g) and P2(g)
from T.C.R.A.S.
IN1<G> THERMODATA
IN1<G>
New Assessment (H_form and S only)
IN1P1<G> CHATILLON(1994 March)
IN1P1<G>
ASSESSED DATA BY C. CHATILLON MARCH 1994. In(g) and P2(g)
from T.C.R.A.S.
GA1P1 S.G.T.E.
GA1P1 Gap GAP
GALLIUM PHOSPHIDE. Calphad, 18, 2, 177-222 (1994).
GA1 S.G.T.E. **
GA1 Ga
GALLIUM
Data from SGTE Unary DB , based on 81GLU/GUR (Ivtan Vol. 3)
20080211 BC Tref 200 -> 298.15
IN1P1 I. BARIN 3rd. Edition
IN1P1 INP InP
INDIUM MONOPHOSPHIDE. Data taken from Calphad, 18, 2, 177-222
(1994)
IN1 S.G.T.E. **
IN1 In
INDIUM
Data from SGTE Unary DB
-OK-
Pressure /100000/: 100000
Low temperature limit /298.15/: 298.15
High temperature limit /2000/: 2000
Step in temperature /100/: 100

Output file /tcex12a/: tcex12b
Graphical output? /Y/: Y
Plot column? /2/: 2

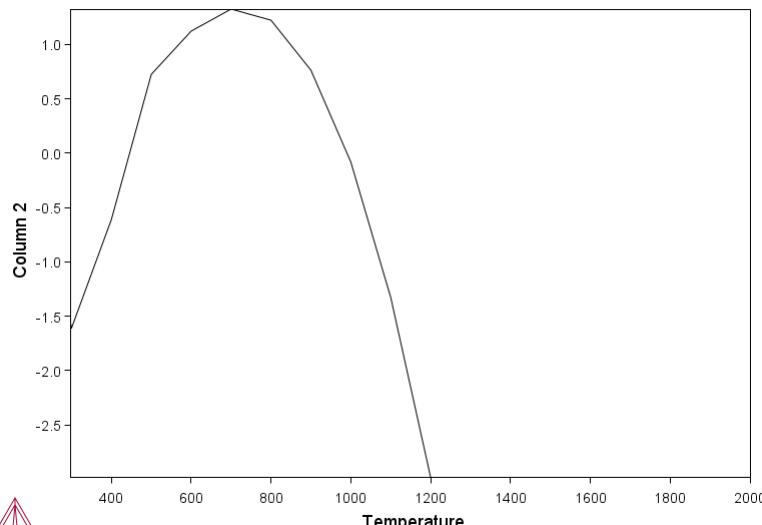
O U T P U T   F R O M   T H E R M O - C A L C
2023. 4.27          15.38.47

Column 6: fef      (G-H298 )/T
Reaction: GA+IN1P1=IN+GA1P1
GA stable as GA_S
IN1P1 stable as IN1P1_S
IN stable as IN_S
GA1P1 stable as GA1P1_S
*****
T     Delta-Cp    Delta-H    Delta-S    Delta-G      fef
(K)   (Joule/K)  (Joule)   (Joule/K)  (Joule)
*****
298.15 -1.56785E+00 -4.01610E+04  4.46600E+00 -4.14925E+04 -4.46600E+00
300.00 -1.60915E+00 -4.01639E+04  4.45617E+00 -4.15008E+04 -4.46597E+00
302. ---- GA becomes GA_L ,delta-H = 5589.80
400.00 -6.09329E-01 -4.59820E+04 -1.46756E+01 -4.01118E+04  1.23002E-01
430. ---- IN becomes IN_L ,delta-H = 3283.00
500.00  7.26020E-01 -4.26605E+04 -6.95385E+00 -3.91835E+04  1.95492E+00
600.00  1.12393E+00 -4.25671E+04 -6.78469E+00 -3.84963E+04  2.77457E+00
700.00  1.32655E+00 -4.24423E+04 -6.59282E+00 -3.78274E+04  3.33376E+00
800.00  1.22407E+00 -4.23120E+04 -6.41862E+00 -3.71771E+04  3.72988E+00
900.00  7.64029E-01 -4.22095E+04 -6.29733E+00 -3.65419E+04  4.02125E+00
1000.00 -8.12013E-01 -4.21720E+04 -6.25712E+00 -3.59149E+04  4.24608E+00
1100.00 -1.32730E+00 -4.22391E+04 -6.32007E+00 -3.52870E+04  4.43091E+00
1200.00 -2.98369E+00 -4.24512E+04 -6.50358E+00 -3.46469E+04  4.59509E+00
Temperature range exceeded for IN1P1

... the command in full is QUICK_EXPERIMENTAL_PLOT
... the command in full is SET_SCALING_STATUS
... the command in full is PLOT_DIAGRAM

```

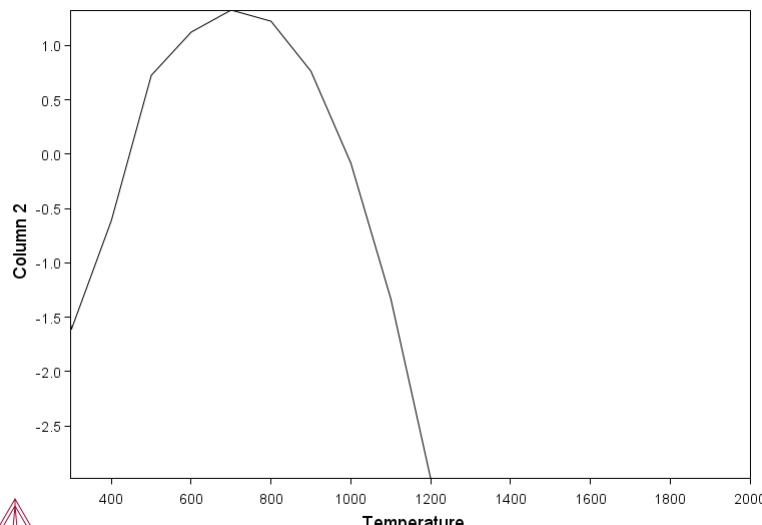
example 12a



```

POST:
POST: set-title example 12b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE EXPERIMENTAL_DATAFILE
*** ERROR 3004 IN LPOSTP: NO AXIS DEFINED
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
example 12b

```



```

POST:
POST: Hit RETURN to continue
POST: back
TAB:
TAB:
TAB: @@ By default a species in a gas is not included in
TAB: @@ a tabulation, you must specify <GAS> if you want that
TAB: t-r n
... the command in full is TABULATEREACTION
Reaction: INP<gas>+GA=GAP+IN;
... the command in full is REJECT
VA DEFINED
REINITIATING GES .....
... the command in full is DEFINE_SPECIES
GA IN1P1 IN
GA1P1 DEFINED
... the command in full is GET_DATA
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS .....

```

List of references for assessed data

```

GA1<G> T.C.R.A.S. Class: 1
GA1<G> Ga<G>
GALLIUM <GAS>
GA1P1<G> S.G.T.E.
GA1P1<G> GaP<G>
GALLIUM PHOSPHIDE <GAS>
ASSESSSED DATA BY C. CHATILLON MARCH 1994. Ga(g) and P2(g)
from T.C.R.A.S.
IN1<G> THERMODATA
IN1<G>
New Assessment (H_form and S only)

```

IN1P1<G> CHATILLON(1994 March)
 IN1P1<G>
 ASSESSED DATA BY C. CHATILLON MARCH 1994. In(g) and P2(g)
 from T.C.R.A.S.
 GA1P1 S.G.T.E.
 GA1P1 Gap GAP
 GALLIUM PHOSPHIDE. Calphad, 18, 2, 177-222 (1994).
 GA1 S.G.T.E. **
 GA1 Ga
 GALLIUM
 Data from SGTE Unary DB , based on 81GLU/GUR (Ivtan Vol. 3)
 20080211 BC Tref 200 -> 298.15
 IN1P1 I. BARIN 3rd. Edition
 IN1P1 INP InP
 INDIUM MONOPHOSPHIDE. Data taken from Calphad, 18, 2, 177-222
 (1994)
 IN1 S.G.T.E. **
 IN1 In
 INDIUM
 Data from SGTE Unary DB
 -OK-

Pressure /100000/: 100000
Low temperature limit /298.15/: 1000
High temperature limit /2000/: 2000
Step in temperature /100/: 100

Output file /tcex12b/:
Graphical output? /Y/: N

O U T P U T F R O M T H E R M O - C A L C
 2023. 4.27 15.39.34

Column 6: fef (G-H298) /T
 Reaction: GA+IN1P1<G>=IN+GA1P1
 GA stable as GA_L
 IN1P1<GAS>
 IN1P1<GAS>
 IN stable as IN_L
 GA1P1 stable as GA1P1_S

| T | Delta-Cp | Delta-H | Delta-S | Delta-G | fef |
|---------|-------------|--------------|--------------|--------------|-------------|
| (K) | (Joule/K) | (Joule) | (Joule/K) | (Joule) | |
| 1000.00 | 1.57503E+01 | -4.65760E+05 | -1.78780E+02 | -2.86980E+05 | 1.86368E+02 |
| 1100.00 | 1.60263E+01 | -4.64172E+05 | -1.77266E+02 | -2.69179E+05 | 1.85608E+02 |
| 1200.00 | 1.63030E+01 | -4.62555E+05 | -1.75860E+02 | -2.51523E+05 | 1.84854E+02 |
| 1300.00 | 1.65828E+01 | -4.60911E+05 | -1.74544E+02 | -2.34004E+05 | 1.84111E+02 |
| 1400.00 | 1.68674E+01 | -4.59238E+05 | -1.73305E+02 | -2.16612E+05 | 1.83383E+02 |
| 1500.00 | 1.71578E+01 | -4.57537E+05 | -1.72131E+02 | -1.99341E+05 | 1.82672E+02 |
| 1600.00 | 1.74548E+01 | -4.55807E+05 | -1.71014E+02 | -1.82184E+05 | 1.81978E+02 |
| 1700.00 | 1.77582E+01 | -4.54046E+05 | -1.69947E+02 | -1.65136E+05 | 1.81301E+02 |

Temperature range exceeded for GA1P1

TAB: Hit RETURN to continue
TAB: @@ =====
TAB: @@ You can list substances in the database
TAB: li-sub
 ... the command in full is LIST_SUBSTANCES
 ... the command in full is REJECT
VA DEFINED
REINITIATING GES
 ... the command in full is DEFINE_SPECIES
AG DEFINED
 ... the command in full is GET_DATA
ELEMENTS
SPECIES
PHASES
PARAMETERS ...
FUNCTIONS

List of references for assessed data

AG1<G> THERMODATA
 AG1<G> Ag<G>
 SILVER <GAS>
 Modified ThermoData new assessment
 AG1 HULTGREN SELECTED VAL. SGTE **
 AG1 Ag
 SILVER
 CODATA KEY VALUE.MPT=1234.93K.
 --U.D. 30/10/85 .
 Cp from 0 to 298.5 : Hultgren 1973, Li 2007

-OK-

With elements /*/: IN P

Exclusively with those elements? /Y/:

| | | |
|-----|----|-------|
| IN | P | IN1P1 |
| IN2 | P2 | P3 |
| P4 | | |

TAB: @@ or all substances with Fe

TAB: li-sub

... the command in full is LIST_SUBSTANCES

With elements /*/: FE

Exclusively with those elements? /Y/: N

| | | |
|-----------|-------------|-------------|
| FE | AL1CL6FE1 | AL2FE1O4 |
| AS1FE1O4 | AS2FE3O8 | B1FE1 |
| B1FE2 | BA1FE1ND1O4 | BA1FE2ND2O7 |
| BR1FE1 | BR2FE1 | BR3FE1 |
| BR4FE2 | BR6FE2 | C1FE1O3 |
| C1FE3 | C5FE1O5 | CA1FE1O6SI2 |
| CA1FE2O4 | CA2FE2O5 | CD1FE2O4 |
| CL1FE1 | CL1FE1O1 | CL2FE1 |
| CL3FE1 | CL4FE2 | CL6FE2 |
| CO1FE2O4 | CR2FE1O4 | CU1FE1O2 |
| CU1FE1S2 | CU1FE2O4 | CU2FE2O4 |
| CU5FE1S4 | F1FE1 | F2FE1 |
| F3FE1 | F4FE2 | F6FE2 |
| FE0.875S1 | FE0.947O1 | FE1.04SE1 |
| FE1/+1 | FE1/-1 | FE1H1 |
| FE1H1O1 | FE1H1O2 | FE1H2O2 |
| FE1H3O3 | FE1H4O6P1 | FE1II1 |
| FE1I2 | FE1I3 | FE1K1O2 |
| FE1K2O2 | FE1K4O3 | FE1LI1O2 |
| FE1L1S04 | FE1M01O4 | FE1NA1O2 |
| FE1O1 | FE1O2 | FE1O3SI1 |

```

FE1O3TI1      FE1O4P1      FE1O4S1
FE1O4V2      FE1O4W1      FE1O6V2
FE1P1       FE1P2       FE1S1
FE1S2       FE1SE0..96   FE1SE1
FE1SE2      FE1SI1      FE1SI2..33
FE1SI2      FE1TE0..9    FE1TE1
FE1TE2       FE1TI1      FE2
FE2H2O4      FE2I4       FE2I6
FE2LI204     FE2MG104    FE2MN104
FE2N1       FE2NB1      FE2NI104
FE2O12S3     FE2O3       FE2O4SI1
FE2O4TI1     FE2O4ZN1    FE2P1
FE2TA1       FE2TI1      FE2U1
FE3LI205     FE3M02      FE3O4
FE3P1        FE3W2       FE4N1
FE5LI108

TAB:
TAB: Hit RETURN to continue
TAB: @@ =====
TAB: @@ You can also tabulate data for a substance or phase. This is equivalent
TAB: @@ to those you can find in NIST-JANAF thermochemical tables for example
TAB: t-sub IN1P1
... the command in full is TABULATE_SUBSTANCE
... the command in full is REJECT
VA DEFINED
REINITIATING GES .....
... the command in full is DEFINE_SPECIES
IN1P1 DEFINED
... the command in full is GET_DATA
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS .....
FUNCTIONS .....

List of references for assessed data
```

```

IN1P1<G> CHATILLON(1994 March)
IN1P1<G>
ASSESSED DATA BY C. CHATILLON MARCH 1994. In(g) and P2(g)
from T.C.R.A.S.
IN1P1 I. BARIN 3rd. Edition
IN1P1 INP InP
INDIUM MONOPHOSPHIDE. Data taken from Calphad, 18, 2, 177-222
(1994)

-OK-
Pressure /100000/: 100000
Low temperature limit /1000/: 300
High temperature limit /2000/: 1300
Step in temperature /100/: 100
Output file /tce12b/: tce12c
Graphical output? /Y/: Y
Plot column? /2/: 2
```

```

O U T P U T   F R O M   T H E R M O - C A L C
2023. 4.27           15.39.34
```

```

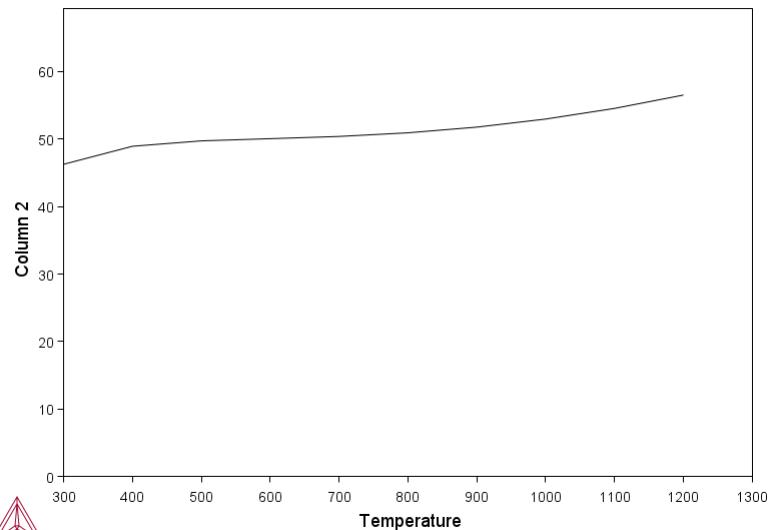
Column 6: fef      (G-H298 )/T

Phase : IN1P1_S          Pressure :      100000.00
Specie: IN1P1

*****
T      Cp            H            S            G            fef
(K)    (Joule/K)      (Joule)      (Joule/K)      (Joule)
*****
300.00  4.62734E+01  -7.44015E+04  6.42060E+01  -9.36633E+04  -6.39209E+01
400.00  4.89412E+01  -6.96137E+04  7.79614E+01  -1.00798E+05  -6.57782E+01
500.00  4.97376E+01  -6.46723E+04  8.89845E+01  -1.09165E+05  -6.93552E+01
600.00  5.00615E+01  -5.96811E+04  9.80837E+01  -1.18531E+05  -7.34072E+01
700.00  5.03923E+01  -5.46595E+04  1.05824E+02  -1.28736E+05  -7.74989E+01
800.00  5.09302E+01  -4.95956E+04  1.12585E+02  -1.39664E+05  -8.14708E+01
900.00  5.117709E+01  -4.44633E+04  1.18629E+02  -1.51229E+05  -8.52694E+01
1000.00 5.29647E+01  -3.92297E+04  1.24142E+02  -1.63372E+05  -8.88848E+01
1100.00 5.45403E+01  -3.38577E+04  1.29261E+02  -1.76045E+05  -9.23252E+01
1200.00 5.65148E+01  -2.83083E+04  1.34088E+02  -1.89214E+05  -9.56061E+01

Temperature range exceeded
... the command in full is QUICK_EXPERIMENTAL_PLOT
... the command in full is PLOT_DIAGRAM
```

example 12b



```

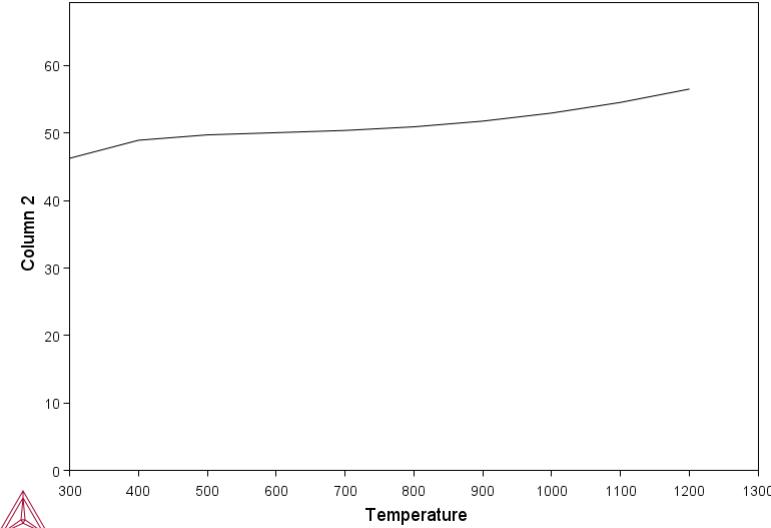
POST:Hit RETURN to continue
POST:
```

```

POST: set-title example 12c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE EXPERIMENTAL_DATAFI
*** ERROR 3004 IN LPOSTP: NO AXIS DEFINED
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 12c



```

POST:
POST: Hit RETURN to continue
POST: back

TAB: @@ =====
TAB: @@ In order to obtain the partial pressure of a species in
TAB: @@ the gas in its pure condensed state you can enter a reaction
TAB: @@ like this for KOH. The partial pressure is entered as a
TAB: @@ function exp(-G/R/T)
TAB: e-fun
... the command in full is ENTER_FUNCTION
Name: pp
Function: exp(-g/r/t);
TAB:
TAB: tab-r n K1O1H1=K1H1O1<g>
... the command in full is TABULATEREACTION
&
... the command in full is REJECT
VA DEFINED
REINITIATING GES ....
... the command in full is DEFINE_SPECIES
H1K1O1 DEFINED
... the command in full is GET_DATA
ELEMENTS ....
SPECIES ....
PHASES ....
PARAMETERS ...
FUNCTIONS ...

List of references for assessed data

H1K1O1<G> J. Phys. Chem. Ref. Data
H1K1O1<G>
Data taken from JPCRD, 26, 4 1031-1110 (1997)
H1K1O1 J. Phys. Chem. Ref. Data
H1K1O1
Data taken from JPCRD, 26, 4 1031-1110 (1997)

-OK-
Pressure /100000/: 100000
Low temperature limit /300/: 300
High temperature limit /1300/: 2000
Step in temperature /100/: 100

Output file /tcex12c/: tcex12d
Graphical output? /Y/: Y
Plot column? /2/: 6

```

```

O U T P U T   F R O M   T H E R M O - C A L C
2023. 4.27           15.40.21

```

```

Column 6: pp      EXP(-G/R/T )
Reaction: H1K1O1=H1K1O1<G>
H1K1O1 stable as H1K1O1_S
H1K1O1<GAS>

*****
T   Delta-Cp   Delta-H   Delta-S   Delta-G   pp
(K)   (Joule/K)   (Joule)   (Joule/K)   (Joule)
*****
300.00 -1.97899E+01  1.92543E+05  1.56915E+02  1.45469E+05  4.70147E-26
400.00 -2.31294E+01  1.90409E+05  1.50797E+02  1.30090E+05  1.02900E-17
500.00 -2.73216E+01  1.87890E+05  1.45195E+02  1.15293E+05  9.03075E-13
517. ---- H1K1O1 becomes H1K1O1_S2 ,delta-H = 5600.00
600.00 -2.71797E+01  1.79542E+05  1.29351E+02  1.01932E+05  1.33747E-09
680. ---- H1K1O1 becomes H1K1O1_L ,delta-H = 7900.00
700.00 -3.36564E+01  1.68804E+05  1.13354E+02  8.94566E+04  2.11269E-07
800.00 -3.31914E+01  1.65462E+05  1.08890E+02  7.83499E+04  7.66317E-06
900.00 -3.27453E+01  1.62165E+05  1.05007E+02  6.76592E+04  1.18375E-04
1000.00 -3.22973E+01  1.58913E+05  1.01580E+02  5.73333E+04  1.01226E-03

```

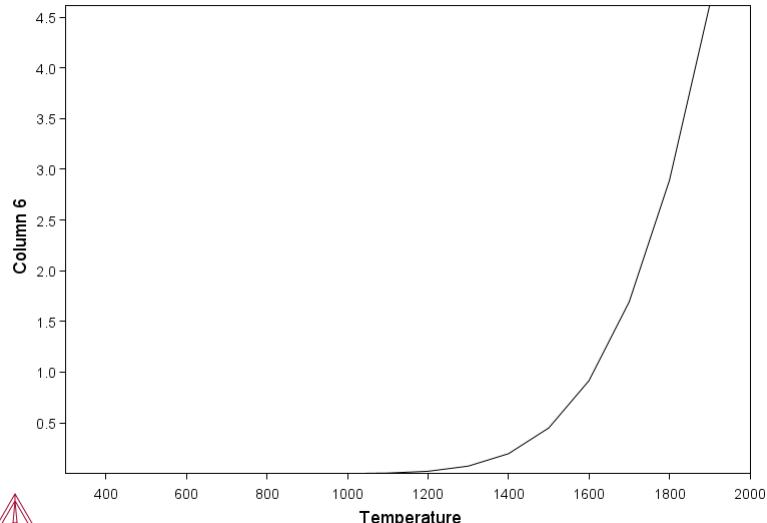
```

1100.00 -3.18358E+01 1.55706E+05 9.85231E+01 4.73310E+04 5.65583E-03
1200.00 -3.13536E+01 1.52547E+05 9.57735E+01 3.76185E+04 2.30437E-02
1300.00 -3.08482E+01 1.49436E+05 9.32837E+01 2.81676E+04 7.38312E-02
1400.00 -3.03294E+01 1.46378E+05 9.10171E+01 1.89543E+04 1.96257E-01
1500.00 -2.98854E+01 1.43368E+05 8.89402E+01 9.95788E+03 4.50033E-01
1600.00 -2.94990E+01 1.40399E+05 8.70240E+01 1.16091E+03 9.16434E-01
1700.00 -2.91580E+01 1.37467E+05 8.52461E+01 -7.45152E+03 1.69415E+00
1800.00 -2.88535E+01 1.34567E+05 8.35882E+01 -1.58923E+04 2.89182E+00
1900.00 -2.85787E+01 1.31695E+05 8.20357E+01 -2.41727E+04 4.61888E+00
Temperature range exceeded for H1K1O1

```

... the command in full is QUICK_EXPERIMENTAL_PLOT
 ... the command in full is SET_SCALING_STATUS
 ... the command in full is PLOT_DIAGRAM

example 12c

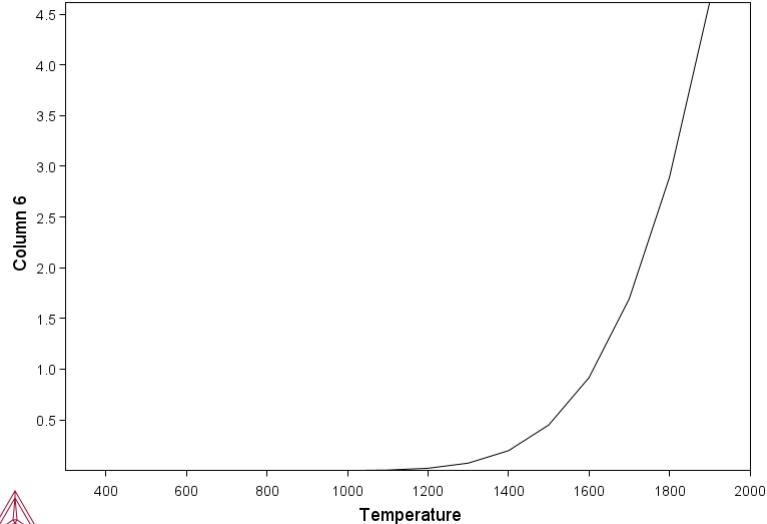


```

POST:
POST: set-title example 12d
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE EXPERIMENTAL_DATAFI
*** ERROR 3004 IN LPOSTP: NO AXIS DEFINED
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 12d

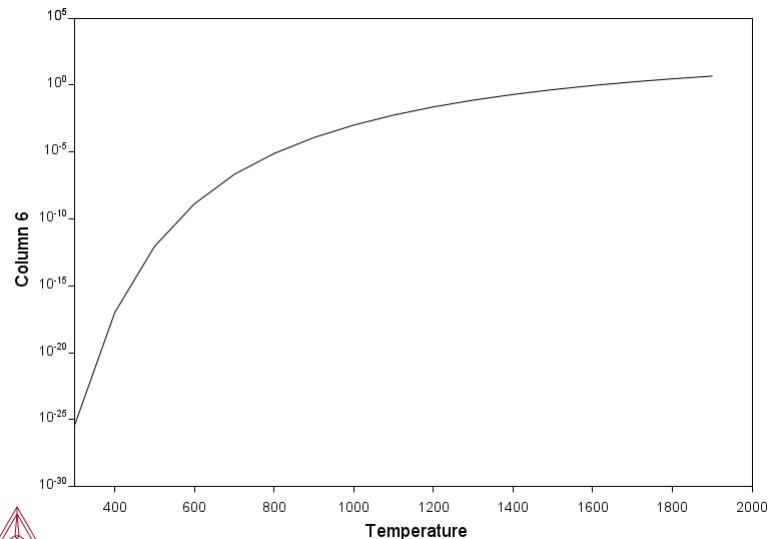


```

POST:
POST: Hit RETURN to continue
POST: s-a-t-y y
... the command in full is SET_AXIS_TYPE
AXIS TYPE /LINEAR/: log
POST: set-title example 12e
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE EXPERIMENTAL_DATAFI
*** ERROR 3004 IN LPOSTP: NO AXIS DEFINED
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 12e



POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:

tce13**SYS:About**

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce13\tce13.TCM"

SYS: set-echo

SYS: @@ Calculating the binary Al-Ti phase diagram and its G curve

SYS: @@ This example calculates an Al-Ti binary phase diagram and

SYS: @@ G curve using the BINARY module.

SYS: set-log ex13,,,

SYS: GO BIN

... the command in full is GOTO_MODULE

 THERMODYNAMIC DATABASE module

 Database folder: C:\jenkins\workspace\generate_console_examples\databases\data
 Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

Simple binary phase diagram calculation module

Database: /TCBIN/: TCBIN

Current database: TC Binary Solutions v1.1

VA /- DEFINED

BCC_B2 FCC_L12 FCC_L102

First element: ?

The following assessed systems

AG-AL AG-AU AG-BI AG-CU AG-GE AG-IN AG-IR AG-MG AG-OS AG-PB AG-PD AG-PT
AG-RH AG-RU AG-SB AG-SI AG-SN AG-TL AG-ZN AG-ZR AL-AS AL-AU AL-B
AL-BI AL-C AL-CA AL-CE AL-CO AL-CR AL-CU AL-FE AL-GA AL-GE AL-IN AL-LI
AL-MG AL-MN AL-MO AL-N AL-NB AL-ND AL-NI AL-O AL-P AL-PB AL-SB AL-SI
AL-SN AL-TA AL-TI AL-V AL-W AL-Y AL-ZN AL-ZR AS-AU AS-CU AS-FE AS-GA
AS-GE AS-IN AS-P AS-SB AU-BI AU-C AU-CR AU-CU AU-GE AU-IN AU-PB AU-PD
AU-RH AU-RU AU-SB AU-SI AU-TL B-C B-CO B-CR B-FE B-HF B-MG
B-MO B-N B-ND B-NI B-SC B-SI B-TI B-V B-W BA-CU BA-EU BA-SR
BA-Y BI-CU BI-GA BI-GE BI-HG BI-IN BI-K BI-MG BI-O BI-PB BI-SB BI-SI
BI-SN BI-TI BI-ZN C-CO C-CR C-CU C-FE C-HF C-MN C-MO C-NB C-NI
C-PB C-SI C-TA C-TI C-V C-W C-Y C-ZR CA-CU CA-MG CA-PB CA-SI
CA-ZN CD-GA CD-GE CD-HG CD-IN CD-PB CD-SB CD-SN CD-TE CD-ZN CE-MG CO-CR
CO-CU CO-DY CO-EF CO-IN CO-MN CO-MO CO-N CO-NB CO-NI CO-PD CO-PT CO-SI
CO-TA CO-TI CO-V CO-W CR-CU CR-FE CR-MG CR-MN CR-NO CR-NB CR-NI
CR-P CR-PD CR-PT CR-SI CR-SN CR-TA CR-TI CR-V CR-W CR-ZN CR-ZR CS-K
CS-NA CS-RB CU-FE CU-GE CU-IN CU-LI CU-MG CU-MN CU-N CU-NB CU-NI CU-O
CU-P CU-PB CU-S CU-SI CU-SN CU-SR CU-TI CU-TL CU-V CU-Y CU-ZN
CU-ZR DY-ER DY-HO ER-TB FE-MG FE-MN FE-MO FE-N FE-NB FE-ND FE-NI
FE-O FE-P FE-PB FE-PD FE-PR FE-PT FE-S FE-SI FE-SN FE-TI FE-V FE-W
FE-ZN FE-ZR GA-GE GA-HG GA-IN GA-P GA-PB GA-SB GA-SN GA-TE GA-ZN GE-IN
GE-PB GE-SE GE-SI GE-SN GE-TE GE-TL GE-ZN H-NB H-ZR HF-TA HF-SI HF-TI
HG-PB HO-TB IN-P IN-PB IN-SB IN-SI IN-SN IN-ZN IR-PD K-RB LA-NI LI-MG
LI-ZR MG-MN MG-NI MG-O MG-SC MG-SI MG-Y MG-ZN MG-ZR MN-MO MN-N MN-O
MN-PB MN-SI MN-TI MN-V MN-Y MN-ZR MO-N MO-NB MO-NI MO-SI MO-TA MO-TI
MO-W N-NB N-NI N-TA N-TI N-V N-W NA-RB NB-NI NB-O NB-TI NB-V
NB-W NB-ZR ND-PR ND-SB NI-P NI-PD NI-SI NI-TA NI-TI NI-V NI-W NI-Y
NI-ZR O-PB O-SN O-SR O-TI O-Y O-ZR P-SB P-SI PB-PD PB-SB PB-SI
PB-SN PB-TL PB-ZN PD-RU PD-SN PR-SB PT-RH PT-RU RE-TA RE-W SB-SI SB-SN
SB-ZN SE-NN SE-TE SE-TL SI-SN SI-TA SI-TE SI-TI SI-U SI-V SI-W SI-Y
SI-ZN SI-ZR SN-TI SN-ZN SN-ZR TA-TI TA-V TA-W TA-ZR TE-ZN TI-V TI-W
TI-ZR U-ZR V-ZR Y-ZR

First element: AL TI

Phase Diagram, Phase fraction (F), G- or A-curves (G/A): /Phase_Diagram/:

... the command in full is REJECT

VA /- DEFINED

BCC_B2 FCC_L12 FCC_L102

D021_HCP REJECTED

REINITIATING GES

... the command in full is DEFINE_ELEMENTS

| | | |
|------------|----------------|---------------|
| AL | TI | DEFINED |
| GAS:G | LQUID:L | IONIC_LQUID:Y |
| FCC_A1 | BCC_A2 | A2_BCC |
| HCP_A3 | HCP_ZN | DIAMOND_A4 |
| BCT_A5 | CBCC_A12 | CUB_A13 |
| B11_CUTI | B32_ALLI | C14_LAVES |
| C15_LAVES | C16_AL2CU | C36_LAVES |
| D019_ALIM3 | D019_SNTI3 | D022_AL3M1 |
| D1A_CU4TI | DS13_AL3N12 | D88_SI3TI5 |
| L10_ALTI | AL11TI5 | AL2TI |
| AL5FB4 | ALCE_AMORPHOUS | MT12 |

REJECTED

LQUID:L RESTORED

AL11TI5 RESTORED

AL2TI RESTORED

D022_AL3M1 RESTORED

D019_ALIM3 RESTORED

L10_ALTI RESTORED

A2_BCC RESTORED

BCC_B2 RESTORED

FCC_A1 RESTORED

HCP_A3 RESTORED

... the command in full is GET_DATA

15:42:47,004 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

ELEMENTS

SPECIES

PHASES

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION

```

... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ....
FUNCTIONS ....

List of references for assessed data

'A T Dinsdale, SGTE Data for Pure Elements, Calphad 15(1991)4 p 317-425; '
'A T Dinsdale, SGTE Data for Pure Elements, update 2001'
'N Saunders, COST 507 (1998) ISBN 92-828-3902-8 p 89-94; Al-Ti'
'N. Dupin, I. Ansara, Z. metallkd., Vol 90 (1999) p 76-85; Al-Ni'
'A V Davydov et al, Metall Mater Trans 32A (2001)9 p 2175-2186; Co-Ti'
-OK-
... the command in full is SET_CONDITION
... the command in full is SET_AXIS_VARIABLE
The condition X(TI)=.1234 created
... the command in full is SET_AXIS_VARIABLE
The condition T=1319.08 created
... the command in full is SET_REFERENCE_STATE
... the command in full is SET_REFERENCE_STATE
... the command in full is SAVE_WORKSPACES

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

... the command in full is SET_CONDITION
... the command in full is SET_ALL_START_VALUES
Forcing automatic start values
Automatic start values will be set
... the command in full is COMPUTE_EQUILIBRIUM
... the command in full is COMPUTE_EQUILIBRIUM
Start points provided by database
... the command in full is SAVE_WORKSPACES
Version S mapping is selected

Organizing start points

Generating start point 1
Generating start point 2

Phase region boundary 1 at: 4.169E-01 1.704E+03
    LIQUID
    ** L10_ALTI
Calculated.          7 equilibria

Phase region boundary 2 at: 3.454E-01 1.652E+03
    LIQUID
    ** AL11T15
    ** L10_ALTI

Phase region boundary 3 at: 3.153E-01 1.652E+03
    LIQUID
    ** AL11T15
Calculated.          3 equilibria

Phase region boundary 4 at: 3.016E-01 1.646E+03
    LIQUID
    ** AL11T15
    ** D022_AL3M1

Phase region boundary 5 at: 2.797E-01 1.646E+03
    LIQUID
    ** D022_AL3M1
Calculated.          36 equilibria

Phase region boundary 6 at: 1.254E-01 9.380E+02
    LIQUID
    ** D022_AL3M1
    ** FCC_A1

Phase region boundary 7 at: 4.025E-03 9.380E+02
    LIQUID
    ** FCC_A1
Calculated.          12 equilibria

Phase region boundary 8 at: 1.287E-01 9.380E+02
    D022_AL3M1
    ** FCC_A1
Calculated..         27 equilibria
Terminating at axis limit.

Phase region boundary 9 at: 2.981E-01 1.646E+03
    AL11T15
    ** D022_AL3M1
Calculated.          17 equilibria

Phase region boundary 10 at: 2.871E-01 1.269E+03
    AL11T15
    ** AL2TT
    ** D022_AL3M1

Phase region boundary 11 at: 3.267E-01 1.269E+03
    AL11T15
    ** AL2TI
Calculated.          9 equilibria

Phase region boundary 12 at: 3.267E-01 1.454E+03
    AL11T15
    ** AL2TI
    ** L10_ALTI

Phase region boundary 13 at: 3.539E-01 1.454E+03
    AL11T15
    ** L10_ALTI
Calculated.          9 equilibria
Terminating at known equilibrium

Phase region boundary 14 at: 3.605E-01 1.454E+03
    AL2TI
    ** L10_ALTI
Calculated..         48 equilibria
Terminating at axis limit.

Phase region boundary 15 at: 2.937E-01 1.269E+03
    ** AL2TI

```

```

D022_AL3M1
Calculated..          40 equilibria
Terminating at axis limit.

Phase region boundary 16 at: 3.454E-01 1.652E+03
    LIQUID
    ** L10_ALTI
Calculated.           9 equilibria

Phase region boundary 17 at: 4.476E-01 1.717E+03
    LIQUID
    ** HCP_A3
    ** L10_ALTI

Phase region boundary 18 at: 4.672E-01 1.717E+03
    LIQUID
    ** HCP_A3
Calculated.           4 equilibria

Phase region boundary 19 at: 5.157E-01 1.776E+03
    LIQUID
    ** BCC_B2
    ** HCP_A3

Phase region boundary 20 at: 5.233E-01 1.776E+03
    LIQUID
    ** BCC_B2
Calculated.           43 equilibria

Phase region boundary 21 at: 5.477E-01 1.776E+03
    ** BCC_B2
    HCP_A3
Calculated.           41 equilibria

Phase region boundary 22 at: 4.784E-01 1.717E+03
    ** HCP_A3
    L10_ALTI
Calculated.           14 equilibria

Phase region boundary 23 at: 5.545E-01 1.399E+03
    ** D019_AL1M3
    ** HCP_A3
    L10_ALTI

Phase region boundary 24 at: 5.596E-01 1.399E+03
    ** D019_AL1M3
    L10_ALTI
Calculated..          45 equilibria
Terminating at axis limit.

Phase region boundary 25 at: 5.977E-01 1.399E+03
    ** D019_AL1M3
    HCP_A3
Calculated..          63 equilibria
Terminating at axis limit.

Phase region boundary 26 at: 4.169E-01 1.704E+03
    LIQUID
    ** L10_ALTI
Calculated.           4 equilibria
Terminating at known equilibrium
*** BUFFER SAVED ON FILE: C:\Users\azureuser\AppData\Local\Temp\BINARY_002.POLY3
CPU time for mapping          4 seconds
POSTPROCESSOR VERSION 3.2

```

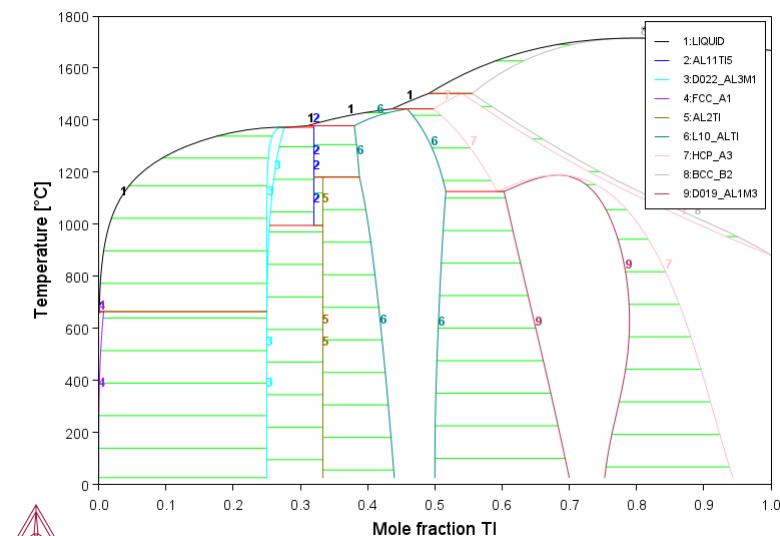
Setting automatic diagram axes

POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

... the command in full is SET_TIELINE_STATUS
... the command in full is SET_LABEL_CURVE_OPTION
... the command in full is PLOT_DIAGRAM

AL TI



POST: @@ Set some phase labels

POST: ADD

... the command in full is ADD_LABEL_TEXT

Give X coordinate in axis units: .7 1400

Automatic phase labels? /Y/:

Automatic labelling not always possible

Using global minimization procedure

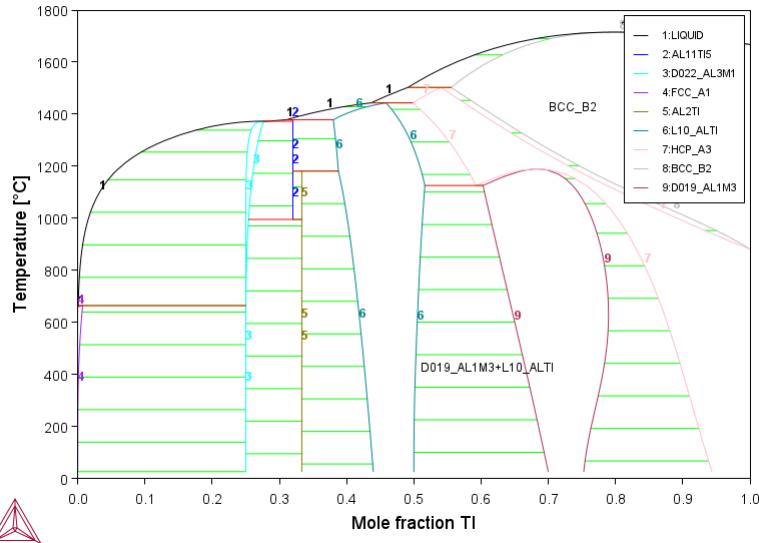
Calculated 6074 grid points in 0 s

```

Found the set of lowest grid points in          0 s
Calculated POLY solution      0 s, total time 0 s
Stable phases are: BCC_B2
Text size: /.36/:
POST: ADD
... the command in full is ADD_LABEL_TEXT
Give X coordinate in axis units: .51 400
Automatic phase labels? /Y/:
Automatic labelling not always possible
Using global minimization procedure
Calculated      6074 grid points in          0 s
Found the set of lowest grid points in          0 s
Calculated POLY solution      0 s, total time 0 s
Stable phases are: D019_AL1M3+L10_ALTI
Text size: /.36/:
POST: set-title example 13a
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 13a

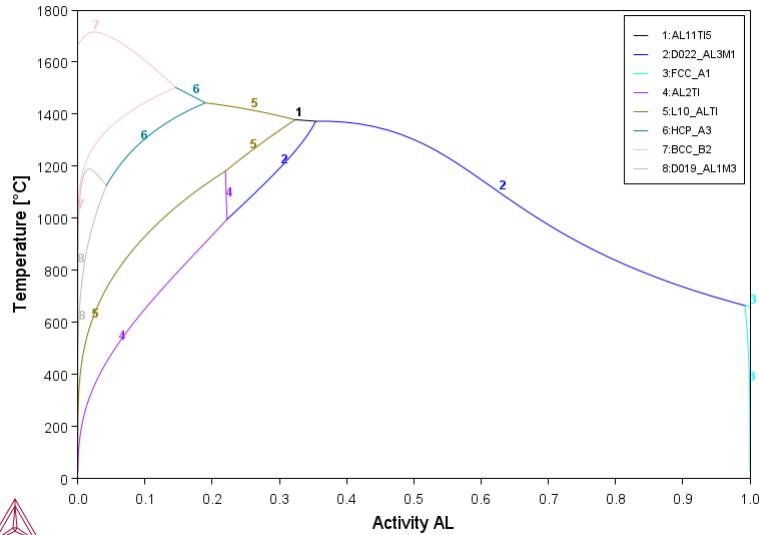


```

POST:
POST:Hit RETURN to continue
POST: @@ Plot the activites, too
POST: S-D-A
... the command in full is SET_DIAGRAM_AXIS
AXIS (X, Y OR Z) : X
VARIABLE : AC
FOR COMPONENT : AL
POST: s-l e
... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 13b
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 13b

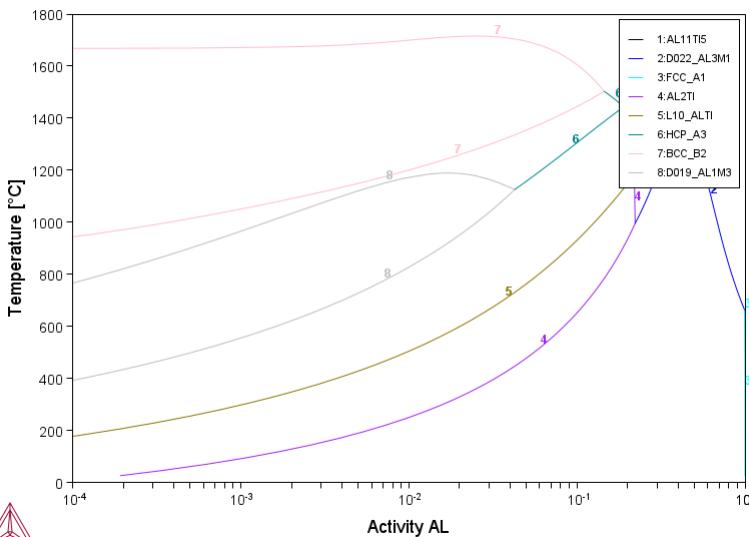


```

POST:
POST:Hit RETURN to continue
POST: S-A-TY X
... the command in full is SET_AXIS_TYPE
AXIS TYPE /LINEAR/: LOG
POST: S-S X N 1E-4 1
... the command in full is SET_SCALING_STATUS
POST: set-title example 13c
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 13c

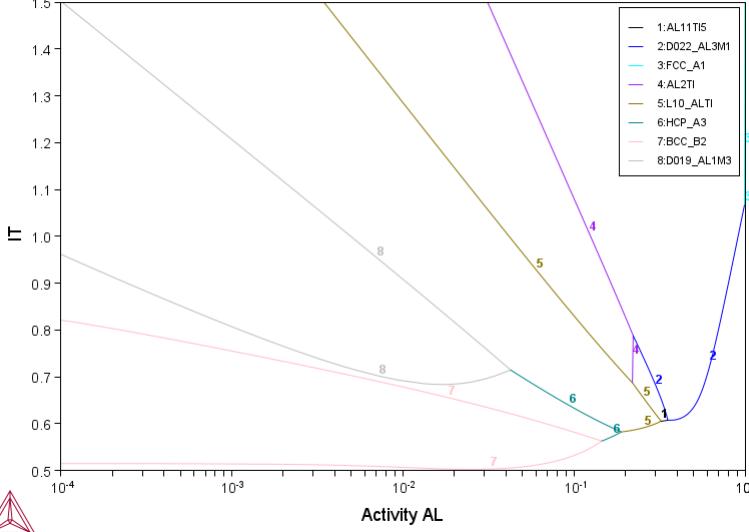


```

POST:
POST:Hit RETURN to continue
POST: @@ Now use inverse of T as y axis
POST: ent fun it=1000/T;
... the command in full is ENTER_SYMBOL
POST: s-d-a y it
... the command in full is SET_DIAGRAM_AXIS
POST: s-s y n .5 1.5
... the command in full is SET_SCALING_STATUS
POST: set-title example 13d
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 13d



```

POST:
POST:Hit RETURN to continue
POST: @@ Now the G curves for the same system
POST: BA
... the command in full is BACK
Current database: Steels/Fe-Alloys v11.0

VA           /- DEFINED
DICTRA_FCC_A1 REJECTED
SYS: GO BIN
... the command in full is GOTO_MODULE
Current database: Steels/Fe-Alloys v11.0

VA           /- DEFINED
DICTRA_FCC_A1 REJECTED

Simple binary phase diagram calculation module

Database: /TCBIN/: TCBIN
Current database: TC Binary Solutions v1.1

VA           /- DEFINED
BCC_B2      FCC_L12          FCC_L102
D021_HCP   REJECTED
First element: AL TI
Phase Diagram, Phase fraction (F), G- or A-curves (G/A): /Phase_Diagram/: G
Temperature (C): /1000/: 1000
... the command in full is REJECT
VA           /- DEFINED
BCC_B2      FCC_L12          FCC_L102
D021_HCP   REJECTED
REINITIATING GES .....
... the command in full is DEFINE_ELEMENTS
AL           TI  DEFINED
GAS:G        LIQUID:L        IONIC_LIQUID:Y

```

```

FCC_A1          BCC_A2          A2_BCC
HCP_A3          HCP_ZN          DIAMOND_A4
BCT_A5          CBCC_A12        CUB_A13
B11_CUTI        B32_ALLI        C14_LAVES
C15_LAVES       C16_AL2CU        C36_LAVES
D019_AL1M3      D019_SNTI3      D022_AL3M1
D1A_CU4TI       DS13_AL3NI2      D88_SI3TI5
L10_ALTI        AL11TI5        AL2TI
AL5FE4          ALCE_AMORPHOUS MT12

REJECTED
LIQUID:L RESTORED
AL11TI5 RESTORED
AL2TI RESTORED
D022_AL3M1 RESTORED
D019_AL1M3 RESTORED
L10_ALTI RESTORED
A2_BCC RESTORED
BCC_B2 RESTORED
FCC_A1 RESTORED
HCP_A3 RESTORED
... the command in full is GET_DATA
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS .....
FUNCTIONS .....

List of references for assessed data

'A T Dinsdale, SGTE Data for Pure Elements, Calphad 15(1991)4 p 317-425; '
'A T Dinsdale, SGTE Data for Pure Elements, update 2001'
'N Saunders, COST 507 (1998) ISBN 92-828-3902-8 p 89-94; Al-Ti'
'N. Dupin, I. Ansara, Z. metallkd., Vol 90 (1999) p 76-85; Al-Ni'
'A V Davydov et al, Metall Mater Trans 32A (2001)9 p 2175-2186; Co-Ti'
-OK-
... the command in full is SET_CONDITION
... the command in full is SET_AXIS_VARIABLE
The condition X(TI)=.1234 created
... the command in full is SET_CONDITION
... the command in full is COMPUTE_EQUILIBRIUM
... the command in full is SET_REFERENCE_STATE
... the command in full is SET_REFERENCE_STATE
... the command in full is SAVE_WORKSPACES
... the command in full is SET_ALL_START_VALUES
Forcing automatic start values
Automatic start values will be set
... the command in full is COMPUTE_EQUILIBRIUM
... the command in full is COMPUTE_EQUILIBRIUM
... the command in full is SAVE_WORKSPACES
... the command in full is STEP_WITH_OPTIONS

Phase Region from 0.502463 for:
 LIQUID
 BCC_B2
 D019_AL1M3
 FCC_A1
 HCP_A3
 L10_ALTI

Phase Region from 0.502463 for:
 LIQUID
 BCC_B2
 D019_AL1M3
 FCC_A1
 HCP_A3
 L10_ALTI

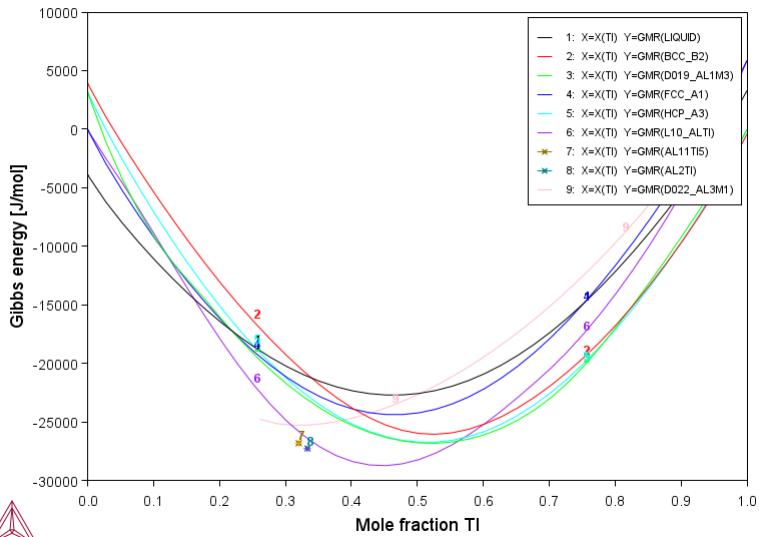
Phase Region from 0.320000 for:
 AL11TI5

Phase Region from 0.333333 for:
 AL2TI

Phase Region from 0.636878 for:
 D022_AL3M1
*** Buffer saved on file *** C:\Users\azureuser\AppData\Local\Temp\GCURVE_002.POLY3
POSTPROCESSOR VERSION 3.2
... the command in full is SET_TIELINE_STATUS
... the command in full is SET_LABEL_CURVE_OPTION
... the command in full is PLOT_DIAGRAM

```

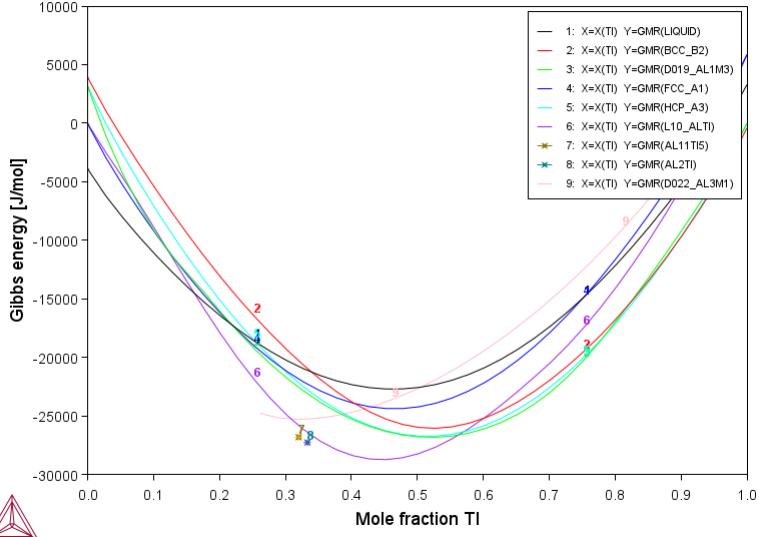
AL TI



```

POST: set-label F
POST: ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 13e
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
example 13e

```



```

POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:

```

tce14

SYS:About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

```
SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce14\tce14.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Variations in solidification of an Al-Mg-Si alloy
SYS:
SYS: @@ This example calculates the heat and heat capacity
SYS: @@ variations during solidification of an Al-Mg-Si alloy.
SYS:
SYS: set-log ex14,....
SYS: go da
... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module
Database folder: C:\jenkins\workspace\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA           /* DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE11: sw ALDEMO
... the command in full is SWITCH_DATABASE
Current database: Aluminum Demo Database v4.1

VA           /* DEFINED
TDB_ALDEMO: d-sys al cu si
... the command in full is DEFINE_SYSTEM
AL          CU          SI
DEFINED
TDB_ALDEMO: l-s c
... the command in full is LIST_SYSTEM
LIQUID:L   :AL CU SI:
AL2CU_C16  :AL:AL CU SI:
ALCU_DEL   :AL:CU:
ALCU_EPS   :AL CU:CU:
ALCU_ETA   :AL CU:CU:
ALCU_ZETA  :AL:CU:
ALZR2_B82  :AL VA:VA:
BCC_A2     :AL CU SI VA:VA:
BCC_B2     :AL CU SI VA:AL CU SI VA:VA:
C14_LAVES  :AL CU:AL CU:
C15_LAVES  :AL CU SI:AL CU SI:
C36_LAVES  :AL CU:AL CU:
CU15SI4_EPSILON :CU:AL SI:
CU33SI7_DELTA :CU:SI:
CU56SI11_GAMMA :CU SI:SI:
CUSI_ETA    :CU:SI:
DIAMOND_A4  :AL SI:
FCC_A1      :AL CU SI:VA:
GAMMA_D83  :AL SI:AL CU SI:CU:
GAMMA_H    :AL:AL CU:CU:
HCP_A3     :AL CU SI:VA:
TDB_ALDEMO: get
... the command in full is GET_DATA
15:44:15,100 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES ....
ELEMENTS ....
SPECIES ....
PHASES ....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ...

List of references for assessed data

'A. Dinsdale, Calphad,15 317-425 (1991)'
'Volume data from TCFE4, 2006'
'H-L Chen, in TCAL7.0, Evaluation and modeling of electrical resistivity
thermal conductivity'
'M J Assael, High Temp High Press 41 (2012); Sb, Pb, Bi, Ni, Ag'
'M Ghasemi, Thermo-Calc Software AB (2020)'
'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
Molar volumes'
'M J Assael, J Phys Chem Ref Data 39 (2010) 033105; Cu, Sn'
'M J Assael, J Phys Chem Ref Data 41 (2012) 033101; Cd, Co, Ga, In, Hg, Si,
Ti, Zn'
'I. Ansara (Editor), COST 507, (1998)'
'M Ghasemi, Thermo-Calc Software AB (2019)'
'C.-Y. He, Calphad, 33,200-210 (2009),Al-Cu-Si,
J. Groebner,Calphad,20(2)247-254(1996),Al-C-Si'
'X.Y. Yan,J. Alloy and Compd. 308, 221-229 (2000),Cu-Si'
'L. Kjellqvist, Thermo-Calc Software AB, Stockholm, 2010; Unassessed
parameter, linear combination of unary volume data'
'H-L Chen, in TCAL3.0, Assessment, extrapolation and assumption'
'Hai-Lin Chen, electrical resistivity
thermal conductivity (2020)'
'L. Kjellqvist, Thermo-Calc Software AB, Sweden 2012; Molar volumes'
'H-L Chen, Evaluation of molar volume'
'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
'N. Dupin, Calphad, 25(2)279-298(2001),Al-Cr-Ni'
'Natalie Dupin, in TCNI6.0, Refinement of Al-Ni'
'Volume data, N. Dupin 2008'
'H-L Chen, in TCAL2.0, Assessment, extrapolation and assumption'
'J.R.Zhao, Y.Du, to be submitted, 2010,Sn-Sr,Cu-Mg-Si'
'W.H. Sun, unpublished (2010),Cu-Si-Zn,Cu-Ni-Zn'
'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
'H-L Chen, in TCAL1.2, assessment of Al-Cu-Mg-Si'
-OK-
```

```

TDB_ALDEMO: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY: @@ The composition

POLY: s-c w(si)=.09,w(cu)=.10,t=1000,p=1e5,n=1
... the command in full is SET_CONDITION
POLY: l-c
... the command in full is LIST CONDITIONS
W(SI)=9E-2, W(CU)=0.1, T=1000, P=100000, N=1
DEGREES OF FREEDOM 0
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 17676 grid points in 4 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 4 s
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /WVCS/: WVCS
Output from POLY-3, equilibrium = 1, label A0 , database: ALDEMO

Conditions:
W(SI)=9E-2, W(CU)=0.1, T=1000, P=100000, N=1
DEGREES OF FREEDOM 0

Temperature 1000.00 K ( 726.85 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 2.87371E+01
Total Gibbs energy -4.64558E+04, Enthalpy 3.21074E+04, Volume 1.11601E-05

Component Moles W-Fraction Activity Potential Ref.stat
AL 8.6269E-01 8.1000E-01 5.0275E-03 -4.4007E+04 SER
CU 4.5223E-02 1.0000E-01 3.2656E-06 -1.0503E+05 SER
SI 9.2090E-02 9.0000E-02 7.5475E-03 -4.0629E+04 SER

LIQUID Status ENTERED Driving force 0.0000E+00
Moles 1.0000E+00, Mass 2.8737B+01, Volume fraction 1.0000E+00 Mass fractions:
AL 8.1000E-01 CU 1.0000E-01 SI 9.0000E-02
POLY:Hit RETURN to continue
POLY: @@ Set temperature as axis
POLY: s-a-v
... the command in full is SET_AXIS_VARIABLE
Axis number: /1/: 1
Condition /NONE/: t
Min value /0/: 500
Max value /1/: 1000
Increment /12.5/: 12.5
POLY: save tcex14 y
... the command in full is SAVE_WORKSPACES
POLY: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 1000.00
...OK

Phase Region from 1000.00 for:
LIQUID
Global test at 9.20000E+02 .... OK
Global check of adding phase at 8.41997E+02
Calculated 18 equilibria

Phase Region from 841.997 for:
LIQUID
FCC_A1
Global check of adding phase at 8.28102E+02
Calculated 5 equilibria

Phase Region from 828.102 for:
LIQUID
DIAMOND_A4
FCC_A1
Global check of adding phase at 7.94799E+02
Calculated 6 equilibria

Phase Region from 794.799 for:
LIQUID
AL2CU_C16
DIAMOND_A4
FCC_A1
Calculated 2 equilibria

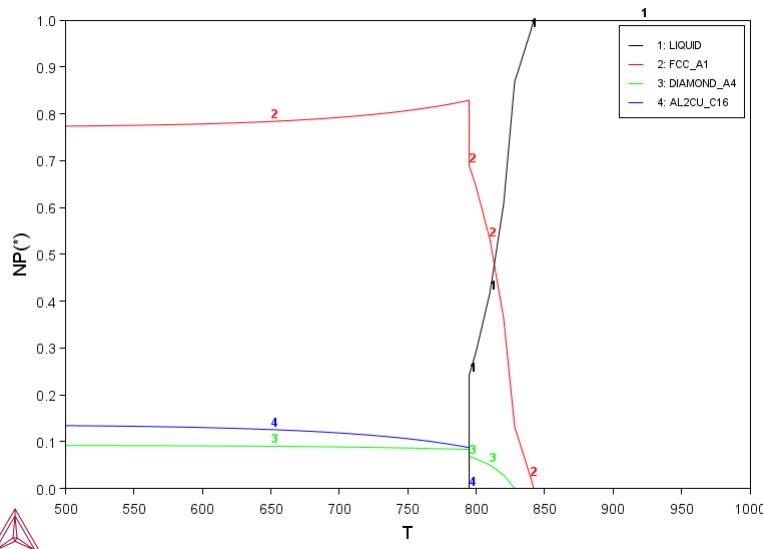
Phase Region from 794.799 for:
AL2CU_C16
DIAMOND_A4
FCC_A1
Global test at 7.20000E+02 .... OK
Global test at 6.20000E+02 .... OK
Global test at 5.20000E+02 .... OK
Terminating at 500.000
Calculated 33 equilibria
*** Buffer saved on file: c:\jenkins\workspace\generate_console_examples\examples\tcex14\tcex14.POLY3
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

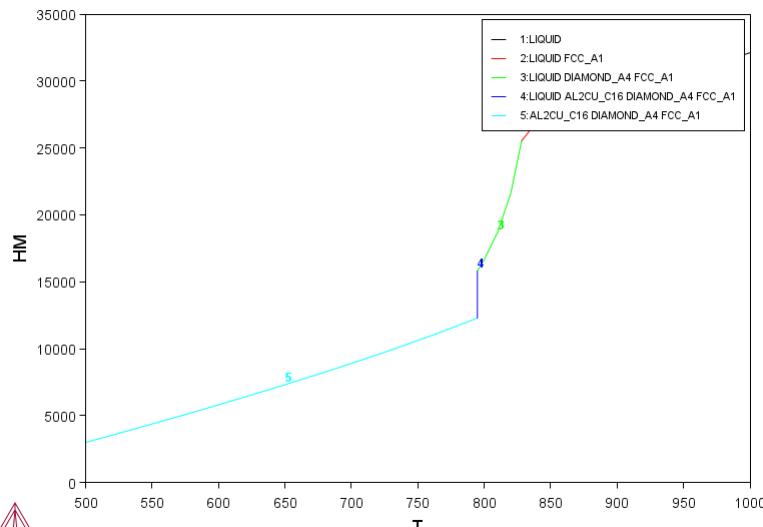
POST: @@ Plot phase fractions
POST: S-D-A X T
... the command in full is SET_DIAGRAM_AXIS
POST: S-D-A Y NP(*)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*:
POST: S-LAB D
... the command in full is SET_LABEL_CURVE_OPTION
POST:
POST: set-title example 14a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:

```

POST: plot
... the command in full is PLOT_DIAGRAM
example 14a

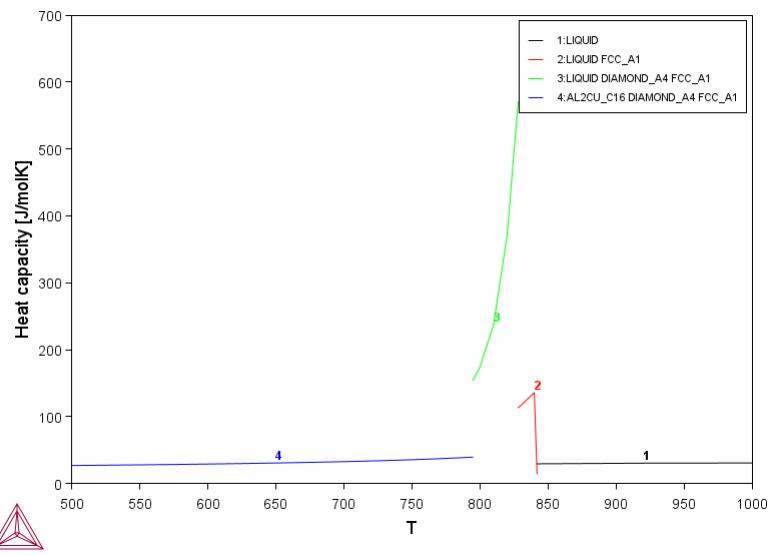


POST:
POST: Hit RETURN to continue
POST: @@ Plot the total enthalpy (heat)
POST: S-D-A Y HM
... the command in full is SET_DIAGRAM_AXIS
POST: S-LAB B
... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 14b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
example 14b



POST:
POST: Hit RETURN to continue
POST: @@ Plot the heat capacity. First this must be entered because
POST: @@ a function as derivatives cannot be plotted directly.
POST:
POST: ENT FUN CP=HM.T;
... the command in full is ENTER_SYMBOL
POST: S-D-A Y CP
... the command in full is SET_DIAGRAM_AXIS
POST: S-S
... the command in full is SET_SCALING_STATUS
AXIS (X, Y OR Z) : Y
AUTOMATIC SCALING (Y OR N) /N/ : N
MIN VALUE : 0
MAX VALUE : 700
POST: S-A-T-S
... the command in full is SET_AXIS_TEXT_STATUS
AXIS (X, Y OR Z) : Y
AUTOMATIC AXIS TEXT (Y OR N) /N/ : N
AXIS TEXT : Heat capacity [J/molK]
POST: set-title example 14c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:

POST: plot
... the command in full is PLOT_DIAGRAM
example 14c



POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:

tce15

SYS:About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce15\tce15.TCM.test"

SYS: SET_ECHO

SYS:

SYS: @@ Simulating the solidification of a Cr-Ni alloy with

SYS: @@ the Scheil module

SYS:

SYS: @@ This is an example of a solidification simulation

SYS: @@ of a Cr-Ni alloy. There is no back diffusion in the

SYS: @@ solid, i.e. Scheil-Gulliver model is used.

SYS:

SYS: GO SCHEIL

SCHEIL: TEMPERATURE-STEP

Temperature step (C) /1/: 5

SCHEIL: START-WIZARD

THERMODYNAMIC DATABASE module

Database folder: C:\jenkins\workspace\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC A1 REJECTED

Database /TCFE11/: FEDEMO

Current database: Iron Demo Database v4.0

VA /- DEFINED

Major element or alloy: cr

Composition input in mass (weight) percent? /Y/: n

Composition will be taken to be in mole percent

1st alloying element: ni

Mole percent /1/: 10

2nd alloying element:

Temperature (C) /2000/: 2000

VA /- DEFINED

REINITIATING GES

CR DEFINED

NI DEFINED

This database has following phases for the defined system

| | | |
|----------|---------|-----------------|
| LIQUID:L | BCC_A2 | LAVES_PHASE_C14 |
| CBCC_A12 | CHI_A12 | CUB_A13 |
| FCC_A1 | HCP_A3 | SIGMA |

Reject phase(s) /NONE/: *

| | | |
|----------|---------|-----------------|
| LIQUID:L | BCC_A2 | LAVES_PHASE_C14 |
| CBCC_A12 | CHI_A12 | CUB_A13 |
| FCC_A1 | HCP_A3 | SIGMA |

REJECTED

Restore phase(s):: liq bcc fcc

| | | |
|----------|--------|--------|
| LIQUID:L | BCC_A2 | FCC_A1 |
|----------|--------|--------|

RESTORED

Restore phase(s): /NONE/: NONE

The following phases are retained in this system:

| | | |
|----------|--------|--------|
| LIQUID:L | BCC_A2 | FCC_A1 |
|----------|--------|--------|

OK? /Y/: y

15:45:37,121 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

FUNCTIONS

List of references for assessed data

'A.T. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
'M. Ghasemi, Thermo-Calc Software AB, Sweden, 2020; Unifying liquid volume
database'
'M. Ghasemi, Thermo-Calc Software AB, Sweden, 2019; Viscosity of metallic
liquid'
'M Ghasemi, Thermo-Calc Software AB: assessing the surface tension of
metallic liquid'
'Y. Tang, in TCCU2, Thermo-Calc Software AB, Stockholm, Sweden'
'M. J. Assael, High Temp. High Press., 41 (2012); Sb, Pb, Bi, Ni, Ag'
'B.J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
'X.G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
volumes'
'X.G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
'A.T. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); CR -NI'
-OK-

Should any phase have a miscibility gap check? /N/:

LIQUID PHASE NAME: LIQUID

Fast diffusing components: /NONE/:

This command is a combination of CHANGE_STATUS and SET_CONDITION
to calculate directly when a phase may form by releasing one condition.
You must release one of these conditions
T=2273.15, X(NI)=0.1, P=100000, N=1 DEGREES OF FREEDOM 0
PHASE CHANGE AT 2058.59459939

BCC_A2#1 forms

Testing POLY result by global minimization procedure

Calculated 627 grid points in 0 s

CALCULATING USING NORMAL EQUILIBRIUM CONDITIONS

...OK

```
Phase Region from 2058.68 for:  
LIQUID  
Terminating at 2058.78  
Calculated 4 equilibria  
  
Phase Region from 2058.68 for:  
LIQUID  
Global check of adding phase at 2.05859E+03  
Calculated 3 equilibria  
  
Phase Region from 2058.59 for:  
LIQUID  
BCC_A2  
Global test at 2.01868E+03 .... OK  
Global test at 1.96868E+03 .... OK  
Global test at 1.91868E+03 .... OK  
Global check of removing phase at 1.89734E+03  
Calculated 35 equilibria  
  
Phase Region from 1897.34 for:  
BCC_A2  
Calculated 4 equilibria  
*** Buffer saved on file: C:\Users\azureuser\AppData\Local\Temp\SCHEIL_4012.POLY3  
POSTPROCESSOR VERSION 3.2
```

Setting automatic diagram axes

POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

An EXP file C:\Users\AZUREU~1\AppData\Local\Temp\SCHEIL_EQ_4012.EXP
has been created to store the equilibrium solidification results.

CALCULATING SCHEIL SOLIDIFICATION

| T(C) | fraction solid |
|----------|----------------|
| 1785.535 | 0.000000 |
| 1785.375 | 0.92399712E-03 |
| 1780.375 | 0.6494391E-01 |
| 1775.375 | 0.1226644 |
| 1770.375 | 0.1749130 |
| 1765.375 | 0.2223831 |
| 1760.375 | 0.2656597 |
| 1755.375 | 0.3052393 |
| 1750.375 | 0.3415456 |
| 1745.375 | 0.3749422 |
| 1740.375 | 0.4057426 |
| 1735.375 | 0.4342186 |
| 1730.375 | 0.4606065 |
| 1725.375 | 0.4851127 |
| 1720.375 | 0.5079185 |
| 1715.375 | 0.5291833 |
| 1710.375 | 0.5490480 |
| 1705.375 | 0.5676374 |
| 1700.375 | 0.5850626 |
| 1695.375 | 0.6014224 |
| 1690.375 | 0.6168054 |
| 1685.375 | 0.6312910 |
| 1680.375 | 0.6449504 |
| 1675.375 | 0.6578480 |
| 1670.375 | 0.6700418 |
| 1665.375 | 0.6815843 |
| 1660.375 | 0.6925233 |
| 1655.375 | 0.7029020 |
| 1650.375 | 0.7127599 |
| 1645.375 | 0.7221332 |
| 1640.375 | 0.7310546 |
| 1635.375 | 0.7395545 |
| 1630.375 | 0.7476604 |
| 1625.375 | 0.7553979 |
| 1620.375 | 0.7627903 |
| 1615.375 | 0.7698592 |
| 1610.375 | 0.7766247 |
| 1605.375 | 0.7831051 |
| 1600.375 | 0.7893176 |
| 1595.375 | 0.7952779 |
| 1590.375 | 0.8010009 |
| 1585.375 | 0.8065002 |
| 1580.375 | 0.8117885 |
| 1575.375 | 0.8168779 |
| 1570.375 | 0.8217793 |
| 1565.375 | 0.8265033 |
| 1560.375 | 0.8310595 |
| 1555.375 | 0.8354570 |
| 1550.375 | 0.8397046 |
| 1545.375 | 0.8438103 |
| 1540.375 | 0.8477816 |
| 1535.375 | 0.8516258 |
| 1530.375 | 0.8553497 |
| 1525.375 | 0.8589602 |
| 1520.375 | 0.8624627 |
| 1515.375 | 0.8658633 |
| 1510.375 | 0.8691676 |
| 1505.375 | 0.8723809 |
| 1500.375 | 0.8755083 |
| 1495.375 | 0.8785546 |
| 1490.375 | 0.8815245 |
| 1485.375 | 0.8844227 |
| 1480.375 | 0.8872536 |
| 1475.375 | 0.8900213 |
| 1470.375 | 0.8927303 |
| 1465.375 | 0.8953845 |
| 1460.375 | 0.8979881 |
| 1455.375 | 0.9005451 |
| 1450.375 | 0.9030587 |
| 1445.375 | 0.9055346 |
| 1440.375 | 0.9079761 |
| 1435.375 | 0.9103873 |
| 1430.375 | 0.9127724 |
| 1425.375 | 0.9151359 |
| 1420.375 | 0.9174820 |
| 1415.375 | 0.9198153 |
| 1410.375 | 0.9221406 |

```

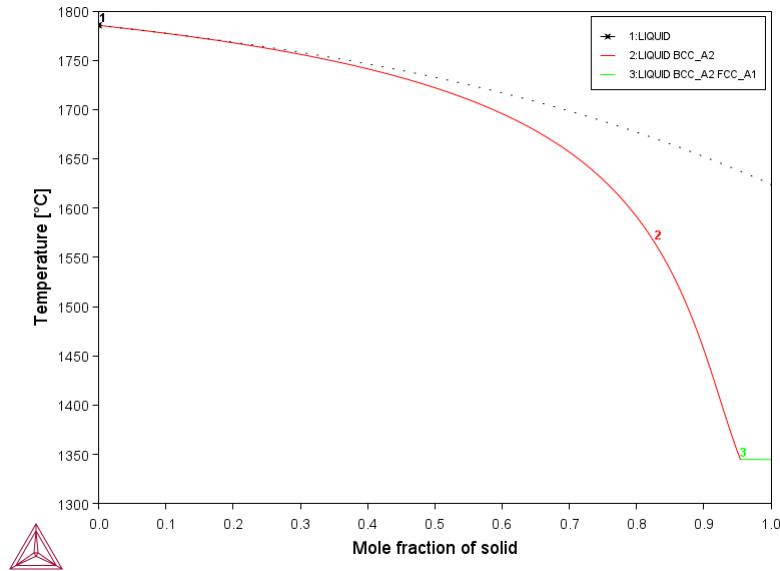
1405.375 0.9244628
1400.375 0.9267870
1395.375 0.9291184
1390.375 0.9314626
1385.375 0.9338254
1380.375 0.9362126
1375.375 0.9386303
1370.375 0.9410850
1365.375 0.9435828
1360.375 0.9461303
1355.375 0.9487336
1350.375 0.9513987
1345.375 0.9541312
1344.897 0.9543838

```

PHASE REGION:BCC_A2 + FCC_A1
T(C) fraction solid

1344.738 1.000000

Calculating properties ...
Liquidus temperature: 2058.595 K
Solidus temperature: 1617.888 K



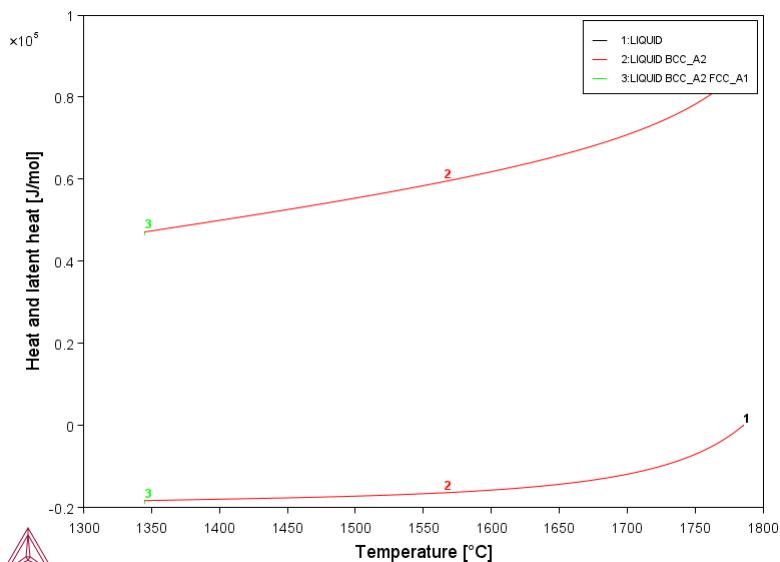
The following axis variables are available

T - Temperature in Celsius
NL/BL/VL - Mole/mass/volume fraction of liquid
NS/BS/VS - Mole/mass/volume fraction of all solid phases
NS(ph)/BS(ph) - Mole/mass fraction of a solid phase
VS(ph) - Volume fraction of a solid phase
W(ph,el) - Weight fraction of an element in a phase
X(ph,el) - Mole fraction of an element in a phase
Y(ph,el) - Site fraction of an element in a phase
NN(ph,el) - Distribution of an element in a phase
NH/BH - Heat release and Latent heat per mole/gram
CP/BCP - Apparent heat capacity per mole/gram
NV/NV(ph) - Molar volume of the system or a phase
DS/DS(ph) - Average density of the system or a phase
BT - Apparent volumetric TEC of the system
DVIS(ph) - Dynamic viscosity of a phase
KVIS(ph) - Kinematic viscosity of a phase
SURF(ph) - Surface tension of a liquid phase
ELRS/ELRS(ph) - Electrical resistivity of the system or a phase
ELCD/ELCD(ph) - Electrical conductivity of the system or a phase
THCD/THCD(ph) - Thermal conductivity of the system or a phase
THRS/THRS(ph) - Thermal resistivity of the system or a phase
THDF/THDF(ph) - Thermal diffusivity of the system or a phase
DGV - Driving force for evaporation
DHV - Evaporation enthalpy
MMG - Molar mass of gas
XAVG(el) - Mole fraction of an element in solid phases
WAVG(el) - Mass fraction of an element in solid phases

"el" and "ph" are name of element and phase, respectively
"**" can be used as a wild character for "el" and "ph"

```

POST:Hit RETURN to continue
POST: s-d-a x t
POST: s-d-a y nh
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot,,,,,,,,,,
```



POST: set-inter
POST:

tce16

SYS:About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

```
SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce16\tce16.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Second order transition of the Al-Fe system
SYS:
SYS: @@ This example calculates the second order transition
SYS: @@ line in the Bcc field of the Al-Fe system.
SYS:
SYS: @@ Note that an SSOL database license is required to run
SYS: @@ the example.
SYS:
SYS: SET-LOG ex16.,
SYS: GO DA
... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module
Database folder: C:\jenkins\workspace\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA           /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE11: SW SSOL7
... the command in full is SWITCH_DATABASE
Current database: SGTE Alloy Solutions v7.0

VA   DEFINED
BCC_B2          FCC_L12          FCC_4SL
HCP_ORD         GAS:G          REJECTED
A2_BCC          B2_BCC          REJECTED
TDE_SSOL7: D-SYS AL FE
... the command in full is DEFINE_SYSTEM
AL             FE  DEFINED
TDB_SSOL7: REJ PH /ALL
... the command in full is REJECT
LIQUID:L        FCC_A1          BCC_A2
B2             HCP_A3          HCP_ZN
DHCP            DIAMOND_A4      BCT_A5
TETRAGONAL_U   CUBC_A12        CUB_A13
ORTORHOMBIC_A20 RHOMBO_C19      LAVES_C14
C14_LAVES      LAVES_C15        LAVES_C36
M4N             ALM_D019        ALCE_AMORPHOUS
ALCR2_C11B    ALCU_THETA      AL2FE
AL5FE2          AL5FE4          AL13FE4
ALLI            AL4MN           AL6MN
AL11MN4         AL12MN          ALNB3
AL3NB           AL3NI2          AL3PD2_D513
ALPD_B2         AL2PD5          ALPD2_C37
ALPT3           ALTI            CRSSI_A15
D_GAMMA          FEPD            FEPD3
FESB            FEU6             FEU2
FE23Y6          FE2Y            FEUZR_DELTA
FEZR2           FEZR3          REJECTED
TDB_SSOL7: @@ The BCC phase has B2 ordering in this system.
TDE_SSOL7: @@ Note that this is modelled with two sublattices with
TDB_SSOL7: @@ both components in both sublattices
TDB_SSOL7:
TDE_SSOL7: REST PH LIQ BCC_B2 BCC_A2
... the command in full is RESTORE
LIQUID:L        BCC_B2          BCC_A2
RESTORED
TDE_SSOL7: LI-SYS
... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/:
LIQUID:L :AL FE:
BCC_A2 :AL FE:VA:
BCC_B2 :AL FE:AL FE:VA:
TDE_SSOL7: GET
... the command in full is GET_DATA
15:47:21,816 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
Creating a new composition set BCC_B2#2
PARAMETERS .....
FUNCTIONS .....

List of references for assessed data

'Unpublished assessment of M Seiersten published in the COST507 final
report; COST507 Thermochemical database for light metal alloys, Volume
2 eds I Ansara, A T Dinsdale and M H Rand, July 1998, EUR18499 >> Al
-Fe '
-OK-
TDB_SSOL7: GO P-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY: li-st p
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES
PHASE           STATUS      DRIVING FORCE    MOLES
BCC_B2#2       ENTERED    0.000000E+00  0.000000E+00
BCC_B2#1       ENTERED    0.000000E+00  0.000000E+00
```

LIQUID ENTERED 0.000000E+00 0.000000E+00

POLY:

POLY: advanced global_minimization y 10000
... the command in full is ADVANCED_OPTIONS
Settings for global minimization:

POLY:

POLY: @@ Set conditions where the BCC phase should be ordered

POLY: SET-COND P=1E5,N=1,T=400,X(AL)=.4
... the command in full is SET_CONDITION

POLY: COMP-EQ
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure

Calculated 10026 grid points in 4 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 4 s

POLY: @@ Use option N in order to see how Al and Fe distribute

POLY: @@ on the sublattices

POLY:

POLY: LIST-EQ
... the command in full is LIST_EQUILIBRIUM

OUTPUT TO SCREEN OR FILE /SCREEN/:

Options /VWCS/: N
Output from POLY-3, equilibrium = 1, label A0 , database: SSOL7

Conditions:
P=100000, N=1, T=400, X(AL)=0.4
DEGREES OF FREEDOM 0

Temperature 400.00 K (126.85 C), Pressure 1.000000E+05
Number of moles of components 1.000000E+00, Mass in grams 4.43010E+01
Total Gibbs energy -3.81486E+04, Enthalpy -2.55850E+04, Volume 0.000000E+00

| Component | Moles | W-Fraction | Activity | Potential | Ref.stat |
|-----------|------------|------------|------------|-------------|----------|
| AL | 4.0000E-01 | 2.4362E-01 | 4.1973E-08 | -5.6493E+04 | SER |
| FE | 6.0000E-01 | 7.5638E-01 | 4.1248E-04 | -2.5919E+04 | SER |

BCC_B2#2 ORD Status ENTERED Driving force 0.0000E+00
Moles 1.0000E+00, Mass 4.4301E+01, Volume fraction 0.0000E+00 Mass fractions:
FE 7.56376E-01 AL 2.43624E-01

Constitution:
Sublattice 1, Number of sites 5.0000E-01
AL 7.99996E-01 FE 2.00004E-01
Sublattice 2, Number of sites 5.0000E-01
FE 9.99996E-01 AL 4.22881E-06
Sublattice 3, Number of sites 3.0000E+00
VA 1.00000E+00

POLY: Hit RETURN to continue

POLY: @@ Change the condition of the Al amount so that the site-fractions in the two sublattices will have a certain difference. If they are the same, the BCC phase is disordered. BCC_B2#2 is the default

POLY: @@ ordered phase.

POLY:

POLY: SET-COND X(AL)=NONE
... the command in full is SET_CONDITION

POLY: SET-COND Y(BCC_B2#2,FE#1)-Y(BCC_B2#2,FE#2)=-0.1
... the command in full is SET_CONDITION

POLY: C-S P BCC_B2#1=SUS
... the command in full is CHANGE_STATUS

POLY: COMP-EQ
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
26 ITS, CPU TIME USED 0 SECONDS

POLY: LIST-EQ
... the command in full is LIST_EQUILIBRIUM

OUTPUT TO SCREEN OR FILE /SCREEN/:

Options /VWN/: Hit RETURN to continue

Options /VWN/: @@ Set a smaller difference. This is as close to the

Output from POLY-3, equilibrium = 1, label A0 , database: SSOL7

Conditions:
P=100000, N=1, T=400, Y(BCC_B2#2,FE)-Y(BCC_B2#2,FE#2)=-0.1
DEGREES OF FREEDOM 0

Temperature 400.00 K (126.85 C), Pressure 1.000000E+05
Number of moles of components 1.000000E+00, Mass in grams 5.36842E+01
Total Gibbs energy -1.86969E+04, Enthalpy -4.69474E+03, Volume 0.000000E+00

| Component | Moles | W-Fraction | Activity | Potential | Ref.stat |
|-----------|------------|------------|------------|-------------|----------|
| AL | 7.4926E-02 | 3.7658E-02 | 7.3790E-14 | -1.0056E+05 | SER |
| FE | 9.2507E-01 | 9.6234E-01 | 2.6569E-02 | -1.2066E+04 | SER |

BCC_B2#2 ORD Status ENTERED Driving force 0.0000E+00
Moles 1.0000E+00, Mass 5.3684E+01, Volume fraction 0.0000E+00 Mass fractions:
FE 9.62342E-01 AL 3.76585E-02

Constitution:
Sublattice 1, Number of sites 5.0000E-01
FE 8.75074E-01 AL 1.24926E-01
Sublattice 2, Number of sites 5.0000E-01
FE 9.75074E-01 AL 2.49265E-02
Sublattice 3, Number of sites 3.0000E+00
VA 1.00000E+00

POLY: @@ second order transition as it is possible to be

POLY:

POLY: SET-COND Y(BCC_B2#2,FE#1)-Y(BCC_B2#2,FE#2)=1E-4
... the command in full is SET_CONDITION

POLY: COMP-EQ
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Using already calculated grid
14 ITS, CPU TIME USED 0 SECONDS

POLY: @@ Now vary the temperature using these conditions

POLY: SET-AXIS-VAR 1
... the command in full is SET_AXIS_VARIABLE

Condition /NONE/: T
Min value /0/: 400
Max value /1/: 2000
Increment /40/: 10

POLY: @@ Always save before STEP or MAP (unless you want to

POLY: @@ overlay the new results on some previous results)

POLY:

```

POLY: SAVE tcex16 Y
... the command in full is SAVE_WORKSPACES
POLY: STEP NORMAL
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 400.000
...OK

Phase Region from 400.000 for:
BCC_B2#2
Global test at 4.80000E+02 .... OK
Global test at 5.80000E+02 .... OK
Global test at 6.80000E+02 .... OK
Global test at 7.80000E+02 .... OK
Global test at 8.80000E+02 .... OK
Global test at 9.80000E+02 .... OK
Global test at 1.08000E+03 .... OK
Global test at 1.18000E+03 .... OK
Global test at 1.28000E+03 .... OK
Global test at 1.38000E+03 .... OK
Global test at 1.48000E+03 .... OK
Global test at 1.58000E+03 .... OK
Global check of adding phase at 1.64515E+03
Calculated 127 equilibria

Phase Region from 1645.15 for:
LIQUID
BCC_B2#2
Global check of removing phase at 1.64515E+03
Calculated 3 equilibria

Phase Region from 1645.15 for:
BCC_B2#2
Global check of adding phase at 1.64515E+03
Calculated 3 equilibria

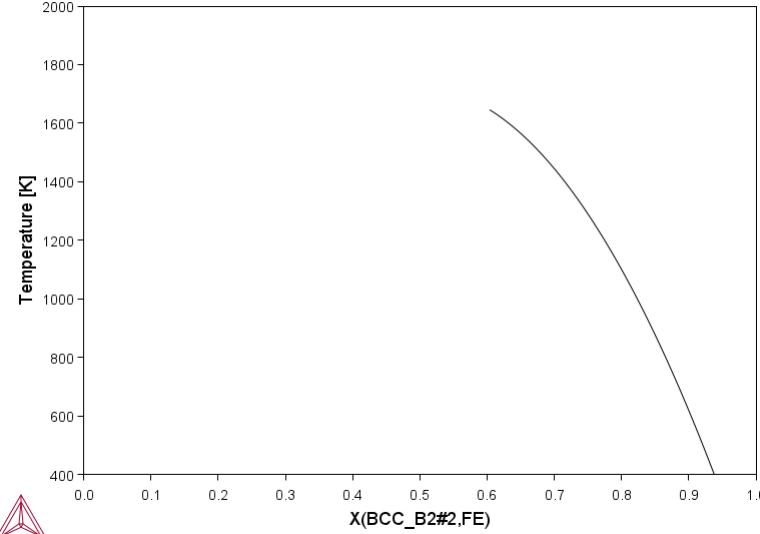
Phase Region from 1645.15 for:
LIQUID
BCC_B2#2
Calculated 3 equilibria
Sorry cannot continue 0 189 1 1.6451539E+03
*** Buffer saved on file: c:\jenkins\workspace\generate_console_examples\examples\tcex16\tcex16.POLY3
POLY: POST
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: SET-DIA-AXIS X X(BCC_B2#2,FE)
... the command in full is SET_DIAGRAM_AXIS
POST: SET-DIA-AXIS Y T-K
... the command in full is SET_DIAGRAM_AXIS
POST: SET-SCAL X N 0 1
... the command in full is SET_SCALING_STATUS
POST: SET-SCAL Y N 400 2000
... the command in full is SET_SCALING_STATUS
POST:
POST: set-title example 16a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: PLOT
... the command in full is PLOT_DIAGRAM

```

example 16a



POST:
POST: Hit RETURN to continue
POST: @@ Write on file to plot with a phase diagram
POST: MAKE_TCEX16
 ... the command in full is MAKE_EXPERIMENTAL_DATAFI
 POST:
POST: BACK
POLY: GO DA
 ... the command in full is GOTO_MODULE
TDB_SSOL7: @@ Get data for all phases stable in Al-Fe
TDB_SSOL7: REJ-SYS
 ... the command in full is REJECT
 VA_DEFINED
 BCC_B2 FCC_L12 FCC_4SL
 HCP_ORD GAS:G REJECTED
 A2_BCC B2_BCC REJECTED

REINITIATING GES

TDB_SSOL7: D-SYS AL FE
... the command in full is DEFINE_SYSTEM
AL FE DEFINED

TDB_SSOL7: L-SYS
... the command in full is LIST_SYSTEM

ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENTS:/ CONSTITUENT

| | |
|-----------------|---------------|
| LIQUID:L | :AL FE: |
| FCC_A1 | :AL FE:VA: |
| BCC_A2 | :AL FE:VA: |
| B2 | :AL:VA: |
| HCP_A3 | :AL FE:VA: |
| HCP_ZN | :AL FE:VA: |
| DHCP | :AL:VA: |
| DIAMOND_A4 | :AL: |
| BCT_A5 | :AL: |
| TETRAGONAL_U | :FE: |
| CBCC_A12 | :AL FE:VA: |
| CUB_A13 | :AL FE:VA: |
| ORTORHOMBIC_A20 | :FE: |
| RHOMBO_C19 | :AL: |
| LAVES_C14 | :AL FE:AL FE: |
| C14_LAVES | :FE:FE: |
| LAVES_C15 | :AL FE:AL FE: |
| LAVES_C36 | :AL:AL: |
| M4N | :FE:VA: |
| ALM_D019 | :AL:AL: |
| ALCE_AMORPHOUS | :AL: |
| ALCR2_C11B | :AL:AL: |
| ALCU_THETA | :AL:AL: |
| AL2FE | :AL:FE: |
| AL5FE2 | :AL:FE: |
| AL5FE4 | :AL FE: |
| AL13FE4 | :AL:FE:AL VA: |
| ALLI | :AL:VA: |
| AL4MN | :AL:FE: |
| AL6MN | :AL:FE: |
| AL11MN4 | :AL:FE: |
| AL12MN | :AL:FE: |
| ALNB3 | :AL:AL: |
| AL3NB | :AL:AL: |
| AL3NI2 | :AL:AL:VA: |
| AL3PD2_D513 | :AL:AL: |
| ALPD_B2 | :AL:VA: |
| AL2PD5 | :AL:AL: |
| ALPD2_C37 | :AL:AL: |
| ALPT3 | :AL:AL: |
| ALTI | :AL:AL: |
| CR3SI_A15 | :FE:AL:VA: |
| D_GAMMA | :AL: |
| FEPD | :FE:FE: |
| FEPD3 | :FE:FE: |
| FESB | :FE:FE: |
| FEU6 | :FE:FE: |
| FE2U | :FE:FE: |
| FE23Y6 | :FE:FE: |
| FE2Y | :FE:FE: |
| FEUZR_DELTA | :FE:FE: |
| FEZR2 | :FE:FE: |
| FEZR3 | :FE:FE: |

TDB_SSOL7: REJ PH /ALL
... the command in full is REJECT

| | | |
|-----------------|------------|----------------|
| LIQUID:L | FCC_A1 | BCC_A2 |
| B2 | HCP_A3 | HCP_ZN |
| DHCP | DIAMOND_A4 | BCT_A5 |
| TETRAGONAL_U | CBCC_A12 | CUB_A13 |
| ORTORHOMBIC_A20 | RHOMBO_C19 | LAVES_C14 |
| C14_LAVES | LAVES_C15 | LAVES_C36 |
| M4N | ALM_D019 | ALCE_AMORPHOUS |
| ALCR2_C11B | ALCU_THETA | AL2FE |
| AL5FE2 | AL5FE4 | AL13FE4 |
| ALLI | AL4MN | AL6MN |
| AL11MN4 | AL12MN | ALNB3 |
| AL3NB | AL3NI2 | AL3PD2_D513 |
| ALPD_B2 | AL2PD5 | ALPD2_C37 |
| ALPT3 | ALTI | CR3SI_A15 |
| D_GAMMA | FEPD | FEPD3 |
| FESB | FEU6 | FE2U |
| FE23Y6 | FE2Y | FEUZR_DELTA |
| FEZR2 | FEZR3 | REJECTED |

TDB_SSOL7: REST PH LIQ BCC_B2 FCC_A1 BCC_A2 AL13FE4 AL2FE AL5FE2 AL5FE4
... the command in full is RESTORE

| | | |
|----------|---------|----------|
| LIQUID:L | BCC_B2 | FCC_A1 |
| BCC_A2 | AL13FE4 | AL2FE |
| AL5FE2 | AL5FE4 | RESTORED |

TDB_SSOL7: GET
... the command in full is GET_DATA

REINITIATING GES

ELEMENTS

SPECIES

PHASES

... the command in full is AMEND_PHASE_DESCRIPTION

Creating a new composition set BCC_B2#2

PARAMETERS ...

FUNCTIONS ...

List of references for assessed data

'Unpublished assessment of M Seiersten published in the COST507 final report; COST507 Thermochemical database for light metal alloys, Volume 2 eds I Ansara, A T Dinsdale and M H Rand, July 1998, EUR18499 >> Al -Fe '

-OK-

TDB_SSOL7: GO P-3
... the command in full is GOTO_MODULE

POLY version 3.32

POLY: @@ Calculate an equilibrium where BCC is ordered

POLY: S-C T=1300,P=1E5,N=1,X(AL)=.3
... the command in full is SET_CONDITION

POLY: C-E

```

... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated          10655 grid points in           1 s
Found the set of lowest grid points in           0 s
Calculated POLY solution      0 s, total time   1 s
POLY: @@ List the equilibrium. Note that option N gives the
POLY: @@ constitution of the BCC phase and this shows that the
POLY: @@ site-fractions are different in the two sublattices,
POLY: @@ i.e. the BCC is ordered
POLY:
POLY: L-E
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWNS/: N
Output from POLY-3, equilibrium =      1, label A0 , database: SSOL7

Conditions:
T=1300, P=100000, N=1, X(AL)=0.3
DEGREES OF FREEDOM 0

Temperature 1300.00 K ( 1026.85 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 4.71875E+01
Total Gibbs energy -8.63003E+04, Enthalpy 1.26381E+04, Volume 0.00000E+00

Component       Moles      W-Fraction Activity Potential Ref.stat
AL            3.0000E-01  1.7154E-01 3.1606E-05 -1.1200E+05 SER
FE            7.0000E-01  8.2846E-01 9.4427E-04 -7.5285E+04 SER

BCC_B2#2          ORD     Status ENTERED Driving force 0.0000E+00
Moles 1.0000E+00, Mass 4.71875E+01, Volume fraction 0.0000E+00 Mass fractions:
FE 8.28459E-01 AL 1.71541E-01
Constitution:
Sublattice 1, Number of sites 5.0000E-01
FE 5.22550E-01 AL 4.77450E-01
Sublattice 2, Number of sites 5.0000E-01
FE 8.77450E-01 AL 1.22550E-01
Sublattice 3, Number of sites 3.0000E+00
VA 1.00000E+00
POLY:Hit RETURN to continue
POLY: @@ Set axis
POLY: S-A-V 1 X(AL)
... the command in full is SET_AXIS_VARIABLE
Min value /0/: 0
Max value /1/: 1
Increment /.025/: .025
POLY: S-A-V 2 T
... the command in full is SET_AXIS_VARIABLE
Min value /0/: 400
Max value /1/: 2000
Increment /40/: 25
POLY: SAVE tceex16 Y
... the command in full is SAVE_WORKSPACES

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

POLY: MAP
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Trying global minimization! 3
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Trying global minimization! 3
Generating start point 27
Generating start point 28

Phase region boundary 1 at: 5.828E-01 4.100E+02
** AL2FE
BCC_B2#2
Calculated..           2 equilibria
Terminating at axis limit.

```

```

Phase region boundary  2 at:  5.829E-01  4.000E+02
  ** AL2FE
  BCC_B2#2
Calculated.          40 equilibria

Phase region boundary  3 at:  6.023E-01  1.368E+03
  ** AL2FE
  ** AL5FE4
  BCC_B2#2
Calculated.          7 equilibria

Phase region boundary  4 at:  5.672E-01  1.368E+03
  ** AL5FE4
  BCC_B2#2
Calculated.          7 equilibria

Phase region boundary  5 at:  5.452E-01  1.496E+03
  ** LIQUID
  ** AL5FE4
  BCC_B2#2
Calculated.          50 equilibria

Phase region boundary  6 at:  5.550E-01  1.496E+03
  ** LIQUID
  BCC_B2#2
Calculated.          50 equilibria

Phase region boundary  7 at:  5.842E-01  1.496E+03
  ** LIQUID
  AL5FE4
Calculated.          6 equilibria

Phase region boundary  8 at:  6.593E-01  1.430E+03
  ** LIQUID
  ** AL5FE2
  AL5FE4
Calculated.          2 equilibria

Phase region boundary  9 at:  6.744E-01  1.430E+03
  ** AL5FE2
  AL5FE4
Calculated.          2 equilibria

Phase region boundary 10 at:  6.740E-01  1.428E+03
  ** AL2FE
  ** AL5FE2
  AL5FE4
Calculated.          4 equilibria
Terminating at known equilibrium

Phase region boundary 12 at:  6.905E-01  1.428E+03
  ** AL2FE
  AL5FE2
Calculated..         43 equilibria
Terminating at axis limit.

Phase region boundary 13 at:  6.993E-01  1.430E+03
  LIQUID
  ** AL5FE2
Calculated.          12 equilibria

Phase region boundary 14 at:  7.362E-01  1.424E+03
  LIQUID
  ** AL13FE4
  ** AL5FE2
Calculated.          24 equilibria

Phase region boundary 15 at:  7.556E-01  1.424E+03
  LIQUID
  ** AL13FE4
Calculated.          24 equilibria

Phase region boundary 16 at:  8.723E-01  9.271E+02
  LIQUID
  ** AL13FE4
  ** FCC_A1
Calculated.          10 equilibria

Phase region boundary 17 at:  9.955E-01  9.271E+02
  LIQUID
  ** FCC_A1
Calculated..         23 equilibria
Terminating at axis limit.

Phase region boundary 19 at:  7.337E-01  1.424E+03
  ** AL13FE4
  AL5FE2
Calculated..         42 equilibria
Terminating at axis limit.

Phase region boundary 20 at:  5.828E-01  4.100E+02
  ** AL2FE
  BCC_B2#2
Calculated.          40 equilibria
Terminating at known equilibrium

Phase region boundary 21 at:  8.364E-03  1.237E+03
  BCC_B2#1
  ** FCC_A1
Calculated.          19 equilibria

Phase region boundary 22 at:  8.364E-03  1.237E+03
  BCC_B2#1
  ** FCC_A1
Calculated.          28 equilibria

Phase region boundary 23 at:  3.562E-01  1.702E+03
  ** LIQUID
  BCC_B2#1
Calculated.          35 equilibria

Phase region boundary 24 at:  3.562E-01  1.702E+03

```

```

** LIQUID
BCC_B2#1
Calculated.          17 equilibria
Terminating at known equilibrium

Phase region boundary 25 at: 5.828E-01 4.100E+02
** AL2FE
BCC_B2#2
Calculated..          2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 26 at: 5.828E-01 4.100E+02
** AL2FE
BCC_B2#2
Calculated.          40 equilibria
Terminating at known equilibrium

Phase region boundary 27 at: 8.825E-01 4.100E+02
** AL13FE4
FCC_A1
Calculated..          2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 28 at: 8.825E-01 4.100E+02
** AL13FE4
FCC_A1
Calculated..          22 equilibria
Terminating at known equilibrium

Phase region boundary 29 at: 8.825E-01 4.100E+02
** AL13FE4
FCC_A1
Calculated..          2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 30 at: 8.825E-01 4.100E+02
** AL13FE4
FCC_A1
Calculated..          22 equilibria
Terminating at known equilibrium

Phase region boundary 31 at: 5.820E-01 9.367E+02
** AL2FE
BCC_B2#2
Calculated..          23 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 32 at: 5.820E-01 9.367E+02
** AL2FE
BCC_B2#2
Calculated..          19 equilibria
Terminating at known equilibrium

Phase region boundary 33 at: 8.765E-01 9.367E+02
LIQUID
** AL13FE4
Calculated..          2 equilibria
Terminating at known equilibrium

Phase region boundary 34 at: 8.765E-01 9.367E+02
LIQUID
** AL13FE4
Calculated..          27 equilibria
Terminating at known equilibrium

Phase region boundary 35 at: 1.862E-02 1.463E+03
** BCC_B2#1
FCC_A1
Calculated..          28 equilibria

Phase region boundary 36 at: 1.862E-02 1.463E+03
** BCC_B2#1
FCC_A1
Calculated..          12 equilibria

Phase region boundary 37 at: 6.298E-01 1.463E+03
LIQUID
** AL5FE4
Calculated..          3 equilibria
Terminating at known equilibrium

Phase region boundary 38 at: 6.298E-01 1.463E+03
LIQUID
** AL5FE4
Calculated..          7 equilibria
Calculated..          7 equilibria

Phase region boundary 39 at: 6.298E-01 1.463E+03
LIQUID
** AL5FE4
Calculated..          6 equilibria
Terminating at known equilibrium

Phase region boundary 40 at: 1.032E-02 1.813E+03
LIQUID
** BCC_B2#1
Calculated..          13 equilibria

Phase region boundary 41 at: 1.032E-02 1.813E+03
LIQUID
** BCC_B2#1
Calculated..          44 equilibria
Calculated..          44 equilibria

Phase region boundary 42 at: 1.032E-02 1.813E+03
LIQUID
** BCC_B2#1
Calculated..          47 equilibria
Terminating at known equilibrium

Phase region boundary 43 at: 3.201E-01 1.728E+03
LIQUID

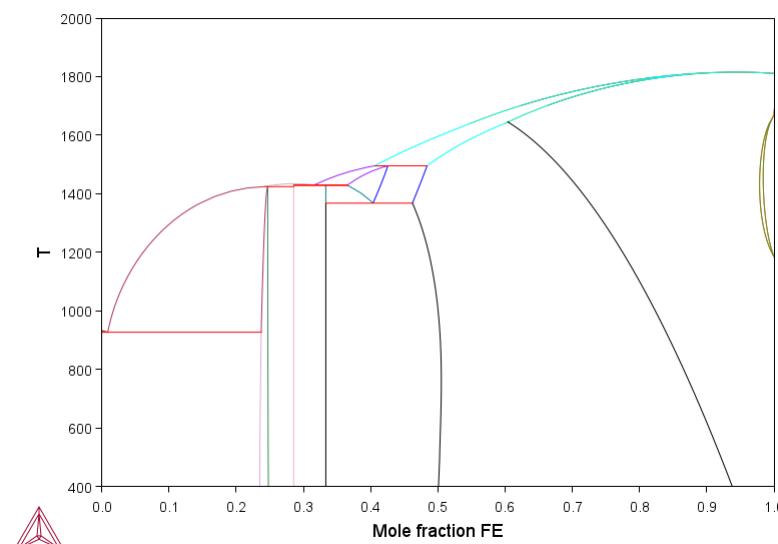
```

```

** BCC_B2#1
Calculated                         34 equilibria
Phase region boundary 44 at:   3.201E-01  1.728E+03
    LIQUID
** BCC_B2#1
Calculated.                      20 equilibria
Calculated.                      20 equilibria
Phase region boundary 45 at:   3.201E-01  1.728E+03
    LIQUID
** BCC_B2#1
Calculated.                      19 equilibria
Phase region boundary 46 at:   6.421E-01  1.451E+03
    LIQUID
** AL5FE4
Calculated.                      7 equilibria
Calculated.                      7 equilibria
Phase region boundary 47 at:   6.421E-01  1.451E+03
    LIQUID
** AL5FE4
Calculated.                      6 equilibria
Terminating at known equilibrium
Phase region boundary 48 at:   6.421E-01  1.451E+03
    LIQUID
** AL5FE4
Calculated.                      3 equilibria
Terminating at known equilibrium
Phase region boundary 49 at:   8.763E-01  9.396E+02
    LIQUID
** AL13FE4
Calculated.                      28 equilibria
Terminating at known equilibrium
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\generate_console_examples\examples\tcex16\tcex16.POLY3
CPU time for mapping               9 seconds
POLY:
POLY: POST
POLY-3 POSTPROCESSOR VERSION 3.2
Setting automatic diagram axes
POST:
POST: S-D-A X M-F FE
... the command in full is SET_DIAGRAM_AXIS
POST: S-D-A Y T
... the command in full is SET_DIAGRAM_AXIS
POST: @@ Append the previous line for the 2nd order transition
POST: A-E-D Y TCEx16
... the command in full is APPEND_EXPERIMENTAL_DATA
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 1
POST: set-title example 16b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 16b



```

POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:

```

tce17

SYS:About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

```
SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce17\tce17.TCM.test"
SYS: set-echo
SYS:
SYS: @@ The pseudo-binary system - CaO-SiO2
SYS:
SYS: @@ This example calculates the pseudo-binary system
SYS: @@ CaO-SiO2 using the Oxide Demo database.
SYS:
SYS: set-log ex17,,
SYS: go da
... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module
Database folder: C:\jenkins\workspace\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA           /* DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE11: @@ This database can be used both for pseudobinary
TDE_TCFE11: @@ systems like the one in this case, CaO-SiO2, or
TDE_TCFE11: @@ for full ternary systems like Ca-Fe-O.
TDB_TCFE11:
TDE_TCFE11: sw OXDEMO
... the command in full is SWITCH_DATABASE
Current database: Oxide Demo Database v4.0

VA           /* DEFINED
TDB_OXDEMO: @@ Note that /* represents the electron.
TDB_OXDEMO: d-sys ca si o
... the command in full is DEFINE_SYSTEM
CA           SI           O
DEFINED
TDB_OXDEMO: l-sys
... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/: CONSTITUENTS
BCC_A2      :CA SI:O VA:
#Body-Centered Cubic (W, A2, bcc) #ci2 #Im-3m # #602e7f15105f8553a825b4e4
CA2SiO4_ALPHA_A:I :CA+2:CA+2:SiO4-4:
#Ca2SiO4 #P24 #P6 3/mmc #This is 2CaO.SiO2 and 3CaO.P2O5.
#602eac57674ba8b79b43f865
CA2SiO4_ALPHA_PRIME:I :CA+2:CA+2:SiO4-4:
#K2CoCl4 #P84 #Pna2_1 #This is 2CaO.SiO2. #602eacaf674ba8b79b43f866
CRISTOBALITE:I :SI+4:SiO4-4:
#Ideal beta-Cristobalite (SiO2, C9) #cF24 #Fd-3m #SiO2 with AlPO4
solubility. #602e7f15105f8553a825b559
DIAMOND_FCC_A4 :SI:VA O:
#Diamond (A4) #cF8 #Fd-3m #This is Silicon #602e7f15105f8553a825b4e8
FCC_A1      :CA Si:O VA:
#Face-Centered Cubic (Cu, A1, fcc) #cF4 #Fm-3m #This is FCC_A1 solid
solution and TiO and VO cubic oxides. #602e7f15105f8553a825b4d9
GAS:G       :CA CA1O1 CA2 O O1Si1 O2 O2Si1 O2Si2 O3 SI SI2 SI3:
#Gas # # # #6038cfccf41046d48150aa2e6
HALITE:I   :CA+2:VA:O-2:
#Rock Salt (NaCl, B1) #cF8 #Fm-3m #This is CaO, CoO, FeO, MgO, MnO and
NiO #602e7f15105f8553a825b4f8
HATRURITE:I :CA+2:SiO4-4:O-2:
#Ca3(SiO4)O-b #hR81 #R3m #This is 3CaO.SiO2 #602eadc3674ba8b79b43f86a
HCP_A3      :CA SI:O VA:
#Hexagonal Close Packed (Mg, A3, hcp) #hP2 #P6 3/mmc #HCP_A3 also
describes hexagonal carbides and nitrides. #602e7f15105f8553a825b4e6
IONIC_LIQ:Y :CA+2 SI+4:O-2 SiO4-4 VA SiO2:
#Liquid # # #Liquid metal and slag mixture. #6038cfda41046d48150aa2e7
LARNITE:I  :CA+2:Si+4:O-2:
#Parawollastonite (CaSiO3, S33(II)) #mP60 #P2_1/c #This is 2CaO.SiO2
(in metastable at 1 atm) #602e7f15105f8553a825b68e
OLIVINE:I  :CA+2:CA+2:Si+4:O-2:
#Forsterite (Mg2SiO4, S12) #oP28 #Pnma #This is Calcio-olivine (Ca2SiO4)
- Co2SiO4 - Fayalite (Fe2SiO4) - Forsterite (Mg2SiO4) - Tephroite
(Mn2SiO4) - Ni2SiO4 - Kirschsteinite (CaFeSiO4) - Monticellite (CaMgSiO4)
solid solution dissolving Cr and Cu. #602e7f15105f8553a825b684
PROTO_PYROXENE:I :CA+2:Si+4:O-2:
#MgSiO3 #oP40 #Pbcn #This is proto-enstatite (MgSiO3) and proto-diopside
(CaMgSi2O6) dissolving Co, Cr, and Fe. #602ead24674ba8b79b43f867
PSEUDO_WOLLASTONITE:I :CA+2:Si+4:O-2:
#CaSiO3 #mS120 #C2/c #This is CaO.SiO2 #602ead45674ba8b79b43f868
QUARTZ:I   :Si+4:SiO4-4:
#alpha-Quartz (low Quartz) #hP9 #P3_121 #SiO2 with AlPO4 solubility.
#602e7f15105f8553a825b6e2
RANKINITE:I :CA+2:Si+4:O-2:
#3CaO.2SiO2 #nP48 #P2_1/c # #602eaf3286932e6d2e4f532d
TRIDYMITE:I :Si+4:SiO4-4:
#Monoclinic (Cc) Low Tridymite (SiO2) #mS144 #Cc #SiO2 with AlPO4
solubility. #602e7f15105f8553a825b82e
WOLLASTONITE:I :CA+2:Si+4:O-2:
#Wollastonite (CaSiO3) #aP30 #P-1 #This is CaO.SiO2
#602e7f15105f8553a825b913
TDB_OXDEMO: @@ If we want to calculate a pseudobinary system
TDB_OXDEMO: @@ we must take away all phases and constituents that
TDB_OXDEMO: @@ make it possible for the phase to exist outside the
TDB_OXDEMO: @@ composition line from CaO to SiO2.
TDB_OXDEMO:
TDB_OXDEMO: @@ This means that for the IONIC_LIQ phase the
TDB_OXDEMO: @@ constituent Va should be suspended for systems with
TDB_OXDEMO: @@ no degree of freedom with respect to oxygen.
TDB_OXDEMO:
TDB_OXDEMO: rej const
... the command in full is REJECT
PHASE: ion
```

```

SUBLATTICE NUMBER: 2
CONSTITUENT: va
VA IN IONIC_LIQ:Y SUBLATTICE 2 REJECTED
CONSTITUENT:
TDB_OXDEMO: l-sys
... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENTS/: CONSTITUENTS
BCC_A2 :CA Si:O VA:
#Body-Centered Cubic (W, A2, bcc) #cI2 #Im-3m # #602e7f15105f8553a825b4e4
CA2SiO4_ALPHA_A:I :CA+2:CA+2:SiO4-4:
#Ca2SiO4 #hp24 #P6_3/mmc #This is 2CaO.SiO2 and 3CaO.P2O5.
#602eac57674ba8b79b43f865
CA2SiO4_ALPHA_PRIME:I :CA+2:CA+2:SiO4-4:
#K2CoCl4 #oP84 #Pna2_1 #This is 2CaO.SiO2. #602eacaf674ba8b79b43f866
CRISTOBALITE:I :Si+4:SiO4-4:
#Ideal beta-Cristobalite (SiO2, C9) #cF24 #Fd-3m #SiO2 with AlPO4
solubility. #602e7f15105f8553a825b559
DIAMOND_FCC_A4 :Si:VA O:
#Diamond (A4) #cF8 #Fd-3m #This is Silicon #602e7f15105f8553a825b4e8
FCC_A1 :CA Si:O VA:
#Face-Centered Cubic (Cu, A1, fcc) #cF4 #Fm-3m #This is FCC_A1 solid
solution and TiO and VO cubic oxides. #602e7f15105f8553a825b4d9
GAS:G :CA CA101 CA2 O O1Si1 O2 O2Si1 O2Si2 O3 SI SI2 SI3:
#Gas # # #6038cfef41046d48150aa2e6
HALITE:I :CA+2 VA:O-2:
#Rock Salt (NaCl, B1) #cF8 #Fm-3m #This is CaO, CoO, FeO, MgO, MnO and
NiO #602e7f15105f8553a825b4f8
HATRURITE:I :CA+2:SiO4-4:O-2:
#Ca3(SiO4)O-b #hR81 #Fm-3m #This is 3CaO.SiO2 #602eadc3674ba8b79b43f86a
HCP_A3 :CA Si:O VA:
#Hexagonal Close Packed (Mg, A3, hcp) #hP2 #P6_3/mmc #HCP_A3 also
describes hexagonal carbides and nitrides. #602e7f15105f8553a825b4e6
IONIC_LIQ:Y :CA+2 Si:O-4:O-2:
#Liquid # # #Liquid metal and slag mixture. #6038cfda41046d48150aa2e7
LARNITE:I :CA+2:Si:O-2:
#Parawollastonite (Casio3, S33(II)) #mP60 #P2_1/c #This is 2CaO.SiO2
(metastable at 1 atm) #602e7f15105f8553a825b68e
OLIVINE:I :CA+2:CA+2:Si:O-2:
#Forsterite (Mg2SiO4, S12) #oP28 #Pnma #This is Calcio-olivine (Ca2SiO4)
- Co2SiO4 - Fayalite (Fe2SiO4) - Forsterite (Mg2SiO4) - Tephrorite
(Mn2SiO4) - Ni2SiO4 - Kirschsteinite (CaFeSiO4) - Monticellite (CaMgSiO4)
solid solution dissolving Cr and Cu. #602e7f15105f8553a825b684
PROTO_PYROXENE:I :CA+2:Si:O-2:
#MgSiO3 #oP40 #Pbcn #This is proto-enstatite (MgSiO3) and proto-diopside
(CaMgSi2O6) dissolving Co, Cr, and Fe. #602ead24674ba8b79b43f867
PSEUDO_WOLLASTONITE:I :CA+2:Si:O-2:
#CaSiO3 #mS120 #C2/c #This is CaO.SiO2 #602ead45674ba8b79b43f868
QUARTZ:I :Si:O-4:
#alpha-Quartz (low Quartz) #hP9 #P3_121 #SiO2 with AlPO4 solubility.
#602e7f15105f8553a825b6e2
RANKINITE:I :CA+2:Si:O-2:
#3CaO.2SiO2 #mP48 #P2_1/c # #602eaf3286932e6d2e4f532d
TRIDYMITE:I :Si:O-4:
#Monoclinic (Cc) Low Tridymite (SiO2) #mS144 #Cc #SiO2 with AlPO4
solubility. #602e7f15105f8553a825b82e
WOLLASTONITE:I :CA+2:Si:O-2:
#Wollastonite (Casio3) #oP30 #P-1 #This is CaO.SiO2
#602e7f15105f8553a825b913
TDB_OXDEMO: Hit RETURN to continue
TDB_OXDEMO: @@ The phase names may seem unfamiliar but this is due
TDB_OXDEMO: @@ to the attempt to create a general database. Thus lime
TDB_OXDEMO: @@ (CaO) is called HALITE which is the generic phase name
TDB_OXDEMO: @@ for this structure. HALITE is also the wudstite phase
TDB_OXDEMO: @@ (FeO) and the periclase phase (MgO).
TDB_OXDEMO:
TDB_OXDEMO: @@ Note also that many phases are modelled with
TDB_OXDEMO: @@ sublattices and vacancies in order to allow for
TDB_OXDEMO: @@ non-stoichiometry in higher order systems.
TDB_OXDEMO:
TDB_OXDEMO: @@ For simplicity reject all phases except those we know
TDB_OXDEMO: @@ should be stable in this system.
TDB_OXDEMO:
TDB_OXDEMO: rej ph /all
... the command in full is REJECT
BCC_A2 CA2SiO4_ALPHA_A:I CA2SiO4_ALPHA_PRIME:I
CRISTOBALITE:I DIAMOND_FCC_A4 FCC_A1
GAS:G HALITE:I HATRURITE:I
HCP_A3 IONIC_LIQ:Y LARNITE:I
OLIVINE:I PROTO_PYROXENE:I PSEUDO_WOLLASTONITE:I
QUARTZ:I RANKINITE:I TRIDYMITE:I
WOLLASTONITE:I REJECTED
TDB_OXDEMO: rest ph ionic_liq ca2si04_alpha ca2si04_alpha_prime cristobalite halite hatrurite
... the command in full is RESTORE
*** ERROR CA2SiO4_ALPHA INPUT IGNORED
IONIC_LIQ:Y CA2SiO4_ALPHA_PRIME:I CRISTOBALITE:I
HALITE:I HATRURITE:I RESTORED
TDB_OXDEMO: rest ph larnite olivine pseudo_wollastonite quartz rankinite
... the command in full is RESTORE
LARNITE:I OLIVINE:I PSEUDO_WOLLASTONITE:I
QUARTZ:I RANKINITE:I RESTORED
TDB_OXDEMO: rest ph tridymite wollastonite
... the command in full is RESTORE
TRIDYMITE:I WOLLASTONITE:I RESTORED
TDB_OXDEMO: @@ To avoid complications also reject the Si+4 in the
TDB_OXDEMO: @@ first sublattice in the liquid phase. When there is
TDB_OXDEMO: @@ oxygen present all Si will form SiO2 or SiO4-/4.
TDB_OXDEMO: @@ The Si+4 ion is needed only for the liquid in systems
TDB_OXDEMO: @@ without oxygen.
TDB_OXDEMO:
TDB_OXDEMO: rej const ionic_liq
... the command in full is REJECT
SUBLATTICE NUMBER: 1
CONSTITUENT: si+4
SI+4 IN IONIC_LIQ:Y SUBLATTICE 1 REJECTED
CONSTITUENT:
TDB_OXDEMO: l-sys
... the command in full is LIST SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENTS/: CONSTITUENTS
CA2SiO4_ALPHA_PRIME:I :CA+2:CA+2:SiO4-4:
#K2CoCl4 #oP84 #Pna2_1 #This is 2CaO.SiO2. #602eacaf674ba8b79b43f866
CRISTOBALITE:I :Si:O-4:
#Ideal beta-Cristobalite (SiO2, C9) #cF24 #Fd-3m #SiO2 with AlPO4
solubility. #602e7f15105f8553a825b559
HALITE:I :CA+2 VA:O-2:

```

```

#Rock Salt (NaCl, B1) #cF8 #Fm-3m #This is CaO, CoO, FeO, MgO, MnO and
NiO #602e7f15105f8553a825b4f8
HATRURITE:I :CA+2:SiO4-4:0-2:
#Ca3(SiO4)O-b #hr81 #R3m #This is 3CaO.SiO2 #602eadc3674ba8b79b43f86a
IONIC_LIQ:Y :CA+2:O-2 SiO4-4 SiO2:
#Liquid # #Liquid metal and slag mixture. #6038cfda41046d48150aa2e7
LARNITE:I :CA+2:Si+4:0-2:
#Parawollastonite (CaSiO3, S33(II)) #mP60 #P2_1/c #This is 2CaO.SiO2
(metastable at 1 atm) #602e7f15105f8553a825b68e
OLIVINE:I :CA+2:CA+2:Si+4:0-2:
#Forsterite (Mg2SiO4, S12) #oP28 #Pnma #This is Calcio-olivine (Ca2SiO4)
- Co2SiO4 - Fayalite (Fe2SiO4) - Forsterite (Mg2SiO4) - Tephroite
(Mn2SiO4) - Ni2SiO4 - Kirschsteinite (CaFeSiO4) - Monticellite (CaMgSiO4)
solid solution dissolving Ca and Cu. #602e7f15105f8553a825b684
PSEUDO_WOLLASTONITE:I :CA+2:Si+4:0-2:
#CaSiO3 #mS120 #C2/c #This is CaO.SiO2 #602ead45674ba8b79b43f868
QUARTZ:I :Si+4:SiO4-4:
#alpha-Quartz (low Quartz) #hP9 #P3_121 #SiO2 with AlPO4 solubility.
#602e7f15105f8553a825b6e2
RANKINITE:I :CA+2:Si+4:0-2:
#3CaO.2SiO2 #nP48 #P2_1/c # #602eaf3286932e6d2e4f532d
TRIDYMITE:I :Si+4:SiO4-4:
#Monoclinic (Cc) Low Tridymite (SiO2) #mS144 #Cc #SiO2 with AlPO4
solubility. #602e7f15105f8553a825b82e
WOLLASTONITE:I :CA+2:Si+4:0-2:
#Wollastonite (CaSiO3) #aP30 #P-1 #This is CaO.SiO2
#602e7f15105f8553a825b913
TDB_OXDEMO:Hit RETURN to continue
TDE_OXDEMO:
TDB_OXDEMO: get
... the command in full is GET_DATA
15:48:54,832 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
VA IN HALITE:I SUBLATTICE 1 REJECTED
... the command in full is AMEND_PHASE_DESCRIPTION
Creating a new composition set IONIC_LIQ#2
PARAMETERS .....
FUNCTIONS .....

List of references for assessed data

'R. Zhang, Molar volumes for oxide liquid in TCOX, Thermo-Calc Software AB,
Sweden, 2018-2022'
'A. Dinsdale, Private Communication; liquid and solid Al2O3, CaO, MgO'
'R. Zhang, Viscosity of liquid oxides, Thermo-Calc Software AB, 2018-2022'
'R. Zhang, Surface tensions for oxide liquid in TCOX, Thermo-Calc Software
AB, Sweden, 2020-2022'
'H. Mao, B. Sundman, Z. Wang and S.K. Saxena, J. Alloys Compd., 327, 2001,
253-262'
'T.I. Barry, NPL, Unpublished work (1987); liquid and solid SiO2'
'W. Huang, M. Hillert and X. Wang, Metall. Mater. Trans. A 26 (1995) 2293
-2231; CaO-MgO-SiO2'
'M. Hillert, B. Sundman and X. Wang, Metall. Trans. B 21 (1990) 303-312;
CaO-SiO2'
'M. Hillert, B. Sundman and X. Wang, Calphad 15 (1991) 53-58; CaO-SiO2'
-OK-
TDB_OXDEMO: @@ There is a miscibility gap in the ionic liquid close to SiO2.
TDE_OXDEMO: @@ In this database two composition sets are created
TDB_OXDEMO: @@ automatically and one has SiO2 as a major constituent
TDE_OXDEMO:
TDB_OXDEMO: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY:

POLY: @@ Define more convenient components than the elements
POLY:
POLY: list-stat cps
... the command in full is LIST_STATUS
*** STATUS FOR ALL COMPONENTS
COMPONENT STATUS REF. STATE T(K) P(Pa)
VA ENTERED SER
CA ENTERED SER
O ENTERED SER
SI ENTERED SER
*** STATUS FOR ALL PHASES
PHASE STATUS DRIVING FORCE MOLES
WOLLASTONITE ENTERED 0.000000E+00 0.000000E+00
TRIDYMITE ENTERED 0.000000E+00 0.000000E+00
RANKINITE ENTERED 0.000000E+00 0.000000E+00
QUARTZ ENTERED 0.000000E+00 0.000000E+00
PSEUDO_WOLLASTONITE ENTERED 0.000000E+00 0.000000E+00
OLIVINE ENTERED 0.000000E+00 0.000000E+00
LARNITE ENTERED 0.000000E+00 0.000000E+00
HATRURITE ENTERED 0.000000E+00 0.000000E+00
HALITE ENTERED 0.000000E+00 0.000000E+00
CRISTOBALITE ENTERED 0.000000E+00 0.000000E+00
CA2SiO4_ALPHA_PRIME ENTERED 0.000000E+00 0.000000E+00
IONIC_LIQ#2 ENTERED 0.000000E+00 0.000000E+00
IONIC_LIQ#1 ENTERED 0.000000E+00 0.000000E+00
*** STATUS FOR ALL SPECIES
CA ENTERED O-2 ENTERED O3 ENTERED SiO2 ENTERED
CA+2 ENTERED O1Si1 ENTERED SI ENTERED SiO4-4 ENTERED
CA1O1 ENTERED O2 ENTERED SI+4 ENTERED VA ENTERED
CA2 ENTERED O2Si1 ENTERED SI2 ENTERED
O ENTERED O2Si2 ENTERED SI3 ENTERED
POLY: def-com cao siO2 o
... the command in full is DEFINE_COMPONENTS
POLY: l-st cps
... the command in full is LIST_STATUS
*** STATUS FOR ALL COMPONENTS
COMPONENT STATUS REF. STATE T(K) P(Pa)
VA ENTERED SER
CAO ENTERED SER
SiO2 ENTERED SER
O ENTERED SER
*** STATUS FOR ALL PHASES
PHASE STATUS DRIVING FORCE MOLES
WOLLASTONITE ENTERED 0.000000E+00 0.000000E+00
TRIDYMITE ENTERED 0.000000E+00 0.000000E+00
RANKINITE ENTERED 0.000000E+00 0.000000E+00

```

```

QUARTZ          ENTERED    0.000000E+00  0.000000E+00
PSEUDO_WOLLASTONITE  ENTERED    0.000000E+00  0.000000E+00
OLIVINE         ENTERED    0.000000E+00  0.000000E+00
LARNITE         ENTERED    0.000000E+00  0.000000E+00
HATRURITE       ENTERED    0.000000E+00  0.000000E+00
HALITE          ENTERED    0.000000E+00  0.000000E+00
CRISTOBALITE    ENTERED    0.000000E+00  0.000000E+00
CA2SiO4_ALPHA_PRIME  ENTERED    0.000000E+00  0.000000E+00
IONIC_LIQ#2      ENTERED    0.000000E+00  0.000000E+00
IONIC_LIQ#1      ENTERED    0.000000E+00  0.000000E+00
*** STATUS FOR ALL SPECIES
CA      ENTERED    O      ENTERED    O2Si2  ENTERED    SI3   ENTERED
CA+2    ENTERED    O-2    ENTERED    O3     ENTERED    SIO2  ENTERED
CA1O1   ENTERED    O1Si1  ENTERED    SI     ENTERED    SIO4-4 ENTERED
CA2    ENTERED    O2     ENTERED    SI+4   ENTERED    VA    ENTERED
CAO    ENTERED    O2Si1  ENTERED    SI2    ENTERED

POLY:Hit RETURN to continue
POLY: s-c t=2000,p=1e5,n=1,w(sio2)=.9
... the command in full is SET_CONDITION
POLY: l-c
... the command in full is LIST_CONDITIONS
T=2000, P=100000, N=1, W(SIO2)=0.9
DEGREES OF FREEDOM 1
POLY: @@ There is one degree of freedom due to the oxygen. As the
POLY: @@ oxygen content is determined by the Ca/Si ration there is no
POLY: @@ possibility to vary the oxygen content in this system
POLY: @@ independently. Thus the oxygen potential can be set to any
POLY: @@ value (larger than zero).
POLY:
POLY: s-c ac(o)=1
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
15:48:56,370 [Thread-0] INFO Database: Preparing system for use: OXDEMO_MODIFIED_168261053524717
15:48:57,749 [Thread-0] INFO Phase: Preparing phase for use: IONIC_LIQ
15:48:58,283 [Thread-0] INFO Phase: Preparing phase for use: CA2SiO4_ALPHA_PRIME
15:48:58,668 [Thread-0] INFO Phase: Preparing phase for use: CRISTOBALITE
15:48:59,032 [Thread-0] INFO Phase: Preparing phase for use: HALITE
15:48:59,419 [Thread-0] INFO Phase: Preparing phase for use: HATRURITE
15:48:59,818 [Thread-0] INFO Phase: Preparing phase for use: LARNITE
15:49:00,165 [Thread-0] INFO Phase: Preparing phase for use: OLIVINE
15:49:00,524 [Thread-0] INFO Phase: Preparing phase for use: PSEUDO_WOLLASTONITE
15:49:00,886 [Thread-0] INFO Phase: Preparing phase for use: QUARTZ
15:49:01,228 [Thread-0] INFO Phase: Preparing phase for use: RANKINITE
15:49:01,576 [Thread-0] INFO Phase: Preparing phase for use: TRIDYMITE
15:49:01,916 [Thread-0] INFO Phase: Preparing phase for use: WOLLASTONITE
Testing POLY result by global minimization procedure
Calculated      1976 grid points in           0 s
      35 ITS, CPU TIME USED 17 SECONDS
POLY:
POLY: @@ Option N is used to include information on the
POLY: @@ constitution of the phases.
POLY: l-e screen
... the command in full is LIST_EQUILIBRIUM
Options /WCFS: n
Output from POLY-3, equilibrium =      1, label A0 , database: OXDEMO

Conditions:
T=2000, P=100000, N=1, W(SIO2)=0.9, AC(O)=1
DEGREES OF FREEDOM 0

Temperature 2000.00 K ( 1726.85 C), Pressure 1.000000E+05
Number of moles of components 1.000000E+00, Mass in grams 5.96568E+01
Total Gibbs energy -1.10541E+06, Enthalpy -7.53273E+05, Volume 2.62576E-05

Component      Moles      W-Fraction Activity Potential Ref.stat
CAO            1.0638E-01  1.0000E-01 6.4224E-25 -9.2632E+05 SER
SIO2           8.9362E-01  9.0000E-01 3.7467E-30 -1.1267E+06 SER
O              0.0000E+00  0.0000E+00 1.0000E+00  0.0000E+00 SER

IONIC_LIQ#1      Status ENTERED      Driving force 0.0000E+00
Moles 6.7244E-01, Mass 4.0313E+01, Volume fraction 6.9347E-01 Mass fractions:
SIO2 9.69165E-01 CAO 3.08355E-02 O 0.00000E+00
Constitution:
Sublattice 1, Number of sites 6.8156E-02
CA+2 1.00000E+00
Sublattice 2, Number of sites 2.00000E+00
SIO2 9.82793E-01 SIO4-4 1.68709E-02 O-2 3.36172E-04

IONIC_LIQ#2      Status ENTERED      Driving force 0.0000E+00
Moles 3.2756E-01, Mass 1.9344E+01, Volume fraction 3.0653E-01 Mass fractions:
SIO2 7.55858E-01 CAO 2.44142E-01 O 0.00000E+00
Constitution:
Sublattice 1, Number of sites 6.9176E-01
CA+2 1.00000E+00
Sublattice 2, Number of sites 2.00000E+00
SIO2 8.26780E-01 SIO4-4 1.72662E-01 O-2 5.57209E-04
POLY:Hit RETURN to continue
POLY: @@ The result shows the expected miscibility gap. However,
POLY: @@ in some cases the first calculation may fail. In such
POLY: @@ cases try to simplify the calculation by suspending
POLY: @@ all phases but the important ones. Save the results.
POLY:
POLY: save tceox17 y
... the command in full is SAVE_WORKSPACES
POLY: @ Set the axis
POLY: s-a-v 1 w(sio2)
... the command in full is SET_AXIS_VARIABLE
Min value /0/: 0
Max value /1/: 1
Increment /0.025/: .025
POLY: s-a-v 2 t
... the command in full is SET_AXIS_VARIABLE
Min value /0/: 1500
Max value /1/: 3500
Increment /50/: 20
POLY: save tceox17 Y
... the command in full is SAVE_WORKSPACES
POLY: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3

```

```

Generating start equilibrium  4
Generating start equilibrium  5
Generating start equilibrium  6
Generating start equilibrium  7
Generating start equilibrium  8
Generating start equilibrium  9
Generating start equilibrium 10
Generating start equilibrium 11

Organizing start points

Using ADDED start equilibria

Generating start point  1
Generating start point  2
Generating start point  3
Generating start point  4
Generating start point  5
Generating start point  6
Generating start point  7
Generating start point  8
Generating start point  9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26

Phase region boundary  1 at:  1.765E-01  1.510E+03
 ** CA2SIO4_ALPHA_PRIME
    HALITE
Calculated..          2 equilibria
Terminating at axis limit.

Phase region boundary  2 at:  1.765E-01  1.500E+03
 ** CA2SIO4_ALPHA_PRIME
    HALITE
Calculated.          3 equilibria

Phase region boundary  3 at:  1.765E-01  1.525E+03
 ** CA2SIO4_ALPHA_PRIME
    HALITE
    ** HATRURITE

Phase region boundary  4 at:  1.327E-01  1.525E+03
    HALITE
    ** HATRURITE
Calculated.          46 equilibria

Phase region boundary  5 at:  1.327E-01  2.422E+03
    ** IONIC_LIQ#2
    HALITE
    ** HATRURITE

Phase region boundary  6 at:  1.433E-01  2.422E+03
    ** IONIC_LIQ#2
    HALITE
Calculated.          53 equilibria

Phase region boundary  7 at:  2.736E-01  2.422E+03
    ** IONIC_LIQ#2
    HATRURITE
Calculated.          7 equilibria

Phase region boundary  8 at:  2.946E-01  2.321E+03
    ** IONIC_LIQ#2
    ** CA2SIO4_ALPHA_PRIME
    HATRURITE

Phase region boundary  9 at:  3.061E-01  2.321E+03
    ** CA2SIO4_ALPHA_PRIME
    HATRURITE
Calculated.          41 equilibria
Terminating at known equilibrium

Phase region boundary 10 at:  3.336E-01  2.321E+03
    IONIC_LIQ#2
    ** CA2SIO4_ALPHA_PRIME
Calculated.          54 equilibria

Phase region boundary 11 at:  3.953E-01  1.732E+03
    IONIC_LIQ#2
    ** CA2SIO4_ALPHA_PRIME
    ** RANKINITE

Phase region boundary 12 at:  4.291E-01  1.732E+03
    IONIC_LIQ#2
    ** RANKINITE
Calculated.          2 equilibria

Phase region boundary 13 at:  4.309E-01  1.727E+03
    IONIC_LIQ#2
    ** PSEUDO_WOLLASTONITE
    ** RANKINITE

Phase region boundary 14 at:  4.813E-01  1.727E+03
    IONIC_LIQ#2
    ** PSEUDO_WOLLASTONITE
Calculated.          29 equilibria

Phase region boundary 15 at:  5.740E-01  1.714E+03
    IONIC_LIQ#2

```

```

** PSEUDO_WOLLASTONITE
** TRIDYMITE

Phase region boundary 16 at: 8.175E-01 1.714E+03
  ** IONIC_LIQ#2
  ** TRIDYMITE
Calculated.          3 equilibria

Phase region boundary 17 at: 8.222E-01 1.744E+03
  ** IONIC_LIQ#2
  ** CRISTOBALITE
  ** TRIDYMITE
Calculated.          12 equilibria

Phase region boundary 18 at: 8.222E-01 1.744E+03
  ** IONIC_LIQ#2
  ** CRISTOBALITE
Calculated.          12 equilibria

Phase region boundary 19 at: 8.695E-01 1.959E+03
  ** IONIC_LIQ#1
  ** IONIC_LIQ#2
  ** CRISTOBALITE
Calculated.          57 equilibria
Terminating at known equilibrium

Phase region boundary 21 at: 9.882E-01 1.959E+03
  ** IONIC_LIQ#1
  ** CRISTOBALITE
Calculated.          24 equilibria

Phase region boundary 22 at: 1.000E+00 1.744E+03
  ** CRISTOBALITE
  ** TRIDYMITE
Calculated.          12 equilibria
Terminating at axis limit.

Phase region boundary 23 at: 7.627E-01 1.714E+03
  ** PSEUDO_WOLLASTONITE
  ** TRIDYMITE
Calculated..         12 equilibria
Terminating at axis limit.

Phase region boundary 24 at: 4.671E-01 1.727E+03
  ** PSEUDO_WOLLASTONITE
  ** RANKINITE
Calculated..         13 equilibria
Terminating at axis limit.

Phase region boundary 25 at: 3.828E-01 1.732E+03
  ** CA2SiO4_ALPHA_PRIME
  ** RANKINITE
Calculated..         13 equilibria
Terminating at axis limit.

Phase region boundary 26 at: 1.765E-01 1.510E+03
  ** CA2SiO4_ALPHA_PRIME
  ** HALITE
Calculated.          2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 27 at: 1.765E-01 1.510E+03
  ** CA2SiO4_ALPHA_PRIME
  ** HALITE
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 28 at: 1.765E-01 1.510E+03
  ** CA2SiO4_ALPHA_PRIME
  ** HALITE
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 29 at: 1.765E-01 1.510E+03
  ** CA2SiO4_ALPHA_PRIME
  ** HALITE
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 30 at: 1.765E-01 1.510E+03
  ** CA2SiO4_ALPHA_PRIME
  ** HALITE
Calculated..         2 equilibria
Terminating at known equilibrium

Phase region boundary 31 at: 7.627E-01 1.510E+03
  ** PSEUDO_WOLLASTONITE
  ** TRIDYMITE
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 32 at: 7.627E-01 1.510E+03
  ** PSEUDO_WOLLASTONITE
  ** TRIDYMITE
Calculated..         13 equilibria
Calculated.          13 equilibria

Phase region boundary 33 at: 7.627E-01 1.510E+03
  ** PSEUDO_WOLLASTONITE
  ** TRIDYMITE
Calculated..         12 equilibria
Terminating at known equilibrium

Phase region boundary 34 at: 7.627E-01 1.510E+03
  ** PSEUDO_WOLLASTONITE
  ** TRIDYMITE
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 35 at: 7.627E-01 1.510E+03
  ** PSEUDO_WOLLASTONITE

```

TRIDYMITE
 Calculated. 13 equilibria
 Calculated 13 equilibria
 Phase region boundary 36 at: 7.627E-01 1.510E+03
 ** PSEUDO_WOLLASTONITE
 TRIDYMITE
 Calculated. 12 equilibria
 Terminating at known equilibrium
 Phase region boundary 37 at: 7.627E-01 1.510E+03
 ** PSEUDO_WOLLASTONITE
 TRIDYMITE
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.
 Phase region boundary 38 at: 7.627E-01 1.510E+03
 ** PSEUDO_WOLLASTONITE
 TRIDYMITE
 Calculated. 13 equilibria
 Calculated 13 equilibria
 Phase region boundary 39 at: 7.627E-01 1.510E+03
 ** PSEUDO_WOLLASTONITE
 TRIDYMITE
 Calculated. 12 equilibria
 Terminating at known equilibrium
 Phase region boundary 40 at: 3.705E-01 2.170E+03
 IONIC_LIQ#1
 ** CA2SiO4_ALPHA_PRIME
 Calculated. 23 equilibria
 Terminating at known equilibrium
 Phase region boundary 41 at: 3.705E-01 2.170E+03
 IONIC_LIQ#1
 ** CA2SiO4_ALPHA_PRIME
 Calculated. 39 equilibria
 Terminating at known equilibrium
 Phase region boundary 42 at: 9.886E-02 2.830E+03
 IONIC_LIQ#1
 ** HALITE
 Calculated. 22 equilibria
 Terminating at known equilibrium
 Phase region boundary 43 at: 9.886E-02 2.830E+03
 IONIC_LIQ#1
 ** HALITE
 Calculated 30 equilibria
 Phase region boundary 44 at: 9.886E-02 2.830E+03
 IONIC_LIQ#1
 ** HALITE
 Calculated. 22 equilibria
 Terminating at known equilibrium
 Phase region boundary 45 at: 9.886E-02 2.830E+03
 IONIC_LIQ#1
 ** HALITE
 Calculated 30 equilibria
 Phase region boundary 46 at: 5.002E-03 3.162E+03
 IONIC_LIQ#1
 ** HALITE
 Calculated 9 equilibria
 Phase region boundary 47 at: 5.002E-03 3.162E+03
 IONIC_LIQ#1
 ** HALITE
 Calculated. 40 equilibria
 Terminating at known equilibrium
 Phase region boundary 48 at: 3.428E-01 2.374E+03
 IONIC_LIQ#1
 ** CA2SiO4_ALPHA_PRIME
 Calculated. 4 equilibria
 Terminating at known equilibrium
 Phase region boundary 49 at: 3.428E-01 2.374E+03
 IONIC_LIQ#1
 ** CA2SiO4_ALPHA_PRIME
 Calculated. 58 equilibria
 Terminating at known equilibrium
 Phase region boundary 50 at: 8.337E-01 1.812E+03
 IONIC_LIQ#1
 ** CRISTOBALITE
 Calculated. 5 equilibria
 Terminating at known equilibrium
 Phase region boundary 51 at: 8.337E-01 1.812E+03
 IONIC_LIQ#1
 ** CRISTOBALITE
 Calculated 10 equilibria
 Phase region boundary 52 at: 8.337E-01 1.812E+03
 IONIC_LIQ#1
 ** CRISTOBALITE
 Calculated. 9 equilibria
 Terminating at known equilibrium
 Phase region boundary 53 at: 9.950E-01 1.978E+03
 IONIC_LIQ#1
 ** CRISTOBALITE
 Calculated 10 equilibria
 Phase region boundary 54 at: 9.950E-01 1.978E+03
 IONIC_LIQ#1
 ** CRISTOBALITE
 Calculated. 2 equilibria
 Terminating at known equilibrium
 Phase region boundary 55 at: 9.950E-01 1.978E+03
 IONIC_LIQ#1

```

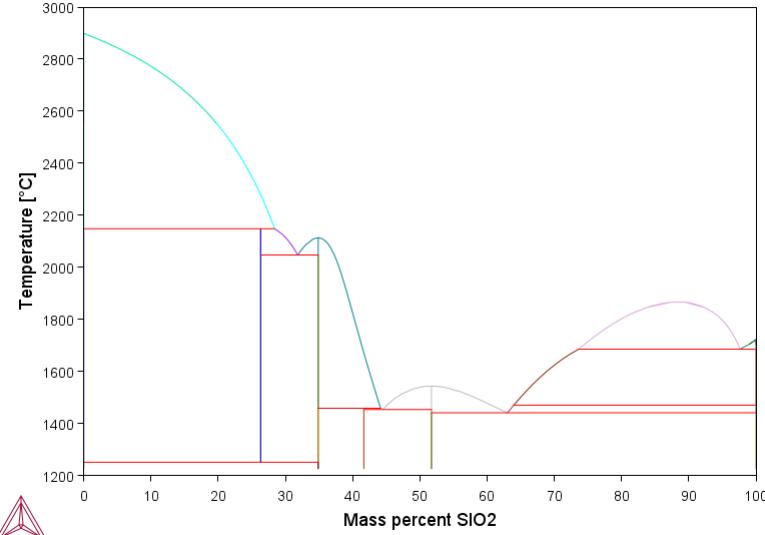
** CRISTOBALITE
Calculated                         18 equilibria
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\generate_console_examples\examples\tcex17\tcex17.POLY3
CPU time for mapping                 4 seconds
POLY:
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: s-d-a x w-p sio2
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t-c
... the command in full is SET_DIAGRAM_AXIS
POST:
POST: set-title example 17a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 17a



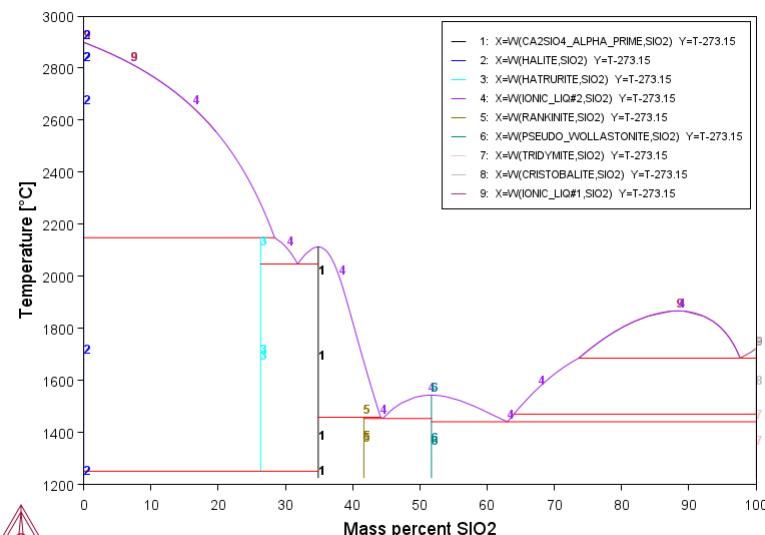
POST:

```

POST: Hit RETURN to continue
POST: @@ Identify the phases with labels
POST: s-lab
... the command in full is SET_LABEL_CURVE_OPTION
CURVE LABEL OPTION (A, B, C, D, E, F OR N) /N: f
POST:
POST: set-title example 17b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 17b



POST:

```

POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:

```

tce18

SYS:About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce18\tce18.TCM.test"

SYS: set-echo
SYS:
SYS: @@ A3 temperature of a steel
SYS:
SYS: @@ This example calculates the A3 temperature of a steel
SYS: @@ and the influence of each alloying element on
SYS: @@ this temperature
SYS:
SYS: @@ A3 temperature is the temperature where ferrite starts to
SYS: @@ form from austenite. You can easily read A3 from an Fe-C
SYS: @@ phase diagram. But for complex multicomponent steels, no
SYS: @@ simple diagram can be used.
SYS:
SYS: @@ Using POLY, it is easy to find out the influence of each
SYS: @@ alloying element on A3 temperature. This information is
SYS: @@ useful if you want to modify the compositions of a steel
SYS: @@ but keep A3 unchanged.
SYS:
SYS: @@ Note that a TCFE database license is required to run
SYS: @@ the example.
SYS:
SYS: set-log ex18,,
SYS: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32

POLY: def-mat
... the command in full is DEFINE_MATERIAL
THERMODYNAMIC DATABASE module
Database folder: C:\jenkins\workspace\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED
DICTRA_FCC_A1 REJECTED
Database /TCFE11/: tcfe11
Major element or alloy: fe
Composition input in mass (weight) percent? /Y/
1st alloying element: cr 1.5 mn .5 c .3 si .3 nb .1
Next alloying element:
Temperature (C) /1000/: 1100
VA /- DEFINED
DICTRA_FCC_A1 REJECTED
REINITIATING GES
... the command in full is DEFINE_ELEMENTS
FE DEFINED
... the command in full is DEFINE_ELEMENTS
CR DEFINED
... the command in full is DEFINE_ELEMENTS
MN DEFINED
... the command in full is DEFINE_ELEMENTS
C DEFINED
... the command in full is DEFINE_ELEMENTS
SI DEFINED
... the command in full is DEFINE_ELEMENTS
NB DEFINED

This database has following phases for the defined system

| | | |
|--------------|----------------|-------------|
| GAS:G | LIQUID:L | BCC_A2 |
| A2_BCC | BCC_B2 | FCC_A1 |
| A1_FCC | FCC_L12 | HCP_A3 |
| CBCC_A12 | CUB_A13 | DIAMOND_A4 |
| GRAPHITE_A9 | CEMENTITE_D011 | M23C6_D84 |
| M7C3_D101 | M6C_E93 | M5C2 |
| M3C2_D510 | KSI_CARBIDE | Z_PHASE |
| FE4N_LP1 | SIGMA_D8B | HIGH_SIGMA |
| MU_D85 | CHI_A12 | C14_LAVES |
| C15_LAVES | M3SI | MN9Si2 |
| MN11Si19 | MN6Si | G_PHASE |
| CR3Si_A15 | FESI2_H | FESI2_L |
| MSI_B20 | M5Si3_D88 | NBNi3_D0A |
| NB3Si | NB5Si3_D8L | NB5Si3_D8M |
| MSI2_C40 | CRNBSI | M11Si8 |
| M6Si5 | FENBSI2 | FE4Nb4Si7 |
| FENBSI_C23 | FE3Nb4Si5 | FENB2Si2 |
| FENB4Si | AL4C3_D71 | FE8Si2C |
| SIC_B3 | MN5SiC | CRZN17 |
| CUZN_EPSILON | AL5Fe4 | MNP_B31 |
| M2P_C22 | FLUORITE_C1:I | ZRO2_TETR:I |
| M2O3C_D53:I | M2O3H_D52:I | NI3Si12 |
| CO2Si_C37 | M2Si_TETA | NiSi_B31 |
| NI3Si2 | CR5Si3_D8M | DELTA_TiH2 |
| NBH_BETA | | |

Reject phase(s) /NONE/: ?

FILE SYSTEM ERROR IN FILHLP
ERROR 1717 READING HELP FILE

Reject phase(s) /NONE/: *

| | | |
|-------------|----------------|------------|
| GAS:G | LIQUID:L | BCC_A2 |
| A2_BCC | BCC_B2 | FCC_A1 |
| A1_FCC | FCC_L12 | HCP_A3 |
| CBCC_A12 | CUB_A13 | DIAMOND_A4 |
| GRAPHITE_A9 | CEMENTITE_D011 | M23C6_D84 |
| M7C3_D101 | M6C_E93 | M5C2 |
| M3C2_D510 | KSI_CARBIDE | Z_PHASE |
| FE4N_LP1 | SIGMA_D8B | HIGH_SIGMA |

```

MU_D85          CHI_A12          C14_LAVES
C15_LAVES       M3SI             MN9SI2
MN115SI19      MN6SI             G_PHASE
CR3SI_A15       FESI2_H          FESI2_L
MSI_B20         MSSI3_D88        NBNI3_D0A
NB3SI          NB5SI3_D8L        NBSSI3_D8M
MSI2_C40        CRNBSI          M11SI8
M6SI5          FENBSI2         FE4NB4SI7
FENBSI_C23     FB3NB4SI5        FENB2SI2
FENB4SI        AL4C3_D71        FE8SI2C
SIC_B3          MN5SIIC          CRZN17
CUZN_EPSILON    AL5FE4           MNP_B31
M2P_C22         FLUORITE_C1:I   ZR02_TETR:I
M203C_D52:I    M203H_D52:I      NI3SI1I2
CO2SI_C37      M2SI_TETA        NISI_B3I
NI3SI2         CR5SI3_D8M        DELTA_TIH2
NBH_BETA        REJECTED

Restore phase(s):: liq fcc_a1 bcc_a2 hcp_a3 graphite cementite m23 m7
LIQUID:L          FCC_A1          BCC_A2
HCP_A3          GRAPHITE_A9      CEMENTITE_D011
*** ERROR M7 INPUT IGNORED
M23C6_D84 RESTORED
Restore phase(s): /NONE:

.....
```

The following phases are retained in this system:

```

LIQUID:L          BCC_A2          FCC_A1
HCP_A3          GRAPHITE_A9      CEMENTITE_D011
M23C6_D84
```

```

OK? /Y/: Y
15:50:23,300 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
Creating a new composition set FCC_A1#2
... the command in full is AMEND_PHASE_DESCRIPTION
Creating a new composition set HCP_A3#2
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS .....
FUNCTIONS .....
```

List of references for assessed data

```

'A.T. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121-127; Molar
    volumes'
'M. Ghasemi, Thermo-Calc Software AB, Sweden, 2020; Unifying liquid volume
    database'
'X.G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
'X.G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
    volumes'
'Y. Tang, in TCCU2, Thermo-Calc Software AB, Stockholm, Sweden'
'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
'A.V. Khvan, B. Hallstedt, K. Chang, CALPHAD, 39, 54-61(2012); C-Cr-Nb'
'J-O. Andersson, CALPHAD, 11 (1987) 271-276; TRITA 0314; C-CR'
'J. Bratberg, Z. Metallkd., 96 (2005) 335-344; Fe-Cr-Mo-C'
'B.J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
'C. Qui, ISIJ International, 32 (1992), 1117-1127; Trita-MAC 482 (1992)
    Revision; C-Cr-Fe-Mo'
'P. Gustafson, Metall. Trans. A, 19A (1988) 2547-2554; TRITA-MAC 348,
    (1987); C-CR-FE-W'
'P. Villars, L.D. Calvert. Pearson's handbook of crystallographic data for
    intermetallic phases, Metals park, Ohio 1985: American society for
    metals'
'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
'J-O. Andersson, CALPHAD, 12 (1988) 9-23; TRITA 0321 (1986); C-FE-MO'
'H. Gohring, O. Fabrichnaya, A. Leineweber, E.J. Mittemeijer, Metall.
    Mater. Trans. A, 47A, 6173-86(2016); Fe-N, and Fe-C-N'
'B. Hallstedt, D. Djurovic, J. von Appen, R. Dronskowski, A. Dick, F.
    Koermann, T. Hickel, J. Neugebauer, CALPHAD, 34, 129-33(2010); Fe-C'
'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, Calphad 35.4
    (2011) 479-491; Fe-Mn-C'
'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, CALPHAD, 34, 279
    -85(2010); Mn-C'
'W. Huang, Metall. Trans. A, 21A (1990) 2115-2123; TRITA-MAC 411 (Rev
    1989); C-FE-MN'
'B.J. Lee, Met Mat. Trans. A, 32A, 2423-2439, 2001; C-Fe-N-Nb-Ti'
'A.V. Khvan, B. Hallstedt, CALPHAD, 40, 10-15(2013); Fe-Nb, Nb-C, Nb-N, Fe
    -Mn-Nb, Fe-Nb-C, Fe-Nb-N, Nb-C-N, Fe-Mn-Nb-C, Fe-Mn-Nb-N'
'R. Naraghi, Thermo-Calc Software AB, Volume data updated for TCFE9
    database (TCFE v9.1, June, 2019).'
'J. Grobner, H.L. Lukas, F. Aldinger, Calphad, 1996, 20 (2), 247-254; Al-C,
    Si-C, Al-Si-C'
'P. Franke; revision of C-Si, Fe-Si and C-Fe-Si'
'J. Lacaze and B. Sundman, Metall. Mater. Trans. A, 22A (1991) 2211-2223;
    Fe-Si and Fe-Si-C'
'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; Cementite'
'B.J. Lee, CALPHAD, 17 (1993) 251-268; revision of Fe-Cr and Fe-Ni liquid'
'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270
    (1986); CR-FE'
'K. Frisk, Metall. Trans. A, 21A (1990) 2477-2488; TRITA 0409 (1989); CR
    -FE-N'
'B.J. Lee, Metall. Trans. A, 24A (1993) 1919-1933; Cr-Mn, Fe-Cr-Mn'
'K. Frisk, CALPHAD, 17 (1993) 335-349; Cr-Mn-N'
'J.G. Costa Neto, S.G. Fries, H.L. Lukas, S. Gama and G. Effenberg,
    CALPHAD, 17 (1993) 219-228; Cr-Nb'
'Same or similar interaction as in the corresponding stable phase'
'Y.Du and J.C.Schuster, J. Phase Equilibria, 21(3) 281-86(2000); Cr-Si'
'W. Huang, CALPHAD, 13 (1989) 243-252; TRITA-MAC 388 (rev 1989); FE-MN'
'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
'A. V. Khvan, B. Hallstedt, CALPHAD, 39 (2012) 62-69; Fe-Nb'
'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; Molar volume Fe-Mn-Si
    and Al-Fe-Mn'
'S. Cotes, A.F. Guillermet, M. Sade, J. Alloys Compd., 208(1998) 168-177'
'S. Liu, B. Hallstedt, D. Music, Y. Du, CALPHAD, 38 (2012) 43-58; Mn-Nb
    and Fe-Mn-Nb'
'W. Zheng, J. Alloys Compd., 632 (2015) 661-675'
'P.B. Fernandes, G. C. Coelho, F. Ferreira, C. A. Nunes, and B. Sundman,
```

Intermetallics, 10 (2002) 993-999; Nb-Si'
 'A.V. Khvan, B. Hallstedt, C. Broeckmann, CALPHAD, 46, 24-33(2014); Cr-Fe-C'
 'J-O. Andersson, Metall. Trans. A, 19A (1988) 627-636 TRITA 0207 (1986); C
 -CR-Fe'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2016; FCC Fe-Cr-C and C-Cr-Ni'
 'B.J. Lee, Metall. Trans. A, 24A (1993) 1017-1025; Fe-Cr-Mn-C'
 'J. Bratberg, Thermo-Calc Software AB, Sweden, 2008; Fe-Cr-Mo-Nb-V-C-N'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; C-Cr-Si'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; Adjusting hcp'
 'S. Canderdyd, Report IM-2005-109, Stockholm, Sweden; Fe-Nb-C'
 'W. Huang, Z. Metallkd., 81 (1990) 397-404; TRITA-MAC 390 (1989); FE-NB, C
 -FE-NB'
 'J. Miettinen and B. Hallstedt, CALPHAD, 22 (1998) 231-256; Fe-Si and Fe
 -Si-C'
 'W. Zheng et al., J. Iron Steel Res. Int. 24(2)(2017) 190-197'
 'R. Naraghi, Thermo-Calc Software AB, Sweden (2015); FROST project'
 'C. Qiu, Metall. Trans. A, 24A (1993) 2393-2409; Cr-Fe-Mn-N'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2019; Cr-Fe-Nb'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; Cr-Fe-Si'
 'M. Lindholm, J. Phase Equilib., 18.5 (1997) 432; Cr-Fe-Si'
 'A. Forsberg and J. Agren, J. Phase Equilib., 14 (1993) 354-363; Fe-Mn-Si'
 'M. Ghasemi, Thermo-Calc Software AB, Sweden, 2019; Viscosity of metallic
 liquid'
 'M. J. Assael, J. Phys. Chem. Ref. Data 35 (2006) 285; Fe, Al'
 'M. J. Assael, J. Phys. Chem. Ref. Data 41 (2012) 033101; Cd, Co, Ga, In,
 Hg, Si, Ti, Zn'
 'M Ghasemi, Thermo-Calc Software AB: assessing the surface tension of
 metallic liquid'

-OK-

Should any phase have a miscibility gap check? /N/: N

Using global minimization procedure
 Calculated 9014 grid points in 6 s
 Found the set of lowest grid points in 0 s
 Calculated POLY solution 2 s, total time 8 s

POLY:

POLY: @@ In the TCFE database the number of phases is very large.
POLY: @@ It is strongly recommended that you reject all phases
POLY: @@ that you know should not be stable
POLY:
POLY: l-e,,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: TCFE11

Conditions:

T=1373.15, W(CR)=1.5E-2, W(MN)=5E-3, W(C)=3E-3, W(SI)=3E-3, W(NB)=1E-3,
P=100000, N=1
DEGREES OF FREEDOM 0

Temperature 1373.15 K (1100.00 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 5.50374E+01
Total Gibbs energy -7.21959E+04, Enthalpy 4.05733E+04, Volume 7.32300E-06

| Component | Moles | W-Fraction | Activity | Potential | Ref.stat |
|-----------|------------|------------|------------|-------------|----------|
| C | 1.3747E-02 | 3.0000E-03 | 1.0856E-02 | -5.1639E+04 | SER |
| CR | 1.5877E-02 | 1.5000E-02 | 1.3440E-04 | -1.0178E+05 | SER |
| FE | 9.5890E-01 | 9.7300E-01 | 2.0383E-03 | -7.0736E+04 | SER |
| MN | 5.0091E-03 | 5.0000E-03 | 4.2390E-06 | -1.4124E+05 | SER |
| NB | 5.9240E-04 | 1.0000E-03 | 1.3165E-07 | -1.8088E+05 | SER |
| SI | 5.8790E-03 | 3.0000E-03 | 1.1486E-08 | -2.0873E+05 | SER |

FCC_A1#1 Status ENTERED Driving force 0.0000E+00
Moles 9.9897E-01, Mass 5.4983E+01, Volume fraction 9.9902E-01 Mass fractions:
FE 9.73957E-01 MN 5.00491E-03 C 2.89335E-03
CR 1.50123E-02 SI 3.00297E-03 NB 1.29814E-04

FCC_A1#2 Status ENTERED Driving force 0.0000E+00
Moles 1.0273E-03, Mass 5.4472E-02, Volume fraction 9.8186E-04 Mass fractions:
NB 8.79352E-01 FE 7.32744E-03 MN 4.50186E-05
C 1.10654E-01 CR 2.62187E-03 SI 1.29638E-09

POLY:hit RETURN to continue

POLY: @@ Two FCC phases are stable, one with mainly Fe and
POLY: @@ one with mainly Nb and C, which is the NbC carbide.
POLY: @@ The second fcc is called FCC#2. The number after # is
POLY: @@ called composition set but can be ignored if it is unity.
POLY:

POLY: li-st

... the command in full is LIST_STATUS

Option /CPS/: CPS

*** STATUS FOR ALL COMPONENTS

| COMPONENT | STATUS | REF. | STATE | T (K) | P (Pa) |
|-----------|---------|------|-------|-------|--------|
| VA | ENTERED | SER | | | |
| C | ENTERED | SER | | | |
| CR | ENTERED | SER | | | |
| FE | ENTERED | SER | | | |
| MN | ENTERED | SER | | | |
| NB | ENTERED | SER | | | |
| SI | ENTERED | SER | | | |

*** STATUS FOR ALL PHASES

| PHASE | STATUS | DRIVING FORCE | MOLES |
|----------------|---------|---------------|--------------|
| FCC_A1#2 | ENTERED | 0.000000E+00 | 1.027344E-03 |
| FCC_A1#1 | ENTERED | 0.000000E+00 | 9.989727E-01 |
| BCC_A2 | ENTERED | -1.865997E-02 | 0.000000E+00 |
| Liquid | ENTERED | -2.122724E-01 | 0.000000E+00 |
| HCP_A3#2 | ENTERED | -3.255375E-01 | 0.000000E+00 |
| HCP_A3#1 | ENTERED | -3.255375E-01 | 0.000000E+00 |
| M23C6_D84 | ENTERED | -4.182898E-01 | 0.000000E+00 |
| CEMENTITE_D011 | ENTERED | -4.735993E-01 | 0.000000E+00 |
| GRAPHITE_A9 | ENTERED | -2.493896E+00 | 0.000000E+00 |

*** STATUS FOR ALL SPECIES

| C | ENTERED | C60 | ENTERED | FE+2 | ENTERED | MN+3 | ENTERED | SI | ENTERED |
|----|---------|------|---------|------|---------|------|---------|------|---------|
| C2 | ENTERED | CR | ENTERED | FE+3 | ENTERED | MN+4 | ENTERED | SI+4 | ENTERED |
| C3 | ENTERED | CR+2 | ENTERED | FE+4 | ENTERED | NB | ENTERED | VA | ENTERED |
| C4 | ENTERED | CR+3 | ENTERED | MN | ENTERED | NB+2 | ENTERED | | |
| C5 | ENTERED | FE | ENTERED | MN+2 | ENTERED | NB+4 | ENTERED | | |

POLY:

POLY: @@ Fcc appears twice in the list. The HCP phase also has
POLY: @@ two composition sets.

POLY:

POLY: @@ This result looks reasonable; save it to file

POLY: save tcecx18 y

... the command in full is SAVE_WORKSPACES

POLY:

POLY: @@ Now calculate when bcc (ferrite) begins to form

POLY: @@ using the COMPUTE-TRANSITION command

```

POLY: c-t
... the command in full is COMPUTE_TRANSITION
This command is a combination of CHANGE_STATUS and SET_CONDITION
to calculate directly when a phase may form by releasing one condition.
Phase to form: bcc_a2
You must release one of these conditions
T=1073.15, W(CR)=1.5E-2, W(MN)=5E-3, W(C)=3E-3, W(SI)=3E-3, W(NB)=1E-3,
P=100000, N=1 DEGREES OF FREEDOM 0
Give the state variable to be removed /T/: t
Testing POLY result by global minimization procedure
Calculated 9014 grid points in 0 s
To form BCC A2 the condition is set to T=1071.58417272
POLY:Hit RETURN to continue
POLY: @@ We may expect BCC to form at a lower temperature, because
POLY: @@ sometimes a higher temperature is found as there is a
POLY: @@ delta-ferrite stable at high temperatures.
POLY:
POLY: @@ Calculate the equilibrium at lower temperature again. You
POLY: @@ can do this with a SET-COND T=... command but then the
POLY: @@ temperature must be given in Kelvin. You can use the
POLY: @@ DEF-MAT command to do this in Celsius
POLY:
POLY: def-mat
... the command in full is DEFINE_MATERIAL
Same elements as before? /Y/: Y
Mass (weight) percent of C /.3/: .3
Mass (weight) percent of CR /1.5/: 1.5
Mass (weight) percent of MN /.5/: .5
Mass (weight) percent of NB /.1/: .1
Mass (weight) percent of SI /.3/: .3
Temperature (C) /798/: 800
Using global minimization procedure
Calculated 9014 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY: l-e,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: TCFE11

Conditions:
T=1073.15, W(CR)=1.5E-2, W(MN)=5E-3, W(C)=3E-3, W(SI)=3E-3, W(NB)=1E-3,
P=100000, N=1
DEGREES OF FREEDOM 0

Temperature 1073.15 K ( 800.00 C), Pressure 1.000000E+05
Number of moles of components 1.000000E+00, Mass in grams 5.50374E+01
Total Gibbs energy -4.87853E+04, Enthalpy 3.03165E+04, Volume 7.17930E-06

Component Moles W-Fraction Activity Potential Ref.stat
C 1.3747E-02 3.0000E-03 4.4628E-02 -2.7744E+04 SER
CR 1.5877E-02 1.5000E-02 3.6747E-04 -7.0568E+04 SER
FE 9.5890E-01 9.7300E-01 4.8655E-03 -4.7519E+04 SER
MN 5.0091E-03 5.0000E-03 8.1198E-06 -1.0458E+05 SER
NB 5.9240E-04 1.0000E-03 2.9346E-09 -1.7530E+05 SER
SI 5.8790E-03 3.0000E-03 9.3983E-10 -1.8546E+05 SER

FCC_A1#1 Status ENTERED Driving force 0.0000E+00
Moles 9.9869E-01, Mass 5.4971E+01, Volume fraction 9.9877E-01 Mass fractions:
FE 9.74162E-01 MN 5.00593E-03 C 2.86276E-03
CR 1.49637E-02 SI 3.00363E-03 NB 1.46017E-06

FCC_A1#2 Status ENTERED Driving force 0.0000E+00
Moles 1.3082E-03, Mass 6.6495E-02, Volume fraction 1.2288E-03 Mass fractions:
NB 8.26485E-01 CR 4.49696E-02 MN 9.44662E-05
C 1.16454E-01 FE 1.19978E-02 SI 1.91601E-10
POLY:
POLY: @@ Try a slightly different COMPUTE-TRANSITION command.
POLY: @@ This finds the first phase change in the specified
POLY: @@ direction.
POLY:
POLY: c-t
... the command in full is COMPUTE_TRANSITION
This command is a combination of CHANGE_STATUS and SET_CONDITION
to calculate directly when a phase may form by releasing one condition.
Phase to form: any
You must release one of these conditions
T=1073.15, W(CR)=1.5E-2, W(MN)=5E-3, W(C)=3E-3, W(SI)=3E-3, W(NB)=1E-3,
P=100000, N=1 DEGREES OF FREEDOM 0
Give the state variable to be removed /T/: t
Estimated change (with sign) /1/: ?
FILE SYSTEM ERROR IN FILHLP
Estimated change (with sign) /1/: -1
Lowering smallest site-fraction from 0.10000E-11 to 0.10000E-12
and recalculating equilibrium
PHASE CHANGE AT 1071.5841681
BCC_A2#1 forms
Testing POLY result by global minimization procedure
Calculated 9014 grid points in 0 s
POLY: show t
... the command in full is SHOW_VALUE
T=1071.5842
POLY: @@ The transition temperature to form BCC is the same.
POLY: @@ If we want it in Celsius enter a function.
POLY: enter fun tc=t-273;
... the command in full is ENTER_SYMBOL
POLY: show tc
... the command in full is SHOW_VALUE
TC=798.58417
POLY:
POLY:Hit RETURN to continue
POLY: @@ This is the minimum temperature for hardening because
POLY: @@ below this temperature ferrite will form from austenite.
POLY: @@ Check how a small change of the composition can change
POLY: @@ this temperature. We must then set bcc as Fix and
POLY: @@ release the condition on the temperature.
POLY:
POLY: c-st p bcc_a2=fix 0
... the command in full is CHANGE_STATUS
POLY: s-c t=None
... the command in full is SET_CONDITION
POLY: @@ The change of the calculated temperature for a small
POLY: @@ change of the amount of a component can be calculated
POLY: @@ as a derivative using the dot "." between the

```

```

POLY: @@ calculated variable and the condition.
POLY:
POLY: sh t.w(mn)
... the command in full is SHOW_VALUE
T.W(MN)=-2584.6297
POLY: sh t.w(cr)
... the command in full is SHOW_VALUE
T.W(CR)=-784.00263
POLY: sh t.w(nb)
... the command in full is SHOW_VALUE
T.W(NB)=3035.5587
POLY: sh t.w(c)
... the command in full is SHOW_VALUE
T.W(C)=-21859.659
POLY: sh t.w(si)
... the command in full is SHOW_VALUE
T.W(SI)=3012.5853
POLY:Hit RETURN to continue
POLY: @@ A negative value means the temperature decreases
POLY: @@ if the amount is increased. Check for Mn
POLY:
POLY: s-c w(mn)
... the command in full is SET_CONDITION
Value /.00500000172/: .01
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated      9014 grid points in          0 s
    9 ITS, CPU TIME USED   0 SECONDS
POLY: sh t
... the command in full is SHOW_VALUE
T=1058.9736
POLY:Hit RETURN to continue
POLY: @@ The temperature decreased from 1072 to 1059
POLY: @@ i.e. 13 degrees. According to the derivatives calculated
POLY: @@ above, you can increase the temperature the same
POLY: @@ amount by increasing the amount of Si
POLY: @@ 2592/2990=0.8669 times of the change in Mn
POLY: @@ i.e. from 0.3 to 0.733 %
POLY:
POLY: s-c w(si)
... the command in full is SET_CONDITION
Value /.003/: .00733
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated      9014 grid points in          0 s
    10 ITS, CPU TIME USED  0 SECONDS
POLY: sh t
... the command in full is SHOW_VALUE
T=1070.8718
POLY: @@ Being able to calculate these derivatives is a powerful
POLY: @@ feature in order to find the best way to obtain a
POLY: @@ specific property of a material.
POLY:
POLY: set-inter
... the command in full is SET_INTERACTIVE
POLY:

```

tce19A**SYS:About**

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

```
SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce19A\tce19A.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Mapping of univariant equilibria with the liquid in Al-Cu-Si
SYS:
SYS: @@ This is the first part of a two part example showing how
SYS: @@ to map univariant equilibria with the liquid in Al-Cu-Si.
SYS: @@ Part A. Step-by-step calculation using the POLY-3 module.
SYS:
SYS: set-log ex19a.,
SYS: go da
... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module
Database folder: C:\jenkins\workspace\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA           /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE11: sw USER tce19_cost2
... the command in full is SWITCH_DATABASE
Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

VA           /- DEFINED
15:51:47,724 [Thread-0] INFO TDBfileParser: USER_505823337_14, number of lines read: 470
15:51:47,965 [Thread-0] INFO DatabaseUtils: Parsing of USER_505823337_14 completed in 288 ms
TDB_USER: d-sys
... the command in full is DEFINE_SYSTEM
ELEMENTS: cu al si
CU           AL           SI
DEFINED
TDB_USER: l-s c
... the command in full is LIST_SYSTEM
LIQUID:L   :AL CU SI:
ALCE_AMORPHOUS :AL:
ALCUZN_T    :AL:CU VA:
ALCU_DELTA  :AL:CU:
ALCU_EPSILON :AL CU:CU:
ALCU_ETA    :AL CU:CU:
ALCU_PRIME  :AL:CU:
ALCU_THETA  :AL:AL CU:
ALCU_ZETA   :AL:CU:
ALLI        :AL:VA:
ALMO        :AL:AL:
ALM_D019    :AL:AL:
ALND_AMORPHOUS :AL:
ALTI        :AL:AL:
BCC_A2      :AL CU SI:VA:
BCC_B2      :AL CU SI:AL CU SI:VA:
BCT_A5      :AL:
CBCC_A12   :AL SI:VA:
CR3SI_A15   :SI:AL SI:
CRS12_     :SI:SI:
CU19SI6_ETA :CU:SI:
CU33SI7_DELTA :CU:SI:
CU4SI_EPSILON :CU:SI:
CU56SI11_GAMMA :CU:SI:
CU6Y        :CU:CU2:
CUB_A13    :AL SI:VA:
CUB_A15    :SI:AL SI:
DIAMOND_A4 :AL SI:
FCC_A1      :AL CU SI:VA:
GAMMA_D83  :AL:AL CU:CU:
GAMMA_H     :AL:AL CU:CU:
HCP_A3      :AL CU SI:VA:
HCP_ZN     :AL CU SI:VA:
LAVES_C14   :AL CU:AL CU:
LAVES_C15   :AL CU SI:AL CU SI:
LAVES_C36   :AL CU:AL CU:
SIV3        :SI:SI:
TDB_USER: get
... the command in full is GET_DATA
15:51:48,056 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS .....
FUNCTIONS .....

List of references for assessed data

'COST2 - TCOST507 Light Alloys Database (Version 2.1), provided by TCSAB,
1999/2003.'
'COST (1998): COST 507 -- Definition of Thermochemical and Thermophysical
Properties to Provide a Database for the Development of New Light
Alloys. European Cooperation in the Field of Scientific and Technical
Research, European Commission. Vol 1. Proceedings of the Final
Workshop of COST 507, Vaals, the Netherlands, 1997; Vol 2.
Thermochemical Database for Light Metal Alloys (Eds. Ansara I.,
Dinsdale A.T., and Rand M.H.); Vol 3. Critical Evaluation of Ternary
Systems (Ed. Effenberg G.).'
-OK-
TDB_USER: go p-3
```

```

... the command in full is GOTO_MODULE

POLY version 3.32
POLY: s-c t=1300,p=101325,n=1
... the command in full is SET_CONDITION
POLY: l-c
... the command in full is LIST_CONDITIONS
T=1300, P=101325, N=1
DEGREES OF FREEDOM 2
POLY: s-c x(si)=.25,x(al)=.2
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
15:51:48,691 [Thread-0] INFO Database: Preparing system for use: USER_505823337_14
15:51:49,531 [Thread-0] INFO Phase: Preparing phase for use: LIQUID
15:51:50,032 [Thread-0] INFO Phase: Preparing phase for use: ALCU_AMORPHOUS
15:51:50,400 [Thread-0] INFO Phase: Preparing phase for use: ALCUZN_T
15:51:50,759 [Thread-0] INFO Phase: Preparing phase for use: ALCU_DELTA
15:51:51,167 [Thread-0] INFO Phase: Preparing phase for use: ALCU_EPSILON
15:51:51,551 [Thread-0] INFO Phase: Preparing phase for use: ALCU_ETA
15:51:51,906 [Thread-0] INFO Phase: Preparing phase for use: ALCU_PRIME
15:51:52,272 [Thread-0] INFO Phase: Preparing phase for use: ALCU_THETA
15:51:52,629 [Thread-0] INFO Phase: Preparing phase for use: ALCU_ZETA
15:51:52,977 [Thread-0] INFO Phase: Preparing phase for use: ALLI
15:51:53,325 [Thread-0] INFO Phase: Preparing phase for use: ALMO
15:51:53,672 [Thread-0] INFO Phase: Preparing phase for use: ALM_D019
15:51:54,019 [Thread-0] INFO Phase: Preparing phase for use: ALND_AMORPHOUS
15:51:54,368 [Thread-0] INFO Phase: Preparing phase for use: ALTI
15:51:54,719 [Thread-0] INFO Phase: Preparing phase for use: BCC_B2
15:51:55,063 [Thread-0] INFO Phase: Preparing phase for use: BCC_A2
15:51:55,427 [Thread-0] INFO Phase: Preparing phase for use: BCT_A5
15:51:55,769 [Thread-0] INFO Phase: Preparing phase for use: CBCC_A12
15:51:56,117 [Thread-0] INFO Phase: Preparing phase for use: CR3SI_A15
15:51:56,459 [Thread-0] INFO Phase: Preparing phase for use: CRSI2
15:51:56,805 [Thread-0] INFO Phase: Preparing phase for use: CU19SI6_ETA
15:51:57,153 [Thread-0] INFO Phase: Preparing phase for use: CU33SI7_DELTA
15:51:57,498 [Thread-0] INFO Phase: Preparing phase for use: CU4SI_EPSILON
15:51:57,847 [Thread-0] INFO Phase: Preparing phase for use: CU56SI11_GAMMA
15:51:58,188 [Thread-0] INFO Phase: Preparing phase for use: CU6Y
15:51:58,534 [Thread-0] INFO Phase: Preparing phase for use: CUB_A13
15:51:58,874 [Thread-0] INFO Phase: Preparing phase for use: CUB_A15
15:51:59,217 [Thread-0] INFO Phase: Preparing phase for use: DIAMOND_A4
15:51:59,559 [Thread-0] INFO Phase: Preparing phase for use: FCC_A1
15:51:59,910 [Thread-0] INFO Phase: Preparing phase for use: GAMMA_D83
15:52:00,255 [Thread-0] INFO Phase: Preparing phase for use: GAMMA_H
15:52:00,597 [Thread-0] INFO Phase: Preparing phase for use: HCP_A3
15:52:00,946 [Thread-0] INFO Phase: Preparing phase for use: HCP_ZN
15:52:01,294 [Thread-0] INFO Phase: Preparing phase for use: LAVES_C14
15:52:01,639 [Thread-0] INFO Phase: Preparing phase for use: LAVES_C15
15:52:01,984 [Thread-0] INFO Phase: Preparing phase for use: LAVES_C36
15:52:02,335 [Thread-0] INFO Phase: Preparing phase for use: SIV3
Calculated 16744 grid points in 22 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 22 s
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /WCFS: vwcs
Output from POLY-3, equilibrium = 1, label A0 , database: USER

Conditions:
T=1300, P=101325, N=1, X(SI)=0.25, X(AL)=0.2
DEGREES OF FREEDOM 0

Temperature 1300.00 K ( 1026.85 C), Pressure 1.013250E+05
Number of moles of components 1.00000E+00, Mass in grams 4.73680E+01
Total Gibbs energy -8.02595E+04, Enthalpy 3.22931E+04, Volume 0.00000E+00

Component Moles W-Fraction Activity Potential Ref.stat
AL 2.0000E-01 1.1393E-01 5.1836E-05 -1.0665E+05 SER
CU 5.5000E-01 7.3785E-01 4.1349E-04 -8.4211E+04 SER
SI 2.5000E-01 1.4823E-01 9.3957E-03 -5.0450E+04 SER

LIQUID Status ENTERED Driving force 0.0000E+00
Moles 1.0000E+00, Mass 4.7368E+01, Volume fraction 0.0000E+00 Mass fractions:
CU 7.37847E-01 SI 1.48228E-01 AL 1.13925E-01
POLY: Hit RETURN to continue
POLY: @@ We want to calculate the monovariant lines with liquid.

POLY: @@ Select two compositions and the temperature as the axis.
POLY: s-a-v 1 x(al)
... the command in full is SET_AXIS_VARIABLE
Min value /0/: 0
Max value /1/: 1
Increment /.025/: .01
POLY: s-a-v 2 x(si)
... the command in full is SET_AXIS_VARIABLE
Min value /0/: 0
Max value /1/: 1
Increment /.025/: .01
POLY: s-a-v 3 t 500 2000 25
... the command in full is SET_AXIS_VARIABLE
POLY: @@ Set liquid as "present", otherwise all monovariant lines
POLY: @@ are calculated.
POLY: adva
... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: ?
EQUILIBRIUM_CALCUL NEW_COMPOSITION_SET STABILITY_CHECK
GLOBAL_MINIMIZATION OUTPUT_FILE_FOR_SHOW STEP_AND_MAP
IGNORE_COMPOSI_SET_ORDER PARAEQUILIBRIUM T-ZERO_TEMPERATURE
KEEP_COMP_SET_NUMBERS PHASE_ADDITION TOGGLE_ALTERNATE_MODE
LIST_PHASE_ADDITION PRESENT_PHASE
MAJOR_CONSTITUENTS SHOW_FOR_T=
Which option? /STEP_AND_MAP/: present
Phase name /NONE/: liquid
POLY:
POLY: save tcex19a1 y
... the command in full is SAVE_WORKSPACES
POLY: map
Version R mapping is selected

Organizing start points

```

NO INITIAL EQUILIBRIUM ADDED, TRYING TO FIX ONE
 Generating start point 1
 Generating start point 2
 Phase region boundary 1 at: 8.426E-02 2.500E-01 1.182E+03
 LIQUID
 ** BCC_B2
 ** DIAMOND_A4
 *** Buffer saved on file:
 c:\jenkins\workspace\generate_console_examples\examples\tcex19A\tcex19a1.POLY3
 CALCULATED 35 EQUILIBRIA
 Phase region boundary 2 at: 4.045E-01 1.269E-01 9.785E+02
 LIQUID
 ALCU_EPSILON
 ** BCC_B2
 ** DIAMOND_A4
 SKIPPING LINE WITHOUT LIQUID#1
 Phase region boundary 2 at: 4.045E-01 1.269E-01 9.785E+02
 LIQUID
 ** ALCU_EPSILON
 ** BCC_B2
 Terminating at diagram limit
 CALCULATED 18 EQUILIBRIA
 Phase region boundary 2 at: 4.045E-01 1.269E-01 9.785E+02
 LIQUID
 ** ALCU_EPSILON
 ** DIAMOND_A4
 CALCULATED 20 EQUILIBRIA
 Phase region boundary 2 at: 5.755E-01 8.764E-02 8.678E+02
 LIQUID
 ** ALCU_EPSILON
 ALCU_ETA
 ** DIAMOND_A4
 SKIPPING LINE WITHOUT LIQUID#1
 Phase region boundary 2 at: 5.755E-01 8.764E-02 8.678E+02
 LIQUID
 ** ALCU_EPSILON
 ** ALCU_ETA
 Terminating at diagram limit
 CALCULATED 16 EQUILIBRIA
 Phase region boundary 2 at: 5.755E-01 8.764E-02 8.678E+02
 LIQUID
 ** ALCU_ETA
 ** DIAMOND_A4
 CALCULATED 8 EQUILIBRIA
 Phase region boundary 2 at: 6.299E-01 7.685E-02 8.291E+02
 LIQUID
 ** ALCU_ETA
 ALCU_THETA
 ** DIAMOND_A4
 SKIPPING LINE WITHOUT LIQUID#1
 Phase region boundary 2 at: 6.299E-01 7.685E-02 8.291E+02
 LIQUID
 ** ALCU_ETA
 ** ALCU_THETA
 Terminating at diagram limit
 CALCULATED 13 EQUILIBRIA
 Phase region boundary 2 at: 6.299E-01 7.685E-02 8.291E+02
 LIQUID
 ** ALCU_THETA
 ** DIAMOND_A4
 CALCULATED 18 EQUILIBRIA
 Phase region boundary 2 at: 7.774E-01 7.282E-02 7.852E+02
 LIQUID
 ** ALCU_THETA
 ** DIAMOND_A4
 FCC_A1
 SKIPPING LINE WITHOUT LIQUID#1
 Phase region boundary 2 at: 7.774E-01 7.282E-02 7.852E+02
 LIQUID
 ** ALCU_THETA
 ** FCC_A1
 Terminating at diagram limit
 CALCULATED 12 EQUILIBRIA
 Phase region boundary 2 at: 7.774E-01 7.282E-02 7.852E+02
 LIQUID
 ** DIAMOND_A4
 ** FCC_A1
 *** SORRY CANNOT CONTINUE *** 4
 CALCULATED 18 EQUILIBRIA
 Phase region boundary 2 at: 8.426E-02 2.500E-01 1.182E+03
 LIQUID
 ** BCC_B2
 ** DIAMOND_A4
 CALCULATED 8 EQUILIBRIA
 Phase region boundary 2 at: 3.577E-02 2.616E-01 1.025E+03
 LIQUID
 ** BCC_B2
 CU19SI6_ETA
 ** DIAMOND_A4
 SKIPPING LINE WITHOUT LIQUID#1
 Phase region boundary 2 at: 3.577E-02 2.616E-01 1.025E+03
 LIQUID
 ** BCC_B2
 ** CU19SI6_ETA
 Terminating at diagram limit
 CALCULATED 12 EQUILIBRIA
 Phase region boundary 2 at: 3.577E-02 2.616E-01 1.025E+03
 LIQUID

```

** CU19SI6_ETA
** DIAMOND_A4
Terminating at diagram limit
CALCULATED 9 EQUILIBRIA
*** LAST BUFFER SAVED ON FILE: c:\jenkins\workspace\generate_console_examples\examples\tcex19A\tcex19a1.POLY3
CPU time for mapping 1 seconds
POLY:
POLY: @@ The monovariant line FCC/BCC/LIQ in the Cu corner is not
POLY: @@ connected, so add a start point. This is different from a
POLY: @@ MAP with two axes, where all connected or non-connected
POLY: @@ lines can be found automatically.
POLY:
POLY: read tcex19a1
... the command in full is READ_WORKSPACES
POLY:
POLY: s-c x(al)=.1 x(si)=.1
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 16744 grid points in 1 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 1 s
POLY: adva
... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /LIQUID#1/: Liquid
POLY:
POLY: map
Version R mapping is selected

Organizing start points

NO INITIAL EQUILIBRIUM ADDED, TRYING TO FIX ONE
Generating start point 1
Generating start point 2

Phase region boundary 1 at: 4.390E-02 1.000E-01 1.285E+03
    LIQUID
    ** BCC_B2
    ** FCC_A1
Terminating at diagram limit
CALCULATED 18 EQUILIBRIA

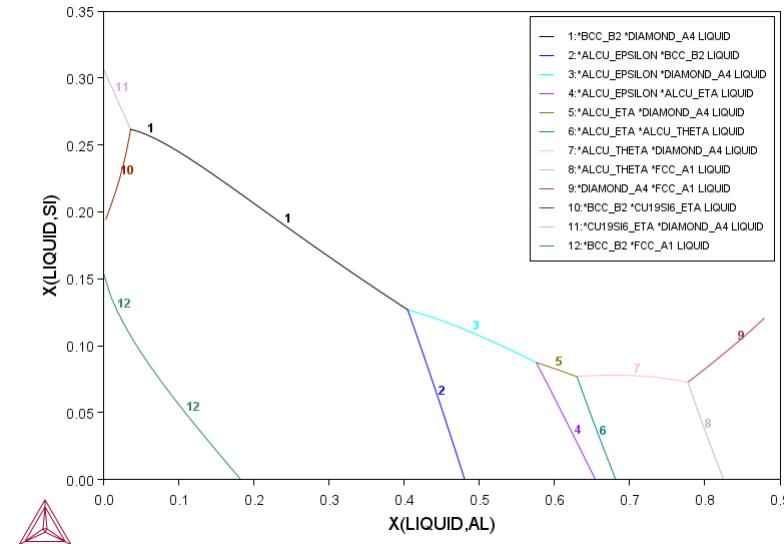
Phase region boundary 2 at: 4.390E-02 1.000E-01 1.285E+03
    LIQUID
    ** BCC_B2
    ** FCC_A1
Terminating at diagram limit
CALCULATED 9 EQUILIBRIA
*** LAST BUFFER SAVED ON FILE: c:\jenkins\workspace\generate_console_examples\examples\tcex19A\tcex19a1.POLY3
CPU time for mapping 0 seconds
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: @@ We want the liquid compositions only
POST: s-d-a x (liquid,al)
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y x (liquid,si)
... the command in full is SET_DIAGRAM_AXIS
POST: s-lab b
... the command in full is SET_LABEL_CURVE_OPTION
POST:
POST: set-title example 19Aa
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 19Aa



```

POST:
POST: Hit RETURN to continue
POST: @@ Make it triangular and scale the axis
POST: s-d-t
... the command in full is SET_DIAGRAM_TYPE
TRIANGULAR DIAGRAM (Y OR N) /N/: y,....,
POST: s-sc y n 0 1

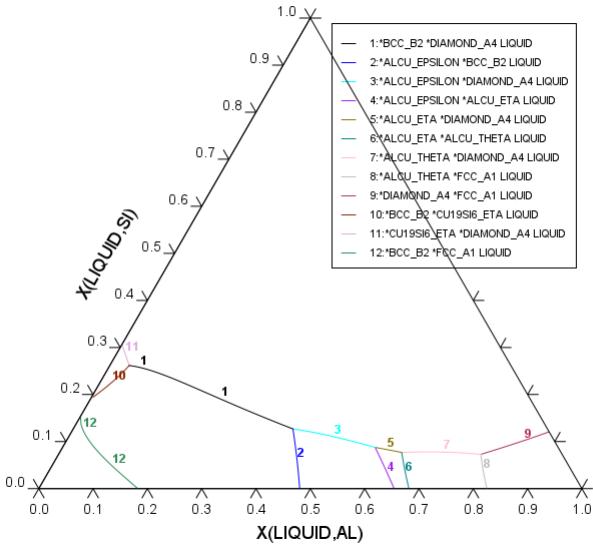
```

```

... the command in full is SET_SCALING_STATUS
POST: s-sc x n 0 1
... the command in full is SET_SCALING_STATUS
POST: @@ Plot the phases stable along the lines
POST: s-lab b
... the command in full is SET_LABEL_CURVE_OPTION
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples/unite/distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAIFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 19Aa

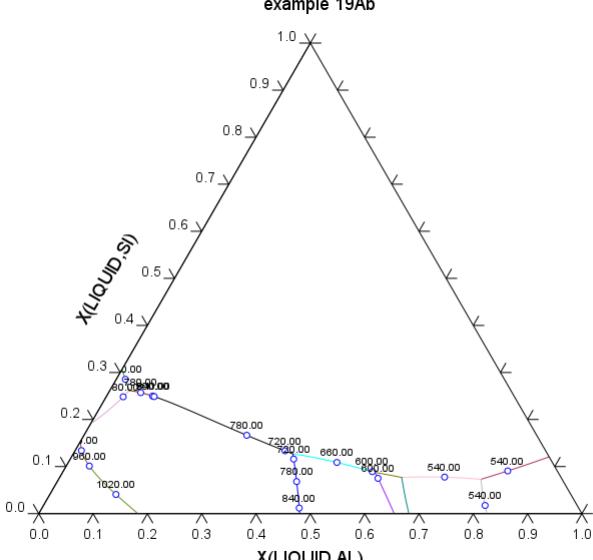


```

POST:
POST:Hit RETURN to continue
POST: @@ Take away the phase labels and add tic
POST: @@ marks along the lines (the Z axis)
POST:
POST: s-lab n
... the command in full is SET_LABEL_CURVE_OPTION
POST: s-d-a z t-c
... the command in full is SET_DIAGRAM_AXIS
POST: s-sc z n 500 1000
... the command in full is SET_SCALING_STATUS
POST: set-title example 19Ab
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples/unite/distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAIFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT DIAGRAM

```

example 19Ab



```

POLY: s-a-v 3
... the command in full is SET_AXIS_VARIABLE
Condition /T/: none
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 16744 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY: save tce19a2.y
... the command in full is SAVE_WORKSPACES
POLY: l-c
... the command in full is LIST_CONDITIONS
T=1300, P=101325, N=1, X(SI)=0.25, X(AL)=0.2
DEGREES OF FREEDOM 0
POLY: s-c x(al)
... the command in full is SET_CONDITION
Value /2/: .10
POLY: @@ Use ADD to have several start points at different
POLY: @@ temperatures. But do not use default direction as
POLY: @@ that creates many start points. Increasing the SI
POLY: @@ content makes a solid phase stable.
POLY:
POLY: adva
... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /LIQUID#1/: liquid
POLY: add 2
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY: add -2
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY:
POLY:
POLY: @@ You can have initial equilibria for different conditions
POLY: @@ at the same time. Just the axis variables have to be
POLY: @@ the same. To make nice isothermal curves is not easy;
POLY: @@ try with several start points to find all curve sections.
POLY:
POLY: s-c t
... the command in full is SET_CONDITION
Value /1300/: 1200
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 16744 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY: adva
... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /LIQUID#1/: liquid
POLY: add 2
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY: add -2
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY:
POLY:
POLY: s-c t
... the command in full is SET_CONDITION
Value /1200/: 1100
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 16744 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 1 s, total time 1 s
POLY: adva
... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /LIQUID#1/: liquid
POLY: add 2
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY: add -2
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY:
POLY:
POLY: @@ This line exists only in the Al rich corner
POLY: s-c x(al)=.5 x(si)=.1
... the command in full is SET_CONDITION
POLY: s-c t
... the command in full is SET_CONDITION
Value /1100/: 1000
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 16744 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY: adva
... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /LIQUID#1/: liquid
POLY: add 2
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY: add -2
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY:
POLY: @@ A start point in the low melting Al corner too
POLY:
POLY: s-c x(al)=.9 x(si)=.01 t=900
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 16744 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY: adva
... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /LIQUID#1/: liquid
POLY: add 1

```

```

... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY: add -1
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY:
POLY:
POLY: map
Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard

Phase region boundary 1 at: 5.000E-02 6.891E-01
    LIQUID
    ** DIAMOND_A4
Calculated                      10 equilibria

Phase region boundary 2 at: 5.000E-02 6.891E-01
    LIQUID
    ** DIAMOND_A4
Calculated                      52 equilibria

Phase region boundary 3 at: 1.004E-01 3.055E-02
    LIQUID
    ** FCC_A1
Calculated                      21 equilibria

Phase region boundary 4 at: 1.004E-01 3.055E-02
    LIQUID
    ** FCC_A1
Calculated                      5 equilibria

Phase region boundary 5 at: 1.373E-01 1.932E-02
    LIQUID
    ** BCC_B2
    ** FCC_A1
Calculated                      51 equilibria

Phase region boundary 6 at: 1.463E-01 2.848E-02
    LIQUID
    ** BCC_B2
Calculated                      51 equilibria

Phase region boundary 7 at: 1.373E-01 1.932E-02
    LIQUID
    ** FCC_A1
Calculated                      27 equilibria

Phase region boundary 8 at: 5.000E-02 6.515E-01
    LIQUID
    ** DIAMOND_A4
Calculated                      43 equilibria

Phase region boundary 9 at: 5.000E-02 6.515E-01
    LIQUID
    ** DIAMOND_A4
Calculated                      52 equilibria

Phase region boundary 10 at: 1.081E-01 1.639E-01
    LIQUID
    ** BCC_B2
Calculated                      16 equilibria

Phase region boundary 11 at: 2.872E-02 1.169E-01
    LIQUID
    ** BCC_B2
    ** FCC_A1
Calculated                      13 equilibria

Phase region boundary 12 at: 2.764E-02 9.624E-02
    LIQUID
    ** FCC_A1
Calculated                      13 equilibria

Phase region boundary 13 at: 2.872E-02 1.169E-01
    LIQUID
    ** BCC_B2
Calculated                      70 equilibria

Phase region boundary 14 at: 1.081E-01 1.639E-01
    LIQUID
    ** BCC_B2
Calculated                      44 equilibria

Phase region boundary 15 at: 5.000E-02 6.262E-01
    LIQUID
    ** DIAMOND_A4
Calculated                      38 equilibria

Phase region boundary 16 at: 5.000E-02 6.262E-01
    LIQUID
    ** DIAMOND_A4
Calculated                      56 equilibria

Phase region boundary 17 at: 1.116E-01 1.999E-01

```

```

LIQUID
** BCC_B2
Calculated           23 equilibria

Phase region boundary 18 at: 1.116E-01 1.999E-01
    LIQUID
    ** BCC_B2
Calculated.          34 equilibria

Phase region boundary 19 at: 4.370E-01 1.765E-02
    LIQUID
    ** ALCU_EPSILON
    ** BCC_B2
Calculated.          18 equilibria

Phase region boundary 20 at: 4.453E-01 1.265E-02
    LIQUID
    ** ALCU_EPSILON
Calculated.          43 equilibria

Phase region boundary 21 at: 4.370E-01 1.765E-02
    LIQUID
    ** BCC_B2
Calculated.          43 equilibria

Phase region boundary 22 at: 2.106E-02 1.939E-01
    LIQUID
    ** BCC_B2
    ** CU19SI6_ETA
Calculated.          24 equilibria

Phase region boundary 23 at: 7.190E-03 2.263E-01
    LIQUID
    ** CU19SI6_ETA
Calculated.          8 equilibria

Phase region boundary 24 at: 2.500E-01 5.691E-01
    LIQUID
    ** DIAMOND_A4
Calculated.          8 equilibria

Phase region boundary 25 at: 1.890E-01 5.683E-01
    LIQUID
    ** BCC_B2
    ** DIAMOND_A4
Calculated.          5 equilibria

Phase region boundary 26 at: 3.667E-01 1.003E-01
    LIQUID
    ** BCC_B2
Calculated.          5 equilibria

Phase region boundary 27 at: 3.979E-01 7.953E-02
    LIQUID
    ** ALCU_EPSILON
    ** BCC_B2
Calculated.          28 equilibria

Phase region boundary 28 at: 4.219E-01 5.542E-02
    LIQUID
    ** ALCU_EPSILON
Calculated.          28 equilibria

Phase region boundary 29 at: 1.890E-01 5.683E-01
    LIQUID
    ** DIAMOND_A4
Calculated.          42 equilibria

Phase region boundary 30 at: 2.500E-01 5.691E-01
    LIQUID
    ** DIAMOND_A4
Calculated.          49 equilibria

Phase region boundary 31 at: 4.698E-01 3.348E-02
    LIQUID
    ** ALCU_EPSILON
Calculated.          6 equilibria
Terminating at known equilibrium

Phase region boundary 32 at: 4.698E-01 3.348E-02
    LIQUID
    ** ALCU_EPSILON
Calculated.          27 equilibria

Phase region boundary 33 at: 9.694E-01 5.516E-03
    LIQUID
    ** FCC_A1
Calculated.          12 equilibria

Phase region boundary 34 at: 9.694E-01 5.516E-03
    LIQUID
    ** FCC_A1
Calculated.          16 equilibria

Phase region boundary 35 at: 5.506E-01 5.000E-03
    LIQUID
    ** ALCU_EPSILON
Calculated.          18 equilibria

Phase region boundary 36 at: 5.506E-01 5.000E-03
    LIQUID
    ** ALCU_EPSILON
Calculated.          10 equilibria

Phase region boundary 37 at: 4.954E-01 4.888E-02
    LIQUID
    ** ALCU_EPSILON
    ** DIAMOND_A4
Calculated.          35 equilibria

Phase region boundary 38 at: 2.690E-01 5.489E-01
    LIQUID
    ** DIAMOND_A4
Calculated.          35 equilibria

Phase region boundary 39 at: 4.954E-01 4.888E-02
    LIQUID
    ** ALCU_EPSILON
Calculated.          22 equilibria
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\generate_console_examples\examples\tcex19A\tcex19a2.POLY3
CPU time for mapping          10 seconds

```

POLY: post

POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: s-d-a x x(liquid,al)

... the command in full is SET_DIAGRAM_AXIS

POST: s-d-a y x(liquid,si)

... the command in full is SET_DIAGRAM_AXIS

POST: s-d-ty y,,,

... the command in full is SET_DIAGRAM_TYPE

POST:

POST:

POST: set-title example 19Ac

POST:

POST:

POST: SET_EXP_FILE_FORMAT 5

POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y

... the command in full is MAKE_EXPERIMENTAL_DATAFI

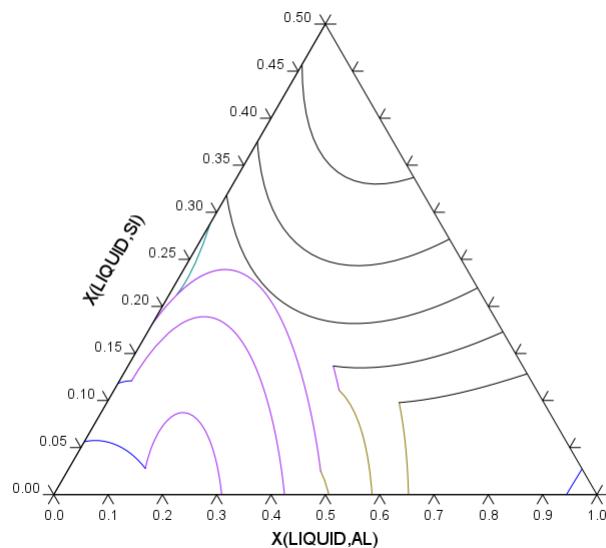
POST: SET_EXP_FILE_FORMAT 10

POST:

POST: plot

... the command in full is PLOT_DIAGRAM

example 19Ac



POST:

POST: Hit RETURN to continue

POST: a-e-d y tcex19a

... the command in full is APPEND_EXPERIMENTAL_DATA

PROLOGUE NUMBER: /0/: 0

DATASET NUMBER(s): /-1/: 1

POST: set-title example 19Ad

POST:

POST:

POST: SET_EXP_FILE_FORMAT 5

POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y

... the command in full is MAKE_EXPERIMENTAL_DATAFI

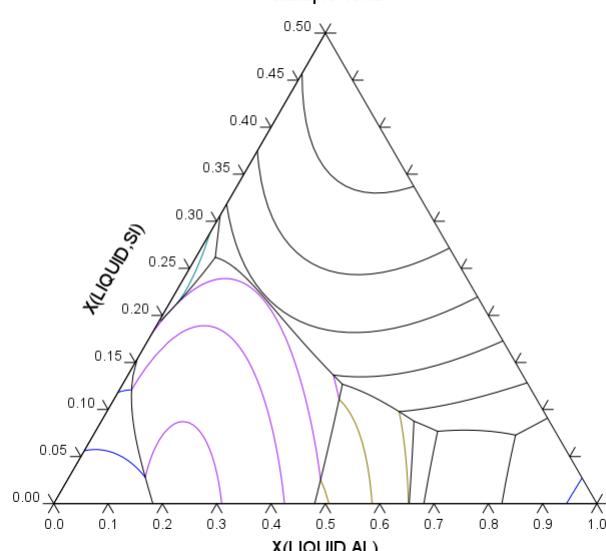
POST: SET_EXP_FILE_FORMAT 10

POST:

POST: plot

... the command in full is PLOT_DIAGRAM

example 19Ad



POST:

POST: Hit RETURN to continue

POST: add .1 .4 n 1300 K

... the command in full is ADD_LABEL_TEXT

Text size: /.36/:

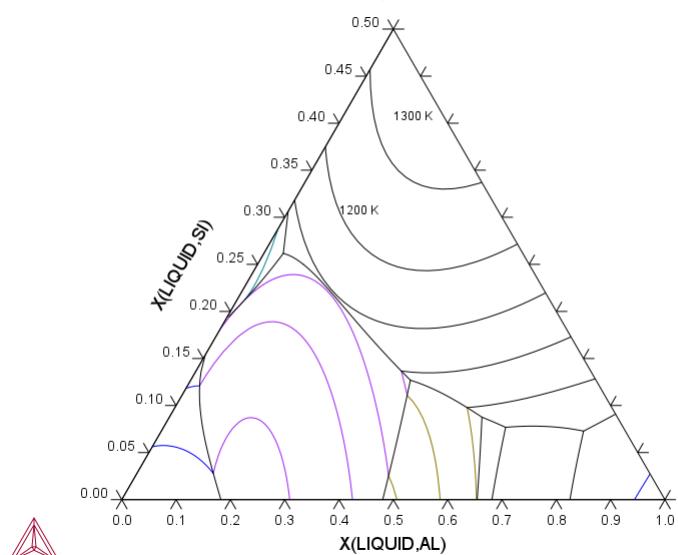
POST:

POST: add .1 .3 n 1200 K

... the command in full is ADD_LABEL_TEXT

```
Text size: /.36/:  
POST:  
POST: set-title example 19Ae  
POST:  
POST:  
POST: SET_EXP_FILE_FORMAT 5  
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y  
... the command in full is MAKE_EXPERIMENTAL_DATAFILE  
POST: SET_EXP_FILE_FORMAT 10  
POST:  
POST: plot  
... the command in full is PLOT_DIAGRAM
```

example 19Ae



```
POST:  
POST: set-inter  
... the command in full is SET_INTERACTIVE_MODE  
POST:
```

tce19B

SYS:About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

```
SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce19B\tce19B.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Mapping of univariant equilibria with the liquid in Al-Cu-Si
SYS:
SYS: @@ This is the second part of a two part example showing how
SYS: @@ to map univariant equilibria with the liquid in Al-Cu-Si.
SYS: @@ Part B. Using the Ternary module, you can get the
SYS: @@ information on invariant reactions, such as temperature
SYS: @@ and compositions.
SYS:
SYS: set-log ex19b.,
SYS: go ter
... the command in full is GOTO_MODULE

Quick ternary phase diagram calculation module

THERMODYNAMIC DATABASE module
Database folder: C:\jenkins\workspace\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA           /* DEFINED
DICTRA_FCC_A1 REJECTED
Current database: Iron Demo Database v4.0

VA           /* DEFINED
Database: /FEDEMO/: user tce19_cost2.TDB
Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

VA           /* DEFINED
15:53:33,679 [Thread-0] INFO TDBfileParser: USER_1502895690_14, number of lines read: 470
15:53:33,901 [Thread-0] INFO DatabaseUtils: Parsing of USER_1502895690_14 completed in 271 ms
First element: al cu si
Phase Diagram, Monovariants, or Liquidus Surface: /Phase_Diagram/: L
Min temperature, C /25/: 25
Max temperature, C /2500/: 2500
Temperature interval /100/: 100
Global minimization on: /N/: N
VA           /* DEFINED
REINITIATING GES .....
AL          CU          SI
DEFINED
*** ERROR GAS INPUT IGNORED

*****
* WARNING: This database has no list of assessed systems *
*           The diagram may be wrong. *
*****


Quit? /Y/: N
15:53:33,990 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS .....
FUNCTIONS .....

List of references for assessed data
'COST2 - TCOST507 Light Alloys Database (Version 2.1), provided by TCSAB,
1999/2003. '
'COST (1998): COST 507 -- Definition of Thermochemical and Thermophysical
Properties to Provide a Database for the Development of New Light
Alloys. European Cooperation in the Field of Scientific and Technical
Research, European Commission. Vol 1. Proceedings of the Final
Workshop of COST 507, Vals, the Netherlands, 1997; Vol 2.
Thermochemical Database for Light Metal Alloys (Eds. Ansara I.,
Dinsdale A.T., and Rand M.H.); Vol 3. Critical Evaluation of Ternary
Systems (Ed. Effenberg G.). '
-OK-
Forcing automatic start values
Automatic start values will be set
15:53:34,531 [Thread-0] INFO Database: Preparing system for use: USER_1502895690_14
15:53:35,335 [Thread-0] INFO Phase: Preparing phase for use: LIQUID
15:53:35,829 [Thread-0] INFO Phase: Preparing phase for use: ALCU_AMORPHOUS
15:53:36,221 [Thread-0] INFO Phase: Preparing phase for use: ALCUZN_T
15:53:36,617 [Thread-0] INFO Phase: Preparing phase for use: ALCU_DELTA
15:53:37,081 [Thread-0] INFO Phase: Preparing phase for use: ALCU_EPSILON
15:53:37,486 [Thread-0] INFO Phase: Preparing phase for use: ALCU_ETA
15:53:37,879 [Thread-0] INFO Phase: Preparing phase for use: ALCU_PRIME
15:53:38,268 [Thread-0] INFO Phase: Preparing phase for use: ALCU_THETA
15:53:38,656 [Thread-0] INFO Phase: Preparing phase for use: ALCU_ZETA
15:53:39,038 [Thread-0] INFO Phase: Preparing phase for use: ALLI
15:53:39,420 [Thread-0] INFO Phase: Preparing phase for use: ALMO
15:53:39,794 [Thread-0] INFO Phase: Preparing phase for use: ALM_D019
15:53:40,170 [Thread-0] INFO Phase: Preparing phase for use: ALND_AMORPHOUS
15:53:40,546 [Thread-0] INFO Phase: Preparing phase for use: ALTI
15:53:40,929 [Thread-0] INFO Phase: Preparing phase for use: BCC_B2
15:53:41,304 [Thread-0] INFO Phase: Preparing phase for use: BCC_A2
15:53:41,676 [Thread-0] INFO Phase: Preparing phase for use: BCT_A5
15:53:42,050 [Thread-0] INFO Phase: Preparing phase for use: CBCC_A12
15:53:42,426 [Thread-0] INFO Phase: Preparing phase for use: CR3SI_A15
```

```
15:53:42,799 [Thread-0] INFO Phase: Preparing phase for use: CRSI2
15:53:43,169 [Thread-0] INFO Phase: Preparing phase for use: CU19SI6_ETA
15:53:43,546 [Thread-0] INFO Phase: Preparing phase for use: CU33SI7_DELTA
15:53:43,921 [Thread-0] INFO Phase: Preparing phase for use: CU4SI_EPSILON
15:53:44,298 [Thread-0] INFO Phase: Preparing phase for use: CU56SI11_GAMMA
15:53:44,678 [Thread-0] INFO Phase: Preparing phase for use: CU6Y
15:53:45,053 [Thread-0] INFO Phase: Preparing phase for use: CUB_A13
15:53:45,425 [Thread-0] INFO Phase: Preparing phase for use: CUB_A15
15:53:45,799 [Thread-0] INFO Phase: Preparing phase for use: DIAMOND_A4
15:53:46,173 [Thread-0] INFO Phase: Preparing phase for use: FCC_A1
15:53:46,551 [Thread-0] INFO Phase: Preparing phase for use: GAMMA_D83
15:53:46,926 [Thread-0] INFO Phase: Preparing phase for use: GAMMA_H
15:53:47,301 [Thread-0] INFO Phase: Preparing phase for use: HCP_A3
15:53:47,674 [Thread-0] INFO Phase: Preparing phase for use: HCP_ZN
15:53:48,047 [Thread-0] INFO Phase: Preparing phase for use: LAVES_C14
15:53:48,423 [Thread-0] INFO Phase: Preparing phase for use: LAVES_C15
15:53:48,798 [Thread-0] INFO Phase: Preparing phase for use: LAVES_C36
15:53:49,175 [Thread-0] INFO Phase: Preparing phase for use: SIV3
Forcing automatic start values
Automatic start values will be set
Forcing automatic start values
Automatic start values will be set
T = 1673.15 K
Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2

Phase region boundary 1 at: 7.327E-03 9.853E-01
    LIQUID
    ** DIAMOND_A4
Calculated                15 equilibria

Phase region boundary 2 at: 7.327E-03 9.853E-01
    LIQUID
    ** DIAMOND_A4
Calculated                15 equilibria
*** BUFFER SAVED ON FILE: C:\Users\azureuser\AppData\Local\Temp\MONOVAR_002.POLY3
CPU time for mapping      1 seconds
T = 1573.15 K

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2

Phase region boundary 1 at: 7.453E-02 8.883E-01
    LIQUID
    ** DIAMOND_A4
Calculated                23 equilibria

Phase region boundary 2 at: 7.453E-02 8.883E-01
    LIQUID
    ** DIAMOND_A4
Calculated                25 equilibria
*** BUFFER SAVED ON FILE: C:\Users\azureuser\AppData\Local\Temp\MONOVAR_002.POLY3
CPU time for mapping      0 seconds
T = 1473.15 K

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2

Phase region boundary 1 at: 1.372E-01 7.942E-01
    LIQUID
    ** DIAMOND_A4
Calculated                30 equilibria

Phase region boundary 2 at: 1.372E-01 7.942E-01
    LIQUID
    ** DIAMOND_A4
Calculated                22 equilibria
*** BUFFER SAVED ON FILE: C:\Users\azureuser\AppData\Local\Temp\MONOVAR_002.POLY3
CPU time for mapping      1 seconds
T = 1373.15 K

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2

Phase region boundary 1 at: 1.926E-01 7.111E-01
    LIQUID
    ** DIAMOND_A4
Calculated                28 equilibria

Phase region boundary 2 at: 1.926E-01 7.111E-01
```

```
LIQUID
** DIAMOND_A4
Calculated          32 equilibria
*** BUFFER SAVED ON FILE: C:\Users\azureuser\AppData\Local\Temp\MONOVAR_002.POLY3
CPU time for mapping      0 seconds
T = 1273.15 K

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point  1
Generating start point  2

Phase region boundary  1 at:  6.652E-01  9.329E-03
    LIQUID
    ** BCC_B2
Calculated.           2 equilibria

Phase region boundary  2 at:  6.645E-01  6.795E-03
    LIQUID
    ** BCC_B2
    ** GAMMA_H
Calculated.           12 equilibria

Phase region boundary  3 at:  6.653E-01  4.077E-03
    LIQUID
    ** GAMMA_H
Calculated.           12 equilibria

Phase region boundary  4 at:  6.645E-01  6.795E-03
    LIQUID
    ** BCC_B2
Calculated.           29 equilibria

Phase region boundary  5 at:  8.419E-01  6.666E-02
    LIQUID
    ** BCC_B2
    ** FCC_A1
Calculated.           25 equilibria

Phase region boundary  6 at:  8.633E-01  4.917E-02
    LIQUID
    ** FCC_A1
Calculated.           25 equilibria

Phase region boundary  7 at:  6.652E-01  9.329E-03
    LIQUID
    ** BCC_B2
Calculated.           30 equilibria
Terminating at known equilibrium
*** BUFFER SAVED ON FILE: C:\Users\azureuser\AppData\Local\Temp\MONOVAR_002.POLY3
CPU time for mapping      0 seconds

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point  1
Generating start point  2

Phase region boundary  1 at:  2.311E-01  6.535E-01
    LIQUID
    ** DIAMOND_A4
Calculated.           34 equilibria

Phase region boundary  2 at:  2.311E-01  6.535E-01
    LIQUID
    ** DIAMOND_A4
Calculated.           34 equilibria
*** BUFFER SAVED ON FILE: C:\Users\azureuser\AppData\Local\Temp\MONOVAR_002.POLY3
CPU time for mapping      0 seconds
T = 1173.15 K

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point  1
Generating start point  2

Phase region boundary  1 at:  5.840E-01  7.591E-03
    LIQUID
    ** BCC_B2
Calculated.           9 equilibria

Phase region boundary  2 at:  5.840E-01  7.591E-03
    LIQUID
    ** BCC_B2
Calculated.           39 equilibria

Phase region boundary  3 at:  8.543E-01  1.296E-01
    LIQUID
    ** BCC_B2
    ** FCC_A1

Phase region boundary  4 at:  8.749E-01  1.099E-01
    LIQUID
    ** FCC_A1
Calculated.           24 equilibria
```

```

Phase region boundary  5 at:   8.543E-01  1.296E-01
    LIQUID
    ** BCC_B2
Calculated              54 equilibria
*** BUFFER SAVED ON FILE: C:\Users\azureuser\AppData\Local\Temp\MONOVAR_002.POLY3
CPU time for mapping      1 seconds

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point  1
Generating start point  2

Phase region boundary  1 at:   2.562E-01  6.158E-01
    LIQUID
    ** DIAMOND_A4
Calculated              39 equilibria

Phase region boundary  2 at:   2.562E-01  6.158E-01
    LIQUID
    ** DIAMOND_A4
Calculated              37 equilibria
*** BUFFER SAVED ON FILE: C:\Users\azureuser\AppData\Local\Temp\MONOVAR_002.POLY3
CPU time for mapping      0 seconds
T = 1073.15 K

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point  1
Generating start point  2

Phase region boundary  1 at:   5.198E-01  5.412E-03
    LIQUID
    ** ALCU_EPSILON
Calculated              11 equilibria

Phase region boundary  2 at:   5.198E-01  5.412E-03
    LIQUID
    ** ALCU_EPSILON
Calculated              5 equilibria

Phase region boundary  3 at:   5.361E-01  2.533E-02
    LIQUID
    ** ALCU_EPSILON
    ** BCC_B2

Phase region boundary  4 at:   5.383E-01  3.569E-02
    LIQUID
    ** BCC_B2
Calculated.              12 equilibria

Phase region boundary  5 at:   5.962E-01  1.431E-01
    LIQUID
    ** BCC_B2
    ** DIAMOND_A4

Phase region boundary  6 at:   2.789E-01  5.911E-01
    LIQUID
    ** DIAMOND_A4
Calculated.              41 equilibria

Phase region boundary  7 at:   5.361E-01  2.533E-02
    LIQUID
    ** ALCU_EPSILON
Calculated.              16 equilibria
*** BUFFER SAVED ON FILE: C:\Users\azureuser\AppData\Local\Temp\MONOVAR_002.POLY3
CPU time for mapping      1 seconds

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point  1
Generating start point  2

Phase region boundary  1 at:   7.337E-01  2.597E-01
    LIQUID
    ** CU19SI6_ETA
Calculated.              4 equilibria

Phase region boundary  2 at:   7.478E-01  2.387E-01
    LIQUID
    ** BCC_B2
    ** CU19SI6_ETA

Phase region boundary  3 at:   7.525E-01  2.105E-01
    LIQUID
    ** BCC_B2
Calculated.              8 equilibria

Phase region boundary  4 at:   6.917E-01  2.112E-01
    LIQUID
    ** BCC_B2
    ** DIAMOND_A4

```

```

Phase region boundary  5 at:  3.329E-01  6.250E-01
    LIQUID
    ** DIAMOND_A4
Calculated.          14 equilibria

Phase region boundary  6 at:  3.469E-01  6.529E-01
    LIQUID
    ** CU19SI6_ETA
    ** DIAMOND_A4

Phase region boundary  7 at:  7.269E-01  2.729E-01
    LIQUID
    ** CU19SI6_ETA
Calculated.          6 equilibria
Terminating at known equilibrium

Phase region boundary  8 at:  7.337E-01  2.597E-01
    LIQUID
    ** CU19SI6_ETA
Calculated.          3 equilibria
Terminating at known equilibrium
*** BUFFER SAVED ON FILE: C:\Users\azureuser\AppData\Local\Temp\MONOVAR_002.POLY3
CPU time for mapping      0 seconds
T =   973.15 K

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point  1
Generating start point  2

Phase region boundary  1 at:  4.736E-01  5.113E-03
    LIQUID
    ** ALCU_EPSILON
Calculated.          12 equilibria

Phase region boundary  2 at:  4.736E-01  5.113E-03
    LIQUID
    ** ALCU_EPSILON
Calculated.          11 equilibria

Phase region boundary  3 at:  5.106E-01  6.209E-02
    LIQUID
    ** ALCU_EPSILON
    ** DIAMOND_A4

Phase region boundary  4 at:  2.273E-01  5.621E-01
    LIQUID
    ** DIAMOND_A4
Calculated.          36 equilibria

Phase region boundary  5 at:  5.106E-01  6.209E-02
    LIQUID
    ** ALCU_EPSILON
Calculated.          24 equilibria
*** BUFFER SAVED ON FILE: C:\Users\azureuser\AppData\Local\Temp\MONOVAR_002.POLY3
CPU time for mapping      0 seconds
T =   873.15 K

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point  1
Generating start point  2

Phase region boundary  1 at:  3.646E-02  1.803E-02
    LIQUID
    ** FCC_A1
Calculated.          15 equilibria

Phase region boundary  2 at:  3.646E-02  1.803E-02
    LIQUID
    ** FCC_A1
Calculated.          33 equilibria
*** BUFFER SAVED ON FILE: C:\Users\azureuser\AppData\Local\Temp\MONOVAR_002.POLY3
CPU time for mapping      1 seconds

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point  1
Generating start point  2

Phase region boundary  1 at:  4.151E-01  5.493E-03
    LIQUID
    ** ALCU_ETA
Calculated.          8 equilibria

Phase region boundary  2 at:  4.151E-01  5.493E-03
    LIQUID
    ** ALCU_ETA
Calculated.          6 equilibria

Phase region boundary  3 at:  4.241E-01  3.756E-02

```

```

LIQUID
** ALCU_EPSILON
** ALCU_ETA
Phase region boundary 4 at: 4.398E-01 3.756E-02
LIQUID
** ALCU_EPSILON
Calculated.          2 equilibria

Phase region boundary 5 at: 4.420E-01 4.464E-02
LIQUID
** ALCU_EPSILON
** DIAMOND_A4

Phase region boundary 6 at: 1.706E-01 5.446E-01
LIQUID
** DIAMOND_A4
Calculated          27 equilibria

Phase region boundary 7 at: 4.241E-01 3.756E-02
LIQUID
** ALCU_ETA
Calculated          17 equilibria
*** BUFFER SAVED ON FILE: C:\Users\azureuser\AppData\Local\Temp\MONOVAR_002.POLY3
CPU time for mapping      0 seconds
T = 773.15 K

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

T = 1773.15 K
Version R mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2

Phase region boundary 1 at: 3.379E-01 7.512E-02 8.731E+02
LIQUID
** ALCU_EPSILON
** ALCU_ETA
CALCULATED        4 EQUILIBRIA

Phase region boundary 2 at: 3.369E-01 8.764E-02 8.678E+02
LIQUID
** ALCU_EPSILON
** ALCU_ETA
DIAMOND_A4
SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary 2 at: 3.369E-01 8.764E-02 8.678E+02
LIQUID
** ALCU_EPSILON
** DIAMOND_A4
CALCULATED        25 EQUILIBRIA

Phase region boundary 2 at: 4.686E-01 1.269E-01 9.785E+02
LIQUID
** ALCU_EPSILON
BCC_B2
** DIAMOND_A4
SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary 2 at: 4.686E-01 1.269E-01 9.785E+02
LIQUID
** ALCU_EPSILON
** BCC_B2
Terminating at diagram limit
CALCULATED        34 EQUILIBRIA

Phase region boundary 2 at: 4.686E-01 1.269E-01 9.785E+02
LIQUID
** BCC_B2
** DIAMOND_A4
CALCULATED        43 EQUILIBRIA

Phase region boundary 2 at: 7.026E-01 2.616E-01 1.025E+03
LIQUID
** BCC_B2
** CU19SI6_ETA
** DIAMOND_A4
SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary 2 at: 7.026E-01 2.616E-01 1.025E+03
LIQUID
** BCC_B2
** CU19SI6_ETA
Terminating at known equilibrium
CALCULATED        37 EQUILIBRIA

Phase region boundary 2 at: 7.026E-01 2.616E-01 1.025E+03
LIQUID
** CU19SI6_ETA
** DIAMOND_A4
*** SORRY CANNOT CONTINUE ***      4

CALCULATED        16 EQUILIBRIA

Phase region boundary 2 at: 3.369E-01 8.764E-02 8.678E+02
LIQUID
** ALCU_ETA
** DIAMOND_A4
CALCULATED        9 EQUILIBRIA

Phase region boundary 2 at: 2.933E-01 7.685E-02 8.291E+02
LIQUID
** ALCU_ETA
ALCU_THETA
** DIAMOND_A4
SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary 2 at: 2.933E-01 7.685E-02 8.291E+02

```



```

Forcing automatic start values
Automatic start values will be set
Forcing automatic start values
Automatic start values will be set
Forcing automatic start values
Automatic start values will be set
Forcing automatic start values
Automatic start values will be set
Forcing automatic start values
Automatic start values will be set
Forcing automatic start values
Automatic start values will be set

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

Version R mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6

Phase region boundary 1 at: 3.379E-01 7.512E-02 8.731E+02
    LIQUID
** ALCU_EPSILON
** ALCU_ETA
CALCULATED      4 EQUILIBRIA

Phase region boundary 2 at: 3.369E-01 8.764E-02 8.678E+02
    LIQUID
** ALCU_EPSILON
** ALCU_ETA
    DIAMOND_A4
SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary 2 at: 3.369E-01 8.764E-02 8.678E+02
    LIQUID
** ALCU_EPSILON
** DIAMOND_A4
CALCULATED      25 EQUILIBRIA

Phase region boundary 2 at: 4.686E-01 1.269E-01 9.785E+02
    LIQUID
** ALCU_EPSILON
    BCC_B2
** DIAMOND_A4
SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary 2 at: 4.686E-01 1.269E-01 9.785E+02
    LIQUID
** ALCU_EPSILON
    BCC_B2
Terminating at diagram limit
CALCULATED      34 EQUILIBRIA

Phase region boundary 2 at: 4.686E-01 1.269E-01 9.785E+02
    LIQUID
** BCC_B2
** DIAMOND_A4
CALCULATED      43 EQUILIBRIA

Phase region boundary 2 at: 7.026E-01 2.616E-01 1.025E+03
    LIQUID
** BCC_B2
    CU19SI6_ETA
** DIAMOND_A4
SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary 2 at: 7.026E-01 2.616E-01 1.025E+03
    LIQUID
** BCC_B2
    CU19SI6_ETA
Terminating at known equilibrium
CALCULATED      37 EQUILIBRIA

Phase region boundary 2 at: 7.026E-01 2.616E-01 1.025E+03
    LIQUID
** CU19SI6_ETA
** DIAMOND_A4
*** SORRY CANNOT CONTINUE ***      4
CALCULATED      16 EQUILIBRIA

Phase region boundary 2 at: 3.369E-01 8.764E-02 8.678E+02
    LIQUID
** ALCU_ETA
** DIAMOND_A4
CALCULATED      9 EQUILIBRIA

Phase region boundary 2 at: 2.933E-01 7.685E-02 8.291E+02
    LIQUID
** ALCU_ETA
    ALCU_THETA
** DIAMOND_A4
SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary 2 at: 2.933E-01 7.685E-02 8.291E+02
    LIQUID
** ALCU_ETA
    ALCU_THETA
Terminating at diagram limit
CALCULATED      14 EQUILIBRIA

Phase region boundary 2 at: 2.933E-01 7.685E-02 8.291E+02
    LIQUID
** ALCU_THETA
** DIAMOND_A4
CALCULATED      17 EQUILIBRIA

Phase region boundary 2 at: 1.498E-01 7.282E-02 7.852E+02

```



```

Generating start point 26
Generating start point 27
Generating start point 28
Generating start point 29
Generating start point 30
Generating start point 31
Generating start point 32
Generating start point 33
Generating start point 34
Generating start point 35
Working hard

Phase region boundary 1 at: 4.398E-01 3.756E-02
    LIQUID
    ** ALCU_EPSILON
Calculated.                2 equilibria

Phase region boundary 2 at: 4.420E-01 4.464E-02
    LIQUID
    ** ALCU_EPSILON
    ** DIAMOND_A4

Phase region boundary 3 at: 1.706E-01 5.446E-01
    LIQUID
    ** DIAMOND_A4
Calculated.                30 equilibria

Phase region boundary 4 at: 4.420E-01 4.464E-02
    LIQUID
    ** ALCU_EPSILON
Calculated.                2 equilibria

Phase region boundary 5 at: 4.398E-01 3.756E-02
    LIQUID
    ** ALCU_EPSILON
    ** ALCU_ETA

Phase region boundary 6 at: 4.241E-01 3.756E-02
    LIQUID
    ** ALCU_ETA
Calculated.                19 equilibria

Phase region boundary 7 at: 4.241E-01 3.756E-02
    LIQUID
    ** ALCU_ETA
Calculated.                19 equilibria

Phase region boundary 8 at: 8.419E-01 6.666E-02
    LIQUID
    ** BCC_B2
Calculated.                28 equilibria

Phase region boundary 9 at: 6.645E-01 6.795E-03
    LIQUID
    ** BCC_B2
    ** GAMMA_H

Phase region boundary 10 at: 6.653E-01 4.077E-03
    LIQUID
    ** GAMMA_H
Calculated.                12 equilibria

Phase region boundary 11 at: 6.645E-01 6.795E-03
    LIQUID
    ** BCC_B2
Calculated.                26 equilibria

Phase region boundary 12 at: 8.419E-01 6.666E-02
    LIQUID
    ** BCC_B2
    ** FCC_A1

Phase region boundary 13 at: 8.633E-01 4.917E-02
    LIQUID
    ** FCC_A1
Calculated.                25 equilibria

Phase region boundary 14 at: 8.633E-01 4.917E-02
    LIQUID
    ** FCC_A1
Calculated.                25 equilibria

Phase region boundary 15 at: 6.645E-01 6.795E-03
    LIQUID
    ** BCC_B2
Calculated.                26 equilibria
Terminating at known equilibrium

Phase region boundary 16 at: 6.653E-01 4.077E-03
    LIQUID
    ** GAMMA_H
Calculated.                12 equilibria

Phase region boundary 17 at: 7.327E-03 9.853E-01
    LIQUID
    ** DIAMOND_A4
Calculated.                15 equilibria

Phase region boundary 18 at: 7.327E-03 9.853E-01
    LIQUID
    ** DIAMOND_A4
Calculated.                15 equilibria

Phase region boundary 19 at: 7.453E-02 8.883E-01
    LIQUID
    ** DIAMOND_A4
Calculated.                23 equilibria

Phase region boundary 20 at: 7.453E-02 8.883E-01
    LIQUID
    ** DIAMOND_A4
Calculated.                25 equilibria

Phase region boundary 21 at: 1.372E-01 7.942E-01
    LIQUID
    ** DIAMOND_A4

```

Calculated 30 equilibria
 Phase region boundary 22 at: 1.372E-01 7.942E-01
 LIQUID
 ** DIAMOND_A4
 Calculated 22 equilibria
 Phase region boundary 23 at: 1.926E-01 7.111E-01
 LIQUID
 ** DIAMOND_A4
 Calculated 28 equilibria
 Phase region boundary 24 at: 1.926E-01 7.111E-01
 LIQUID
 ** DIAMOND_A4
 Calculated 32 equilibria
 Phase region boundary 25 at: 6.652E-01 9.329E-03
 LIQUID
 ** BCC_B2
 Calculated. 2 equilibria
 Terminating at known equilibrium
 Phase region boundary 26 at: 6.652E-01 9.329E-03
 LIQUID
 ** BCC_B2
 Calculated. 30 equilibria
 Terminating at known equilibrium
 Phase region boundary 27 at: 2.311E-01 6.535E-01
 LIQUID
 ** DIAMOND_A4
 Calculated 34 equilibria
 Phase region boundary 28 at: 2.311E-01 6.535E-01
 LIQUID
 ** DIAMOND_A4
 Calculated 40 equilibria
 Phase region boundary 29 at: 5.840E-01 7.591E-03
 LIQUID
 ** BCC_B2
 Calculated 9 equilibria
 Phase region boundary 30 at: 5.840E-01 7.591E-03
 LIQUID
 ** BCC_B2
 Calculated. 39 equilibria
 Phase region boundary 31 at: 8.543E-01 1.296E-01
 LIQUID
 ** BCC_B2
 ** FCC_A1
 Calculated 24 equilibria
 Phase region boundary 32 at: 8.749E-01 1.099E-01
 LIQUID
 ** FCC_A1
 Calculated 24 equilibria
 Phase region boundary 33 at: 8.543E-01 1.296E-01
 LIQUID
 ** BCC_B2
 Calculated 54 equilibria
 Phase region boundary 34 at: 2.562E-01 6.158E-01
 LIQUID
 ** DIAMOND_A4
 Calculated 39 equilibria
 Phase region boundary 35 at: 2.562E-01 6.158E-01
 LIQUID
 ** DIAMOND_A4
 Calculated 37 equilibria
 Phase region boundary 36 at: 5.198E-01 5.412E-03
 LIQUID
 ** ALCU_EPSILON
 Calculated 11 equilibria
 Phase region boundary 37 at: 5.198E-01 5.412E-03
 LIQUID
 ** ALCU_EPSILON
 Calculated. 5 equilibria
 Phase region boundary 38 at: 5.361E-01 2.533E-02
 LIQUID
 ** ALCU_EPSILON
 ** BCC_B2
 Calculated. 12 equilibria
 Phase region boundary 39 at: 5.383E-01 3.569E-02
 LIQUID
 ** BCC_B2
 Calculated. 12 equilibria
 Phase region boundary 40 at: 5.962E-01 1.431E-01
 LIQUID
 ** BCC_B2
 ** DIAMOND_A4
 Calculated 41 equilibria
 Phase region boundary 41 at: 2.789E-01 5.911E-01
 LIQUID
 ** DIAMOND_A4
 Calculated 41 equilibria
 Phase region boundary 42 at: 5.361E-01 2.533E-02
 LIQUID
 ** ALCU_EPSILON
 Calculated 16 equilibria
 Phase region boundary 43 at: 7.337E-01 2.597E-01
 LIQUID
 ** CU19SI6_ETA
 Calculated. 4 equilibria
 Phase region boundary 44 at: 7.478E-01 2.387E-01
 LIQUID

```

** BCC_B2
** CU19SI6_ETA

Phase region boundary 45 at: 7.525E-01 2.105E-01
    LIQUID
    ** BCC_B2
Calculated.          8 equilibria

Phase region boundary 46 at: 6.917E-01 2.112E-01
    LIQUID
    ** BCC_B2
    ** DIAMOND_A4

Phase region boundary 47 at: 3.329E-01 6.250E-01
    LIQUID
    ** DIAMOND_A4
Calculated.          14 equilibria

Phase region boundary 48 at: 3.469E-01 6.529E-01
    LIQUID
    ** CU19SI6_ETA
    ** DIAMOND_A4

Phase region boundary 49 at: 7.269E-01 2.729E-01
    LIQUID
    ** CU19SI6_ETA
Calculated.          6 equilibria
Terminating at known equilibrium

Phase region boundary 50 at: 7.337E-01 2.597E-01
    LIQUID
    ** CU19SI6_ETA
Calculated.          3 equilibria
Terminating at known equilibrium

Phase region boundary 51 at: 4.736E-01 5.113E-03
    LIQUID
    ** ALCU_EPSILON
Calculated.          12 equilibria

Phase region boundary 52 at: 4.736E-01 5.113E-03
    LIQUID
    ** ALCU_EPSILON
Calculated.          11 equilibria

Phase region boundary 53 at: 5.106E-01 6.209E-02
    LIQUID
    ** ALCU_EPSILON
    ** DIAMOND_A4

Phase region boundary 54 at: 2.273E-01 5.621E-01
    LIQUID
    ** DIAMOND_A4
Calculated.          36 equilibria

Phase region boundary 55 at: 5.106E-01 6.209E-02
    LIQUID
    ** ALCU_EPSILON
Calculated.          24 equilibria

Phase region boundary 56 at: 3.646E-02 1.803E-02
    LIQUID
    ** FCC_A1
Calculated.          15 equilibria

Phase region boundary 57 at: 3.646E-02 1.803E-02
    LIQUID
    ** FCC_A1
Calculated.          33 equilibria

Phase region boundary 58 at: 4.151E-01 5.493E-03
    LIQUID
    ** ALCU_ETA
Calculated.          8 equilibria

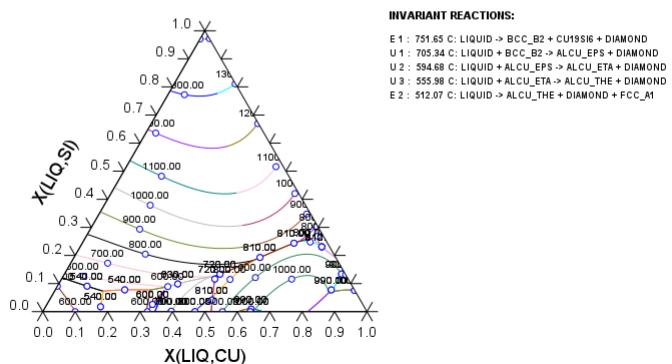
Phase region boundary 59 at: 4.151E-01 5.493E-03
    LIQUID
    ** ALCU_ETA
Calculated.          6 equilibria
Terminating at known equilibrium
*** BUFFER SAVED ON FILE: C:\Users\azureuser\AppData\Local\Temp\MONOVAR_002.POLY3
CPU time for mapping          8 seconds
POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes
POSTPROCESSOR VERSION 3.2
Setting automatic diagram axes

INVARIANT REACTIONS:
E 1: 751.65 C: LIQUID -> BCC_B2 + CU19SI6 + DIAMOND
U 1: 705.34 C: LIQUID + BCC_B2 -> ALCU_EPS + DIAMOND
U 2: 594.68 C: LIQUID + ALCU_EPS -> ALCU_ETA + DIAMOND
U 3: 555.98 C: LIQUID + ALCU_ETA -> ALCU_THE + DIAMOND
E 2: 512.07 C: LIQUID -> ALCU_THE + DIAMOND + FCC_A1

```

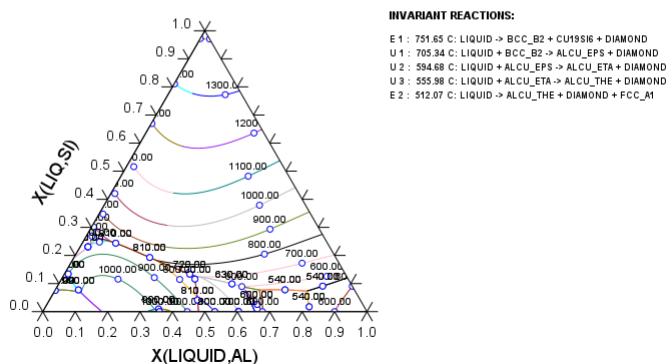
AL-CU-SI (600C/1400C/100C)



```

POST: s-d-a x (liquid,al)
... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 19B
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
example 19B

```



```

POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:

```

tce20

SYS:About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce20\tce20.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Adiabatic decompression in a geological system
SYS:
SYS: @@ This example calculates the adiabatic decompression
SYS: @@ in a geological system using the geochemical
SYS: @@ database (PGEO.TDB)
SYS:
SYS: set-log ex20,,
SYS: go da
... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module
Database folder: C:\jenkins\workspace\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0
VA /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFC11: sw user PGEO.TDB
... the command in full is SWITCH_DATABASE
Current database: User defined Database
O VA DEFINED
STEAM OXYGEN HYDROGEN
REJECTED
CARBON_MONOXIDE CARBON_DIOXIDE METHANE
REJECTED
15:55:52,552 [Thread-0] INFO TDBfileParser: USER_693609315_14, number of lines read: 3095
15:55:53,370 [Thread-0] INFO DatabaseUtils: Parsing of USER_693609315_14 completed in 867 ms
TDB_USER: d-sys mg si
... the command in full is DEFINE_SYSTEM
MG SI DEFINED
TDB_USER: l-sys
... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT:/
GAS:G :O2:
> Gaseous Mixture with C-H-O species, using ideal gas model
A_QUARTZ :SI1O2:
B_QUARTZ :SI1O2:
CRISTOBALITE :SI1O2:
TRIDYMITE :SI1O2:
COESITE :SI1O2:
STISHOVITE :SI1O2:
PERICLASE :Mg1O1:
FORSTERITE :SI1Mg2O4:
BETA_FORSTERITE :SI1Mg2O4:
GAMMA_FORSTERITE :SI1Mg2O4:
ILMENITE_MG :SI1Mg1O3:
MG_PEROVSKITE :SI1Mg1O3:
CLINOENSTATITE :SI1Mg1O3:
ORTHOENSTATITE :SI1Mg1O3:
PROTOENSTATITE :SI1Mg1O3:
CLINOENSTHP :SI1Mg1O3:
GARNET_MG :SI1Mg1O3:
TDB_USER: rej ph gas proto
... the command in full is REJECT
GAS:G PROTOENSTATITE REJECTED
TDB_USER: get
... the command in full is GET_DATA
15:55:53,756 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
ELEMENTS
SPECIES
PHASES
PARAMETERS ...
FUNCTIONS
-OK-
TDB_USER: go p-3
... the command in full is GOTO_MODULE
POLY version 3.32
POLY: @@ Define more convenient components
POLY: def-com mgo o sio2
... the command in full is DEFINE_COMPONENTS
POLY: l-st
... the command in full is LIST_STATUS
Option /CPS/: CPS
*** STATUS FOR ALL COMPONENTS

| COMPONENT | STATUS | REF. | STATE | T (K) | P (Pa) |
|-----------|---------|------|-------|-------|--------|
| VA | ENTERED | SER | | | |
| MGO | ENTERED | SER | | | |
| O | ENTERED | SER | | | |
| SIO2 | ENTERED | SER | | | |

*** STATUS FOR ALL PHASES

| PHASE | STATUS | DRIVING FORCE | MOLES |
|------------------|---------|---------------|--------------|
| TRIDYMITE | ENTERED | 0.000000E+00 | 0.000000E+00 |
| STISHOVITE | ENTERED | 0.000000E+00 | 0.000000E+00 |
| PERICLASE | ENTERED | 0.000000E+00 | 0.000000E+00 |
| ORTHOENSTATITE | ENTERED | 0.000000E+00 | 0.000000E+00 |
| MG_PEROVSKITE | ENTERED | 0.000000E+00 | 0.000000E+00 |
| ILMENITE_MG | ENTERED | 0.000000E+00 | 0.000000E+00 |
| GARNET_MG | ENTERED | 0.000000E+00 | 0.000000E+00 |
| GAMMA_FORSTERITE | ENTERED | 0.000000E+00 | 0.000000E+00 |
| FORSTERITE | ENTERED | 0.000000E+00 | 0.000000E+00 |
| CRISTOBALITE | ENTERED | 0.000000E+00 | 0.000000E+00 |
| COESITE | ENTERED | 0.000000E+00 | 0.000000E+00 |
| CLINOENSTHP | ENTERED | 0.000000E+00 | 0.000000E+00 |

```

CLINOENSTATITE      ENTERED      0.000000E+00  0.000000E+00
B_QUARTZ            ENTERED      0.000000E+00  0.000000E+00
BETA_FORSTERITE    ENTERED      0.000000E+00  0.000000E+00
A_QUARTZ            ENTERED      0.000000E+00  0.000000E+00
*** STATUS FOR ALL SPECIES
MG     ENTERED      O     ENTERED      SI1MG1O3 ENTERED      SIO2      ENTERED
MG1O1   ENTERED      O2    ENTERED      SI1MG2O4 ENTERED      VA       ENTERED
MGO    ENTERED      SI     ENTERED      SI1O2     ENTERED
POLY:Hit RETURN to continue
POLY: @@ and specify a composition assumed
POLY: @@ to be present in the Earth's mantle
POLY:
POLY: s-i-a n(mgo)=80
... the command in full is SET_INPUT_AMOUNTS
POLY: s-i-a n(simg1o3)=100
... the command in full is SET_INPUT_AMOUNTS
POLY: l-c
... the command in full is LIST_CONDITIONS
N(MGO)=180, N(SIO2)=100
DEGREES OF FREEDOM 3
POLY:Hit RETURN to continue
POLY: @@ There is an error if MgSiO3 is used instead of the
POLY: @@ defined Si1Mg1O3, since MgSiO3 is not defined as
POLY: @@ a species.
POLY:
POLY: s-c t=2200,p=2e10
... the command in full is SET_CONDITION
POLY: save tce20 y
... the command in full is SAVE_WORKSPACES
POLY: @@ There is no degree of freedom with respect
POLY: @@ to oxygen so set its activity to unity (or
POLY: @@ any positive number)
POLY:
POLY: s-c ac(o)=1
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
15:55:55,237 [Thread-0] INFO Database: Preparing system for use: USER_693609315_14_MODIFIED_168261095400417
15:55:57,793 [Thread-0] INFO Phase: Preparing phase for use: A_QUARTZ
15:55:58,256 [Thread-0] INFO Phase: Preparing phase for use: BETA_FORSTERITE
15:55:58,659 [Thread-0] INFO Phase: Preparing phase for use: B_QUARTZ
15:55:59,030 [Thread-0] INFO Phase: Preparing phase for use: CLINOENSTATITE
15:55:59,437 [Thread-0] INFO Phase: Preparing phase for use: CLINOENSTHP
15:55:59,796 [Thread-0] INFO Phase: Preparing phase for use: COESITE
15:56:00,155 [Thread-0] INFO Phase: Preparing phase for use: CRISTOBALITE
15:56:00,545 [Thread-0] INFO Phase: Preparing phase for use: FORSTERITE
15:56:00,917 [Thread-0] INFO Phase: Preparing phase for use: GAMMA_FORSTERITE
15:56:01,279 [Thread-0] INFO Phase: Preparing phase for use: GARNET_MG
15:56:01,666 [Thread-0] INFO Phase: Preparing phase for use: ILMENITE_MG
15:56:02,025 [Thread-0] INFO Phase: Preparing phase for use: MG_PEROVSKITE
15:56:02,383 [Thread-0] INFO Phase: Preparing phase for use: ORTHOENSTATITE
15:56:02,739 [Thread-0] INFO Phase: Preparing phase for use: PERICLASE
15:56:03,097 [Thread-0] INFO Phase: Preparing phase for use: STISHOVITE
15:56:03,454 [Thread-0] INFO Phase: Preparing phase for use: TRIDYMITE
Testing POLY result by global minimization procedure
Calculated          16 grid points in          0 s
 31 ITS, CPU TIME USED 23 SECONDS
POLY: save tce20 y
... the command in full is SAVE_WORKSPACES
POLY: l-st p
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES
PHASE           STATUS      DRIVING FORCE      MOLES
GARNET_MG        ENTERED      0.000000E+00  4.000000E+01
BETA_FORSTERITE  ENTERED      0.000000E+00  2.400000E+02
GAMMA_FORSTERITE ENTERED      -5.946730E-03 0.000000E+00
MG_PEROVSKITE    ENTERED      -2.558352E-02 0.000000E+00
ILMENITE_MG      ENTERED      -4.828445E-02 0.000000E+00
PERICLASE         ENTERED      -9.575143E-02 0.000000E+00
CLINOENSTHP      ENTERED      -1.541632E-01 0.000000E+00
ORTHOENSTATITE   ENTERED      -2.197450E-01 0.000000E+00
CLINOENSTATITE   ENTERED      -2.394369E-01 0.000000E+00
FORSTERITE        ENTERED      -2.417190E-01 0.000000E+00
STISHOVITE        ENTERED      -3.053984E-01 0.000000E+00
COESITE           ENTERED      -3.775316E+00 0.000000E+00
ENTERED PHASES WITH DRIVING FORCE LESS THAN -7.835592E+00
A_QUARTZ B_QUARTZ TRIDYMITE CRISTOBALITE
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /WVCS/: X
Output from POLY-3, equilibrium = 1, label A0 , database: USER

Conditions:
N(MGO)=180, N(SIO2)=100, T=2200, P=2E10, AC(O)=1
DEGREES OF FREEDOM 0

Temperature 2200.00 K ( 1926.85 C), Pressure 2.000000E+10
Number of moles of components 2.80000E+02, Mass in grams 1.32632E+04
Total Gibbs energy -1.80863E+08, Enthalpy -9.91578E+07, Volume 3.55512E-03

Component      Moles      M-Fraction Activity Potential Ref.stat
MGO            1.8000E+02  6.4286E-01 7.6674E-14 -5.5240E+05 SER
O              0.0000E+00  0.0000E+00 1.0000E+00  0.0000E+00 SER
SIO2           1.0000E+02  3.5714E-01 4.6393E-20 -8.1430E+05 SER

BETA_FORSTERITE      Status ENTERED      Driving force 0.0000E+00
Moles 2.4000E+02, Mass 1.1255E+04, Volume fraction 8.5320E-01 Mole fractions:
MGO 6.66667E-01 SIO2 3.33333E-01 O 0.00000E+00

GARNET_MG      Status ENTERED      Driving force 0.0000E+00
Moles 4.0000E+01, Mass 2.0078E+03, Volume fraction 1.4680E-01 Mole fractions:
MGO 5.0000E-01 SIO2 5.00000E-01 O 0.00000E+00
POLY:Hit RETURN to continue
POLY:
POLY: ent fun dens=1e-3*bm/vm;
... the command in full is ENTER_SYMBOL
POLY: sh dens
... the command in full is SHOW_VALUE
DENS=3730.7358
POLY: @@ We have found the equilibrium at this pressure.
POLY: @@ Now assume this system is decompressed
POLY: @@ adiabatically. What will the new temperature become?

```

```

POLY:
POLY: s-c h
... the command in full is SET_CONDITION
Value /-99157833.21/:
POLY: s-c t
... the command in full is SET_CONDITION
Value /2200/: none
POLY: l-c
... the command in full is LIST CONDITIONS
N(MGO)=180, N(SIO2)=100, P=2E10, AC(O)=1, H=-99157833.21
DEGREES OF FREEDOM 0
POLY:Hit RETURN to continue
POLY: @@ Now t is independent, calculate the equilibrium and get t
POLY:
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Using already calculated grid
 6 ITS, CPU TIME USED 0 SECONDS
POLY: sh t
... the command in full is SHOW_VALUE
T=2200.
POLY:Hit RETURN to continue
POLY: @@ It's the same temperature. Now change pressure
POLY:
POLY: s-c p
... the command in full is SET_CONDITION
Value /2E+10/: 150e8
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated 16 grid points in 0 s
 17 ITS, CPU TIME USED 0 SECONDS
POLY: sh t
... the command in full is SHOW_VALUE
T=2977.6276
POLY:Hit RETURN to continue
POLY: @@ We will also have a new density and another set of
POLY: @@ stable phases.
POLY:
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VXCS/:
Output from POLY-3, equilibrium = 1, label A0 , database: USER

Conditions:
N(MGO)=180, N(SIO2)=100, P=1.5E10, AC(O)=1, H=-99157833.21
DEGREES OF FREEDOM 0

Temperature 2977.63 K ( 2704.48 C), Pressure 1.500000E+10
Number of moles of components 2.80000E+02, Mass in grams 1.32632E+04
Total Gibbs energy -2.30661E+08, Enthalpy -9.91578E+07, Volume 3.59115E-03

Component Moles M-Fraction Activity Potential Ref.stat
MGO 1.8000E+02 6.4286E-01 4.6875E-13 -7.0283E+05 SER
O 0.0000E+00 0.0000E+00 1.0000E+00 0.0000E+00 SER
SIO2 1.0000E+02 3.5714E-01 5.3688E-19 -1.0415E+06 SER

GARNET_MG Status ENTERED Driving force 0.0000E+00
Moles 2.0000E+02, Mass 1.0039E+04, Volume fraction 7.4847E-01 Mole fractions:
MGO 5.00000E-01 SIO2 5.00000E-01 O 0.00000E+00

PERICLASE Status ENTERED Driving force 0.0000E+00
Moles 8.0000E+01, Mass 3.2244E+03, Volume fraction 2.5153E-01 Mole fractions:
MGO 1.00000E+00 SIO2 0.00000E+00 O 0.00000E+00

POLY: sh dens
... the command in full is SHOW_VALUE
DENS=3693.3029
POLY: sh v
... the command in full is SHOW_VALUE
V=3.5911547E-3
POLY: sh vm
... the command in full is SHOW_VALUE
VM=1.2825553E-5
POLY:
POLY: set-inter
... the command in full is SET_INTERACTIVE
POLY:

```

tce21

SYS:About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

```
SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce21\tce21.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Calculating a ternary isotherm in Fe-Cr-Ni
SYS:
SYS: @@ This example calculates a ternary isotherm
SYS: @@ in Fe-Cr-Ni with a user-defined database.
SYS:
SYS: set-log ex21,,
SYS: go da
... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module
Database folder: C:\jenkins\workspace\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA           /* DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE11: sw user tce21
... the command in full is SWITCH_DATABASE
Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

VA DEFINED
15:57:20,318 [Thread-0] INFO TDBFileParser: USER_1699311230_14, number of lines read: 195
15:57:20,472 [Thread-0] INFO DatabaseUtils: Parsing of USER_1699311230_14 completed in 203 ms
TDB_USER: def-sys *
... the command in full is DEFINE_SYSTEM
/-          VA          CR
FE          NI  DEFINED
TDB_USER: li-sys
... the command in full is LIST SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/:
LIQUID:L :CR FE NI:
BCC A2 :CR FE NI:VA:
FCC A1 :CR FE NI:VA:
HCP_A3 :CR FE NI:VA:
SIGMA :FE NI:CR:CR FE NI:
TDB_USER:Hit RETURN to continue
TDB_USER: get
... the command in full is GET_DATA
15:57:20,558 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS .....
FUNCTIONS .....

List of references for assessed data

'A.T. Dinsdale, SGTE Data for Pure Elements, Calphad 15(1991)4, p 317-425; '
'J.O. Andersson, B. Sundman, Calphad 11(1987)1 p 83-92 TRITA-MAC 270
(1986); Cr-Fe'
'Byeong-Joo Lee, unpublished revision (1991); C-Cr-Fe-Ni'
'Byeong-Joo Lee, Calphad 16(1992)2, p 121-149; carbides'
'A. Dinsdale, T. Chart, MTDS NPL, unpublished work (1986); Fe-Ni'
'A. Dinsdale, T. Chart, MTDS NPL, unpublished work (1986); Cr-Ni'
'A.F. Guillermet, Z. Metallkde. 79(1988)8 p 524-536, TRITA-MAC 362 (1988);
C-Co-Ni, C-Co-Fe-Ni'
'K. Frisk, Metall. Trans. 21A (1990)9 p 2477-2488, Cr-Fe-N'
'Unassessed parameter, linear combination of unary data.'
'P. Gustafson, Calphad 12(1987)3 p 277-292, Cr-Ni-W '
-OK-
TDB_USER: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY: @@ With 3 components we must set 5 conditions

POLY: s-c t=1073 p=1e5 n=1 x(cr)=.2 x(ni)=.2
... the command in full is SET_CONDITION
POLY: l-c
... the command in full is LIST_CONDITIONS
T=1073, P=100000, N=1, X(CR)=0.2, X(NI)=0.2
DEGREES OF FREEDOM 0
POLY:
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
15:57:21,778 [Thread-0] INFO Database: Preparing system for use: USER_1699311230_14
15:57:22,662 [Thread-0] INFO Phase: Preparing phase for use: LIQUID
15:57:23,161 [Thread-0] INFO Phase: Preparing phase for use: BCC_A2
15:57:23,629 [Thread-0] INFO Phase: Preparing phase for use: FCC_A1
15:57:24,035 [Thread-0] INFO Phase: Preparing phase for use: HCP_A3
15:57:24,475 [Thread-0] INFO Phase: Preparing phase for use: SIGMA
Calculated      9684 grid points in          8 s
Found the set of lowest grid points in          0 s
Calculated POLY solution      0 s, total time     8 s
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
Output from POLY-3, equilibrium =      1, label A0 , database: USER

Conditions:
T=1073, P=100000, N=1, X(CR)=0.2, X(NI)=0.2
```

DEGREES OF FREEDOM 0

Temperature 1073.00 K (799.85 C), Pressure 1.000000E+05
 Number of moles of components 1.00000E+00, Mass in grams 5.56454E+01
 Total Gibbs energy -5.39559E+04, Enthalpy 3.01555E+04, Volume 0.00000E+00

Component Moles W-Fraction Activity Potential Ref.stat
 CR 2.0000E-01 1.8688E-01 5.8626E-03 -4.5849E+04 SER
 FE 6.0000E-01 6.0217E-01 3.1002E-03 -5.1533E+04 SER
 NI 2.0000E-01 2.1094E-01 4.2164E-04 -6.9332E+04 SER

FCC_A1 Status ENTERED Driving force 0.0000E+00
 Moles 1.0000E+00, Mass 5.5645E+01, Volume fraction 0.0000E+00 Mass fractions:
 FE 6.02174E-01 NI 2.10943E-01 CR 1.86883E-01

POLY:Hit RETURN to continue

POLY: @@ Define axis
POLY: s-a-v 1 x(cr) 0 1,,
 ... the command in full is SET_AXIS_VARIABLE
POLY: s-a-v 2 x(ni) 0 1,,
 ... the command in full is SET_AXIS_VARIABLE
POLY: save tcez21 y
 ... the command in full is SAVE_WORKSPACES

POLY: map

Version S mapping is selected
 Generating start equilibrium 1
 Generating start equilibrium 2
 Generating start equilibrium 3
 Generating start equilibrium 4
 Generating start equilibrium 5
 Generating start equilibrium 6
 Generating start equilibrium 7
 Generating start equilibrium 8
 Generating start equilibrium 9

Organizing start points

Using ADDED start equilibria

Generating start point 1
 Generating start point 2
 Generating start point 3
 Generating start point 4
 Generating start point 5
 Generating start point 6
 ERROR 1611 when calculating equilibrium
 Generating start point 7
 Generating start point 8
 Generating start point 9
 Generating start point 10
 Working hard
 Generating start point 11
 Generating start point 12
 Generating start point 13
 Generating start point 14
 Generating start point 15
 Generating start point 16
 Generating start point 17
 Generating start point 18

Phase region boundary 1 at: 3.521E-02 1.510E-02
 BCC_A2
 ** FCC_A1
 Calculated. 20 equilibria

Phase region boundary 2 at: 2.615E-01 6.190E-02
 BCC_A2
 ** FCC_A1
 ** SIGMA

Phase region boundary 3 at: 3.723E-01 3.566E-02
 BCC_A2
 ** SIGMA
 Calculated. 21 equilibria

Phase region boundary 4 at: 3.168E-01 6.107E-02
 FCC_A1
 ** SIGMA
 Calculated. 20 equilibria

Phase region boundary 5 at: 4.140E-01 2.295E-01
 ** BCC_A2
 FCC_A1
 ** SIGMA

Phase region boundary 6 at: 5.304E-01 1.820E-01
 ** BCC_A2
 FCC_A1
 Calculated. 43 equilibria

Phase region boundary 7 at: 6.616E-01 7.178E-02
 ** BCC_A2
 SIGMA
 Calculated. 31 equilibria

Phase region boundary 8 at: 2.615E-01 6.190E-02
 BCC_A2
 ** FCC_A1
 Calculated. 33 equilibria

Phase region boundary 9 at: 3.521E-02 1.510E-02
 BCC_A2
 ** FCC_A1
 Calculated. 15 equilibria

Phase region boundary 10 at: 1.095E-02 2.044E-02
 BCC_A2
 ** FCC_A1
 Calculated. 18 equilibria

Phase region boundary 11 at: 1.095E-02 2.044E-02
 BCC_A2
 ** FCC_A1
 Calculated. 22 equilibria

Terminating at known equilibrium

Phase region boundary 12 at: 3.838E-01 1.780E-02

```

      BCC_A2
      ** SIGMA
Calculated.          2 equilibria
Terminating at known equilibrium

Phase region boundary 13 at: 3.838E-01 1.780E-02
      BCC_A2
      ** SIGMA
Calculated.          21 equilibria

Phase region boundary 14 at: 5.848E-01 2.838E-02
      BCC_A2
      ** SIGMA
Calculated.          32 equilibria

Phase region boundary 15 at: 5.848E-01 2.838E-02
      BCC_A2
      ** SIGMA
Calculated.          8 equilibria
Terminating at known equilibrium

Phase region boundary 16 at: 5.404E-01 9.033E-03
      BCC_A2
      ** SIGMA
Calculated.          12 equilibria

Phase region boundary 17 at: 5.404E-01 9.033E-03
      BCC_A2
      ** SIGMA
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 18 at: 4.123E-01 2.273E-01
      FCC_A1
      ** SIGMA
Calculated.          19 equilibria
Terminating at known equilibrium

Phase region boundary 19 at: 4.123E-01 2.273E-01
      FCC_A1
      ** SIGMA
Calculated.          2 equilibria
Terminating at known equilibrium

Phase region boundary 20 at: 9.183E-03 2.090E-02
      ** BCC_A2
      FCC_A1
Calculated.          13 equilibria

Phase region boundary 21 at: 9.183E-03 2.090E-02
      ** BCC_A2
      FCC_A1
Calculated.          22 equilibria
Terminating at known equilibrium

Phase region boundary 22 at: 6.363E-01 2.710E-01
      ** BCC_A2
      FCC_A1
Calculated.          16 equilibria
Terminating at known equilibrium

Phase region boundary 23 at: 6.363E-01 2.710E-01
      ** BCC_A2
      FCC_A1
Calculated.          26 equilibria

Phase region boundary 24 at: 6.789E-01 3.114E-01
      ** BCC_A2
      FCC_A1
Calculated.          22 equilibria
Terminating at known equilibrium

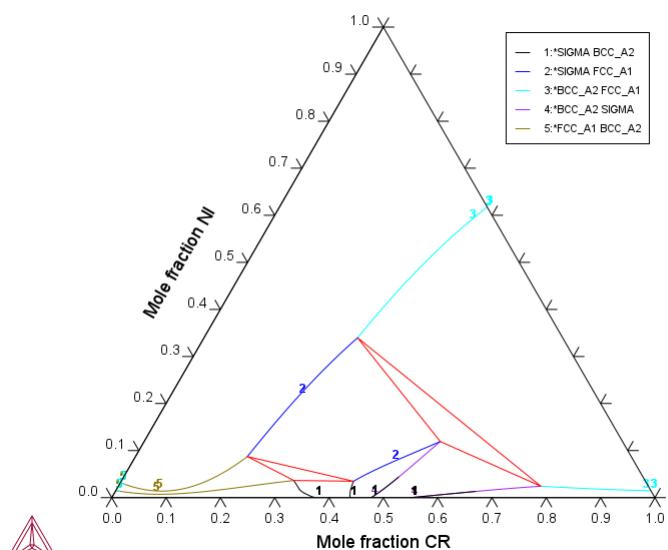
Phase region boundary 25 at: 6.789E-01 3.114E-01
      ** BCC_A2
      FCC_A1
Calculated.          16 equilibria
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\generate_console_examples\examples\tcex21\tcex21.POLY3
CPU time for mapping           3 seconds
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST:
POST: set-title example 21a
POST: se-d-tv Y,,,
... the command in full is SET_DIAGRAM_TYPE
POST: s-l b
... the command in full is SET_LABEL_CURVE_OPTION
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 21a



POST:
POST: Hit RETURN to continue

POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:

SYS:About

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Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

```
SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce22\tce22.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Calculating an adiabatic flame temperature
SYS:
SYS: @@ This example examines a heat balance when C3H8 is burned
SYS: @@ in oxygen by calculating the adiabatic flame temperature.
SYS: @@ Note that a SSUB database license is required to run
SYS: @@ the example.
SYS:
SYS: set-log ex22.,
SYS: go da
... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module
Database folder: C:\jenkins\workspace\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA           /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE11: sw ssub6
... the command in full is SWITCH_DATABASE
Current database: SGTE Substances v6.0

VA DEFINED
TDB_SSUB6: def-sys c o h
... the command in full is DEFINE_SYSTEM
C          O          H
DEFINED
TDB_SSUB6: get
... the command in full is GET_DATA
15:58:44,568 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS .....

List of references for assessed data

C1<G> T.C.R.A.S. Class: 1
C1<G> C<G>
C1H1<G> T.C.R.A.S. Class: 2
C1H1<G> CH<G>
C1H1O1<G> T.C.R.A.S. Class: 4
C1H1O1<G> HCO<G>
FORMYL <GAS>
C1H1O2<G> T.C.R.A.S. Class: 6
C1H1O2<G>
C1H2<G> T.C.R.A.S. Class: 5
METHYLENE
METHYLENE <GAS>
C1H2O1<G> T.C.R.A.S. Class: 5
C1H2O1<G> CH2O<G>
FORMALDEHYDE <GAS>
C1H2O2_CIS<G> T.C.R.A.S. Class: 5
C1H2O2_CIS<G>
C1H2O2_DIOXIRANE<G> T.C.R.A.S. Class: 6
C1H2O2_DIOXIRANE<G>
S298 corrected and cp refitted
due to corrected data in IVTAN2000 7/2002
C1H2O2_TRANS<G> T.C.R.A.S. Class: 5
C1H2O2_TRANS<G>
C1H3<G> T.C.R.A.S. Class: 5
METHYL Gaseous Standard State.
METHYL <GAS>
C1H3O1_CH2OH<G> T.C.R.A.S. Class: 6
C1H3O1_CH2OH<G>
C1H3O1_CH3O<G> T.C.R.A.S. Class: 5
C1H3O1_CH3O<G>
C1H4<G> T.C.R.A.S. Class: 5
METHANE. Gaseous Standard State.
METHANE <GAS>
C1H4O1<G> T.C.R.A.S. Class: 5
C1H4O1<G> CH3OH<G>
METHANOL <GAS>
C1O1<G> JANAF THERMOCHEMICAL TABLES SGTE **
C1O1<G> CO<G>
CARBON MONOXIDE <GAS>
STANDARD STATE : CODATA KEY VALUE. /CP FROM JANAF PUB. 9/65
C1O2<G> T.C.R.A.S. Class: 2
C1O2<G> CO2<G>
CARBON DIOXIDE <GAS>
C2<G> T.C.R.A.S. Class: 2
CARBON Diatomic Gas.
CARBON <DIATOMIC GAS>
C2H1<G> T.C.R.A.S. Class: 6
C2H1<G> C2H<G>
CCH RADICAL <GAS>
C2H2<G> T.C.R.A.S. Class: 2
ACETYLENE (ETYNE). Gaseous Standard State.
ACETYLENE <GAS>
C2H2O1<G> T.C.R.A.S. Class: 6
C2H2O1<G>
OXIRENE
S298 corrected and cp refitted
due to corrected data in IVTAN2000 7/2002
C2H3<G> T.C.R.A.S. Class: 6
```

DICARBON TRIHYDRIDE Gaseous Standard State.
C2H4<G> T.C.R.A.S. Class: 6
ETHYLENE. Gaseous Standard State.
ETHYLENE <GAS>
C2H4O1_ACETALDEHYDE<G> T.C.R.A.S. Class: 5
C2H4O1_ACETALDEHYDE<G>
C2H4O1_OXIRANE<G> T.C.R.A.S. Class: 6
C2H4O1_OXIRANE<G>
S298 corrected and cp refitted
due to corrected data in IVTAN2000 7/2002
C2H4O2_ACETICACID<G> T.C.R.A.S. Class: 5
C2H4O2_ACETICACID<G>
C2H4O2_DIOXETANE<G> T.C.R.A.S. Class: 6
C2H4O2_DIOXETANE<G>
S298 corrected and cp refitted
due to corrected data in IVTAN2000 7/2002
typing error corrected 12/06
C2H4O3_123TRIOXOLANE<G> T.C.R.A.S. Class: 7
C2H4O3_123TRIOXOLANE<G>
S298 corrected and cp refitted
due to corrected data in IVTAN2000 7/2002
typing error corrected 12/06
C2H5<G> T.C.R.A.S. Class: 6
ETHYL radical. Gaseous Standard State.
C2H6<G> T.C.R.A.S. Class: 6
ETHANE. Gaseous Standard State.
C2H6O1_1<G> THERMODATA 04/98 TC
ETHANOL. Gaseous Standard State.
C2H6O1_2<G> THERMODATA 04/98 TC
DIMETHYL ETHER. Gaseous Standard State.
C2H6O2<G> THERMODATA
C2H6O2<G>
E-GLYCOL <GAS>. Data revised by THDA.
C2O1<G> T.C.R.A.S. Class: 5
C2O1<G>
C3<G> T.C.R.A.S. Class: 6
CARBON triatomic gas.
CARBON <TRIATOMIC GAS>
C3H1<G> T.C.R.A.S. Class: 6
C3H1<G>
2-PROPYNYLIDYNE
S298 corrected and cp refitted
due to corrected data in IVTAN2000 7/2002
C3H4_1<G> STULL WESTRUM SINKE 1969 SGTE
C3H4_1<G>
ALLENE = 1,2-PROPADIENE
EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.
C3H4_2<G> STULL WESTRUM SINKE 1969 SGTE
C3H4_2<G>
PROPYNE (METHYLACETYLENE)
EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.
C3H6O1_1<G> THERMODATA 04/98 TC
2-PROPENOL (ALLYL ALCOHOL). Gaseous Standard State.
C3H6O1_2<G> THERMODATA 04/98 TC
DL-METHYLOXIRANE. Gaseous Standard State.
C3H6_1<G> T.C.R.A.S. Class: 6 4.09.85
C3H6(G) Cyclopropane
C3H6_2<G> STULL WESTRUM SINKE 1969 SGTE
PROPENE
PROPENE
EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.
C3H8<G> THERMODATA SGTE
PROPANE. Gaseous Standard State.
PROPANE <GAS>
PROPANE
C3O2<G> T.C.R.A.S. Class: 6
C3O2<G>
C4<G>
C4<G>
C4H1<G> T.C.R.A.S Class: 6
1,3-BUTADIYNYL Gaseous Standard State.
1,3-BUTADIYNYL. Data provided by T.C.R.A.S. in 2000
C4H10_1<G> T.C.R.A.S Class: 4
BUTANE Gaseous Standard State.
BUTANE. Data provided by T.C.R.A.S. in 2000
C4H10_2<G> T.C.R.A.S Class: 4
METHYLPROPANE N-BUTANE Gaseous Standard State.
METHYLPROPANE N-BUTANE. Data provided by T.C.R.A.S. in 2000
C4H2_1<G> THERMODATA 1978 ST
1,3-BUTADIYNE. Gaseous Standard State.
C4H2_2<G> THERMODATA 06/93 ST
BUTADIYNE(BIACETYLENE). Gaseous Standard State.
C4H4_1<G> T.C.R.A.S Class: 6
1,3-CYCLOBUTADIENE Gaseous Standard State.
1,3-CYCLOBUTADIENE. Data provided by T.C.R.A.S. in 2000
C4H4_2<G> STULL WESTRUM SINKE 1969 SGTE
1-BUTEN-3-YNE VINYLACETYLENE. Gaseous Standard State.
1-BUTEN-3-YNE VINYLACETYLENE
EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.
C4H6_1<G> STULL WESTRUM SINKE 1969 SGTE
C4H6_1<G>
1,2-BUTADIENE
EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.
C4H6_2<G> STULL WESTRUM SINKE 1969 SGTE
C4H6_2<G>
1,3-BUTADIENE
EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.
C4H6_3<G> STULL WESTRUM SINKE 1969 SGTE
C4H6_3<G>
1-BUTYNE ETHYLACETYLENE
EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.
C4H6_4<G> STULL WESTRUM SINKE 1969 SGTE
C4H6_4<G>
2-BUTYNE DIMETHYLACETYLENE
EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.
C4H6_5<G> T.C.R.A.S Class: 6
C4H6_5<G>
CYCLOBUTENE. Data provided by T.C.R.A.S. in 2000
C4H8_1<G> THERMODATA 04/98 TC
1-BUTENE. Gaseous Standard State.
C4H8_2<G> THERMODATA 04/98 TC
(E)-2-BUTENE. Gaseous Standard State.

C4H8_3<G> THERMODATA 04/98 TC
 (Z)-2-BUTENE. Gaseous Standard State.
 C4H8_4<G> THERMODATA 04/98 TC
 CYCLOBUTANE. Gaseous Standard State.
 C4H8_5<G> THERMODATA 04/98 TC
 2-METHYLPROPENE. Gaseous Standard State.
 C4H8_6<G> THERMODATA 04/98 TC
 METHYLCYCLOPROPANE. Gaseous Standard State.
 C5<G> T.C.R.A.S. Class: 7
 C5<G>
 C60<G> MHR-95
 C60<G>
 Data processed from [94Kor/Sid] M.V. Korobov, L.N. sidorov,
 J. Chem. Thermo., 26, 61-73 (1994). Recalculated from the rotational
 data in [91McK] and vibration frequencies in [94Kor/Sid]. Note that
 a frequency with degeneracy 5 is missing from list in [94Kor/Sid];
 taken to be 419 cm-1, which gives very good, though not exact,
 agreement with values quoted in [94Kor/Sid]. Note discrepancy
 between calculated DrS(298) = -8943.5 J mol K-1 for the reaction
 $60<g>+C60<g>$ and that given by [94Kor/Sid] in their Table 5,
-8950 J mol K-1. Enthalpy of formation: DfH = 2588 kJ/mol from
DsubH(298.15K) = 166 +/- 11 kJ mol-1 [94Kor/Sid]. Vapour pressure
values reproduced very well.
[91McK] J.T. McKinnon, J. Phys. Chem. 95 8941(1993).
C6H6<G> T.C.R.A.S Class: 5
BENZENE. Gaseous Standard State.
BENZENE. Data provided by T.C.R.A.S. in 2000
C6H6O1<G> THERMODATA 01/93
C6H6O1<G>
PHENOL
28/01/93
H1<G> JANAF 1982; ASSESSMENT DATED 3/77 SGTE **
H1<G> H<G>
HYDROGEN <MONATOMIC GAS>
H1O1<G> T.C.R.A.S. Class: 1
H1O1<G> OH<G>
H1O2<G> T.C.R.A.S. Class: 4
H1O2<G>
H2<G> JANAF THERMOCHEMICAL TABLES SGTE **
H2<G> H2<G>
HYDROGEN<G>
STANDARD STATE FROM CODATA KEY VALUES. CP FROM JANAF PUB. 3/61
H2O1<G> T.C.R.A.S. Class: 1
H2O1<G> H2O<G>
WATER <GAS>
H2O2<G> JANAF SECOND EDIT SGTE
H2O2<G> H2O2<G>
HYDROGEN PEROXIDE <GAS>
O1<G> TCRAS 02/06/80
O1 Gaseous Standard State.
O2<G> TCRAS 21/06/90
OXYGEN Gaseous Standard State.
O3<G> TCRAS 02/06/80
OZONE Gaseous Standard State.
C1H2O2<L> THERMODATA 01/93
C1H2O2 HCOOH
FORMIC ACID MONOMERIC
28/01/93
C1H4O1<L> I. BARIN 3rd. Edition
C1H4O1 CH3OH
METHANOL. H298 and S298 modified.
C1H4<L> THERMODATA 04/99 HH
METHANE Liquid Standard State.
C2H4O2<L> THERMODATA 01/93
C2H4O2
ACETIC ACID
28/01/93 Tb=389K.
C2H6O1<L> THERMODATA 01/93
C2H6O1 C2H6O
ETHANOL
28/01/93
C2H6O2<L> THERMODATA
C2H6O2
E-GLYCOL
Data revised by THDA.
C2H6<L> THERMODATA 04/99 HH
ETHANE Liquid Standard State.
C3H6<L> THERMODATA 03/05 HH
CYCLOPROPANE. Liquid Standard State.
C3H8<L> THERMODATA 04/99 HH
PROPANE Liquid Standard State
C4H8<L> THERMODATA 04/99 HH
CYCLOBUTANE. Liquid Standard State.
C60 MHR-95
C60
Data processed from [94Kor/Sid] M.V. Korobov, L.N. sidorov, J. Chem.
The
Fitted to the data in [94Kor/Sid], who took the phase transition at
257K
that [94Kor/Sid] do not give an explicit value for S(298.15K).
S(298.15K) = 422.6 J mol K-1 was calculated from S(300) = 425.8 and Cp
e
calculated from DrS(298) for 60C<graphite>=C60 given by [94Kor/Sid]
in their Table 5, which gives S(298.15K) = 425.4 J mol K-1.
Enthalpy of formation: DfH = +2422 +/- 14 kJ/mol from [92Ste/Chi],
the value preferred, if obliquely, by [94Kor/Sid].
[92Ste/Chi] W.V. Steele, R.D. Chirico, N.K. Smith, W.e. Billups,
P.R. Elmore, A.E. Wheeler, J. Phys. Chem. 96 4731 (1993).
C6H6<L> THERMODATA 04/99 BC
BENZENE. Liquid Standard State. Tm=278.6K
C1 S.G.T.E. **
GRAPHITE
Data from SGTE Unary DB, pressure dependent data added by atd 7/9/95
C1<DIAMOND> S.G.T.E. **
C1<DIAMOND> <DIAMOND>
DIAMOND
Data from SGTE Unary DB, data added by atd 7/9/95, H298-H0 taken
from 1994 database (ex THERMODATA 01/93)
H2O1<L> T.C.R.A.S. Class: 4
H2O1 H2O
WATER
T.C.R.A.S. Class: 4 cp modified by atd 12/9/94 and 5/7/2002
H2O2<L> THERMODATA 01/93
H2O2 H2O2
HYDROGEN PEROXIDE
28/01/93

-OK-

TOB_SSUB6: go p-3

... the command in full is GOTO_MODULE

POLY version 3.32

POLY: l-st

... the command in full is LIST_STATUS

Option /CPS/:

*** STATUS FOR ALL COMPONENTS

| COMPONENT | STATUS | REF. | STATE | T (K) | P (Pa) |
|-----------|---------|------|-------|-------|--------|
| VA | ENTERED | SER | | | |
| C | ENTERED | SER | | | |
| H | ENTERED | SER | | | |
| O | ENTERED | SER | | | |

*** STATUS FOR ALL PHASES

| PHASE | STATUS | DRIVING FORCE | MOLES |
|----------|---------|---------------|--------------|
| H2O2_L | ENTERED | 0.000000E+00 | 0.000000E+00 |
| H2O1_L | ENTERED | 0.000000E+00 | 0.000000E+00 |
| DIAMOND | ENTERED | 0.000000E+00 | 0.000000E+00 |
| C_S | ENTERED | 0.000000E+00 | 0.000000E+00 |
| C_L | ENTERED | 0.000000E+00 | 0.000000E+00 |
| C6H6_L | ENTERED | 0.000000E+00 | 0.000000E+00 |
| C60_S | ENTERED | 0.000000E+00 | 0.000000E+00 |
| C4H8_L | ENTERED | 0.000000E+00 | 0.000000E+00 |
| C3H8_L | ENTERED | 0.000000E+00 | 0.000000E+00 |
| C3H6_L | ENTERED | 0.000000E+00 | 0.000000E+00 |
| C2H6_L | ENTERED | 0.000000E+00 | 0.000000E+00 |
| C2H6O2_L | ENTERED | 0.000000E+00 | 0.000000E+00 |
| C2H6O1_L | ENTERED | 0.000000E+00 | 0.000000E+00 |
| C2H4O2_L | ENTERED | 0.000000E+00 | 0.000000E+00 |
| C1H4_L | ENTERED | 0.000000E+00 | 0.000000E+00 |
| C1H4O1_L | ENTERED | 0.000000E+00 | 0.000000E+00 |
| C1H2O2_L | ENTERED | 0.000000E+00 | 0.000000E+00 |
| GAS | ENTERED | 0.000000E+00 | 0.000000E+00 |

*** STATUS FOR ALL SPECIES

| | | | |
|----------------------|---------|----------|---------|
| C | ENTERED | C3H6 | ENTERED |
| C1H1 | ENTERED | C3H6O1_1 | ENTERED |
| C1H1O1 | ENTERED | C3H6O1_2 | ENTERED |
| C1H1O2 | ENTERED | C3H6_1 | ENTERED |
| C1H2 | ENTERED | C3H6_2 | ENTERED |
| C1H2O1 | ENTERED | C3H8 | ENTERED |
| C1H2O2 | ENTERED | C3O2 | ENTERED |
| C1H2O2_CIS | ENTERED | C4 | ENTERED |
| C1H2O2_DIOXIRANE | ENTERED | C4H1 | ENTERED |
| C1H2O2_TRANS | ENTERED | C4H10_1 | ENTERED |
| C1H3 | ENTERED | C4H10_2 | ENTERED |
| C1H3O1_CH2OH | ENTERED | C4H2_1 | ENTERED |
| C1H3O1_CH3O | ENTERED | C4H2_2 | ENTERED |
| C1H4 | ENTERED | C4H4_1 | ENTERED |
| C1H4O1 | ENTERED | C4H4_2 | ENTERED |
| C1O1 | ENTERED | C4H6_1 | ENTERED |
| C1O2 | ENTERED | C4H6_2 | ENTERED |
| C2 | ENTERED | C4H6_3 | ENTERED |
| C2H1 | ENTERED | C4H6_4 | ENTERED |
| C2H2 | ENTERED | C4H6_5 | ENTERED |
| C2H2O1 | ENTERED | C4H8 | ENTERED |
| C2H3 | ENTERED | C4H8_1 | ENTERED |
| C2H4 | ENTERED | C4H8_2 | ENTERED |
| C2H4O1_ACETALDEHYDE | ENTERED | C4H8_3 | ENTERED |
| C2H4O1_OXIRANE | ENTERED | C4H8_4 | ENTERED |
| C2H4O2 | ENTERED | C4H8_5 | ENTERED |
| C2H4O2_ACETICACID | ENTERED | C4H8_6 | ENTERED |
| C2H4O2_DIOXETANE | ENTERED | C5 | ENTERED |
| C2H4O3_123TRIOXOLANE | ENTERED | C60 | ENTERED |
| C2H4O3_124TRIOXOLANE | ENTERED | C6H6 | ENTERED |
| C2H5 | ENTERED | C6H6O1 | ENTERED |
| C2H6 | ENTERED | H | ENTERED |
| C2H6O1 | ENTERED | H1O1 | ENTERED |
| C2H6O1_1 | ENTERED | H1O2 | ENTERED |
| C2H6O1_2 | ENTERED | H2 | ENTERED |
| C2H6O2 | ENTERED | H2O1 | ENTERED |
| C2O1 | ENTERED | H2O2 | ENTERED |
| C3 | ENTERED | O | ENTERED |
| C3H1 | ENTERED | O2 | ENTERED |
| C3H4_1 | ENTERED | O3 | ENTERED |
| C3H4_2 | ENTERED | VA | ENTERED |

POLY: @@ We need to know the heat content of C3H8<G> at room

POLY: @@ temperature. This is a simple number to look up in a

POLY: @@ table but actually quite tricky to calculate as pure

POLY: @@ C3H8 at room temperature does not represent an

POLY: @@ equilibrium state. However, you can get it as follows.

POLY:

POLY: s-c t=298.15,p=1e5,n(o)=1e-10

... the command in full is SET_CONDITION

POLY: s-i-a n(c3h8)=1

... the command in full is SET_INPUT_AMOUNTS

POLY: c-s p *=sus

... the command in full is CHANGE_STATUS

POLY: c-s p gas

... the command in full is CHANGE_STATUS

Status: /ENTERED/

Start value, number of mole formula units /0/:

POLY: c-e

... the command in full is COMPUTE_EQUILIBRIUM

Using global minimization procedure

Calculated 76 grid points in 0 s

Found the set of lowest grid points in 0 s

Calculated POLY solution 1 s, total time 1 s

POLY: @@ The equilibrium state at room temperature is listed

POLY: l-e,,,

... the command in full is LIST_EQUILIBRIUM

Output from POLY-3, equilibrium = 1, label A0 , database: SSUB6

Conditions:

T=298.15, P=100000, N(O)=1E-10, N(C)=3, N(H)=8

DGREES OF FREEDOM 0

Temperature 298.15 K (25.00 C), Pressure 1.000000E+05

Number of moles of components 1.10000E+01, Mass in grams 4.40962E+01

Total Gibbs energy -2.20108E+05, Enthalpy -1.06064E+05, Volume 4.99502E-02

| Component | Moles | W-Fraction | Activity | Potential | Ref.stat |
|-----------|------------|------------|------------|-------------|----------|
| C | 3.0000E+00 | 8.1715E-01 | 1.1356E+07 | 4.0271E+04 | SER |
| H | 8.0000E+00 | 1.8285E-01 | 3.4211E-08 | -4.2615E+04 | SER |

O 1.0000E-10 3.6282E-11 1.2651E-49 -2.7911E+05 SER

GAS Status ENTERED Driving force 0.0000E+00
Moles 1.1000E+01, Mass 4.4096E+01, Volume fraction 1.0000E+00 Mass fractions:
C 8.17145E-01 H 1.82855E-01 O 3.62820E-11

Constitution:

| | Moles | Status | Driving force | Ref.stat |
|--------------|-------------|--------------|---------------|--------------------------|
| C1H4 | 9.90348E-01 | C1H2O1 | 4.96084E-27 | C4H6_3 1.00000E-30 |
| C60 | 8.16678E-03 | C1H2O2_CIS | 4.88436E-27 | C2H4O1_OXIRA 1.00000E-30 |
| C6H6 | 1.38456E-03 | C4H6_4 | 3.94602E-28 | C4H6_5 1.00000E-30 |
| C2H6 | 1.00313E-04 | C3H4_2 | 6.04110E-29 | C5 1.00000E-30 |
| C3H8 | 5.44582E-07 | C2H5 | 1.32230E-29 | C2H3 1.00000E-30 |
| C4H10_2 | 3.84975E-08 | C1H2O2_TRANS | 6.61825E-30 | C2H2O1 1.00000E-30 |
| H2 | 7.83769E-09 | C3H4_1 | 2.45341E-30 | C2H2 1.00000E-30 |
| C4H10_1 | 6.16323E-09 | C4H6_1 | 2.07866E-30 | C2H1 1.00000E-30 |
| C1O2 | 2.32090E-11 | C | 1.00000E-30 | C2 1.00000E-30 |
| H2O1 | 2.50979E-12 | C3O2 | 1.00000E-30 | H 1.00000E-30 |
| C1O1 | 7.01016E-13 | C4 | 1.00000E-30 | H1O1 1.00000E-30 |
| C4H8_5 | 6.29486E-14 | C3H6O1_2 | 1.00000E-30 | H1O2 1.00000E-30 |
| C3H6_2 | 5.52670E-14 | C3H6O1_1 | 1.00000E-30 | H2O2 1.00000E-30 |
| C2H4 | 3.33175E-14 | C4H1 | 1.00000E-30 | C1H3O1_CH3O 1.00000E-30 |
| C4H8_2 | 7.83367E-15 | C4H2_1 | 1.00000E-30 | C1H3O1_CH2OH 1.00000E-30 |
| C4H6_3 | 3.33692E-15 | C3H1 | 1.00000E-30 | C1H3 1.00000E-30 |
| C4H8_1 | 4.53470E-16 | C3 | 1.00000E-30 | O 1.00000E-30 |
| C6H6O1 | 1.02341E-18 | C2O1 | 1.00000E-30 | C1H2O2_DIOXI 1.00000E-30 |
| C3H6_1 | 2.70389E-21 | C2H6O2 | 1.00000E-30 | O2 1.00000E-30 |
| C4H8_6 | 1.07592E-21 | C2H6O1_2 | 1.00000E-30 | O3 1.00000E-30 |
| C4H6_2 | 4.91032E-22 | C4H2_2 | 1.00000E-30 | C1H2 1.00000E-30 |
| C2H4O1_ACETA | 1.25014E-22 | C4H4_1 | 1.00000E-30 | C1H1O2 1.00000E-30 |
| C4H8_4 | 2.10624E-23 | C4H4_2 | 1.00000E-30 | C1H1O1 1.00000E-30 |
| C2H4O2_ACETI | 9.64309E-24 | C2H4O3_124TR | 1.00000E-30 | C1H1 1.00000E-30 |
| C2H6O1_1 | 1.76369E-24 | C2H4O3_123TR | 1.00000E-30 | |
| C1H4O1 | 1.08754E-24 | C2H4O2_DIOXE | 1.00000E-30 | |

POLY: @@ The enthalpy for the system is
POLY: sh h
... the command in full is SHOW_VALUE
H=-106064.27

POLY:Hit RETURN to continue

POLY: @@ But we want a gas with just C3H8.
POLY: @@ Use the Set-All-Startvalues command.

POLY: s-a-s
... the command in full is SET_ALL_START_VALUES

Automatic start values for phase constituents? /N/: n
Should GAS be stable? /Y/: 1
Major constituent(s): C3H8

POLY: sh h
... the command in full is SHOW_VALUE
H=-99431.45

POLY: @@ The difference in H for the two calculations is actually
POLY: @@ not very large. The value is approximate but good as the
POLY: @@ enthalpy is calculated for the following gas constitution

POLY: l-e,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: SSUB6

Conditions:
T=298.15, P=100000, N(O)=1E-10, N(C)=3, N(H)=8
DEGREES OF FREEDOM 0

Temperature 298.15 K (25.00 C), Pressure 1.000000E+05
Number of moles of components 1.07458E+01, Mass in grams 4.32993E+01
Total Gibbs energy -1.78580E+05, Enthalpy -9.94314E+04, Volume 2.43005E-02

| Component | Moles | W-Fraction | Activity | Potential | Ref.stat |
|-----------|------------|------------|------------|-------------|----------|
| C | 2.9417E+00 | 8.1602E-01 | 1.1356E+07 | 4.0271E+04 | SER |
| H | 7.7974E+00 | 1.8150E-01 | 3.4211E-08 | -4.2615E+04 | SER |
| O | 6.7105E-03 | 2.4795E-03 | 1.2651E-49 | -2.7911E+05 | SER |

GAS Status ENTERED Driving force 0.0000E+00
Moles 1.07464E+01, Mass 4.32998E+01, Volume fraction 1.0000E+00 Mass fractions:
C 8.16017E-01 H 1.81504E-01 O 2.47953E-03

Constitution:

| | Moles | Status | Driving force | Ref.stat |
|--------|-------------|--------------|---------------|--------------------------|
| C3H8 | 9.70396E-01 | C4H4_1 | 1.31579E-04 | C2H4O2_ACETI 1.31579E-04 |
| C | 1.31579E-04 | C4H2_2 | 1.31579E-04 | C2H4O1_OXIRA 1.31579E-04 |
| O2 | 1.31579E-04 | C4H2_1 | 1.31579E-04 | C2H4O1_ACETA 1.31579E-04 |
| O | 1.31579E-04 | C4H10_2 | 1.31579E-04 | C2H4 1.31579E-04 |
| H2O2 | 1.31579E-04 | C4H10_1 | 1.31579E-04 | C2H3 1.31579E-04 |
| H2O1 | 1.31579E-04 | C4H1 | 1.31579E-04 | C2H2O1 1.31579E-04 |
| H2 | 1.31579E-04 | C4 | 1.31579E-04 | C2H2 1.31579E-04 |
| H1O2 | 1.31579E-04 | C3O2 | 1.31579E-04 | C2H1 1.31579E-04 |
| H1O1 | 1.31579E-04 | O3 | 1.31579E-04 | C2 1.31579E-04 |
| H | 1.31579E-04 | C3H6_2 | 1.31579E-04 | C1O2 1.31579E-04 |
| C6H6O1 | 1.31579E-04 | C3H6_1 | 1.31579E-04 | C1O1 1.31579E-04 |
| C6H6 | 1.31579E-04 | C3H6O1_2 | 1.31579E-04 | C1H4O1 1.31579E-04 |
| C6O | 1.31579E-04 | C3H6O1_1 | 1.31579E-04 | C1H4 1.31579E-04 |
| C5 | 1.31579E-04 | C3H4_2 | 1.31579E-04 | C1H3O1_CH3O 1.31579E-04 |
| C4H8_6 | 1.31579E-04 | C3H4_1 | 1.31579E-04 | C1H3O1_CH2OH 1.31579E-04 |
| C4H8_5 | 1.31579E-04 | C3H1 | 1.31579E-04 | C1H3 1.31579E-04 |
| C4H8_4 | 1.31579E-04 | C3 | 1.31579E-04 | C1H2O2_TRANS 1.31579E-04 |
| C4H8_3 | 1.31579E-04 | C2O1 | 1.31579E-04 | C1H2O2_DIOXI 1.31579E-04 |
| C4H8_2 | 1.31579E-04 | C2H6O2 | 1.31579E-04 | C1H2O2_CIS 1.31579E-04 |
| C4H8_1 | 1.31579E-04 | C2H6O1_2 | 1.31579E-04 | C1H2O1 1.31579E-04 |
| C4H6_5 | 1.31579E-04 | C2H6O1_1 | 1.31579E-04 | C1H2 1.31579E-04 |
| C4H6_4 | 1.31579E-04 | C2H6 | 1.31579E-04 | C1H1O2 1.31579E-04 |
| C4H6_3 | 1.31579E-04 | C2H5 | 1.31579E-04 | C1H1O1 1.31579E-04 |
| C4H6_2 | 1.31579E-04 | C2H4O3_124TR | 1.31579E-04 | C1H1 1.31579E-04 |
| C4H6_1 | 1.31579E-04 | C2H4O3_123TR | 1.31579E-04 | |
| C4H4_2 | 1.31579E-04 | C2H4O2_DIOXE | 1.31579E-04 | |

POLY:Hit RETURN to continue

POLY: @@ We now have the initial amount of heat. Assuming an excess
POLY: @@ of oxygen we can calculate the temperature where the
POLY: @@ heat content would be the same

POLY:
POLY: sh h
... the command in full is SHOW_VALUE
H=-99431.45

POLY: @@ H is just 11 times HM as there are 11 atoms in C3H8.
POLY: @@ Save that value in a variable

POLY:
POLY: enter var h298=h;
... the command in full is ENTER_SYMBOL
POLY: sh h298
... the command in full is SHOW_VALUE
H298=-99431.45

```

POLY: @@ If all carbon and hydrogen react with oxygen we need 7
POLY: @@ oxygen atoms to form 3 moles ClO and 4 moles of H2O.
POLY: @@ Add some oxygen in excess
POLY:
POLY: s-c n(o)=9
... the command in full is SET_CONDITION
POLY: @@ Set the heat content as a condition and remove the
POLY: @@ condition on t
POLY:
POLY: s-c h=h298
... the command in full is SET_CONDITION
POLY: s-c t
... the command in full is SET_CONDITION
Value /298.15/: none
POLY: l-c
... the command in full is LIST_CONDITIONS
P=100000, N(O)=9, N(C)=3, N(H)=8, H=H298
DEGREES OF FREEDOM 0
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated 76 grid points in 0 s
152 ITS, CPU TIME USED 0 SECONDS
POLY: l-e,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: SSUB6

Conditions:
P=100000, N(O)=9, N(C)=3, N(H)=8, H=H298
DEGREES OF FREEDOM 0

Temperature 3103.37 K ( 2830.22 C), Pressure 1.000000E+05
Number of moles of components 2.000000E+01, Mass in grams 1.88087E+02
Total Gibbs energy -7.70691E+06, Enthalpy -9.94314E+04, Volume 2.20472E+00

Component Moles W-Fraction Activity Potential Ref.stat
C 3.0000E+00 1.9158E-01 9.3982E-09 -4.7691E+05 SER
H 8.0000E+00 4.2869E-02 7.7626E-06 -3.0360E+05 SER
O 9.0000E+00 7.6555E-01 6.3815E-08 -4.2748E+05 SER

GAS Status ENTERED Driving force 0.0000E+00
Moles 2.0000E+01, Mass 1.8809E+02, Volume fraction 1.0000E+00 Mass fractions:
O 7.65554E-01 C 1.91576E-01 H 4.28695E-02
Constitution:
H2O1 3.17918E-01 C1H2O2_DIOXI 7.89694E-16 C3H6O1_2 1.00000E-30
C1O1 2.27799E-01 C2H1 8.90508E-17 C3H6_1 1.00000E-30
C1O2 1.23305E-01 C3O2 8.73154E-17 C3H6_2 1.00000E-30
H1O1 8.75243E-02 C2 1.57966E-17 C3H8 1.00000E-30
H2 7.66545E-02 C2H2O1 2.52104E-18 C4 1.00000E-30
O2 6.61854E-02 C2H3 2.72613E-19 C4H1 1.00000E-30
H 5.95645E-02 C2H4O1_ACETA 1.22421E-20 C4H10_1 1.00000E-30
O 4.10043E-02 C2H4 1.12666E-20 C4H10_2 1.00000E-30
H1O2 4.23460E-05 C2H4O2_ACETI 7.64173E-21 C4H4_1 1.00000E-30
H2O2 1.60571E-06 C3H1 9.69741E-23 C4H8_4 1.00000E-30
C1H1O1 9.35079E-07 C3 6.41061E-23 C4H8_5 1.00000E-30
C1H1O2 6.80240E-07 C2H4O1_OXIRA 1.10545E-23 C4H4_2 1.00000E-30
O3 3.00641E-08 C2H5 2.16426E-24 C4H6_1 1.00000E-30
C1H2O2_CIS 1.60533E-08 C2H6 2.32872E-26 C4H6_2 1.00000E-30
C1H2O2_TRANS 8.97486E-09 C2H6O1_1 6.05817E-27 C4H6_3 1.00000E-30
C1H2O1 7.25807E-09 C2H6O2 8.46558E-28 C4H6_4 1.00000E-30
C 5.41880E-11 C3H4_2 5.36473E-28 C4H8_6 1.00000E-30
C1H1 5.71334E-12 C3H4_1 2.88191E-28 C4H6_5 1.00000E-30
C1H2 2.82748E-12 C2H6O1_2 7.51593E-29 C5 1.00000E-30
C1H3 2.09122E-12 C2H4O2_DIOXE 1.26866E-29 C6O 1.00000E-30
C2O1 1.16897E-12 C2H4O3_124TR 2.44145E-30 C4H8_1 1.00000E-30
C1H3O1_CH2OH 8.94424E-13 C4H2_1 2.38485E-30 C6H6 1.00000E-30
C1H4 1.80436E-13 C4H2_2 2.37831E-30 C6H6O1 1.00000E-30
C1H3O1_CH3O 1.92548E-14 C4H8_3 1.00000E-30 C4H8_2 1.00000E-30
C1H4O1 9.77820E-15 C2H4O3_123TR 1.00000E-30
C2H2 1.14657E-15 C3H6O1_1 1.00000E-30

POLY: @@ The adiabatic temperature is
POLY: sh t
... the command in full is SHOW_VALUE
T=3103.3658
POLY:Hit RETURN to continue
POLY: @@ Now calculate how the adiabatic temperature varies
POLY: @@ with the amount of oxygen
POLY:
POLY: s-a-v 1 n(o) 5 10
... the command in full is SET_AXIS_VARIABLE
Increment /.125/:
POLY: save tcex22 y
... the command in full is SAVE_WORKSPACES
POLY: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 9.00000
...OK

Phase Region from 9.00000 for:
  GAS
Global test at 1.000000E+01 .... OK
Terminating at 10.0000
Calculated 11 equilibria

Phase Region from 9.00000 for:
  GAS
Global test at 8.000000E+00 .... OK
Global test at 6.750000E+00 .... OK
Global test at 5.500000E+00 .... OK
Terminating at 5.00000
Calculated 35 equilibria
*** Buffer saved on file: c:\jenkins\workspace\generate_console_examples\examples\tcex22\tcex22.POLY3
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2
POST:
POST: s-d-a x n(o)
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t
... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 22a
POST:
POST: SET_EXP_FILE_FORMAT 5

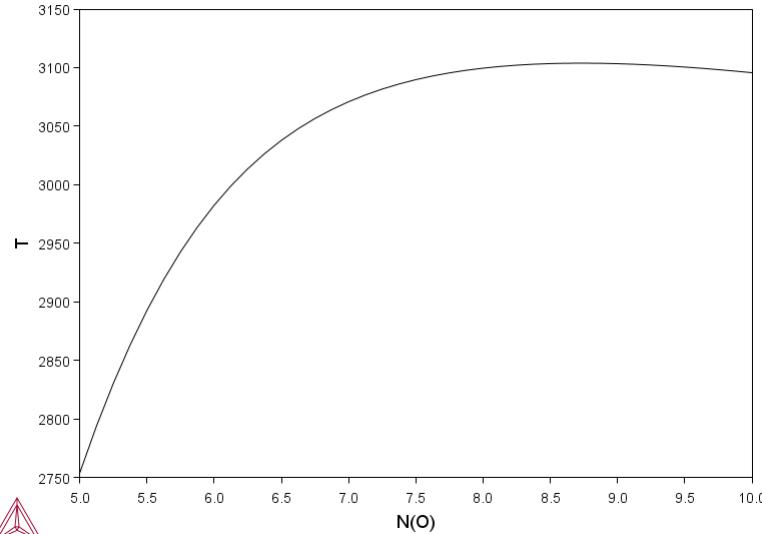
```

```

POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 22a

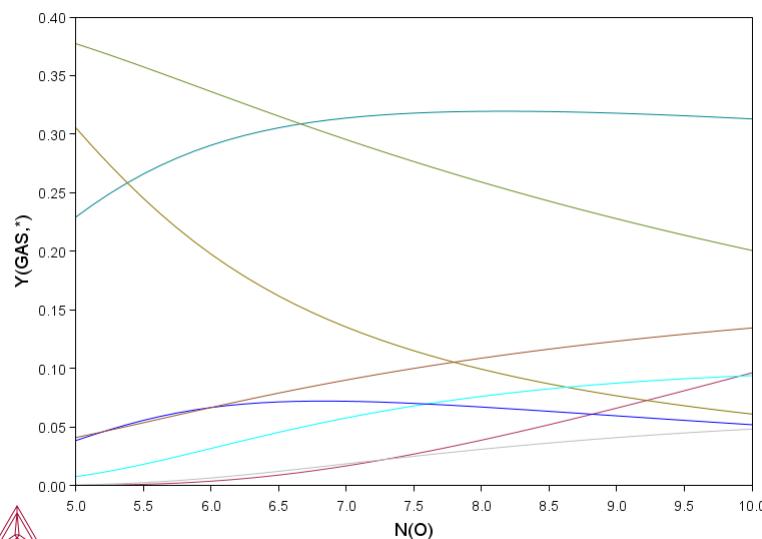


```

POST:
POST:Hit RETURN to continue
POST: @@ Plot how the gas constitution changes
POST: s-d-a y y(gas,*)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*:
POST: set-title example 22b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 22b

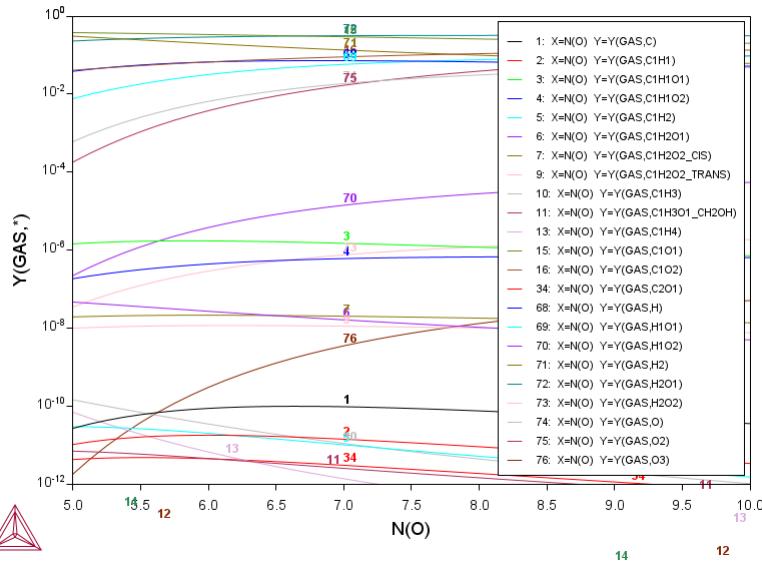


```

POST:
POST:Hit RETURN to continue
POST: @@ Add labels and a logarithmic fraction scale
POST: s-lab d
... the command in full is SET_LABEL_CURVE_OPTION
POST: s-a-ty y log
... the command in full is SET_AXIS_TYPE
POST: s-s y n 1e-12 1
... the command in full is SET_SCALING_STATUS
POST: set-title example 22c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

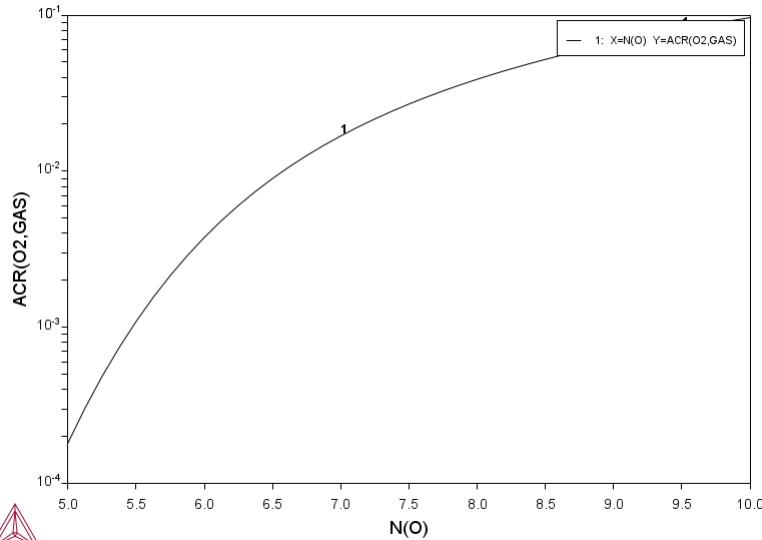
example 22c



POST:
POST: Hit RETURN to continue

POST: @@ Plot how the oxygen partial pressure changes
POST: s-d-a y acr(o2,gas)
... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 22d
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

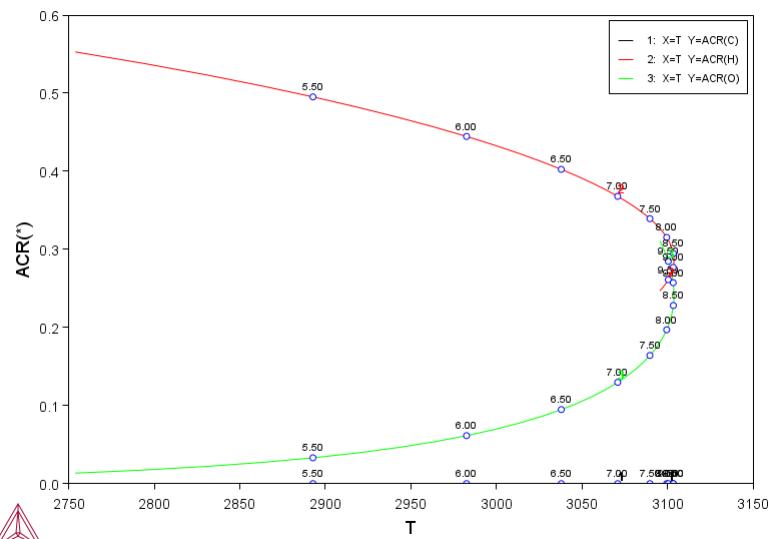
example 22d



POST:
POST: Hit RETURN to continue

POST: @@ Plot how the activities of the components change
POST: @@ with temperature. Note that the oxygen content
POST: @@ also changes. Set the reference states
POST:
POST: set-ref-state o gas * 1e5
... the command in full is SET_REFERENCE_STATE
You should set-diagram-axis for the activity/potential after this!
POST: set-ref-state h gas * 1e5
... the command in full is SET_REFERENCE_STATE
You should set-diagram-axis for the activity/potential after this!
POST: set-ref-state c c_s * 1e5
... the command in full is SET_REFERENCE_STATE
You should set-diagram-axis for the activity/potential after this!
POST: s-d-a x t
... the command in full is SET_DIAGRAM_AXIS
POST: s-a-ty y lin
... the command in full is SET_AXIS_TYPE
POST: s-d-a z n(o)
... the command in full is SET_DIAGRAM_AXIS
POST: s-s z n 5 10
... the command in full is SET_SCALING_STATUS
POST: s-d-a y acr(*)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*:
POST: set-title example 22e
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI

```
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
example 22e
```



```
POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:
```

tce23**SYS:About**

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce23\tce23.TCM.test"

SYS: set-echo

SYS:

SYS: @@ Calculating a paraequilibrium and the

SYS: @@ T0 temperature in a low alloyed steel

SYS:

SYS: @@ Note that a TCFE database license is required to run

SYS: @@ the example.

SYS:

SYS: set-log ex23,,,

SYS: go p-3

... the command in full is GOTO_MODULE

POLY version 3.32

POLY: @@ Define the material

POLY: def-mat

... the command in full is DEFINE_MATERIAL

THERMODYNAMIC DATABASE module

Database folder: C:\jenkins\workspace\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

Database /TCFE11/: tcfe11

Major element or alloy: fe

Composition input in mass (weight) percent? /Y/: Y

1st alloying element: mn 1.5

2nd alloying element: si .3

Next alloying element: c .3

Next alloying element:

Temperature (C) /1000/: 700

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

REINITIATING GES

... the command in full is DEFINE_ELEMENTS

FE DEFINED

... the command in full is DEFINE_ELEMENTS

MN DEFINED

... the command in full is DEFINE_ELEMENTS

SI DEFINED

... the command in full is DEFINE_ELEMENTS

C DEFINED

This database has following phases for the defined system

| | | |
|--------------|----------------|-------------|
| GAS:G | LIQUID:L | BCC_A2 |
| A2_BCC | BCC_B2 | FCC_A1 |
| A1_FCC | FCC_L12 | HCP_A3 |
| CBCC_A12 | CUB_A13 | DIAMOND_A4 |
| GRAPHITE_A9 | CEMENTITE_D011 | M23C6_D84 |
| M7C3_D101 | M5C2 | KSI_CARBIDE |
| FE4N_LP1 | C14_LAVES | C15_LAVES |
| M3SI | MN9Si2 | MN11Si19 |
| MN6Si | G_PHASE | CR3Si_A15 |
| FESI2_H | FESI2_L | MSI_B20 |
| M5Si3_D88 | NBNi3_D0A | AL4C3_D71 |
| FE8Si2C | SIC_B3 | MN5SiC |
| CUZN_EPSILON | AL5Fe4 | MNP_B31 |
| M2P_C22 | FLUORITE_C1:I | ZRO2_TETR:I |
| M2O3C_D53:I | M2O3H_D52:I | NI31Si12 |
| CO2Si_C37 | M2Si_TETA | NiSi_B31 |
| NI3Si2 | CR5Si3_D8M | |

Reject phase(s) /NONE/: NONE

Restore phase(s): /NONE/: NONE

.....
The following phases are retained in this system:

| | | |
|--------------|----------------|-------------|
| GAS:G | LIQUID:L | BCC_A2 |
| A2_BCC | BCC_B2 | FCC_A1 |
| A1_FCC | FCC_L12 | HCP_A3 |
| CBCC_A12 | CUB_A13 | DIAMOND_A4 |
| GRAPHITE_A9 | CEMENTITE_D011 | M23C6_D84 |
| M7C3_D101 | M5C2 | KSI_CARBIDE |
| FE4N_LP1 | C14_LAVES | C15_LAVES |
| M3SI | MN9Si2 | MN11Si19 |
| MN6Si | G_PHASE | CR3Si_A15 |
| FESI2_H | FESI2_L | MSI_B20 |
| M5Si3_D88 | NBNi3_D0A | AL4C3_D71 |
| FE8Si2C | SIC_B3 | MN5SiC |
| CUZN_EPSILON | AL5Fe4 | MNP_B31 |
| M2P_C22 | FLUORITE_C1:I | ZRO2_TETR:I |
| M2O3C_D53:I | M2O3H_D52:I | NI31Si12 |
| CO2Si_C37 | M2Si_TETA | NiSi_B31 |
| NI3Si2 | CR5Si3_D8M | |

.....
OK? /Y/: Y

16:00:17,739 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

ELEMENTS

SPECIES

PHASES

... the command in full is AMEND_PHASE_DESCRIPTION

... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION
 ... the command in full is AMEND_PHASE_DESCRIPTION
 Suspending FLUORITE_C1 as it has net charge
 Suspending M203C_D53 as it has net charge
 Suspending M203H_D52 as it has net charge
 Suspending ZRO2_TETR as it has net charge
 PARAMETERS ...
 FUNCTIONS ...

 List of references for assessed data

 'A.T. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
 'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121-127; Molar volumes'
 'X.G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
 'Y. Tang, in TCCU2, Thermo-Calc Software AB, Stockholm, Sweden'
 'X.G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar volumes'
 'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equilib., 19 (1998) 441-448; Fe-Ti'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; C14_LAVES'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, Volume data updated for TCFE9 database (TCFE v9.0, Jan, 2017).'
 'N. Dupin, introduction of Nb to NI15VA-4SL'
 'N. Dupin, Private communication, (2008); Volume data'
 'H. Gohring, O. Fabrichnaya, A. Leineweber, E.J. Mittemeijer, Metall. Mater. Trans. A, 47A, 6173-86(2016); FE-N, and Fe-C-N'
 'Unassessed parameter; Linear combination of unary data'
 'N. Saunders, COST 507 Report (1998); Mn-Ti'
 'W. Zheng, J. Alloys Compd., 632 (2015) 661-675'
 'L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2012; Molar volumes'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; FE4N'
 'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
 'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; C14_LAVES'
 'I. Ansara, unpublished work (1991); Cr-Si'
 'M. Seiersten, Unpublished work (1989); Al-Fe'
 'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FI'
 'M. Ghasemi, Thermo-Calc Software AB, Sweden, 2020; Unifying liquid volume database'
 'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
 'J-O. Andersson, CALPHAD, 12 (1988) 9-23; TRITA 0321 (1986); C-FE-MO'
 'B. Hallstedt, D. Djurovic, J. von Appen, R. Dronskowski, A. Dick, F. Koermann, T. Hichel, J. Neugebauer, CALPHAD, 34, 129-33(2010); Fe-C'
 'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, Calphad 35.4 (2011) 479-491; Fe-Mn-C'
 'P. Villars, L.D. Calvert. Pearson's handbook of crystallographic data for intermetallic phases, Metals park, Ohio 1985: American society for metals'
 'W. Huang, Metall. Trans. A, 21A (1990) 2115-2123; TRITA-MAC 411 (Rev 1989); C-FE-MN'
 'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, CALPHAD, 34, 279-85 (2010); Mn-C'
 'J. Grobner, H.L. Lukas, F. Aldinger, Calphad, 1996, 20 (2), 247-254; Al-C, Si-C, Al-Si-C'
 'P. Franke; revision of C-Si, Fe-Si and C-Fe-Si'
 'J. Lacaze and B. Sundman, Metall. Mater. Trans. A, 22A (1991) 2211-2223; Fe-Si and Fe-Si-C'
 'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; Cementite'
 'R. Naraghi, Thermo-Calc Software AB, Volume data updated for TCFE9 database (TCFE v9.1, June, 2019).'
 'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; SIGMA and M7C3'
 'Thermo-Calc Software, Sweden, 2008; Volume data updated for STCFE6 database (TCFE v6, April, 2008).'
 'NPL, Unpublished work (1989); C-Mn-Si'
 'W. Huang, CALPHAD, 13 (1989) 243-252; TRITA-MAC 388 (rev 1989); FE-MN'
 'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
 'S. Liu, B. Hallstedt, D. Music, Y. Du, CALPHAD, 38 (2012) 43-58; Mn-Nb and Fe-Mn-Nb'
 'A. Markstrom, Thermo-Calc software AB, Sweden, 2011'
 'L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2013; Reassessed solubility of Al, Cr, Fe, Ni in Mn203. When Mn203 is modelled as the same phase as cubic Y2O3 (M203C).'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; Molar volume Fe-Mn-Si and Al-Fe-Mn'
 'S. Cotes, A.F. Guillermet, M. Sade, J. Alloys Compd., 208(1998) 168-177'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2019; Cr-Fe-Nb-Si'
 'N. Dupin, Private communication; Si systems'
 'L. Kjellqvist, Thermo-Calc Software AB, Stockholm, 2010; Unassessed parameter, linear combination of unary volume data'
 'A. Forsberg and J. Agren, J. Phase Equilib., 14 (1993) 354-363; Fe-Mn-Si'
 'R. Naraghi, Thermo-Calc Software AB, Sweden (2019); Fe-Ni-Si'
 'J. Miettinen, G. Vassilev, J. Phase Equilib. Diffus., 37(5) 2016, 283-290; Fe-P-Si'
 'B.J. Lee, KRISS, unpublished research, during 1993-1995'
 'M. Chen, B. Hallstedt, L. J. Gauckler, J. Alloys Compd., 393 (2005) 114-21; Mn-Y-O'
 'M. Chen, B. Hallstedt, L.J. Gauckler, Solid State Ionics, 176 (2005) 1457-64; Mn-Zr-O, Mn-Y-Zr-O'
 'J. Miettinen, CALPHAD, 28 (2004) 313-320; Mn-Zn'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, Volume data updated for TCFE8 database (TCFE v8, May, 2015).'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; Adjusting hcp'
 'J. Miettinen and B. Hallstedt, CALPHAD, 22 (1998) 231-256; Fe-Si and Fe-Si-C'
 'W. Zheng et al., J. Iron Steel Res. Int. 24(2)(2017) 190-197'
 'M. Ghasemi, Thermo-Calc Software AB, Sweden, 2019; Viscosity of metallic liquid'
 'M. J. Assael, J. Phys. Chem. Ref. Data 35 (2006) 285; Fe, Al'
 'M. J. Assael, J. Phys. Chem. Ref. Data 41 (2012) 033101; Cd, Co, Ga, In, Hg, Si, Ti, Zn'
 'Q. Chen, Thermo-Calc Software AB (2014), L12 constraints'
 'M. Ghasemi, Thermo-Calc Software AB: assessing the surface tension of metallic liquid'
 -OK-

-OK-

Should any phase have a miscibility gap check? /N/: N

Using global minimization procedure

Calculated 31546 grid points in 13 s
 Found the set of lowest grid points in 0 s
 Calculated POLY solution 1 s, total time 14 s
POLY: l-e
 ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
 Output from POLY-3, equilibrium = 1, label A0 , database: TCFE11
Conditions:
 T=973.15, W(MN)=1.5E-2, W(SI)=3E-3, W(C)=3E-3, P=100000, N=1
 DEGREES OF FREEDOM 0
 Temperature 973.15 K (700.00 C), Pressure 1.000000E+05
 Number of moles of components 1.000000E+00, Mass in grams 5.50671E+01
 Total Gibbs energy -4.16107E+04, Enthalpy 2.38957E+04, Volume 7.24171E-06
 Component Moles W-Fraction Activity Potential Ref.stat
 C 1.3754E-02 3.0000E-03 2.2665E-01 -1.2010E+04 SER
 FE 9.6533E-01 9.7900E-01 6.6047E-03 -4.0618E+04 SER
 MN 1.5035E-02 1.5000E-02 6.4361E-05 -7.8089E+04 SER
 SI 5.8822E-03 3.0000E-03 2.0473E-10 -1.8051E+05 SER
 BCC_A2 Status ENTERED Driving force 0.0000E+00
 Moles 7.3879E-01, Mass 4.1107E+01, Volume fraction 7.4524E-01 Mass fractions:
 FE 9.87914E-01 MN 8.77859E-03 SI 3.19709E-03 C 1.10316E-04
 FCC_A1 Status ENTERED Driving force 0.0000E+00
 Moles 2.5523E-01, Mass 1.3888E+01, Volume fraction 2.5031E-01 Mass fractions:
 FE 9.57680E-01 MN 3.34919E-02 C 6.39600E-03 SI 2.43217E-03
 GRAPHITE A9 Status ENTERED Driving force 0.0000E+00
 Moles 5.9809E-03, Mass 7.1837E-02, Volume fraction 4.4546E-03 Mass fractions:
 C 1.000000E+00 SI 0.000000E+00 MN 0.000000E+00 FE 0.000000E+00
POLY: @@ Suspend some phases that normally never appear
POLY: ch-st p gra m5c2=sus
 ... the command in full is CHANGE_STATUS
POLY:Hit RETURN to continue
POLY: @@ Set axis for T-w(c) phase diagram
POLY: s-a-v 1 w(c)
 ... the command in full is SET_AXIS_VARIABLE
Min value /0/: 0
Max value /1/: .01
Increment /2.5E-04/: 2.5E-04
POLY: s-a-v 2 t
 ... the command in full is SET_AXIS_VARIABLE
Min value /0/: 800
Max value /1/: 1200
Increment /10/: 30
POLY: save toex23a y
 ... the command in full is SAVE_WORKSPACES
POLY: map
 Version S mapping is selected
 Generating start equilibrium 1
 Generating start equilibrium 2
 Generating start equilibrium 3
 Generating start equilibrium 4
 Generating start equilibrium 5
 Generating start equilibrium 6
 Generating start equilibrium 7
 Generating start equilibrium 8
 Generating start equilibrium 9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12
 Organizing start points
 Using ADDED start equilibria
 Tie-lines not in the plane of calculation
 Generating start point 1
 Generating start point 2
 Generating start point 3
 Generating start point 4
 Generating start point 5
 Generating start point 6
 Generating start point 7
 Generating start point 8
 Generating start point 9
 Generating start point 10
 Working hard
 Generating start point 11
 Generating start point 12
 Generating start point 13
 Generating start point 14
 Generating start point 15
 Generating start point 16
 Generating start point 17
 Generating start point 18
 Generating start point 19
 Generating start point 20
 Working hard
 Generating start point 21
 Generating start point 22
 Generating start point 23
 Generating start point 24
 Phase region boundary 1 at: 2.500E-04 9.472E+02
 BCC_A2
 CEMENTITE_D011
 ** FCC_A1
 Calculated. 2 equilibria
 Phase region boundary 2 at: 6.572E-05 9.454E+02
 BCC_A2
 ** CEMENTITE_D011
 ** FCC_A1
 Calculated 24 equilibria
 Phase region boundary 3 at: 6.572E-05 9.454E+02
 BCC_A2
 ** FCC_A1
 Calculated 24 equilibria
 Phase region boundary 4 at: 6.572E-05 9.454E+02

```

        BCC_A2
** CEMENTITE_D011
Calculated..          11 equilibria
Terminating at axis limit.

Phase region boundary  5 at:   6.572E-05  9.454E+02
        BCC_A2
** CEMENTITE_D011
        FCC_A1
Calculated.          31 equilibria

Phase region boundary  6 at:   7.062E-03  9.920E+02
        ** BCC_A2
        ** CEMENTITE_D011
        FCC_A1
Calculated..          17 equilibria
Terminating at axis limit.

Phase region boundary  7 at:   7.062E-03  9.920E+02
        ** CEMENTITE_D011
        FCC_A1
Calculated..          17 equilibria
Terminating at axis limit.

Phase region boundary  8 at:   7.062E-03  9.920E+02
        ** BCC_A2
        FCC_A1
Calculated.          42 equilibria

Phase region boundary  9 at:   7.062E-03  9.920E+02
        ** BCC_A2
        CEMENTITE_D011
        FCC_A1
Calculated..          13 equilibria
Terminating at axis limit.

Phase region boundary 10 at:   6.572E-05  9.454E+02
        BCC_A2
        CEMENTITE_D011
        ** FCC_A1
Calculated..          42 equilibria
Terminating at axis limit.

Phase region boundary 11 at:   2.500E-04  9.472E+02
        BCC_A2
        CEMENTITE_D011
        ** FCC_A1
Calculated..          41 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 12 at:   3.417E-03  9.669E+02
        BCC_A2
        CEMENTITE_D011
        ** FCC_A1
Calculated.          15 equilibria
Terminating at known equilibrium

Phase region boundary 13 at:   3.417E-03  9.669E+02
        BCC_A2
        CEMENTITE_D011
        ** FCC_A1
Calculated..          28 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 14 at:   6.583E-03  9.764E+02
        BCC_A2
        CEMENTITE_D011
        ** FCC_A1
Calculated..          28 equilibria
Terminating at known equilibrium

Phase region boundary 15 at:   6.583E-03  9.764E+02
        BCC_A2
        CEMENTITE_D011
        ** FCC_A1
Calculated..          16 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 16 at:   5.319E-06  8.100E+02
        BCC_A2
        CEMENTITE_D011
Calculated..          2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 17 at:   5.319E-06  8.100E+02
        BCC_A2
        CEMENTITE_D011
Calculated..          10 equilibria
Terminating at known equilibrium

Phase region boundary 18 at:   9.750E-03  9.821E+02
        BCC_A2
        CEMENTITE_D011
        ** FCC_A1
Calculated..          40 equilibria
Terminating at known equilibrium

Phase region boundary 19 at:   9.750E-03  9.821E+02
        BCC_A2
        CEMENTITE_D011
        ** FCC_A1
Calculated..          3 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 20 at:   5.765E-05  9.367E+02
        BCC_A2
        CEMENTITE_D011
Calculated..          11 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 21 at:   5.765E-05  9.367E+02
        BCC_A2

```

```

** CEMENTITE_D011
Calculated.          2 equilibria
Terminating at known equilibrium

Phase region boundary 22 at:  2.646E-03  1.063E+03
** BCC_A2
FCC_A1
Calculated.          19 equilibria
Terminating at known equilibrium

Phase region boundary 23 at:  2.646E-03  1.063E+03
** BCC_A2
FCC_A1
Calculated.          24 equilibria

Phase region boundary 24 at:  8.894E-03  1.063E+03
** CEMENTITE_D011
FCC_A1
Calculated.          11 equilibria
Terminating at known equilibrium

Phase region boundary 25 at:  8.894E-03  1.063E+03
** CEMENTITE_D011
FCC_A1
Calculated..         7 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 26 at:  2.500E-04  1.128E+03
** BCC_A2
FCC_A1
Calculated.          4 equilibria

Phase region boundary 27 at:  2.500E-04  1.128E+03
** BCC_A2
FCC_A1
Calculated.          29 equilibria
Terminating at known equilibrium

Phase region boundary 28 at:  3.417E-03  1.048E+03
** BCC_A2
FCC_A1
Calculated.          26 equilibria

Phase region boundary 29 at:  3.417E-03  1.048E+03
** BCC_A2
FCC_A1
Calculated.          16 equilibria
Terminating at known equilibrium

Phase region boundary 30 at:  6.583E-03  9.982E+02
** BCC_A2
FCC_A1
Calculated.          38 equilibria

Phase region boundary 31 at:  6.583E-03  9.982E+02
** BCC_A2
FCC_A1
Calculated.          3 equilibria
Terminating at known equilibrium

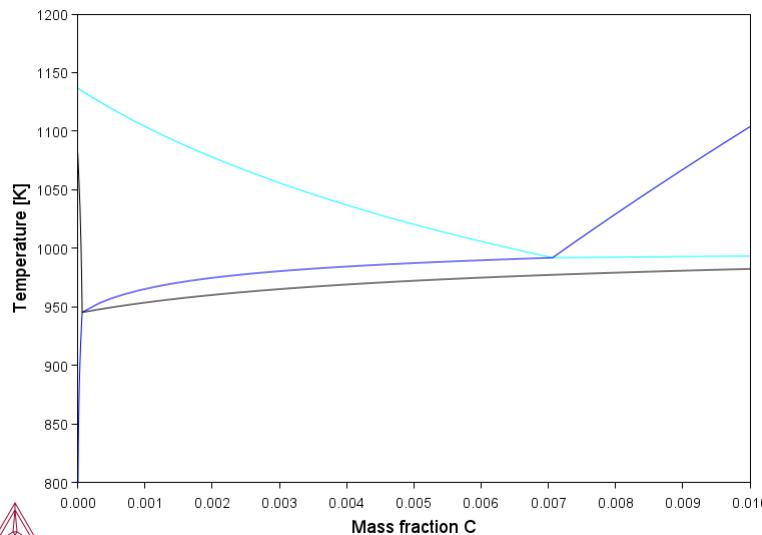
Phase region boundary 32 at:  9.750E-03  1.095E+03
** CEMENTITE_D011
FCC_A1
Calculated.          12 equilibria
Terminating at known equilibrium

Phase region boundary 33 at:  9.750E-03  1.095E+03
** CEMENTITE_D011
FCC_A1
Calculated..         3 equilibria
Terminating at known equilibrium
Terminating at axis limit.
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\generate_console_examples\examples\tcex23\tcex23a.POLY3
CPU time for mapping   15 seconds
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2
  Setting automatic diagram axes

POST:
POST: set-title example 23a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

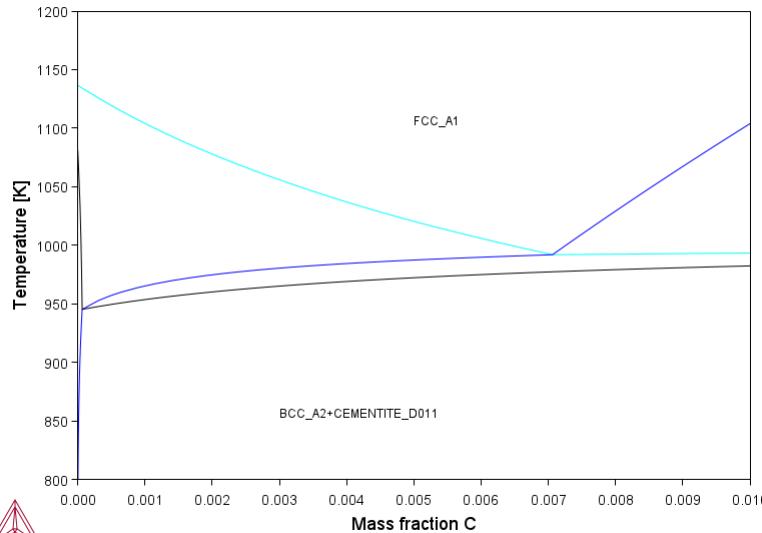
```

example 23a



```
POST:  
POST:Hit RETURN to continue  
POST: @@ Add labels  
POST: add  
... the command in full is ADD_LABEL_TEXT  
Give X coordinate in axis units: .005  
Give Y coordinate in axis units: 1100  
Automatic phase labels? /Y/: Y  
Automatic labelling not always possible  
Using global minimization procedure  
Calculated 31336 grid points in 1 s  
Found the set of lowest grid points in 0 s  
Calculated POLY solution 0 s, total time 1 s  
Stable phases are: FCC_A1  
Text size: /.36/: .34  
POST: add  
... the command in full is ADD_LABEL_TEXT  
Give X coordinate in axis units: .003  
Give Y coordinate in axis units: 850  
Automatic phase labels? /Y/: Y  
Automatic labelling not always possible  
Using global minimization procedure  
Calculated 31336 grid points in 0 s  
Found the set of lowest grid points in 0 s  
Calculated POLY solution 0 s, total time 0 s  
Stable phases are: BCC_A2+CEMENTITE_D011  
Text size: /.36/: .34  
POST: set-title example 23b  
POST:  
POST:  
POST: SET_EXP_FILE_FORMAT 5  
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y  
... the command in full is MAKE_EXPERIMENTAL_DATAFI  
POST: SET_EXP_FILE_FORMAT 10  
POST:  
POST: plot  
... the command in full is PLOT_DIAGRAM
```

example 23b



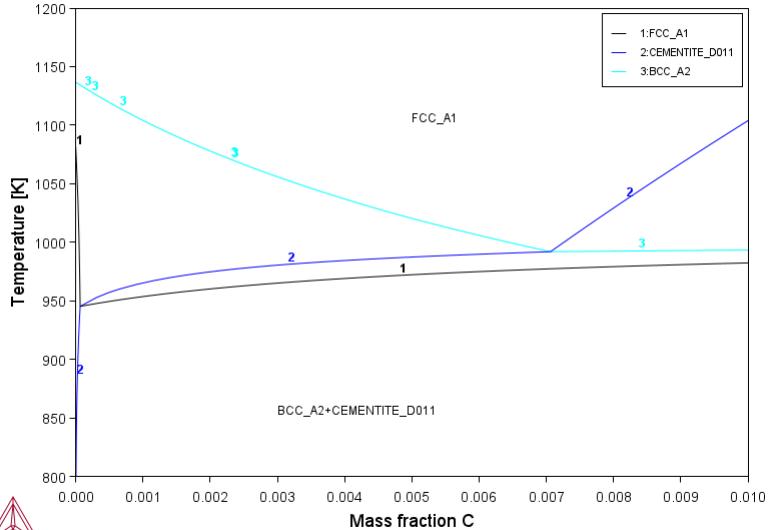
```
POST:  
POST:Hit RETURN to continue  
POST: s-lab  
... the command in full is SET_LABEL_CURVE_OPTION  
CURVE LABEL OPTION (A, B, C, D, E, F OR N) /N/: ?  
THE OPTIONS MEANS:  
A LIST STABLE PHASES ALONG LINE  
B AS A BUT CURVES WITH SAME FIX PHASE HAVE SAME NUMBER  
C LIST AXIS QUANTITIES  
D AS C BUT CURVES WITH SAME QUANTITIES HAVE SAME NUMBER  
E AS B WITH CHANGING COLORS
```

```

F      AS D WITH CHANGING COLORS
N      NO LABELS
CURVE LABEL OPTION (A, B, C, D, E, F OR N) /N/: e
POST: set-title example 23c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAIFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 23c



```

POST:
POST:Hit RETURN to continue
POST: ba
... the command in full is BACK
POLY: @@ Now calculate the T-zero temperature for the steel
POLY: read tce23a
... the command in full is READ_WORKSPACES
POLY: advanced-options
Which option? /STEP_AND_MAP/: ?
EQUILIBRIUM_CALCUL    NEW_COMPOSITION_SET      STABILITY_CHECK
GLOBAL_MINIMIZATION    OUTPUT_FILE_FOR_SHOW   STEP_AND_MAP
IGNORE_COMPOSI_SET_ORDER PARAEQUILIBRIUM       T-ZERO_TEMPERATURE
KEEP_COMP_SET_NUMBERS   PHASE_ADDITION        TOGGLE_ALTERNATE_MODE
LIST_PHASE_ADDITION    PRESENT_PHASE
MAJOR_CONSTITUENTS     SHOW_FOR_T=
Which option? /STEP_AND_MAP/: t-z

```

This command calculates the temperature when two phases have the same Gibbs energy. You must calculate an equilibrium at an estimated temperature first.

Name of first phase: fcc_a1

Name of second phase: bcc_a2

```

The T0 temperature is 922.16 K
Note: LIST-EQUILIBRIUM is not relevant
POLY:Hit RETURN to continue
POLY: @@ Calculate the T-zero line, remove the T-axis
POLY: l-ax
... the command in full is LIST_AXIS_VARIABLE
Axis No 1: W(C)          Min: 0           Max: 1E-2        Inc: 2.5E-4
Axis No 2: T              Min: 800         Max: 1200       Inc: 30

```

```

POLY: s-a-v 2 none
... the command in full is SET_AXIS_VARIABLE
POLY: save tce23b y
... the command in full is SAVE_WORKSPACES

```

```

POLY: step
... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/: ?

```

The following options are available:

| | |
|--------------------|---|
| NORMAL | Stepping with given conditions |
| INITIAL_EQUILIBRIA | An initial equilibrium stored at every step |
| EVALUATE | Specified variables evaluated after each step |
| SEPARATE_PHASES | Each phase calculated separately |
| T-ZERO | T0 line calculation |
| PARAEQUILIBRIUM | Paraequilibrium diagram |
| MIXED_SCHEIL | Scheil with fast diffusing elements |
| ONE_PHASE_AT_TIME | One phase at a time |

Option? /NORMAL/: t-z

Name of first phase: fcc_a1

Name of second phase: bcc_a2

Phase Region from 0.300000E-02 for:

| | |
|-------------|---------|
| BCC_A2 | |
| FCC_A1 | |
| 3.00000E-03 | 922.16 |
| 2.75000E-03 | 932.50 |
| 2.50000E-03 | 943.20 |
| 2.25000E-03 | 954.33 |
| 2.00000E-03 | 965.99 |
| 1.75000E-03 | 978.35 |
| 1.50000E-03 | 991.63 |
| 1.25000E-03 | 1006.24 |
| 1.00000E-03 | 1022.92 |
| 7.50000E-04 | 1041.84 |
| 5.00000E-04 | 1063.23 |
| 2.50000E-04 | 1087.65 |
| 2.50000E-10 | 1115.87 |

Phase Region from 0.169768E-02 for:

```

BCC_A2
FCC_A1
1.697680E-03 980.98
1.947680E-03 968.46
2.197680E-03 956.66
2.447680E-03 945.44
2.697680E-03 934.65
2.947680E-03 924.24
3.197680E-03 914.14
3.447680E-03 904.29
3.697680E-03 894.67
3.947680E-03 885.23
4.197680E-03 875.97
4.447680E-03 866.85
4.697680E-03 857.86
4.947680E-03 848.99
5.197680E-03 840.23
5.447680E-03 831.55
5.697680E-03 822.95
5.947680E-03 814.43
6.197680E-03 805.98
6.447680E-03 797.58
6.697680E-03 789.24
6.947680E-03 780.94
7.197680E-03 772.69
7.447680E-03 764.47
7.697680E-03 756.29
7.947680E-03 748.14
8.197680E-03 740.01
8.447680E-03 731.91
8.697680E-03 723.82
8.947680E-03 715.76
9.197680E-03 707.70
9.447680E-03 699.65
9.697680E-03 691.62
9.947680E-03 683.59
1.000000E-02 681.91
*** Buffer saved on file c:\jenkins\WORKSP~1\GENERA~1\examples\tcex23\tcex23b.POLY3

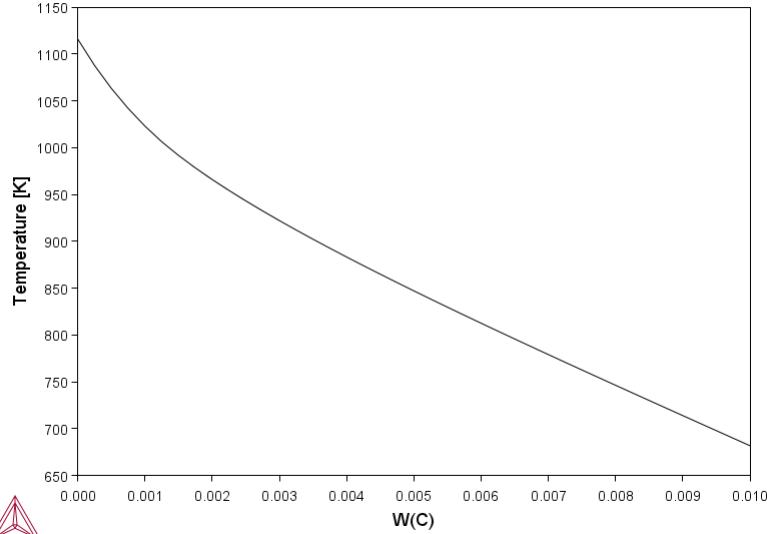
```

```

POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2
POST:
POST: set-title example 23d
POST: s-d-a x w(c)
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t-k
... the command in full is SET_DIAGRAM_AXIS
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 23d




POST:
POST: Hit RETURN to continue
POST: @@ Write the line on a data file
POST: make tcex23b y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: back
POLY: @@ Plot together with a phase diagram
POLY: read tcex23a
... the command in full is READ_WORKSPACES
POLY: post

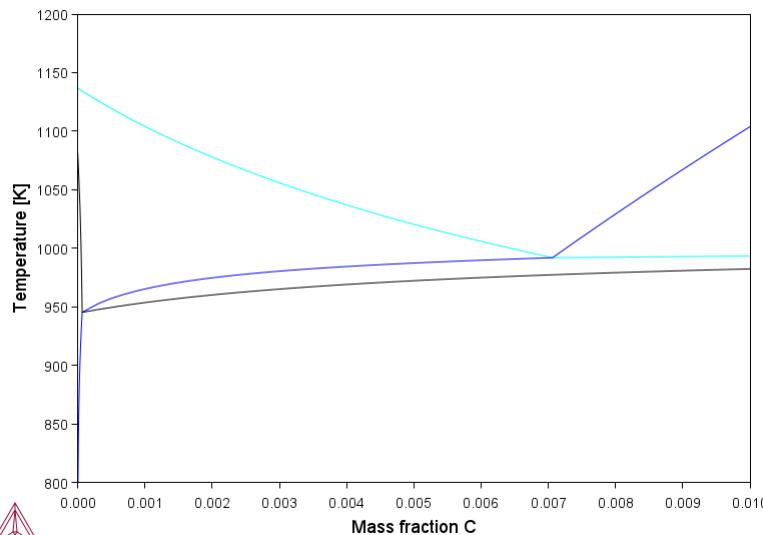
```

POLY-3 POSTPROCESSOR VERSION 3.2
Setting automatic diagram axes

POST:
POST: set-title example 23e
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

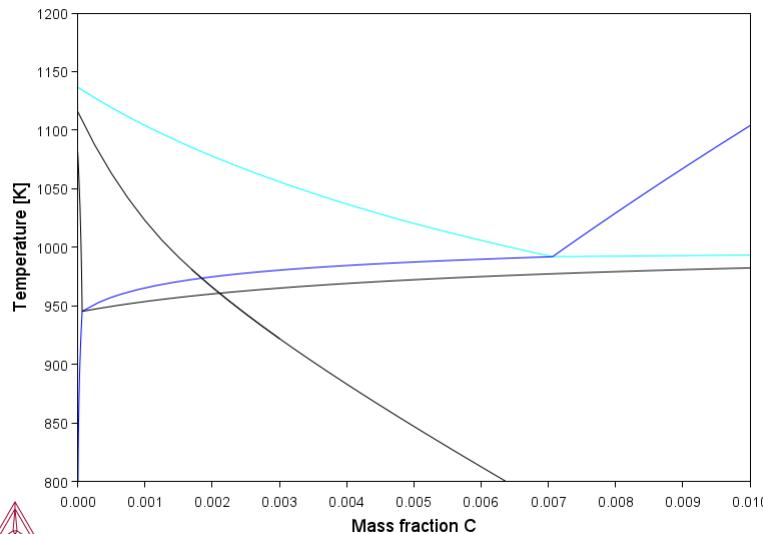
example 23e



```

POST:
POST:Hit RETURN to continue
POST: a-e-d y tce23b
... the command in full is APPEND_EXPERIMENTAL_DATA
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 1
POST: set-title example 23f
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
example 23f

```



```

POST:
POST:Hit RETURN to continue
POST: back
POLY: @@ Now calculate the paraequilibrium for the steel.
POLY: @@ At paraequilibrium only C is mobile, the other
POLY: @@ alloying elements have the same compositions in
POLY: @@ both phases
POLY:
POLY: read tce23a
... the command in full is READ_WORKSPACES
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated          31336 grid points in           0 s
Found the set of lowest grid points in           0 s
Calculated POLY solution      0 s, total time   0 s
POLY: l-e,,,
... the command in full is LIST EQUILIBRIUM
Output from POLY-3, equilibrium =      1, label A0 , database: TCFE11

```

Conditions:
 $T=973.15$ K (700.00 C), Pressure $1.000000E+05$
 $W(MN)=1.5E-2$, $W(SI)=3E-3$, $W(C)=3E-3$, $P=100000$, $N=1$
DEGREES OF FREEDOM 0

Temperature 973.15 K (700.00 C), Pressure 1.000000E+05
Number of moles of components 1.000000E+00, Mass in grams 5.50671E+01
Total Gibbs energy -4.16101E+04, Enthalpy 2.36448E+04, Volume 7.22672E-06

| Component | Moles | W-Fraction | Activity | Potential | Ref.stat |
|-----------|------------|------------|------------|-------------|----------|
| C | 1.3754E-02 | 3.0000E-03 | 2.3005E-01 | -1.1890E+04 | SER |
| FE | 9.6533E-01 | 9.7900E-01 | 6.6052E-03 | -4.0617E+04 | SER |
| MN | 1.5035E-02 | 1.5000E-02 | 6.3288E-05 | -7.8225E+04 | SER |

```

SI 5.8822E-03 3.0000E-03 2.0682E-10 -1.8043E+05 SER

BCC_A2 Status ENTERED Driving force 0.0000E+00
Moles 7.9472E-01, Mass 4.4217E+01, Volume fraction 8.0329E-01 Mass fractions:
FE 9.88037E-01 MN 8.63083E-03 SI 3.22040E-03 C 1.11809E-04

FCC_A1 Status ENTERED Driving force 0.0000E+00
Moles 1.7204E-01, Mass 9.3596E+00, Volume fraction 1.6904E-01 Mass fractions:
FE 9.58089E-01 MN 3.30180E-02 C 6.45696E-03 SI 2.43634E-03

CEMENTITE_D011 Status ENTERED Driving force 0.0000E+00
Moles 3.3244E-02, Mass 1.4900E+00, Volume fraction 2.7670E-02 Mass fractions:
FE 8.42175E-01 MN 9.08298E-02 C 6.69948E-02 SI 4.69956E-13

POLY: advance para
... the command in full is ADVANCED_OPTIONS

This command calculates a paraequilibrium between two phases.
You must calculate an equilibrium with the overall composition first.
Name of first phase: fcc_a1
Name of second phase: bcc_a2
Fast diffusing component: /C/: c
Fast diffusing component: /NONE/:
NP(FCC_A1) = 0.4278 with U-fractions C = 3.17321E-02
NP(BCC_A2) = 0.5722 with U-fractions C = 6.47641E-04
All other compositions the same in both phases
Note: LIST-EQUILIBRIUM is not relevant

POLY:
POLY: Hit RETURN to continue
POLY:
POLY:
POLY: @@ Now calculate the paraequilibrium for the steel
POLY: @@ at varying temperatures
POLY:
POLY: s-a-v 1 t 800 1200 20
... the command in full is SET_AXIS_VARIABLE
POLY: s-a-v 2 none
... the command in full is SET_AXIS_VARIABLE
POLY: save tcex23c y
... the command in full is SAVE_WORKSPACES
POLY: step para
... the command in full is STEP_WITH_OPTIONS

This command calculates a paraequilibrium between two phases.
You must calculate an equilibrium with the overall composition first.
Name of first phase: fcc_a1
Name of second phase: bcc_a2
Fast diffusing component: /C/: c
Fast diffusing component: /NONE/:
Output during stepping is:
axis value, phase amounts, u-fractions of interstitial(s) in phase 1 and 2,
and LNACR value(s) of interstitial(s)

Phase Region from 973.150 for:
  BCC_A2
  FCC_A1
  9.731500E+02 0.428 0.572 3.173207E-02 6.476405E-04 -1.294536E+00
  9.531500E+02 0.345 0.655 3.908147E-02 7.295252E-04 -8.709572E-01
  9.331500E+02 0.285 0.715 4.698753E-02 8.034098E-04 -4.581102E-01
  9.131500E+02 0.240 0.760 5.533663E-02 8.670323E-04 -5.291004E-02
  8.931500E+02 0.206 0.794 6.403530E-02 9.189130E-04 3.476369E-01
  8.731500E+02 0.180 0.820 7.300677E-02 9.581551E-04 7.462385E-01
  8.531500E+02 0.160 0.840 8.218895E-02 9.843379E-04 1.145330E+00
  8.331500E+02 0.143 0.857 9.153169E-02 9.974272E-04 1.547112E+00
  8.131500E+02 0.129 0.871 1.009946E-01 9.977113E-04 1.953612E+00
  8.000000E+02 0.122 0.878 1.072659E-01 9.911826E-04 2.224380E+00

Phase Region from 973.150 for:
  BCC_A2
  FCC_A1
  9.731500E+02 0.428 0.572 3.169128E-02 6.466406E-04 -1.296235E+00
  9.931500E+02 0.547 0.453 2.503573E-02 5.600526E-04 -1.733345E+00
  1.013150E+03 0.718 0.282 1.922849E-02 4.734693E-04 -2.184104E+00
  1.033150E+03 0.974 0.026 1.430536E-02 3.893313E-04 -2.652658E+00
  1.053150E+03 1.403 -0.403 1.002992E-02 3.022701E-04 -3.169313E+00
  1.073150E+03 2.250 -1.250 6.316301E-03 2.110002E-04 -3.783482E+00
  1.093150E+03 4.635 -3.635 3.098720E-03 1.147920E-04 -4.638561E+00
  1.113150E+03 45.140 -44.140 3.218793E-04 1.322260E-05 -7.038177E+00
*** Buffer saved on file c:\jenkins\workspace\generatex\examples\tcex23\tcex23c.POLY3
*** ERROR 8 IN NS01AD: Numerical error

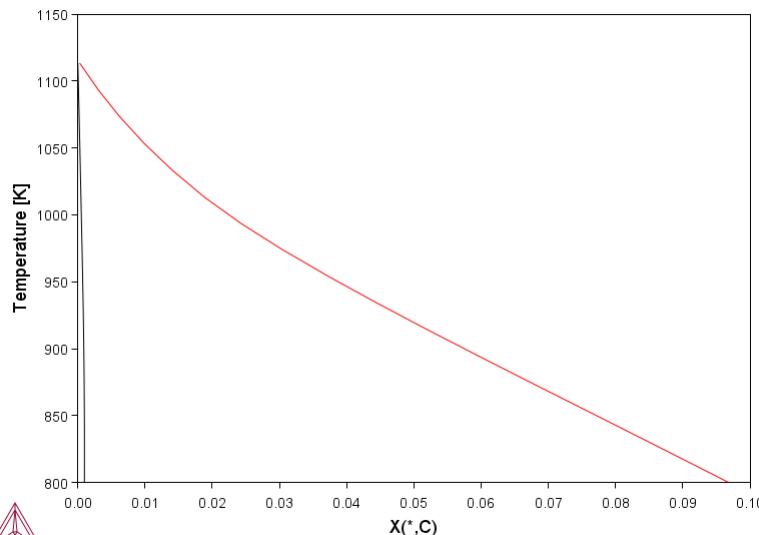
POLY:
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST:
POST:
POST: set-title example 23g
POST: s-d-a x x(*,c)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER */:
POST: s-d-a y t-k
... the command in full is SET_DIAGRAM_AXIS
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generatex\examples\tcex23\tcex23c.POLY3
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 23g



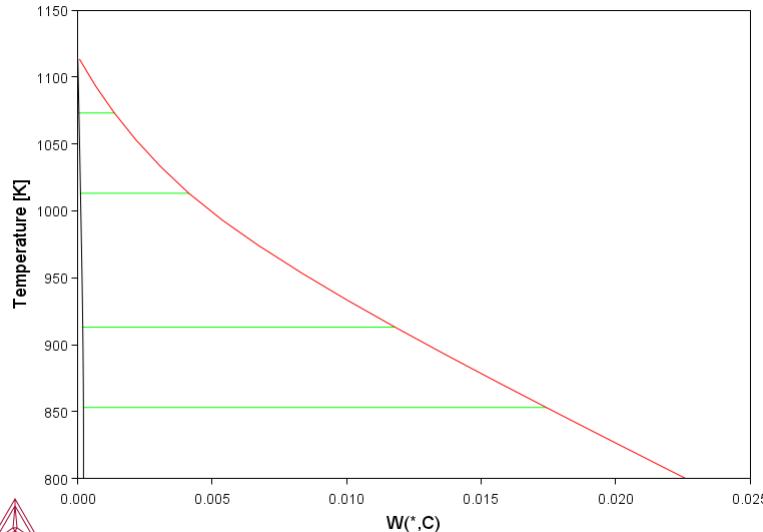
POST:
POST: Hit RETURN to continue
POST: s-d-a x w(*,c)

... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER */:
POST:

POST: s-t-s 3
... the command in full is SET_TIELINE_STATUS
POST: set-title example 23h
POST:

POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

example 23h



POST:
POST: Hit RETURN to continue
POST: make tce23c y

... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: back

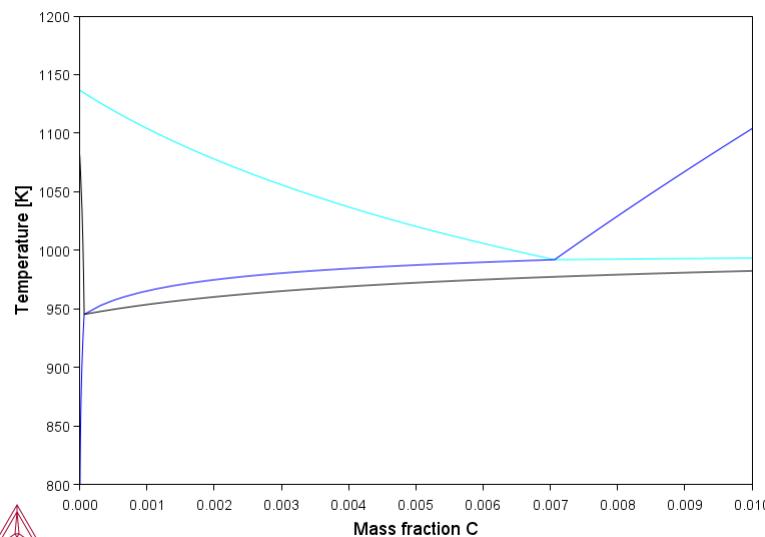
POLY: read tce23a
... the command in full is READ_WORKSPACES

POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

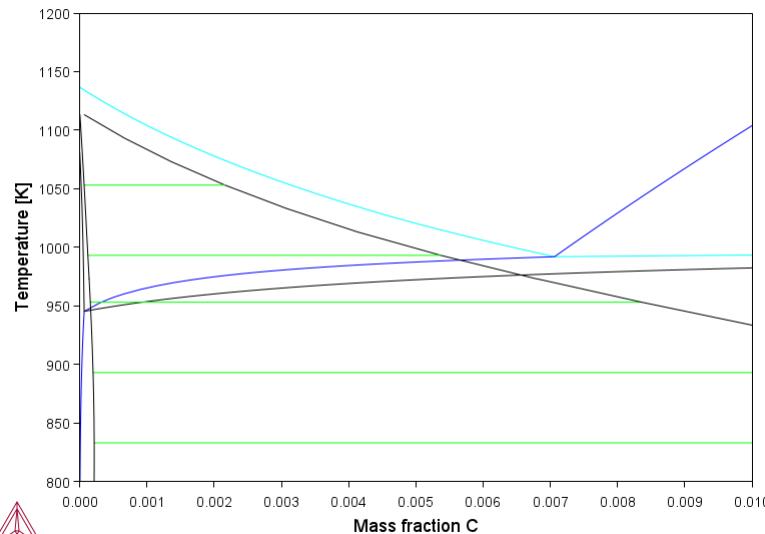
POST:
POST:
POST: set-title example 23i
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

example 23i



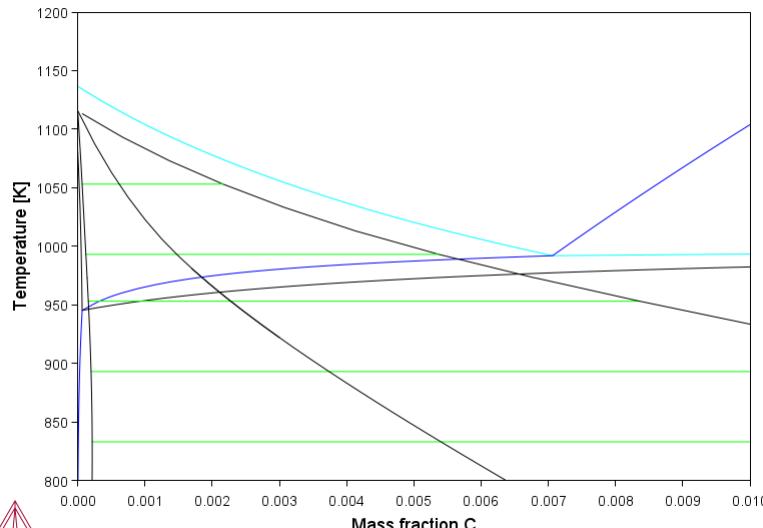
```
POST:  
POST:Hit RETURN to continue  
POST: a-e-d y tcex23c  
... the command in full is APPEND_EXPERIMENTAL_DATA  
PROLOGUE NUMBER: /0/: 0  
DATASET NUMBER(s): /-1/: 1  
POST: set-title example 23j  
POST:  
POST:  
POST: SET_EXP_FILE_FORMAT 5  
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y  
... the command in full is MAKE_EXPERIMENTAL_DATAFI  
POST: SET_EXP_FILE_FORMAT 10  
POST:  
POST: plot  
... the command in full is PLOT_DIAGRAM
```

example 23j



```
POST:  
POST:Hit RETURN to continue  
POST: a-e-d y tcex23b.exp tcex23c.exp 0; 1; 0; 1;  
... the command in full is APPEND_EXPERIMENTAL_DATA  
POST:  
POST: set-title example 23k  
POST:  
POST:  
POST: SET_EXP_FILE_FORMAT 5  
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y  
... the command in full is MAKE_EXPERIMENTAL_DATAFI  
POST: SET_EXP_FILE_FORMAT 10  
POST:  
POST: plot  
... the command in full is PLOT_DIAGRAM
```

example 23k



POST:
POST: Hit RETURN to continue
POST: back

POLY: @@ Now calculate both a normal and paraequilibrium
POLY: @@ for the steel at 1000 K.
POLY:
POLY: @@ Note that a paraequilibrium does not always exist
POLY: @@ for the given conditions. The calculated results
POLY: @@ are the amounts of the two phases. This indicates
POLY: @@ how much of the phases can be tranformed at
POLY: @@ paraequilibrium conditions. The carbon content of
POLY: @@ the phases are also listed; the other alloying
POLY: @@ elements have the same fractions in both phases
POLY:
POLY: read tcecx23a.POLY3
... the command in full is READ_WORKSPACES
POLY: s-c T=1000
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 31336 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY: l-e,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: TCFE11

Conditions:
T=1000, W(MN)=1.5E-2, W(SI)=3E-3, W(C)=3E-3, P=100000, N=1
DEGREES OF FREEDOM 0

Temperature 1000.00 K (726.85 C), Pressure 1.000000E+05
Number of moles of components 1.000000E+00, Mass in grams 5.50671E+01
Total Gibbs energy -4.34569E+04, Enthalpy 2.63111E+04, Volume 7.20719E-06

| Component | Moles | W-Fraction | Activity | Potential | Ref.stat |
|-----------|------------|------------|------------|-------------|----------|
| C | 1.3754E-02 | 3.0000E-03 | 1.6697E-01 | -1.4883E+04 | SER |
| FE | 9.6533E-01 | 9.7900E-01 | 6.1069E-03 | -4.2390E+04 | SER |
| MN | 1.5035E-02 | 1.5000E-02 | 4.0529E-05 | -8.4089E+04 | SER |
| SI | 5.8822E-03 | 3.0000E-03 | 3.3223E-10 | -1.8147E+05 | SER |

FCC_A1 Status ENTERED Driving force 0.0000E+00
Moles 5.3724E-01, Mass 2.9327E+01, Volume fraction 5.3051E-01 Mass fractions:
FE 9.69681E-01 MN 2.22412E-02 C 5.52941E-03 SI 2.54873E-03

BCC_A2 Status ENTERED Driving force 0.0000E+00
Moles 4.6276E-01, Mass 2.5740E+01, Volume fraction 4.6949E-01 Mass fractions:
FE 9.89618E-01 MN 6.74998E-03 SI 3.51414E-03 C 1.18192E-04

POLY: advanced
... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: para

This command calculates a paraequilibrium between two phases.
You must calculate an equilibrium with the overall composition first.

Name of first phase: fcc_a1
Name of second phase: bcc_a2
Fast diffusing component: /C/: c
Fast diffusing component: /NONE/:
NP(FCC_A1) = 0.5976 with U-fractions C = 2.29802E-02
NP(BCC_A2) = 0.4024 with U-fractions C = 5.31092E-04

All other compositions the same in both phases
Note: LIST-EQUILIBRIUM is not relevant

POLY:
POLY:Hit RETURN to continue
POLY: @@ Now calculate an isothermal phase diagram at 1000 K
POLY: s-a-v 2 w(mn) 0 .1,,,
... the command in full is SET_AXIS_VARIABLE
POLY:Hit RETURN to continue
POLY: save tcecx23d y
... the command in full is SAVE_WORKSPACES

POLY: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8

```

Generating start equilibrium  9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Tie-lines not in the plane of calculation
Generating start point  1
Generating start point  2
Generating start point  3
Generating start point  4
Generating start point  5
Generating start point  6
Generating start point  7
Generating start point  8
Generating start point  9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Generating start point 27
Generating start point 28
Generating start point 29
Generating start point 30
Working hard
Generating start point 31
Generating start point 32

Phase region boundary  1 at:  2.521E-03  2.500E-03
  BCC_A2
  ** CEMENTITE_D011
  FCC_A1
Calculated.          11 equilibria

Phase region boundary  2 at:  1.815E-04  1.155E-03
  BCC_A2
  ** CEMENTITE_D011
  ** FCC_A1
Calculated          10 equilibria

Phase region boundary  3 at:  1.815E-04  1.155E-03
  BCC_A2
  ** CEMENTITE_D011
Calculated          10 equilibria

Phase region boundary  4 at:  1.815E-04  1.155E-03
  BCC_A2
  ** FCC_A1
Calculated          32 equilibria

Phase region boundary  5 at:  1.815E-04  1.155E-03
  BCC_A2
  CEMENTITE_D011
  ** FCC_A1
Calculated..        41 equilibria
Terminating at axis limit.

Phase region boundary  6 at:  1.815E-04  1.155E-03
  BCC_A2
  ** CEMENTITE_D011
  FCC_A1
Calculated.          30 equilibria

Phase region boundary  7 at:  7.338E-03  6.999E-03
  ** BCC_A2
  ** CEMENTITE_D011
  FCC_A1
Calculated..        39 equilibria
Terminating at axis limit.

Phase region boundary  8 at:  7.338E-03  6.999E-03
  ** CEMENTITE_D011
  FCC_A1
Calculated..        39 equilibria
Terminating at axis limit.

Phase region boundary  9 at:  7.338E-03  6.999E-03
  ** BCC_A2
  FCC_A1
Calculated.          42 equilibria

Phase region boundary 10 at:  7.338E-03  6.999E-03
  ** BCC_A2
  CEMENTITE_D011
  FCC_A1
Calculated..        13 equilibria
Terminating at axis limit.

Phase region boundary 11 at:  2.521E-03  2.500E-03
  BCC_A2
  ** CEMENTITE_D011
  FCC_A1
Calculated.          21 equilibria
Terminating at known equilibrium

Phase region boundary 12 at:  2.500E-04  5.820E-02
  ** BCC_A2
  FCC_A1
Calculated.          22 equilibria

Phase region boundary 13 at:  2.500E-04  5.820E-02

```

```

** BCC_A2
FCC_A1
Calculated.          30 equilibria
Terminating at known equilibrium

Phase region boundary 14 at: 3.417E-03 3.130E-03
BCC_A2
** CEMENTITE_D011
FCC_A1
Calculated.          14 equilibria
Terminating at known equilibrium

Phase region boundary 15 at: 3.417E-03 3.130E-03
BCC_A2
** CEMENTITE_D011
FCC_A1
Calculated.          17 equilibria
Terminating at known equilibrium

Phase region boundary 16 at: 6.583E-03 6.081E-03
BCC_A2
** CEMENTITE_D011
FCC_A1
Calculated.          27 equilibria
Terminating at known equilibrium

Phase region boundary 17 at: 6.583E-03 6.081E-03
BCC_A2
CEMENTITE_D011
** FCC_A1
Calculated.          5 equilibria
Terminating at known equilibrium

Phase region boundary 18 at: 6.969E-03 2.500E-03
BCC_A2
CEMENTITE_D011
** FCC_A1
Calculated.          29 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 19 at: 6.969E-03 2.500E-03
BCC_A2
CEMENTITE_D011
** FCC_A1
Calculated..         14 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 20 at: 9.750E-03 3.142E-03
BCC_A2
CEMENTITE_D011
** FCC_A1
Calculated.          40 equilibria
Terminating at known equilibrium

Phase region boundary 21 at: 9.750E-03 3.142E-03
BCC_A2
CEMENTITE_D011
** FCC_A1
Calculated..         3 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 22 at: 4.029E-03 3.417E-02
BCC_A2
FCC_A1
Calculated.          22 equilibria
Terminating at known equilibrium

Phase region boundary 23 at: 4.029E-03 3.417E-02
BCC_A2
FCC_A1
Calculated.          36 equilibria

Phase region boundary 24 at: 7.086E-03 3.417E-02
BCC_A2
CEMENTITE_D011
FCC_A1
Calculated.          12 equilibria
Terminating at known equilibrium

Phase region boundary 25 at: 7.086E-03 3.417E-02
BCC_A2
CEMENTITE_D011
FCC_A1
Calculated..         28 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 26 at: 6.838E-03 6.583E-02
BCC_A2
CEMENTITE_D011
FCC_A1
Calculated.          25 equilibria
Terminating at known equilibrium

Phase region boundary 27 at: 6.838E-03 6.583E-02
BCC_A2
CEMENTITE_D011
FCC_A1
Calculated..         15 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 28 at: 6.838E-03 6.583E-02
BCC_A2
CEMENTITE_D011
FCC_A1
Calculated.          25 equilibria
Terminating at known equilibrium

Phase region boundary 29 at: 6.838E-03 6.583E-02
BCC_A2
CEMENTITE_D011
FCC_A1
Calculated..         15 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 30 at: 6.634E-03 9.750E-02
BCC_A2
CEMENTITE_D011
FCC_A1

```

```

Calculated.          38 equilibria
Terminating at known equilibrium

Phase region boundary 31 at: 6.634E-03 9.750E-02
** CEMENTITE_D011
FCC_A1
Calculated..          3 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 32 at: 2.500E-04 5.820E-02
** BCC_A2
FCC_A1
Calculated          4 equilibria

Phase region boundary 33 at: 2.500E-04 5.820E-02
** BCC_A2
FCC_A1
Calculated.          30 equilibria
Terminating at known equilibrium

Phase region boundary 34 at: 3.417E-03 3.851E-02
** BCC_A2
FCC_A1
Calculated          26 equilibria

Phase region boundary 35 at: 3.417E-03 3.851E-02
** BCC_A2
FCC_A1
Calculated.          17 equilibria
Terminating at known equilibrium

Phase region boundary 36 at: 6.583E-03 1.378E-02
** BCC_A2
FCC_A1
Calculated          38 equilibria

Phase region boundary 37 at: 6.583E-03 1.378E-02
** BCC_A2
FCC_A1
Calculated.          5 equilibria
Terminating at known equilibrium

Phase region boundary 38 at: 6.634E-03 9.750E-02
** CEMENTITE_D011
FCC_A1
Calculated.          38 equilibria
Terminating at known equilibrium

Phase region boundary 39 at: 6.634E-03 9.750E-02
** CEMENTITE_D011
FCC_A1
Calculated..          3 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 40 at: 9.750E-03 7.763E-03
** BCC_A2
CEMENTITE_D011
FCC_A1
Calculated.          11 equilibria
Terminating at known equilibrium

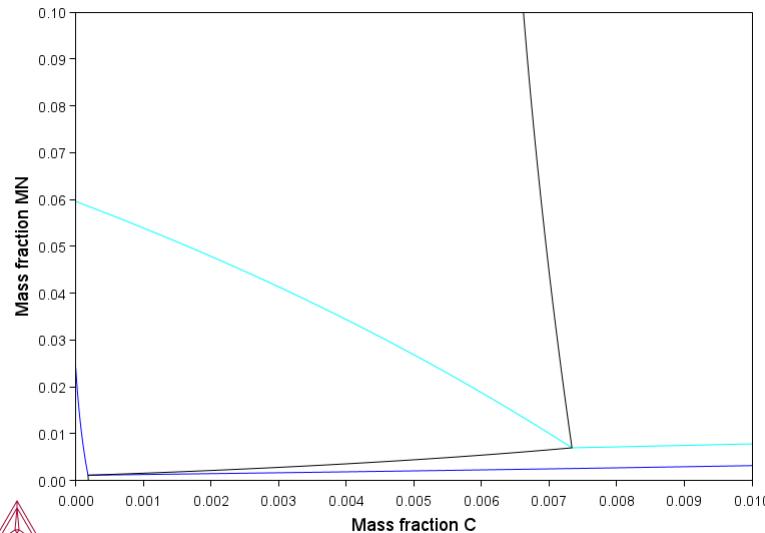
Phase region boundary 41 at: 9.750E-03 7.763E-03
** BCC_A2
CEMENTITE_D011
FCC_A1
Calculated..          3 equilibria
Terminating at known equilibrium
Terminating at axis limit.
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\generate_console_examples\examples\tcex23\tcex23d.POLY3
CPU time for mapping      12 seconds
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST:
POST:
POST: set-title example 231
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

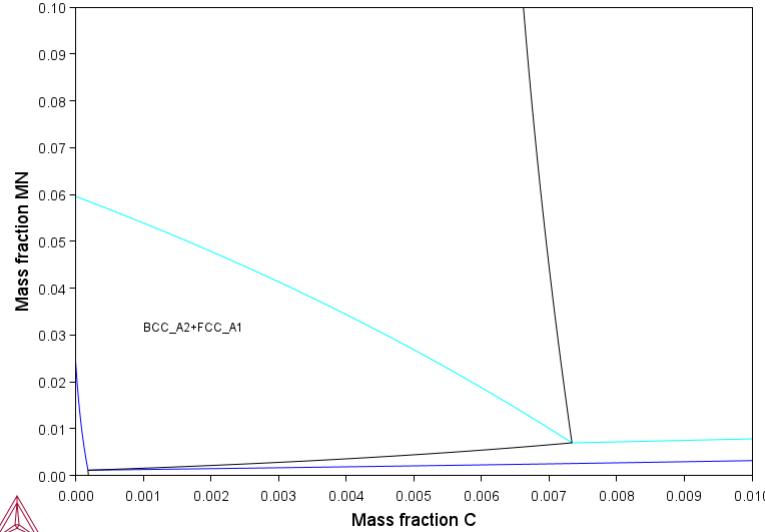
```

example 23l



```
POST:  
POST:Hit RETURN to continue  
POST: add .001 .03,,,  
... the command in full is ADD_LABEL_TEXT  
Automatic labelling not always possible  
Using global minimization procedure  
Using already calculated grid  
Found the set of lowest grid points in      0 s  
Calculated POLY solution    0 s, total time    0 s  
Stable phases are: BCC_A2+FCC_A1  
POST: set-title example 23m  
POST:  
POST:  
POST: SET_EXP_FILE_FORMAT 5  
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y  
... the command in full is MAKE_EXPERIMENTAL_DATAFI  
POST: SET_EXP_FILE_FORMAT 10  
POST:  
POST: plot  
... the command in full is PLOT_DIAGRAM
```

example 23m



```
POST:  
POST:Hit RETURN to continue  
POST: back  
POLY: @@ Calculate the corresponding paraequilibrium diagram  
POLY: @@ where fcc and bcc have the same alloy composition.  
POLY:  
POLY: read tce23d  
... the command in full is READ_WORKSPACES  
POLY: @@ Only one axis is set, the interstitial  
POLY: @@ composition must not be an axis  
POLY:  
POLY: s-a-v 1 w(mn) 0 .1,,  
... the command in full is SET_AXIS_VARIABLE  
POLY: s-a-v 2 none  
... the command in full is SET_AXIS_VARIABLE  
POLY: save tce23e y  
... the command in full is SAVE_WORKSPACES  
POLY: step  
... the command in full is STEP_WITH_OPTIONS  
Option? /NORMAL/: ?  
The following options are available:  
NORMAL          Stepping with given conditions  
INITIAL_EQUILIBRIA An initial equilibrium stored at every step  
EVALUATE        Specified variables evaluated after each step  
SEPARATE_PHASES Each phase calculated separately  
T-ZERO          T0 line calculation  
PARAEQUILIBRIUM Paraequilibrium diagram  
MIXED_SCHEIL   Scheil with fast diffusing elements
```

```

ONE_PHASE_AT_TIME One phase at a time
Option? /NORMAL/: para

This command calculates a paraequilibrium between two phases.
You must calculate an equilibrium with the overall composition first.
Name of first phase: fcc_a1
Name of second phase: bcc_a2
Fast diffusing component: /C/: c
Fast diffusing component: /NONE/:
Output during stepping is:
axis value, phase amounts, u-fractions of interstitial(s) in phase 1 and 2,
and LNACR value(s) of interstitial(s)

Phase Region from 0.150000E-01 for:
  BCC_A2
  FCC_A1
1.500000E-02    0.598    0.402    2.298022E-02    5.310923E-04   -1.884317E+00
1.250000E-02    0.541    0.459    2.526500E-02    5.938109E-04   -1.755858E+00
1.000000E-02    0.494    0.506    2.755370E-02    6.585896E-04   -1.635468E+00
7.500000E-03    0.454    0.546    2.984541E-02    7.254514E-04   -1.521908E+00
5.000000E-03    0.420    0.580    3.213933E-02    7.944190E-04   -1.414210E+00
2.500000E-03    0.390    0.610    3.443471E-02    8.655154E-04   -1.311599E+00
2.500000E-09    0.363    0.637    3.673089E-02    9.387636E-04   -1.213448E+00

Phase Region from 0.150000E-01 for:
  BCC_A2
  FCC_A1
1.500000E-02    0.597    0.403    2.298398E-02    5.312222E-04   -1.883912E+00
1.750000E-02    0.666    0.334    2.070420E-02    4.705375E-04   -2.022034E+00
2.000000E-02    0.751    0.249    1.843022E-02    4.118621E-04   -2.172021E+00
2.250000E-02    0.860    0.140    1.616367E-02    3.551844E-04   -2.336856E+00
2.500000E-02    1.003    -0.003    1.390572E-02    3.004774E-04   -2.520888E+00
2.750000E-02    1.201    -0.201    1.165535E-02    2.476621E-04   -2.730954E+00
3.000000E-02    1.493    -0.493    9.402954E-03    1.964659E-04   -2.979282E+00
3.250000E-02    1.971    -0.971    7.146299E-03    1.468099E-04   -3.287374E+00
3.500000E-02    2.894    -1.894    4.884077E-03    9.864283E-05   -3.701739E+00
3.750000E-02    5.421    -4.421    2.614914E-03    5.191598E-05   -4.360340E+00
4.000000E-02    42.141   -41.141   3.373635E-04    6.583378E-06   -6.442132E+00
*** Buffer saved on file c:\jenkins\WORKSP~1\GENERA~1\examples\tcex23\tcex23e.POLY3
*** ERROR      3 IN NS01AD: Numerical error
```

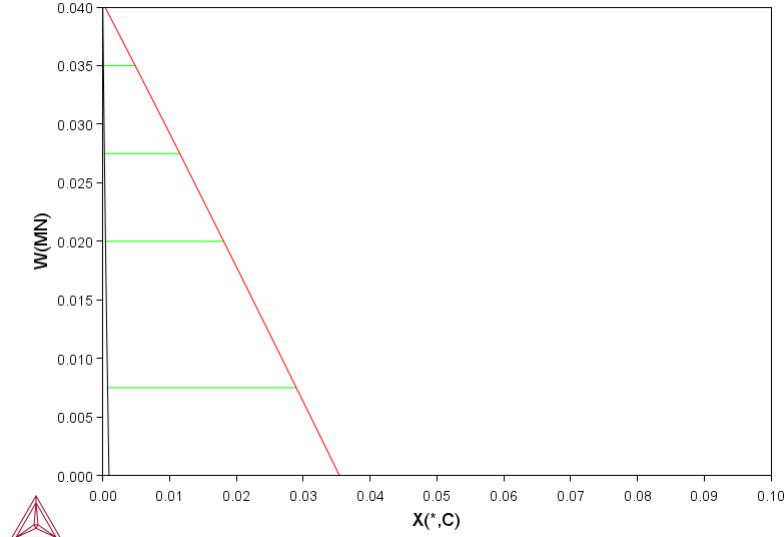
POLY:
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

```

POST:
POST:
POST: s-t-s 3
... the command in full is SET_TIELINE_STATUS
POST: set-title example 23n
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
```

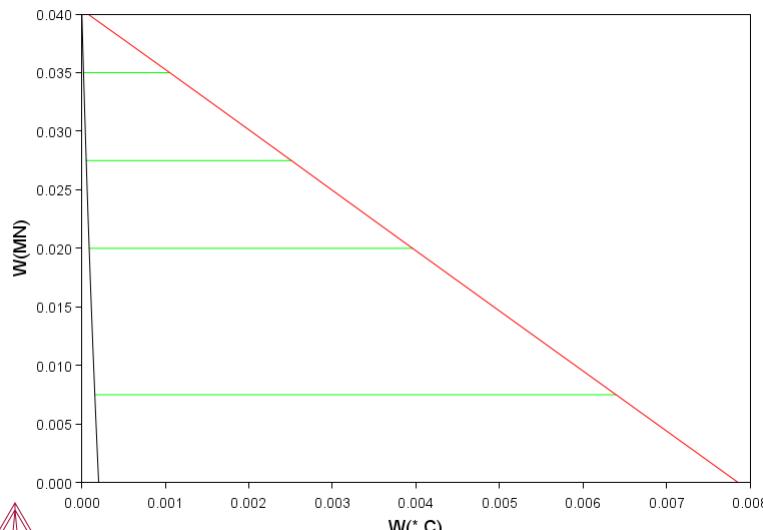
example 23n



```

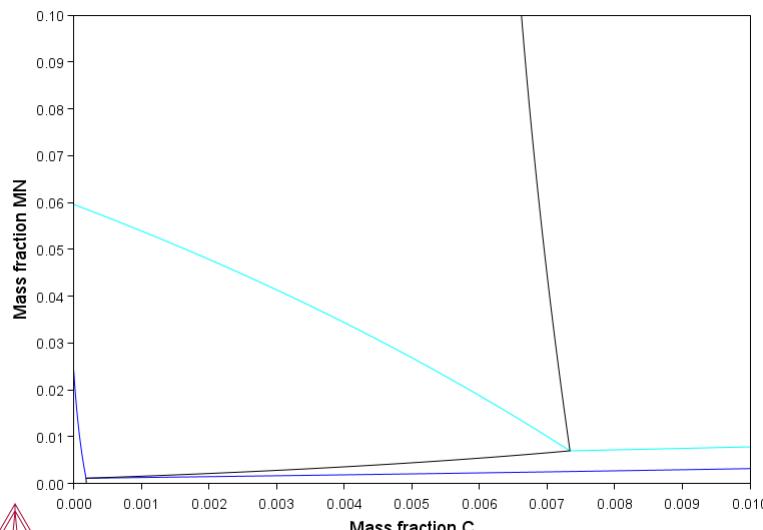
POST:
POST:Hit RETURN to continue
POST: s-d-a x w(*,c)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*:
POST:
POST: set-title example 23o
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
```

example 23o



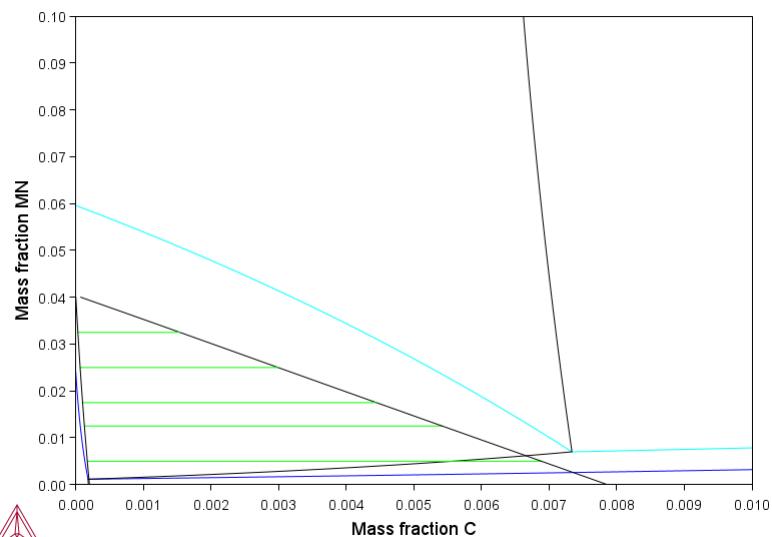
```
POST:  
POST: make tcex23e y  
... the command in full is MAKE_EXPERIMENTAL_DATAFI  
POST:Hit RETURN to continue  
POST: back  
POLY: @@ Now overlay the two diagrams  
POLY: read tcex23d  
... the command in full is READ_WORKSPACES  
POLY: post  
POLY-3 POSTPROCESSOR VERSION 3.2  
Setting automatic diagram axes  
  
POST:  
POST:  
POST: set-title example 23p  
POST:  
POST:  
POST: SET_EXP_FILE_FORMAT 5  
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y  
... the command in full is MAKE_EXPERIMENTAL_DATAFI  
POST: SET_EXP_FILE_FORMAT 10  
POST:  
POST: plot  
... the command in full is PLOT_DIAGRAM
```

example 23p



```
POST:  
POST:Hit RETURN to continue  
POST: a-e-d y tcex23e  
... the command in full is APPEND_EXPERIMENTAL_DATA  
PROLOGUE NUMBER: /0/: 0  
DATASET NUMBER(s): /-1/: 1  
POST: set-title example 23q  
POST:  
POST:  
POST: SET_EXP_FILE_FORMAT 5  
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y  
... the command in full is MAKE_EXPERIMENTAL_DATAFI  
POST: SET_EXP_FILE_FORMAT 10  
POST:  
POST: plot  
... the command in full is PLOT_DIAGRAM
```

example 23q



POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:

SYS:About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

```
SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce24\tce24.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Simulation of the silicon arc furnace using the REACTOR module
SYS:
SYS: @@ This is a simple reactor model with output of gases at the top
SYS: @@ and output of condensed phases at the bottom. The gas phase
SYS: @@ from one segment flows to higher segments, 80% reacts in the
SYS: @@ first above, 15% in the second above and 5 % in the third
SYS: @@ above. The condensed phases flow downwards and all of it goes
SYS: @@ to the next lowest segment.
SYS:
SYS: @@ Heat can be added at any module. The only way to specify the
SYS: @@ initial state of the reactants added to the reactor is to
SYS: @@ specify the heat content.
SYS:
SYS: @@ Note that a SSUB database license is required to run
SYS: @@ the example.
SYS:
SYS: @@ First fetch data
SYS: GO DAT
THERMODYNAMIC DATABASE module
Database folder: C:\jenkins\workspace\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA           /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE11: SW SSUB6
Current database: SGTE Substances v6.0

VA DEFINED
TDB_SSUB6:
TDB_SSUB6: @@ Define-species means that data for just these species is
TDB_SSUB6: @@ retrieved. Define-system means that data for all
TDB_SSUB6: @@ combinations of the elements would be retrieved and this
TDB_SSUB6: @@ is not necessary.
TDB_SSUB6: DEFINED
TDB_SSUB6: DEF-SPECIES C C1O1 C1O2 C1Si1 C2 C3 N1O1 N2 N4Si3
C          C1O1          C1O2
C1Si1      C2          C3
N1O1      N2          N4Si3
TDB_SSUB6: DEFINED
TDB_SSUB6: DEF-SP O O2 SI O1Si1 O2Si1
O          O2          SI
O1Si1      O2Si1  DEFINED
TDB_SSUB6: GET
16:02:38,445 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ...

List of references for assessed data

C1<G> T.C.R.A.S. Class: 1
C1<G> C<G>
C1O1<G> JANAF THERMOCHEMICAL TABLES SGTE **
C1O1<G> CO<G>
CARBON MONOXIDE <GAS>
STANDARD STATE : CODATA KEY VALUE. /CP FROM JANAF PUB. 9/65
C1O2<G> T.C.R.A.S. Class: 2
C1O2<G> CO2<G>
CARBON DIOXIDE <GAS>
C1Si1<G> T.C.R.A.S. Class: 5
C1Si1<G> SiC<G>
SILICON CARBIDE <GAS>
C2<G> T.C.R.A.S. Class: 2
CARBON Diatomic Gas.
CARBON <DIATOMIC GAS>
C3<G> T.C.R.A.S. Class: 6
CARBON triatomic gas.
CARBON <TRIATOMIC GAS>
N1O1<G> T.C.R.A.S. Class: 1
N1O1<G> NO<G>
NITRIC OXIDE <GAS>
N2<G> JANAF THERMOCHEMICAL TABLES SGTE **
N2<G> N2<G>
NITROGEN <DIATOMIC GAS>
PUBLISHED BY JANAF AT 09/65
O1<G> TCRAS 02/06/80
O1 Gaseous Standard State.
O1Si1<G> T.C.R.A.S. Class: 1
O1Si1<G> SiO<G>
SILICON <MONOXIDE GAS>
O2<G> TCRAS 21/06/90
OXYGEN Gaseous Standard State.
O2Si1<G> T.C.R.A.S. Class: 5
O2Si1<G> SiO2<G>
SILICON DIOXIDE <GAS>
Si1<G> T.C.R.A.S. Class: 1
Si1<G> Si<G>
SILICON <GAS>
O2Si1<BETA-QUARTZ> N.P.L.
O2Si1<BETA_QUARTZ> SiO2<BETA_QUARTZ>
Data from an assessment by T I Barry, reported in paper on CaO-SiO2
```

system by J R Taylor and A T Dinsdale, CALPHAD, 1990, 19(1), 71-88
C1Si1<ALPHA> JANAF THERMOCHEMICAL TABLES SGTE **
C1Si1<C1Si1_ALPHA> SiC<ALPHA>
N CARBIDE <ALPHA>
ALPHA-SIC . HEX.FORM . PUBL. BY JANAF AT 3/67 .LESS STABLE THAN
SIC BETA UP TO 2200K. Decomposes to complex vapour at about 3259K.
C1Si1<BETA> JANAF THERMOCHEMICAL TABLES SGTE
C1Si1<C1Si1_BETA> SiC<BETA>
N CARBIDE <BETA>
CUBIC FORM OF TYPE ZNS. STABLE WITH RESPECT TO SIC-ALPHA UP TO 2200K.
PUBL. BY JANAF 03/67
O2Si1<CRISTOBALITE> N.P.L.
O2Si1<CRISTOBALITE> SiO2<CRISTOBALITE>
Data from an assessment by T I Barry, reported in paper on CaO-SiO2
syst
by J R Taylor and A T Dinsdale, CALPHAD, 1990, 19(1), 71-88
C1 S.G.T.E. **
GRAPHITE
Data from SGTE Unary DB, pressure dependent data added by atd 7/9/95
C1<DIAMOND> S.G.T.E. **
C1<DIAMOND> <DIAMOND>
DIAMOND
Data from SGTE Unary DB, data added by atd 7/9/95, H298-H0 taken
from 1994 database (ex THERMODATA 01/93)
N4Si3 CHATILLON(1997)
N4Si3 Si3N4 N4Si3
Gurvich V.V., Veyts I.V., Alcock C.B., Thermodynamical Properties of
Individual Substances, 4th ed. Vol 1 and 2 English Ed (1990). S(298)
corrected according to Koshchenko V.I., Grindberg Ya. Zh. Inorg.
Mater.
18(6) 903-5 (1982). Recent calorimetric determination par O'Hare et
al., J. Mater. Res., 12 (1997) 3203-3205. Enthalpy of transformation
alpha to beta very small(1 ± 4 kJ/mol) but no knowledge of T trans.
according to them.
O2Si1<> N.P.L.
O2Si1<LIQUID_O2Si> SiO2<LIQUID>
Data from an assessment by T I Barry, reported in paper on CaO-SiO2
syst
by J R Taylor and A T Dinsdale, CALPHAD, 1990, 19(1), 71-88
O2Si1<QUARTZ> N.P.L.
O2Si1<QUARTZ> SiO2<QUARTZ> SiO2<quartz>
Data from an assessment by T I Barry, reported in paper on CaO-SiO2
syst
by J R Taylor and A T Dinsdale, CALPHAD, 1990, 19(1), 71-88
S11 JANAF THERMOCHEMICAL TABLES SGTE **
S11 Si
SILICON
PUBLISHED BY JANAF AT 12/66 . MPT FROM NBS BULL. (IPTS-68)
--U.D. 31/10/85
O2Si1<TRIDYMITE> N.P.L.
O2Si1<TRIDYMITE> SiO2<TRIDYMITE>
Data from an assessment by T I Barry, reported in paper on CaO-SiO2
syst
by J R Taylor and A T Dinsdale, CALPHAD, 1990, 19(1), 71-88
-OK-
TDB_SSUB6: GO G
GIBBS ENERGY SYSTEM
GES6: CH-ST EL Y VA
ELEMENT VA SUSPENDED
SPECIES VA SUSPENDED
GES6: L-ST
GAS CONSTANT IN USER ENERGY UNITS: 8.31451000E+00
1 BAR IN USER PRESSURE UNITS: 1.00000000E+05
CURRENT VALUE OF TEMPERATURE (KELVIN): 298.15
CURRENT VALUE OF PRESSURE (PASCAL): 1.00000000E+05
CURRENT NUMBER OF ELEMENT 4

| ELEMENT | STABLE ELEMENT | REFERENCE | MASS | H298-H0 | S298 |
|---------|------------------|-----------|------------|------------|---------------------|
| -1 /- | ELECTRON_GAS | | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 E0000000 |
| 0 VA | VACUUM | | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 E0000000 |
| 1 C | GRAPHITE | | 1.2011E+01 | 1.0540E+03 | 5.7400E+00 08000000 |
| 2 N | 1/2 MOLE_N2(GAS) | | 1.4007E+01 | 4.3350E+03 | 9.5751E+01 08000000 |
| 3 O | 1/2 MOLE_O2(GAS) | | 1.5999E+01 | 4.3410E+03 | 1.0252E+02 08000000 |
| 4 SI | DIAMOND_A4 | | 2.8085E+01 | 3.2175E+03 | 1.8820E+01 08000000 |

CURRENT NUMBER OF PHASE 17

| PHASE | STATUS | SUBLATTICES |
|--------------------|--------|-------------|
| 1 GAS | | 88200000 1 |
| 2 BETA_QUARTZ | | 82200000 1 |
| 3 C1Si1_ALPHA | | 82200000 1 |
| 4 C1Si1_BETA | | 82200000 1 |
| 5 CRISTOBALITE | | 82200000 1 |
| 6 C_L | | 82200000 1 |
| 7 C_S | | 82200000 1 |
| 8 DIAMOND | | 82200000 1 |
| 9 N4Si3_S | | 82200000 1 |
| 10 O2Si1_L | | 82200000 1 |
| 11 O2Si1_QUARTZ | | 82200000 1 |
| 12 O2Si1_QUARTZ_S2 | | 82200000 1 |
| 13 SI_L | | 82200000 1 |
| 14 SI_S | | 82200000 1 |
| 15 TRIDYMITE | | 82200000 1 |
| 16 TRIDYMITE_S2 | | 82200000 1 |
| 17 TRIDYMITE_S3 | | 82200000 1 |

CURRENT NUMBER OF SPECIES 15

| SPECIES | STOICHIOMETRY |
|----------|---------------|
| 1 C | C |
| 2 C1O1 | C1O1 |
| 3 C1O2 | C1O2 |
| 4 C1Si1 | C1Si1 |
| 5 C2 | C2 |
| 6 C3 | C3 |
| 7 N | N |
| 8 N1O1 | N1O1 |
| 9 N2 | N2 |
| 10 N4Si3 | N4Si3 |
| 11 O | O |
| 12 O1Si1 | O1Si1 |
| 13 O2 | O2 |
| 14 O2Si1 | O2Si1 |
| 15 SI | SI |
| 16 VA | VA |

GES6: GO R

Thermo-Calc REACTOR version 1.0

REACTOR: ?

| | | |
|---------------------|-----------------------|------------------|
| AMEND_INPUT | CREATE_STAGE_BOXES | LIST_RECORDS |
| AMEND_RECORD | EQUILIBRATE | MACRO-FILE-OPEN |
| BACK | EXECUTE_POLY3_COMMAND | READ_WORKSPACE |
| CHANGE_SURROUNDINGS | EXIT | SAVE_WORKSPACE |
| CONTINUE_SIMULATION | GOTO_MODULE | SET_INTERACTIVE |
| CREATE_DIVIDERS | HELP | SHOW_PROBE |
| CREATE_PIPES | INFORMATION | START_SIMULATION |
| CREATE_PROBE | LIST_DESIGN | |

REACTOR: @@ Create a reactor with 4 segments which is heat controlled.

REACTOR: @@ At the top segment 1 mole of quartz (SiO2) and 1.8 mole of graphite (C) is added. A small amount of N is also added to

REACTOR: @@ simplify calculations. The reactants have room temperature.

REACTOR: @@ In the other three segments only heat is added.

REACTOR:

REACTOR: @@ A guess of the initial temperature in each segment must be provided.

REACTOR:

REACTOR: CREATE_STAGE

NUMBER OF STAGE BOXES /4/: 4

YOU MUST FIRST DEFINE FEED FROM SURROUNDINGS!

GIVE FEED TO SYSTEM: N(C)=1.8

Input temperature /298.15/:

GIVE FEED TO SYSTEM: N(O₂S1)=1

Input temperature /298.15/:

GIVE FEED TO SYSTEM: H=876000

GIVE FEED TO SYSTEM: N(N₂)=4e-4

Input temperature /298.15/:

GIVE FEED TO SYSTEM:

GIVE FOR STAGE BOX 1

NAME: /SEGMENT_1/:

TYPE OF BOX /EQUILIBRIUM/: EQUILIBRIUM

Is the stage heat controlled? /Y/: Y

Initial guess of temperature? /1000/: 1750

Give initial amount:

Each phase may have a separate output, give these

Phase name /REST/: gas

Phase name /REST/: REST

GIVE FOR STAGE BOX 2

NAME: /SEGMENT_2/:

TYPE OF BOX /EQUILIBRIUM/: EQUILIBRIUM

Is the stage heat controlled? /Y/: Y

Initial guess of temperature? /1000/: 1900

Give initial amount:

Each phase may have a separate output, give these

Phase name /REST/: gas

Phase name /REST/: REST

GIVE FOR STAGE BOX 3

NAME: /SEGMENT_3/:

TYPE OF BOX /EQUILIBRIUM/: EQUILIBRIUM

Is the stage heat controlled? /Y/: Y

Initial guess of temperature? /1000/: 2050

Give initial amount:

Each phase may have a separate output, give these

Phase name /REST/: gas

Phase name /REST/: REST

GIVE FOR STAGE BOX 4

NAME: /SEGMENT_4/:

TYPE OF BOX /EQUILIBRIUM/: EQUILIBRIUM

Is the stage heat controlled? /Y/: Y

Initial guess of temperature? /1000/: 2200

Give initial amount:

Each phase may have a separate output, give these

Phase name /REST/: gas

Phase name /REST/: REST

REACTOR: l-r

Number: 0 name: SURROUNDINGS stage box at: 23,
Feed of C with 1.8000E+00 mol to record: -1
Feed of O₂S1 with 1.0000E+00 mol to record: -1
Feed of heat 8.7600E+05 J to record: -1
Feed of N₂ with 4.0000E-04 mol to record: -1

Number: 1 name: SEGMENT_1 stage box at: 72, H controlled
Output for phase GAS to record: -1
Output for phase REST to record: -1

Number: 2 name: SEGMENT_2 stage box at: 114, H controlled
Output for phase GAS to record: -1
Output for phase REST to record: -1

Number: 3 name: SEGMENT_3 stage box at: 156, H controlled
Output for phase GAS to record: -1
Output for phase REST to record: -1

Number: 4 name: SEGMENT_4 stage box at: 198, H controlled
Output for phase GAS to record: -1
Output for phase REST to record: -1

REACTOR: @@ Create dividers, one for distributing the gas from segment

REACTOR: @@ 2 to 4, one for splitting the heat feed, and one for splitting

REACTOR: @@ the feed on N₂

REACTOR:

REACTOR: create-div

Number of dividers /4/: 5

Number of outputs for divider 1: /3/: 2

Percent of input to output 1: /100/: 80

Number of outputs for divider 2: /3/: 3

Percent of input to output 1: /100/: 80 15

Number of outputs for divider 3: /3/: 3

Percent of input to output 1: /100/: 80 15

Number of outputs for divider 4: /3/: 3

Percent of input to output 1: /100/: 85 10

Number of outputs for divider 5: /3/: 4

Percent of input to output 1: /100/: 25 25 25

REACTOR: 1-r

Number: 0 name: SURROUNDINGS stage box at: 23,
 Feed of C with 1.8000E+00 mol to record: -1
 Feed of O2SI1 with 1.0000E+00 mol to record: -1
 Feed of heat 8.7600E+05 J to record: -1
 Feed of N2 with 4.0000E-04 mol to record: -1

Number: 1 name: SEGMENT_1 stage box at: 72, H controlled
 Output for phase GAS to record: -1
 Output for phase REST to record: -1

Number: 2 name: SEGMENT_2 stage box at: 114, H controlled
 Output for phase GAS to record: -1
 Output for phase REST to record: -1

Number: 3 name: SEGMENT_3 stage box at: 156, H controlled
 Output for phase GAS to record: -1
 Output for phase REST to record: -1

Number: 4 name: SEGMENT_4 stage box at: 198, H controlled
 Output for phase GAS to record: -1
 Output for phase REST to record: -1

Number: 5 name: DIVIDER_5 divider at: 240
 80 % of input to record: -1
 20 % of input to record: -1

Number: 6 name: DIVIDER_6 divider at: 268
 80 % of input to record: -1
 15 % of input to record: -1
 5 % of input to record: -1

Number: 7 name: DIVIDER_7 divider at: 301
 80 % of input to record: -1
 15 % of input to record: -1
 5 % of input to record: -1

Number: 8 name: DIVIDER_8 divider at: 334
 85 % of input to record: -1
 10 % of input to record: -1
 5 % of input to record: -1

Number: 9 name: DIVIDER_9 divider at: 367
 25 % of input to record: -1
 25 % of input to record: -1
 25 % of input to record: -1
 25 % of input to record: -1

REACTOR: @@ Finally create the pipes between the segments first for the feed
REACTOR: c-pipe 0 1 1 8 9

Feed of C
 Feed of O2SI1
 Feed of heat
 Input set to this divider
 Feed of N2
 Input set to this divider
 NO MORE OUTPUT RECORDS

REACTOR: @@ All solid phases are assumed to go down one segment
REACTOR: @@ The gas phase is assumed to go up, 80% to the next segment,
REACTOR: @@ 15% to the second next and 5% to the third segment above.
REACTOR: @@ Output from stage boxes

REACTOR: c-pipe 1 0 2
 Output record for phase GAS
 Output record for phase REST
 NO MORE OUTPUT RECORDS

REACTOR: c-pipe 2 5 3
 Output record for phase GAS
 Input set to this divider
 Output record for phase REST
 NO MORE OUTPUT RECORDS

REACTOR: c-pipe 3 6 4
 Output record for phase GAS
 Input set to this divider
 Output record for phase REST
 NO MORE OUTPUT RECORDS

REACTOR: c-pipe 4 7 0
 Output record for phase GAS
 Input set to this divider
 Output record for phase REST
 NO MORE OUTPUT RECORDS

REACTOR: @@ Output from dividers

REACTOR: c-pipe 5 1 0
 Output record for 80 % of input
 Output record for 20 % of input
 NO MORE OUTPUT RECORDS

REACTOR: c-pipe 6 2 1 0
 Output record for 80 % of input
 Output record for 15 % of input
 Output record for 5 % of input
 NO MORE OUTPUT RECORDS

REACTOR: c-pipe 7 3 2 1
 Output record for 80 % of input
 Output record for 15 % of input
 Output record for 5 % of input
 NO MORE OUTPUT RECORDS

REACTOR: c-pipe 8 4 3 2
 Output record for 85 % of input
 Output record for 10 % of input
 Output record for 5 % of input
 NO MORE OUTPUT RECORDS

REACTOR: c-pipe 9 1 2 3 4
 Output record for 25 % of input
 NO MORE OUTPUT RECORDS

REACTOR: 1-r

Number: 0 name: SURROUNDINGS stage box at: 23,
 Feed of C with 1.8000E+00 mol to record: 1
 Feed of O2SI1 with 1.0000E+00 mol to record: 1
 Feed of heat 8.7600E+05 J to record: 8
 Feed of N2 with 4.0000E-04 mol to record: 9

```

Number: 1 name: SEGMENT_1          stage box at:    72, H controlled
Output for phase GAS              to record:    0
Output for phase REST             to record:    2

Number: 2 name: SEGMENT_2          stage box at:   114, H controlled
Output for phase GAS              to record:    5
Output for phase REST             to record:    3

Number: 3 name: SEGMENT_3          stage box at:   156, H controlled
Output for phase GAS              to record:    6
Output for phase REST             to record:    4

Number: 4 name: SEGMENT_4          stage box at:   198, H controlled
Output for phase GAS              to record:    7
Output for phase REST             to record:    0

Number: 5 name: DIVIDER_5          divider at:   240
 80 % of input to record:    1
 20 % of input to record:    0

Number: 6 name: DIVIDER_6          divider at:   268
 80 % of input to record:    2
 15 % of input to record:    1
  5 % of input to record:    0

Number: 7 name: DIVIDER_7          divider at:   301
 80 % of input to record:    3
 15 % of input to record:    2
  5 % of input to record:    1

Number: 8 name: DIVIDER_8          divider at:   334
 85 % of input to record:    4
 10 % of input to record:    3
  5 % of input to record:    2

Number: 9 name: DIVIDER_9          divider at:   367
 25 % of input to record:    1
 25 % of input to record:    2
 25 % of input to record:    3
 25 % of input to record:    4

REACTOR: save tcex24 y
REACTOR: @@ Now start the process
REACTOR: read tcex24
REACTOR:
REACTOR: @@ The output for each iteration consists of the conditions set in
REACTOR: @@ each segment, and you can also select some state variables,
REACTOR: @@ in this case NP($) meaning moles of stable phases.
REACTOR: @@ After each loop the temperatures in all segments are listed
REACTOR:
REACTOR: @@ We want to achieve a reactor where only Si<L> leaves at the bottom.
REACTOR: START
Max number of loops: /10/: 50
OUTPUT TO SCREEN OR FILE /SCREEN/:
Output conditions? /Y/:
Output variables: /BP($)/: T BP($)
>>> DATA AT ITERATION 1 FROM STAGE 1
T=1750, P=100000, N(C)=1.8, N(N)=2E-4, N(O)=2, N(SI)=1
DEGREES OF FREEDOM 0
T= 1.750000E+03
BP(GAS)=8.3899239E-3, BP(C1SI1_BETA)=3.9560636E-3,
BP(CRISTOBALITE)=60.077021, BP(C_S)=21.616235
>>> DATA AT ITERATION 1 FROM STAGE 2
T=1900, P=100000, N(C)=1.799801831, N(N)=2E-4, N(O)=1.999800965,
N(SI)=0.9999991472
DEGREES OF FREEDOM 0
T= 1.900000E+03
BP(GAS)=35.781375, BP(C1SI1_BETA)=23.515817, BP(CRISTOBALITE)=22.402821
>>> DATA AT ITERATION 1 FROM STAGE 3
T=2050, P=100000, N(C)=0.5864878616, N(N)=2E-4, N(O)=0.7457290951,
N(SI)=0.9593524091
DEGREES OF FREEDOM 0
T= 2.050000E+03
BP(GAS)=1.1001909E-2, BP(C1SI1_BETA)=23.51327, BP(O2SI1_L)=22.396537,
BP(SI_L)=6.3106228E-4
>>> DATA AT ITERATION 1 FROM STAGE 4
T=2200, P=100000, N(C)=0.58644243231, N(N)=2E-4, N(O)=0.74551992,
N(SI)=0.9592067528
DEGREES OF FREEDOM 0
T= 2.200000E+03
BP(GAS)=27.369406, BP(C1SI1_BETA)=9.7781171, BP(SI_L)=8.7657159
=====
>>> DATA AT ITERATION 2 FROM STAGE 1
H=-969231.6342, P=100000, N(C)=2.78778854, N(N)=4E-4, N(O)=3.040564868,
N(SI)=1.052700505
DEGREES OF FREEDOM 0
T= 1.098651E+03
BP(GAS)=25.395955, BP(BETA_QUARTZ)=63.249404, BP(C_S)=23.055463
>>> DATA AT ITERATION 2 FROM STAGE 2
H=-837416.4877, P=100000, N(C)=1.970963345, N(N)=3.9E-4, N(O)=2.217396337,
N(SI)=1.113300827
DEGREES OF FREEDOM 0
T= 1.764644E+03
BP(GAS)=2.5771879E-2, BP(C1SI1_BETA)=0.19891753, BP(CRISTOBALITE)=66.592185,
BP(C_S)=23.605007
>>> DATA AT ITERATION 2 FROM STAGE 3
H=-772456.8489, P=100000, N(C)=2.24428875, N(N)=3.6E-4, N(O)=2.813089043,
N(SI)=1.435877836
DEGREES OF FREEDOM 0
T= 1.785830E+03
BP(GAS)=28.121362, BP(C1SI1_BETA)=21.054185, BP(CRISTOBALITE)=54.435284,
BP(C_S)=8.6836041
>>> DATA AT ITERATION 2 FROM STAGE 4
H=33660.30349, P=100000, N(C)=1.248065358, N(N)=2E-4, N(O)=1.812002861,
N(SI)=1.431095835
DEGREES OF FREEDOM 0
T= 2.447572E+03
BP(GAS)=60.210326, BP(C1SI1_BETA)=0.55847709, BP(SI_L)=23.407071
=====
>>> DATA AT ITERATION 3 FROM STAGE 1
H=-922751.4701, P=100000, N(C)=2.011716301, N(N)=5.76E-4, N(O)=2.241341655,
N(SI)=1.029906422
DEGREES OF FREEDOM 0
T= 8.124883E+02
BP(GAS)=4.0693569, BP(C_S)=23.005715, BP(O2SI1_QUARTZ)=61.879868
>>> DATA AT ITERATION 3 FROM STAGE 2

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H=-903970.2067, P=100000, N(C)=2.89748639, N(N)=5.18E-4, N(O)=3.13248222,
N(SI)=1.12129161
DEGREES OF FREEDOM 0
T= 1.746338E+03
BP(GAS)=25.042951, BP(CRISTOBALITE)=67.278274, BP(C_S)=24.095798
>>> DATA AT ITERATION 3 FROM STAGE 3
H=-804917.287, P=100000, N(C)=2.993453661, N(N)=3.6E-4, N(O)=3.689113428,
N(SI)=1.586740033
DEGREES OF FREEDOM 0
T= 1.785838E+03
BP(GAS)=55.589668, BP(C1SI1_BETA)=28.960504, BP(CRISTOBALITE)=51.37138,
BP(C_S)=3.6235824
>>> DATA AT ITERATION 3 FROM STAGE 4
H=-61307.1432, P=100000, N(C)=1.023967769, N(N)=2E-4, N(O)=1.7100138,
N(SI)=1.57728602
DEGREES OF FREEDOM 0
T= 2.594647E+03
BP(GAS)=59.391022, BP(SI_L)=24.567245
=====
>>> DATA AT ITERATION 4 FROM STAGE 1
H=-975672.9943, P=100000, N(C)=2.859695045, N(N)=6.784E-4, N(O)=3.096742498,
N(SI)=1.037773929
DEGREES OF FREEDOM 0
T= 1.067994E+03
BP(GAS)=27.303365, BP(BETA_QUARTZ)=62.352571, BP(C_S)=23.392027
>>> DATA AT ITERATION 4 FROM STAGE 2
H=-926156.1401, P=100000, N(C)=3.676734224, N(N)=5.18E-4, N(O)=3.915329631,
N(SI)=1.150718125
DEGREES OF FREEDOM 0
T= 1.785833E+03
BP(GAS)=48.987037, BP(C1SI1_BETA)=2.2730167, BP(CRISTOBALITE)=65.232008,
BP(C_S)=22.635726
>>> DATA AT ITERATION 4 FROM STAGE 3
H=-759974.2115, P=100000, N(C)=2.760446561, N(N)=3.6E-4, N(O)=3.53940754,
N(SI)=1.704419532
DEGREES OF FREEDOM 0
T= 1.856422E+03
BP(GAS)=54.420155, BP(C1SI1_BETA)=34.739066, BP(CRISTOBALITE)=48.497149
>>> DATA AT ITERATION 4 FROM STAGE 4
H=97718.13169, P=100000, N(C)=0.8663972889, N(N)=2E-4, N(O)=1.614338479,
N(SI)=1.673565628
DEGREES OF FREEDOM 0
T= 2.773504E+03
BP(GAS)=58.669424, BP(SI_L)=24.569593
=====
>>> DATA AT ITERATION 5 FROM STAGE 1
H=-1013577.447, P=100000, N(C)=3.515796758, N(N)=6.784E-4, N(O)=3.764623788,
N(SI)=1.0512292
DEGREES OF FREEDOM 0
T= 1.163508E+03
BP(GAS)=45.980219, BP(C_S)=22.850503, BP(TRIDYMITE_S3)=63.161004
>>> DATA AT ITERATION 5 FROM STAGE 2
H=-913270.225, P=100000, N(C)=3.547663629, N(N)=5.18E-4, N(O)=3.884664421,
N(SI)=1.195722123
DEGREES OF FREEDOM 0
T= 1.785833E+03
BP(GAS)=49.603255, BP(C1SI1_BETA)=5.1279345, BP(CRISTOBALITE)=63.651652,
BP(C_S)=19.968004
>>> DATA AT ITERATION 5 FROM STAGE 3
H=-720022.7647, P=100000, N(C)=2.483485629, N(N)=3.6E-4, N(O)=3.410261538,
N(SI)=1.826276239
DEGREES OF FREEDOM 0
T= 1.974923E+03
BP(GAS)=54.11176, BP(C1SI1_BETA)=33.932787, BP(CRISTOBALITE)=47.641383
>>> DATA AT ITERATION 5 FROM STAGE 4
H=121546.0245, P=100000, N(C)=0.846288591, N(N)=2E-4, N(O)=1.585852345,
N(SI)=1.639214763
DEGREES OF FREEDOM 0
T= 2.880121E+03
BP(GAS)=58.994116, BP(SI_L)=22.582856
=====
>>> DATA AT ITERATION 6 FROM STAGE 1
H=-1010753.26, P=100000, N(C)=3.493730651, N(N)=6.784E-4, N(O)=3.765652929,
N(SI)=1.076563738
DEGREES OF FREEDOM 0
T= 1.245814E+03
BP(GAS)=44.984991, BP(C_S)=22.786504, BP(TRIDYMITE_S3)=64.683179
>>> DATA AT ITERATION 6 FROM STAGE 2
H=-907819.023, P=100000, N(C)=3.33837247, N(N)=5.18E-4, N(O)=3.850532682,
N(SI)=1.351481693
DEGREES OF FREEDOM 0
T= 1.785834E+03
BP(GAS)=49.986925, BP(C1SI1_BETA)=12.328795, BP(CRISTOBALITE)=62.215898,
BP(C_S)=15.079393
>>> DATA AT ITERATION 6 FROM STAGE 3
H=-689981.5848, P=100000, N(C)=2.239978012, N(N)=3.6E-4, N(O)=3.339680256,
N(SI)=2.011081244
DEGREES OF FREEDOM 0
T= 2.024859E+03
BP(GAS)=55.901308, BP(C1SI1_BETA)=33.947222, BP(O2SI1_L)=46.973649
>>> DATA AT ITERATION 6 FROM STAGE 4
H=142731.8648, P=100000, N(C)=0.8466486045, N(N)=2E-4, N(O)=1.563625286,
N(SI)=1.628461247
DEGREES OF FREEDOM 0
T= 2.939413E+03
BP(GAS)=59.078725, BP(SI_L)=21.844948
=====
>>> DATA AT ITERATION 7 FROM STAGE 1
H=-1008944.095, P=100000, N(C)=3.468043928, N(N)=6.784E-4, N(O)=3.768216951,
N(SI)=1.106725752
DEGREES OF FREEDOM 0
T= 1.360090E+03
BP(GAS)=43.509997, BP(C_S)=23.028873, BP(TRIDYMITE_S3)=66.495403
>>> DATA AT ITERATION 7 FROM STAGE 2
H=-908459.8575, P=100000, N(C)=3.15897605, N(N)=5.179999999E-4,
N(O)=3.868839264, N(SI)=1.540418611
DEGREES OF FREEDOM 0
T= 1.785834E+03
BP(GAS)=51.714963, BP(C1SI1_BETA)=20.759109, BP(CRISTOBALITE)=60.91749,
BP(C_S)=9.7183714
>>> DATA AT ITERATION 7 FROM STAGE 3
H=-668400.831, P=100000, N(C)=2.00417664, N(N)=3.6E-4, N(O)=3.278678122,
N(SI)=2.212140735
DEGREES OF FREEDOM 0
T= 2.054719E+03
BP(GAS)=58.391064, BP(C1SI1_BETA)=34.178134, BP(O2SI1_L)=46.091554

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>>> DATA AT ITERATION    7 FROM STAGE      4
H=157520.1355, P=100000, N(C)=0.8524075704, N(N)=2E-4, N(O)=1.53426275,
N(SI)=1.619538945
DEGREES OF FREEDOM 0
T= 2.970399E+03
BP(GAS)=58.350805, BP(SI_L)=21.921685
=====
>>> DATA AT ITERATION    8 FROM STAGE      1
H=-1010260.226, P=100000, N(C)=3.481080374, N(N)=6.784E-4, N(O)=3.81122454,
N(SI)=1.137875423
DEGREES OF FREEDOM 0
T= 1.482989E+03
BP(GAS)=43.00392, BP(C_S)=23.382924, BP(TRIDYMITE_S3)=68.366927
>>> DATA AT ITERATION    8 FROM STAGE      2
H=-910878.3295, P=100000, N(C)=-2.996068863, N(N)=-5.18E-4, N(O)=-3.901421157,
N(SI)=1.737804825
DEGREES OF FREEDOM 0
T= 1.785834E+03
BP(GAS)=53.791867, BP(C1SI1_BETA)=29.488661, BP(CRISTOBALITE)=59.674774,
BP(C_S)=4.2628222
>>> DATA AT ITERATION    8 FROM STAGE      3
H=-655233.1078, P=100000, N(C)=1.772287341, N(N)=3.6E-4, N(O)=3.213821477,
N(SI)=2.399849981
DEGREES OF FREEDOM 0
T= 2.072919E+03
BP(GAS)=59.871551, BP(C1SI1_BETA)=34.480045, BP(O2SI1_L)=45.758107
>>> DATA AT ITERATION    8 FROM STAGE      4
H=163921.0653, P=100000, N(C)=0.859937269, N(N)=2E-4, N(O)=1.523163186,
N(SI)=1.621518862
DEGREES OF FREEDOM 0
T= 2.980408E+03
BP(GAS)=57.971021, BP(SI_L)=22.269932
=====
>>> DATA AT ITERATION    9 FROM STAGE      1
H=-1012646.88, P=100000, N(C)=3.504415438, N(N)=6.784E-4, N(O)=3.861764807,
N(SI)=1.165496436
DEGREES OF FREEDOM 0
T= 1.587698E+03
BP(GAS)=42.882392, BP(C_S)=23.711015, BP(TRIDYMITE_S3)=70.024972
>>> DATA AT ITERATION    9 FROM STAGE      2
H=-913275.5573, P=100000, N(C)=2.83297897, N(N)=5.18E-4, N(O)=3.911942365,
N(SI)=1.912421221
DEGREES OF FREEDOM 0
T= 1.813659E+03
BP(GAS)=54.528551, BP(C1SI1_BETA)=36.500133, BP(CRISTOBALITE)=59.302998
>>> DATA AT ITERATION    9 FROM STAGE      3
H=-654500.852, P=100000, N(C)=1.598268366, N(N)=3.6E-4, N(O)=3.1925664,
N(SI)=2.560193536
DEGREES OF FREEDOM 0
T= 2.082775E+03
BP(GAS)=61.270688, BP(C1SI1_BETA)=34.761698, BP(O2SI1_L)=46.150363
>>> DATA AT ITERATION    9 FROM STAGE      4
H=160038.1016, P=100000, N(C)=0.8669617393, N(N)=2E-4, N(O)=1.536220325,
N(SI)=1.635071902
DEGREES OF FREEDOM 0
T= 2.968716E+03
BP(GAS)=58.16585, BP(SI_L)=22.749012
=====
>>> DATA AT ITERATION   10 FROM STAGE      1
H=-1011746.004, P=100000, N(C)=3.491172416, N(N)=6.784E-4, N(O)=3.875588138,
N(SI)=1.192089346
DEGREES OF FREEDOM 0
T= 1.688378E+03
BP(GAS)=41.819001, BP(C_S)=24.015589, BP(TRIDYMITE_S3)=71.592748
>>> DATA AT ITERATION   10 FROM STAGE      2
H=-917570.6538, P=100000, N(C)=2.714555789, N(N)=5.18E-4, N(O)=3.938638187,
N(SI)=2.055421364
DEGREES OF FREEDOM 0
T= 1.931654E+03
BP(GAS)=54.443862, BP(C1SI1_BETA)=37.245342, BP(CRISTOBALITE)=61.663362
>>> DATA AT ITERATION   10 FROM STAGE      3
H=-675805.5219, P=100000, N(C)=1.622473584, N(N)=3.6E-4, N(O)=3.281582211,
N(SI)=2.615260062
DEGREES OF FREEDOM 0
T= 2.082796E+03
BP(GAS)=62.678066, BP(C1SI1_BETA)=35.07906, BP(O2SI1_L)=47.687059
>>> DATA AT ITERATION   10 FROM STAGE      4
H=140324.5929, P=100000, N(C)=0.8748767964, N(N)=2E-4, N(O)=1.587372775,
N(SI)=1.668563184
DEGREES OF FREEDOM 0
T= 2.917962E+03
BP(GAS)=59.278419, BP(SI_L)=23.490502
=====
>>> DATA AT ITERATION   11 FROM STAGE      1
H=-1003110.741, P=100000, N(C)=3.384404635, N(N)=6.784E-4, N(O)=3.842325843,
N(SI)=1.263783677
DEGREES OF FREEDOM 0
T= 1.785825E+03
BP(GAS)=40.181408, BP(C1SI1_BETA)=2.0429771, BP(CRISTOBALITE)=72.460052,
BP(C_S)=22.941885
>>> DATA AT ITERATION   11 FROM STAGE      2
H=-922616.7773, P=100000, N(C)=2.690333937, N(N)=5.18E-4, N(O)=4.005471932,
N(SI)=2.139132245
DEGREES OF FREEDOM 0
T= 1.964263E+03
BP(GAS)=56.690326, BP(C1SI1_BETA)=37.355783, BP(CRISTOBALITE)=62.435823
>>> DATA AT ITERATION   11 FROM STAGE      3
H=-699253.1695, P=100000, N(C)=1.631560023, N(N)=3.6E-4, N(O)=3.348217301,
N(SI)=2.636542748
DEGREES OF FREEDOM 0
T= 2.082357E+03
BP(GAS)=62.812323, BP(C1SI1_BETA)=34.943937, BP(O2SI1_L)=49.460881
>>> DATA AT ITERATION   11 FROM STAGE      4
H=117365.2449, P=100000, N(C)=0.8715068208, N(N)=2E-4, N(O)=1.646418501,
N(SI)=1.694716071
DEGREES OF FREEDOM 0
T= 2.855981E+03
BP(GAS)=60.986548, BP(SI_L)=23.421073
=====
>>> DATA AT ITERATION   12 FROM STAGE      1
H=-1003449.781, P=100000, N(C)=3.364523602, N(N)=6.784E-4, N(O)=3.879313025,
N(SI)=1.318964335
DEGREES OF FREEDOM 0
T= 1.785826E+03
BP(GAS)=41.745844, BP(C1SI1_BETA)=4.6200258, BP(CRISTOBALITE)=71.897831,
BP(C_S)=21.265337

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>>> DATA AT ITERATION 12 FROM STAGE 2
H=-923111.7484, P=100000, N(C)=2.624481147, N(N)=5.18E-4, N(O)=4.001685486,
N(SI)=2.194444401
DEGREES OF FREEDOM 0
T= 1.981583E+03
BP(GAS)=56.956866, BP(C1SI1_BETA)=37.363041, BP(CRISTOBALITE)=62.863929
>>> DATA AT ITERATION 12 FROM STAGE 3
H=-719678.5628, P=100000, N(C)=1.629045072, N(N)=3.6E-4, N(O)=3.409704374,
N(SI)=2.666749026
DEGREES OF FREEDOM 0
T= 2.082497E+03
BP(GAS)=63.219191, BP(C1SI1_BETA)=34.784905, BP(O2SI1_L)=51.014914
=====>
>>> DATA AT ITERATION 12 FROM STAGE 4
H=97299.17323, P=100000, N(C)=0.8675405342, N(N)=2E-4, N(O)=1.698148022,
N(SI)=1.716614545
DEGREES OF FREEDOM 0
T= 2.791245E+03
BP(GAS)=62.594967, BP(SI_L)=23.207654
=====
>>> DATA AT ITERATION 13 FROM STAGE 1
H=-1002049.949, P=100000, N(C)=3.311715933, N(N)=6.784E-4, N(O)=3.868933584,
N(SI)=1.360090087
DEGREES OF FREEDOM 0
T= 1.785826E+03
BP(GAS)=41.782601, BP(C1SI1_BETA)=6.503078, BP(CRISTOBALITE)=71.546701,
BP(C_S)=20.051341
>>> DATA AT ITERATION 13 FROM STAGE 2
H=-924576.1055, P=100000, N(C)=2.570937218, N(N)=5.18E-4, N(O)=4.005562772,
N(SI)=2.246634772
DEGREES OF FREEDOM 0
T= 1.994519E+03
BP(GAS)=57.417427, BP(C1SI1_BETA)=37.390387, BP(CRISTOBALITE)=63.260705
>>> DATA AT ITERATION 13 FROM STAGE 3
H=-737399.6998, P=100000, N(C)=1.626554057, N(N)=3.6E-4, N(O)=3.464295587,
N(SI)=2.697632851
DEGREES OF FREEDOM 0
T= 2.082731E+03
BP(GAS)=63.654311, BP(C1SI1_BETA)=34.710227, BP(O2SI1_L)=52.365328
=====>
>>> DATA AT ITERATION 13 FROM STAGE 4
H=79895.15778, P=100000, N(C)=0.8656780545, N(N)=2E-4, N(O)=1.743099655,
N(SI)=1.737227882
DEGREES OF FREEDOM 0
T= 2.721648E+03
BP(GAS)=64.038962, BP(SI_L)=23.039395
=====
>>> DATA AT ITERATION 14 FROM STAGE 1
H=-1001186.959, P=100000, N(C)=3.268147774, N(N)=6.784E-4, N(O)=3.865162854,
N(SI)=1.398884527
DEGREES OF FREEDOM 0
T= 1.785826E+03
BP(GAS)=41.977201, BP(C1SI1_BETA)=8.2717563, BP(CRISTOBALITE)=71.225272,
BP(C_S)=18.915409
>>> DATA AT ITERATION 14 FROM STAGE 2
H=-925814.1594, P=100000, N(C)=2.519691745, N(N)=5.18E-4, N(O)=4.009317679,
N(SI)=2.297603162
DEGREES OF FREEDOM 0
T= 2.001975E+03
BP(GAS)=56.899726, BP(C1SI1_BETA)=37.678344, BP(O2SI1_L)=64.366461
>>> DATA AT ITERATION 14 FROM STAGE 3
H=-753439.8042, P=100000, N(C)=1.632245752, N(N)=3.6E-4, N(O)=3.537064524,
N(SI)=2.744501863
DEGREES OF FREEDOM 0
T= 2.083146E+03
BP(GAS)=65.32767, BP(SI_L)=22.875374
=====>
>>> DATA AT ITERATION 15 FROM STAGE 1
H=-999862.6593, P=100000, N(C)=3.222315839, N(N)=6.784E-4, N(O)=3.845817455,
N(SI)=1.424659955
DEGREES OF FREEDOM 0
T= 1.785826E+03
BP(GAS)=41.607103, BP(C1SI1_BETA)=9.4314277, BP(CRISTOBALITE)=71.039976,
BP(C_S)=18.17504
>>> DATA AT ITERATION 15 FROM STAGE 2
H=-928208.0513, P=100000, N(C)=2.491890776, N(N)=5.18E-4, N(O)=4.036544188,
N(SI)=2.349766658
DEGREES OF FREEDOM 0
T= 2.011374E+03
BP(GAS)=58.095637, BP(C1SI1_BETA)=37.727938, BP(O2SI1_L)=64.687648
>>> DATA AT ITERATION 15 FROM STAGE 3
H=-766271.3227, P=100000, N(C)=1.63303438, N(N)=3.6E-4, N(O)=3.578304454,
N(SI)=2.770582586
DEGREES OF FREEDOM 0
T= 2.083324E+03
BP(GAS)=65.468306, BP(C1SI1_BETA)=34.724896, BP(O2SI1_L)=54.487322
>>> DATA AT ITERATION 15 FROM STAGE 4
H=52615.99449, P=100000, N(C)=0.8660438827, N(N)=2E-4, N(O)=1.813735059,
N(SI)=1.772911412
DEGREES OF FREEDOM 0
T= 2.575864E+03
BP(GAS)=66.468904, BP(SI_L)=22.746114
=====
>>> DATA AT ITERATION 16 FROM STAGE 1
H=-1000065.826, P=100000, N(C)=3.199111233, N(N)=6.784E-4, N(O)=3.861986524,
N(SI)=1.463551792
DEGREES OF FREEDOM 0
T= 1.785826E+03
BP(GAS)=42.375409, BP(C1SI1_BETA)=11.209864, BP(CRISTOBALITE)=70.703913,
BP(C_S)=17.036615
>>> DATA AT ITERATION 16 FROM STAGE 2
H=-928526.6601, P=100000, N(C)=2.441492278, N(N)=5.18E-4, N(O)=4.03725716,
N(SI)=2.39893458
DEGREES OF FREEDOM 0
T= 2.020037E+03
BP(GAS)=58.591617, BP(C1SI1_BETA)=37.771358, BP(O2SI1_L)=64.9352
>>> DATA AT ITERATION 16 FROM STAGE 3
H=-776567.9187, P=100000, N(C)=1.634858189, N(N)=3.6E-4, N(O)=3.612504622,
N(SI)=2.793188421
DEGREES OF FREEDOM 0
T= 2.083472E+03
BP(GAS)=65.828605, BP(C1SI1_BETA)=34.789072, BP(O2SI1_L)=55.266805

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>>> DATA AT ITERATION 16 FROM STAGE 4
H=42605.34955, P=100000, N(C)=0.8676444641, N(N)=2E-4, N(O)=1.839681934,
N(SI)=1.78485431
DEGREES OF FREEDOM 0
T= 2.507706E+03
BP(GAS)=67.422078, BP(SI_L)=22.6366
=====
>>> DATA AT ITERATION 17 FROM STAGE 1
H=-999180.6617, P=100000, N(C)=3.158039639, N(N)=6.784E-4, N(O)=3.858499968,
N(SI)=1.500852128
DEGREES OF FREEDOM 0
T= 1.785826E+03
BP(GAS)=42.570551, BP(C1SI1_BETA)=12.913321, BP(CRISTOBALITE)=70.390442,
BP(C_S)=15.94975
>>> DATA AT ITERATION 17 FROM STAGE 2
H=-928656.1632, P=100000, N(C)=2.39392504, N(N)=5.18E-4, N(O)=4.037317203,
N(SI)=2.445398188
DEGREES OF FREEDOM 0
T= 2.027376E+03
BP(GAS)=59.074263, BP(C1SI1_BETA)=37.816728, BP(O2SI1_L)=65.141744
>>> DATA AT ITERATION 17 FROM STAGE 3
H=-784668.481, P=100000, N(C)=1.637270199, N(N)=3.6E-4, N(O)=3.640137416,
N(SI)=2.812536338
DEGREES OF FREEDOM 0
T= 2.083598E+03
BP(GAS)=66.144586, BP(C1SI1_BETA)=34.875519, BP(O2SI1_L)=55.878832
>>> DATA AT ITERATION 17 FROM STAGE 4
H=34757.51226, P=100000, N(C)=0.8698004514, N(N)=2E-4, N(O)=1.860054655,
N(SI)=1.799827779
DEGREES OF FREEDOM 0
T= 2.447965E+03
BP(GAS)=68.189742, BP(SI_L)=22.567411
=====
>>> DATA AT ITERATION 18 FROM STAGE 1
H=-998330.5256, P=100000, N(C)=3.119226814, N(N)=6.784E-4, N(O)=3.855155414,
N(SI)=1.536158792
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=42.754619, BP(C1SI1_BETA)=14.526163, BP(CRISTOBALITE)=70.093081,
BP(C_S)=14.922323
>>> DATA AT ITERATION 18 FROM STAGE 2
H=-928546.6446, P=100000, N(C)=2.349118499, N(N)=5.18E-4, N(O)=4.036282847,
N(SI)=2.488498889
DEGREES OF FREEDOM 0
T= 2.033605E+03
BP(GAS)=59.522044, BP(C1SI1_BETA)=37.858508, BP(O2SI1_L)=65.307946
>>> DATA AT ITERATION 18 FROM STAGE 3
H=-790949.9947, P=100000, N(C)=1.640036998, N(N)=3.6E-4, N(O)=3.661967998,
N(SI)=2.828189292
DEGREES OF FREEDOM 0
T= 2.083688E+03
BP(GAS)=66.403735, BP(C1SI1_BETA)=34.965077, BP(O2SI1_L)=56.352237
>>> DATA AT ITERATION 18 FROM STAGE 4
H=28693.24488, P=100000, N(C)=0.8720340547, N(N)=2E-4, N(O)=1.875813018,
N(SI)=1.809940564
DEGREES OF FREEDOM 0
T= 2.398231E+03
BP(GAS)=68.793576, BP(SI_L)=22.526539
=====
>>> DATA AT ITERATION 19 FROM STAGE 1
H=-997507.364, P=100000, N(C)=3.082739634, N(N)=6.784E-4, N(O)=3.851600756,
N(SI)=1.569002212
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=42.913712, BP(C1SI1_BETA)=16.026794, BP(CRISTOBALITE)=69.816123,
BP(C_S)=13.966846
>>> DATA AT ITERATION 19 FROM STAGE 2
H=-928272.7034, P=100000, N(C)=2.307755901, N(N)=5.18E-4, N(O)=4.034285186,
N(SI)=2.527482593
DEGREES OF FREEDOM 0
T= 2.038832E+03
BP(GAS)=59.919123, BP(C1SI1_BETA)=37.894909, BP(O2SI1_L)=65.440556
>>> DATA AT ITERATION 19 FROM STAGE 3
H=-795775.4787, P=100000, N(C)=1.642731724, N(N)=3.6E-4, N(O)=3.678988929,
N(SI)=2.8405587
DEGREES OF FREEDOM 0
T= 2.083751E+03
BP(GAS)=66.611155, BP(C1SI1_BETA)=35.046899, BP(O2SI1_L)=56.715074
>>> DATA AT ITERATION 19 FROM STAGE 4
H=24048.6439, P=100000, N(C)=0.8740746979, N(N)=2E-4, N(O)=1.887890878,
N(SI)=1.818020137
DEGREES OF FREEDOM 0
T= 2.358284E+03
BP(GAS)=69.261142, BP(SI_L)=22.503632
=====
>>> DATA AT ITERATION 20 FROM STAGE 1
H=-996726.5575, P=100000, N(C)=3.049123425, N(N)=6.784E-4, N(O)=3.847816589,
N(SI)=1.598785439
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.042147, BP(C1SI1_BETA)=17.38765, BP(CRISTOBALITE)=69.565063,
BP(C_S)=13.10077
>>> DATA AT ITERATION 20 FROM STAGE 2
H=-927908.7494, P=100000, N(C)=2.270418325, N(N)=5.18E-4, N(O)=4.031694211,
N(SI)=2.562010124
DEGREES OF FREEDOM 0
T= 2.043175E+03
BP(GAS)=60.262858, BP(C1SI1_BETA)=37.925514, BP(O2SI1_L)=65.546008
>>> DATA AT ITERATION 20 FROM STAGE 3
H=-799465.3621, P=100000, N(C)=1.645127528, N(N)=3.6E-4, N(O)=3.6921614,
N(SI)=2.850193241
DEGREES OF FREEDOM 0
T= 2.083795E+03
BP(GAS)=66.774913, BP(C1SI1_BETA)=35.116375, BP(O2SI1_L)=56.991949
>>> DATA AT ITERATION 20 FROM STAGE 4
H=20506.07963, P=100000, N(C)=0.8758074288, N(N)=2E-4, N(O)=1.897107301,
N(SI)=1.824361079
DEGREES OF FREEDOM 0
T= 2.326901E+03
BP(GAS)=69.620224, BP(SI_L)=22.490901
=====
>>> DATA AT ITERATION 21 FROM STAGE 1
H=-996006.4808, P=100000, N(C)=3.01882883, N(N)=6.784E-4, N(O)=3.84398989,
N(SI)=1.625226511
DEGREES OF FREEDOM 0
T= 1.785827E+03

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BP(GAS)=43.142842, BP(C1SI1_BETA)=18.595739, BP(CRISTOBALITE)=69.342397,
BP(C_S)=12.332158
>>> DATA AT ITERATION 21 FROM STAGE 2
H=-927507.9381, P=100000, N(C)=2.23734628, N(N)=5.18E-4, N(O)=4.02882958,
N(SI)=2.592088084
DEGREES OF FREEDOM 0
T= 2.046761E+03
BP(GAS)=60.555657, BP(C1SI1_BETA)=37.950681, BP(O2SI1_L)=65.629722
>>> DATA AT ITERATION 21 FROM STAGE 3
H=-802280.7014, P=100000, N(C)=1.647141377, N(N)=3.6E-4, N(O)=3.702321175,
N(SI)=2.85764962
DEGREES OF FREEDOM 0
T= 2.083827E+03
BP(GAS)=66.903688, BP(C1SI1_BETA)=35.172896, BP(O2SI1_L)=57.2028
>>> DATA AT ITERATION 21 FROM STAGE 4
H=17809.13326, P=100000, N(C)=0.8772170856, N(N)=2E-4, N(O)=1.904125951,
N(SI)=1.829280061
DEGREES OF FREEDOM 0
T= 2.302568E+03
BP(GAS)=69.894824, BP(SI_L)=22.483673
=====
>>> DATA AT ITERATION 22 FROM STAGE 1
H=-995357.8295, P=100000, N(C)=2.992030175, N(N)=6.784E-4, N(O)=3.840290978,
N(SI)=1.64831152
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.220495, BP(C1SI1_BETA)=19.650412, BP(CRISTOBALITE)=69.148216,
BP(C_S)=11.661298
>>> DATA AT ITERATION 22 FROM STAGE 2
H=-927105.1479, P=100000, N(C)=2.208490987, N(N)=5.18E-4, N(O)=4.025931494,
N(SI)=2.617966256
DEGREES OF FREEDOM 0
T= 2.049708E+03
BP(GAS)=60.802623, BP(C1SI1_BETA)=37.971114, BP(O2SI1_L)=65.696164
>>> DATA AT ITERATION 22 FROM STAGE 3
H=-804426.6999, P=100000, N(C)=1.648778713, N(N)=3.6E-4, N(O)=3.710147757,
N(SI)=2.863406141
DEGREES OF FREEDOM 0
T= 2.083850E+03
BP(GAS)=67.00497, BP(C1SI1_BETA)=35.217744, BP(O2SI1_L)=57.363226
>>> DATA AT ITERATION 22 FROM STAGE 4
H=15757.61961, P=100000, N(C)=0.8783355821, N(N)=2E-4, N(O)=1.909466093,
N(SI)=1.833068629
DEGREES OF FREEDOM 0
T= 2.283844E+03
BP(GAS)=70.1044348, BP(SI_L)=22.479422
=====
>>> DATA AT ITERATION 23 FROM STAGE 1
H=-994784.2916, P=100000, N(C)=2.968672003, N(N)=6.784E-4, N(O)=3.836843152,
N(SI)=1.668213894
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.280015, BP(C1SI1_BETA)=20.559619, BP(CRISTOBALITE)=68.980974,
BP(C_S)=11.083055
>>> DATA AT ITERATION 23 FROM STAGE 2
H=-926721.1849, P=100000, N(C)=2.183606756, N(N)=5.18E-4, N(O)=4.023154643,
N(SI)=2.640023859
DEGREES OF FREEDOM 0
T= 2.052127E+03
BP(GAS)=61.00957, BP(C1SI1_BETA)=37.987587, BP(O2SI1_L)=65.748921
>>> DATA AT ITERATION 23 FROM STAGE 3
H=-806061.8922, P=100000, N(C)=1.650084342, N(N)=3.6E-4, N(O)=3.716176003,
N(SI)=2.867846986
DEGREES OF FREEDOM 0
T= 2.083867E+03
BP(GAS)=67.084741, BP(C1SI1_BETA)=35.252803, BP(O2SI1_L)=57.485244
>>> DATA AT ITERATION 23 FROM STAGE 4
H=14197.51797, P=100000, N(C)=0.8792099779, N(N)=2E-4, N(O)=1.913527759,
N(SI)=1.835973858
DEGREES OF FREEDOM 0
T= 2.269500E+03
BP(GAS)=70.264027, BP(SI_L)=22.476822
=====
>>> DATA AT ITERATION 24 FROM STAGE 1
H=-994284.2894, P=100000, N(C)=2.948544358, N(N)=6.784E-4, N(O)=3.833714836,
N(SI)=1.685209092
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.325564, BP(C1SI1_BETA)=21.335979, BP(CRISTOBALITE)=68.838273,
BP(C_S)=10.589354
>>> DATA AT ITERATION 24 FROM STAGE 2
H=-926367.3416, P=100000, N(C)=2.162341333, N(N)=5.18E-4, N(O)=4.020587037,
N(SI)=2.658689475
DEGREES OF FREEDOM 0
T= 2.054109E+03
BP(GAS)=61.182135, BP(C1SI1_BETA)=38.000817, BP(O2SI1_L)=65.790851
>>> DATA AT ITERATION 24 FROM STAGE 3
H=-807307.862, P=100000, N(C)=1.651113825, N(N)=3.6E-4, N(O)=3.720821065,
N(SI)=2.871273073
DEGREES OF FREEDOM 0
T= 2.083880E+03
BP(GAS)=70.385646, BP(SI_L)=22.47517
=====
>>> DATA AT ITERATION 25 FROM STAGE 1
H=-993853.0717, P=100000, N(C)=2.931354723, N(N)=6.784E-4, N(O)=3.830932009,
N(SI)=1.69961397
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.360421, BP(C1SI1_BETA)=21.99399, BP(CRISTOBALITE)=68.717389,
BP(C_S)=10.170943
>>> DATA AT ITERATION 25 FROM STAGE 2
H=-926048.81, P=100000, N(C)=2.144299888, N(N)=5.18E-4, N(O)=4.018271202,
N(SI)=2.674393791
DEGREES OF FREEDOM 0
T= 2.055734E+03
BP(GAS)=61.325481, BP(C1SI1_BETA)=38.011423, BP(O2SI1_L)=65.824208
>>> DATA AT ITERATION 25 FROM STAGE 3
H=-808257.3892, P=100000, N(C)=1.651920278, N(N)=3.6E-4, N(O)=3.724402802,
N(SI)=2.873917453
DEGREES OF FREEDOM 0

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T= 2.083891E+03
BP(GAS)=67.197432, BP(C1SI1_BETA)=35.300889, BP(O2SI1_L)=57.648628
>>> DATA AT ITERATION 25 FROM STAGE 4
H=12108.9087, P=100000, N(C)=0.8804092457, N(N)=2E-4, N(O)=1.918966368,
N(SI)=1.83989243
DEGREES OF FREEDOM 0
T= 2.250176E+03
BP(GAS)=70.478235, BP(SI_L)=22.474083
=====
>>> DATA AT ITERATION 26 FROM STAGE 1
H=-993484.3106, P=100000, N(C)=2.916778756, N(N)=6.784E-4, N(O)=3.82849335,
N(SI)=1.711750609
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.387117, BP(C1SI1_BETA)=22.548385, BP(CRISTOBALITE)=68.615573,
BP(C_S)=9.8184381
>>> DATA AT ITERATION 26 FROM STAGE 2
H=-925766.9251, P=100000, N(C)=2.129084013, N(N)=5.18E-4, N(O)=4.016220304,
N(SI)=2.68754445
DEGREES OF FREEDOM 0
T= 2.057064E+03
BP(GAS)=61.444186, BP(C1SI1_BETA)=38.019917, BP(O2SI1_L)=65.850776
>>> DATA AT ITERATION 26 FROM STAGE 3
H=-808981.0832, P=100000, N(C)=1.652549579, N(N)=3.6E-4, N(O)=3.727166692,
N(SI)=2.875959646
DEGREES OF FREEDOM 0
T= 2.083989E+03
BP(GAS)=67.236831, BP(C1SI1_BETA)=35.316945, BP(O2SI1_L)=57.702306
>>> DATA AT ITERATION 26 FROM STAGE 4
H=11422.82717, P=100000, N(C)=0.8808096844, N(N)=2E-4, N(O)=1.920753173,
N(SI)=1.841186271
DEGREES OF FREEDOM 0
T= 2.243802E+03
BP(GAS)=70.548705, BP(SI_L)=22.473348
=====
>>> DATA AT ITERATION 27 FROM STAGE 1
H=-993171.1032, P=100000, N(C)=2.904490933, N(N)=6.784E-4, N(O)=3.826381052,
N(SI)=1.721926174
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.407586, BP(C1SI1_BETA)=23.013203, BP(CRISTOBALITE)=68.530222,
BP(C_S)=9.5228987
>>> DATA AT ITERATION 27 FROM STAGE 2
H=-925520.6929, P=100000, N(C)=2.116314075, N(N)=5.18E-4, N(O)=4.014428885,
N(SI)=2.698513221
DEGREES OF FREEDOM 0
T= 2.058154E+03
BP(GAS)=61.54221, BP(C1SI1_BETA)=38.026721, BP(O2SI1_L)=65.871965
>>> DATA AT ITERATION 27 FROM STAGE 3
H=-809532.8183, P=100000, N(C)=1.653039624, N(N)=3.6E-4, N(O)=3.729301458,
N(SI)=2.877538028
DEGREES OF FREEDOM 0
T= 2.083905E+03
BP(GAS)=67.268068, BP(C1SI1_BETA)=35.329239, BP(O2SI1_L)=57.743144
>>> DATA AT ITERATION 27 FROM STAGE 4
H=10900.92137, P=100000, N(C)=0.8811163038, N(N)=2E-4, N(O)=1.922112528,
N(SI)=1.842172568
DEGREES OF FREEDOM 0
T= 2.238945E+03
BP(GAS)=70.602347, BP(SI_L)=22.472838
=====
>>> DATA AT ITERATION 28 FROM STAGE 1
H=-992906.5612, P=100000, N(C)=2.894182072, N(N)=6.784E-4, N(O)=3.824567939,
N(SI)=1.730422343
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.423288, BP(C1SI1_BETA)=23.401316, BP(CRISTOBALITE)=68.458958,
BP(C_S)=9.2761351
>>> DATA AT ITERATION 28 FROM STAGE 2
H=-925307.8308, P=100000, N(C)=2.105641595, N(N)=5.18E-4, N(O)=4.012880936,
N(SI)=2.707631055
DEGREES OF FREEDOM 0
T= 2.059046E+03
BP(GAS)=61.622967, BP(C1SI1_BETA)=38.032171, BP(O2SI1_L)=65.888879
>>> DATA AT ITERATION 28 FROM STAGE 3
H=-809953.5935, P=100000, N(C)=1.65342085, N(N)=3.6E-4, N(O)=3.730951974,
N(SI)=2.878759038
DEGREES OF FREEDOM 0
T= 2.083910E+03
BP(GAS)=67.292881, BP(C1SI1_BETA)=35.338636, BP(O2SI1_L)=57.774212
>>> DATA AT ITERATION 28 FROM STAGE 4
H=10503.8989, P=100000, N(C)=0.8813506666, N(N)=2E-4, N(O)=1.923146703,
N(SI)=1.842924018
DEGREES OF FREEDOM 0
T= 2.235247E+03
BP(GAS)=70.643173, BP(SI_L)=22.472477
=====
>>> DATA AT ITERATION 29 FROM STAGE 1
H=-992684.1788, P=100000, N(C)=2.885569092, N(N)=6.784E-4, N(O)=3.823023314,
N(SI)=1.737491302
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.435345, BP(C1SI1_BETA)=23.724244, BP(CRISTOBALITE)=68.399659,
BP(C_S)=9.0708184
>>> DATA AT ITERATION 29 FROM STAGE 2
H=-925125.3489, P=100000, N(C)=2.096754056, N(N)=5.18E-4, N(O)=4.011555221,
N(SI)=2.715188257
DEGREES OF FREEDOM 0
T= 2.059777E+03
BP(GAS)=61.689365, BP(C1SI1_BETA)=38.03654, BP(O2SI1_L)=65.902398
>>> DATA AT ITERATION 29 FROM STAGE 3
H=-810274.5957, P=100000, N(C)=1.653717297, N(N)=3.6E-4, N(O)=3.732229339,
N(SI)=2.879704451
DEGREES OF FREEDOM 0
T= 2.083913E+03
BP(GAS)=67.312613, BP(C1SI1_BETA)=35.345812, BP(O2SI1_L)=57.797853
>>> DATA AT ITERATION 29 FROM STAGE 4
H=10201.80757, P=100000, N(C)=0.8815296235, N(N)=2E-4, N(O)=1.923933665,
N(SI)=1.843496456
DEGREES OF FREEDOM 0
T= 2.232430E+03
BP(GAS)=70.674249, BP(SI_L)=22.472217
=====
>>> DATA AT ITERATION 30 FROM STAGE 1
H=-992497.996, P=100000, N(C)=2.878398466, N(N)=6.784E-4, N(O)=3.82171563,
N(SI)=1.743354918

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DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.444613, BP(C1SI1_BETA)=23.99212, BP(CRISTOBALITE)=68.350461,
BP(C_S)=8.9005039
>>> DATA AT ITERATION 30 FROM STAGE 2
H=-924969.9915, P=100000, N(C)=2.089375883, N(N)=5.18E-4, N(O)=4.010427918,
N(SI)=2.721435928
DEGREES OF FREEDOM 0
T= 2.060375E+03
BP(GAS)=61.743862, BP(C1SI1_BETA)=38.040042, BP(O2SI1_L)=65.91321
>>> DATA AT ITERATION 30 FROM STAGE 3
H=-810519.5139, P=100000, N(C)=1.653947803, N(N)=3.6E-4, N(O)=3.733218791,
N(SI)=2.880437076
DEGREES OF FREEDOM 0
T= 2.083916E+03
BP(GAS)=67.328324, BP(C1SI1_BETA)=35.351286, BP(O2SI1_L)=57.815842
>>> DATA AT ITERATION 30 FROM STAGE 4
H=9971.960415, P=100000, N(C)=0.8816661409, N(N)=2E-4, N(O)=1.924532479,
N(SI)=1.84393238
DEGREES OF FREEDOM 0
T= 2.230286E+03
BP(GAS)=70.697901, BP(SI_L)=22.472028
=====
>>> DATA AT ITERATION 31 FROM STAGE 1
H=-992342.668, P=100000, N(C)=2.872446979, N(N)=6.784E-4, N(O)=3.820614418,
N(SI)=1.748205868
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.451747, BP(C1SI1_BETA)=24.213745, BP(CRISTOBALITE)=68.309748,
BP(C_S)=8.7595956
>>> DATA AT ITERATION 31 FROM STAGE 2
H=-924838.4834, P=100000, N(C)=2.083267294, N(N)=5.18E-4, N(O)=4.009475034,
N(SI)=2.726589423
DEGREES OF FREEDOM 0
T= 2.060864E+03
BP(GAS)=61.788518, BP(C1SI1_BETA)=38.042851, BP(O2SI1_L)=65.921865
>>> DATA AT ITERATION 31 FROM STAGE 3
H=-810706.4279, P=100000, N(C)=1.654127081, N(N)=3.6E-4, N(O)=3.73398594,
N(SI)=2.881005315
DEGREES OF FREEDOM 0
T= 2.083919E+03
BP(GAS)=67.340847, BP(C1SI1_BETA)=35.355459, BP(O2SI1_L)=57.829532
>>> DATA AT ITERATION 31 FROM STAGE 4
H=9797.067657, P=100000, N(C)=0.8817702251, N(N)=2E-4, N(O)=1.924988162,
N(SI)=1.844264306
DEGREES OF FREEDOM 0
T= 2.228654E+03
BP(GAS)=70.715903, BP(SI_L)=22.471889
=====
>>> DATA AT ITERATION 32 FROM STAGE 1
H=-992213.475, P=100000, N(C)=2.86752054, N(N)=6.784E-4, N(O)=3.819691136,
N(SI)=1.752209665
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.457241, BP(C1SI1_BETA)=24.396675, BP(CRISTOBALITE)=68.276134,
BP(C_S)=8.6432877
>>> DATA AT ITERATION 32 FROM STAGE 2
H=-924727.7131, P=100000, N(C)=2.078221938, N(N)=5.18E-4, N(O)=4.008673643,
N(SI)=2.730831868
DEGREES OF FREEDOM 0
T= 2.061265E+03
BP(GAS)=61.825058, BP(C1SI1_BETA)=38.045106, BP(O2SI1_L)=65.928798
>>> DATA AT ITERATION 32 FROM STAGE 3
H=-810849.1092, P=100000, N(C)=1.65426658, N(N)=3.6E-4, N(O)=3.734581289,
N(SI)=2.881446451
DEGREES OF FREEDOM 0
T= 2.083921E+03
BP(GAS)=67.350839, BP(C1SI1_BETA)=35.358639, BP(O2SI1_L)=57.83995
>>> DATA AT ITERATION 32 FROM STAGE 4
H=9663.982869, P=100000, N(C)=0.8818495484, N(N)=2E-4, N(O)=1.925334945,
N(SI)=1.844517021
DEGREES OF FREEDOM 0
T= 2.227411E+03
BP(GAS)=70.729605, BP(SI_L)=22.471786
=====
>>> DATA AT ITERATION 33 FROM STAGE 1
H=-992106.3108, P=100000, N(C)=2.863452262, N(N)=6.784E-4, N(O)=3.818920005,
N(SI)=1.755507396
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.461477, BP(C1SI1_BETA)=24.547355, BP(CRISTOBALITE)=68.248438,
BP(C_S)=8.547484
>>> DATA AT ITERATION 33 FROM STAGE 2
H=-924634.808, P=100000, N(C)=2.074063626, N(N)=5.18E-4, N(O)=4.008002576,
N(SI)=2.734318075
DEGREES OF FREEDOM 0
T= 2.061592E+03
BP(GAS)=61.854916, BP(C1SI1_BETA)=38.046916, BP(O2SI1_L)=65.934358
>>> DATA AT ITERATION 33 FROM STAGE 3
H=-810958.0678, P=100000, N(C)=1.654375201, N(N)=3.6E-4, N(O)=3.73504378,
N(SI)=2.881789255
DEGREES OF FREEDOM 0
T= 2.083922E+03
BP(GAS)=67.358817, BP(C1SI1_BETA)=35.361063, BP(O2SI1_L)=57.84788
>>> DATA AT ITERATION 33 FROM STAGE 4
H=9562.691135, P=100000, N(C)=0.8819099934, N(N)=2E-4, N(O)=1.925598909,
N(SI)=1.844709448
DEGREES OF FREEDOM 0
T= 2.226466E+03
BP(GAS)=70.740035, BP(SI_L)=22.471709
=====
>>> DATA AT ITERATION 34 FROM STAGE 1
H=-992017.6334, P=100000, N(C)=2.860099732, N(N)=6.784E-4, N(O)=3.818278077,
N(SI)=1.758218521
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.464743, BP(C1SI1_BETA)=24.671239, BP(CRISTOBALITE)=68.225659,
BP(C_S)=8.4687164
>>> DATA AT ITERATION 34 FROM STAGE 2
H=-924557.1796, P=100000, N(C)=2.070642959, N(N)=5.18E-4, N(O)=4.007442756,
N(SI)=2.73717822
DEGREES OF FREEDOM 0
T= 2.061859E+03
BP(GAS)=61.879292, BP(C1SI1_BETA)=38.04837, BP(O2SI1_L)=65.938813
>>> DATA AT ITERATION 34 FROM STAGE 3
H=-811041.2387, P=100000, N(C)=1.654459801, N(N)=3.6E-4, N(O)=3.735403256,

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N(SI)=2.882055783
DEGREES OF FREEDOM 0
T= 2.083924E+03
BP(GAS)=67.365194, BP(C1SI1_BETA)=35.362908, BP(O2SI1_L)=57.853911
>>> DATA AT ITERATION 34 FROM STAGE 4
H=9485.65643, P=100000, N(C)=0.8819560019, N(N)=2E-4, N(O)=1.925799679,
N(SI)=1.844855841
DEGREES OF FREEDOM 0
T= 2.225746E+03
BP(GAS)=70.747969, BP(SI_L)=22.471651
=====
>>> DATA AT ITERATION 35 FROM STAGE 1
H=-991944.4167, P=100000, N(C)=2.857342293, N(N)=6.784E-4, N(O)=3.817745422,
N(SI)=1.760443763
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.46727, BP(C1SI1_BETA)=24.772928, BP(CRISTOBALITE)=68.206955,
BP(C_S)=8.4040602
>>> DATA AT ITERATION 35 FROM STAGE 2
H=-924492.5133, P=100000, N(C)=2.067833775, N(N)=5.18E-4, N(O)=4.006977224,
N(SI)=2.739521408
DEGREES OF FREEDOM 0
T= 2.062077E+03
BP(GAS)=61.899164, BP(C1SI1_BETA)=38.049539, BP(O2SI1_L)=65.942392
>>> DATA AT ITERATION 35 FROM STAGE 3
H=-811104.7821, P=100000, N(C)=1.654525761, N(N)=3.6E-4, N(O)=3.735682999,
N(SI)=2.88226326
DEGREES OF FREEDOM 0
T= 2.083924E+03
BP(GAS)=67.370291, BP(C1SI1_BETA)=35.364313, BP(O2SI1_L)=57.858503
>>> DATA AT ITERATION 35 FROM STAGE 4
H=9427.014726, P=100000, N(C)=0.8819910534, N(N)=2E-4, N(O)=1.925952529,
N(SI)=1.844967318
DEGREES OF FREEDOM 0
T= 2.225198E+03
BP(GAS)=70.75401, BP(SI_L)=22.471608
=====
>>> DATA AT ITERATION 36 FROM STAGE 1
H=-991884.0753, P=100000, N(C)=2.855078011, N(N)=6.784E-4, N(O)=3.817304372,
N(SI)=1.762267391
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.469219, BP(C1SI1_BETA)=24.856268, BP(CRISTOBALITE)=68.19162,
BP(C_S)=8.3510693
>>> DATA AT ITERATION 36 FROM STAGE 2
H=-924438.813, P=100000, N(C)=2.065530416, N(N)=5.18E-4, N(O)=4.006591217,
N(SI)=2.741438457
DEGREES OF FREEDOM 0
T= 2.062255E+03
BP(GAS)=61.915353, BP(C1SI1_BETA)=38.050477, BP(O2SI1_L)=65.945263
>>> DATA AT ITERATION 36 FROM STAGE 3
H=-811153.313, P=100000, N(C)=1.654577215, N(N)=3.6E-4, N(O)=3.735900835,
N(SI)=2.882424867
DEGREES OF FREEDOM 0
T= 2.083925E+03
BP(GAS)=67.37437, BP(C1SI1_BETA)=35.365383, BP(O2SI1_L)=57.861996
>>> DATA AT ITERATION 36 FROM STAGE 4
H=9382.407402, P=100000, N(C)=0.8820177299, N(N)=2E-4, N(O)=1.92606881,
N(SI)=1.845052135
DEGREES OF FREEDOM 0
T= 2.224782E+03
BP(GAS)=70.758605, BP(SI_L)=22.471575
=====
>>> DATA AT ITERATION 37 FROM STAGE 1
H=-991834.4392, P=100000, N(C)=2.853221644, N(N)=6.784E-4, N(O)=3.816940168,
N(SI)=1.763759895
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.470728, BP(C1SI1_BETA)=24.92448, BP(CRISTOBALITE)=68.179065,
BP(C_S)=8.3076968
>>> DATA AT ITERATION 37 FROM STAGE 2
H=-924394.3263, P=100000, N(C)=2.063644393, N(N)=5.18E-4, N(O)=4.006271958,
N(SI)=2.743005034
DEGREES OF FREEDOM 0
T= 2.062401E+03
BP(GAS)=61.928527, BP(C1SI1_BETA)=38.051233, BP(O2SI1_L)=65.94757
>>> DATA AT ITERATION 37 FROM STAGE 3
H=-811190.4098, P=100000, N(C)=1.654617396, N(N)=3.6E-4, N(O)=3.73607066,
N(SI)=2.882550894
DEGREES OF FREEDOM 0
T= 2.083926E+03
BP(GAS)=67.377635, BP(C1SI1_BETA)=35.366198, BP(O2SI1_L)=57.864656
>>> DATA AT ITERATION 37 FROM STAGE 4
H=9348.452196, P=100000, N(C)=0.8820380469, N(N)=2E-4, N(O)=1.926157334,
N(SI)=1.845116714
DEGREES OF FREEDOM 0
T= 2.224464E+03
BP(GAS)=70.762104, BP(SI_L)=22.47155
=====
>>> DATA AT ITERATION 38 FROM STAGE 1
H=-991793.6711, P=100000, N(C)=2.851701749, N(N)=6.784E-4, N(O)=3.816639943,
N(SI)=1.764979854
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.471895, BP(C1SI1_BETA)=24.980239, BP(CRISTOBALITE)=68.168798,
BP(C_S)=8.2722419
>>> DATA AT ITERATION 38 FROM STAGE 2
H=-924357.5632, P=100000, N(C)=2.062102102, N(N)=5.18E-4, N(O)=4.006008515,
N(SI)=2.744283771
DEGREES OF FREEDOM 0
T= 2.062519E+03
BP(GAS)=61.939243, BP(C1SI1_BETA)=38.05184, BP(O2SI1_L)=65.949421
>>> DATA AT ITERATION 38 FROM STAGE 3
H=-811218.749, P=100000, N(C)=1.654648786, N(N)=3.6E-4, N(O)=3.736203116,
N(SI)=2.882649215
DEGREES OF FREEDOM 0
T= 2.083926E+03
BP(GAS)=67.38025, BP(C1SI1_BETA)=35.366817, BP(O2SI1_L)=57.866678
>>> DATA AT ITERATION 38 FROM STAGE 4
H=9322.629957, P=100000, N(C)=0.8820535025, N(N)=2E-4, N(O)=1.926224663,
N(SI)=1.845165834
DEGREES OF FREEDOM 0
T= 2.224223E+03
BP(GAS)=70.764765, BP(SI_L)=22.471532
=====
>>> DATA AT ITERATION 39 FROM STAGE 1

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H=-991760.2394, P=100000, N(C)=2.85045897, N(N)=6.784E-4, N(O)=3.816393014,
N(SI)=1.76597595
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.472801, BP(C1SI1_BETA)=25.025769, BP(CRISTOBALITE)=68.160411,
BP(C_S)=8.2432907
>>> DATA AT ITERATION 39 FROM STAGE 2
H=-924327.2395, P=100000, N(C)=2.060842307, N(N)=5.18E-4, N(O)=4.005791549,
N(SI)=2.745326542
DEGREES OF FREEDOM 0
T= 2.062616E+03
BP(GAS)=61.947949, BP(C1SI1_BETA)=38.052328, BP(O2SI1_L)=65.950911
>>> DATA AT ITERATION 39 FROM STAGE 3
H=-811240.419, P=100000, N(C)=1.654673335, N(N)=3.6E-4, N(O)=3.736306546,
N(SI)=2.882726013
DEGREES OF FREEDOM 0
T= 2.083927E+03
BP(GAS)=67.382346, BP(C1SI1_BETA)=35.367289, BP(O2SI1_L)=57.868218
>>> DATA AT ITERATION 39 FROM STAGE 4
H=9302.976885, P=100000, N(C)=0.8820652704, N(N)=2E-4, N(O)=1.926275913,
N(SI)=1.845203227
DEGREES OF FREEDOM 0
T= 2.224040E+03
BP(GAS)=70.766791, BP(SI_L)=22.471517
=====
>>> DATA AT ITERATION 40 FROM STAGE 1
H=-991732.8574, P=100000, N(C)=2.849443892, N(N)=6.784E-4, N(O)=3.816190178,
N(SI)=1.766788398
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.473501, BP(C1SI1_BETA)=25.062907, BP(CRISTOBALITE)=68.153568,
BP(C_S)=8.2196755
>>> DATA AT ITERATION 40 FROM STAGE 2
H=-924302.2787, P=100000, N(C)=2.05981439, N(N)=5.18E-4, N(O)=4.005613195,
N(SI)=2.74617608
DEGREES OF FREEDOM 0
T= 2.062694E+03
BP(GAS)=61.955019, BP(C1SI1_BETA)=38.052721, BP(O2SI1_L)=65.952107
>>> DATA AT ITERATION 40 FROM STAGE 3
H=-811256.9836, P=100000, N(C)=1.654692546, N(N)=3.6E-4, N(O)=3.736387359,
N(SI)=2.882786033
DEGREES OF FREEDOM 0
T= 2.083927E+03
BP(GAS)=67.384025, BP(C1SI1_BETA)=35.367648, BP(O2SI1_L)=57.869389
>>> DATA AT ITERATION 40 FROM STAGE 4
H=9288.029243, P=100000, N(C)=0.882074223, N(N)=2E-4, N(O)=1.926314898,
N(SI)=1.845231672
DEGREES OF FREEDOM 0
T= 2.223900E+03
BP(GAS)=70.768332, BP(SI_L)=22.471507
=====
>>> DATA AT ITERATION 41 FROM STAGE 1
H=-991710.4603, P=100000, N(C)=2.848615708, N(N)=6.784E-4, N(O)=3.816023867,
N(SI)=1.767450444
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.474046, BP(C1SI1_BETA)=25.093171, BP(CRISTOBALITE)=68.147989,
BP(C_S)=8.2004307
>>> DATA AT ITERATION 41 FROM STAGE 2
H=-924281.7645, P=100000, N(C)=2.05897647, N(N)=5.18E-4, N(O)=4.005466814,
N(SI)=2.746867618
DEGREES OF FREEDOM 0
T= 2.062758E+03
BP(GAS)=61.960758, BP(C1SI1_BETA)=38.053037, BP(O2SI1_L)=65.953068
>>> DATA AT ITERATION 41 FROM STAGE 3
H=-811269.6466, P=100000, N(C)=1.654707588, N(N)=3.6E-4, N(O)=3.736450544,
N(SI)=2.882832975
DEGREES OF FREEDOM 0
T= 2.083927E+03
BP(GAS)=67.385371, BP(C1SI1_BETA)=35.367921, BP(O2SI1_L)=57.87028
>>> DATA AT ITERATION 41 FROM STAGE 4
H=9276.662867, P=100000, N(C)=0.8820810323, N(N)=2E-4, N(O)=1.926344547,
N(SI)=1.845253306
DEGREES OF FREEDOM 0
T= 2.223794E+03
BP(GAS)=70.769504, BP(SI_L)=22.471498
=====
>>> DATA AT ITERATION 42 FROM STAGE 1
H=-991692.1603, P=100000, N(C)=2.847940643, N(N)=6.784E-4, N(O)=3.815887678,
N(SI)=1.767989464
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.474468, BP(C1SI1_BETA)=25.117813, BP(CRISTOBALITE)=68.143446,
BP(C_S)=8.184761
>>> DATA AT ITERATION 42 FROM STAGE 2
H=-924264.9307, P=100000, N(C)=2.058294034, N(N)=5.18E-4, N(O)=4.00534685,
N(SI)=2.747430101
DEGREES OF FREEDOM 0
T= 2.062810E+03
BP(GAS)=61.965412, BP(C1SI1_BETA)=38.053291, BP(O2SI1_L)=65.95384
>>> DATA AT ITERATION 42 FROM STAGE 3
H=-811279.3277, P=100000, N(C)=1.654719375, N(N)=3.6E-4, N(O)=3.736499982,
N(SI)=2.882869714
DEGREES OF FREEDOM 0
T= 2.083928E+03
BP(GAS)=67.38645, BP(C1SI1_BETA)=35.368129, BP(O2SI1_L)=57.870957
>>> DATA AT ITERATION 42 FROM STAGE 4
H=9268.021681, P=100000, N(C)=0.8820862103, N(N)=2E-4, N(O)=1.92636709,
N(SI)=1.845269755
DEGREES OF FREEDOM 0
T= 2.223713E+03
BP(GAS)=70.770395, BP(SI_L)=22.471492
=====
>>> DATA AT ITERATION 43 FROM STAGE 1
H=-991677.2235, P=100000, N(C)=2.847390873, N(N)=6.784E-4, N(O)=3.815776292,
N(SI)=1.768427968
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.474797, BP(C1SI1_BETA)=25.137861, BP(CRISTOBALITE)=68.139748,
BP(C_S)=8.1720125
>>> DATA AT ITERATION 43 FROM STAGE 2
H=-924251.1362, P=100000, N(C)=2.057738688, N(N)=5.18E-4, N(O)=4.005248664,
N(SI)=2.747887281
DEGREES OF FREEDOM 0
T= 2.062852E+03
BP(GAS)=61.969186, BP(C1SI1_BETA)=38.053496, BP(O2SI1_L)=65.954461

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>>> DATA AT ITERATION 43 FROM STAGE 3
H=-811286.7244, P=100000, N(C)=1.654728613, N(N)=3.6E-4, N(O)=3.736538678,
N(SI)=2.882898478
DEGREES OF FREEDOM 0
T= 2.083928E+03
BP(GAS)=67.387316, BP(C1SI1_BETA)=35.368286, BP(O2SI1_L)=57.871471
>>> DATA AT ITERATION 43 FROM STAGE 4
H=9261.459285, P=100000, N(C)=0.8820901433, N(N)=2E-4, N(O)=1.926384214,
N(SI)=1.84528225
DEGREES OF FREEDOM 0
T= 2.223652E+03
BP(GAS)=70.771072, BP(SI_L)=22.471487
=====
>>> DATA AT ITERATION 44 FROM STAGE 1
H=-991665.0436, P=100000, N(C)=2.846943512, N(N)=6.784E-4, N(O)=3.815685307,
N(SI)=1.768784445
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.475053, BP(C1SI1_BETA)=25.154159, BP(CRISTOBALITE)=68.136741,
BP(C_S)=8.1616482
>>> DATA AT ITERATION 44 FROM STAGE 2
H=-924239.8456, P=100000, N(C)=2.057287096, N(N)=5.18E-4, N(O)=4.005168397,
N(SI)=2.748258629
DEGREES OF FREEDOM 0
T= 2.062886E+03
BP(GAS)=61.972243, BP(C1SI1_BETA)=38.05366, BP(O2SI1_L)=65.95496
>>> DATA AT ITERATION 44 FROM STAGE 3
H=-811292.3803, P=100000, N(C)=1.654735863, N(N)=3.6E-4, N(O)=3.736568996,
N(SI)=2.882921021
DEGREES OF FREEDOM 0
T= 2.083928E+03
BP(GAS)=67.388011, BP(C1SI1_BETA)=35.368406, BP(O2SI1_L)=57.871862
>>> DATA AT ITERATION 44 FROM STAGE 4
H=9256.47258, P=100000, N(C)=0.8820931328, N(N)=2E-4, N(O)=1.926397228,
N(SI)=1.845291747
DEGREES OF FREEDOM 0
T= 2.223605E+03
BP(GAS)=70.771586, BP(SI_L)=22.471484
=====
>>> DATA AT ITERATION 45 FROM STAGE 1
H=-991655.1199, P=100000, N(C)=2.846579745, N(N)=6.784E-4, N(O)=3.815611044,
N(SI)=1.769074031
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.475251, BP(C1SI1_BETA)=25.1674, BP(CRISTOBALITE)=68.134298,
BP(C_S)=8.1532281
>>> DATA AT ITERATION 45 FROM STAGE 2
H=-924230.6165, P=100000, N(C)=2.056920145, N(N)=5.18E-4, N(O)=4.005102855,
N(SI)=2.748560063
DEGREES OF FREEDOM 0
T= 2.062914E+03
BP(GAS)=61.974719, BP(C1SI1_BETA)=38.053792, BP(O2SI1_L)=65.955362
>>> DATA AT ITERATION 45 FROM STAGE 3
H=-811296.7057, P=100000, N(C)=1.654741556, N(N)=3.6E-4, N(O)=3.73659277,
N(SI)=2.882938703
DEGREES OF FREEDOM 0
T= 2.083928E+03
BP(GAS)=67.388568, BP(C1SI1_BETA)=35.368497, BP(O2SI1_L)=57.872159
>>> DATA AT ITERATION 45 FROM STAGE 4
H=9252.684225, P=100000, N(C)=0.8820954043, N(N)=2E-4, N(O)=1.926407116,
N(SI)=1.845298962
DEGREES OF FREEDOM 0
T= 2.223570E+03
BP(GAS)=70.771977, BP(SI_L)=22.471481
=====
>>> DATA AT ITERATION 46 FROM STAGE 1
H=-991647.0416, P=100000, N(C)=2.846284169, N(N)=6.784E-4, N(O)=3.815550497,
N(SI)=1.769309127
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.475406, BP(C1SI1_BETA)=25.178149, BP(CRISTOBALITE)=68.132314,
BP(C_S)=8.146392
>>> DATA AT ITERATION 46 FROM STAGE 2
H=-924223.0806, P=100000, N(C)=2.056622167, N(N)=5.18E-4, N(O)=4.005049392,
N(SI)=2.748804602
DEGREES OF FREEDOM 0
T= 2.062937E+03
BP(GAS)=61.976723, BP(C1SI1_BETA)=38.053899, BP(O2SI1_L)=65.955685
>>> DATA AT ITERATION 46 FROM STAGE 3
H=-811300.0138, P=100000, N(C)=1.654746029, N(N)=3.6E-4, N(O)=3.736611425,
N(SI)=2.882952581
DEGREES OF FREEDOM 0
T= 2.083928E+03
BP(GAS)=67.389015, BP(C1SI1_BETA)=35.368567, BP(O2SI1_L)=57.872385
>>> DATA AT ITERATION 46 FROM STAGE 4
H=9249.807181, P=100000, N(C)=0.8820971299, N(N)=2E-4, N(O)=1.926414627,
N(SI)=1.845304444
DEGREES OF FREEDOM 0
T= 2.223543E+03
BP(GAS)=70.772274, BP(SI_L)=22.471479
=====
>>> DATA AT ITERATION 47 FROM STAGE 1
H=-991640.4706, P=100000, N(C)=2.846044161, N(N)=6.784E-4, N(O)=3.81550118,
N(SI)=1.769499874
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.475527, BP(C1SI1_BETA)=25.186871, BP(CRISTOBALITE)=68.130703,
BP(C_S)=8.1408452
>>> DATA AT ITERATION 47 FROM STAGE 2
H=-924216.9334, P=100000, N(C)=2.056380344, N(N)=5.18E-4, N(O)=4.005005824,
N(SI)=2.749002879
DEGREES OF FREEDOM 0
T= 2.062955E+03
BP(GAS)=61.978345, BP(C1SI1_BETA)=38.053985, BP(O2SI1_L)=65.955944
>>> DATA AT ITERATION 47 FROM STAGE 3
H=-811302.5476, P=100000, N(C)=1.654749548, N(N)=3.6E-4, N(O)=3.736626081,
N(SI)=2.882963487
DEGREES OF FREEDOM 0
T= 2.083928E+03
BP(GAS)=67.389374, BP(C1SI1_BETA)=35.368619, BP(O2SI1_L)=57.872557
>>> DATA AT ITERATION 47 FROM STAGE 4
H=9247.619408, P=100000, N(C)=0.8820984425, N(N)=2E-4, N(O)=1.92642034,
N(SI)=1.845308613
DEGREES OF FREEDOM 0
T= 2.223522E+03
BP(GAS)=70.7725, BP(SI_L)=22.471478

```

```

=====
>>> DATA AT ITERATION 48 FROM STAGE 1
H=-991635.1295, P=100000, N(C)=2.845849388, N(N)=6.784E-4, N(O)=3.815461034,
N(SI)=1.769654547
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.47562, BP(C1SI1_BETA)=25.193944, BP(CRISTOBALITE)=68.129397,
BP(C_S)=8.1363472
>>> DATA AT ITERATION 48 FROM STAGE 2
H=-924211.9246, P=100000, N(C)=2.056184213, N(N)=5.18E-4, N(O)=4.004970353,
N(SI)=2.74916356
DEGREES OF FREEDOM 0
T= 2.062970E+03
BP(GAS)=61.97965, BP(C1SI1_BETA)=38.054054, BP(O2SI1_L)=65.956153
>>> DATA AT ITERATION 48 FROM STAGE 3
H=-811304.4822, P=100000, N(C)=1.654752315, N(N)=3.6E-4, N(O)=3.736637589,
N(SI)=2.882972053
DEGREES OF FREEDOM 0
T= 2.083928E+03
BP(GAS)=67.389662, BP(C1SI1_BETA)=35.368659, BP(O2SI1_L)=57.872687
>>> DATA AT ITERATION 48 FROM STAGE 4
H=9245.962626, P=100000, N(C)=0.8820994364, N(N)=2E-4, N(O)=1.926424668,
N(SI)=1.84531177
DEGREES OF FREEDOM 0
T= 2.223507E+03
BP(GAS)=70.772671, BP(SI_L)=22.471476
=====
>>> DATA AT ITERATION 49 FROM STAGE 1
H=-991630.7915, P=100000, N(C)=2.845691425, N(N)=6.784E-4, N(O)=3.815428401,
N(SI)=1.769779915
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.475694, BP(C1SI1_BETA)=25.199677, BP(CRISTOBALITE)=68.128338,
BP(C_S)=8.1327012
>>> DATA AT ITERATION 49 FROM STAGE 2
H=-924207.8451, P=100000, N(C)=2.056025209, N(N)=5.18E-4, N(O)=4.004941492,
N(SI)=2.749293722
DEGREES OF FREEDOM 0
T= 2.062982E+03
BP(GAS)=61.980718, BP(C1SI1_BETA)=38.054109, BP(O2SI1_L)=65.956321
>>> DATA AT ITERATION 49 FROM STAGE 3
H=-811305.9618, P=100000, N(C)=1.654754494, N(N)=3.6E-4, N(O)=3.736646635,
N(SI)=2.882978789
DEGREES OF FREEDOM 0
T= 2.083928E+03
BP(GAS)=67.389893, BP(C1SI1_BETA)=35.368689, BP(O2SI1_L)=57.872785
>>> DATA AT ITERATION 49 FROM STAGE 4
H=9244.706005, P=100000, N(C)=0.8821001905, N(N)=2E-4, N(O)=1.926427951,
N(SI)=1.845314166
DEGREES OF FREEDOM 0
T= 2.223495E+03
BP(GAS)=70.772801, BP(SI_L)=22.471475
=====
>>> DATA AT ITERATION 50 FROM STAGE 1
H=-991627.2695, P=100000, N(C)=2.845563367, N(N)=6.784E-4, N(O)=3.815401874,
N(SI)=1.769881476
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.475751, BP(C1SI1_BETA)=25.204322, BP(CRISTOBALITE)=68.127479,
BP(C_S)=8.1297474
>>> DATA AT ITERATION 50 FROM STAGE 2
H=-924204.5258, P=100000, N(C)=2.055896374, N(N)=5.18E-4, N(O)=4.004918028,
N(SI)=2.74939911
DEGREES OF FREEDOM 0
T= 2.062992E+03
BP(GAS)=61.981575, BP(C1SI1_BETA)=38.054154, BP(O2SI1_L)=65.956456
>>> DATA AT ITERATION 50 FROM STAGE 3
H=-811307.0965, P=100000, N(C)=1.654756211, N(N)=3.6E-4, N(O)=3.736653759,
N(SI)=2.882984094
DEGREES OF FREEDOM 0
T= 2.083928E+03
BP(GAS)=67.390079, BP(C1SI1_BETA)=35.368712, BP(O2SI1_L)=57.87286
>>> DATA AT ITERATION 50 FROM STAGE 4
H=9243.750271, P=100000, N(C)=0.8821007644, N(N)=2E-4, N(O)=1.926430448,
N(SI)=1.845315989
DEGREES OF FREEDOM 0
T= 2.223486E+03
BP(GAS)=70.772899, BP(SI_L)=22.471475
=====
REACTOR: @@ Use POLY-3 to list the constitution in each segment
REACTOR: GO P-3
POLY: L-E
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS: VWCS
Output from POLY-3, equilibrium = 1004, label A0 , database: SSUB6

Conditions:
H=9243.750271, P=100000, N(C)=0.8821007644, N(N)=2E-4, N(O)=1.926430448,
N(SI)=1.845315989
DEGREES OF FREEDOM 0

Temperature 2223.49 K ( 1950.34 C), Pressure 1.000000E+05
Number of moles of components 4.65405E+00, Mass in grams 9.32444E+01
Total Gibbs energy -1.35902E+06, Enthalpy 9.24375E+03, Volume 3.56321E-01

Component Moles W-Fraction Activity Potential Ref.stat
C 8.8210E-01 1.1363E-01 5.0908E-03 -9.7618E+04 SER
N 2.0000E-04 3.0044E-05 8.4815E-09 -3.4359E+05 SER
O 1.9264E+00 3.3054E-01 1.4658E-13 -5.4632E+05 SER
SI 1.8453E+00 5.5581E-01 1.5639E-03 -1.1944E+05 SER

GAS Status ENTERED Driving force 0.0000E+00
Moles 3.8539E+00, Mass 7.0773E+01, Volume fraction 1.0000E+00 Mass fractions:
O 4.35491E-01 SI 4.14766E-01 C 1.49703E-01 N 3.95829E-05
Constitution:
O1SI1 5.41812E-01 C1O2 2.03423E-05 C 2.35264E-10 O2 9.78900E-14
C1O1 4.57645E-01 O2SI1 1.70445E-06 N1O1 7.37248E-11
SI 4.69580E-04 C1SI1 3.44146E-09 C3 4.10890E-12
N2 5.18835E-05 O 9.79789E-10 C2 3.46788E-12

SI_L Status ENTERED Driving force 0.0000E+00
Moles 8.0012E-01, Mass 2.2471E+01, Volume fraction 0.0000E+00 Mass fractions:
O 1.0000E+00 C 0.0000E+00 O 0.0000E+00 N 0.0000E+00
POLY: @@ This equilibrium is valid for the fourth segment. Note it is

```

POLY: @@ identified with number 1004. The other have numbers 1001,
POLY: @@ 1002 and 1003.
POLY:
POLY: go sys
SYS: set-inter
SYS:

tce26

SYS:About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

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Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce26\tce26.TCM.test"

SYS: set-echo

SYS:

SYS: @@ The As-Ga phase diagram: Plotting the partial pressures

SYS: @@ of a gas species

SYS:

SYS: @@ This is an example of plotting the partial pressures

SYS: @@ of a gas species along the solubility lines in the As-Ga

SYS: @@ phase diagram. The calculation makes it possible to monitor

SYS: @@ the input gases to a process of depositing solid As-Ga.

SYS:

SYS: set-log ex26,,,

SYS: go da

... the command in full is GOTO_MODULE

THERMODYNAMIC DATABASE module

Database folder: C:\jenkins\workspace\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

TDB_TCFE11: @@ The data is taken from the pg35 database

TDB_TCFE11:

TDB_TCFE11: sw

... the command in full is SWITCH_DATABASE

Use one of these databases

TCFE11 = Steels/Fe-Alloys v11.0

TCFE9 = Steels/Fe-Alloys v9.3

SSOL7 = SGTE Alloy Solutions v7.0

SSOL6 = SGTE Alloy Solutions v6.0

SSUB6 = SGTE Substances v6.0

TCOX11 = Metal Oxide Solutions v11.1

FEDEMO = Iron Demo Database v4.0

ALDEMO = Aluminum Demo Database v4.1

OXDEMO = Oxide Demo Database v4.0

SUBDEMO = Substance Demo Database v1.0

PAQ2 = Public Aqueous Solution (SIT) v2.5

PG35 = PG35 Binary Semi-Conductors v1.3

MALDEMO = Al-Alloys Mobility demo database v2.0.1

USER = User defined Database

DATABASE NAME /TCFE11/: pg35

Current database: PG35 Binary Semi-Conductors v1.3

VA DEFINED

AL1G AL2G ALASG

ALPG ALP2G ALSBG

REJECTED

AS1G ASGAG ASING

AS2G AS3G AS4G

REJECTED

GA1G GA2G GAPG

GA1SBG GA1SB2G REJECTED

IN1G IN2G INPG

INSBG INSB2G REJECTED

P1G P2G P4G

SB1G SB2G SB3G

SB4G REJECTED

TDB_PG35: d-sys as ga

... the command in full is DEFINE_SYSTEM

AS GA DEFINED

TDB_PG35: @@ Reject all but the stable phases in this system

TDB_PG35: rej ph /all

... the command in full is REJECT

GAS:G LIQUID FCC_A1

HCP_A3 FCC_B3 BCT_A5

BCT_A6 P_RED ASP

RHOMBO_A7 ORTHO GA_GAMMA

REJECTED

TDB_PG35: rest ph liq rhom ortho fcc_b3 gas:g

... the command in full is RESTORE

LIQUID RHOMBO_A7 ORTHO

FCC_B3 GAS:G RESTORED

TDB_PG35: l-sys

... the command in full is LIST_SYSTEM

ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/: CONSTITUENTS

GAS:G :AS1 AS2 AS3 AS4 AS1GA1 GA1 GA2:

> Gaseous mixture phase: using the Ideal EOS & Mixing Model

LIQUID :AS GA:

> Liquid mixture phase: Metallic species Al-As-Ga-In-P-Sb

FCC_B3 :GA:AS:

> FCC_B3 solution phase: for the complete Al-As-Ga-In-P-Sb system

RHOMBO_A7 :AS:

> RHOMBO_A7 solution phase: for the As-Sb binary join only

ORTHO :GA:

TDB_PG35: Hit RETURN to continue

TDB_PG35: get

... the command in full is GET_DATA

16:04:01,451 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

REINITIATING GES

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

FUNCTIONS

List of references for assessed data

'PG35 - ISC Group III-V Binary Semiconductors Database (V1.2), developed by Informal scientific Collaboration Group (Ansara I., Chatillon C., Lukas H.L., Nishizawa T., Ohtani H., Ishida K., Hillert M., Sundman B., Argent B.B., Watson A., Chart T. G., and Anderson T.), 1994, as published data [A Binary Database for III-V Compound Semiconductor Systems, Calphad, 18, 177-222] and provided by Thermo-Calc Software (May 2003/June 2008). '

-OK-

TDB_PG35: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32

POLY: @@ Set conditions at the As rich side of the system. We want

POLY: @@ to calculate the metastable system without gas phase but
POLY: @@ then plot the gas constitution. Set gas to be dormant.

POLY:

POLY: s-c t=1200 p=1e5 n=1 x(ga)=.3

... the command in full is SET_CONDITION

POLY: c-s p gas=dorm

... the command in full is CHANGE_STATUS

POLY: c-e

... the command in full is COMPUTE_EQUILIBRIUM

Using global minimization procedure

Calculated 212 grid points in 1 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 1 s

POLY: l-e

... the command in full is LIST_EQUILIBRIUM

OUTPUT TO SCREEN OR FILE /SCREEN/:

Options /VWCS/: x

Output from POLY-3, equilibrium = 1, label A0 , database: PG35

Conditions:

T=1200, P=100000, N=1, X(GA)=0.3

Degrees of Freedom 0

Temperature 1200.00 K (926.85 C), Pressure 1.000000E+05

Number of moles of components 1.000000E+00, Mass in grams 7.33623E+01

Total Gibbs energy -8.75968E+04, Enthalpy 1.20850E+04, Volume 0.000000E+00

| Component | Moles | M-Fraction | Activity | Potential | Ref.stat |
|-----------|------------|------------|------------|-------------|----------|
| AS | 7.0000E-01 | 7.0000E-01 | 1.2211E-03 | -6.6929E+04 | SER |
| GA | 3.0000E-01 | 3.0000E-01 | 1.2244E-06 | -1.3582E+05 | SER |

| GAS | Status | DORMANT | Driving force | 8.1507E-01 |
|---|--------|---------|---------------|-----------------|
| Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 | | | | Mole fractions: |
| AS 1.000000E+00 GA 9.09718E-11 | | | | |

Constitution:

| AS4 | 9.80210E-01 | AS3 | 2.00768E-03 | GA1 | 3.55191E-10 | GA2 | 1.87160E-17 |
|-----|-------------|-----|-------------|--------|-------------|-----|-------------|
| AS2 | 1.77817E-02 | AS1 | 2.30505E-07 | AS1GA1 | 5.27773E-12 | | |

| Liquid | Status | ENTERED | Driving force | 0.0000E+00 |
|---|--------|---------|---------------|-----------------|
| Moles 5.0575E-01, Mass 3.7617E+01, Volume fraction 0.0000E+00 | | | | Mole fractions: |
| AS 8.95449E-01 GA 1.04551E-01 | | | | |

| FCC_B3 | Status | ENTERED | Driving force | 0.0000E+00 |
|---|--------|---------|---------------|-----------------|
| Moles 4.9425E-01, Mass 3.5745E+01, Volume fraction 0.0000E+00 | | | | Mole fractions: |
| AS 5.00000E-01 GA 5.00000E-01 | | | | |

POLY: Hit RETURN to continue

POLY: @@ Note that the gas would like to be stable (driving force
@@ positive) but it is not allowed to form as it is dormant.

POLY:

POLY: l-st ph

... the command in full is LIST_STATUS

*** STATUS FOR ALL PHASES

| Phase | Status | Driving Force | Moles |
|-----------|---------|---------------|--------------|
| LIQUID | ENTERED | 0.000000E+00 | 5.057539E-01 |
| FCC_B3 | ENTERED | 0.000000E+00 | 4.942461E-01 |
| RHOMBO_A7 | ENTERED | -4.059045E-01 | 0.000000E+00 |
| ORTHO | ENTERED | -6.644230E+00 | 0.000000E+00 |
| GAS | DORMANT | 8.150658E-01 | |

POLY: @@ The phase diagram is calculated with the composition and

POLY: @@ temperature on the axis as usual

POLY: s-a-v 1 x(ga)

... the command in full is SET_AXIS_VARIABLE

Min value /0/: 0

Max value /1/: 1

Increment /0.025/: .025

POLY: s-a-v 2 t

... the command in full is SET_AXIS_VARIABLE

Min value /0/: 300

Max value /1/: 2000

Increment /42.5/: 25

POLY: @@ For an explanation of these symbols see below

POLY: ent fun pas1=0.4343*lnacr(as1,gas);

... the command in full is ENTER_SYMBOL

POLY: ent fun pas2=0.4343*lnacr(as2,gas);

... the command in full is ENTER_SYMBOL

POLY: ent fun pas3=0.4343*lnacr(as3,gas);

... the command in full is ENTER_SYMBOL

POLY: ent fun pas4=0.4343*lnacr(as4,gas);

... the command in full is ENTER_SYMBOL

POLY: ent fun pasga=0.4343*lnacr(as1ga1,gas);

... the command in full is ENTER_SYMBOL

POLY: ent fun pg1=0.4343*lnacr(ga1,gas);

... the command in full is ENTER_SYMBOL

POLY: ent tab pp

... the command in full is ENTER_SYMBOL

Variable(s): pas1 pas2 pas3 pas4 pasga pg1;

POLY:

POLY: l-sym

... the command in full is LIST_SYMBOLS

DEFINED FUNCTIONS AND VARIABLES%

PAS1=.4343*LNACR(AS1,GAS)

PAS2=.4343*LNACR(AS2,GAS)

PAS3=.4343*LNACR(AS3,GAS)

PAS4=.4343*LNACR(AS4,GAS)

PASGA=.4343*LNACR(AS1GA1,GAS)

PGA1=.4343*LNACR(GA1,GAS)

DEFINED TABLES

PP=PAS1, PAS2, PAS3, PAS4, PASGA, PGA1

POLY: Hit RETURN to continue

```

POLY: ent fun dd=0.4343*dgf(gas);
... the command in full is ENTER_SYMBOL
POLY: ent fun qas1=log10(y(gas,as1))+dd;
... the command in full is ENTER_SYMBOL
POLY: ent fun qas2=log10(y(gas,as2))+dd;
... the command in full is ENTER_SYMBOL
POLY: ent fun qas3=log10(y(gas,as3))+dd;
... the command in full is ENTER_SYMBOL
POLY: ent fun qas4=log10(y(gas,as4))+dd;
... the command in full is ENTER_SYMBOL
POLY: ent fun qasga=log10(y(gas,as1ga))+dd;
... the command in full is ENTER_SYMBOL
POLY: ent fun qga1=log10(y(gas,ga1))+dd;
... the command in full is ENTER_SYMBOL
POLY: ent tab qq
... the command in full is ENTER_SYMBOL
Variable(s): qas1 qas2 qas3 qas4 qasga qga1;
POLY:
POLY: ent fun it=1000/T;
... the command in full is ENTER_SYMBOL
POLY: save tceix26 y
... the command in full is SAVE_WORKSPACES
POLY: l-sym
... the command in full is LIST_SYMBOLS
DEFINED FUNCTIONS AND VARIABLES%
PAS1=.4343*LNACR(AS1,GAS)
PAS2=.4343*LNACR(AS2,GAS)
PAS3=.4343*LNACR(AS3,GAS)
PAS4=.4343*LNACR(AS4,GAS)
PASGA=.4343*LNACR(AS1GA1,GAS)
PGA1=.4343*LNACR(GA1,GAS)
DD=.4343*DGF(GAS)
QAS1= LOG10(Y(GAS,AS1) )+DD
QAS2= LOG10(Y(GAS,AS2) )+DD
QAS3= LOG10(Y(GAS,AS3) )+DD
QAS4= LOG10(Y(GAS,AS4) )+DD
QASGA= LOG10(Y(GAS,AS1GA1) )+DD
QGA1= LOG10(Y(GAS,GA1) )+DD
IT=1000/T
DEFINED TABLES
PP=PAS1, PAS2, PAS3, PAS4, PASGA, PGA1
QQ=QAS1, QAS2, QAS3, QAS4, QASGA, QGA1
POLY: Hit RETURN to continue
POLY: @@ Map follows all lines in the phase diagram
POLY: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Generating start point 27
Generating start point 28

Phase region boundary 1 at: 2.500E-01 3.100E+02
** FCC_B3
   RHOMBO_A7
Calculated..          2 equilibria
Terminating at axis limit.

Phase region boundary 2 at: 2.500E-01 3.000E+02
** FCC_B3
   RHOMBO_A7
Calculated..          32 equilibria

Phase region boundary 3 at: 2.500E-01 1.067E+03
** FCC_B3
** LIQUID
   RHOMBO_A7
Calculated..          10 equilibria
Phase region boundary 4 at: 2.345E-02 1.067E+03
** LIQUID
   RHOMBO_A7
Calculated..          10 equilibria

```

```

Phase region boundary  5 at:  2.734E-01  1.067E+03
  ** FCC_B3
  ** LIQUID
Calculated.          101 equilibria

Phase region boundary  6 at:  7.500E-01  3.029E+02
  ** FCC_B3
  ** LIQUID
  ** ORTHO
Calculated..         2 equilibria
Terminating at axis limit.

Phase region boundary  7 at:  7.500E-01  3.029E+02
  ** FCC_B3
  ** ORTHO
Calculated..         2 equilibria
Terminating at axis limit.

Phase region boundary  8 at:  1.000E+00  3.029E+02
  ** LIQUID
  ** ORTHO
Calculated.          12 equilibria

Phase region boundary  9 at:  2.500E-01  3.100E+02
  ** FCC_B3
  ** RHOMBO_A7
Calculated..         32 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 10 at:  2.500E-01  3.100E+02
  ** FCC_B3
  ** RHOMBO_A7
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 11 at:  2.500E-01  3.100E+02
  ** FCC_B3
  ** RHOMBO_A7
Calculated..         32 equilibria
Terminating at known equilibrium

Phase region boundary 12 at:  2.500E-01  3.100E+02
  ** FCC_B3
  ** RHOMBO_A7
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 13 at:  2.500E-01  3.100E+02
  ** FCC_B3
  ** RHOMBO_A7
Calculated..         32 equilibria
Terminating at known equilibrium

Phase region boundary 14 at:  7.500E-01  3.100E+02
  ** FCC_B3
  ** LIQUID
Calculated..         2 equilibria
Terminating at known equilibrium

Phase region boundary 15 at:  7.500E-01  3.100E+02
  ** FCC_B3
  ** LIQUID
Calculated..         100 equilibria
Terminating at known equilibrium

Phase region boundary 16 at:  7.500E-01  3.100E+02
  ** FCC_B3
  ** LIQUID
Calculated..         2 equilibria
Terminating at known equilibrium

Phase region boundary 17 at:  7.500E-01  3.100E+02
  ** FCC_B3
  ** LIQUID
Calculated..         100 equilibria
Terminating at known equilibrium

Phase region boundary 18 at:  7.500E-01  3.100E+02
  ** FCC_B3
  ** LIQUID
Calculated..         2 equilibria
Terminating at known equilibrium

Phase region boundary 19 at:  7.500E-01  3.100E+02
  ** FCC_B3
  ** LIQUID
Calculated..         100 equilibria
Terminating at known equilibrium

Phase region boundary 20 at:  2.500E-01  8.700E+02
  ** FCC_B3
  ** RHOMBO_A7
Calculated..         24 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 21 at:  2.500E-01  8.700E+02
  ** FCC_B3
  ** RHOMBO_A7
Calculated..         9 equilibria
Terminating at known equilibrium

Phase region boundary 22 at:  7.492E-01  8.700E+02
  ** FCC_B3
  ** LIQUID
Calculated..         24 equilibria
Terminating at known equilibrium

Phase region boundary 23 at:  7.492E-01  8.700E+02
  ** FCC_B3
  ** LIQUID
Calculated..         81 equilibria
Terminating at known equilibrium

Phase region boundary 24 at:  3.939E-01  1.430E+03
  ** FCC_B3

```

```

LIQUID
Calculated.          18 equilibria
Terminating at known equilibrium

Phase region boundary 25 at: 3.939E-01 1.430E+03
** FCC_B3
LIQUID
Calculated.          87 equilibria
Terminating at known equilibrium

Phase region boundary 26 at: 6.143E-01 1.430E+03
** FCC_B3
LIQUID
Calculated.          50 equilibria
Terminating at known equilibrium

Phase region boundary 27 at: 6.143E-01 1.430E+03
** FCC_B3
LIQUID
Calculated.          55 equilibria
Terminating at known equilibrium

Phase region boundary 28 at: 5.000E-03 1.086E+03
LIQUID
** RHOMBO_A7
Calculated.          15 equilibria
Terminating at known equilibrium

Phase region boundary 29 at: 5.000E-03 1.086E+03
LIQUID
** RHOMBO_A7
Calculated.          3 equilibria
Terminating at known equilibrium

Phase region boundary 30 at: 4.183E-01 1.463E+03
** FCC_B3
LIQUID
Calculated.          21 equilibria
Terminating at known equilibrium

Phase region boundary 31 at: 4.183E-01 1.463E+03
** FCC_B3
LIQUID
Calculated.          67 equilibria
Terminating at known equilibrium

Phase region boundary 32 at: 5.817E-01 1.468E+03
** FCC_B3
LIQUID
Calculated.          34 equilibria
Terminating at known equilibrium

Phase region boundary 33 at: 5.817E-01 1.468E+03
** FCC_B3
LIQUID
Calculated.          54 equilibria
Terminating at known equilibrium

Phase region boundary 34 at: 7.450E-01 9.995E+02
** FCC_B3
LIQUID
Calculated.          74 equilibria
Terminating at known equilibrium

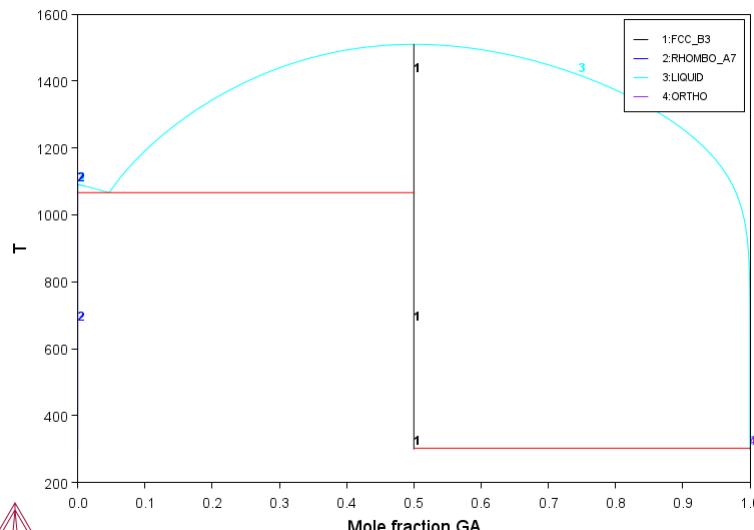
Phase region boundary 35 at: 7.450E-01 9.995E+02
** FCC_B3
LIQUID
Calculated.          29 equilibria
Terminating at known equilibrium
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\generate_console_examples\examples\tcex26\tcex26.POLY3
CPU time for mapping      5 seconds
POLY: @@ Now we plot this in the post processor
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: s-d-a x m-f ga
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t
... the command in full is SET_DIAGRAM_AXIS
POST: s-l d
... the command in full is SET_LABEL_CURVE_OPTION
POST:
POST: set-title example 26a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 26a

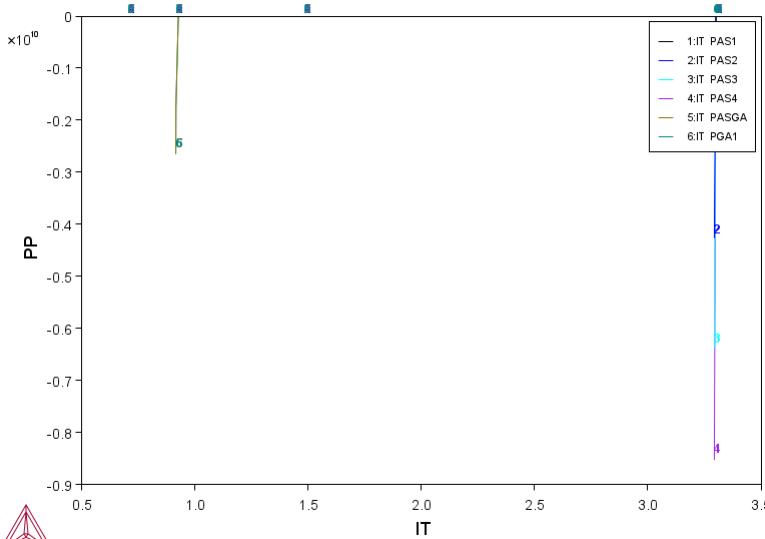


```

POST:
POST:Hit RETURN to continue
POST: @@ This is the traditional phase diagram.
POST:
POST: @@ Now those who work with this system is interesting to
POST: @@ know the partial pressures of the different gas species
POST: @@ along the solubility lines. As Thermo-Calc saves the
POST: @@ complete description of all tie-lines calculated in a
POST: @@ MAP or STEP command, even for dormant phases, we can
POST: @@ now plot these.
POST:
POST: @@ The partial pressures of a species in the gas is equal
POST: @@ to the fraction of that species if the gas is stable
POST: @@ (Dalton's law). If the gas is not stable then add the
POST: @@ driving force per formula unit of the gas (the formula
POST: @@ unit depends on the species).
POST:
POST: @@ We can directly get the activity of a gas species using
POST: @@ the state variable acr(species,gas) which has as
POST: @@ reference state a pure gas of the species itself. The
POST: @@ state variable lnacr(species,gas) is the natural logarithm
POST: @@ of this quantity. To make it into log10, multiply by 0.4343
POST:
POST: s-d-a y pp
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*:
POST: @@ Plot against the inverse of temperature
POST: s-d-a x it
... the command in full is SET_DIAGRAM_AXIS
POST: l-sy
... the command in full is LIST_SYMBOLS
DEFINED CONSTANTS
ZERO=0
DEFINED FUNCTIONS AND VARIABLES%
PAS1=.4343*LNACR(AS1,GAS)
PAS2=.4343*LNACR(AS2,GAS)
PAS3=.4343*LNACR(AS3,GAS)
PAS4=.4343*LNACR(AS4,GAS)
PASGA=.4343*LNACR(AS1GA1,GAS)
PGA1=.4343*LNACR(GA1,GAS)
DD=.4343*DGF(GAS)
QAS1= LOG10(Y(GAS,AS1) )+DD
QAS2= LOG10(Y(GAS,AS2) )+DD
QAS3= LOG10(Y(GAS,AS3) )+DD
QAS4= LOG10(Y(GAS,AS4) )+DD
QASGA= LOG10(Y(GAS,AS1GA1) )+DD
QGA1= LOG10(Y(GAS,GA1) )+DD
IT=1000/T
TEMP_C=T-273.15
DEFINED TABLES
PP=PAS1, PAS2, PAS3, PAS4, PASGA, PGA1
QQ=QAS1, QAS2, QAS3, QAS4, QASGA, QGA1
POST: set-title example 26b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFILE
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 26b

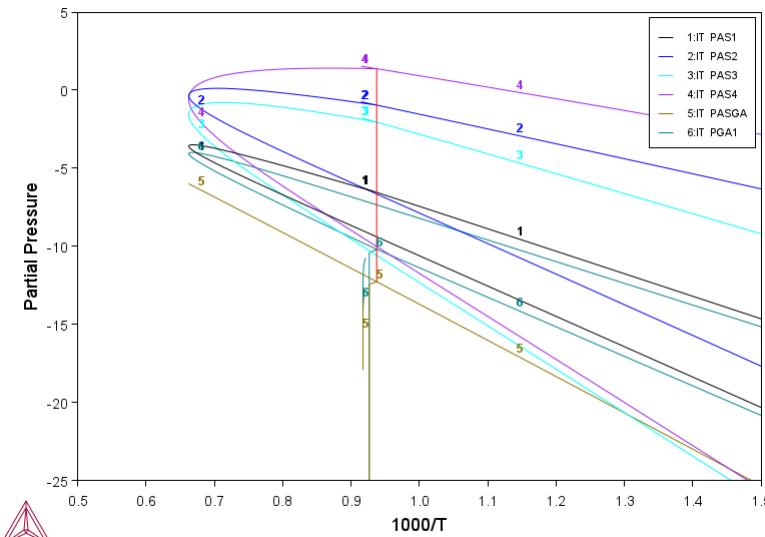


```

POST:
POST:Hit RETURN to continue
POST: @@ Now make the plot readable by adding axis text and labels
POST: s-s x n 0.5 1.5
... the command in full is SET_SCALING_STATUS
POST: s-s y n -25 5
... the command in full is SET_SCALING_STATUS
POST: s-a-text x n 1000/T
... the command in full is SET_AXIS_TEXT_STATUS
POST: s-a-text y n Partial Pressure
... the command in full is SET_AXIS_TEXT_STATUS
POST: s-lab d
... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 26c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFILE
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 26c



```

POST:
POST: set-interactive
... the command in full is SET_INTERACTIVE_MODE
POST:

```

SYS:About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

```
SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce27\tce27.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Calculating chemical vapor depositions (CVD)
SYS:
SYS: @@ Note that a SSUB database license is required
SYS: @@ to run the example.
SYS:
SYS: @@ Get data from the database
SYS: set-log ex27,....
SYS: go da
... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module
Database folder: C:\jenkins\workspace\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA           /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFC11: sw ssusb6
... the command in full is SWITCH_DATABASE
Current database: SGTE Substances v6.0

VA   DEFINED
TDB_SSUSB6:
TDB_SSUSB6: d-sys h cl ar w si
... the command in full is DEFINE_SYSTEM
H             CL          AR
W             SI          DEFINED
TDB_SSUSB6: get
... the command in full is GET_DATA
16:05:23,673 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS .....

List of references for assessed data

AR1<G> HULTGREN SELECTED VAL 1973 SGTE **
AR1<G> Ar<G>
ARGON <GAS>
STANDARD STATE : CODATA KEY VALUE .
CL1<G> T.C.R.A.S. Class: 1
CL1<G> Cl<G>
CHLORINE <MONATOMIC GAS>
CL10W2<G> JANAF THERMOCHEMICAL TABLES SGTE
CL10W2<G> W2C110<G>
TUNGSTEN PENTACHLORIDE <GAS>
PUBLISHED BY JANAF AT 12/66
CL1H1<G> T.C.R.A.S. Class: 1
CL1H1<G> HCl<G>
HYDROGEN CHLORIDE <GAS>
CL1H1S1<G> T.C.R.A.S. Class: 5
CL1H1S1<G>
CL1H3S1<G> R.W.T.H.-91 SGTE **
CL1H3S1<G> SiH3Cl<G>
MOLWT(G/M) : 66.5630
CL1Si1<G> T.C.R.A.S. Class: 1
CL1Si1<G> SiCl<G>
SILICON MONOCHLORIDE <GAS>
CL1W1<G> T.C.R.A.S. Class: 3
CL1W1<G> WC1<G>
TUNGSTEN MONOCHLORIDE <GAS>
CL2<G> T.C.R.A.S. Class: 1
CL2<G> Chlorine
CHLORINE <DIATOMIC GAS>
CL2H2Si1<G> THERMODATA 01/93
CL2H2Si1<G> SiH2Cl2<G>
DICHLOROSILANE
28/01/93 DICHLOROSILANE.
CL2Si1<G> T.C.R.A.S. Class: 5
CL2Si1<G> SiCl2<G>
SILICON DICHLORIDE <GAS>
CL2W1<G> JANAF THERMOCHEMICAL TABLES SGT
CL2W1<G> WC12<G>
TUNGSTEN DICHLORIDE <GAS>
PUBLISHED BY JANAF AT 12/66
CL3H1S1<G> THERMODATA 01/93
CL3H1S1<G> SiHCl3<G>
28/01/93
CL3Si1<G> T.C.R.A.S. Class: 6
CL3Si1<G> SiCl3<G>
SILICON TRICHLORIDE <GAS>
CL3W1<G> T.C.R.A.S. Class: 6
CL3W1<G>
CL4Si1<G> T.C.R.A.S. Class: 6
CL4Si1<G> SiCl4<G>
SILICON TETRACHLORIDE <GAS>
CL4W1<G> JANAF THERMOCHEMICAL TABLES SGTE
CL4W1<G> WC14<G>
TUNGSTEN TETRACHLORIDE <GAS>
PUBLISHED BY JANAF AT 12/66
CL5W1<G> JANAF THERMOCHEMICAL TABLES SGTE
CL5W1<G> WC15<G>
TUNGSTEN PENTACHLORIDE <GAS>
PUBLISHED BY JANAF AT 12/66
```

CL6W1<G> JANAF THERMOCHEMICAL TABLES SGTE
 CL6W1<G> WC16<G>
 TUNGSTEN HEXACHLORIDE <GAS>
 PUBLISHED BY JANAF AT 12/66
 H1<G> JANAF 1982; ASSESSMENT DATED 3/77 SGTE **
 H1<G> H<G>
 HYDROGEN <MONATOMIC GAS>
 H1Si1<G> T.C.R.A.S. Class: 2
 H1Si1<G> SiH<G>
 SILICON MONOHYDRIDE <GAS>
 H2<G> JANAF THERMOCHEMICAL TABLES SGTE **
 H2<G> H2<G>
 HYDROGEN<G>
 STANDARD STATE FROM CODATA KEY VALUES. CP FROM JANAF PUB. 3/61
 H2Si1<G> T.C.R.A.S. Class: 6
 H2Si1<G>
 H3Si1<G> T.C.R.A.S. Class: 5
 H3Si1<G>
 H4Si1<G> JANAF 1978; ASSESSMENT DATED 6/76 SGTE
 H4Si1<G> SiH4<G>
 SILANE <GAS>
 H6Si2<G> THERMODATA 01/93
 H6Si2<G> Si2H6<G>
 DISILANE <GAS>
 28/01/93
 Si1<G> T.C.R.A.S. Class: 1
 Si1<G> Si<G>
 SILICON <GAS>
 Si2<G> T.C.R.A.S. Class: 5
 Si2<G> Si2<G>
 SILICON <DIATOMIC GAS>
 Si3<G> T.C.R.A.S. Class: 6
 Si3<G> Si3<G>
 SILICON <TRIATOMIC GAS>
 W1<G> T.C.R.A.S. Class: 4
 W1<G> W<G>
 TUNGSTEN <GAS>
 CL2W1 JANAF THERMOCHEMICAL TABLES SGTE **
 CL2W1 WC12
 TUNGSTEN DICHLORIDE
 PUBLISHED BY JANAF AT 12/66
 Decomposes and sublimes to complex vapour at about 860K.
 CL3W1 T.C.R.A.S. Class: 7
 CL3W1
 CL4Si1<L> N.P.L. SGTE **
 CL4Si1 SiCl4
 SILICON TETRACHLORIDE
 ESTIM.COEF.FOR CP .MELTING PT. AT 203.15 K. LF=1850(#100)CAL/MOL FOR
 GAS
 SEE Si1Cl4<G> ABOVE 331 K.
 CL4W1 JANAF THERMOCHEMICAL TABLES SGTE
 CL4W1 WC14
 TUNGSTEN TETRACHLORIDE
 PUBLISHED BY JANAF AT 12/66
 Decomposes at 771K to WC12(s) and WC15(g).
 CL5W1 JANAF THERMOCHEMICAL TABLES SGTE
 CL5W1 WC15
 TUNGSTEN PENTACHLORIDE
 PUBLISHED BY JANAF AT 12/66
 CL6W1 THERMODATA 01/93
 CL6W1 WC16
 TUNGSTEN HEXACHLORIDE
 28/01/93 Tb = 613.6 K
 H6Si2 THERMODATA 06/86 BK
 DISILANE. Solid Standard State.
 Si2W1 VAHLAS ET AL **
 Si2W1 WSi2
 from Vahlas et al Calphad 13(3) (1989) 273
 Si3W5 VAHLAS ET AL **
 Si3W5 W5Si3
 from Vahlas et al Calphad 13(3) (1989) 273
 Si1 JANAF THERMOCHEMICAL TABLES SGTE **
 Si1 Si
 SILICON
 PUBLISHED BY JANAF AT 12/66 . MPT FROM NBS BULL. (IPTS-68)
 --U.D. 31/10/85
 W1 S.G.T.E. **
 W1 W
 Data from SGTE Unary DB
 -OK-

TDB_SSUB6:
TDB_SSUB6: @@ Calculations are made in POLY-3 module
TDB_SSUB6: go p-3
 ... the command in full is GOTO_MODULE

POLY version 3.32
POLY:

POLY: @@ Very many stoichiometric phases can make equilibrium calculations
POLY: @@ difficult. Setting a very high maximum number of grid points can
POLY: @@ avoid this.
POLY: adv g y 10000000
 ... the command in full is ADVANCED_OPTIONS
 Settings for global minimization:
POLY:

POLY: @@ In POLY-3 you define new components
POLY: def-com ar cl4w1 cl2h2si1 h2 cl1h1
 ... the command in full is DEFINE_COMPONENTS
POLY: l-st c
 ... the command in full is LIST_STATUS
 *** STATUS FOR ALL COMPONENTS

| COMPONENT | STATUS | REF. | STATE | T (K) | P (Pa) |
|-----------|---------|------|-------|-------|--------|
| VA | ENTERED | SER | | | |
| AR | ENTERED | SER | | | |
| CL4W1 | ENTERED | SER | | | |
| CL2H2SI1 | ENTERED | SER | | | |
| H2 | ENTERED | SER | | | |
| CL1H1 | ENTERED | SER | | | |

POLY: Hit RETURN to continue
POLY:

POLY: @@ Set conditions for input of gases. The best way is
POLY: @@ to set amounts equal to moles/minutes, for example.
POLY: @@ In this case we had initial partial pressures of
POLY: @@ argon 0.9 atm, WCL4 1e-5..0.1 SiH2Cl2 1e-5..0.1 unknown
POLY: @@ pressure of H2. Should be no addition of HCl nor Cl but

```

POLY: @@ added a small addition of CL1H1 to get equilibrium to
POLY: @@ converge.
POLY: s-c n=1 x(ar)=.9 x(cl2h2si)=1e-3 x(cl4w)=.001 x(cl1h1)=1e-12
... the command in full is SET_CONDITION
POLY:
POLY: @@ At the reaction zone T=1000 and total pressure is 1 atm
POLY: s-c t=1000 p=101325
... the command in full is SET_CONDITION
POLY: l-c
... the command in full is LIST_CONDITIONS
N=1, X(AR)=0.9, X(CL2H2SI1)=1E-3, X(CL4W1)=1E-3, X(CL1H1)=1E-12, T=1000,
P=101325
DEGREES OF FREEDOM 0
POLY:
POLY: @@ Save the file, then calculate and list the results
POLY: save tce27 y
... the command in full is SAVE_WORKSPACES
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 8347817 grid points in 87 s
Found the set of lowest grid points in 1 s
Calculated POLY solution 1 s, total time 89 s
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /WVCS/: WVCS
Output from POLY-3, equilibrium = 1, label A0 , database: SSUB6

Conditions:
N=1, X(AR)=0.9, X(CL2H2SI1)=1E-3, X(CL4W1)=1E-3, X(CL1H1)=1E-12, T=1000,
P=101325
DEGREES OF FREEDOM 0

Temperature 1000.00 K ( 726.85 C), Pressure 1.013250E+05
Number of moles of components 1.00000E+00, Mass in grams 3.65774E+01
Total Gibbs energy -1.67561E+05, Enthalpy 1.45855E+04, Volume 8.21892E-02

Component Moles W-Fraction Activity Potential Ref.stat
AR 9.0000E-01 9.8293E-01 2.0867E-09 -1.6619E+05 SER
CL4W1 1.0000E-03 8.9034E-03 8.9672E-57 -1.0730E+06 SER
CL2H2SI1 1.0000E-03 2.7615E-03 1.5207E-40 -7.6231E+05 SER
H2 9.8000E-02 5.4008E-03 2.4479E-09 -1.6486E+05 SER
CL1H1 1.0022E-12 9.9901E-13 1.9600E-18 -3.3901E+05 SER

GAS Status ENTERED Driving force 0.0000E+00
Moles 1.0016E+00, Mass 3.6377E+01, Volume fraction 1.0000E+00 Mass fractions:
AR 9.88357E-01 CL1H1 5.21203E-03 CL4W1 1.31332E-10
H2 5.31980E-03 CL2H2SI1 1.11068E-03

Constitution:
AR 8.98562E-01 CL 3.03070E-11 H1SI1 1.54528E-17
H2 9.65533E-02 CL1H1SI1 2.25619E-11 SI 2.70199E-19
CL1H1 4.48535E-03 CL2W1 1.46463E-11 H6SI2 1.36833E-22
CL4SI1 3.16220E-04 H4SI1 6.03281E-12 CL5W1 4.37795E-24
CL3H1SI1 7.81990E-05 CL1SI1 1.41372E-12 SI2 1.26468E-26
CL1H3SI1 4.29796E-06 CL2 6.15724E-15 CL1W1 1.35601E-30
CL2H2SI1 3.50040E-07 H3SI1 4.22110E-16 SI3 1.15600E-30
CL2SI1 2.90182E-07 H2SI1 3.80095E-16 W 1.00000E-30
CL3SI1 3.29494E-09 CL4W1 1.12601E-16 CL10W2 1.00000E-30
H 7.01220E-10 CL3W1 1.62069E-17 CL6W1 1.00000E-30

SI3W5_S Status ENTERED Driving force 0.0000E+00
Moles-1.6000E-03, Mass 2.0070E-01, Volume fraction 0.0000E+00 Mass fractions:
CL4W1 1.62262E+00 H2 2.00876E-02 CL1H1 -9.44672E-01
CL2H2SI1 3.01962E-01 AR 0.00000E+00
POLY:Hit RETURN to continue
POLY: @@ Now set axis to vary along the input amounts of WC14
POLY: @@ and SiH2Cl2. Use a logarithmic step as the magnitudes
POLY: @@ vary. Note that a limit equal to zero should not be
POLY: @@ used with log.axis
POLY:
POLY: s-a-v 1 x(cl2h2si)
... the command in full is SET_AXIS_VARIABLE
Min value /0/: 1e-8
Max value /1/: 0.02
Increment /4.9999975E-04/: 2.0*
Logarithmic step set
POLY: s-a-v 2 x(cl4w)
... the command in full is SET_AXIS_VARIABLE
Min value /0/: 1e-8
Max value /1/: 0.02
Increment /4.9999975E-04/: 2.0*
Logarithmic step set
POLY: @@ Add with both direction and continuation ">" to be
POLY: @@ sure to get all lines
POLY: add
... the command in full is ADD_INITIAL_EQUILIBRIUM
Direction /Default/: 2>
POLY: add -2>
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY: l-ax
... the command in full is LIST_AXIS_VARIABLE
Axis No 1: X(CL2H2SI1) Min: 1E-8 Max: 2E-2 Inc: 2*
Axis No 2: X(CL4W1) Min: 1E-8 Max: 2E-2 Inc: 2*
POLY: li-in
... the command in full is LIST_INITIAL_EQUILIBRIA
No 1 +2> N=1, X(AR)=0.9, X(CL2H2SI1)=1E-3, X(CL4W1)=1E-3,
X(CL1H1)=1.0022113E-12, T=1000, P=101325
No 2 -2> N=1, X(AR)=0.9, X(CL2H2SI1)=1E-3, X(CL4W1)=1E-3,
X(CL1H1)=1.0021619E-12, T=1000, P=101325
POLY:Hit RETURN to continue
POLY: @@
POLY: @@ Save again with the start point before mapping
POLY: save tce27 y
... the command in full is SAVE_WORKSPACES
POLY: map
Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Tie-lines not in the plane of calculation
Generating start point 1

```

```

Generating start point  2
Generating start point  3
Generating start point  4
Generating start point  5
Generating start point  6
Generating start point  7
Generating start point  8
Generating start point  9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18

Phase region boundary  1 at:  1.435E-02  1.970E-03
    GAS
    SI2W1_S
    ** SI_S
Calculated              79 equilibria

Phase region boundary  2 at:  1.435E-02  1.970E-03
    GAS
    SI2W1_S
    ** SI_S
Calculated..           2 equilibria
Terminating at axis limit.

Phase region boundary  3 at:  2.000E-02  2.810E-03
    GAS
    SI2W1_S
    ** SI_S
Calculated              68 equilibria

Phase region boundary  4 at:  9.344E-03  1.970E-03
    GAS
    SI2W1_S
    ** SI3W5_S
Calculated              80 equilibria

Phase region boundary  5 at:  9.344E-03  1.970E-03
    GAS
    SI2W1_S
    ** SI3W5_S
Calculated..           3 equilibria
Terminating at axis limit.

Phase region boundary  6 at:  2.000E-02  3.793E-03
    GAS
    SI2W1_S
    ** SI3W5_S
Calculated              82 equilibria

Phase region boundary  7 at:  4.095E-03  1.970E-03
    GAS
    ** SI2W1_S
    SI3W5_S
Calculated..           65 equilibria
Terminating at axis limit.

Phase region boundary  8 at:  4.095E-03  1.970E-03
    GAS
    ** SI2W1_S
    SI3W5_S
Calculated..           4 equilibria
Terminating at axis limit.

Phase region boundary  9 at:  2.000E-02  7.114E-03
    GAS
    ** SI2W1_S
    SI3W5_S
Calculated              70 equilibria

Phase region boundary 10 at:  2.938E-03  1.970E-03
    GAS
    SI3W5_S
    ** W_S
Calculated              83 equilibria

Phase region boundary 11 at:  2.938E-03  1.970E-03
    GAS
    SI3W5_S
    ** W_S
Calculated..           4 equilibria
Terminating at axis limit.

Phase region boundary 12 at:  2.000E-02  7.879E-03
    GAS
    SI3W5_S
    ** W_S
Calculated              85 equilibria

Phase region boundary 13 at:  1.000E-03  1.970E-03
    GAS
    ** SI3W5_S
    W_S
Calculated              91 equilibria

Phase region boundary 14 at:  1.000E-03  1.970E-03
    GAS
    ** SI3W5_S
    W_S
Calculated..           6 equilibria
Terminating at axis limit.

Phase region boundary 15 at:  2.000E-02  1.266E-02
    GAS
    ** SI3W5_S
    W_S
Calculated              97 equilibria

Phase region boundary 16 at:  1.000E-03  1.970E-03
    GAS

```

```

** SI3W5_S
W_S
Calculated          36 equilibria
Phase region boundary 17 at: 1.000E-03 1.970E-03
  GAS
** SI3W5_S
W_S
Calculated..       7 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 18 at: 1.000E-03 1.037E-03
  GAS
  SI3W5_S
** W_S
Calculated          35 equilibria
Phase region boundary 19 at: 1.000E-03 1.037E-03
  GAS
  SI3W5_S
** W_S
Calculated..       6 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 20 at: 1.000E-03 3.753E-04
  GAS
  SI2W1_S
** SI3W5_S
Calculated          33 equilibria
Phase region boundary 21 at: 1.000E-03 3.753E-04
  GAS
  SI2W1_S
** SI3W5_S
Calculated..       6 equilibria
Terminating at known equilibrium
Terminating at axis limit.

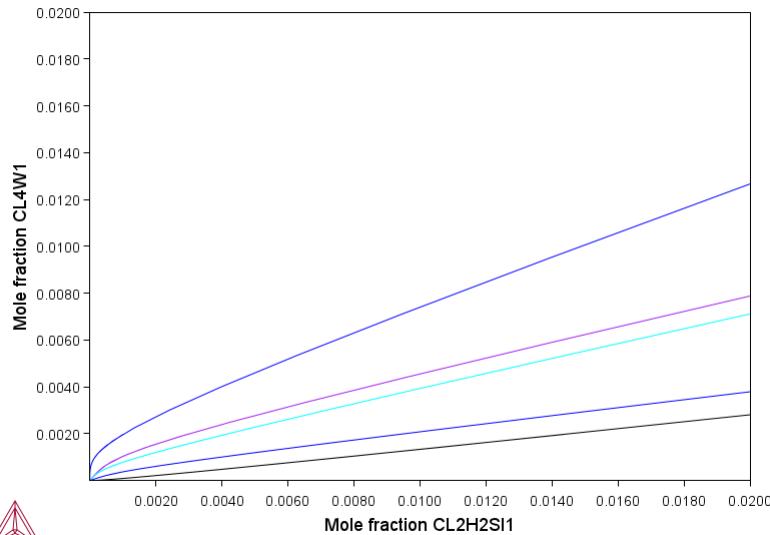
Phase region boundary 22 at: 1.000E-03 7.855E-04
  GAS
** SI2W1_S
SI3W5_S
Calculated          33 equilibria
Phase region boundary 23 at: 1.000E-03 7.855E-04
  GAS
** SI2W1_S
SI3W5_S
Calculated..       6 equilibria
Terminating at known equilibrium
Terminating at axis limit.
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\generate_console_examples\examples\tcex27\tcex27.POLY3
CPU time for mapping           22 seconds
POLY: @@
POLY: @@ Plot the diagram in the Post module
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST:
POST: set-title example 27a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 27a

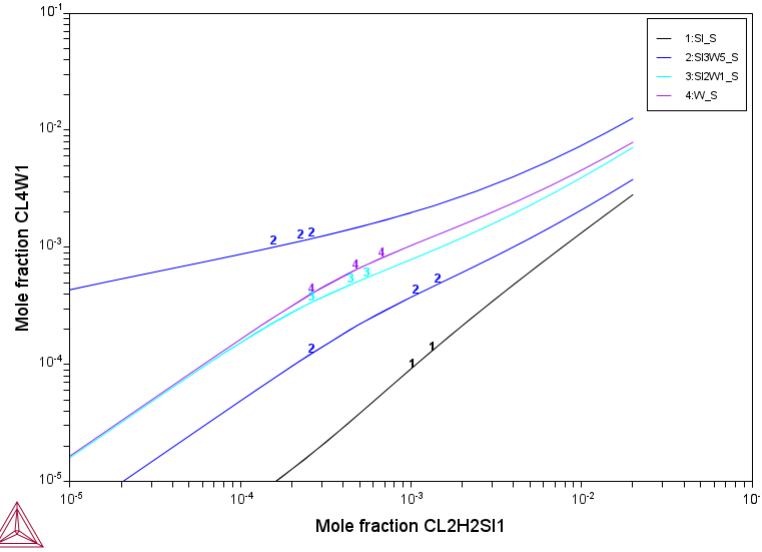


POST:
POST:Hit RETURN to continue
POST: @@ Better with logarithmic axis
POST: s-a-ty x log
... the command in full is SET_AXIS_TYPE
POST: s-a-ty y log
... the command in full is SET_AXIS_TYPE
POST: s-s x n 1e-5 .01
... the command in full is SET_SCALING_STATUS
POST: s-s y n 1e-5 .01

```

... the command in full is SET_SCALING_STATUS
POST: s-lab b
... the command in full is SET_LABEL_CURVE_OPTION
POST: @@
POST: set-title example 27b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAIFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
example 27b

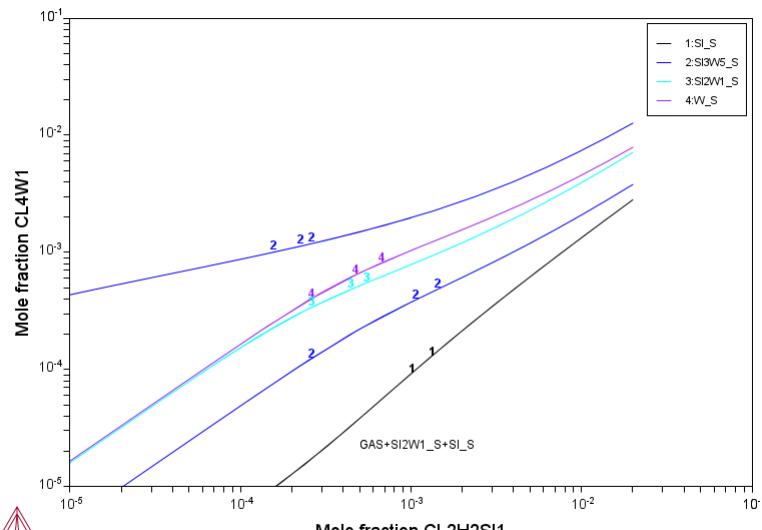
```



```

POST:
POST:Hit RETURN to continue
POST: @@Identify one of the phase regions
POST: add .0005 2e-5
... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
Automatic labelling not always possible
Using global minimization procedure
Using already calculated grid
Found the set of lowest grid points in           1 s
Calculated POLY solution      0 s, total time   1 s
Stable phases are: GAS+SI2W1_S+SI_S
Text size: /.36/:
POST: set-title example 27c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAIFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
example 27c

```



```

POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:

```

SYS:About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

```
SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce28\tce28.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Pitting Resistance Equivalence (PRE)
SYS: @@ for a duplex stainless steel.
SYS:
SYS: @@ Note that a TCFE database license is required
SYS: @@ to run the example.
SYS:
SYS: set-log ex28,,
SYS: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY: @@ Set the nominal composition

POLY: def-mat
... the command in full is DEFINE_MATERIAL
THERMODYNAMIC DATABASE module
Database folder: C:\jenkins\workspace\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA
      /- DEFINED
DICTRA_FCC_A1 REJECTED
Database /TCFE11/: tcfe11
Major element or alloy: fe
Composition input in mass (weight) percent? /Y/:
1st alloying element: cr 25 ni 7 mo 4 c .002 n .27 si .3 mn .3
Next alloying element:
Temperature (C) /1000/: 1050
VA
      /- DEFINED
DICTRA_FCC_A1 REJECTED
REINITIATING GES ....
... the command in full is DEFINE_ELEMENTS
FE DEFINED
... the command in full is DEFINE_ELEMENTS
CR DEFINED
... the command in full is DEFINE_ELEMENTS
NI DEFINED
... the command in full is DEFINE_ELEMENTS
MO DEFINED
... the command in full is DEFINE_ELEMENTS
C DEFINED
... the command in full is DEFINE_ELEMENTS
N DEFINED
... the command in full is DEFINE_ELEMENTS
SI DEFINED
... the command in full is DEFINE_ELEMENTS
MN DEFINED

... the command in full is DEFINE_ELEMENTS
```

This database has following phases for the defined system

| | | |
|--------------|----------------|-------------|
| GAS:G | LIQUID:L | BCC_A2 |
| A2_BCC | BCC_B2 | FCC_A1 |
| A1_FCC | FCC_L12 | HCP_A3 |
| CBCC_A12 | CUB_A13 | DIAMOND_A4 |
| GRAPHITE_A9 | CEMENTITE_D011 | M23C6_D84 |
| M7C3_D101 | M6C_E93 | M5C2 |
| M3C2_D510 | MC_ETA | MC_SHP |
| KSI_CARBIDE | Z_PHASE | FE4N_LP1 |
| PI_A13 | SIGMA_D8B | HIGH_SIGMA |
| MU_D85 | P_PHASE | R_PHASE |
| CHI_A12 | C14_LAVES | C15_LAVES |
| M3SI | MN9SI2 | MN11SI19 |
| MN6SI | G_PHASE | ETA_M5SIN |
| CR3SI_A15 | FESI2_H | FESI2_L |
| MSI_B20 | M5SI3_D88 | NBN13_D0A |
| NI3TI_D024 | MOSI2_C11B | MO5SI3_D8M |
| NB5SI3_D8L | MSI2_C40 | M11SI8 |
| M6SI5 | AL4C3_D71 | FE8SI2C |
| SIC_B3 | MN5SIC | CRZN17 |
| CUZN_EPSILON | NIZN_B2 | NIZN_L10 |
| NI2ZN11_D82 | AL5FE4 | SI3N4 |
| MN3N2 | MN6N5 | MNP_B31 |
| M2P_C22 | FLUORITE_C1:I | ZRO2_TETR:I |
| M2O3C_D53:I | M2O3H_D52:I | M4Si1_G3 |
| NI3Si12 | CO2Si_C37 | M2Si1_TETA |
| NISI_B31 | NI3Si2 | CR5Si3_D8M |

Reject phase(s) /NONE/: *

| | | |
|-------------|----------------|------------|
| GAS:G | LIQUID:L | BCC_A2 |
| A2_BCC | BCC_B2 | FCC_A1 |
| A1_FCC | FCC_L12 | HCP_A3 |
| CBCC_A12 | CUB_A13 | DIAMOND_A4 |
| GRAPHITE_A9 | CEMENTITE_D011 | M23C6_D84 |
| M7C3_D101 | M6C_E93 | M5C2 |
| M3C2_D510 | MC_ETA | MC_SHP |
| KSI_CARBIDE | Z_PHASE | FE4N_LP1 |
| PI_A13 | SIGMA_D8B | HIGH_SIGMA |
| MU_D85 | P_PHASE | R_PHASE |
| CHI_A12 | C14_LAVES | C15_LAVES |
| M3SI | MN9SI2 | MN11SI19 |
| MN6SI | G_PHASE | ETA_M5SIN |
| CR3SI_A15 | FESI2_H | FESI2_L |
| MSI_B20 | M5SI3_D88 | NBN13_D0A |
| NI3TI_D024 | MOSI2_C11B | MO5Si3_D8M |
| NB5Si3_D8L | MSI2_C40 | M11Si8 |
| M6Si5 | AL4C3_D71 | FE8Si2C |

```

SIC_B3          MN5SIC          CRZN17
CUZN_EPSILON    NIZN_B2          NIZN_L10
NI2ZN11_D82     AL5FE4           SI3N4
MN3N2          MN6N5            MNP_B31
M2P_C22         FLUORITE_C1:I   ZRO2_TETR:I
M203C_D53:I    M203H_D52:I    M4Si1_G3
NI31Si12       CO2Si_C37      M2Si_TETA
NISI_B31        NI3Si2          CR5Si3_D8M
REJECTED

Restore phase(s):: fcc_a1 bcc_a2 hcp_a3 m23 sigma
FCC_A1          BCC_A2          HCP_A3
M23C6_D84       SIGMA_D8B      RESTORED
Restore phase(s): /NONE:

.....
```

The following phases are retained in this system:

```

BCC_A2          FCC_A1          HCP_A3
M23C6_D84       SIGMA_D8B
```

OK? //:

```

16:07:50,847 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
Creating a new composition set FCC_A1#2
... the command in full is AMEND_PHASE_DESCRIPTION
Creating a new composition set HCP_A3#2
PARAMETERS .....
FUNCTIONS .....
```

List of references for assessed data

```

'A.T. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
'X.G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
'X.G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
    volumes'
'B. Sundman et al., Report EUR 20315, Contract No 7210-PR/050, 2002; New
    Sigma model'
'A.F. Guillermet, Z. Metallkd., 79 (1988) 524-536, TRITA-MAC 362 (1988); C
    -CO-NI AND C-CO-FE-NI'
'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
'J-O. Andersson, CALPHAD, 11 (1987) 271-276; TRITA 0314; C-CR'
'J. Bratberg, Z. Metallkd., 96 (2005) 335-344; Fe-Cr-Mo-C'
'B.J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
'C. Qui, ISIJ International, 32 (1992), 1117-1127; TRITA-MAC 482 (1992)
    Revision; C-Cr-Fe-Mo'
'P. Gustafson, Metall. Trans. A, 19A (1988) 2547-2554; TRITA-MAC 348,
    (1987); C-CR-FE-W'
'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
'J-O. Andersson, CALPHAD, 12 (1988) 9-23; TRITA 0321 (1986); C-FE-MO'
'H. Gohring, O. Fabrichnaya, A. Leineweber, E.J. Mittemeijer, Metall.
    Mater. Trans. A, 47A, 6173-86(2016); FE-N, and Fe-C-N'
'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, Calphad 35.4
    (2011) 479-491; Fe-Mn-C'
'W. Huang, Metall. Trans. A, 21A (1990) 2115-2123; TRITA-MAC 411 (Rev
    1989); C-FE-MN'
'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, CALPHAD, 34, 279
    -85(2010); Mn-C'
'J.H. Shim, C.S. Oh, D.N. Lee, Metall. Mater. Trans. B, 27 (1996) 955-966;
    Ti-Mo-C'
'P. Villars, L.D. Calvert. Pearson's handbook of crystallographic data for
    intermetallic phases, Metals park, Ohio 1985: American society for
    metals'
'A. Gabriel, C. Chatillon, and I. Ansara, published in High Temp. Sci.
    (Parameters listed in CALPHAD, 11 (1987) 203-218); C-NI'
'P. Franke; revision of C-Si, Fe-Si and C-Fe-Si'
'J. Lacaze and B. Sundman, Metall. Mater. Trans. A, 22A (1991) 2211-2223;
    Fe-Si and Fe-Si-C'
'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270
    (1986); CR-FE'
'K. Frisk, Metall. Trans. A, 21A (1990) 2477-2488; TRITA 0409 (1989); CR
    -FE-N'
'B.J. Lee, Metall. Trans. A, 24A (1993) 1919-1933; Cr-Mn, Fe-Cr-Mn'
'K. Frisk, CALPHAD, 17 (1993) 335-349; Cr-Mn-N'
'K. Frisk, KTH Report D 60 (1984); CR-MO'
'B. Sundman, Private communication; FCC parameter same as BCC; Cr-Mo'
'J-O. Andersson, TRITA-MAC 323 (1986); C-CR-FE-MO'
'K. Frisk, CALPHAD, 15 (1991) 79-106; TRITA-MAC 393 (1989); CR-N, FE-N, MO
    -N, CR-MO-N'
'A.T. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); CR-NI'
'L.L. Zhu, H.Y. Qi, L. Jiang, Z.P. Jin, J.C. Zhao, Intermetallics. 64
    (2015) 86-95; Cr-Ru and Cr-Ni-Ru'
'Y.Du and J.C.Schuster, J. Phase Equilibria, 21(3) 281-86(2000); Cr-Si'
'W. Huang, CALPHAD, 13 (1989) 243-252; TRITA-MAC 388 (rev 1989); FE-MN'
'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
'A.F. Guillermet, CALPHAD, 6 (1982) 127-140; (sigma phase revised 1986);
    TRITA-MAC 200 (1982); FE-MO'
'H. Du, J. Phase Equilib., 14, 682-93(1993); Fe-N, Fe-C-N'
'A.T. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); FE-NI'
'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; Molar volume Fe-Mn-Si
    and Al-Fe-Mn'
'S. Cotes, A.F. Guillermet, M. Sade, J. Alloys Compd., 208(1998) 168-177'
'B.J. Lee, KRISS, unpublished research, during 1993-1995'
'C. Qiu and A.F. Guillermet, Z. Metallkd., 84 (1993) 11-12; Mn-N'
'Shuhong Liu, unpublished work (2010),Mn-Ni,Al-Mn-Ni,Mn-Ni-Zn, Al-Cu-Fe-Mg
    -Mn-Si'
'C.P. Guo, Intermetallics,13(5),525-534,(2005),Mn-Ni'
'W. Zheng, J. Alloys Compd., 632 (2015) 661-675'
'K. Frisk, CALPHAD, 14 (1990) 311-320; MO-NI'
'Y. Liu, G. Shao, P. Tsakirooulos, Intermatallics 8 (200) 953-962; Mo-Si,
    Al-Mo-Si'
'R. Naraghi, Thermo-Calc Software AB, Sweden (2015); FROST project'
'K. Frisk, Z. Metallkd., 82 (1991) 59-66; TRITA-MAC 414 (1989); Fe-Ni-N'
'K. Frisk, Int. J. Thermophys., 12 (1990) 417-431; TRITA-MAC 419 (1990); N
    -NI'
'N. Dupin, Private communication; Si systems'
'Same or similar interaction as in the corresponding stable phase'
'A.V. Khvan, B. Hallstedt, C. Broeckmann, CALPHAD, 46, 24-33(2014); Cr-Fe-C'
'J-O. Andersson, Metall. Trans. A, 19A (1988) 627-636 TRITA 0207 (1986); C
```

-CR-FE'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2016; FCC Fe-Cr-C and C-Cr-Ni'
 'B.J. Lee, Metall. Trans. A, 24A (1993) 1017-1025; Fe-Cr-Mn-C'
 'J. Bratberg, Thermo-Calc Software AB, Sweden, 2008; Fe-Cr-Mo-V-W-C'
 'P. Gustafson, Inst. Met. Res. (Sweden) (1990); Estimations of C-CR-FE-V,
 C-CR-FE-MO-V-W, FE-N-W, FE-MN-N, FE-N-SI, CR-N-V, C-CR-N, FE-MO-N, CR
 -N-W, CR-TI-N'
 'NPL, unpublished work (1989); C-Cr-Ni'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; Adjusting hcp'
 'A. Gabriel, P. Gustafson, and I. Ansara, CALPHAD, 11 (1987) 203-218;
 TRITA-MAC 285 (1986); C-FE-NI'
 'J. Miettinen and B. Hallstedt, CALPHAD, 22 (1998) 231-256; Fe-Si and Fe
 -Si-C'
 'C. Qiu, Metall. Trans. A, 24A (1993) 2393-2409; Cr-Fe-Mn-N'
 'B.J. Lee, Private communication, (2000); Estimated parameter'
 'B.J. Lee, CALPHAD, 17 (1993) 251-268; revision of Fe-Cr and Fe-Ni liquid'
 'M. Lindholm, J. Phase Equilib., 18.5 (1997) 432; Cr-Fe-Si'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; Cr-Fe-Si'
 'J. Kunze, P. Broz,
 I. Stloukal, Steel Research 67(1996) 279-284.'
 'B. Sundman, Private communication, 2(1999); Estimated parameter'
 'B. Sundman, estimated parameter (2000); Cr-Ni-Mo'
 'K. Frisk, TRITA-MAC 422 (1990); Cr-FE-N-NI'
 'J.C. Schuster and Y.Du, Metall. Mater. Trans.A, 31A(7) 1795-803(2000); Cr
 -Ni-Si.'
 'R. Naraghi, Thermo-Calc Software AB, Sweden (2019); Cr-Ni-Si'
 'C. Qiu, Metall. Trans. A, 24A (1993) 629-645; Fe-Mn-N'
 'L.J. Zhang, Int.J. Mater. Res.,100(2) 160-175 (2009),Fe-Mn-Ni'
 'W. Zheng et al., J. Iron Steel Res. Int. 24(2)(2017) 190-197'
 'A. Forsberg and J. Agren, J. Phase Equilib., 14 (1993) 354-363; Fe-Mn-Si'
 'K. Frisk, TRITA-MAC 433 (1990); FE-CR-MO-MO-NI-N'
 'K. Frisk, TRITA-MAC 428 (1990); FE-MO-NI'
 'J. Miettinen, CALPHAD, 22 (1998) 275-300; Fe-Mo-Si'
 'R. Naraghi, Thermo-Calc Software AB, Sweden (2019); Fe-Ni-Si'
 'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; Carbonitrides and
 M23C6'

-OK-

Should any phase have a miscibility gap check? /N/: N

Using global minimization procedure

Calculated 7296 grid points in 6 s
 Found the set of lowest grid points in 0 s
 Calculated POLY solution 2 s, total time 8 s

POLY:

POLY: save tcex28 y
 ... the command in full is SAVE_WORKSPACES

POLY: l-e

 ... the command in full is LIST_EQUILIBRIUM

OUTPUT TO SCREEN OR FILE /SCREEN/:

Options /VWCS/: VWCS

Output from POLY-3, equilibrium = 1, label A0 , database: TCFE11

Conditions:

T=1323.15, W(CR)=0.25, W(NI)=7E-2, W(MO)=4E-2, W(C)=2E-5, W(N)=2.7E-3,
 W(SI)=3E-3, W(MN)=3E-3, P=100000, N=1

DEGREES OF FREEDOM 0

Temperature 1323.15 K (1050.00 C), Pressure 1.000000E+05

Number of moles of components 1.000000E+00, Mass in grams 5.53180E+01

Total Gibbs energy -7.36566E+04, Enthalpy 3.92934E+04, Volume 7.43528E-06

| Component | Moles | W-Fraction | Activity | Potential | Ref.stat |
|-----------|------------|------------|------------|-------------|----------|
| C | 9.2112E-05 | 2.0000E-05 | 3.4290E-05 | -1.1310E+05 | SER |
| CR | 2.6597E-01 | 2.5000E-01 | 2.5349E-03 | -6.5761E+04 | SER |
| FE | 6.2530E-01 | 6.3128E-01 | 1.6027E-03 | -7.0806E+04 | SER |
| MN | 3.0208E-03 | 3.0000E-03 | 2.8578E-06 | -1.4044E+05 | SER |
| MO | 2.3064E-02 | 4.0000E-02 | 6.4306E-04 | -8.0852E+04 | SER |
| N | 1.0663E-02 | 2.7000E-03 | 4.3489E-07 | -1.6115E+05 | SER |
| NI | 6.5978E-02 | 7.0000E-02 | 1.1328E-04 | -9.9955E+04 | SER |
| SI | 5.9090E-03 | 3.0000E-03 | 2.8769E-09 | -2.1636E+05 | SER |

| FCC_A1#1 | Status | ENTERED | Driving force | 0.0000E+00 |
|---|--------|---------|---------------|-----------------|
| Moles 5.6930E-01, Mass 3.1283E+01, Volume fraction 5.6483E-01 | | | | Mass fractions: |
| FE 6.38111E-01 NI 8.52508E-02 N 4.38243E-03 SI 3.16161E-03 | | | | |
| CR 2.34121E-01 MO 3.17006E-02 MN 3.24360E-03 C 2.81314E-05 | | | | |

| BCC_A2 | Status | ENTERED | Driving force | 0.0000E+00 |
|---|--------|---------|---------------|-----------------|
| Moles 4.3070E-01, Mass 2.4035E+01, Volume fraction 4.3517E-01 | | | | Mass fractions: |
| FE 6.22389E-01 MO 5.08020E-02 SI 2.78966E-03 N 5.10240E-04 | | | | |
| CR 2.70667E-01 NI 5.01505E-02 MN 2.68295E-03 C 9.41666E-06 | | | | |

POLY:

POLY:Hit RETURN to continue

POLY: @@ Calculate the temperature for an equal amount

POLY: c-s p bcc_a2=fix .5

 ... the command in full is CHANGE_STATUS

POLY: s-c t=none

 ... the command in full is SET_CONDITION

POLY: c-e

 ... the command in full is COMPUTE_EQUILIBRIUM

Normal POLY minimization, not global

Testing POLY result by global minimization procedure

Calculated 7296 grid points in 0 s
 12 ITS, CPU TIME USED 0 SECONDS

POLY: sh t

 ... the command in full is SHOW_VALUE

T=1382.2188

POLY: l-e,,,,

 ... the command in full is LIST_EQUILIBRIUM

Output from POLY-3, equilibrium = 1, label A0 , database: TCFE11

Conditions:

W(CR)=0.25, W(NI)=7E-2, W(MO)=4E-2, W(C)=2E-5, W(N)=2.7E-3, W(SI)=3E-3,
 W(MN)=3E-3, P=100000, N=1

FIXED PHASES

BCC_A2=.5

DEGREES OF FREEDOM 0

Temperature 1382.22 K (1109.07 C), Pressure 1.000000E+05

Number of moles of components 1.000000E+00, Mass in grams 5.53180E+01

Total Gibbs energy -7.87487E+04, Enthalpy 4.15704E+04, Volume 7.46475E-06

| Component | Moles | W-Fraction | Activity | Potential | Ref.stat |
|-----------|------------|------------|------------|-------------|----------|
| C | 9.2112E-05 | 2.0000E-05 | 3.2717E-05 | -1.1869E+05 | SER |
| CR | 2.6597E-01 | 2.5000E-01 | 2.1012E-03 | -7.0854E+04 | SER |
| FE | 6.2530E-01 | 6.3128E-01 | 1.3662E-03 | -7.5802E+04 | SER |
| MN | 3.0208E-03 | 3.0000E-03 | 2.5263E-06 | -1.4812E+05 | SER |

```

MO          2.3064E-02 4.0000E-02 4.8253E-04 -8.7762E+04 SER
N          1.0663E-02 2.7000E-03 6.2930E-07 -1.6410E+05 SER
NI         6.5978E-02 7.0000E-02 1.0285E-04 -1.0553E+05 SER
SI         5.9090E-03 3.0000E-03 4.1845E-09 -2.2171E+05 SER

BCC_A2          Status FIXED      Driving force 0.0000E+00
Moles 5.0146E-01, Mass 2.7959E+01, Volume fraction 5.0593E-01 Mass fractions:
FE 6.25815E-01 NI 5.42157E-02 SI 2.86526E-03 N 7.17191E-04
CR 2.64835E-01 MO 4.88074E-02 MN 2.73452E-03 C 1.01462E-05

FCC_A1#1          Status ENTERED     Driving force 0.0000E+00
Moles 4.9854E-01, Mass 2.7359E+01, Volume fraction 4.9407E-01 Mass fractions:
FE 6.36865E-01 NI 8.61301E-02 N 4.72624E-03 SI 3.13769E-03
CR 2.34840E-01 MO 3.09997E-02 MN 3.27129E-03 C 3.00697E-05

POLY: @@ Enter the PRE functions
POLY: ent fun pffcc
... the command in full is ENTER_SYMBOL
Function: 100*w(fcc_a1,cr)+300*w(fcc_a1,mo)+1600*w(fcc_a1,n);
POLY: ent fun prebcc
... the command in full is ENTER_SYMBOL
Function: 100*w(bcc_a2,cr)+300*w(bcc_a2,mo)+1600*w(bcc_a2,n);
POLY: l-sy
... the command in full is LIST_SYMBOLS
DEFINED FUNCTIONS AND VARIABLES%
  PREFCC=100*W(FCC_A1#1,CR)+300*W(FCC_A1#1,MO)+1600*W(FCC_A1#1,N)
  PREBCC=100*W(BCC_A2,CR)+300*W(BCC_A2,MO)+1600*W(BCC_A2,N)
POLY: eval
... the command in full is EVALUATE_FUNCTIONS
Name(s): *
PREFCC=40.345889
PREBCC=42.273231
POLY: Hit RETURN to continue
POLY: @@ Then vary the nitrogen content
POLY: s-a-v 1
... the command in full is SET_AXIS_VARIABLE
Condition /NONE/: w(n)
Min value /0/: .001
Max value /1/: .005
Increment /1E-04/: 1E-04
POLY: li-ax
... the command in full is LIST_AXIS_VARIABLE
Axis No 1: W(N)           Min: 1E-3       Max: 5E-3       Inc: 1E-4
POLY: save tcex28 y
... the command in full is SAVE_WORKSPACES
POLY: step
... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/: NORMAL
No initial equilibrium, using default
Step will start from axis value 0.270000E-02
...OK

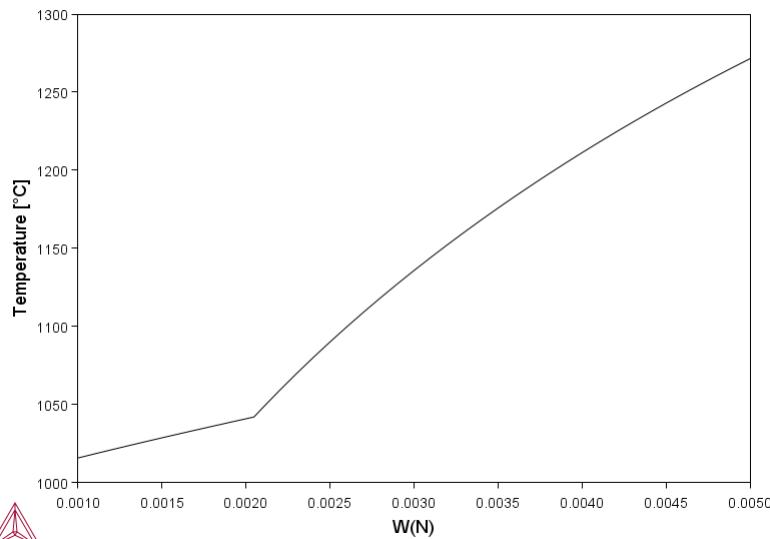
Phase Region from 0.270000E-02 for:
  BCC_A2
  FCC_A1#1
Global test at 3.50000E-03 .... OK
Global test at 4.50000E-03 .... OK
Terminating at 0.500000E-02
Calculated    26 equilibria

Phase Region from 0.270000E-02 for:
  BCC_A2
  FCC_A1#1
Global check of adding phase at 2.04865E-03
Calculated    9 equilibria

Phase Region from 0.204865E-02 for:
  BCC_A2
  FCC_A1#1
  SIGMA_DSB
Global test at 1.30000E-03 .... OK
Terminating at 0.100000E-02
Calculated    14 equilibria
*** Buffer saved on file: c:\jenkins\workspace\generate_console_examples\examples\tcex28\tcex28.POLY3
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2
POST:
POST: @@ First plot how the temperature varies
POST: s-d-a x w(n)
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t-c
... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 28a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFILE
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 28a

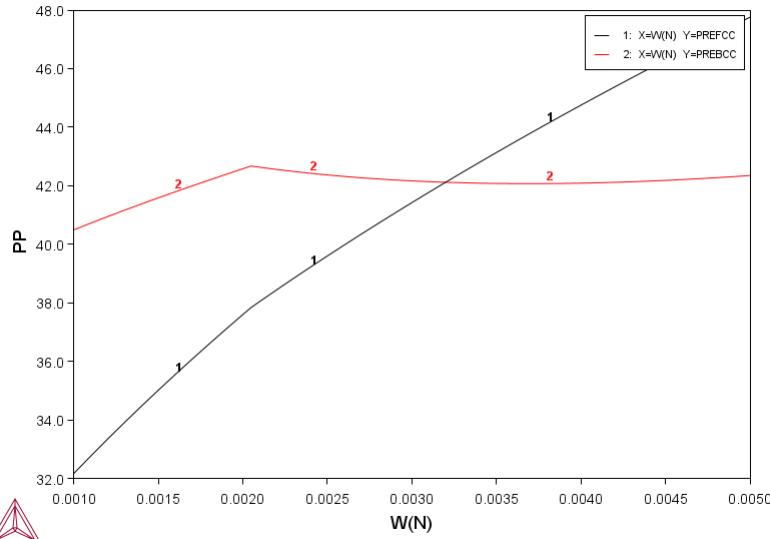


```

POST:
POST: Hit RETURN to continue
POST: @@ Then plot the PRE
POST: ent tab pp
... the command in full is ENTER_SYMBOL
Variable(s): prefcc prebcc
&
POST:
POST: s-d-a y pp
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: s-lab d
... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 28b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 28b

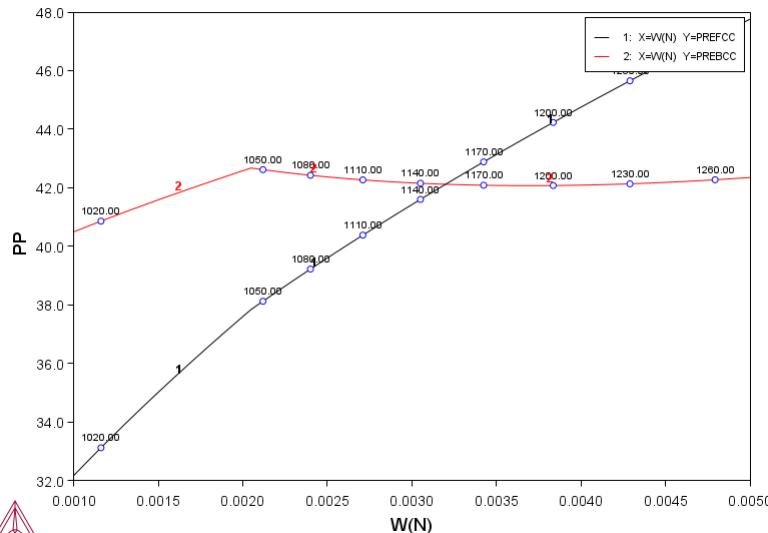


```

POST:
POST: Hit RETURN to continue
POST: @@ Add the temperature as tic marks to the plot
POST: s-d-a z t-c
... the command in full is SET_DIAGRAM_AXIS
POST: s-s z n 800 1300
... the command in full is SET_SCALING_STATUS
POST: set-title example 28c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 28c



```

POST:
POST:Hit RETURN to continue
POST: back
POLY: @@ Check how close we are to form Cr2N
POLY: read tce28
... the command in full is READ_WORKSPACES
POLY:
POLY: @@ Restore BCC as entered
POLY: c-s p bcc_a2=ent 1
... the command in full is CHANGE_STATUS
POLY: s-c t=1323
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 7296 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY: l-e,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: TCFE11

Conditions:
T=1323, W(CR)=0.25, W(NI)=7E-2, W(MO)=4E-2, W(C)=2E-5, W(N)=2.7E-3,
W(SI)=3E-3, W(MN)=3E-3, P=100000, N=1
DEGREES OF FREEDOM 0

Temperature 1323.00 K ( 1049.85 C), Pressure 1.000000E+05
Number of moles of components 1.000000E+00, Mass in grams 5.53180E+01
Total Gibbs energy -7.36438E+04, Enthalpy 3.92877E+04, Volume 7.43521E-06

Component Moles W-Fraction Activity Potential Ref.stat
C 9.2112E-05 2.0000E-05 3.4295E-05 -1.1309E+05 SER
CR 2.6597E-01 2.5000E-01 2.5362E-03 -6.5749E+04 SER
FE 6.2530E-01 6.3128E-01 1.6033E-03 -7.0793E+04 SER
MN 3.0208E-03 3.0000E-03 2.8587E-06 -1.4042E+05 SER
MO 2.3064E-02 4.0000E-02 6.4354E-04 -8.0835E+04 SER
N 1.0663E-02 2.7000E-03 4.3448E-07 -1.6114E+05 SER
NI 6.5978E-02 7.0000E-02 1.1330E-04 -9.9941E+04 SER
SI 5.9090E-03 3.0000E-03 2.8740E-09 -2.1634E+05 SER

FCC_A1#1 Status ENTERED Driving force 0.0000E+00
Moles 5.6946E-01, Mass 3.1291E+01, Volume fraction 5.6499E-01 Mass fractions:
FE 6.38114E-01 NI 8.52488E-02 N 4.38171E-03 SI 3.16166E-03
CR 2.34120E-01 MO 3.17023E-02 MN 3.24354E-03 C 2.81273E-05

BCC_A2 Status ENTERED Driving force 0.0000E+00
Moles 4.3054E-01, Mass 2.4027E+01, Volume fraction 4.3501E-01 Mass fractions:
FE 6.22380E-01 MO 5.08067E-02 SI 2.78946E-03 N 5.09797E-04
CR 2.70682E-01 NI 5.01405E-02 MN 2.68282E-03 C 9.41522E-06

POLY:Hit RETURN to continue
POLY: @@ Find out at which temperature sigma forms
POLY: c-t
... the command in full is COMPUTE_TRANSITION
This command is a combination of CHANGE_STATUS and SET_CONDITION
to calculate directly when a phase may form by releasing one condition.
Phase to form: sigma
You must release one of these conditions
T=1323, W(CR)=0.25, W(NI)=7E-2, W(MO)=4E-2, W(C)=2E-5, W(N)=2.7E-3,
W(SI)=3E-3, W(MN)=3E-3, P=100000, N=1 DEGREES OF FREEDOM 0
Give the state variable to be removed /T/: t
Testing POLY result by global minimization procedure
Calculated 7296 grid points in 0 s
To form SIGMA the condition is set to T=1319.86319867
POLY:Hit RETURN to continue
POLY: @@ Find the temperature for Cr2N, set the start
POLY: @@ constitution. but first make sure hcp#2 is nitride
POLY: s-s-c hcp_a3#2 *
... the command in full is SET_START_CONSTITUTION
POLY: c-t
... the command in full is COMPUTE_TRANSITION
This command is a combination of CHANGE_STATUS and SET_CONDITION
to calculate directly when a phase may form by releasing one condition.
Phase to form: hcp_a3#2
You must release one of these conditions
T=1319.863199, W(NI)=7E-2, W(MO)=4E-2, W(C)=2E-5, W(N)=2.7E-3,
W(SI)=3E-3, W(MN)=3E-3, P=100000, N=1 DEGREES OF FREEDOM 0
Give the state variable to be removed /T/: t
Testing POLY result by global minimization procedure
Calculated 7296 grid points in 0 s
To form HCP_A3 the condition is set to T=1252.900841

```

POLY: l-e,,,
 ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium = 1, label A0 , database: TCFE11
 Conditions:
 T=1252.900841, W(CR)=0.25, W(NI)=7E-2, W(MO)=4E-2, W(C)=2E-5, W(N)=2.7E-3,
 W(SI)=3E-3, W(MN)=3E-3, P=100000, N=1
 DEGREES OF FREEDOM 0
 Temperature 1252.90 K (979.75 C), Pressure 1.000000E+05
 Number of moles of components 1.000000E+00, Mass in grams 5.53180E+01
 Total Gibbs energy -6.77519E+04, Enthalpy 3.59731E+04, Volume 7.34852E-06

| Component | Moles | W-Fraction | Activity | Potential | Ref.stat |
|-----------|------------|------------|------------|-------------|----------|
| C | 9.2112E-05 | 2.0000E-05 | 3.8787E-05 | -1.0581E+05 | SER |
| CR | 2.6597E-01 | 2.5000E-01 | 3.1477E-03 | -6.0015E+04 | SER |
| FE | 6.2530E-01 | 6.3128E-01 | 1.9955E-03 | -6.4763E+04 | SER |
| MN | 3.0208E-03 | 3.0000E-03 | 3.3609E-06 | -1.3129E+05 | SER |
| MO | 2.3064E-02 | 4.0000E-02 | 6.6368E-04 | -7.6230E+04 | SER |
| N | 1.0663E-02 | 2.7000E-03 | 2.6467E-07 | -1.5777E+05 | SER |
| NI | 6.5978E-02 | 7.0000E-02 | 1.1846E-04 | -9.4182E+04 | SER |
| SI | 5.9090E-03 | 3.0000E-03 | 2.0069E-09 | -2.0862E+05 | SER |

FCC_A1#1 Status ENTERED Driving force 0.0000E+00
 Moles 7.8161E-01, Mass 4.2894E+01, Volume fraction 7.8081E-01 Mass fractions:
 FE 6.59812E-01 NI 7.97879E-02 SI 3.76583E-03 MN 3.27146E-03
 CR 2.26955E-01 MO 2.29001E-02 N 3.48207E-03 C 2.57931E-05

SIGMA_D8B Status ENTERED Driving force 0.0000E+00
 Moles 2.1839E-01, Mass 1.2424E+01, Volume fraction 2.1919E-01 Mass fractions:
 FE 5.32777E-01 MO 9.90356E-02 MN 2.06282E-03 C 0.00000E+00
 CR 3.29560E-01 NI 3.62083E-02 SI 3.56050E-04 N 0.00000E+00

HCP_A3#2 Status ENTERED Driving force 0.0000E+00
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mass fractions:
 CR 8.27428E-01 MO 3.71106E-02 MN 1.14771E-03 C 2.81566E-04
 N 1.08349E-01 FE 2.45758E-02 NI 1.10769E-03 SI 1.87756E-08
POLY: @@ Rapid cooling is needed to avoid these phases.
POLY: set-inter
... the command in full is SET_INTERACTIVE
POLY:

tce29

SYS:About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

```
SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce29\tce29.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Calculating the speciation of a gas
SYS:
SYS: @@ Note that a SSUB database license is required
SYS: @@ to run the example.
SYS:
SYS: set-log ex29,,
SYS: go da
... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module
Database folder: C:\jenkins\workspace\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA           /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE11: sw ssusb6
... the command in full is SWITCH_DATABASE
Current database: SGTE Substances v6.0

VA DEFINED
TDB_SSUB6: d-sys c o h s
... the command in full is DEFINE_SYSTEM
C          O          H
S DEFINED
TDB_SSUB6: l-sys
... the command in full is LIST SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/: CONSTITUENT
GAS:G      :C C1H1 C1H1O1 C1H1O2 C1H2 C1H2O1 C1H2O2_CIS C1H2O2_DIOXIRANE
C1H2O2_TRANS C1H3 C1H3O1_CH2O1 C1H3O1_CH3O C1H4 C1H4O1 C1H4S1 C1O1 C1O1S1
C1O2 C1S1 C1S2 C2 C2H1 C2H2 C2H2O1 C2H3 C2H4 C2H4O1_ACETALDEHYDE
C2H4O1_OXIRANE C2H4O2_ACETICACID C2H4O2_DIOXETANE C2H4O3_123TRIOXOLANE
C2H4O3_124TRIOXOLANE C2H5 C2H6 C2H6O1_1 C2H6O1_2 C2H6O2 C2O1 C3 C3H1
C3H4_1 C3H4_2 C3H6_1 C3H6_2 C3H6O1_1 C3H6O1_2 C3H8 C3O2 C4 C4H1 C4H10_1
C4H10_2 C4H2_1 C4H2_2 C4H4_1 C4H4_2 C4H6_1 C4H6_2 C4H6_3 C4H6_4 C4H6_5
C4H8_1 C4H8_2 C4H8_3 C4H8_4 C4H8_5 C4H8_6 C5 C60 C6H6 C6H6O1 H H1O1
H1O1S1_HSO H1O1S1_SOH H1O2 H1S1 H2 H2O1_H2O1S1_H2SO H2O1S1_HSOH H2O2
H2O4S1_H2S1 H2S2 O O1S1 O1S2 O2 O2S1 O3 O3S1 S S2 S3 S4 S5 S6 S7 S8:
C_S          :C:
C_L          :C:
DIAMOND      :C:
C1H2O2_L     :C1H2O2:
C1H2S3_L     :C1H2S3:
C1H4_L       :C1H4:
C1H4O1_L     :C1H4O1:
C1H4S1_L     :C1H4S1:
C1S2_L       :C1S2:
C2H4O2_L     :C2H4O2:
C2H6_L       :C2H6:
C2H6O1_L     :C2H6O1:
C2H6O2_L     :C2H6O2:
C3H6_L       :C3H6:
C3H8_L       :C3H8:
C4H8_L       :C4H8:
C6O_S        :C6O:
C6H6_L       :C6H6:
H1O08S1_L    :H1O08S1:
H15O10_5S1_L :H15O10.5S1:
H2O1_L       :H2O1:
H2O2_L       :H2O2:
H2O4S1_L     :H2O4S1:
H2S1_L       :H2S1:
H2S2_L       :H2S2:
H4O5S1_L     :H4O5S1:
H6O6S1_L     :H6O6S1:
H8O7S1_L     :H8O7S1:
O3S1_L       :O3S1:
S_S          :S:
S_S2         :S:
S_L          :S:
TDB_SSUB6:Hit RETURN to continue
TDB_SSUB6: get
... the command in full is GET_DATA
16:09:20,033 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS .....

List of references for assessed data

C1<G> T.C.R.A.S. Class: 1
  C1<G> C<G>
C1H1<G> T.C.R.A.S. Class: 2
  C1H1<G> CH<G>
C1H1O1<G> T.C.R.A.S. Class: 4
  C1H1O1<G> HCO<G>
  FORMYL <GAS>
C1H1O2<G> T.C.R.A.S. Class: 6
  C1H1O2<G>
C1H2<G> T.C.R.A.S. Class: 5
  METHYLENE
  METHYLENE <GAS>
C1H2O1<G> T.C.R.A.S. Class: 5
```

C1H2O1<G> CH2O<G>
 FORMALDEHYDE <GAS>
 C1H2O2_CIS<G> T.C.R.A.S. Class: 5
 C1H2O2_CIS<G>
 C1H2O2_DIOXIRANE<G> T.C.R.A.S. Class: 6
 C1H2O2_DIOXIRANE<G>
 S298 corrected and cp refitted
 due to corrected data in IVTAN2000 7/2002
 C1H2O2_TRANS<G> T.C.R.A.S. Class: 5
 C1H2O2_TRANS<G>
 C1H3<G> T.C.R.A.S. Class: 5
 METHYL Gaseous Standard State.
 METHYL <GAS>
 C1H3O1_CH2OH<G> T.C.R.A.S. Class: 6
 C1H3O1_CH2OH<G>
 C1H3O1_CH3O<G> T.C.R.A.S. Class: 5
 C1H3O1_CH3O<G>
 C1H4<G> T.C.R.A.S. Class: 5
 METHANE. Gaseous Standard State.
 METHANE <GAS>
 C1H4O1<G> T.C.R.A.S. Class: 5
 C1H4O1<G> CH3OH<G>
 METHANOL <GAS>
 C1H4S1<G> THERMODATA 04/98 TC
 METHANETHIOL. Gaseous Standard State.
 C1O1<G> JANAF THERMOCHEMICAL TABLES SGTE **
 C1O1<G> CO<G>
 CARBON MONOXIDE <GAS>
 STANDARD STATE : CODATA KEY VALUE. /CP FROM JANAF PUB. 9/65
 C1O1S1<G> T.C.R.A.S. Class: 2
 C1O1S1<G> COS<G>
 CARBON OXIDE SULFIDE <GAS>
 C1O2<G> T.C.R.A.S. Class: 2
 C1O2<G> CO2<G>
 CARBON DIOXIDE <GAS>
 C1S1<G> T.C.R.A.S. Class: 1
 C1S1<G> CS<G>
 CARBON MONOSULFIDE <GAS>
 C1S2<G> T.C.R.A.S. Class: 3
 C1S2<G> CS2<G>
 CARBON DISULFIDE <GAS>
 C2<G> T.C.R.A.S. Class: 2
 CARBON diatomic Gas.
 CARBON <DIATOMIC GAS>
 C2H1<G> T.C.R.A.S. Class: 6
 C2H1<G> C2H<G>
 CCH RADICAL <GAS>
 C2H2<G> T.C.R.A.S. Class: 2
 ACETYLENE (ETYNE). Gaseous Standard State.
 ACETYLENE <GAS>
 C2H2O1<G> T.C.R.A.S. Class: 6
 C2H2O1<G>
 OXIRENE
 S298 corrected and cp refitted
 due to corrected data in IVTAN2000 7/2002
 C2H3<G> T.C.R.A.S. Class: 6
 DICARBON TRIHYDRIDE Gaseous Standard State.
 C2H4<G> T.C.R.A.S. Class: 6
 ETHYLENE. Gaseous Standard State.
 ETHYLENE <GAS>
 C2H4O1_ACETALDEHYDE<G> T.C.R.A.S. Class: 5
 C2H4O1_ACETALDEHYDE<G>
 C2H4O1_OXIRANE<G> T.C.R.A.S. Class: 6
 C2H4O1_OXIRANE<G>
 S298 corrected and cp refitted
 due to corrected data in IVTAN2000 7/2002
 C2H4O2_ACETICACID<G> T.C.R.A.S. Class: 5
 C2H4O2_ACETICACID<G>
 C2H4O2_DIOXETANE<G> T.C.R.A.S. Class: 6
 C2H4O2_DIOXETANE<G>
 S298 corrected and cp refitted
 due to corrected data in IVTAN2000 7/2002
 typing error corrected 12/06
 C2H4O3_123TRIOXOLANE<G> T.C.R.A.S. Class: 7
 C2H4O3_123TRIOXOLANE<G>
 S298 corrected and cp refitted
 due to corrected data in IVTAN2000 7/2002
 C2H4O3_124TRIOXOLANE<G> T.C.R.A.S. Class: 7
 C2H4O3_124TRIOXOLANE<G>
 S298 corrected and cp refitted
 due to corrected data in IVTAN2000 7/2002
 typing error corrected 12/06
 C2H5<G> T.C.R.A.S. Class: 6
 ETHYL radical. Gaseous Standard State.
 C2H6<G> T.C.R.A.S. Class: 6
 ETHANE. Gaseous Standard State.
 C2H6O1_1<G> THERMODATA 04/98 TC
 ETHANOL. Gaseous Standard State.
 C2H6O1_2<G> THERMODATA 04/98 TC
 DIMETHYL ETHER. Gaseous Standard State.
 C2H6O2<G> THERMODATA
 C2H6O2<G>
 E-GLYCOL <GAS>. Data revised by THDA.
 C2O1<G> T.C.R.A.S. Class: 5
 C2O1<G>
 C3<G> T.C.R.A.S. Class: 6
 CARBON triatomic gas.
 CARBON <TRIATOMIC GAS>
 C3H1<G> T.C.R.A.S. Class: 6
 C3H1<G>
 2-PROPYNYLIDYNE
 S298 corrected and cp refitted
 due to corrected data in IVTAN2000 7/2002
 C3H4_1<G> STULL WESTRUM SINKE 1969 SGTE
 C3H4_1<G>
 ALLENE = 1,2-PROPADIENE
 EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.
 C3H4_2<G> STULL WESTRUM SINKE 1969 SGTE
 C3H4_2<G>
 PROPYNIE (METHYLACETYLENE)
 EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.
 C3H6O1_1<G> THERMODATA 04/98 TC
 2-PROPENOL (ALLYL ALCOHOL). Gaseous Standard State.
 C3H6O1_2<G> THERMODATA 04/98 TC
 DL-METHYLOXIRANE. Gaseous Standard State.
 C3H6_1<G> T.C.R.A.S. Class: 6 4.09.85

C3H6 (G) Cyclopropane
C3H6_2<G> STULL WESTRUM SINKE 1969 SGTE
PROPENE
PROPENE
EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.
C3H8<G> THERMODATA SGTE
PROPANE. Gaseous Standard State.
PROPANE <GAS>
PROPANE
C3O2<G> T.C.R.A.S. Class: 6
C3O2<G>
C4<G> T.C.R.A.S. Class: 7
C4<G>
C4H1<G> T.C.R.A.S Class: 6
1,3-BUTADIYNYL Gaseous Standard State.
1,3-BUTADIYNYL. Data provided by T.C.R.A.S. in 2000
C4H10_1<G> T.C.R.A.S Class: 4
BUTANE Gaseous Standard State.
BUTANE. Data provided by T.C.R.A.S. in 2000
C4H10_2<G> T.C.R.A.S Class: 4
METHYLPROPANE N-BUTANE Gaseous Standard State.
METHYLPROPANE N-BUTANE. Data provided by T.C.R.A.S. in 2000
C4H2_1<G> THERMODATA 1978 ST
1,3-BUTADIYNE. Gaseous Standard State.
C4H2_2<G> THERMODATA 06/93 ST
BUTADIYNE(BIACETYLENE). Gaseous Standard State.
C4H4_1<G> T.C.R.A.S Class: 6
1,3-CYCLOBUTADIENE Gaseous Standard State.
1,3-CYCLOBUTADIENE. Data provided by T.C.R.A.S. in 2000
C4H4_2<G> STULL WESTRUM SINKE 1969 SGTE
1-BUTEN-3-YNE VINYLACETYLENE. Gaseous Standard State.
1-BUTEN-3-YNE VINYLACETYLENE
EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.
C4H6_1<G> STULL WESTRUM SINKE 1969 SGTE
C4H6_1<G>
1,2-BUTADIENE
EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.
C4H6_2<G> STULL WESTRUM SINKE 1969 SGTE
C4H6_2<G>
1,3-BUTADIENE
EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.
C4H6_3<G> STULL WESTRUM SINKE 1969 SGTE
C4H6_3<G>
1-BUTYNE ETHYLACETYLENE
EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.
C4H6_4<G> STULL WESTRUM SINKE 1969 SGTE
C4H6_4<G>
CYCLOBUTENE. Data provided by T.C.R.A.S. in 2000
C4H8_1<G> THERMODATA 04/98 TC
1-BUTENE. Gaseous Standard State.
C4H8_2<G> THERMODATA 04/98 TC
(E)-2-BUTENE. Gaseous Standard State.
C4H8_3<G> THERMODATA 04/98 TC
(Z)-2-BUTENE. Gaseous Standard State.
C4H8_4<G> THERMODATA 04/98 TC
CYCLOBUTANE. Gaseous Standard State.
C4H8_5<G> THERMODATA 04/98 TC
2-METHYLPROPENE. Gaseous Standard State.
C4H8_6<G> THERMODATA 04/98 TC
METHYLCYCLOPROPANE. Gaseous Standard State.
C5<G> T.C.R.A.S. Class: 7
C5<G>
C60<G> MHR-95
C60<G>
Data processed from [94Kor/Sid] M.V. Korobov, L.N. sidorov,
J. Chem. Thermo., 26, 61-73 (1994). Recalculated from the rotational
data in [91McK] and vibration frequencies in [94Kor/Sid]. Note that
a frequency with degeneracy 5 is missing from list in [94Kor/Sid];
taken to be 419 cm⁻¹, which gives very good, though not exact,
agreement with values quoted in [94Kor/Sid]. Note discrepancy
between calculated DrS(298) = -8943.5 J mol K⁻¹ for the reaction
60<g>=C60<g>and that given by [94Kor/Sid] in their Table 5,
-8950 J mol K⁻¹. Enthalpy of formation: DfH₀ = 2588 kJ/mol from
DsubH(298.15K) = 166 +/- 11 kJ mol⁻¹ [94Kor/Sid]. Vapour pressure
values reproduced very well.
[91McK] J.T. McKinnon, J. Phys. Chem. 95 8941(1993).
C6H6<G> T.C.R.A.S Class: 5
BENZENE. Gaseous Standard State.
BENZENE. Data provided by T.C.R.A.S. in 2000
C6H601<G> THERMODATA 01/93
C6H601<G>
PHENOL
28/01/93
H1<G> JANAF 1982; ASSESSMENT DATED 3/77 SGTE **
H1<G> H<G>
HYDROGEN <MONATOMIC GAS>
H1O1<G> T.C.R.A.S. Class: 1
H1O1<G> OH<G>
H1O1S1_HSO<G> T.C.R.A.S. Class: 4
H1O1S1_HSO<G>
H1O1S1_SOH<G> T.C.R.A.S. Class: 5
H1O1S1_SOH<G>
H1O2<G> T.C.R.A.S. Class: 4
H1O2<G>
H1S1<G> T.C.R.A.S. Class: 2
H1S1<G>
H2<G> H2<G>
HYDROGEN<G>
STANDARD STATE FROM CODATA KEY VALUES. CP FROM JANAF PUB. 3/61
H2O1<G> T.C.R.A.S. Class: 1
H2O1<G> H2O<G>
WATER <GAS>
H2O1S1_H2SO<G> T.C.R.A.S. Class: 4
H2O1S1_H2SO<G>
H2O1S1_HSOH<G> T.C.R.A.S. Class: 4
H2O1S1_HSOH<G>
H2O2<G> JANAF SECOND EDIT SGTE
H2O2<G> H2O2<G>
HYDROGEN PEROXIDE <GAS>
H2O4S1<G> JANAF 1982; ASSESSMENT DATED 9/77 SGTE
H2O4S1<G> H2SO4<G>

SULFURIC ACID <GAS>
 H2S1<G> T.C.R.A.S. Class: 2
 H2S1<G> H2S<G>
 HYDROGEN SULFIDE <GAS>
 H2S2<G> K.C. MILLS SGTE **
 H2S2<G> H2S2<G>
 DIHYDROGEN DISULFIDE <GAS>
 O1<G> TCRAS 02/06/80
 O1 Gaseous Standard State.
 O1S1<G> T.C.R.A.S. Class: 3
 O1S1<G> SO<G>
 SULFUR MONOXIDE <GAS>
 O1S2<G> JANAF THERMOCHEMICAL TABLES SGTE **
 O1S2<G> S2<G>
 DISULFUR MONOXIDE <GAS>
 PUBLISHED BY JANAF AT 9/65
 O2<G> TCRAS 21/06/90
 OXYGEN Gaseous Standard State.
 O2S1<G> JANAF THERMOCHEMICAL TABLES SGTE **
 O2S1<G> SO2<G>
 SULFUR DIOXIDE <GAS>
 PUBLISHED BY JANAF AT 6/61
 O3<G> TCRAS 02/06/80
 OZONE Gaseous Standard State.
 O3S1<G> JANAF THERMOCHEMICAL TABLES SGTE **
 O3S1<G> SO3<G>
 SULFUR TRIOXIDE <GAS>
 PUBLISHED BY JANAF AT 9/65
 S1<G> T.C.R.A.S. Class: 1
 S1<G> S<G>
 SULFUR <GAS>
 S2<G> T.C.R.A.S. Class: 4
 S2<G> S2<G>
 SULFUR <DIATOMIC GAS>
 S3<G> T.C.R.A.S. Class: 5
 S3<G> S3<G>
 SULFUR <3-ATOMIC GAS>
 S4<G> T.C.R.A.S. Class: 6
 S4<G> S4<G>
 SULFUR <4-ATOMIC GAS>
 S5<G> T.C.R.A.S. Class: 6
 S5<G> S5<G>
 SULFUR <5-ATOMIC GAS>
 S6<G> T.C.R.A.S. Class: 6
 S6<G> S6<G>
 SULFUR <6-ATOMIC GAS>
 S7<G> T.C.R.A.S. Class: 7
 S7<G> S7<G>
 SULFUR <7-ATOMIC GAS>
 S8<G> T.C.R.A.S. Class: 7
 S8<G> S8<G>
 SULFUR <OCTATOMIC GAS>
 C1H2O2<L> THERMODATA 01/93
 C1H2O2 HCOOH
 FORMIC ACID MONOMERIC
 28/01/93
 C1H2S3<L> THERMODATA 01/86 BC
 TRITHIO-CARBONIC ACID. Liquid Standard State.
 C1H4O1<L> I. BARIN 3rd. Edition
 C1H4O1 CH3OH
 METHANOL. H298 and S298 modified.
 C1H4S1<L> THERMODATA 04/99 HH
 METHANETHIOL. Liquid Standard State.
 C1H4<L> THERMODATA 04/99 HH
 METHANE Liquid Standard State.
 C1S2<L> KUBASCHEWSKI EVANS ALCOCK 1967 SGTE
 C1S2 CS2
 CARBON DISULFIDE
 C1S2 MELTS AT 161.15K LF=1.05(0.1) KCAL/MOLE
 C2H4O2<L> THERMODATA 01/93
 C2H4O2
 ACETIC ACID
 28/01/93 Tb=389K.
 C2H6O1<L> THERMODATA 01/93
 C2H6O1 C2H6O
 ETHANOL
 28/01/93
 C2H6O2<L> THERMODATA
 C2H6O2
 E-GLYCOL
 Data revised by THDA.
 C2H6<L> THERMODATA 04/99 HH
 ETHANE Liquid Standard State.
 C3H6<L> THERMODATA 03/05 HH
 CYCLOPROPANE. Liquid Standard State.
 C3H8<L> THERMODATA 04/99 HH
 PROPANE Liquid Standard State
 C4H8<L> THERMODATA 04/99 HH
 CYCLOBUTANE. Liquid Standard State.
 C60 MHR-95
 C60
 Data processed from [94Kor/Sid] M.V. Korobov, L.N. sidorov, J. Chem.
 The
 Fitted to the data in [94Kor/Sid], who took the phase transition at
 257K
 that [94Kor/Sid] do not give an explicit value for S(298.15K).
 S(298.15K) = 422.6 J mol K-1 was calculated from S(300) = 425.8 and Cp
 e
 calculated from DrS(298) for 60C<graphite>=C60 given by [94Kor/Sid]
 in their Table 5, which gives S(298.15K) = 425.4 J mol K-1.
 Enthalpy of formation : DfH = +2422 +/- 14 kJ/mol from [92Ste/Chi],
 the value preferred, if obliquely, by [94Kor/Sid].
 [92Ste/Chi]W.V. Steele, R.D. Chirico, N.K. Smith, W.e. Billups,
 P.R. Elmore, A.E. Wheeler, J. Phys. Chem. 96 4731 (1993).
 C6H6<L> THERMODATA 04/99 BC
 BENZENE. Liquid Standard State. Tm=278.6K
 C1 S.G.T.E. **
 GRAPHITE
 Data from SGTE Unary DB, pressure dependent data added by atd 7/9/95
 C1<DIAMOND> S.G.T.E. **
 C1<DIAMOND> <DIAMOND>
 DIAMOND
 Data from SGTE Unary DB, data added by atd 7/9/95, H298-H0 taken
 from 1994 database (ex THERMODATA 01/93)
 H10O8S1<L> THERMODATA 01/93
 H10O8S1

SULFURIC ACID TETRAHYDRATE.
 28/01/93
 H15O10.5S1<L> THERMODATA 01/93
 H15O10.5S1
 SULFURIC ACID HEMIHEXAHYDRATE.
 28/01/93
 H2O1<L> T.C.R.A.S. Class: 4
 H2O1 H2O
 WATER
 T.C.R.A.S. Class: 4 cp modified by atd 12/9/94 and 5/7/2002
 H2O2<L> THERMODATA 01/93
 H2O2 H2O2
 HYDROGEN PEROXIDE
 28/01/93
 H2O4S1<L> THERMODATA 01/93
 H2O4S1 H2SO4
 SULFURIC ACID
 28/01/93 Tb = 553K.
 S298 modified by NPL 24/11/94. Negative value in Thermodata.
 H2S1<L> THERMODATA 12/94 KK
 HYDROGEN SULFIDE. Liquid Standard State.
 H2S2<L> THERMODATA 11/99 KK
 Liquid standard State.
 H4O5S1<L> THERMODATA 01/93
 H4O5S1
 SULFURIC ACID MONOHYDRATE.
 28/01/93
 H6O6S1<L> THERMODATA 01/93
 H6O6S1
 H2SO4-2H2O
 28/01/93
 H8O7S1<L> Janaf 4th. Edition
 H8O7S1 H2SO4.3H2O
 SULFURIC ACID TRIHYDRATE
 O3S1<L> THERMODATA 12/94 KK
 SULFUR OXIDE BETA. Liquid Standard State.
 S1 T.C.R.A.S Class: 5
 S1
 Data provided by T.C.R.A.S. October 1994.
 Data refitted by I.A.

-OK-

TDB_SSUB6: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32

POLY: l-st c

... the command in full is LIST_STATUS

*** STATUS FOR ALL COMPONENTS

| COMPONENT | STATUS | REF. | STATE | T (K) | P (Pa) |
|-----------|---------|------|-------|-------|--------|
| VA | ENTERED | SER | | | |
| C | ENTERED | SER | | | |
| H | ENTERED | SER | | | |
| O | ENTERED | SER | | | |
| S | ENTERED | SER | | | |

POLY: s-i-a n(h2)=10

... the command in full is SET_INPUT_AMOUNTS

POLY: l-c

... the command in full is LIST CONDITIONS

N(H)=20

DEGREES OF FREEDOM 5

POLY: s-i-a n(clo2)=5

... the command in full is SET_INPUT_AMOUNTS

POLY: s-i-a n(o2s1)=0.1

... the command in full is SET_INPUT_AMOUNTS

POLY: l-c

... the command in full is LIST CONDITIONS

N(H)=20, N(C)=5, N(O)=10.2, N(S)=0.1

DEGREES OF FREEDOM 2

POLY: s-c t=1000 p=1e5

... the command in full is SET_CONDITION

POLY: c-e

... the command in full is COMPUTE_EQUILIBRIUM

Using global minimization procedure

| Calculated | 132 grid points in | 4 s |
|--|--------------------|-----|
| Found the set of lowest grid points in | | 0 s |
| Calculated POLY solution | 0 s, total time | 4 s |

POLY: l-e

... the command in full is LIST_EQUILIBRIUM

OUTPUT TO SCREEN OR FILE /SCREEN/:

Options /VWCS/: VWCS

Output from POLY-3, equilibrium = 1, label A0 , database: SSUB6

Conditions:

N(H)=20, N(C)=5, N(O)=10.2, N(S)=0.1, T=1000, P=100000

DEGREES OF FREEDOM 0

Temperature 1000.00 K (726.85 C), Pressure 1.000000E+05

Number of moles of components 3.53000E+01, Mass in grams 2.46609E+02

Total Gibbs energy -4.82824E+06, Enthalpy -1.54921E+06, Volume 1.23971E+00

| Component | Moles | W-Fraction | Activity | Potential | Ref.stat |
|-----------|------------|------------|------------|-------------|----------|
| C | 5.0000E+00 | 2.4352E-01 | 3.4847E-02 | -2.7910E+04 | SER |
| H | 2.0000E+01 | 8.1741E-02 | 1.0525E-04 | -7.6154E+04 | SER |
| O | 1.0200E+01 | 6.6173E-01 | 7.2141E-17 | -3.0903E+05 | SER |
| S | 1.0000E-01 | 1.3003E-02 | 9.1466E-08 | -1.3476E+05 | SER |

| GAS | Status | ENTERED | Driving force | 0.0000E+00 |
|--|--------|---------|-----------------|------------|
| Moles 3.53000E+01, Mass 2.4661E+02, Volume fraction 1.0000E+00 | | | Mass fractions: | |
| O 6.61734E-01 C 2.43523E-01 H 8.17406E-02 S 1.30027E-02 | | | | |

Constitution:

| | | | | | |
|--------------|-------------|--------------|-------------|----------|-------------|
| H2 | 4.42736E-01 | H1O1S1_SOH | 3.35036E-14 | C4H8_6 | 1.82465E-21 |
| H2O1 | 2.15350E-01 | C2H6O1_1 | 2.75193E-14 | O2 | 1.79235E-21 |
| C1O1 | 1.95778E-01 | C2H5 | 2.60816E-14 | C2O1 | 1.66878E-21 |
| C1O2 | 1.36417E-01 | C3H8 | 1.55219E-14 | S5 | 8.95084E-22 |
| H2S1 | 6.57218E-03 | C1H3O1_CH2OH | 7.69302E-15 | C2H2O1 | 5.16353E-22 |
| C1H4 | 3.01187E-03 | H2O1S1_H2SO | 2.59570E-15 | C4H6_5 | 3.26857E-22 |
| C1O1S1 | 1.34465E-04 | C2H3 | 1.30277E-15 | C3H6O1_2 | 9.94895E-23 |
| H1S1 | 5.08063E-08 | C3H4_2 | 1.28184E-15 | C4H8_4 | 5.15316E-23 |
| C1H2O1 | 4.89873E-08 | C3O2 | 7.11139E-16 | H2O4S1 | 1.59729E-23 |
| C1H2O2_CIS | 4.46604E-08 | C3H4_1 | 3.44164E-16 | C4H2_1 | 8.50232E-24 |
| H2S2 | 3.75745E-08 | H1O1S1_HSO | 1.08974E-16 | C4H2_2 | 8.48033E-24 |
| C1S2 | 1.41821E-08 | C3H6_1 | 5.22179E-17 | C6H6O1 | 6.55562E-24 |
| S2 | 1.10500E-08 | C1H3O1_CH3O | 1.80849E-17 | H1O2 | 1.72311E-24 |
| C1H2O2_TRANS | 6.42811E-09 | C2H6O1_2 | 9.96672E-18 | C2H1 | 3.18714E-25 |
| C2H6 | 3.64609E-09 | C2H4O1_OXIRA | 2.11511E-18 | S6 | 2.65463E-26 |

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C2H4      3.02667E-09 C4H6_2      1.29360E-18 C1H1      5.08634E-27
H       1.51148E-09 S4        1.12104E-18 C4H4_1      4.75003E-27
C1H4O1    1.14083E-09 C4H8_5      6.89221E-19 C3H1      9.91558E-28
O2S1      2.26895E-10 C4H8_1      5.18832E-19 C1H2O2_DIOXI 4.40433E-30
C1H3      1.88514E-10 C4H8_2      4.53214E-19 C          1.00000E-30
C1H4S1    1.76437E-10 C4H8_3      3.93010E-19 C2        1.00000E-30
H2O1S1_HSOH 8.67082E-11 C3H6O1_1  2.60648E-19 C2H4O2_DIOXE 1.00000E-30
C2H4O1_ACETA 2.61120E-11 C2H6O2  2.59417E-19 C2H4O3_123TR 1.00000E-30
C2H2      1.43254E-11 C1H2        2.13894E-19 C2H4O3_124TR 1.00000E-30
O1S1      1.05406E-11 C4H10_1     8.31953E-20 C3        1.00000E-30
C1H1O1    9.19785E-12 C4H10_2     4.22679E-20 C4        1.00000E-30
C1S1      5.40802E-12 C6H6        3.95182E-20 C4H1      1.00000E-30
C2H4O2_ACETI 4.53120E-12 H2O2     2.47048E-20 C5        1.00000E-30
H1O1      1.61961E-12 C4H6_4      1.91129E-20 C6O       1.00000E-30
O1S2      9.69426E-13 O3S1        1.73550E-20 O3        1.00000E-30
C1H1O2    9.05180E-13 C4H6_1      1.14077E-20 S7       1.00000E-30
S         7.19264E-13 O          6.65398E-21 S8        1.00000E-30
S3        1.46179E-13 C4H6_3      6.48690E-21
C3H6_2    1.11399E-13 C4H4_2      3.35580E-21

POLY: Hit RETURN to continue
POLY: s-a-v 1 t 500 2000 50
... the command in full is SET_AXIS_VARIABLE
POLY: save tcex29 y
... the command in full is SAVE_WORKSPACES
POLY:

POLY: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 1000.00
...OK

Phase Region from 1000.00 for:
  GAS
Global test at 1.08000E+03 .... OK
Global test at 1.18000E+03 .... OK
Global test at 1.28000E+03 .... OK
Global test at 1.38000E+03 .... OK
Global test at 1.48000E+03 .... OK
Global test at 1.58000E+03 .... OK
Global test at 1.68000E+03 .... OK
Global test at 1.78000E+03 .... OK
Global test at 1.88000E+03 .... OK
Global test at 1.98000E+03 .... OK
Terminating at 2000.00
Calculated 103 equilibria

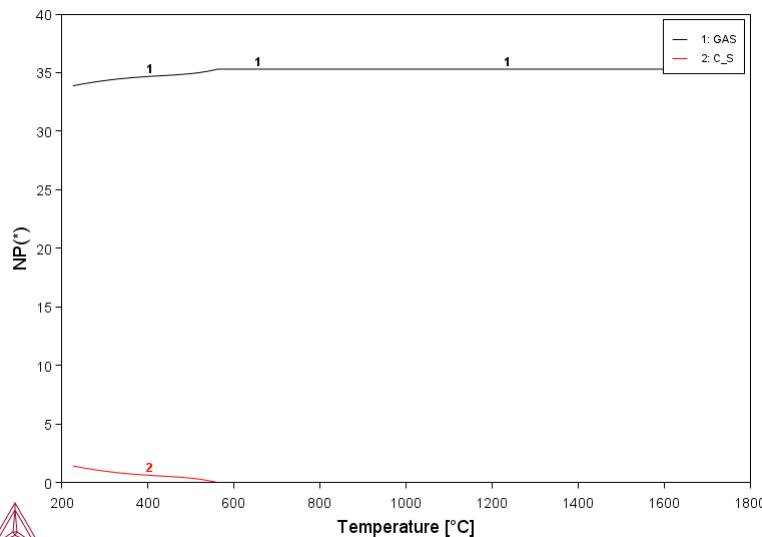
Phase Region from 1000.00 for:
  GAS
Global test at 9.20000E+02 .... OK
Global check of adding phase at 8.35809E+02
Calculated 19 equilibria

Phase Region from 835.809 for:
  GAS
  C_S
Global test at 7.60000E+02 .... OK
Global test at 6.60000E+02 .... OK
Global test at 5.60000E+02 .... OK
Terminating at 500.000
Calculated 37 equilibria
*** Buffer saved on file: c:\jenkins\workspace\generate_console_examples\examples\tcex29\tcex29.POLY3
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2
Setting automatic diagram axes

POST:
POST: @@ Plot the amount of phases (mainly gas)
POST: s-d-a x t-c
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y np(*)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*:
POST: s-l f
... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 29a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 29a

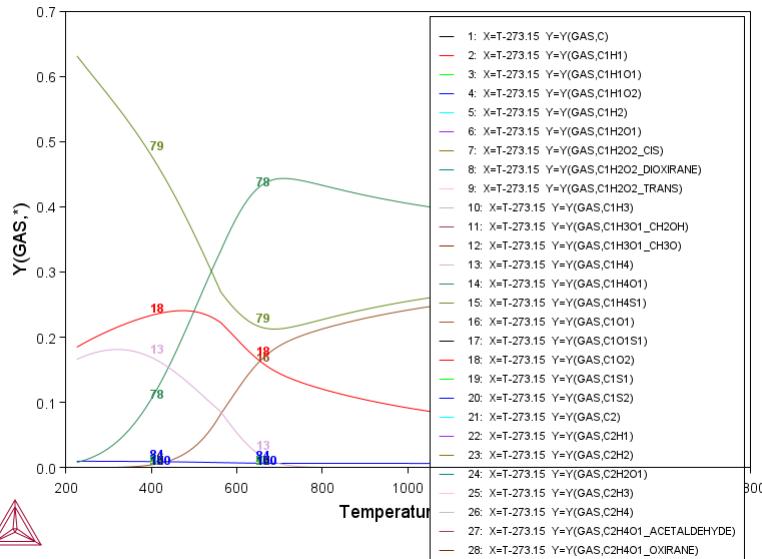


```

POST:
POST:Hit RETURN to continue
POST: @@ Plot gas speciation. y(gas,*) are partial
POST: @@ pressures expressed in bar (as total pressure
POST: @@ is one bar). Set labels on the lines.
POST: s-d-a y y(gas,*)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*:
POST: set-title example 29b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 29b

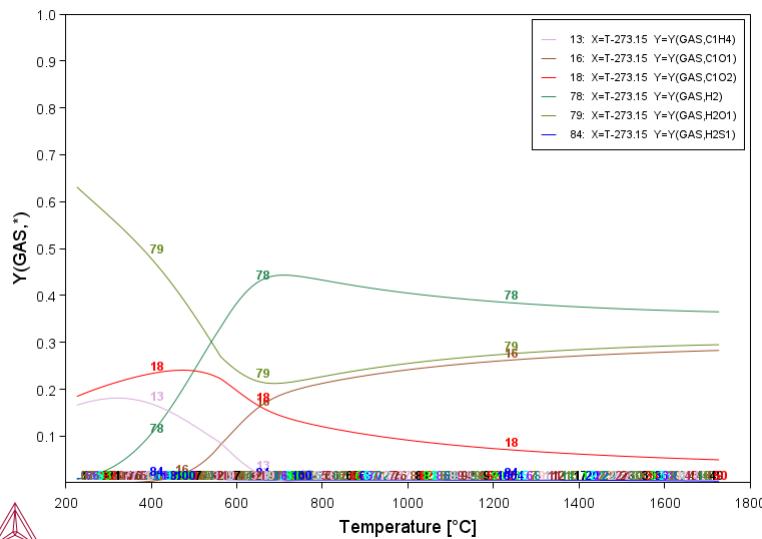


```

POST:Hit RETURN to continue
POST: @@ To avoid cluttered labels, change the scaling
POST: @@ so only major species are visible
POST: s-s y n 0.001 1
... the command in full is SET_SCALING_STATUS
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

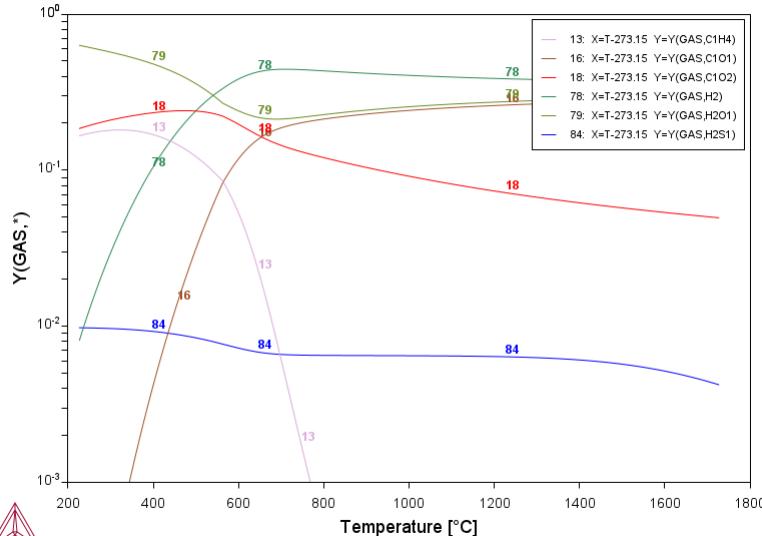
```

example 29b



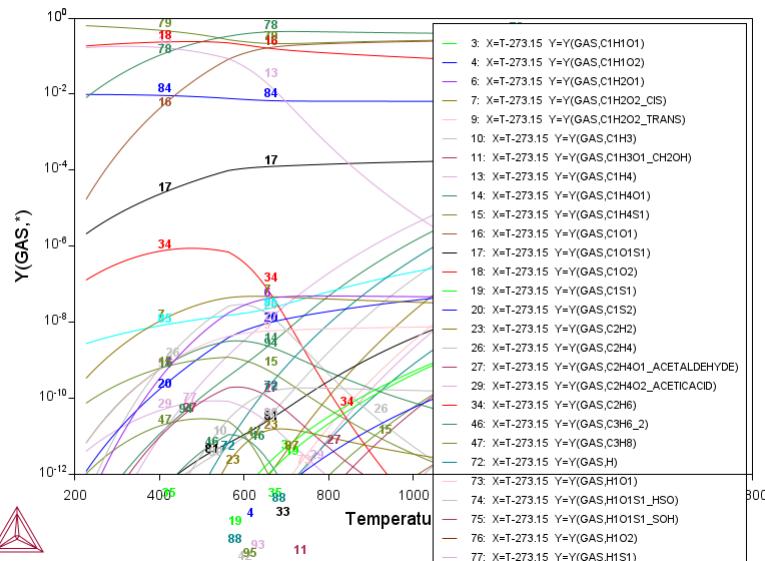
```
POST: Hit RETURN to continue
POST: @@ Set a logarithmic axis
POST: s=ax-ty
... the command in full is SET_AXIS_TYPE
AXIS (X, Y OR Z) : y
AXIS TYPE /LINEAR/: log
POST:
POST: set-title example 29c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
```

example 29c



```
POST:
POST: Hit RETURN to continue
POST: @@ Set scaling
POST: s-s y n 1e-12 1
... the command in full is SET_SCALING_STATUS
POST: set-title example 29d
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
```

example 29d



POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:

tce30A

SYS:About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

```
SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce30A\tce30A.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Scheil calculation for an Al-4Mg-2Si-2Cu alloy
SYS:
SYS: @@ This is the first of two examples showing how to
SYS: @@ do a Scheil calculation for an Al-4Mg-2Si-2Cu alloy.
SYS: @@ In part A, you use the POLY3 module and the
SYS: @@ STEP_WITH_OPTIONS command with an EVALUATE setting.
SYS: @@ Then in part B you use the SCHEIL module commands to
SYS: @@ do the same thing.
SYS:
SYS: go da
THERMODYNAMIC DATABASE module
Database folder: C:\jenkins\workspace\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA          /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE11: sw user tce30_cost2.TDB
Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

VA          /- DEFINED
16:10:52,913 [Thread-0] INFO TDBfileParser: USER_1232666241_14, number of lines read: 880
16:10:53,242 [Thread-0] INFO DatabaseUtils: Parsing of USER_1232666241_14 completed in 378 ms
TDB_USER: def-ele al cu mg si
          CU          MG
SI DEFINED
TDB_USER: get
16:10:53,355 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS .....

List of references for assessed data

'COST2 - TCOST507 Light Alloys Database (Version 2.1), provided by TCSAB,
1999/2003. '
'COST (1998): COST 507 -- Definition of Thermochemical and Thermophysical
Properties to Provide a Database for the Development of New Light
Alloys. European Cooperation in the Field of Scientific and Technical
Research, European Commission. Vol 1. Proceedings of the Final
Workshop of COST 507, Vaals, the Netherlands, 1997; Vol 2.
Thermochemical Database for Light Metal Alloys (Eds. Ansara I.,
Dinsdale A.T., and Rand M.H.); Vol 3. Critical Evaluation of Ternary
Systems (Ed. Effenberg G.). '

-OK-
TDB_USER: go p-3

POLY version 3.32
POLY: s-c p=101325 n=1 t=1000 w(si)=0.02 w(mg)=0.04 w(cu)=0.02
POLY: c-e
Using global minimization procedure
16:10:54,036 [Thread-0] INFO Database: Preparing system for use: USER_1232666241_14
16:10:54,930 [Thread-0] INFO Phase: Preparing phase for use: LIQUID
16:10:55,406 [Thread-0] INFO Phase: Preparing phase for use: AL12MG17
16:10:55,861 [Thread-0] INFO Phase: Preparing phase for use: ALCE_AMORPHOUS
16:10:56,228 [Thread-0] INFO Phase: Preparing phase for use: ALCUZN_T
16:10:56,605 [Thread-0] INFO Phase: Preparing phase for use: ALCU_DELTA
16:10:57,016 [Thread-0] INFO Phase: Preparing phase for use: ALCU_EPSILON
16:10:57,376 [Thread-0] INFO Phase: Preparing phase for use: ALCU_ETA
16:10:57,746 [Thread-0] INFO Phase: Preparing phase for use: ALCU_PRIME
16:10:58,115 [Thread-0] INFO Phase: Preparing phase for use: ALCU_THETA
16:10:58,473 [Thread-0] INFO Phase: Preparing phase for use: ALCU_ZETA
16:10:58,831 [Thread-0] INFO Phase: Preparing phase for use: ALLI
16:10:59,192 [Thread-0] INFO Phase: Preparing phase for use: ALMG_BETA
16:10:59,553 [Thread-0] INFO Phase: Preparing phase for use: ALMG_EPS
16:10:59,907 [Thread-0] INFO Phase: Preparing phase for use: ALMG_GAMMA
16:11:00,271 [Thread-0] INFO Phase: Preparing phase for use: ALMO
16:11:00,628 [Thread-0] INFO Phase: Preparing phase for use: ALM_D019
16:11:00,982 [Thread-0] INFO Phase: Preparing phase for use: ALND_AMORPHOUS
16:11:01,334 [Thread-0] INFO Phase: Preparing phase for use: ALTI
16:11:01,688 [Thread-0] INFO Phase: Preparing phase for use: BCC_B2
16:11:02,043 [Thread-0] INFO Phase: Preparing phase for use: BCC_A2
16:11:02,422 [Thread-0] INFO Phase: Preparing phase for use: BCT_A5
16:11:02,779 [Thread-0] INFO Phase: Preparing phase for use: CBCC_A12
16:11:03,141 [Thread-0] INFO Phase: Preparing phase for use: CR3Si_A15
16:11:03,504 [Thread-0] INFO Phase: Preparing phase for use: CRSI2
16:11:03,863 [Thread-0] INFO Phase: Preparing phase for use: CU19Si6_ETA
16:11:04,219 [Thread-0] INFO Phase: Preparing phase for use: CU33Si7_DELTA
16:11:04,573 [Thread-0] INFO Phase: Preparing phase for use: CU4Si_EPSILON
16:11:04,927 [Thread-0] INFO Phase: Preparing phase for use: CU56Si11_GAMMA
16:11:05,283 [Thread-0] INFO Phase: Preparing phase for use: CU6Y
16:11:05,636 [Thread-0] INFO Phase: Preparing phase for use: CUB_A13
16:11:05,993 [Thread-0] INFO Phase: Preparing phase for use: CUB_A15
16:11:06,348 [Thread-0] INFO Phase: Preparing phase for use: CUMG2
16:11:06,703 [Thread-0] INFO Phase: Preparing phase for use: CUMGSi_SIGMA
16:11:07,059 [Thread-0] INFO Phase: Preparing phase for use: CUMGSi_TAU
16:11:07,411 [Thread-0] INFO Phase: Preparing phase for use: CUZN_GAMMA
16:11:07,760 [Thread-0] INFO Phase: Preparing phase for use: DIAMOND_A4
16:11:08,111 [Thread-0] INFO Phase: Preparing phase for use: FCC_A1
16:11:08,470 [Thread-0] INFO Phase: Preparing phase for use: GAMMA_D83
16:11:08,824 [Thread-0] INFO Phase: Preparing phase for use: GAMMA_H
16:11:09,176 [Thread-0] INFO Phase: Preparing phase for use: HCP_A3
16:11:09,534 [Thread-0] INFO Phase: Preparing phase for use: HCP_ZN
```

```

16:11:09,895 [Thread-0] INFO Phase: Preparing phase for use: LAVES_C14
16:11:10,261 [Thread-0] INFO Phase: Preparing phase for use: LAVES_C15
16:11:10,624 [Thread-0] INFO Phase: Preparing phase for use: LAVES_C36
16:11:10,984 [Thread-0] INFO Phase: Preparing phase for use: MG24Y5
16:11:11,336 [Thread-0] INFO Phase: Preparing phase for use: MG2SI
16:11:11,691 [Thread-0] INFO Phase: Preparing phase for use: MG2Y
16:11:12,048 [Thread-0] INFO Phase: Preparing phase for use: MG2ZN11
16:11:12,402 [Thread-0] INFO Phase: Preparing phase for use: MG2ZN3
16:11:12,752 [Thread-0] INFO Phase: Preparing phase for use: MGY_GAMMA
16:11:13,104 [Thread-0] INFO Phase: Preparing phase for use: MGZN
16:11:13,457 [Thread-0] INFO Phase: Preparing phase for use: PHI
16:11:13,807 [Thread-0] INFO Phase: Preparing phase for use: QPHASE
16:11:14,158 [Thread-0] INFO Phase: Preparing phase for use: SIV3
16:11:14,505 [Thread-0] INFO Phase: Preparing phase for use: SPHASE
16:11:14,852 [Thread-0] INFO Phase: Preparing phase for use: TAU
16:11:15,210 [Thread-0] INFO Phase: Preparing phase for use: VPHASE
Calculated 26538 grid points in 32 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 32 s
POLY: l-e,
Options /VWCS/:
Output from POLY-3, equilibrium = 1, label A0 , database: USER

Conditions:
P=101325, N=1, T=1000, W(SI)=2E-2, W(MG)=4E-2, W(CU)=2E-2
DEGREES OF FREEDOM 0

Temperature 1000.00 K ( 726.85 C), Pressure 1.013250E+05
Number of moles of components 1.00000E+00, Mass in grams 2.71965E+01
Total Gibbs energy -4.56562E+04, Enthalpy 3.06144E+04, Volume 0.00000E+00

Component Moles W-Fraction Activity Potential Ref.stat
AL 9.2731E-01 9.2000E-01 5.4982E-03 -4.3263E+04 SER
CU 8.5596E-03 2.0000E-02 5.9020E-07 -1.1925E+05 SER
MG 4.4759E-02 4.0000E-02 1.0064E-04 -7.6526E+04 SER
SI 1.9367E-02 2.0000E-02 1.1370E-03 -5.6367E+04 SER

LIQUID Status ENTERED Driving force 0.0000E+00
Moles 1.00000E+00, Mass 2.7197E+01, Volume fraction 0.0000E+00 Mass fractions:
AL 9.20000E-01 MG 4.00000E-02 SI 2.00000E-02 CU 2.00000E-02
POLY: @@ calculate liquidus temperature in order to choose

POLY: @@ a starting temperature where only liquid exists
POLY: c-st phase fcc_a1=fix 0
POLY: s-c t=None
POLY: c-e
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated 26538 grid points in 1 s
12 ITS, CPU TIME USED 1 SECONDS
POLY: l-e,
Options /VWCS/:
Output from POLY-3, equilibrium = 1, label A0 , database: USER

Conditions:
P=101325, N=1, W(SI)=2E-2, W(MG)=4E-2, W(CU)=2E-2
FIXED PHASES
FCC_A1=0
DEGREES OF FREEDOM 0

Temperature 897.74 K ( 624.59 C), Pressure 1.013250E+05
Number of moles of components 1.00000E+00, Mass in grams 2.71965E+01
Total Gibbs energy -3.80281E+04, Enthalpy 2.73862E+04, Volume 0.00000E+00

Component Moles W-Fraction Activity Potential Ref.stat
AL 9.2731E-01 9.2000E-01 8.2190E-03 -3.5838E+04 SER
CU 8.5596E-03 2.0000E-02 5.5836E-07 -1.0747E+05 SER
MG 4.4759E-02 4.0000E-02 1.2754E-04 -6.6933E+04 SER
SI 1.9367E-02 2.0000E-02 2.2867E-03 -4.5388E+04 SER

LIQUID Status ENTERED Driving force 0.0000E+00
Moles 1.00000E+00, Mass 2.7197E+01, Volume fraction 0.0000E+00 Mass fractions:
AL 9.20000E-01 MG 4.00000E-02 CU 2.00000E-02 SI 2.00000E-02

FCC_A1 Status FIXED Driving force 0.0000E+00
Moles 0.00000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mass fractions:
AL 9.85194E-01 MG 1.12509E-02 CU 1.91685E-03 SI 1.63879E-03
POLY: show t
T=897.74074
POLY:Hit RETURN to continue
POLY: s-c t
Value /897.7407448/: 900
POLY: c-st phase
Phase name(s): fcc_a1
Status: /ENTERED/: ENTERED
Start value, number of mole formula units /0/: 0
POLY: c-e
Using global minimization procedure
Calculated 26538 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY: l-e,
Options /VWCS/:
Output from POLY-3, equilibrium = 1, label A0 , database: USER

Conditions:
P=101325, N=1, T=900, W(SI)=2E-2, W(MG)=4E-2, W(CU)=2E-2
DEGREES OF FREEDOM 0

Temperature 900.00 K ( 626.85 C), Pressure 1.013250E+05
Number of moles of components 1.00000E+00, Mass in grams 2.71965E+01
Total Gibbs energy -3.81928E+04, Enthalpy 2.74567E+04, Volume 0.00000E+00

Component Moles W-Fraction Activity Potential Ref.stat
AL 9.2731E-01 9.2000E-01 8.1424E-03 -3.5998E+04 SER
CU 8.5596E-03 2.0000E-02 5.5930E-07 -1.0773E+05 SER
MG 4.4759E-02 4.0000E-02 1.2687E-04 -6.7141E+04 SER
SI 1.9367E-02 2.0000E-02 2.2488E-03 -4.5627E+04 SER

LIQUID Status ENTERED Driving force 0.0000E+00
Moles 1.00000E+00, Mass 2.7197E+01, Volume fraction 0.0000E+00 Mass fractions:
AL 9.20000E-01 MG 4.00000E-02 CU 2.00000E-02 SI 2.00000E-02
POLY: s-a-v 1 t
Min value /0/: 750 900 1
POLY:

```

```

POLY: ent var nl=1;
POLY: ent var nfcc=0;
POLY: ent var nl=np(liquid)*nl;
POLY: ent fun ns=1-nl;
POLY: ent var nfcc=nfcc+nl*np(fcc_a1);
POLY: ent var wsi=w(liquid,si);
POLY: ent var wmg=w(liquid,mg);
POLY: ent var wcu=w(liquid,cu);
POLY: ent tab tab1
Variable(s): t nl ns nfcc
&
POLY: s-c w(si)=wsi w(mg)=wmg w(cu)=wcu
POLY: save tcex30a y
POLY:
POLY: step
Option? /NORMAL/: eva
Variable name(s): wsi wmg wcu
No initial equilibrium, using default
...OK

Phase Region from 900.000 for:
    LIQUID
Global check of adding phase at 8.97741E+02
Calculated 5 equilibria

Phase Region from 897.741 for:
    LIQUID
    FCC_A1
Global test at 8.90000E+02 .... OK
Global test at 8.80000E+02 .... OK
Global test at 8.70000E+02 .... OK
Global test at 8.60000E+02 .... OK
Global check of adding phase at 8.57875E+02
Calculated 43 equilibria

Phase Region from 857.875 for:
    LIQUID
    FCC_A1
    MG2SI
Global test at 8.50000E+02 .... OK
Global test at 8.40000E+02 .... OK
Global test at 8.30000E+02 .... OK
Global test at 8.20000E+02 .... OK
Global test at 8.10000E+02 .... OK
Global test at 8.00000E+02 .... OK
Global test at 7.90000E+02 .... OK
Global test at 7.80000E+02 .... OK
Global check of adding phase at 7.78888E+02
Calculated 82 equilibria

Phase Region from 778.888 for:
    LIQUID
    ALCU_THETA
    FCC_A1
    MG2SI
Global check of adding phase at 7.73208E+02
Calculated 8 equilibria

Phase Region from 773.208 for:
    LIQUID
    ALCU_THETA
    DIAMOND_A4
    FCC_A1
    MG2SI
Calculated 2 equilibria

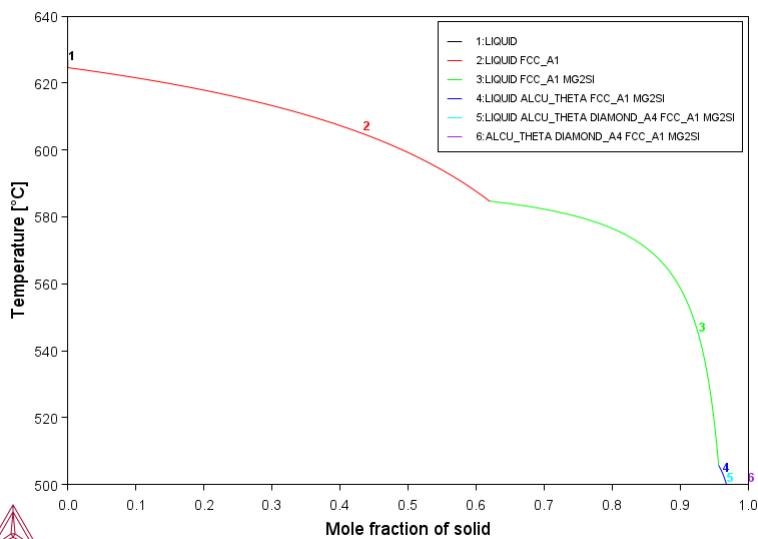
Phase Region from 773.208 for:
    ALCU_THETA
    DIAMOND_A4
    FCC_A1
    MG2SI
Global test at 7.66000E+02 .... OK
Global test at 7.56000E+02 .... OK
Terminating at 750.000
Calculated 27 equilibria
*** Buffer saved on file: c:\jenkins\workspace\generate_console_examples\examples\tcex30A\tcex30a.POLY3
POLY:
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: s-d-a x tab1
COLUMN NUMBER /*:/: 3
POST: s-d-a y t-c
POST:
POST: s-s-s y
AUTOMATIC SCALING (Y OR N) /N/: n
MIN VALUE : 500 640
POST: s-lab b
POST: se-ax-te x n
AXIS TEXT : Mole fraction of solid
POST: set-title example 30Aa
POST: plot

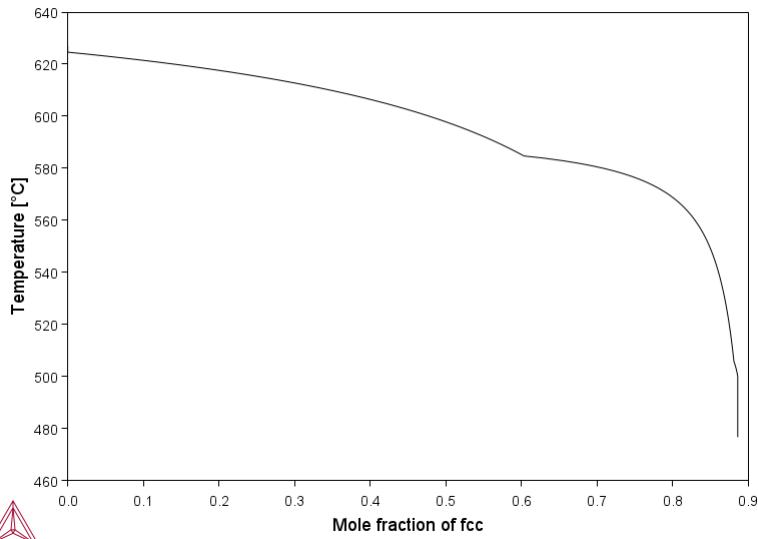
```

example 30Aa



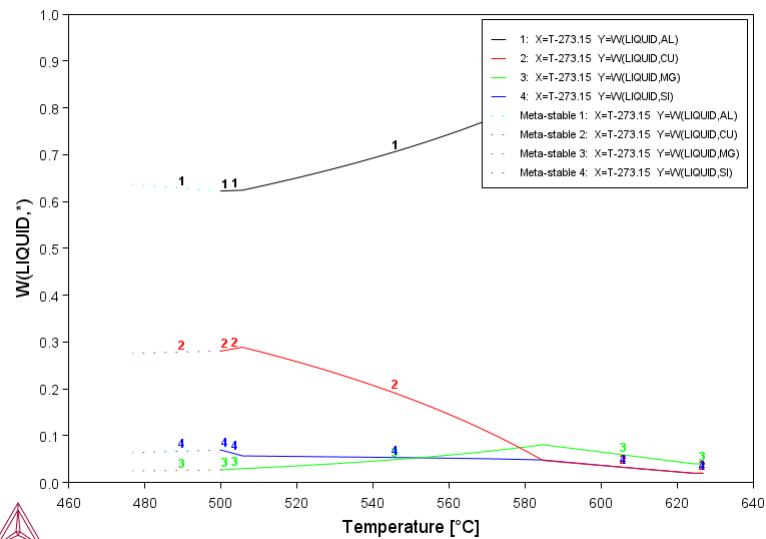
```
POST:  
POST: SET_EXP_FILE_FORMAT 5  
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y  
POST: SET_EXP_FILE_FORMAT 10  
POST:  
POST:  
POST:Hit RETURN to continue  
POST: back  
POLY: read,,  
POLY: po  
POLY-3 POSTPROCESSOR VERSION 3.2  
Setting automatic diagram axes  
POST: s-d-a x tabl  
COLUMN NUMBER /*/: 4  
POST: s-d-a y t-c  
POST: se-ax-te x n  
AXIS TEXT : Mole fraction of fcc  
POST: set-title example 30Ab  
POST:  
POST: plot
```

example 30Ab



```
POST:  
POST: SET_EXP_FILE_FORMAT 5  
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y  
POST: SET_EXP_FILE_FORMAT 10  
POST:  
POST:  
POST:Hit RETURN to continue  
POST: s-d-a x t-c  
POST: s-d-a y w(liquid,*),,  
POST: set-title example 30Ac  
POST: s-l d  
POST:  
POST: plot
```

example 30Ac



POST:

```
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST:
POST: set-inter
POST:
```

tce30B

SYS:About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce30B\tce30B.TCM.test"

SYS: set-echo

SYS:

SYS: @@ Scheil calculation for an Al-4Mg-2Si-2Cu alloy

SYS:

SYS: @@ This is the second of two examples showing how to

SYS: @@ do a Scheil calculation for an Al-4Mg-2Si-2Cu alloy.

SYS: @@ In part A, you used the POLY3 module and the

SYS: @@ STEP_WITH_OPTIONS command with an Evaluate setting.

SYS:

SYS: @@ This is part B where you use the SCHEIL module commands

SYS: @@ to do the same thing.

SYS:

SYS: go scheil

SCHEIL: start

THERMODYNAMIC DATABASE module
Database folder: C:\jenkins\workspace\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

Database /TCFE11/: user tce30_cost2.TDB

Current database: User defined Database

This database does not support the DATABASE_INFORMATION command

VA /- DEFINED

16:13:01,471 [Thread-0] INFO TDBfileParser: USER_235593888_14, number of lines read: 880

16:13:01,793 [Thread-0] INFO DatabaseUtils: Parsing of USER_235593888_14 completed in 371 ms

Major element or alloy: al

Composition input in mass (weight) percent? /Y/:

1st alloying element: mg 4 si 2 cu 2

Next alloying element:

Temperature (C) /2000/: 800

VA /- DEFINED

REINITIATING GES

AL DEFINED

MG DEFINED

SI DEFINED

CU DEFINED

This database has following phases for the defined system

| | | |
|----------------|----------------|----------------|
| LIQUID:L | AL12MG17 | ALCE_AMORPHOUS |
| ALCUZN_T | ALCU_DELTA | ALCU_EPSILON |
| ALCU_ETA | ALCU_PRIME | ALCU_THETA |
| ALCU_ZETA | ALLI | ALMG_BETA |
| ALMG_EPS | ALMG_GAMMA | ALMO |
| ALM_D019 | ALND_AMORPHOUS | ALTI |
| BCC_A2 | BCC_B2 | BCT_A5 |
| CBCC_A12 | CR3SI_A15 | CRSI2 |
| CU19Si6_ETA | CU33Si7_DELTA | CU4Si_EPSILON |
| CU56Si11_GAMMA | CU6Y | CUB_A13 |
| CUB_A15 | CUMG2 | CUMGSI_SIGMA |
| CUMGSI_TAU | CUZN_GAMMA | DIAMOND_A4 |
| FCC_A1 | GAMMA_D83 | GAMMA_H |
| HCP_A3 | HCP_ZN | LAVES_C14 |
| LAVES_C15 | LAVES_C36 | MG24Y5 |
| MG2Si | MG2Y | MG2ZN11 |
| MG2ZN3 | MGY_GAMMA | MGZN |
| PHI | QPHASE | SIV3 |
| SPHASE | TAU | VPHASE |

Reject phase(s) /NONE/: *

| | | |
|----------------|----------------|----------------|
| LIQUID:L | AL12MG17 | ALCE_AMORPHOUS |
| ALCUZN_T | ALCU_DELTA | ALCU_EPSILON |
| ALCU_ETA | ALCU_PRIME | ALCU_THETA |
| ALCU_ZETA | ALLI | ALMG_BETA |
| ALMG_EPS | ALMG_GAMMA | ALMO |
| ALM_D019 | ALND_AMORPHOUS | ALTI |
| BCC_A2 | BCC_B2 | BCT_A5 |
| CBCC_A12 | CR3SI_A15 | CRSI2 |
| CU19Si6_ETA | CU33Si7_DELTA | CU4Si_EPSILON |
| CU56Si11_GAMMA | CU6Y | CUB_A13 |
| CUB_A15 | CUMG2 | CUMGSI_SIGMA |
| CUMGSI_TAU | CUZN_GAMMA | DIAMOND_A4 |
| FCC_A1 | GAMMA_D83 | GAMMA_H |
| HCP_A3 | HCP_ZN | LAVES_C14 |
| LAVES_C15 | LAVES_C36 | MG24Y5 |
| MG2Si | MG2Y | MG2ZN11 |
| MG2ZN3 | MGY_GAMMA | MGZN |
| PHI | QPHASE | SIV3 |
| SPHASE | TAU | VPHASE |

REJECTED

Restore phase(s):: liquid fcc_a1 alcu_th mg2si diamond_a4 al12mg17

| | | |
|----------|------------|------------|
| LIQUID:L | FCC_A1 | ALCU_THETA |
| MG2Si | DIAMOND_A4 | AL12MG17 |

RESTORED

Restore phase(s): /NONE/:

The following phases are retained in this system:

| | | |
|------------|----------|------------|
| LIQUID:L | AL12MG17 | ALCU_THETA |
| DIAMOND_A4 | FCC_A1 | MG2Si |

```

OK? /Y/: Y
16:13:01,922 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS .....

List of references for assessed data

'COST2 - TCOST507 Light Alloys Database (Version 2.1), provided by TCSAB,
1999/2003. '
'COST (1998): COST 507 -- Definition of Thermochemical and Thermophysical
Properties to Provide a Database for the Development of New Light
Alloys. European Cooperation in the Field of Scientific and Technical
Research, European Commission. Vol 1. Proceedings of the Final
Workshop of COST 507, Vlaams, the Netherlands, 1997; Vol 2.
Thermochemical Database for Light Metal Alloys (Eds. Ansara I.,
Dinsdale A.T., and Rand M.H.); Vol 3. Critical Evaluation of Ternary
Systems (Ed. Effenberg G.). '
-OK-
Should any phase have a miscibility gap check? /N/: N
16:13:02,486 [Thread-0] INFO Database: Preparing system for use: USER_235593888_14
16:13:03,375 [Thread-0] INFO Phase: Preparing phase for use: LIQUID
16:13:03,905 [Thread-0] INFO Phase: Preparing phase for use: AL12MG17
16:13:04,297 [Thread-0] INFO Phase: Preparing phase for use: ALCU_THETA
16:13:04,669 [Thread-0] INFO Phase: Preparing phase for use: DIAMOND_A4
16:13:05,090 [Thread-0] INFO Phase: Preparing phase for use: FCC_A1
16:13:05,482 [Thread-0] INFO Phase: Preparing phase for use: MG2SI
    LIQUID PHASE NAME: LIQUID
Fast diffusing components: /NONE/:
This command is a combination of CHANGE_STATUS and SET_CONDITION
to calculate directly when a phase may form by releasing one condition.
You must release one of these conditions
T=1073.15, W(MG)=4E-2, W(SI)=2E-2, W(CU)=2E-2, P=100000, N=1
DEGREES OF FREEDOM 0
PHASE CHANGE AT 897.740742588
FCC_A1#1 forms
Testing POLY result by global minimization procedure
Calculated      5945 grid points in          0 s
    CALCULATING USING NORMAL EQUILIBRIUM CONDITIONS
...OK

Phase Region from     897.831      for:
    LIQUID
Terminating at     897.931
Calculated      4 equilibria

Phase Region from     897.831      for:
    LIQUID
Global check of adding phase at  8.97741E+02
Calculated      3 equilibria

Phase Region from     897.741      for:
    LIQUID
    FCC_A1
Global test at  8.89831E+02 .... OK
Global test at  8.79831E+02 .... OK
Global test at  8.69831E+02 .... OK
Global test at  8.59831E+02 .... OK
Global check of adding phase at  8.57535E+02
Calculated      43 equilibria

Phase Region from     857.535      for:
    LIQUID
    FCC_A1
    MG2SI
Global test at  8.49831E+02 .... OK
Global test at  8.39831E+02 .... OK
Global test at  8.29831E+02 .... OK
Global check of removing phase at  8.26196E+02
Calculated      34 equilibria

Phase Region from     826.196      for:
    FCC_A1
    MG2SI
Calculated      4 equilibria
*** Buffer saved on file: C:\Users\azureuser\AppData\Local\Temp\SCHEIL_3600.POLY3
POSTPROCESSOR VERSION 3.2

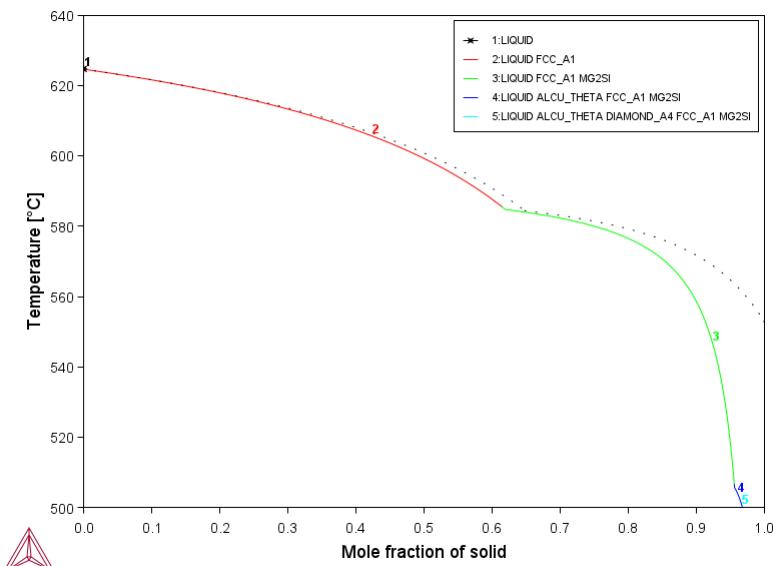
Setting automatic diagram axes
POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

An EXP file C:\Users\AZUREU~1\AppData\Local\Temp\SCHEIL_EQ_3600.EXP
has been created to store the equilibrium solidification results.
CALCULATING SCHEIL SOLIDIFICATION
    T(C)      fraction solid
    624.6807  0.000000
PHASE REGION:LIQUID + FCC_A1
    T(C)      fraction solid
    624.5851  0.2038889E-03
    623.5851  0.3538798E-01
    622.5851  0.6842453E-01
    621.5851  0.9949709E-01
    620.5851  0.1287693
    619.5851  0.1563873
    618.5851  0.1824824
    617.5851  0.2071723
    616.5851  0.2305634
    615.5851  0.2527515
    614.5851  0.2738237
    613.5851  0.2938587
    612.5851  0.3129285
    611.5851  0.3310983
    610.5851  0.3484280
    609.5851  0.3649722
    608.5851  0.3807809
    607.5851  0.3959003
    606.5851  0.4103725
    605.5851  0.4242366
    604.5851  0.4375286
    603.5851  0.4502817

```

602.5851 0.4625266
 601.5851 0.4742918
 600.5851 0.4856038
 599.5851 0.4964872
 598.5851 0.5069647
 597.5851 0.5170577
 596.5851 0.5267860
 595.5851 0.5361681
 594.5851 0.5452213
 593.5851 0.5539619
 592.5851 0.5624050
 591.5851 0.5705648
 590.5851 0.5784547
 589.5851 0.5860871
 588.5851 0.5934739
 587.5851 0.6006261
 586.5851 0.6075542
 585.5851 0.6142679
PHASE REGION:LIQUID + FCC_A1 + MG2SI
 T (C) fraction solid
 584.7245 0.6199090
 583.7245 0.6576760
 582.7245 0.6886411
 581.7245 0.7144754
 580.7245 0.7363465
 579.7245 0.7550939
 578.7245 0.7713365
 577.7245 0.7855406
 576.7245 0.7980640
 575.7245 0.8091857
 574.7245 0.8191265
 573.7245 0.8280633
 572.7245 0.8361395
 571.7245 0.8434725
 570.7245 0.8501596
 569.7245 0.8562816
 568.7245 0.8619067
 567.7245 0.8670925
 566.7245 0.8718879
 565.7245 0.8763351
 564.7245 0.8804703
 563.7245 0.8843250
 562.7245 0.8879265
 561.7245 0.8912987
 560.7245 0.8944628
 559.7245 0.8974371
 558.7245 0.9002382
 557.7245 0.9028806
 556.7245 0.9053773
 555.7245 0.9077400
 554.7245 0.9099790
 553.7245 0.9121039
 552.7245 0.9141230
 551.7245 0.9160440
 550.7245 0.9178738
 549.7245 0.9196187
 548.7245 0.9212845
 547.7245 0.9228765
 546.7245 0.9243993
 545.7245 0.9258573
 544.7245 0.9272547
 543.7245 0.9285951
 542.7245 0.9298819
 541.7245 0.9311183
 540.7245 0.9323071
 539.7245 0.9334511
 538.7245 0.9345527
 537.7245 0.9356142
 536.7245 0.9366378
 535.7245 0.9376256
 534.7245 0.9385793
 533.7245 0.9395007
 532.7245 0.9403914
 531.7245 0.9412529
 530.7245 0.9420867
 529.7245 0.9428941
 528.7245 0.9436762
 527.7245 0.9444344
 526.7245 0.9451697
 525.7245 0.9458831
 524.7245 0.9465756
 523.7245 0.9472482
 522.7245 0.9479016
 521.7245 0.9485367
 520.7245 0.9491543
 519.7245 0.9497551
 518.7245 0.9503399
 517.7245 0.9509091
 516.7245 0.9514636
 515.7245 0.9520038
 514.7245 0.9525303
 513.7245 0.9530437
 512.7245 0.9535444
 511.7245 0.9540330
 510.7245 0.9545099
 509.7245 0.9549755
 508.7245 0.9554302
 507.7245 0.9558745
 506.7245 0.9563086
PHASE REGION:LIQUID + ALCU_THETA + FCC_A1 + MG2SI
 T (C) fraction solid
 505.7364 0.9567319
 504.7364 0.9594803
 503.7364 0.9618348
 502.7364 0.9638799
 501.7364 0.9656767
 500.7364 0.9672706
 500.0670 0.9682413
PHASE REGION:ALCU_THETA + DIAMOND_A4 + FCC_A1 + MG2SI
 T (C) fraction solid
 500.0351 1.000000
 Calculating properties ...
 Liquidus temperature: 897.741 K
 Solidus temperature: 773.185 K



The following axis variables are available

T - Temperature in Celsius
 NL/BL/VL - Mole/mass/volume fraction of liquid
 NS/BS/VS - Mole/mass/volume fraction of all solid phases
 NS(ph)/BS(ph) - Mole/mass fraction of a solid phase
 VS(ph) - Volume fraction of a solid phase
 W(ph,el) - Weight fraction of an element in a phase
 X(ph,el) - Mole fraction of an element in a phase
 Y(ph,el) - Site fraction of an element in a phase
 NN(ph,el) - Distribution of an element in a phase
 NH/BH - Heat release and Latent heat per mole/gram
 CP/BCP - Apparent heat capacity per mole/gram
 NV/NV(ph) - Molar volume of the system or a phase
 DS/DS(ph) - Average density of the system or a phase
 BT - Apparent volumetric TEC of the system
 DVIS(ph) - Dynamic viscosity of a phase
 KVVIS(ph) - Kinematic viscosity of phase
 SURF(ph) - Surface tension of a liquid phase
 ELRS/ELRS(ph) - Electrical resistivity of the system or a phase
 ELCD/ELCD(ph) - Electrical conductivity of the system or a phase
 THCD/THCD(ph) - Thermal conductivity of the system or a phase
 THRS/THRS(ph) - Thermal resistivity of the system or a phase
 THDF/THDF(ph) - Thermal diffusivity of the system or a phase
 DGV - Driving force for evaporation
 DHV - Evaporation enthalpy
 MMG - Molar mass of gas
 XAVG(el) - Mole fraction of an element in solid phases
 WAVG(el) - Mass fraction of an element in solid phases

"el" and "ph" are name of element and phase, respectively
 "*" can be used as a wild character for "el" and "ph"

```

POST:  

POST:Hit RETURN to continue  

POST: s-d-a x t  

POST: s-d-a y w(liquid,*),....  

POST: s-s-s y n 0 0.3  

POST: set-lab F  

POST:  

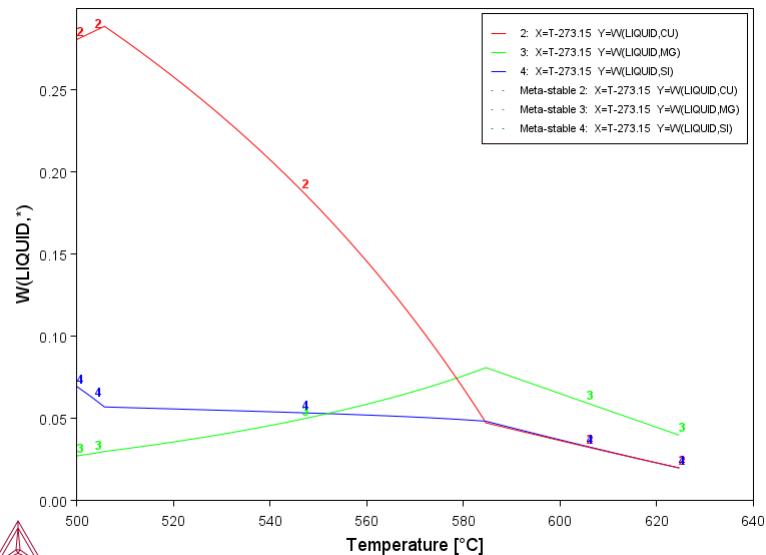
POST: SET_EXP_FILE_FORMAT 5  

POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y  

POST: SET_EXP_FILE_FORMAT 10  

POST:  

POST: plot,....
  
```



POST:
POST: set-inter
POST:

tce31**SYS:About**

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

```
SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce31\tce31.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Using the GES module to calculate CVM
SYS:
SYS: @@ This example calculates the CVM and compares it with the
SYS: @@ sublattices of a fictitious A B system. You also learn how
SYS: @@ to overlay diagrams from two calculations.
SYS:
SYS: @@ This example uses some GES commands that are not yet
SYS: @@ supported by GES6. Therefore, we enforce the use of GES5.
SYS: set-ges-version 5
SYS:
SYS: set-log ex31,,
SYS:
SYS: go g
... the command in full is GOTO_MODULE
GIBBS ENERGY SYSTEM
GES5:
GES5: @@ Enter the elements and the reference states
GES5: e-e A B
... the command in full is ENTER_ELEMENT
THERMODYNAMIC DATABASE module
Database folder: C:\jenkins\workspace\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA          /- DEFINED
DICTRA_FCC_A1 REJECTED
GES5: a-e-d A
... the command in full is AMEND_ELEMENT_DATA
NEW STABLE ELEMENT REFERENCE /UNKNOWN/: FCC
NEW ATOMIC MASS /0/: 10
NEW H(298.15)-H(0) /0/: 0
NEW S(298.15) /0/: 0
Default element reference state symbol index /1/: 1
GES5: a-e-d B
... the command in full is AMEND_ELEMENT_DATA
NEW STABLE ELEMENT REFERENCE /BETA_RHOMBO_B/: FCC
NEW ATOMIC MASS /10.811/: 10
NEW H(298.15)-H(0) /1222/: 0
NEW S(298.15) /5.9/: 0
Default element reference state symbol index /1/: 1
GES5:
GES5: @@ =====
GES5: @@ These species represent the clusters. 4 clusters A3B are
GES5: @@ needed as the B atom can be on 4 different sublattices etc.
GES5:
GES5: e-sp S0 A
... the command in full is ENTER_SPECIES
GES5: e-sp S11 A.75B.25
... the command in full is ENTER_SPECIES
GES5: e-sp S12 A.75B.25
... the command in full is ENTER_SPECIES
GES5: e-sp S13 A.75B.25
... the command in full is ENTER_SPECIES
GES5: e-sp S14 A.75B.25
... the command in full is ENTER_SPECIES
GES5: e-sp S21 A.5B.5
... the command in full is ENTER_SPECIES
GES5: e-sp S22 A.5B.5
... the command in full is ENTER_SPECIES
GES5: e-sp S23 A.5B.5
... the command in full is ENTER_SPECIES
GES5: e-sp S24 A.5B.5
... the command in full is ENTER_SPECIES
GES5: e-sp S25 A.5B.5
... the command in full is ENTER_SPECIES
GES5: e-sp S26 A.5B.5
... the command in full is ENTER_SPECIES
GES5: e-sp S31 A.25B.75
... the command in full is ENTER_SPECIES
GES5: e-sp S32 A.25B.75
... the command in full is ENTER_SPECIES
GES5: e-sp S33 A.25B.75
... the command in full is ENTER_SPECIES
GES5: e-sp S34 A.25B.75
... the command in full is ENTER_SPECIES
GES5: e-sp S4 B
... the command in full is ENTER_SPECIES
GES5:
GES5: @@ =====
GES5: @@ This function describes the bond energy A-B at equiatomic
GES5: @@ composition.
GES5: e-sy fun U1J
... the command in full is ENTER_SYMBOL
LOW TEMPERATURE LIMIT /298.15/: 298.15
FUNCTION: -100*R;
HIGH TEMPERATURE LIMIT /6000/: 6000
ANY MORE RANGES /N/: N
GES5:
GES5: @@ These functions describe the end-member energies at
GES5: @@ A3B, A2B2 and AB3 respectively.
GES5: @@ In the simplest case, like here, they are just the
GES5: @@ bond energy multiplied with 3, 4 and 3, respectively.
GES5:
```

```

GES5: e-sy fun GA3B1,,3*UIJ;,,,
... the command in full is ENTER_SYMBOL
GES5: e-sy fun GA2B2,,4*UIJ;,,,
... the command in full is ENTER_SYMBOL
GES5: e-sy fun GA1B3,,3*UIJ;,,,
... the command in full is ENTER_SYMBOL
GES5:
GES5: @@ =====
GES5: @@ This is the FCC phase with CVM for both LRO and SRO
GES5: e-ph CVM_TET
... the command in full is ENTER_PHASE
TYPE CODE:
NUMBER OF SUBLATTICES /1/: 1
NAME OF CONSTITUENT: S0 S11 S12 S13 S14 S21 S22 S23 S24 S25 S26 S31 S32 S33 S34 S4
NAME OF CONSTITUENT:
WILL YOU ADD CONSTITUENTS LATER /NO/: NO
DO YOU WANT A LIST OF POSSIBLE PARAMETERS /NO/: NO
GES5: E-PAR G(C,S11),,GA3B1;,,,
... the command in full is ENTER_PARAMETER
G(CVM_TET,S11;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)
GES5: E-PAR G(C,S12),,GA3B1;,,,
... the command in full is ENTER_PARAMETER
G(CVM_TET,S12;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)
GES5: E-PAR G(C,S13),,GA3B1;,,,
... the command in full is ENTER_PARAMETER
G(CVM_TET,S13;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)
GES5: E-PAR G(C,S14),,GA3B1;,,,
... the command in full is ENTER_PARAMETER
G(CVM_TET,S14;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)
GES5: E-PAR G(C,S21),,GA2B2;,,,
... the command in full is ENTER_PARAMETER
G(CVM_TET,S21;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES5: E-PAR G(C,S22),,GA2B2;,,,
... the command in full is ENTER_PARAMETER
G(CVM_TET,S22;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES5: E-PAR G(C,S23),,GA2B2;,,,
... the command in full is ENTER_PARAMETER
G(CVM_TET,S23;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES5: E-PAR G(C,S24),,GA2B2;,,,
... the command in full is ENTER_PARAMETER
G(CVM_TET,S24;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES5: E-PAR G(C,S25),,GA2B2;,,,
... the command in full is ENTER_PARAMETER
G(CVM_TET,S25;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES5: E-PAR G(C,S26),,GA2B2;,,,
... the command in full is ENTER_PARAMETER
G(CVM_TET,S26;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES5: E-PAR G(C,S31),,GA1B3;,,,
... the command in full is ENTER_PARAMETER
G(CVM_TET,S31;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0)
GES5: E-PAR G(C,S32),,GA1B3;,,,
... the command in full is ENTER_PARAMETER
G(CVM_TET,S32;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0)
GES5: E-PAR G(C,S33),,GA1B3;,,,
... the command in full is ENTER_PARAMETER
G(CVM_TET,S33;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0)
GES5: E-PAR G(C,S34),,GA1B3;,,,
... the command in full is ENTER_PARAMETER
G(CVM_TET,S34;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0)
GES5: l-d,,,
... the command in full is LIST_DATA

```

1OUTPUT FROM GIBBS ENERGY SYSTEM ON PC/WINDOWS NT DATE 2023- 4-27
FROM DATABASE: User data 2023.04.27

ALL DATA IN SI UNITS
FUNCTIONS VALID FOR 298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED

| ELEMENT | STABLE ELEMENT | REFERENCE | MASS | H298-H0 | S298 |
|---------|----------------|-----------|-------------|-------------|-------------|
| 1 A | FCC | | 1.00000E+01 | 0.00000E+00 | 0.00000E+00 |
| 2 B | FCC | | 1.00000E+01 | 0.00000E+00 | 0.00000E+00 |

| SPECIES | STOICHIOMETRY |
|---------|---------------|
| 1 A | A |
| 2 B | B |
| 3 S0 | A |
| 4 S11 | A0.75B0.25 |
| 5 S12 | A0.75B0.25 |
| 6 S13 | A0.75B0.25 |
| 7 S14 | A0.75B0.25 |
| 8 S21 | A0.5B0.5 |
| 9 S22 | A0.5B0.5 |
| 10 S23 | A0.5B0.5 |
| 11 S24 | A0.5B0.5 |
| 12 S25 | A0.5B0.5 |
| 13 S26 | A0.5B0.5 |
| 14 S31 | A0.25B0.75 |
| 15 S32 | A0.25B0.75 |
| 16 S33 | A0.25B0.75 |
| 17 S34 | A0.25B0.75 |
| 18 S4 | B |

| CVM_TET | CONSTITUENTS: S0,S11,S12,S13,S14,S21,S22,S23,S24,S25,S26,S31,S32,S33,S34, S4 |
|--|---|
| G(CVM_TET,S0;0)-G(FCC,A;0) | = 0.0 |
| G(CVM_TET,S11;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) | = +GA3B1 |
| G(CVM_TET,S12;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) | = +GA3B1 |
| G(CVM_TET,S13;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) | = +GA3B1 |
| G(CVM_TET,S14;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) | = +GA3B1 |
| G(CVM_TET,S21;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) | = +GA2B2 |
| G(CVM_TET,S22;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) | = +GA2B2 |
| G(CVM_TET,S23;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) | = +GA2B2 |
| G(CVM_TET,S24;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) | = +GA2B2 |
| G(CVM_TET,S25;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) | = +GA2B2 |
| G(CVM_TET,S26;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) | = +GA2B2 |
| G(CVM_TET,S31;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) | = +GA1B3 |
| G(CVM_TET,S32;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) | = +GA1B3 |
| G(CVM_TET,S33;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) | = +GA1B3 |

```

G(CVM_TET,S34;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
G(CVM_TET,S4;0)-G(FCC,B;0) = 0.0

SYMBOL      STATUS   VALUE/FUNCTION
FUNCTION R    298.15   8.314510000000000 ; 6000 N REFO !
2 RTLNP    20000000 +RT*T*LN(1E-05*P)
103 UIJ     20000000 -100*R
104 GA3B1   20000000 +3*UIJ
105 GA2B2   20000000 +4*UIJ
106 GA1B3   20000000 +3*UIJ

GES5:
GES5:Hit RETURN to continue
GES5:
GES5: @@ =====
GES5: @@ This is an FCC phase with no SRO but LRO
GES5: @@ described with the sublattice model
GES5:
GES5: E-PH LRO
... the command in full is ENTER_PHASE
TYPE CODE:
NUMBER OF SUBLATTICES /1/: 4
NUMBER OF SITES IN SUBLATTICE 1 /1/: .25
NUMBER OF SITES IN SUBLATTICE 2 /1/: .25
NUMBER OF SITES IN SUBLATTICE 3 /1/: .25
NUMBER OF SITES IN SUBLATTICE 4 /1/: .25
CONSTITUENTS IN SUBLATTICE          1
NAME OF CONSTITUENT: A B;
CONSTITUENTS IN SUBLATTICE          2
NAME OF CONSTITUENT: A B;
CONSTITUENTS IN SUBLATTICE          3
NAME OF CONSTITUENT: A B;
CONSTITUENTS IN SUBLATTICE          4
NAME OF CONSTITUENT: A B;
WILL YOU ADD CONSTITUENTS LATER /NO/: NO
DO YOU WANT A LIST OF POSSIBLE PARAMETERS /NO/: NO
GES5:
GES5: E-PAR G(L,A:A:B),,GA3B1;,,,
... the command in full is ENTER_PARAMETER
G(LRO,A:A:A:B;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)
GES5: E-PAR G(L,A:A:B:A),,GA3B1;,,,
... the command in full is ENTER_PARAMETER
G(LRO,A:A:B:A;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)
GES5: E-PAR G(L,A:B:A:A),,GA3B1;,,,
... the command in full is ENTER_PARAMETER
G(LRO,A:B:A:A;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)
GES5: E-PAR G(L,B:A:A:A),,GA3B1;,,,
... the command in full is ENTER_PARAMETER
G(LRO,B:A:A:A;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)
GES5: E-PAR G(L,A:B:B:B),,GA1B3;,,,
... the command in full is ENTER_PARAMETER
G(LRO,A:B:B:B;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)
GES5: E-PAR G(L,B:B:B:B),,GA1B3;,,,
... the command in full is ENTER_PARAMETER
G(LRO,B:B:B:B;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)
GES5: E-PAR G(L,B:B:B:A),,GA1B3;,,,
... the command in full is ENTER_PARAMETER
G(LRO,B:B:B:A;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)
GES5: E-PAR G(L,B:B:A:B),,GA1B3;,,,
... the command in full is ENTER_PARAMETER
G(LRO,B:B:A:B;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)
GES5: E-PAR G(L,B:B:B:B),,GA1B3;,,,
... the command in full is ENTER_PARAMETER
G(LRO,B:B:B:B;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)
GES5: E-PAR G(L,A:B:B:B),,GA2B2;,,,
... the command in full is ENTER_PARAMETER
G(LRO,A:A:B:B;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES5: E-PAR G(L,A:B:B:A),,GA2B2;,,,
... the command in full is ENTER_PARAMETER
G(LRO,A:B:B:A;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES5: E-PAR G(L,B:A:B:A),,GA2B2;,,,
... the command in full is ENTER_PARAMETER
G(LRO,B:A:B:A;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES5: E-PAR G(L,B:B:A:B),,GA2B2;,,,
... the command in full is ENTER_PARAMETER
G(LRO,B:B:A:B;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES5: E-PAR G(L,B:B:B:A),,GA2B2;,,,
... the command in full is ENTER_PARAMETER
G(LRO,B:B:B:A;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES5: E-PAR G(L,B:B:B:B),,GA2B2;,,,
... the command in full is ENTER_PARAMETER
G(LRO,B:B:B:B;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES5: 1-p-d lro
... the command in full is LIST_PHASE_DATA

LRO
EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
4 SUBLATTICES, SITES .25: .25: .25: .25
CONSTITUENTS: A,B : A,B : A,B : A,B

G(LRO,A:A:A:A;0)-G(FCC,A;0) = 0.0
G(LRO,B:A:A:A;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
G(LRO,A:B:A:A;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
G(LRO,B:B:A:A;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(LRO,A:A:B:A;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
G(LRO,B:A:B:A;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(LRO,B:B:B:A;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
G(LRO,A:A:A:B;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
G(LRO,B:A:A:B;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(LRO,A:B:A:B;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(LRO,B:B:A:B;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
G(LRO,A:A:B:B;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(LRO,B:A:B:B;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
G(LRO,A:B:B:B;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
G(LRO,B:B:B:B;0)-G(FCC,B;0) = 0.0

GES5:
GES5: @@ =====
GES5: @@ This is the FCC phase with no SRO and no LRO. The regular
GES5: @@ parameter is simply 12 times the bond energy as the ;1 and ;2
GES5: @@ parameters cancel when GA1B3=GA3B1=0.75*GA2B2
GES5:
GES5: e-ph fcc_a1
... the command in full is ENTER_PHASE

```

```

TYPE CODE:
NUMBER OF SUBLATTICES /1/: 1
NAME OF CONSTITUENT: A B
NAME OF CONSTITUENT:
WILL YOU ADD CONSTITUENTS LATER /NO/: NO
DO YOU WANT A LIST OF POSSIBLE PARAMETERS /NO/: NO
GES5:
GES5: e-par l(fcc,a,b;0),,GA3B1+1.5*GA2B2+GA1B3;,,,,,
... the command in full is ENTER_PARAMETER
L(FCC_A1,A,B;0)
GES5: e-par l(fcc,a,b;1),,2*GA3B1-2*GA1B3;,,,,,
... the command in full is ENTER_PARAMETER
L(FCC_A1,A,B;1)
GES5: e-par l(fcc,a,b;2),,GA3B1-1.5*GA2B2+GA1B3;,,,,,
... the command in full is ENTER_PARAMETER
L(FCC_A1,A,B;2)
GES5: l-p-d fcc
... the command in full is LIST_PHASE_DATA

FCC_A1
EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
CONSTITUENTS: A,B

G(FCC_A1,A;0)-G(FCC,A;0) = 0.0
G(FCC_A1,B;0)-G(FCC,B;0) = 0.0
L(FCC_A1,A,B;0) = +GA3B1+1.5*GA2B2+GA1B3
L(FCC_A1,A,B;1) = +2*GA3B1-2*GA1B3
L(FCC_A1,A,B;2) = +GA3B1-1.5*GA2B2+GA1B3
GES5:
GES5: @@ Finally, add together the LRO phase with the disordered FCC
GES5: @@ Note that the parameters in LRO give zero contribution
GES5: @@ when the phase is disordered
GES5:
GES5: amend-phase LRO dis FCC
... the command in full is AMEND_PHASE_DESCRIPTION
GES5:
GES5: @@
GES5: @@ This is the way to set CVM entropy calculation
GES5: am-ph cvm stat 02204030
... the command in full is AMEND_PHASE_DESCRIPTION
GES5:
GES5: l-p-d cvm
... the command in full is LIST_PHASE_DATA

CVM_TET
$ CVM-SRO ENTROPY CONTRIBUTION
CONSTITUENTS: S0,S11,S12,S13,S14,S21,S22,S23,S24,S25,S26,S31,S32,S33,S34,
S4

G(CVM_TET,S0;0)-G(FCC,A;0) = 0.0
G(CVM_TET,S11;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
G(CVM_TET,S12;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
G(CVM_TET,S13;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
G(CVM_TET,S14;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
G(CVM_TET,S21;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(CVM_TET,S22;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(CVM_TET,S23;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(CVM_TET,S24;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(CVM_TET,S25;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(CVM_TET,S26;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(CVM_TET,S31;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
G(CVM_TET,S32;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
G(CVM_TET,S33;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
G(CVM_TET,S34;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
G(CVM_TET,S4;0)-G(FCC,B;0) = 0.0
GES5:
GES5: Hit RETURN to continue
GES5:
GES5: @@ We need 3 CVM phases for the L10, L12 and disordered states
GES5: am-ph cvm
... the command in full is AMEND_PHASE_DESCRIPTION
AMEND WHAT /COMPOSITION_SETS/: COMPOSITION_SETS
NEW HIGHEST SET NUMBER 7/2/: 3
Creating a new composition set CVM_TET#2
GIVE FOR COMPOSITION SET 2
Major constituent(s) for sublattice 1: /$/: s11
Creating a new composition set CVM_TET#2
GIVE FOR COMPOSITION SET 3
Major constituent(s) for sublattice 1: /$/: none
GES5:
GES5: am-ph cvm maj
... the command in full is AMEND_PHASE_DESCRIPTION
Composition set /1/: 1
Major constituent(s) for sublattice 1: /S0 S11 S12 S13 S14 S21 S22 S23 S24 S25 S26 S31 S32 S33 S34 S/: S25
GES5:
GES5: @@ Also for the sublattice phase we need 3 composition sets
GES5: am-ph lro
... the command in full is AMEND_PHASE_DESCRIPTION
AMEND WHAT /COMPOSITION_SETS/: COMPOSITION_SETS
NEW HIGHEST SET NUMBER 7/2/: 3
Creating a new composition set LRO#2
GIVE FOR COMPOSITION SET 2
Major constituent(s) for sublattice 1: /A B/: *
Major constituent(s) for sublattice 2: /A B/: *
Major constituent(s) for sublattice 3: /A B/: *
Major constituent(s) for sublattice 4: /A B/: *
Creating a new composition set LRO#2
GIVE FOR COMPOSITION SET 3
Major constituent(s) for sublattice 1: /A B/: A
Major constituent(s) for sublattice 2: /A B/: A
Major constituent(s) for sublattice 3: /A B/: B
Major constituent(s) for sublattice 4: /A B/: B
GES5: am-ph lro
... the command in full is AMEND_PHASE_DESCRIPTION
AMEND WHAT /COMPOSITION_SETS/: maj
Composition set /1/: 1
Major constituent(s) for sublattice 1: /A B/: A
Major constituent(s) for sublattice 2: /A B/: A
Major constituent(s) for sublattice 3: /A B/: A
Major constituent(s) for sublattice 4: /A B/: B
GES5:

```

GES5: l-d,,,
... the command in full is LIST DATA

1OUTPUT FROM GIBBS ENERGY SYSTEM ON PC/WINDOWS NT DATE 2023- 4-27
FROM DATABASE: User data 2023.04.27

ALL DATA IN SI UNITS
FUNCTIONS VALID FOR 298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED

| ELEMENT | STABLE ELEMENT | REFERENCE | MASS | H298-H0 | S298 |
|---------|----------------|-----------|------------|------------|------------|
| 1 A | FCC | | 1.0000E+01 | 0.0000E+00 | 0.0000E+00 |
| 2 B | FCC | | 1.0000E+01 | 0.0000E+00 | 0.0000E+00 |

| SPECIES | STOICHIOMETRY |
|---------|---------------|
| 1 A | A |
| 2 B | B |
| 3 S0 | A |
| 4 S11 | A0.75B0.25 |
| 5 S12 | A0.75B0.25 |
| 6 S13 | A0.75B0.25 |
| 7 S14 | A0.75B0.25 |
| 8 S21 | A0.5B0.5 |
| 9 S22 | A0.5B0.5 |
| 10 S23 | A0.5B0.5 |
| 11 S24 | A0.5B0.5 |
| 12 S25 | A0.5B0.5 |
| 13 S26 | A0.5B0.5 |
| 14 S31 | A0.25B0.75 |
| 15 S32 | A0.25B0.75 |
| 16 S33 | A0.25B0.75 |
| 17 S34 | A0.25B0.75 |
| 18 S4 | B |

CVM_TET
\$ CVM-SRO ENTROPY CONTRIBUTION
CONSTITUENTS: S0,S11,S12,S13,S14,S21,S22,S23,S24,S25,S26,S31,S32,S33,S34,
S4

G(CVM_TET,S0;0)-G(FCC,A;0) = 0.0
G(CVM_TET,S11;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
G(CVM_TET,S12;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
G(CVM_TET,S13;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
G(CVM_TET,S14;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
G(CVM_TET,S21;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(CVM_TET,S22;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(CVM_TET,S23;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(CVM_TET,S24;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(CVM_TET,S25;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(CVM_TET,S26;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(CVM_TET,S31;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
G(CVM_TET,S32;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
G(CVM_TET,S33;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
G(CVM_TET,S34;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
G(CVM_TET,S4;0)-G(FCC,B;0) = 0.0

FCC_A1
\$ THIS PHASE IS THE DISORDERED PART OF LRO
EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
CONSTITUENTS: A,B

G(FCC_A1,A;0)-G(FCC,A;0) = 0.0
G(FCC_A1,B;0)-G(FCC,B;0) = 0.0
L(FCC_A1,A,B;0) = +GA3B1+1.5*GA2B2+GA1B3
L(FCC_A1,A,B;1) = +2*GA3B1-2*GA1B3
L(FCC_A1,A,B;2) = +GA3B1-1.5*GA2B2+GA1B3

LRO
\$ THIS PHASE HAS A DISORDERED CONTRIBUTION FROM FCC_A1
EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
4 SUBLATTICES, SITES .25: .25: .25: .25
CONSTITUENTS: A,B : A,B : A,B : A,B

G(LRO,A:A:A:A;0) = 0.0
G(LRO,B:A:A:A;0) = +GA3B1
G(LRO,A:B:A:A;0) = +GA3B1
G(LRO,B:B:A:A;0) = +GA2B2
G(LRO,A:A:B:A;0) = +GA3B1
G(LRO,B:A:B:A;0) = +GA2B2
G(LRO,A:B:B:A;0) = +GA1B3
G(LRO,A:A:A:B;0) = +GA3B1
G(LRO,B:A:A:B;0) = +GA2B2
G(LRO,A:B:A:B;0) = +GA2B2
G(LRO,B:B:A:B;0) = +GA1B3
G(LRO,A:A:B:B;0) = +GA2B2
G(LRO,B:A:B:B;0) = +GA1B3
G(LRO,A:B:B:B;0) = +GA1B3
G(LRO,B:B:B:B;0) = 0.0

| SYMBOL | STATUS | VALUE/FUNCTION |
|------------|----------|-----------------------------------|
| FUNCTION R | 298.15 | 8.314510000000000 ; 6000 N REF0 ! |
| 2 RTLNP | 20000000 | +RT*T*LN(1E-05*P) |
| 103 UIJ | 20000000 | -100*R |
| 104 GA3B1 | 20000000 | +3*UIJ |
| 105 GA2B2 | 20000000 | +4*UIJ |
| 106 GA1B3 | 20000000 | +3*UIJ |

GES5:Hit RETURN to continue
GES5:
GES5: @@ =====
GES5: @@ Now start the calculation
GES5: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY:

POLY: @@ Turn global minimization off

```

POLY: set-min-op
... the command in full is SET_MINIMIZATION_OPTIONS
This command is DEPRECATED and to be removed in the future!
Settings for global minimization:
Use global minimization /Y/: n
Settings for general calculations:
Force positive definite Phase Hessian /Y/: n
Control minimization step size /Y/:
POLY:
POLY: L-C
... the command in full is LIST_CONDITIONS
DEGREES OF FREEDOM 4
POLY: S-C T=60 P=1E5 N=1 X(B)=.4
... the command in full is SET_CONDITION
POLY: @@
POLY: @@ First calculate just with the full CVM phases
POLY: ch-st ph *=sus
... the command in full is CHANGE_STATUS
POLY: ch-st ph cvm cvm#2 cvm#3=ent 1
... the command in full is CHANGE_STATUS
POLY: @@
POLY: @@ L10 ordering, setting start composition essential
POLY: @@ The initial fraction of each species is basically
POLY: @@ calculated as the product of the site fraction on
POLY: @@ each sublattice.
POLY: s-s-c cvm
... the command in full is SET_START_CONSTITUITION
Y(CVM_TET#1,S0) /1/: .002
Y(CVM_TET#1,S11) /1/: 1.16e-3
Y(CVM_TET#1,S12) /1/: 1.76e-1
Y(CVM_TET#1,S13) /1/: 1.16e-3
Y(CVM_TET#1,S14) /1/: 1.76e-1
Y(CVM_TET#1,S21) /1/: 7.56e-3
Y(CVM_TET#1,S22) /1/: 5e-5
Y(CVM_TET#1,S23) /1/: 7.56e-3
Y(CVM_TET#1,S24) /1/: 7.56e-3
Y(CVM_TET#1,S25) /1/: 6.08e-1
Y(CVM_TET#1,S26) /1/: 7.56e-3
Y(CVM_TET#1,S31) /1/: 1.76e-3
Y(CVM_TET#1,S32) /1/: 2e-5
Y(CVM_TET#1,S33) /1/: 1.76e-3
Y(CVM_TET#1,S34) /1/: 2e-5
Y(CVM_TET#1,S4) /1/: 4e-7
POLY:
POLY: @@ L12 ordering
POLY: s-s-c cvm#2
... the command in full is SET_START_CONSTITUITION
Y(CVM_TET#2,S0) /1/: .002
Y(CVM_TET#2,S11) /1/: .46
Y(CVM_TET#2,S12) /1/: .0078
Y(CVM_TET#2,S13) /1/: .0078
Y(CVM_TET#2,S14) /1/: .0078
Y(CVM_TET#2,S21) /1/: .168
Y(CVM_TET#2,S22) /1/: .168
Y(CVM_TET#2,S23) /1/: .168
Y(CVM_TET#2,S24) /1/: .0012
Y(CVM_TET#2,S25) /1/: .0012
Y(CVM_TET#2,S26) /1/: .0012
Y(CVM_TET#2,S31) /1/: 5e-6
Y(CVM_TET#2,S32) /1/: .002
Y(CVM_TET#2,S33) /1/: .002
Y(CVM_TET#2,S34) /1/: .002
Y(CVM_TET#2,S4) /1/: 1e-6
POLY:
POLY: s-s-c cvm#3 *
... the command in full is SET_START_CONSTITUITION
POLY:
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Global equilibrium calculation turned off, you can turn it on with
ADVANCED OPTIONS GLOBAL_MINIMIZATION Y,....,
15 ITS, CPU TIME USED 0 SECONDS
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: xnp
Output from POLY-3, equilibrium = 1, label A0 , database: User dat

Conditions:
T=60, P=100000, N=1, X(B)=0.4
DEGREES OF FREEDOM 0

Temperature 60.00 K ( -213.15 C), Pressure 1.000000E+05
Number of moles of components 1.000000E+00, Mass in grams 1.000000E+01
Total Gibbs energy -3.10213E+03, Enthalpy -2.96850E+03, Volume 0.000000E+00

Component Moles M-Fraction Activity Potential Ref.stat
A 6.0000E-01 6.0000E-01 2.0465E-02 -1.9401E+03 SER
B 4.0000E-01 4.0000E-01 6.0538E-05 -4.8452E+03 SER

CVM_TET#1 Status ENTERED Driving force 0.0000E+00
Moles 5.6950E-01, Mass 5.6950E+00, Volume fraction 0.0000E+00 Mole fractions:
A 5.89207E-01 B 4.10793E-01
Constitution:
S25 5.78440E-01 S26 1.28068E-02 S31 4.13398E-03 S22 2.56479E-04
S14 1.76120E-01 S24 1.28068E-02 S0 3.76373E-03 S32 1.15932E-04
S12 1.76120E-01 S21 1.28068E-02 S13 2.78465E-03 S34 1.15932E-04
S23 1.28068E-02 S33 4.13398E-03 S11 2.78465E-03 S4 3.67798E-06

CVM_TET#2 Status ENTERED Driving force 0.0000E+00
Moles 4.3050E-01, Mass 4.3050E+00, Volume fraction 0.0000E+00 Mole fractions:
A 6.14278E-01 B 3.85722E-01
Constitution:
S11 4.21306E-01 S12 1.38900E-02 S33 4.69234E-03 S26 3.19866E-03
S21 1.69717E-01 S13 1.38900E-02 S34 4.69234E-03 S24 3.19866E-03
S22 1.69717E-01 S14 1.38900E-02 S0 4.13973E-03 S31 5.05554E-05
S23 1.69717E-01 S32 4.69234E-03 S25 3.19866E-03 S4 8.90403E-06

CVM_TET#3 Status ENTERED Driving force -2.3482E-02
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mole fractions:
A 6.09605E-01 B 3.90395E-01
Constitution:
S11 1.09346E-01 S24 8.57142E-02 S22 8.57142E-02 S33 7.93976E-03

```

```

S14  1.09346E-01  S25  8.57142E-02  S26  8.57142E-02  S34  7.93976E-03
S12  1.09346E-01  S21  8.57142E-02  S0   1.64839E-02  S31  7.93976E-03
S13  1.09346E-01  S23  8.57142E-02  S32  7.93976E-03  S4   8.69093E-05
POLY:Hit RETURN to continue
POLY:
POLY: s-c t=40
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
 14 ITS, CPU TIME USED 0 SECONDS
POLY: s-s-c cvm#3 *
... the command in full is SET_START_CONSTITUITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
 18 ITS, CPU TIME USED 0 SECONDS
POLY: L-E
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VXNP/:
Output from POLY-3, equilibrium = 1, label A0 , database: User dat

Conditions:
T=40, P=100000, N=1, X(B)=0.4
DEGREES OF FREEDOM 0

Temperature      40.00 K ( -233.15 C), Pressure 1.000000E+05
Number of moles of components 1.000000E+00, Mass in grams 1.000000E+01
Total Gibbs energy -3.06232E+03, Enthalpy -2.98938E+03, Volume 0.000000E+00

Component          Moles      M-Fraction    Activity    Potential  Ref.stat
A                 6.0000E-01  6.0000E-01  4.1519E-03  -1.8239E+03  SER
B                 4.0000E-01  4.0000E-01  3.7621E-07  -4.9199E+03  SER

CVM_TET#1          Status ENTERED    Driving force 0.0000E+00
Moles 6.6953E-01, Mass 6.6953E+00, Volume fraction 0.0000E+00 Mole fractions:
A 5.88358E-01  B 4.11642E-01
Constitution:
S25  6.26368E-01  S24  4.57470E-03  S31  6.44301E-04  S22  1.02379E-05
S14  1.76201E-01  S23  4.57470E-03  S33  6.44301E-04  S32  4.02672E-06
S12  1.76201E-01  S26  4.57470E-03  S11  4.60814E-04  S34  4.02672E-06
S21  4.57470E-03  S0   7.03194E-04  S13  4.60814E-04  S4   2.24689E-08

CVM_TET#2          Status ENTERED    Driving force 0.0000E+00
Moles 3.3047E-01, Mass 3.3047E+00, Volume fraction 0.0000E+00 Mole fractions:
A 6.23586E-01  B 3.76414E-01
Constitution:
S11  4.81572E-01  S12  4.56422E-03  S34  7.57611E-04  S26  4.03145E-04
S23  1.66859E-01  S14  4.56422E-03  S32  7.57611E-04  S24  4.03145E-04
S21  1.66859E-01  S13  4.56422E-03  S0   6.77145E-04  S31  4.66624E-07
S22  1.66859E-01  S33  7.57611E-04  S25  4.03145E-04  S4   4.50770E-08

CVM_TET#3          Status ENTERED    Driving force -6.0046E-02
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mole fractions:
A 6.15517E-01  B 3.84483E-01
Constitution:
S24  1.46218E-01  S13  1.44857E-01  S21  2.79748E-02  S32  1.40187E-03
S25  1.46205E-01  S14  1.44849E-01  S11  2.54012E-02  S34  1.40110E-03
S26  1.46097E-01  S22  2.79941E-02  S31  6.70812E-03  S33  1.40093E-03
S12  1.44923E-01  S23  2.79926E-02  S0   6.52643E-03  S4   5.09667E-05
POLY:Hit RETURN to continue
POLY:
POLY: s-a-v 1 x(b) 0 .5,,
... the command in full is SET_AXIS_VARIABLE
POLY: s-a-v 2 t 0 100,,
... the command in full is SET_AXIS_VARIABLE
POLY: save tcex31a y
... the command in full is SAVE_WORKSPACES
POLY: map -
Version R mapping is selected

Organizing start points

NO INITIAL EQUILIBRIUM ADDED, TRYING TO FIX ONE
Generating start point 1
Generating start point 2

Phase region boundary 1 at: 4.116E-01 4.000E+01
  CVM_TET#1
** CVM_TET#2
*** Buffer saved on file:
c:\jenkins\workspace\generate_console_examples\examples\tcex31\tcex31a.POLY3
Terminating at diagram limit
CALCULATED 27 EQUILIBRIA

Phase region boundary 2 at: 4.116E-01 4.000E+01
  CVM_TET#1
** CVM_TET#2
CALCULATED 26 EQUILIBRIA

Phase region boundary 2 at: 4.240E-01 8.061E+01
  CVM_TET#1
** CVM_TET#2
  CVM_TET#3

Phase region boundary 2 at: 4.147E-01 8.061E+01
  CVM_TET#2
  CVM_TET#3
MAPPING TERMINATED 1
CALCULATED 95 EQUILIBRIA

Phase region boundary 2 at: 4.240E-01 8.061E+01
  CVM_TET#1
** CVM_TET#3
Terminating at diagram limit
CALCULATED 24 EQUILIBRIA
*** LAST BUFFER SAVED ON FILE: c:\jenkins\workspace\generate_console_examples\examples\tcex31\tcex31a.POLY3
CPU time for mapping 0 seconds
POLY: po
... the command in full is POST
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: s-d-a x m-f b
... the command in full is SET_DIAGRAM_AXIS

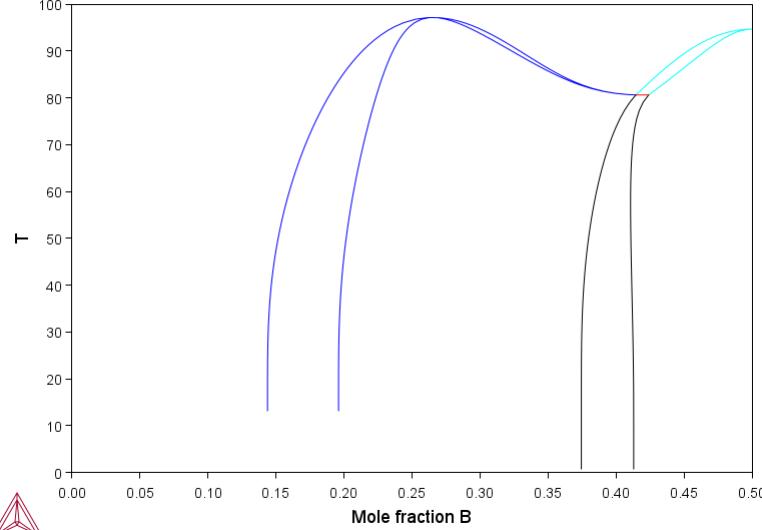
```

```

POST: s-d-a y t
... the command in full is SET_DIAGRAM_AXIS
POST: s-s-s x n 0 0.5
... the command in full is SET_SCALING_STATUS
POST: s-s-s y n 0 100
... the command in full is SET_SCALING_STATUS
POST: set-title example 31a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 31a



```

POST:
POST:
POST:Hit RETURN to continue
POST:
POST: @@ Make an Experimental data file to overlay the next
POST: @@ calculation
POST: make tcex31 y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: back
POLY: @@
POLY: @@ It is interesting to compare with a CEF without any
POLY: @@ SRO contribution. This is the classical FCC ordering
POLY: @@ diagram first calculated manually by W Shockley,
POLY: @@ J Chem Phys, 6, (1938) p 130.
POLY: read tcex31a
... the command in full is READ_WORKSPACES
POLY: list-ini-eq
... the command in full is LIST_INITIAL_EQUILIBRIA
POLY:
POLY:
POLY:
POLY:Hit RETURN to continue
POLY:
POLY: c-st p *=sus
... the command in full is CHANGE_STATUS
POLY: c-st p lro lro#2 lro#3=ent 0
... the command in full is CHANGE_STATUS
POLY: s-c t=70 x(b)=.4
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
29 ITS, CPU TIME USED 0 SECONDS
POLY: l-e,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: User dat

```

Conditions:
T=70, P=100000, N=1., X(B)=0.4
DEGREES OF FREEDOM 0

Temperature 70.00 K (-203.15 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 1.00000E+01
Total Gibbs energy -3.08055E+03, Enthalpy -2.95310E+03, Volume 0.00000E+00

| | | | | | |
|-----------|------------|------------|------------|-------------|----------|
| Component | Moles | M-Fraction | Activity | Potential | Ref.stat |
| A | 6.0000E-01 | 6.0000E-01 | 4.7333E-02 | -1.7755E+03 | SER |
| B | 4.0000E-01 | 4.0000E-01 | 1.7400E-04 | -5.0382E+03 | SER |

LRO#1 ORD Status ENTERED Driving force 0.0000E+00
Moles 2.6762E-01, Mass 2.6762E+00, Volume fraction 0.0000E+00 Mole fractions:
A 6.74559E-01 B 3.25441E-01

Constitution:

| | | | |
|-------------------------------|-------------|---|-------------|
| Sublattice 1, Number of sites | 2.5000E-01 | | |
| A | 8.99309E-01 | B | 1.00691E-01 |
| Sublattice 2, Number of sites | 2.5000E-01 | | |
| A | 8.99309E-01 | B | 1.00691E-01 |
| Sublattice 3, Number of sites | 2.5000E-01 | | |
| A | 8.99309E-01 | B | 1.00691E-01 |
| Sublattice 4, Number of sites | 2.5000E-01 | | |
| B | 9.99692E-01 | A | 3.08116E-04 |

LRO#2 DISORD Status ENTERED Driving force -4.6485E-01
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mole fractions:
A 6.45965E-01 B 3.54035E-01
Constitution:
Sublattice 1, Number of sites 2.5000E-01

```

A 6.45965E-01 B 3.54035E-01
Sublattice 2, Number of sites 2.5000E-01
A 6.45965E-01 B 3.54035E-01
Sublattice 3, Number of sites 2.5000E-01
A 6.45965E-01 B 3.54035E-01
Sublattice 4, Number of sites 2.5000E-01
A 6.45965E-01 B 3.54035E-01

LRO#3          ORD Status ENTERED Driving force 0.0000E+00
Moles 7.3238E-01, Mass 7.3238E+00, Volume fraction 0.0000E+00 Mole fractions:
A 5.72756E-01 B 4.27244E-01
Constitution:
Sublattice 1, Number of sites 2.5000E-01
A 9.99661E-01 B 3.38612E-04
Sublattice 2, Number of sites 2.5000E-01
A 9.99661E-01 B 3.38612E-04
Sublattice 3, Number of sites 2.5000E-01
B 8.54150E-01 A 1.45850E-01
Sublattice 4, Number of sites 2.5000E-01
B 8.54150E-01 A 1.45850E-01
POLY:Hit RETURN to continue
POLY:
POLY: s-s-c lro#3
... the command in full is SET_START_CONSTITUITION
Y(LRO#3,A) /.9996613878:/
Y(LRO#3,B) /3.386121641E-04:/
Y(LRO#3,A#2) /.9996613878:/
Y(LRO#3,B#2) /3.386121641E-04:/
Y(LRO#3,A#3) /.1458499446/: 0.0001
Y(LRO#3,B#3) /.8541500554/: 0.9999
Y(LRO#3,A#4) /.1458499446/: .6
Y(LRO#3,B#4) /.8541500554/: .4
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
19 ITS, CPU TIME USED 0 SECONDS
POLY: l-e,,,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: User dat

Conditions:
T=70, P=100000, N=1., X(B)=0.4
DEGREES OF FREEDOM 0

Temperature 70.00 K (-203.15 C), Pressure 1.000000E+05
Number of moles of components 1.000000E+00, Mass in grams 1.000000E+01
Total Gibbs energy -3.09267E+03, Enthalpy -2.98506E+03, Volume 0.000000E+00

Component Moles M-Fraction Activity Potential Ref.stat
A 6.0000E-01 6.0000E-01 4.1721E-02 -1.8489E+03 SER
B 4.0000E-01 4.0000E-01 1.9961E-04 -4.9583E+03 SER

LRO#1          ORD Status ENTERED Driving force -3.9680E-02
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mole fractions:
A 6.68666E-01 B 3.31334E-01
Constitution:
Sublattice 1, Number of sites 2.5000E-01
A 8.91452E-01 B 1.08548E-01
Sublattice 2, Number of sites 2.5000E-01
A 8.91452E-01 B 1.08548E-01
Sublattice 3, Number of sites 2.5000E-01
A 8.91452E-01 B 1.08548E-01
Sublattice 4, Number of sites 2.5000E-01
B 9.99690E-01 A 3.09940E-04

LRO#2          DISORD Status ENTERED Driving force -4.9687E-01
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mole fractions:
A 6.39146E-01 B 3.60854E-01
Constitution:
Sublattice 1, Number of sites 2.5000E-01
A 6.39146E-01 B 3.60854E-01
Sublattice 2, Number of sites 2.5000E-01
A 6.39146E-01 B 3.60854E-01
Sublattice 3, Number of sites 2.5000E-01
A 6.39146E-01 B 3.60854E-01
Sublattice 4, Number of sites 2.5000E-01
A 6.39146E-01 B 3.60854E-01

LRO#3          ORD Status ENTERED Driving force 0.0000E+00
Moles 1.0000E+00, Mass 1.0000E+01, Volume fraction 0.0000E+00 Mole fractions:
A 6.00000E-01 B 4.00000E-01
Constitution:
Sublattice 1, Number of sites 2.5000E-01
A 9.98449E-01 B 1.55066E-03
Sublattice 2, Number of sites 2.5000E-01
A 9.98449E-01 B 1.55066E-03
Sublattice 3, Number of sites 2.5000E-01
B 9.92271E-01 A 7.72920E-03
Sublattice 4, Number of sites 2.5000E-01
B 6.04628E-01 A 3.95372E-01
POLY:Hit RETURN to continue
POLY:
POLY: s-c x(b)=.33
... the command in full is SET_CONDITION
POLY: s-s-c lro *
... the command in full is SET_START_CONSTITUITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
20 ITS, CPU TIME USED 1 SECONDS
POLY: l-e,,,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: User dat

Conditions:
T=70, P=100000, N=1., X(B)=0.33
DEGREES OF FREEDOM 0

Temperature 70.00 K (-203.15 C), Pressure 1.000000E+05
Number of moles of components 1.000000E+00, Mass in grams 1.000000E+01
Total Gibbs energy -2.85605E+03, Enthalpy -2.74060E+03, Volume 0.000000E+00

Component Moles M-Fraction Activity Potential Ref.stat
A 6.7000E-01 6.7000E-01 5.7336E-02 -1.6639E+03 SER
B 3.3000E-01 3.3000E-01 1.1554E-04 -5.2765E+03 SER

LRO#1          ORD Status ENTERED Driving force 0.0000E+00

```

```

Moles 7.8876E-02, Mass 7.8876E-01, Volume fraction 0.0000E+00 Mole fractions:
A 6.87496E-01 B 3.12504E-01
Constitution:
Sublattice 1, Number of sites 2.5000E-01
A 9.16558E-01 B 8.34422E-02
Sublattice 2, Number of sites 2.5000E-01
A 9.16558E-01 B 8.34422E-02
Sublattice 3, Number of sites 2.5000E-01
A 9.16558E-01 B 8.34422E-02
Sublattice 4, Number of sites 2.5000E-01
B 9.99689E-01 A 3.11152E-04

LRO#2          DISORD Status ENTERED Driving force -4.8130E-01
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mole fractions:
A 6.61498E-01 B 3.38502E-01
Constitution:
Sublattice 1, Number of sites 2.5000E-01
A 6.61498E-01 B 3.38502E-01
Sublattice 2, Number of sites 2.5000E-01
A 6.61498E-01 B 3.38502E-01
Sublattice 3, Number of sites 2.5000E-01
A 6.61498E-01 B 3.38502E-01
Sublattice 4, Number of sites 2.5000E-01
A 6.61498E-01 B 3.38502E-01

LRO#3          ORD Status ENTERED Driving force 0.0000E+00
Moles 9.2112E-01, Mass 9.2112E+00, Volume fraction 0.0000E+00 Mole fractions:
A 6.68502E-01 B 3.31498E-01
Constitution:
Sublattice 1, Number of sites 2.5000E-01
A 9.82295E-01 B 1.77045E-02
Sublattice 2, Number of sites 2.5000E-01
A 9.82295E-01 B 1.77045E-02
Sublattice 3, Number of sites 2.5000E-01
B 9.99255E-01 A 7.44800E-04
Sublattice 4, Number of sites 2.5000E-01
A 7.08671E-01 B 2.91329E-01
POLY:Hit RETURN to continue
POLY:
POLY: s-a-v 2 t 0 250 5
... the command in full is SET_AXIS_VARIABLE
POLY:
POLY: list-init-eq
... the command in full is LIST_INITIAL_EQUILIBRIA
POLY:
POLY:
POLY:Hit RETURN to continue
POLY:
POLY: save tcex31c y
... the command in full is SAVE_WORKSPACES
POLY:
POLY: add -1
... the command in full is ADD_INITIAL_EQUIlibrium
POLY:
POLY:
POLY: list-init-eq
... the command in full is LIST_INITIAL_EQUILIBRIA
No 1 -1 T=70, P=100000, N=1., X(B)=0.33
POLY:
POLY:
POLY:Hit RETURN to continue
POLY:
POLY: map -
Version R mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2

Phase region boundary 1 at: 3.315E-01 7.0000E+01
** LRO#1
LRO#3
*** SORRY CANNOT CONTINUE ***
CALCULATED 41 EQUILIBRIA

Phase region boundary 2 at: 3.315E-01 7.0000E+01
** LRO#1
LRO#3
Terminating at diagram limit
CALCULATED 68 EQUILIBRIA
*** LAST BUFFER SAVED ON FILE: c:\jenkins\workspace\generate_console_examples\examples\tcex31\tcex31c.POLY3
CPU time for mapping 0 seconds
POLY: @@ Add the A2/L1_2 line
POLY: read tcex31c
... the command in full is READ_WORKSPACES
POLY:
POLY:
POLY: list-init-eq
... the command in full is LIST_INITIAL_EQUILIBRIA
POLY:
POLY:
POLY: s-c x(b)=.15 t=110
... the command in full is SET_CONDITION
POLY: s-a-s f
... the command in full is SET_ALL_START_VALUES
Forcing automatic start values
Automatic start values will be set
POLY: c-e
... the command in full is COMPUTE_EQUIlibrium
34 ITC, CPU TIME USED 0 SECONDS
POLY: l-e,,
... the command in full is LIST_EQUIlibrium
Output from POLY-3, equilibrium = 1, label A0 , database: User dat

Conditions:
T=110, P=100000, N=1., X(B)=0.15
DEGREES OF FREEDOM 0

Temperature 110.00 K (-163.15 C), Pressure 1.000000E+05

```

Number of moles of components 1.00000E+00, Mass in grams 1.00000E+01
Total Gibbs energy -1.66707E+03, Enthalpy -1.39975E+03, Volume 0.00000E+00

| Component | Moles | M-Fraction | Activity | Potential | Ref.stat |
|-----------|------------|------------|------------|-------------|----------|
| A | 8.5000E-01 | 8.5000E-01 | 7.3635E-01 | -2.7991E+02 | SER |
| B | 1.5000E-01 | 1.5000E-01 | 2.9909E-05 | -9.5277E+03 | SER |

LRO#1 ORD Status ENTERED Driving force 0.0000E+00
Moles 7.2552E-01, Mass 7.2552E+00, Volume fraction 0.0000E+00 Mole fractions:
A 8.40743E-01 B 1.59257E-01
Constitution:
Sublattice 1, Number of sites 2.5000E-01
A 9.74694E-01 B 2.53056E-02
Sublattice 2, Number of sites 2.5000E-01
A 9.74694E-01 B 2.53056E-02
Sublattice 3, Number of sites 2.5000E-01
A 9.74694E-01 B 2.53056E-02
Sublattice 4, Number of sites 2.5000E-01
B 5.61112E-01 A 4.38888E-01

LRO#2 DISORD Status ENTERED Driving force 0.0000E+00
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mole fractions:
A 8.74469E-01 B 1.25531E-01
Constitution:
Sublattice 1, Number of sites 2.5000E-01
A 8.74469E-01 B 1.25531E-01
Sublattice 2, Number of sites 2.5000E-01
A 8.74469E-01 B 1.25531E-01
Sublattice 3, Number of sites 2.5000E-01
A 8.74469E-01 B 1.25531E-01
Sublattice 4, Number of sites 2.5000E-01
A 8.74469E-01 B 1.25531E-01

LRO#3 DISORD Status ENTERED Driving force 0.0000E+00
Moles 2.7448E-01, Mass 2.7448E+00, Volume fraction 0.0000E+00 Mole fractions:
A 8.74469E-01 B 1.25531E-01
Constitution:
Sublattice 1, Number of sites 2.5000E-01
A 8.74469E-01 B 1.25531E-01
Sublattice 2, Number of sites 2.5000E-01
A 8.74469E-01 B 1.25531E-01
Sublattice 3, Number of sites 2.5000E-01
A 8.74469E-01 B 1.25531E-01
Sublattice 4, Number of sites 2.5000E-01
A 8.74469E-01 B 1.25531E-01

POLY:Hit RETURN to continue
POLY:
POLY: list-init-eq
... the command in full is LIST_INITIAL_EQUILIBRIA
POLY:
POLY:
POLY:Hit RETURN to continue
POLY:
POLY: map -
Version R mapping is selected

Organizing start points

NO INITIAL EQUILIBRIUM ADDED, TRYING TO FIX ONE
Generating start point 1
Generating start point 2

Phase region boundary 1 at: 1.593E-01 1.100E+02
LRO#1
** LRO#3
MAPPING TERMINATED 1
CALCULATED 55 EQUILIBRIA

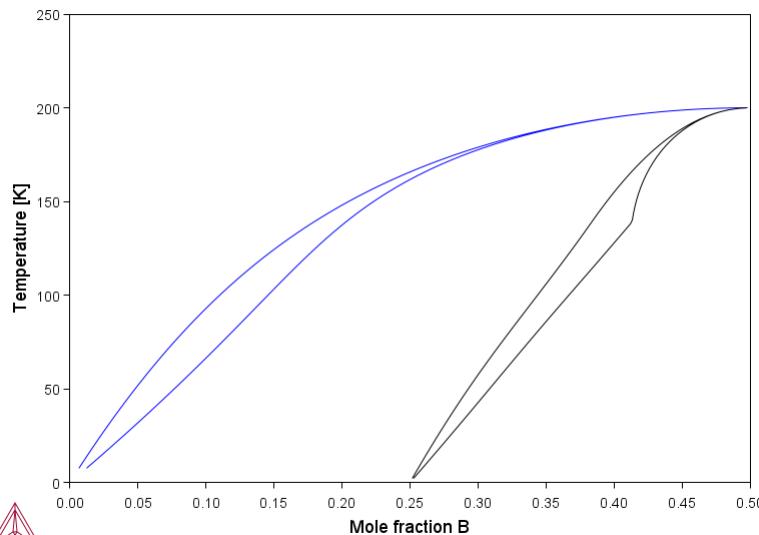
Phase region boundary 2 at: 1.593E-01 1.100E+02
LRO#1
** LRO#3
Terminating at diagram limit
CALCULATED 69 EQUILIBRIA
*** LAST BUFFER SAVED ON FILE: c:\jenkins\workspace\generate_console_examples\examples\tcex31\tcex31c.POLY3
CPU time for mapping 0 seconds

POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

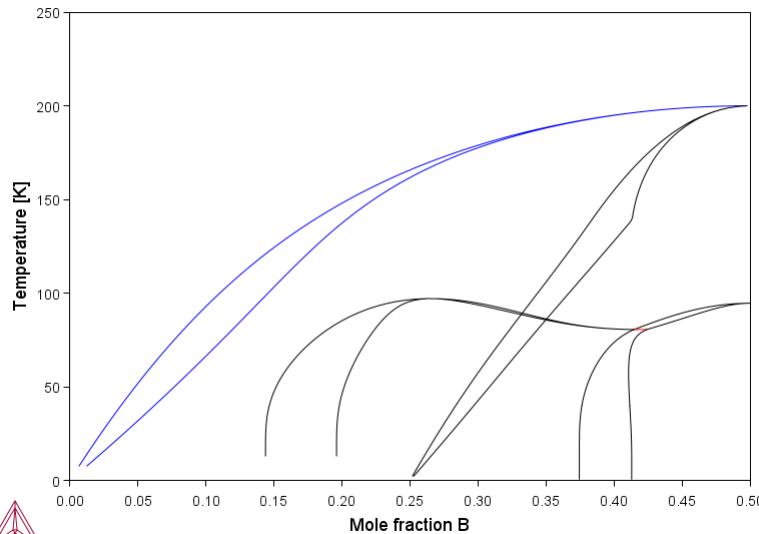
POST: s-s x n 0 .5
... the command in full is SET_SCALING_STATUS
POST: @@ Usually some 2nd order lines also appear
POST: set-title example 31b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

example 31b



```
POST:  
POST:  
POST:Hit RETURN to continue  
POST:  
POST: a-e-d y tce31 0; 1;  
... the command in full is APPEND_EXPERIMENTAL_DATA  
POST:  
POST: set-title example 31c  
POST:  
POST:  
POST: SET_EXP_FILE_FORMAT 5  
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y  
... the command in full is MAKE_EXPERIMENTAL_DATAFI  
POST: SET_EXP_FILE_FORMAT 10  
POST:  
POST: plot  
... the command in full is PLOT_DIAGRAM
```

example 31c



```
POST:  
POST:Hit RETURN to continue  
POST:  
POST: ba  
... the command in full is BACK  
POLY: read tce31c  
... the command in full is READ_WORKSPACES  
POLY: go g  
... the command in full is GOTO_MODULE  
GIBBS ENERGY SYSTEM  
GES5: @@ Now add a reciprocal parameter to LRO which describes  
GES5: @@ the SRO contribution. The default value of this is  
GES5: @@ the bond energy. One can have 3 different parameters  
GES5: @@ depending on if one is at 25%B, 50%B or 75%B. Here  
GES5: @@ we just take the same value.  
GES5:  
GES5: e-sym f GSROAA,,UIJ;.....  
... the command in full is ENTER_SYMBOL  
GES5: e-sym f GSROAB,,UIJ;.....  
... the command in full is ENTER_SYMBOL  
GES5: e-sym f GSROBB,,UIJ;.....  
... the command in full is ENTER_SYMBOL  
GES5:  
GES5: e-par l(lro,a,b:a,b:*),,GSROAB;....  
... the command in full is ENTER_PARAMETER  
L(LRO,A,B:A,B:*)  
GES5: e-par l(lro,a,b:*:a,b:*),,GSROAB;....  
... the command in full is ENTER_PARAMETER  
L(LRO,A,B:*:A,B:*)  
GES5: e-par l(lro,a,b:***:a,b),,GSROAB;....
```

```

... the command in full is ENTER_PARAMETER
L(LRO,A,B::*:A,B;0)
GES5: e-par l(lro,*:a,b:a,b:*),,GSROAB;....
... the command in full is ENTER_PARAMETER
L(LRO,*:A,B:A,B:*;0)
GES5: e-par l(lro,*:a,b::a,b),,GSROAB;....
... the command in full is ENTER_PARAMETER
L(LRO,*::A,B:A,B;0)
GES5: e-par l(lro,*::a,b:a,b),,GSROAB;....
... the command in full is ENTER_PARAMETER
L(LRO,*::A,B:A,B;0)
GES5: l-p-d lro
... the command in full is LIST_PHASE_DATA

LRO
$ THIS PHASE HAS A DISORDERED CONTRIBUTION FROM FCC_A1
EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
4 SUBLATTICES, SITES .25: .25: .25: .25
CONSTITUENTS: A,B : A,B : A,B : A,B

G(LRO,A::A:A:A;0) = 0.0
G(LRO,B::A::A:A;0) = +GA3B1
G(LRO,A:B::A:A;0) = +GA3B1
G(LRO,B:B::A:A;0) = +GA2B2
G(LRO,A:A:B::A;0) = +GA3B1
G(LRO,B::A:B::A;0) = +GA2B2
G(LRO,A:B::A:B;0) = +GA2B2
G(LRO,B:B::A:B;0) = +GA1B3
G(LRO,A:A:B:B;0) = +GA3B1
G(LRO,B:A:B:B;0) = +GA2B2
G(LRO,A:B:A:B;0) = +GA2B2
G(LRO,B:B:A:B;0) = +GA1B3
G(LRO,A:A:B:B;0) = +GA2B2
G(LRO,B:A:B:B;0) = +GA1B3
G(LRO,A:B:B:B;0) = +GA1B3
G(LRO,B:B:B:B;0) = 0.0
G(LRO,A::A::*:0) = 0.0
G(LRO,A::*:A::0) = 0.0
G(LRO,*:A::A::0) = 0.0
G(LRO,*::A::A::0) = 0.0
L(LRO,A,B::*,*:0) = +GSROAB
L(LRO,A,B::*:A,B;0) = +GSROAB
L(LRO,A,B::*:A,B;0) = +GSROAB
L(LRO,*:A,B::A,B;0) = +GSROAB
L(LRO,*::A,B::A,B;0) = +GSROAB
GES5:
GES5:Hit RETURN to continue
GES5:
GES5: @@ These reciprocal parameters do not give any contribution to
GES5: @@ the disordered state as the contribution from the ordered
GES5: @@ phase is zero there. But it is in the disordered state that
GES5: @@ the SRO contribution to the Gibbs energy is most important.
GES5: @@ We must add regular solution parameters to the FCC phase
GES5: @@ giving the same contribution. These can be derived by
GES5: @@ setting all site-fractions for the same element equal,
GES5: @@ i.e. the disordered state.
GES5:
GES5: e-par l(fcc,a,b;0),,GA3B1+1.5*GA2B2+GA1B3+
... the command in full is ENTER_PARAMETER
L(FCC_A1,A,B;0)
& 0.375*GSROAA+.75*GSROAB+0.375*GSROBB;....,
GES5: e-par l(fcc,a,b;1),,2*GA3B1-2*GA1B3+0.75*GSROAA-0.75*GSROBB;....,
... the command in full is ENTER_PARAMETER
L(FCC_A1,A,B;1)
GES5: e-par l(fcc,a,b;2),,GA3B1-1.5*GA2B2+GA1B3-1.5*GSROAB;....,
... the command in full is ENTER_PARAMETER
L(FCC_A1,A,B;2)
GES5: e-par l(fcc,a,b;3),,-0.75*GSROAA+0.75*GSROBB;....,
... the command in full is ENTER_PARAMETER
L(FCC_A1,A,B;3)
GES5: e-par l(fcc,a,b;4),,-0.375*GSROAA+0.75*GSROAB-0.375*GSROBB;....,
... the command in full is ENTER_PARAMETER
L(FCC_A1,A,B;4)
GES5: l-p-d fcc
... the command in full is LIST_PHASE_DATA

FCC_A1
$ THIS PHASE IS THE DISORDERED PART OF LRO
EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
CONSTITUENTS: A,B

G(FCC_A1,A;0)-G(FCC,A;0) = 0.0
G(FCC_A1,B;0)-G(FCC,B;0) = 0.0
L(FCC_A1,A,B;0) = +GA3B1+1.5*GA2B2+GA1B3+.375*GSROAA+.75*GSROAB
+.375*GSROBB
L(FCC_A1,A,B;1) = +2*GA3B1-2*GA1B3+.75*GSROAA-.75*GSROBB
L(FCC_A1,A,B;2) = +GA3B1-1.5*GA2B2+GA1B3-1.5*GSROAB
L(FCC_A1,A,B;3) = -.75*GSROAA-.75*GSROAB
L(FCC_A1,A,B;4) = -.375*GSROAA+.75*GSROAB-.375*GSROBB
GES5:
GES5:Hit RETURN to continue
GES5:
GES5: ba
... the command in full is BACK
POLY: c-st p lro#3=e 0
... the command in full is CHANGE_STATUS
POLY: l-c
... the command in full is LIST_CONDITIONS
T=70, P=100000, N=1., X(B)=0.33
DEGREES OF FREEDOM 0
POLY: s-c t=40
... the command in full is SET_CONDITION
POLY: s-a=s f
... the command in full is SET_ALL_START_VALUES
Forcing automatic start values
Automatic start values will be set
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM

```

```

Global equilibrium calculation turned off, you can turn it on with
ADVANCED_OPTIONS GLOBAL_MINIMIZATION Y,,,...,
 24 ITS, CPU TIME USED 0 SECONDS
POLY: l-e,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: User dat

Conditions:
T=40, P=100000, N=1., X(B)=0.33
DEGREES OF FREEDOM 0

Temperature 40.00 K (-233.15 C), Pressure 1.000000E+05
Number of moles of components 1.000000E+00, Mass in grams 1.000000E+01
Total Gibbs energy -2.81177E+03, Enthalpy -2.73484E+03, Volume 0.000000E+00

Component Moles M-Fraction Activity Potential Ref.stat
A 6.7000E-01 6.7000E-01 5.5303E-03 -1.7286E+03 SER
B 3.3000E-01 3.3000E-01 2.8612E-07 -5.0109E+03 SER

LRO#1 ORD Status ENTERED Driving force 0.00000E+00
Moles 9.1974E-01, Mass 9.1974E+00, Volume fraction 0.0000E+00 Mole fractions:
A 6.79151E-01 B 3.20849E-01
Constitution:
Sublattice 1, Number of sites 2.5000E-01
A 9.05532E-01 B 9.44682E-02
Sublattice 2, Number of sites 2.5000E-01
A 9.05532E-01 B 9.44682E-02
Sublattice 3, Number of sites 2.5000E-01
A 9.05532E-01 B 9.44682E-02
Sublattice 4, Number of sites 2.5000E-01
B 9.99993E-01 A 6.81574E-06

LRO#2 DISORD Status ENTERED Driving force -3.8166E-01
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mole fractions:
A 6.26318E-01 B 3.73682E-01
Constitution:
Sublattice 1, Number of sites 2.5000E-01
A 6.26318E-01 B 3.73682E-01
Sublattice 2, Number of sites 2.5000E-01
A 6.26318E-01 B 3.73682E-01
Sublattice 3, Number of sites 2.5000E-01
A 6.26318E-01 B 3.73682E-01
Sublattice 4, Number of sites 2.5000E-01
A 6.26318E-01 B 3.73682E-01

LRO#3 ORD Status ENTERED Driving force 0.0000E+00
Moles 8.0263E-02, Mass 8.0263E-01, Volume fraction 0.0000E+00 Mole fractions:
A 5.65144E-01 B 4.34856E-01
Constitution:
Sublattice 1, Number of sites 2.5000E-01
A 9.99996E-01 B 4.15407E-06
Sublattice 2, Number of sites 2.5000E-01
A 9.99996E-01 B 4.15407E-06
Sublattice 3, Number of sites 2.5000E-01
B 8.69708E-01 A 1.30292E-01
Sublattice 4, Number of sites 2.5000E-01
B 8.69708E-01 A 1.30292E-01
POLY:Hit RETURN to continue
POLY:
POLY: save tcex31d y
... the command in full is SAVE_WORKSPACES
POLY:
POLY: list-init-eq
... the command in full is LIST_INITIAL_EQUILIBRIA
POLY:
POLY:
POLY:Hit RETURN to continue
POLY:
POLY: map -
Version R mapping is selected

Organizing start points

NO INITIAL EQUILIBRIUM ADDED, TRYING TO FIX ONE
Generating start point 1
Generating start point 2

Phase region boundary 1 at: 3.208E-01 4.0000E+01
  LRO#1
  ** LRO#3
TOO LONG JUMP IN AXIS, SKIPPING NODE
MAPPING TERMINATED 1
CALCULATED 30 EQUILIBRIA

Phase region boundary 2 at: 3.208E-01 4.0000E+01
  LRO#1
  ** LRO#3
CALCULATED 22 EQUILIBRIA

Phase region boundary 2 at: 3.685E-01 7.734E+01
  LRO#1
  LRO#2
  ** LRO#3

Phase region boundary 2 at: 4.193E-01 7.734E+01
  ** LRO#2
  LRO#3
Terminating at diagram limit
CALCULATED 23 EQUILIBRIA

Phase region boundary 2 at: 3.685E-01 7.734E+01
  LRO#1
  ** LRO#2
Terminating at diagram limit
CALCULATED 90 EQUILIBRIA
*** LAST BUFFER SAVED ON FILE: c:\jenkins\workspace\generate_console_examples\examples\tcex31\tcex31d.POLY3
CPU time for mapping 1 seconds
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

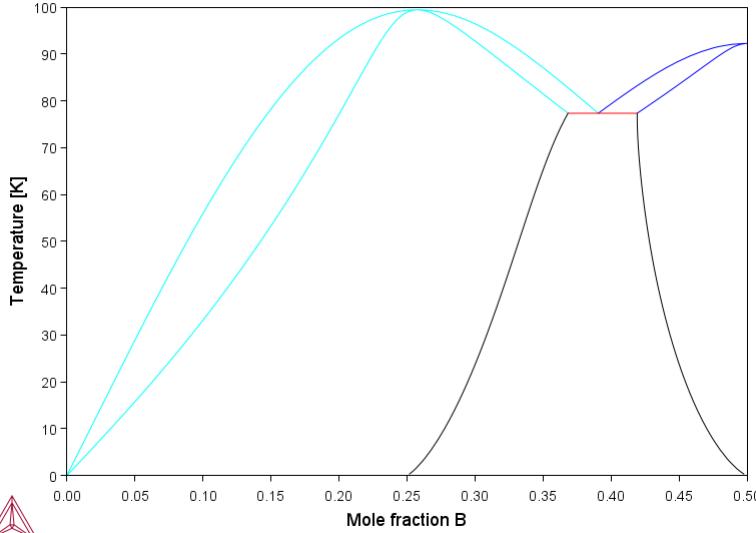
POST: set-title example 31d
POST: s-s y n
... the command in full is SET_SCALING_STATUS

```

```

MIN VALUE : 0 100
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
example 31d

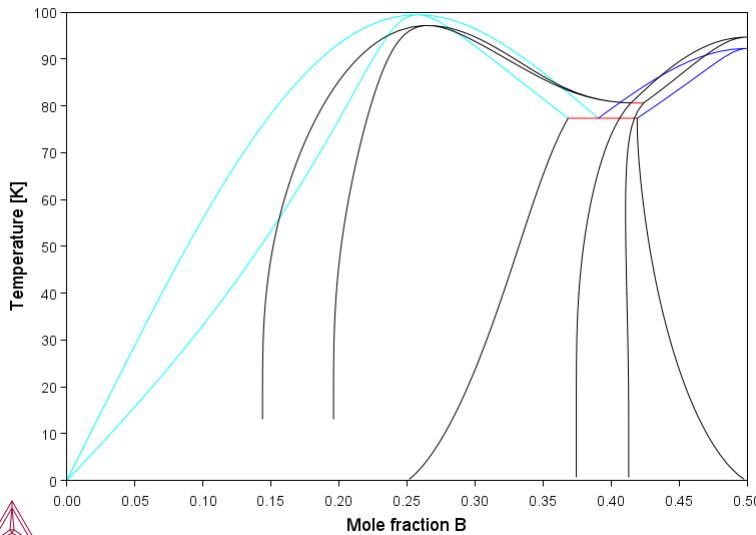
```



```

POST:
POST:Hit RETURN to continue
POST:
POST: a-e-d y tcex31 0; 1;
... the command in full is APPEND_EXPERIMENTAL_DATA
POST: set-title example 31e
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
example 31e

```



```

POST:
POST: @@ It actually turns out, that this is not the stable phase diagram,
POST: @@ but rather a meta-stable diagram. Thanks to Nathalie Dupin for
POST: @@ pointing this out to us :-)
POST: @@ The calculation of the stable diagram is not entirely trivial.
POST: @@ It requires switching GLOBAL on again and also a Global test interval of 1.
POST: @@ This is done like shown below and will noticeably increase calculation time.
POST:
POST:Hit RETURN to continue
POST:
POST: ba
... the command in full is BACK
POLY: s-c x(b)=0.4 t=70
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
17 ITS, CPU TIME USED 0 SECONDS
POLY: adv g y 2000
... the command in full is ADVANCED_OPTIONS
Settings for global minimization:
POLY: adv step,1,...
... the command in full is ADVANCED_OPTIONS

```

Settings for MAP and STEP:
 Settings for MAP:
POLY: s-a=s y
 ... the command in full is SET_ALL_START_VALUES
 Old start values kept
POLY: c-e
 ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated 1360 grid points in 0 s
 Found the set of lowest grid points in 0 s
 Calculated POLY solution 0 s, total time 0 s
POLY: save tceex3le_stable y
 ... the command in full is SAVE_WORKSPACES
POLY: map
 Version S mapping is selected
 Generating start equilibrium 1
 Generating start equilibrium 2
 Generating start equilibrium 3
 Generating start equilibrium 4
 Generating start equilibrium 5
 Generating start equilibrium 6
 Generating start equilibrium 7
 Generating start equilibrium 8
 Generating start equilibrium 9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

 Using ADDED start equilibria

 Trying global minimization! 3
 Working hard
 Working hard
 Trying global minimization! 3
 Working hard
 Trying global minimization! 3
 Working hard
 Working hard
 Working hard
 Working hard
 Generating start point 1
 Generating start point 2
 Generating start point 3
 Generating start point 4
 Generating start point 5
 Generating start point 6
 Trying global minimization! 3
 Generating start point 7
 Generating start point 8
 Generating start point 9
 Generating start point 10
 Working hard
 Generating start point 11
 Generating start point 12

 Phase region boundary 1 at: 1.244E-02 5.000E+00
 LRO#1
 ** LRO#2
 Calculated 6 equilibria

 Phase region boundary 2 at: 1.244E-02 5.000E+00
 LRO#1
 ** LRO#2
 Calculated. 37 equilibria

 Phase region boundary 3 at: 3.796E-01 7.734E+01
 LRO#1
 ** LRO#2
 ** LRO#3
 Calculated.. 16 equilibria
 Terminating at axis limit.

 Phase region boundary 4 at: 4.050E-01 7.734E+01
 LRO#1
 ** LRO#3
 Calculated. 16 equilibria

 Phase region boundary 5 at: 3.939E-01 7.734E+01
 LRO#2
 ** LRO#3
 Calculated 18 equilibria

 Phase region boundary 6 at: 3.796E-01 7.734E+01
 LRO#1
 ** LRO#2
 Calculated 55 equilibria

 Phase region boundary 7 at: 1.244E-02 5.000E+00
 LRO#1
 ** LRO#2
 Calculated 6 equilibria

 Phase region boundary 8 at: 1.244E-02 5.000E+00
 LRO#1
 ** LRO#2
 Calculated. 37 equilibria
 Terminating at known equilibrium

 Phase region boundary 9 at: 1.415E-01 6.228E+01
 ** LRO#1
 LRO#2
 Calculated 35 equilibria

 Phase region boundary 10 at: 1.415E-01 6.228E+01
 ** LRO#1
 LRO#2
 Calculated. 23 equilibria
 Terminating at known equilibrium

 Phase region boundary 11 at: 1.244E-02 5.000E+00
 ** LRO#1
 LRO#2
 Calculated. 37 equilibria
 Terminating at known equilibrium

```

Phase region boundary 12 at: 1.244E-02 5.000E+00
** LRO#1
LRO#2
Calculated. 37 equilibria
Terminating at known equilibrium

Phase region boundary 13 at: 4.840E-01 9.148E+01
** LRO#1
LRO#2
Calculated. 9 equilibria
Terminating at known equilibrium

Phase region boundary 14 at: 4.840E-01 9.148E+01
** LRO#1
LRO#2
Calculated.. 3 equilibria
Terminating at axis limit.

Phase region boundary 15 at: 4.965E-01 9.199E+01
** LRO#1
LRO#2
Calculated. 19 equilibria
Terminating at known equilibrium

Phase region boundary 16 at: 4.430E-01 8.500E+01
** LRO#1
LRO#2
Calculated. 5 equilibria
Terminating at known equilibrium

Phase region boundary 17 at: 4.430E-01 8.500E+01
** LRO#1
LRO#2
Calculated.. 10 equilibria
Terminating at axis limit.

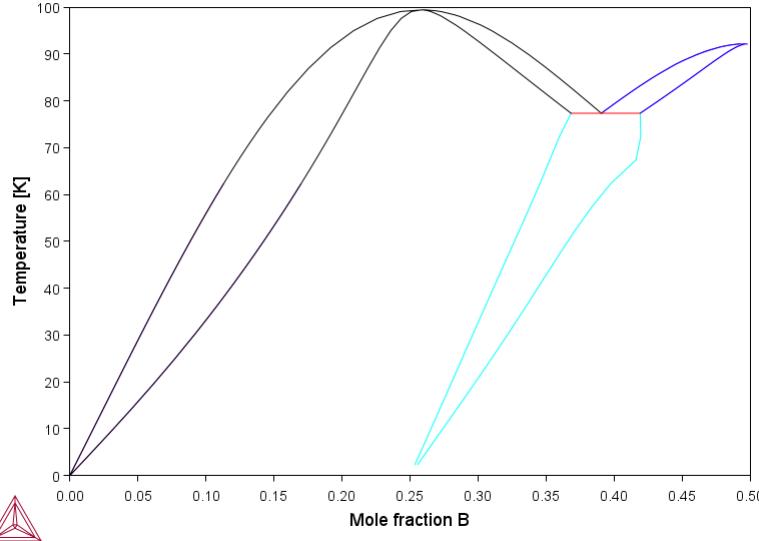
Phase region boundary 18 at: 4.962E-01 9.201E+01
** LRO#1
LRO#2
Calculated. 19 equilibria
Terminating at known equilibrium
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\generate_console_examples\examples\tcex31\tcex31e_stable.POLY3
CPU time for mapping 27 seconds
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: set-title example 31e-stable
POST: s-s-s y n 0 100
... the command in full is SET_SCALING_STATUS
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 31e-stable



```

POST:
POST: @@ There is still a tiny part of the phase diagram missing
POST: @@ At M-F B = 0.25.
POST: @@ This gap can be filled by some more fine tuning:
POST: @@ 1. making a finer step interval in the mapping
POST: @@ 2. increase the gridpoints for GLOBAL to 4000
POST: @@ Note, that there might be other combinations that will
POST: @@ work. Finding good solutions is simply a matter of experience
POST: @@ and trial-and-error... If you find a good solution, you are
POST: @@ always welcomed to let us know: support@thermocalc.com
POST:
POST: Hit RETURN to continue
POST:
POST: ba
... the command in full is BACK
POLY: s-a-v 1 X(B) 0 0.5 0.0005
... the command in full is SET_AXIS_VARIABLE
POLY: s-a-v 2 t 0 100 1
... the command in full is SET_AXIS_VARIABLE
POLY: adv g y 4000
... the command in full is ADVANCED_OPTIONS

```

```

Settings for global minimization:
POLY: adv step,10,,,
... the command in full is ADVANCED_OPTIONS
Settings for MAP and STEP:
Settings for MAP:
POLY: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Trying global minimization! 3
Trying global minimization! 3
Generating start point 5
Generating start point 6
Trying global minimization! 3
Generating start point 7
Generating start point 8
Trying global minimization! 3
Trying global minimization! 3
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Trying global minimization! 3
Generating start point 13
Generating start point 14
Trying global minimization! 3
Generating start point 15
Generating start point 16
Trying global minimization! 3
Generating start point 17
Generating start point 18

Phase region boundary 1 at: 2.493E-03 1.000E+00
** LRO#1
LRO#2
Calculated 19 equilibria

Phase region boundary 2 at: 2.493E-03 1.000E+00
** LRO#1
LRO#2
Calculated. 756 equilibria

Phase region boundary 3 at: 3.796E-01 7.734E+01
** LRO#1
LRO#2
** LRO#3
Calculated 31 equilibria

Phase region boundary 4 at: 3.939E-01 7.734E+01
LRO#2
** LRO#3
Calculated 31 equilibria

Phase region boundary 5 at: 3.939E-01 7.734E+01
LRO#2
** LRO#3
Calculated.. 177 equilibria
Terminating at axis limit.

Phase region boundary 6 at: 4.050E-01 7.734E+01
LRO#1
** LRO#3
Calculated.. 191 equilibria
Terminating at axis limit.

Phase region boundary 7 at: 3.796E-01 7.734E+01
** LRO#1
LRO#2
Calculated 775 equilibria

Phase region boundary 8 at: 1.384E-01 6.081E+01
** LRO#1
LRO#2
Calculated 290 equilibria

Phase region boundary 9 at: 1.384E-01 6.081E+01
** LRO#1
LRO#2
Calculated. 484 equilibria
Terminating at known equilibrium

Phase region boundary 10 at: 2.493E-03 1.000E+00
** LRO#1
LRO#2
Calculated 19 equilibria

Phase region boundary 11 at: 2.493E-03 1.000E+00
** LRO#1
LRO#2
Calculated. 756 equilibria
Terminating at known equilibrium

Phase region boundary 12 at: 4.992E-01 9.224E+01
** LRO#1
LRO#2
Calculated. 190 equilibria
Terminating at known equilibrium

```

```

Phase region boundary 13 at: 4.992E-01 9.224E+01
** LRO#1
LRO#2
Calculated.. 3 equilibria
Terminating at axis limit.

Phase region boundary 14 at: 4.997E-01 9.224E+01
** LRO#1
LRO#2
Calculated. 191 equilibria
Terminating at known equilibrium

Phase region boundary 15 at: 3.158E-01 3.367E+01
** LRO#2
LRO#3
Calculated 145 equilibria

Phase region boundary 16 at: 3.158E-01 3.367E+01
** LRO#2
LRO#3
Calculated. 163 equilibria
Terminating at known equilibrium

Phase region boundary 17 at: 3.158E-01 3.367E+01
LRO#2
** LRO#3
Calculated 150 equilibria

Phase region boundary 18 at: 3.158E-01 3.367E+01
LRO#2
** LRO#3
Calculated. 163 equilibria
Terminating at known equilibrium

Phase region boundary 19 at: 3.815E-01 6.633E+01
LRO#2
** LRO#3
Calculated 269 equilibria

Phase region boundary 20 at: 3.815E-01 6.633E+01
LRO#2
** LRO#3
Calculated. 26 equilibria
Terminating at known equilibrium

Phase region boundary 21 at: 3.212E-01 9.073E+01
LRO#1
** LRO#2
Calculated 653 equilibria

Phase region boundary 22 at: 3.212E-01 9.073E+01
LRO#1
** LRO#2
Calculated. 118 equilibria
Terminating at known equilibrium

Phase region boundary 23 at: 4.996E-01 9.224E+01
LRO#1
** LRO#2
Calculated. 191 equilibria
Terminating at known equilibrium

Phase region boundary 24 at: 4.996E-01 9.224E+01
LRO#1
** LRO#2
Calculated.. 2 equilibria
Terminating at axis limit.

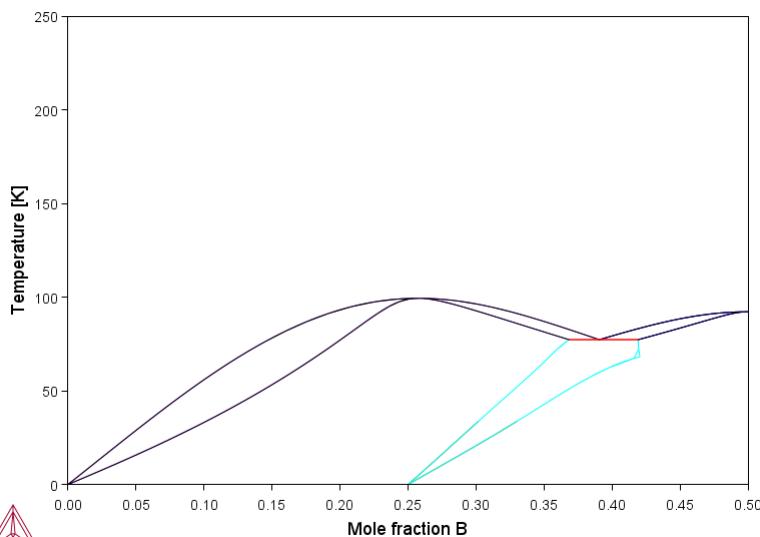
Phase region boundary 25 at: 4.996E-01 9.224E+01
LRO#1
** LRO#2
Calculated. 199 equilibria
Terminating at known equilibrium
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\generate_console_examples\examples\tcex31\tcex31e_stable.POLY3
CPU time for mapping 74 seconds
POLY: po
... the command in full is POST
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: pl,,
... the command in full is PLOT_DIAGRAM

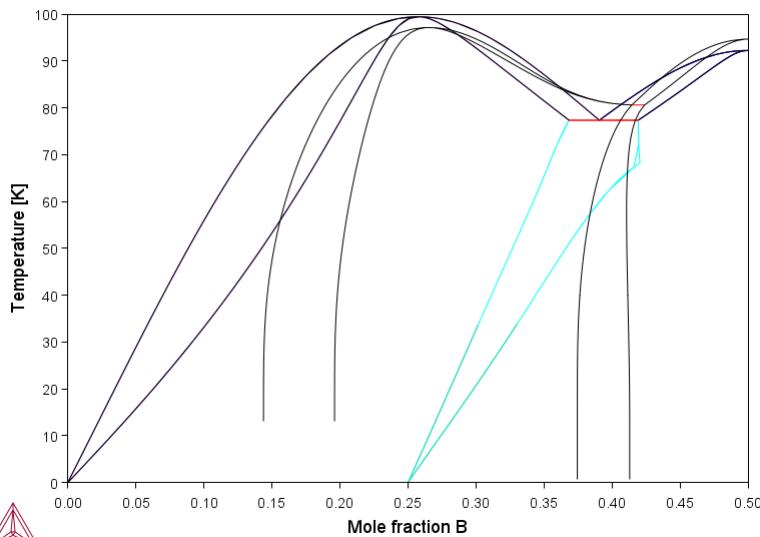
```

example 31e-stable



POST: a-e-d y tcex31 0; 1;
... the command in full is APPEND_EXPERIMENTAL_DATA
POST: s-s-s y n 0 100
... the command in full is SET_SCALING_STATUS
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT DIAGRAM

example 31e-stable



POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:

SYS:About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

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Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

```
SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce32\tce32.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Calculating oxide layers on steel
SYS:
SYS: @@ This example calculates oxide layers on a steel
SYS:
SYS: @@ Note that a TCOX license is
SYS: @@ required to run the example.
SYS:
SYS: set-log ex32,,
SYS: go da
... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module
Database folder: C:\jenkins\workspace\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA           /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE11: sw tcoxi1
... the command in full is SWITCH_DATABASE
Current database: Metal Oxide Solutions v11.1

VA           /- DEFINED
TDB_TCOX11: d-sys fe cr c v mn si o
... the command in full is DEFINE_SYSTEM
FE          CR          C
V           MN          SI
O DEFINED
TDB_TCOX11: get
... the command in full is GET_DATA
16:18:17,922 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES ....
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
Creating a new composition set IONIC_LIQ#2
... the command in full is AMEND_PHASE_DESCRIPTION
Creating a new composition set IONIC_LIQ#3
... the command in full is AMEND_PHASE_DESCRIPTION
MN+4 IN NIMNO3:I SUBLATTICE 1 REJECTED
VA IN NB205:I SUBLATTICE 2 REJECTED
VA IN RUTILE:I SUBLATTICE 2 REJECTED
... the command in full is AMEND_PHASE_DESCRIPTION
Suspending CA2SiO4_ALPHA_A as it has net charge
Suspending CA2SiO4_ALPHA_PRIME as it has net charge
Suspending HATURITE as it has net charge
Suspending K4Al22O35 as it has net charge
Suspending KAl11O17 as it has net charge
Suspending NBO2 as it has net charge
Suspending PSEUDO_BROOKITE as it has net charge
PARAMETERS ...
FUNCTIONS ...

List of references for assessed data

'SGTE Substances Database v6.0 (2017)'
'A.N. Grundy et al., JPED 26 (2005) 131-51; La-Mn-O'
'L. Kjellqvist, Thermo-Calc Software AB (2018), based on Sundman (2008);
Ti-O'
'A. Dinsdale, SGTE Data for Pure Elements, Calphad 15 (1991) 317-425'
'L. Kjellqvist, Thermo-Calc Software AB (2019); C-O-V, C-O-Ti'
'L. Kjellqvist, Thermo-Calc Software AB (2020), tentative vacancy fraction
in pure FCC metals and its carbides.'
'SGTE Unary (Pure Elements) Database V5.1 (2010)'
'TCS, TCMP2 - TCS Materials Processing Database v2 (2004)'
'L. Kjellqvist, Thermo-Calc Software AB (2013); Cr-Zr-O'
'L. Kjellqvist, Thermo-Calc Software AB (2013); Reassessed solubility of
Al, Cr, Fe, Ni in Mn2O3. Mn2O3 is now modelled as the same phase as
cubic Y2O3 (M2O3C).'
'E. Povoden et al., JPED 30 (2009) 12-27; Cr-La-O'
'L. Kjellqvist, Thermo-Calc Software AB (2016); Cr-La-O'
'L. Kjellqvist, Thermo-Calc Software AB (2016); Cr-Nb-O'
'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; FE4N'
'L. Kjellqvist, Thermo-Calc Software AB (2013); Fe-Zr-O'
'E. Povoden et al., JPED 30 (2009) 351-366; Fe-La-O'
'H. Mao, Thermo-Calc Software AB (2015); Fe-Nb-O'
'H. Gohring, O. Fabrichnaya, A. Leineweber, E.J. Mittemeijer, Metall.
Mater. Trans. A 47A (2016) 6173-86; FE-N, and Fe-C-N'
'W. Zheng, J. Alloys Compd., 632 (2015) 661-675; Mn-Si, Fe-Mn-Si'
'M. Chen, B. Hallstedt and L. J. Gauckler, J. Alloys Compd. 393 (2005) 114
-21; Mn-Y-O'
'M. Chen, B. Hallstedt and L.J. Gauckler, Solid State Ionics 176 (2005)
1457-64; Mn-Zr-O, Mn-Y-Zr-O'
'L. Kjellqvist, Thermo-Calc Software AB (2018-19), tentative vacancy
fraction in pure FCC metals.'
'J. Bratberg and Karin Frisk, Calphad 26 (2002) 459-476; Mo-V-C'
'A.V. Khvan, B. Hallstedt and K. Chang, Calphad 39 (2012) 54-61; C-Cr-Nb'
'J. Bratberg, Z. Metallkd. 96 (2005) 335-344; Fe-Cr-Mo-C'
'B-J. Lee, Calphad 16 (1992) 121-149; C-Cr-Fe-Ni'
```

'J.-O. Andersson, Calphad 11 (1987) 271-276; C-Cr'
 'C. Qiu, ISI Int. 32 (1992) 1117-1127; C-Cr-Fe-Mo'
 'P. Gustafson, Metall. Trans. A 19 (1988) 2547-2554; C-Cr-Fe-W'
 'B-J. Lee, Metall. Trans. A 24 (1993) 1017-1025; Fe-Cr-Mn-C'
 'P. Gustafson, Scand. J. Metall. 14 (1985) 259-267; C-Fe'
 'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
 'B. Hallstedt, D. Djurovic, J. von Appen, R. Dronskowsk, A. Dick, F. Koermann, T. Hickel, J. Neugebauer, Calphad 34 (2010) 129-133; Fe-C'
 'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowsk, Calphad 35 (2011) 479-491; Fe-Mn-C'
 'J.-O. Andersson, Calphad 12 (1988) 9-23; C-Fe-Mo'
 'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowsk, Calphad 34 (2010) 279-85; Mn-C'
 'W. Huang, Calphad 13 (1989) 243-252; Fe-Mn'
 'L. Kjellqvist, Thermo-Calc Software AB (2012); Si-O DIAMOND_A4'
 'J. Grobner, H.L. Lukas and F. Aldinger, Calphad 20 (1996) 247-254; Al-C, Si-C and Al-Si-C'
 'J. Lacaze and B. Sundman, Metall. Trans. A 22 (1991) 2211-2223; C-Fe-Si'
 'P. Franke, estimated parameter within SGTE (2008); Fe-Mn-C'
 'Unassessed parameter'
 'T. Godecke, F. Sommer and H.-L. Lukas, unpublished work (1996); Al-Si parameters available from J. Grobner et al. Calphad 20 (1996) 247; Al-Si, C-Si'
 'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; Cementite'
 'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; SIGMA and M7C3'
 'W. Huang, TRITA-MAC 431 (1990); C-V'
 'A. Fernandez Guillerm, Z. Metallkd. 82 (1991) 478-487; C-V, Nb-Zr'
 'A.F. Guillerm and W. Huang, TRITA-MAC 440 (1990); Mn-V-C'
 'B.J. Lee, TRITA-MAC 475 (1991); C-Cr-Fe-V'
 'A. Gabriel, P. Gustafson and I. Ansara, Calphad 11 (1987) 203-218; C-Fe-Ni'
 'J.-O. Andersson and B. Sundman, Calphad 11 (1987) 83-92; CR-Fe'
 'K. Frisk, Metall. Trans. A 21 (1990) 2477-2488; Cr-Fe-N'
 'B-J. Lee, Metall. Trans. A 24 (1993) 1919-1933; Cr-Mn, Fe-Cr-Mn'
 'K. Frisk, Calphad, 17 (1993) 335-349; Cr-Mn-N'
 'SSOL4 - SGTE Alloy Solutions Database v4 (2008)'
 'L. Kjellqvist, Unpublished revision of liquid phase (2010); Cr-Fe-Mn-Ni-O'
 'J.R. Taylor and A.T. Dinsdale, Z. Metallkd. 81 (1990) 354-366; Ni-O, Cr-O and Cr-Ni-O'
 'L. Kjellqvist, Thermo-Calc Software AB (2019), reassessment; Cr-O'
 'M. Kowalski and P.J. Spencer, Calphad 19 (1995) 229-243; Cr-O, Fe-O and Ni-O'
 'J.R. Taylor and A.T. Dinsdale, Z. Metallkd. 84 (1993) 335-345; Cr-Fe-O'
 'L. Kjellqvist, M. Selleby and B. sundman, Calphad 32 (2008) 577-592; Cr-Fe-Ni-O'
 'Y. Du and J.C. Schuster, J. Phase Equilib. 21 (2000) 281-86; Cr-Si'
 'B-J. Lee, TRITA-MAC 474 (1991); Cr-Fe-V'
 'H.K. Danielsen and J. Hald, Calphad 31 (2007) 505-514; Z-PHASE'
 'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
 'L. Kjellqvist, Thermo-Calc Software AB (2016); Columbite, (Ca,Fe,Mg, Mn)Nb206'
 'B. Sundman, J. Phase Equilib. 12 (1991) 127-140; Fe-O'
 'A. Forsberg and J. Agren, J. Phase Equilib. 14 (1993) 354-363; Fe-Mn-Si'
 'W. Huang, TRITA-MAC 432 (Rev 1989,1990); Fe-V, C-Fe-V'
 'J.-O. Andersson, CALPHAD, 7 (1983) 305-315 (Parameters revised 1986 due to new description of V) TRITA 0201 (1982); FE-V'
 'W. Huang, TRITA-MAC 439 (1990) also in W. Huang, CALPHAD, 15, 195-208 (1991); Mn-V, Fe-Mn-V'
 'A.N. Grundy, B. Hallstedt and L.J. Gauckler, J. Phase Equilib. 24 (2003) 21-39; Mn-O'
 'B-J. Lee, KRISS, unpublished research, during 1993-1995'
 'L. Kjellqvist, Thermo-Calc Software AB, Sweden, estimations, 2016'
 'L. Kjellqvist, Thermo-Calc Software AB (2019); Mn-Ti-O'
 'L. Kjellqvist and M. Selleby, JPED 31 (2010) 113-134; Fe-Mn-O'
 'M. Chen, PhD thesis, ETH Zurich (2005); La-Zr-O, Mn-Zr-O, Mn-Y-Zr-O'
 'L. Kjellqvist and M. Selleby, Int. J. Mater. Res. (formerly Z. Metallkd.) 101 (2010) 1222-1231; Mn-Ni-O'
 'W. Huang, TRITA-MAC 441 (1990) also in W. Huang, Metall. Trans. A, 22A, 1911-20 (1991); Fe-Mn-V-C'
 'T.I. Barry, NPL, Unpublished work (1987); liquid and solid SiO2'
 'B. Hallstedt, J. Phase Equilib. 14 (1993) 662-675; Al-Ca-Mg-Si-O'
 'B. Hallstedt, Calphad 16 (1992) 53-61; Si-O'
 'B-J. Lee, estimated parameter (1999)'
 'L. Kjellqvist, Thermo-Calc Software AB (2016); Revised CaO-SiO2-Y2O3'
 'L. Kjellqvist, Thermo-Calc Software AB (2018); Al2O3-P2O5-SiO2'
 'L. Kjellqvist, Thermo-Calc Software AB (2020), estimated; Fe-O-Na2O-SiO2'
 'Y. Yang et al., Calphad 51 (2015) 144-160; O-V'
 'Unassessed Linear combination of parameters'
 'L. Kjellqvist, Thermo-Calc Software AB (2019); V-O, reassessment of VO phase (changed model from HALITE -> FCC_A1'
 'Y. Yang, H. Mao, H-L. Chen, M. Selleby, J. Alloys Compd. 722 (2017) 365-374; Ti-V-O'
 'L. Kjellqvist, Thermo-Calc Software AB (2018), Estimations (No intermetallic compounds modelled); Nb-O-V, O-V-P, O-V-Zr'
 'N. Saunders, COST 507 Report (1998); Al-Nb, Al-Mo, Al-Cu, Al-V, Al-W, Cr-Ti, Mn-Ti, Si-V, Ti-V, Al-Nb-Ti'
 'A.V. Khvan, B. Hallstedt, C. Broeckmann, Calphad 46 (2014) 24-33; Cr-Fe-C'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2016; FCC Fe-Cr-C and C-Cr-Ni'
 'J.-O. Andersson, Metall. Trans. A, 19A (1988) 627-636 TRITA 0207 (1986); C-CR-Fe'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; C-Cr-Si'
 'J. Bratberg, Thermo-Calc Software AB, Sweden (2009); Carbonitrides and M23C6'
 'J. Bratberg, Thermo-Calc Software AB, Sweden, 2008; Fe-Cr-V-C'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; Adjusting hcp'
 'W. Huang, Metall. Trans. A, 21A (1990) 2115-2123; TRITA-MAC 411 (Rev 1989); C-Fe-MN'
 'L. Kjellqvist and M. Selleby, Calphad 33 (2009) 393-397; C-Cr-Fe-Ni-O'
 'J. Miettinen, Calphad 22 (1998) 231-256; Fe-Si and Fe-Si-C'
 'W. Zheng et al., J. Iron Steel Res. Int. 24 (2017) 190-197; C-Mn-Si, Fe-Mn-Si'
 'Y. Yang, H. Mao, M. Selleby, Calphad 56 (2017) 29-40; Ca-V-O'
 'R. Naraghi, Thermo-Calc Software AB, Sweden (2015); FROST project'
 'C. Qiu, Metall. Trans. A 24 (1993) 2393-2409; Cr-Fe-Mn-N'
 'A. Markstrom, Thermo-Calc Software AB (2013), CBCC_A12; Cr-Fe-Mn'
 'L. Kjellqvist, Thermo-Calc Software AB (2019), introducing low-temp miscibility gap; Cr-Fe-O Corundum'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; Cr-Fe-Si'
 'M. Lindholm, J. Phase Equilib. 18 (1997) 432; Cr-Fe-Si'
 'L. Kjellqvist, M. Selleby, J. Alloys Compd. 507 (2010) 84-92; Cr-Mn-O'
 'L. Kjellqvist, Thermo-Calc Software AB (2019), reassessment; Cr-O-Si'
 'L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2013; Cr-Si-O'
 'L. Kjellqvist, Thermo-Calc Software AB (2017); estimated solubility between metals and oxide liquids.'
 'S. Arnout et al., J. Am. Ceram. Soc. 92 (2009) 1831-1839; Cr-O-MgO-SiO2'
 'L. Kjellqvist, Thermo-Calc Software AB (2018); Cr-O-V'
 'L. Kjellqvist, Thermo-Calc Software AB (2018), tentative assessment; Al-O

-V'
 'L. Kjellqvist, Thermo-Calc Software AB (2019), reassessment of solubility
 in M4O7 and V3O5, due to change of model.'
 'L. Kjellqvist, Thermo-Calc Software AB (2020); Fe-O-K2O'
 'M. Selleby, Metall. Mater. Trans. B 28 (1997) 563-576; Fe-O-Si'
 'L. Kjellqvist, Thermo-Calc Software AB (2016); Fe-Mn-O-SiO2'
 'M. Selleby, Metall. Mater. Trans. B 28 (1997) 577-596; Ca-Fe-O-Si'
 'L. Kjellqvist, Thermo-Calc Software AB (2020), reassessment metastable
 FeSiO3 ortho-pyroxene; FeO-SiO2, FeO-MgO-SiO2'
 'L. Kjellqvist, Thermo-Calc Software AB (2014); Fe-O-MgO-SiO2'
 'L. Kjellqvist, Thermo-Calc Software AB (2018); Fe-Ti-O'
 'L. Kjellqvist, Thermo-Calc Software AB (2018); Fe-O-V'
 'L. Kjellqvist, Thermo-Calc Software AB (2019), reassessment of V2O3
 solubility in Halite, due to change of model'
 'L. Kjellqvist, reassessment, Thermo-Calc Software AB (2018); Mn-Si-O, Al
 -Mn-Si-O, Ca-Mn-Si-O, Al2O3-FeO-MnO-SiO2'
 'L. Kjellqvist, Thermo-Calc Software AB, Sweden (2011); Mn-Si-O'
 'L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2014; Reassess liquid
 phase; Mn-Si-O'
 'G. Eriksson et al., Can. Metall. Q. 33 (1994) 13-21; MnO-SiO2'
 'Y. Kang et al., ISIJ Int. 44 (2004) 965-974; CaO-MnO-SiO2, CaO-MnO-Al2O3'
 'L. Kjellqvist, Thermo-Calc Software AB (2018); Mn-O-V'
 'L. Kjellqvist, Thermo-Calc Software AB (2018), tentative assessment; Si-O
 -V'
 'G. Lambotte, P. Chartrand, J. Chem. Thermodynamics 57 (2013) 306-334;
 Al2O3-Na2O-SiO2'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2016; C-Cr-Fe-V'
 'L. Kjellqvist, Thermo-Calc Software AB (2018), Reassessed solubility of
 Fe, Gd, Mg, Mn and Y in CA2SiO4_ALPHA and CA2SiO4_ALPHA_PRIME due to
 change of model'
 'L. Kjellqvist, Thermo-Calc Software, AB, Sweden (2010); Spinels'
 'L. Kjellqvist, Thermo-Calc Software AB (2019), Estimated Cr2O3-FeO-TiO2'
 'L. Kjellqvist, Thermo-Calc Software AB (2017), Garnet; estimated
 solubility between Spessartine and Grossular.'
 'L. Kjellqvist, Thermo-Calc Software AB (2017), estimated cation
 distribution in Olivine (M1,M2)2SiO4 systems.'
 'L. Kjellqvist, Thermo-Calc Software AB (2019); Cr2O3-Mn-O-TiO2'
 'L. Kjellqvist, Thermo-Calc Software AB (2019); Fe-Mn-O-TiO2'
 'D.-G. Kim, B. Konar, I.-H. Jung, Metal. Mater. Trans. B 48B (2017) 2788
 -2803; K2O-MgO-SiO2'
 'M. Ghasemi, Thermo-Calc Software: Unifying liquid volume database, 2020'
 'Volume data for TCFE4, 2006'
 'X.G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
 volumes'
 'Estimated values, 2019'
 'L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2012; Molar volumes'
 'Y.Tang, in TCCU2, Thermo-Calc Software AB, Stockholm, Sweden'
 'N. Dupin, Private communication, (2008); Volume data'
 'X.G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
 'H. Mao, Thermo-Calc Software AB, Sweden, 2013; Molar volumes'
 'R. Zhang, Molar volumes for oxide liquid in TCOX, Thermo-Calc Software AB,
 Sweden, 2018-2020'
 'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
 'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121-127; Molar
 volumes'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, Volume data updated for
 TCFE9 database (TCFE v9.0, Jan, 2017).'
 'P. Villars, L.D. Calvert. Pearson's handbook of crystallographic data for
 intermetallic phases, Metals park, Ohio 1985: American society for
 metals'
 'R. Naraghi, Thermo-Calc Software AB, Volume data updated for TCFE9
 database (TCFE v9.1, June, 2019).'
 'Thermo-Calc Software, Sweden, 2008: Volume data updated for TCFE6
 database (TCFE v6, April, 2008).'
 'A.F. Guillermet and G. Grimvall, J. Phys. Chem. Solids, 1992, 53, 105-125;
 Molar volumes'
 'H. Mao, Thermo-Calc Software AB, Sweden, 2011; Molar volumes'
 'H. Mao, B. Sundman, Z. Wang and S.K. Saxena, J. Alloys Compd., 327, 2001,
 253-262'
 'Yang YANG, Thermo-Calc Software AB, Sweden, 2019; Volume data updated for
 TCT13.0 database (TCTI v3.0, Aug-Oct 2019).'
 'R. Zhang, Viscosity of liquid oxides, Thermo-Calc Software AB, 2018-2020'
 'M. Ghasemi, Viscosity of liquid metals, Thermo-Calc Software AB, 2019'
 'R. Zhang, Surface tensions for oxide liquid in TCOX, Thermo-Calc Software
 AB, Sweden, 2020'

-OK-

TDB TCOX11:

TDB_TCOX11: go p-3
 ... the command in full is GOTO_MODULE

POLY version 3.32

POLY:

POLY: s-c b(cr)=16 b(v)=.1 b(c)=1 b(mn)=.3 b(si)=.3 t=1073 p=1e5 b=100
 ... the command in full is SET_CONDITION

POLY: 1-c

... the command in full is LIST_CONDITIONS

B(CR)=16, B(V)=0.1, B(C)=1, B(MN)=0.3, B(SI)=0.3, T=1073, P=100000, B=100
 DEGREES OF FREEDOM 1

POLY: Hit RETURN to continue

POLY:

POLY: @@ We have atomic oxygen as a component. Later we use the
 @@ partial pressure of O2 as output. The state variable
 @@ LNACR is the chemical potential divided by RT, usual
 @@ values are between -40 and 0

POLY: @@ To improve convergence we first choose a very low value

POLY:

POLY: s-c lnacr(o)=-50
 ... the command in full is SET_CONDITION

POLY: s-r-s o gas * 1e5
 ... the command in full is SET_REFERENCE_STATE

POLY: c-e

... the command in full is COMPUTE_EQUILIBRIUM

Normal POLY minimization, not global

Testing POLY result by global minimization procedure

Calculated 70421 grid points in 1 s
 182 ITS, CPU TIME USED 14 SECONDS

POLY: l-e

... the command in full is LIST_EQUILIBRIUM

OUTPUT TO SCREEN OR FILE /SCREEN/:

Options /VWCS/: VWCS

Output from POLY-3, equilibrium = 1, label A0 , database: TCOX11

Conditions:

B(CR)=16, B(V)=0.1, B(C)=1, B(MN)=0.3, B(SI)=0.3, T=1073, P=100000, B=100,

LNACR(O)=-50
DEGREES OF FREEDOM 0

Temperature 1073.00 K (799.85 C), Pressure 1.000000E+05
Number of moles of components 1.88275E+00, Mass in grams 1.000000E+02
Total Gibbs energy -9.42381E+04, Enthalpy 4.96931E+04, Volume 1.34230E-05

| Component | Moles | W-Fraction | Activity | Potential | Ref.stat |
|-----------|------------|------------|------------|-------------|----------|
| C | 8.3257E-02 | 1.0000E-02 | 6.0029E-03 | -4.5638E+04 | SER |
| CR | 3.0772E-01 | 1.6000E-01 | 2.2693E-03 | -5.4317E+04 | SER |
| FE | 1.4737E+00 | 8.2300E-01 | 4.5659E-03 | -4.8079E+04 | SER |
| MN | 5.4607E-03 | 3.0000E-03 | 8.6742E-06 | -1.0398E+05 | SER |
| O | 4.6959E-12 | 7.5130E-13 | 1.9287E-22 | -4.4607E+05 | GAS |
| SI | 1.0682E-02 | 3.0000E-03 | 6.0839E-10 | -1.8932E+05 | SER |
| V | 1.9631E-03 | 1.0000E-03 | 1.0285E-07 | -1.4355E+05 | SER |

BCC_A2 Status ENTERED Driving force 0.0000E+00
Moles 1.5657E+00, Mass 8.6625E+01, Volume fraction 8.5605E-01 Mass fractions:
FE 9.16292E-01 SI 3.46321E-03 V 1.35768E-04 O 8.67303E-13
CR 7.73672E-02 MN 2.68313E-03 C 5.86710E-05

M7C3_D101 Status ENTERED Driving force 0.0000E+00
Moles 1.8521E-01, Mass 7.4807E+00, Volume fraction 8.1843E-02 Mass fractions:
CR 7.60041E-01 C 8.92121E-02 MN 2.88836E-03 O 0.00000E+00
FE 1.40049E-01 V 7.80948E-03 SI 5.42131E-11

M23C6_D84 Status ENTERED Driving force 0.0000E+00
Moles 1.3181E-01, Mass 5.8944E+00, Volume fraction 6.2107E-02 Mass fractions:
CR 6.12851E-01 C 5.55686E-02 V 5.05875E-03 SI 0.00000E+00
FE 3.18723E-01 MN 7.79845E-03 O 0.00000E+00

POLY:
POLY: @@ The start values of a successful compute-equilibrium are
POLY: @@ used for subsequent calculations, this improves convergence.
POLY: s-c lnacr(o)=-25
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Using already calculated grid
119 ITS, CPU TIME USED 1 SECONDS
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
Output from POLY-3, equilibrium = 1, label A0 , database: TCOX11

Conditions:
B(CR)=16, B(V)=0.1, B(C)=1, B(MN)=0.3, B(SI)=0.3, T=1073, P=100000, B=100,
LNACR(O)=-25
DEGREES OF FREEDOM 0

Temperature 1073.00 K (799.85 C), Pressure 1.000000E+05
Number of moles of components 2.34073E+00, Mass in grams 1.000000E+02
Total Gibbs energy -3.29432E+05, Enthalpy -1.74943E+05, Volume 1.66080E-05

| Component | Moles | W-Fraction | Activity | Potential | Ref.stat |
|-----------|------------|------------|------------|-------------|----------|
| C | 8.3257E-02 | 1.0000E-02 | 1.9686E-01 | -1.4500E+04 | SER |
| CR | 3.0772E-01 | 1.6000E-01 | 2.0598E-07 | -1.3735E+05 | SER |
| FE | 1.2898E+00 | 7.2031E-01 | 4.8275E-03 | -4.7582E+04 | SER |
| MN | 5.4607E-03 | 3.0000E-03 | 1.4312E-10 | -2.0223E+05 | SER |
| O | 6.4186E-01 | 1.0269E-01 | 1.3888E-11 | -2.2304E+05 | GAS |
| SI | 1.0682E-02 | 3.0000E-03 | 1.3875E-15 | -3.0521E+05 | SER |
| V | 1.9631E-03 | 1.0000E-03 | 8.7031E-12 | -2.2721E+05 | SER |

FCC_A1 Status ENTERED Driving force 0.0000E+00
Moles 1.1854E+00, Mass 6.4192E+01, Volume fraction 5.0415E-01 Mass fractions:
FE 9.91403E-01 CR 1.13457E-05 V 1.87290E-08 SI 3.28124E-09
C 8.58597E-03 MN 9.59676E-08 O 1.08471E-08

SPINEL Status ENTERED Driving force 0.0000E+00
Moles 1.0859E+00, Mass 3.4717E+01, Volume fraction 4.6843E-01 Mass fractions:
CR 4.60846E-01 FE 2.41686E-01 V 2.88038E-03 SI 0.00000E+00
O 2.85947E-01 MN 8.64107E-03 C 0.00000E+00

QUARTZ Status ENTERED Driving force 0.0000E+00
Moles 3.2046E-02, Mass 6.4180E-01, Volume fraction 1.5248E-02 Mass fractions:
O 5.32563E-01 C 0.00000E+00 MN 0.00000E+00 CR 0.00000E+00
SI 4.67437E-01 V 0.00000E+00 FE 0.00000E+00

GRAPHITE Status ENTERED Driving force 0.0000E+00
Moles 3.7370E-02, Mass 4.4885E-01, Volume fraction 1.2171E-02 Mass fractions:
C 1.00000E+00 SI 0.00000E+00 MN 0.00000E+00 CR 0.00000E+00
V 0.00000E+00 O 0.00000E+00 FE 0.00000E+00

POLY:
POLY: sh lnacr(o)
... the command in full is SHOW_VALUE
LNACR(O)=-25.
POLY: @@ List the activity of O2
POLY: show lnacr(o2,gas)
... the command in full is SHOW_VALUE
LNACR(O2,GAS)=-50.
POLY: Hit RETURN to continue
POLY:
POLY: @@ Vary the normalized chemical potential of oxygen
POLY: @@ between -20 and -50
POLY: s-a-v 1 lnacr(o)
... the command in full is SET_AXIS_VARIABLE
Min value /0/: -50
Max value /1/: -20
Increment /.75/: 0.5
POLY: save tce32 y
... the command in full is SAVE_WORKSPACES
POLY: step
... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/: NORMAL
No initial equilibrium, using default
Step will start from axis value -25.0000
...OK

Phase Region from -25.0000 for:
FCC_A1
GRAPHITE
QUARTZ
SPINEL

```

Global check of adding phase at -2.32891E+01
Calculated      6 equilibria

Phase Region from   -23.2891    for:
  GAS
  FCC_A1
  GRAPHITE
  QUARTZ
  SPINEL
Global check of removing phase at -2.32891E+01
Calculated      2 equilibria

Phase Region from   -23.2891    for:
  GAS
  FCC_A1
  QUARTZ
  SPINEL
Global check of adding phase at -2.31539E+01
Calculated      3 equilibria

Phase Region from   -23.1539    for:
  GAS
  FCC_A1
  OLIVINE
  QUARTZ
  SPINEL
Global check of removing phase at -2.31434E+01
Calculated      3 equilibria

Phase Region from   -23.1434    for:
  GAS
  FCC_A1
  OLIVINE
  SPINEL
Global check of adding phase at -2.23176E+01
Calculated      5 equilibria

Phase Region from   -22.3176    for:
  GAS
  BCC_A2
  FCC_A1
  OLIVINE
  SPINEL
Global check of removing phase at -2.23176E+01
Calculated      2 equilibria

Phase Region from   -22.3176    for:
  GAS
  BCC_A2
  OLIVINE
  SPINEL
Global check of adding phase at -2.17868E+01
Calculated      6 equilibria

Phase Region from   -21.7868    for:
  GAS
  BCC_A2
  HALITE
  OLIVINE
  SPINEL
Global check of removing phase at -2.17852E+01
Calculated      3 equilibria

Phase Region from   -21.7852    for:
  GAS
  HALITE
  OLIVINE
  SPINEL
Global check of removing phase at -2.09564E+01
Calculated     10 equilibria

Phase Region from   -20.9564    for:
  GAS
  OLIVINE
  SPINEL
Terminating at   -20.0000
Calculated      6 equilibria

Phase Region from   -25.0000    for:
  FCC_A1
  GRAPHITE
  QUARTZ
  SPINEL
Global check of adding phase at -2.67717E+01
Calculated      6 equilibria

Phase Region from   -26.7717    for:
  CORUNDUM
  FCC_A1
  GRAPHITE
  QUARTZ
  SPINEL
Global check of adding phase at -2.81820E+01
Calculated      6 equilibria

Phase Region from   -28.1820    for:
  CEMENTITE_D011
  CORUNDUM
  FCC_A1
  GRAPHITE
  QUARTZ
  SPINEL
Global check of removing phase at -2.81821E+01
Calculated      2 equilibria

Phase Region from   -28.1821    for:
  CEMENTITE_D011
  CORUNDUM
  FCC_A1
  QUARTZ
  SPINEL
Global test at -2.92000E+01 .... OK
Global check of adding phase at -2.93358E+01
Calculated     12 equilibria

Phase Region from   -29.3358    for:

```

```

CEMENTITE_D011
CORUNDUM
FCC_A1
M7C3_D101
QUARTZ
SPINEL
Global check of removing phase at -2.93467E+01
Calculated      3 equilibria

Phase Region from -29.3467      for:
CORUNDUM
FCC_A1
M7C3_D101
QUARTZ
SPINEL
Global check of adding phase at -3.00924E+01
Calculated      9 equilibria

Phase Region from -30.0924      for:
BCC_A2
CORUNDUM
FCC_A1
M7C3_D101
QUARTZ
SPINEL
Global check of removing phase at -3.00952E+01
Calculated      3 equilibria

Phase Region from -30.0952      for:
BCC_A2
CORUNDUM
M23C6_D84
M7C3_D101
QUARTZ
SPINEL
Global check of adding phase at -3.06349E+01
Calculated      8 equilibria

Phase Region from -30.6349      for:
BCC_A2
CORUNDUM
M23C6_D84
M7C3_D101
QUARTZ
SPINEL
Global check of removing phase at -3.06349E+01
Calculated      2 equilibria

Phase Region from -30.6349      for:
BCC_A2
M23C6_D84
M7C3_D101
QUARTZ
SPINEL
Global check of adding phase at -3.14550E+01
Calculated      5 equilibria

Phase Region from -31.4550      for:
BCC_A2
M23C6_D84
M7C3_D101
QUARTZ
RHODONITE
SPINEL
Global check of removing phase at -3.14551E+01
Calculated      2 equilibria

Phase Region from -31.4551      for:
BCC_A2
M23C6_D84
M7C3_D101
RHODONITE
SPINEL
Global check of removing phase at -3.15015E+01
Calculated      3 equilibria

Phase Region from -31.5015      for:
BCC_A2
M23C6_D84
M7C3_D101
RHODONITE
Global check of removing phase at -3.16317E+01
Calculated      3 equilibria

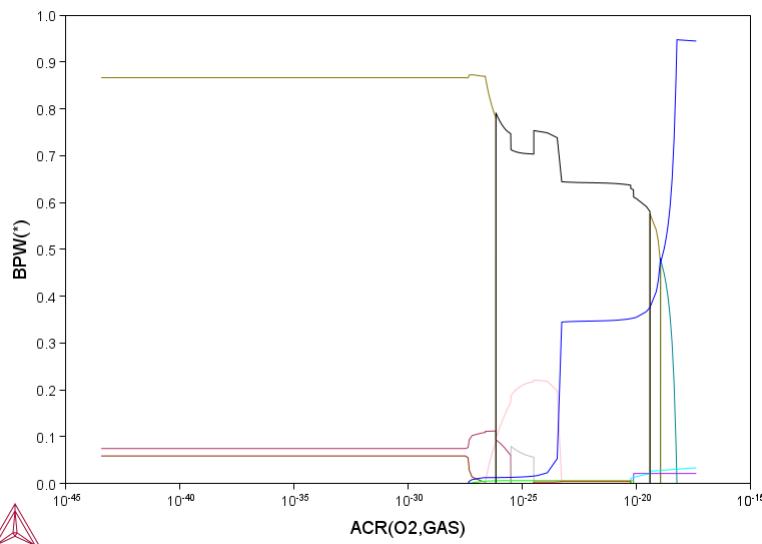
Phase Region from -31.6317      for:
BCC_A2
M23C6_D84
M7C3_D101
Global test at -3.53000E+01 .... OK
Global test at -4.03000E+01 .... OK
Global test at -4.53000E+01 .... OK
Global test at -5.00000E+01 .... OK
Terminating at -50.0000
Calculated      41 equilibria
*** Buffer saved on file: c:\jenkins\workspace\generate_console_examples\examples\tcex32\tcex32.POLY3
POLY:
POLY: po
... the command in full is POST
POLY-3 POSTPROCESSOR VERSION 3.2
POST:
POST: s-d-a x acr(o2,gas)
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y bpw(*)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*: *
POST: s-a-t-y
... the command in full is SET_AXIS_TYPE
AXIS (X, Y OR Z) : x
AXIS TYPE /LINEAR/: log
POST: set-title example 32a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:

```

```

POST: plot
... the command in full is PLOT_DIAGRAM
example 32a

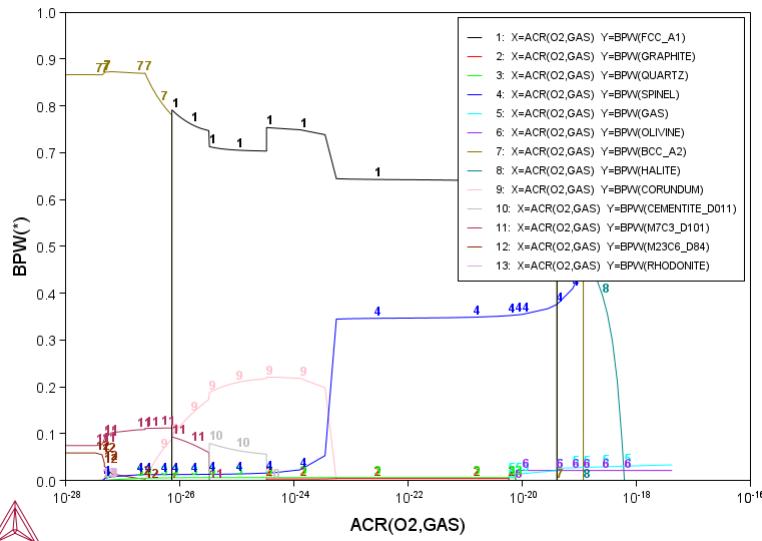
```



```

POST:
POST:Hit RETURN to continue
POST:
POST: s-lab f
... the command in full is SET_LABEL_CURVE_OPTION
POST: s-s x n 1e-28 1e-18
... the command in full is SET_SCALING_STATUS
POST: set-title example 32b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
example 32b

```

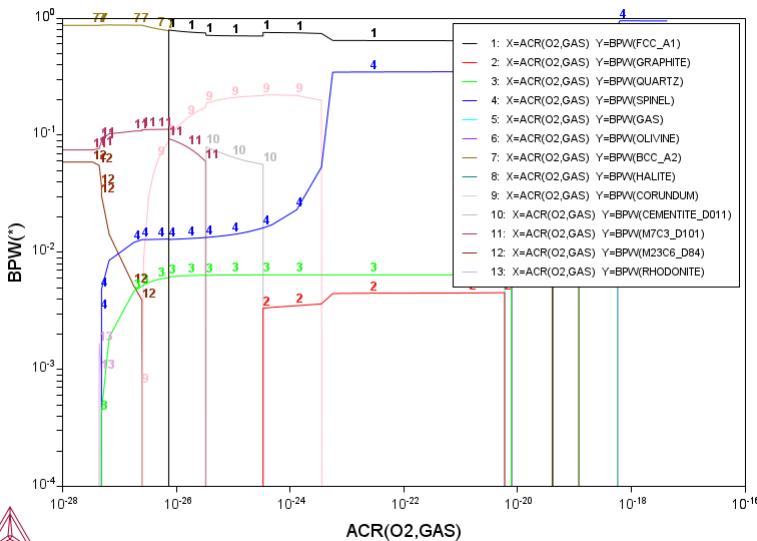


```

POST:
POST:Hit RETURN to continue
POST:
POST: s-a-ty y
... the command in full is SET_AXIS_TYPE
AXIS TYPE /LINEAR/: log
POST: s-s y n 1e-4 1
... the command in full is SET_SCALING_STATUS
POST: set-title example 32c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

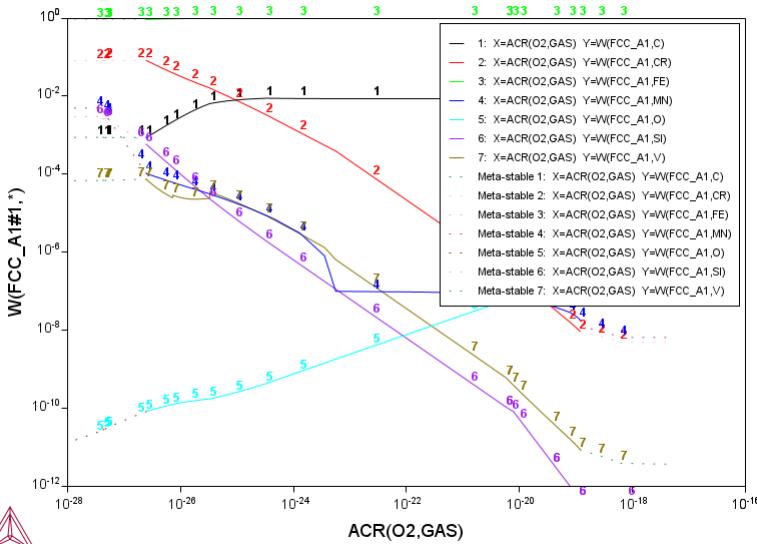
example 32c



```

POST:
POST:Hit RETURN to continue
POST:
POST: @@ Finally plot how the composition of FCC varies.
POST: s-d-a y w(fcc_a1#1,*)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: s-s y n 1e-12 1
... the command in full is SET_SCALING_STATUS
POST: set-title example 32d
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
example 32d

```



```

POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:

```

SYS:About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

```
SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce33\tce33.TCM.test"
SYS: set-echo
SYS: @@
SYS: @@
SYS: @@ Benchmark calculation for Fe-Cr-C isopleth
SYS: @@
SYS: set-log ex33,,
SYS: go da
... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module
Database folder: C:\jenkins\workspace\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA           /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE11: sw FEDEMO
... the command in full is SWITCH_DATABASE
Current database: Iron Demo Database v4.0

VA           /- DEFINED
TDB_FEDEMO: d-sys fe cr c
... the command in full is DEFINE_SYSTEM
FE           CR           C
DEFINED
TDB_FEDEMO: rej ph /all
... the command in full is REJECT
GAS:G          LIQUID:L          BCC_A2
LAVES_PHASE_C14 CBCC_A12        CEMENTITE
CHI_A12        CUB_A13         DIAMOND_FCC_A4
FCC_A1          GRAPHITE        HCP_A3
KSI_CARBIDE    M23C6          M3C2
M5C2           M7C3           SIGMA
REJECTED
TDB_FEDEMO: rest ph liquid fcc_a1 bcc_a2 graphite sigma cementite m23 m7 m3c2
... the command in full is RESTORE
LIQUID:L        FCC_A1          BCC_A2
GRAPHITE       SIGMA          CEMENTITE
M23C6          M7C3           M3C2
RESTORED
TDB_FEDEMO: get
... the command in full is GET_DATA
16:20:09,649 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
Creating a new composition set FCC_A1#2
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS .....
FUNCTIONS .....

List of references for assessed data

'A.T. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121 -127; Molar
  volumes'
'M. Ghasemi, Thermo-Calc Software AB, Sweden, 2019; Viscosity of metallic
  liquid'
'M Ghasemi, Thermo-Calc Software AB: assessing the surface tension of
  metallic liquid'
'M. Ghasemi, Thermo-Calc Software AB, Sweden, 2020; Unifying liquid volume
  database'
'Y. Tang, in TCCU2, Thermo-Calc Software AB, Stockholm, Sweden'
'M. J. Assael, J. Phys. Chem. Ref. Data 35 (2006) 285; Fe, Al'
'A.V. Khvan, B. Hallstedt, K. Chang, CALPHAD, 39, 54-61(2012); C -Cr-Nb'
'A.V. Khvan, B. Hallstedt, C. Broeckmann, CALPHAD, 46, 24 -33(2014); Cr-Fe
  -C'
'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
'B.J. Lee, CALPHAD, 17 (1993) 251-268; revision of Fe-Cr and Fe -Ni liquid'
'J-O. Andersson, CALPHAD, 11 (1987) 271-276; TRITA 0314; C-CR'
'X.G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
'X.G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
  volumes'
'J-O. Andersson, Metall. Trans. A, 19A (1988) 627-636 TRITA 0207 (1986); C
  -CR-FE'
'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270
  (1986); CR-FE'
'B.J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
'P. Villars, L.D. Calvert. Pearson's handbook of crystallographic data for
  intermetallic phases, Metals park, Ohio 1985: American society for
  metals'
'B. Hallstedt, D. Djurovic, J. von Appen, R. Dronskowski, A. Dick, F.
  Koermann, T. Hickel, J. Neugebauer, CALPHAD, 34, 129 -33(2010); Fe-C'
'J. Bratberg, Z. Metalldkd., 96 (2005) 335-344; Fe-Cr-Mo-C'
'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
'R. Naraghi, Thermo-Calc Software AB, Sweden, 2016; FCC Fe-Cr-C and C-Cr-Ni'
'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, Calphad 35.4
  (2011) 479-491; Fe-Mn-C'
'B. Sundman et al., Report EUR 20315, Contract No 7210-PR/050, 2002; New
  Sigma model'
-OK-
TDB_FEDEMO: go p-3
... the command in full is GOTO_MODULE
```

```

POLY: s-c t=1200,p=1e5,n=1 w(cr)=.13 w(c)=.01
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 10193 grid points in 2 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 1 s, total time 3 s
POLY: s-a-v 1 w(c) 0 .02
... the command in full is SET_AXIS_VARIABLE
Increment /5E-04/: 5E-04
POLY: s-a-v 2 t 800 2000
... the command in full is SET_AXIS_VARIABLE
Increment /30/: 30
POLY: save tceex33 y
... the command in full is SAVE_WORKSPACES
POLY: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Tie-lines not in the plane of calculation
Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Generating start point 27
Generating start point 28

Phase region boundary 1 at: 6.615E-03 8.100E+02
  BCC_A2
  M23C6
  ** M7C3
Calculated.. 2 equilibria
Terminating at axis limit.

Phase region boundary 2 at: 6.665E-03 8.000E+02
  BCC_A2
  M23C6
  ** M7C3
Calculated. 11 equilibria

Phase region boundary 3 at: 5.191E-03 1.088E+03
  BCC_A2
  ** FCC_A1#1
  M23C6
  ** M7C3
Calculated. 12 equilibria

Phase region boundary 4 at: 5.191E-03 1.088E+03
  BCC_A2
  ** FCC_A1#1
  M23C6
Calculated. 12 equilibria

Phase region boundary 5 at: 1.203E-04 1.127E+03
  BCC_A2
  ** FCC_A1#1
  M23C6
Calculated.. 14 equilibria
Terminating at axis limit.

Phase region boundary 6 at: 1.203E-04 1.127E+03
  BCC_A2
  ** FCC_A1#1
  M23C6
Calculated.. 14 equilibria
Terminating at axis limit.

Phase region boundary 7 at: 1.203E-04 1.127E+03
  BCC_A2
  ** M23C6
Calculated.. 12 equilibria
Terminating at axis limit.

Phase region boundary 8 at: 1.203E-04 1.127E+03
  BCC_A2
  FCC_A1#1
  ** M23C6
Calculated.. 3 equilibria

Phase region boundary 9 at: 1.027E-03 1.162E+03

```

```

** BCC_A2
FCC_A1#1
** M23C6
Calculated.          9 equilibria

Phase region boundary 10 at:  1.027E-03  1.162E+03
    FCC_A1#1
    ** M23C6
Calculated.          9 equilibria

Phase region boundary 11 at:  3.934E-03  1.328E+03
    FCC_A1#1
    ** M23C6
    ** M7C3
Calculated.          11 equilibria
Terminating at known equilibrium

Phase region boundary 12 at:  3.934E-03  1.328E+03
    FCC_A1#1
    ** M23C6
    M7C3
Calculated.          11 equilibria
Terminating at known equilibrium

Phase region boundary 13 at:  3.934E-03  1.328E+03
    FCC_A1#1
    ** M7C3
Calculated.          19 equilibria

Phase region boundary 14 at:  1.106E-02  1.554E+03
    ** LIQUID
    FCC_A1#1
    ** M7C3
Calculated..         20 equilibria
Terminating at axis limit.

Phase region boundary 15 at:  1.106E-02  1.554E+03
    LIQUID
    FCC_A1#1
    ** M7C3
Calculated..         20 equilibria
Terminating at axis limit.

Phase region boundary 16 at:  1.106E-02  1.554E+03
    ** LIQUID
    FCC_A1#1
Calculated.          16 equilibria

Phase region boundary 17 at:  5.090E-03  1.667E+03
    ** LIQUID
    ** BCC_A2
    FCC_A1#1
Calculated.          8 equilibria

Phase region boundary 18 at:  5.090E-03  1.667E+03
    ** LIQUID
    BCC_A2
    FCC_A1#1
Calculated.          8 equilibria

Phase region boundary 19 at:  2.029E-03  1.685E+03
    ** LIQUID
    BCC_A2
    ** FCC_A1#1
Calculated..         24 equilibria

Phase region boundary 20 at:  2.029E-03  1.685E+03
    ** LIQUID
    BCC_A2
Calculated.          24 equilibria

Phase region boundary 21 at:  2.029E-03  1.685E+03
    BCC_A2
    ** FCC_A1#1
Calculated.          26 equilibria

Phase region boundary 22 at:  2.029E-03  1.685E+03
    LIQUID
    BCC_A2
    ** FCC_A1#1
Calculated.          17 equilibria

Phase region boundary 23 at:  9.895E-03  1.706E+03
    LIQUID
    ** BCC_A2
    ** FCC_A1#1
Calculated.          17 equilibria

Phase region boundary 24 at:  9.895E-03  1.706E+03
    LIQUID
    ** FCC_A1#1
Calculated..         22 equilibria
Terminating at axis limit.

Phase region boundary 25 at:  9.895E-03  1.706E+03
    LIQUID
    ** BCC_A2
Calculated.          32 equilibria

Phase region boundary 26 at:  9.895E-03  1.706E+03
    LIQUID
    ** BCC_A2
    FCC_A1#1
Calculated.          11 equilibria
Terminating at known equilibrium

Phase region boundary 27 at:  5.090E-03  1.667E+03
    ** BCC_A2
    FCC_A1#1
Calculated.          18 equilibria
Terminating at known equilibrium

Phase region boundary 28 at:  1.106E-02  1.554E+03
    ** LIQUID
    FCC_A1#1
    M7C3
Calculated..         20 equilibria
Terminating at axis limit.

Phase region boundary 29 at:  3.934E-03  1.328E+03
    FCC_A1#1
    M23C6
    ** M7C3
Calculated.          9 equilibria

```

```

Terminating at known equilibrium
Phase region boundary 30 at: 1.027E-03 1.162E+03
** BCC_A2
** FCC_A1#1
M23C6
Calculated.. 14 equilibria
Terminating at known equilibrium
Phase region boundary 31 at: 6.464E-03 1.088E+03
** BCC_A2
** FCC_A1#1
M7C3
Calculated.. 29 equilibria
Terminating at axis limit.
Phase region boundary 32 at: 7.028E-03 1.088E+03
** BCC_A2
** FCC_A1#1
M7C3
Calculated.. 28 equilibria
Terminating at axis limit.
Phase region boundary 33 at: 6.464E-03 1.088E+03
** BCC_A2
** M23C6
M7C3
Calculated.. 11 equilibria
Terminating at known equilibrium
Terminating at axis limit.
Phase region boundary 34 at: 6.615E-03 8.100E+02
BCC_A2
M23C6
** M7C3
Calculated.. 11 equilibria
Terminating at known equilibrium
Phase region boundary 35 at: 5.000E-04 1.122E+03
BCC_A2
** FCC_A1#1
M23C6
Calculated.. 2 equilibria
Terminating at known equilibrium
Phase region boundary 36 at: 5.000E-04 1.122E+03
BCC_A2
** FCC_A1#1
M23C6
Calculated.. 11 equilibria
Terminating at known equilibrium
Phase region boundary 37 at: 6.833E-03 1.055E+03
BCC_A2
** M23C6
M7C3
Calculated.. 2 equilibria
Terminating at known equilibrium
Phase region boundary 38 at: 6.833E-03 1.055E+03
BCC_A2
** M23C6
M7C3
Calculated.. 12 equilibria
Terminating at known equilibrium
Terminating at axis limit.
Phase region boundary 39 at: 1.317E-02 1.076E+03
BCC_A2
** FCC_A1#1
M7C3
Calculated.. 15 equilibria
Terminating at known equilibrium
Terminating at axis limit.
Phase region boundary 40 at: 1.317E-02 1.076E+03
BCC_A2
** FCC_A1#1
M7C3
Calculated.. 15 equilibria
Terminating at known equilibrium
Terminating at axis limit.
Phase region boundary 41 at: 1.943E-02 8.100E+02
BCC_A2
M3C2
** M7C3
Calculated.. 3 equilibria
Terminating at axis limit.
Phase region boundary 42 at: 1.941E-02 8.000E+02
BCC_A2
M3C2
** M7C3
Calculated.. 19 equilibria
Phase region boundary 43 at: 1.973E-02 8.151E+02
BCC_A2
** GRAPHITE
M3C2
** M7C3
Calculated.. 2 equilibria
Terminating at axis limit.
Phase region boundary 44 at: 1.973E-02 8.151E+02
BCC_A2
** GRAPHITE
M3C2
Calculated.. 2 equilibria
Terminating at axis limit.
Phase region boundary 45 at: 2.266E-02 8.151E+02
BCC_A2
** GRAPHITE
M7C3
Phase region boundary 46 at: 7.607E-01 8.151E+02
** BCC_A2
GRAPHITE

```

M7C3

Phase region boundary 47 at: 2.266E-02 8.151E+02

BCC_A2
** M3C2
M7C3

Phase region boundary 48 at: 7.607E-01 8.151E+02

GRAPHITE
** M3C2
M7C3

Phase region boundary 49 at: 1.943E-02 8.100E+02

BCC_A2
M3C2
** M7C3

Calculated. 22 equilibria

Terminating at known equilibrium

Phase region boundary 50 at: 1.950E-02 8.204E+02

BCC_A2
M3C2
** M7C3

Calculated.. 7 equilibria

Terminating at known equilibrium

Terminating at axis limit.

Phase region boundary 51 at: 1.950E-02 8.204E+02

BCC_A2
M3C2
** M7C3

Calculated. 8 equilibria

Terminating at known equilibrium

Phase region boundary 52 at: 8.289E-04 1.203E+03

** BCC_A2
FCC_A1#1

Calculated. 3 equilibria

Terminating at known equilibrium

Phase region boundary 53 at: 8.289E-04 1.203E+03

** BCC_A2
FCC_A1#1

Calculated. 17 equilibria

Terminating at known equilibrium

Phase region boundary 54 at: 6.104E-03 1.203E+03

FCC_A1#1
** M23C6
M7C3

Calculated. 5 equilibria

Terminating at known equilibrium

Phase region boundary 55 at: 6.104E-03 1.203E+03

FCC_A1#1
** M23C6
M7C3

Calculated. 7 equilibria

Terminating at known equilibrium

Phase region boundary 56 at: 1.148E-03 1.597E+03

BCC_A2
** FCC_A1#1

Calculated. 26 equilibria

Phase region boundary 57 at: 1.148E-03 1.597E+03

BCC_A2
** FCC_A1#1

Calculated. 4 equilibria

Terminating at known equilibrium

Phase region boundary 58 at: 8.870E-03 1.597E+03

** LIQUID
FCC_A1#1

Calculated. 7 equilibria

Terminating at known equilibrium

Phase region boundary 59 at: 8.870E-03 1.597E+03

** LIQUID
FCC_A1#1

Calculated. 11 equilibria

Terminating at known equilibrium

Phase region boundary 60 at: 5.000E-04 1.788E+03

LIQUID
** BCC_A2

Calculated. 22 equilibria

Phase region boundary 61 at: 5.000E-04 1.788E+03

LIQUID
** BCC_A2

Calculated. 20 equilibria

Terminating at known equilibrium

Phase region boundary 62 at: 6.833E-03 1.733E+03

LIQUID
** BCC_A2

Calculated. 26 equilibria

Phase region boundary 63 at: 6.833E-03 1.733E+03

LIQUID
** BCC_A2

Calculated. 8 equilibria

Terminating at known equilibrium

Phase region boundary 64 at: 1.317E-02 1.688E+03

LIQUID
** FCC_A1#1

Calculated. 8 equilibria

Terminating at known equilibrium

Phase region boundary 65 at: 1.317E-02 1.688E+03

LIQUID
** FCC_A1#1

Calculated.. 15 equilibria

Terminating at known equilibrium

```

Terminating at axis limit.

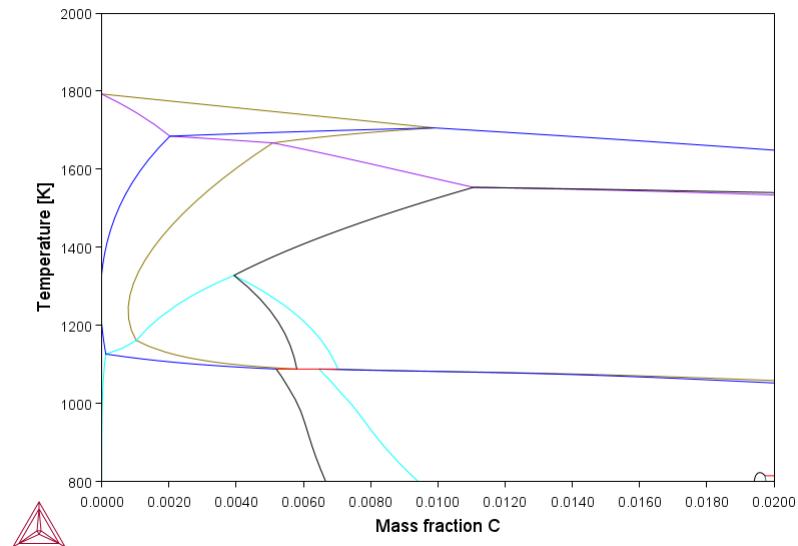
Phase region boundary 66 at: 1.950E-02 1.652E+03
    LIQUID
    ** FCC_A1#1
Calculated..          21 equilibria
Terminating at known equilibrium

Phase region boundary 67 at: 1.950E-02 1.652E+03
    LIQUID
    ** FCC_A1#1
Calculated..          3 equilibria
Terminating at known equilibrium
Terminating at axis limit.
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\generate_console_examples\examples\tcex33\tcex33.POLY3
CPU time for mapping           8 seconds
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST:
POST: set-title example 33a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAIFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
example 33a

```



 **POST:**
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:

tce34

SYS:About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce34\tce34.TCM"

SYS: set-echo

SYS:

SYS: @@ The Al-Zn phase diagram and its G curve

SYS:

SYS: @@ This example uses the BINARY module to calculate

SYS: @@ the phase diagram and G curves in the Al-Zn system.

SYS:

SYS: go bin

 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\generate_console_examples\databases\data
 Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

Simple binary phase diagram calculation module

Database: /TCBIN/: TCBIN

Current database: TC Binary Solutions v1.1

VA /- DEFINED

BCC_B2 FCC_L12 FCC_L102

D021_HCP REJECTED

First element: al zn

Phase Diagram, Phase fraction (F), G- or A-curves (G/A): /Phase_Diagram/: Phase_Diagram

VA /- DEFINED

BCC_B2 FCC_L12 FCC_L102

D021_HCP REJECTED

REINITIATING GES

AL ZN DEFINED

GAS:G LIQUID:L IONIC_LIQUID:Y

FCC_A1 BCC_A2 A2_BCC

HCP_A3 HCP_ZN DIAMOND_A4

BCT_A5 TETRAGONAL_A6 RHOMBOHEDRAL_A7

Cbcc_A12 CUB_A13 B32_ALLI

B3_ZINCLENDE C14_LAVES C15_LAVES

C16_AL2CU C36_LAVES D019_AL1M3

D513_AL3NI2 D82_FEZN_GAMMA L10_ALTI

AGZN_ZETA A15FE4 ALCE_AMORPHOUS

ALCU_ETA FEZN4 FEZN_DELTA

FEZN_ZETA REJECTED

LIQUID:L RESTORED

FCC_A1 RESTORED

HCP_A3 RESTORED

HCP_ZN RESTORED

16:21:33,229 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

FUNCTIONS

List of references for assessed data

'A T Dinsdale, SGTE Data for Pure Elements, Calphad 15(1991)4 p 317-425; '
'A T Dinsdale, SGTE Data for Pure Elements, update 2001'
'S an Mey, Z Metallkde 84(1993)7 p 451-455; Al-Zn'

-OK-

Creating a new composition set FCC_A1#2

The condition X(ZN)=.1234 created

The condition T=612.43 created

This file contains results from a previous STEP or MAP command.

The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

Forcing automatic start values

Automatic start values will be set

Start points provided by database

Version S mapping is selected

Organizing start points

Generating start point 1
Generating start point 2

Phase region boundary 1 at: 5.345E-01 5.000E+02

* * FCC_A1#1

 HCP_ZN

Calculated..

 10 equilibria

Terminating at axis limit.

Phase region boundary 2 at: 5.027E-01 3.000E+02

* * FCC_A1#1

 HCP_ZN

Calculated..

 13 equilibria

Phase region boundary 3 at: 5.626E-01 5.504E+02

* * FCC_A1#1

 HCP_ZN

Calculated..

 13 equilibria

Phase region boundary 4 at: 7.872E-01 5.504E+02

* * FCC_A1#1

 HCP_ZN

Calculated..

 6 equilibria

```

Phase region boundary 5 at: 8.211E-01 6.540E+02
** LIQUID
** FCC_A1#1
HCP_ZN

Phase region boundary 6 at: 9.263E-01 6.540E+02
** LIQUID
HCP_ZN
Calculated 17 equilibria

Phase region boundary 7 at: 7.783E-01 6.540E+02
** LIQUID
FCC_A1#1
Calculated 73 equilibria

Phase region boundary 8 at: 3.658E-01 5.504E+02
** FCC_A1#1
FCC_A1#2
Calculated 28 equilibria

Phase region boundary 9 at: 5.345E-01 5.000E+02
** FCC_A1#1
HCP_ZN
Calculated. 5 equilibria
Terminating at known equilibrium
*** BUFFER SAVED ON FILE: C:\Users\azureuser\AppData\Local\Temp\BINARY_002.POLY3
CPU time for mapping 2 seconds
POSTPROCESSOR VERSION 3.2

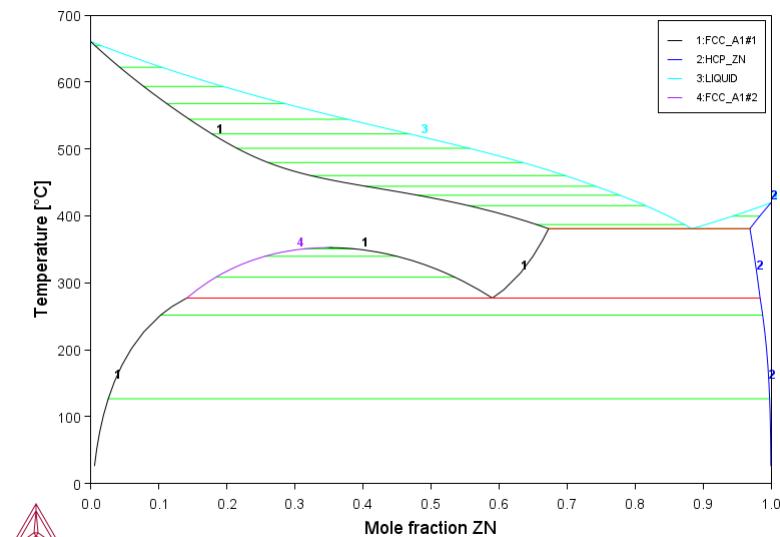
```

Setting automatic diagram axes

POSTPROCESSOR VERSION 3.2

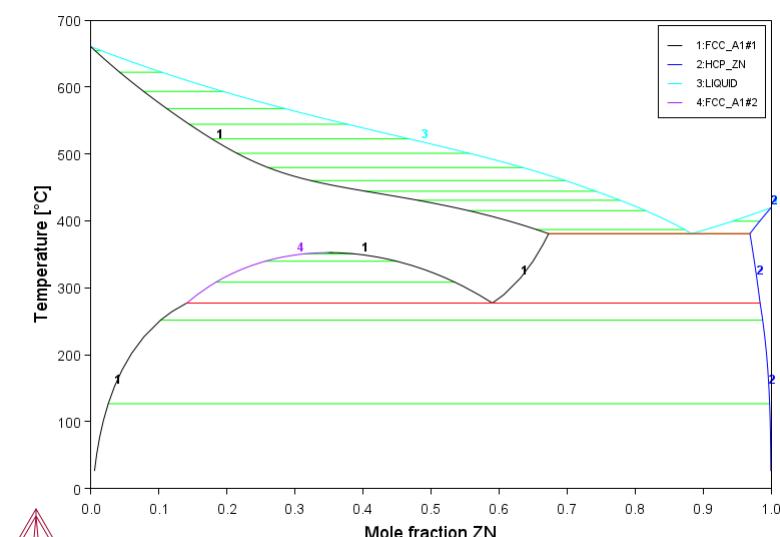
Setting automatic diagram axes

AL ZN



POST: set-title example 34a
POST: plot

example 34a



POST:
POST: Hit RETURN to continue
POST: @@ Now plot a G curve at 573 K!

POST: back

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

SYS: go bin

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED
Simple binary phase diagram calculation module

Database: /TCBIN/: TCBIN
Current database: TC Binary Solutions v1.1

| | | |
|----------|------------|----------|
| VA | /- DEFINED | |
| BCC_B2 | FCC_L12 | FCC_L102 |
| D021_HCP | REJECTED | |

First element: al zn
Phase Diagram, Phase fraction (F), G- or A-curves (G/A): /Phase_Diagram/: G
Temperature (C): /1000/: 300

| | | |
|----------|------------|----------|
| VA | /- DEFINED | |
| BCC_B2 | FCC_L12 | FCC_L102 |
| D021_HCP | REJECTED | |

REINITIATING GES

| | | |
|---------------|----------------|-----------------|
| AL | ZN DEFINED | |
| GAS:G | LIQUID:L | IONIC_LIQUID:Y |
| FCC_A1 | BCC_A2 | A2_BCC |
| HCP_A3 | HCP_ZN | DIAMOND_A4 |
| BCT_A5 | TETRAGONAL_A6 | RHOMBOHEDRAL_A7 |
| CBCC_A12 | CUB_A13 | B32_ALLI |
| B3_ZINCBLENDE | C14_LAVES | C15_LAVES |
| C16_AL2CU | C36_LAVES | D019_AL1M3 |
| D513_AL3NI2 | D82_FEZN_GAMMA | L10_ALTI |
| AGZN_ZETA | AL5FE4 | ALCE_AMORPHOUS |
| ALCU_ETA | FEZN4 | FEZN_DELTA |

FEZN_ZETA REJECTED
LIQUID:L RESTORED
FCC_A1 RESTORED
HCP_A3 RESTORED
HCP_ZN RESTORED
ELEMENTS

SPECIES

PHASES

PARAMETERS

FUNCTIONS

List of references for assessed data

'A T Dinsdale, SGTE Data for Pure Elements, Calphad 15(1991)4 p 317-425; '
'A T Dinsdale, SGTE Data for Pure Elements, update 2001'
'S an Mey, Z Metallkde 84(1993)7 p 451-455; Al-Zn'

-OK-
Creating a new composition set FCC_A1#2
The condition X(ZN)=.1234 created

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

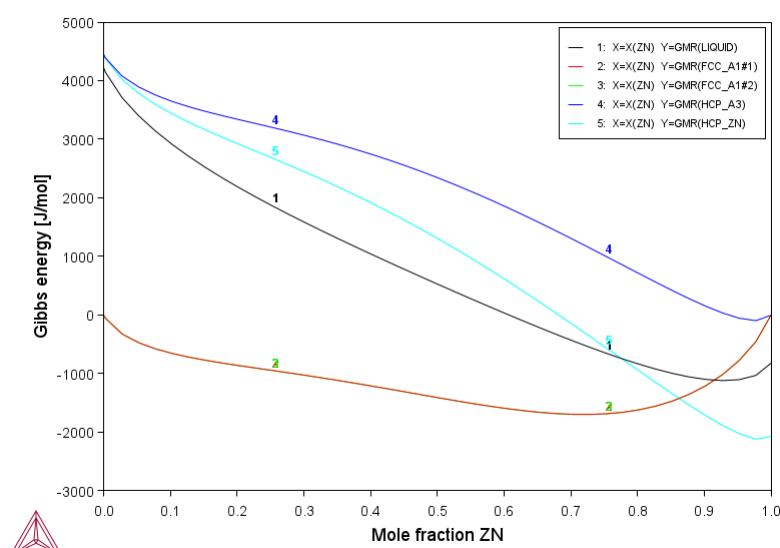
Forcing automatic start values
Automatic start values will be set

Phase Region from 0.502463 for:
LIQUID
FCC_A1#1
FCC_A1#2
HCP_A3
HCP_ZN

Phase Region from 0.502463 for:
LIQUID
FCC_A1#1
FCC_A1#2
HCP_A3
HCP_ZN

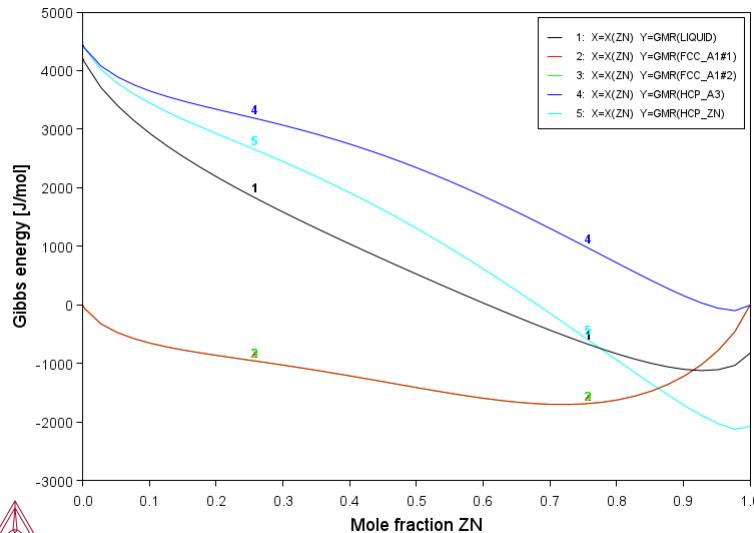
*** Buffer saved on file *** C:\Users\azureuser\AppData\Local\Temp\GCURVE_002.POLY3
POSTPROCESSOR VERSION 3.2

AL ZN



POST:
POST: set-title example 34b
POST:
POST: plot

example 34b



```

POST:
POST:Hit RETURN to continue
POST: @@ Now plot an activity (A) curve at 573 K
POST: back
Current database: Steels/Fe-Alloys v11.0

```

```

VA           /- DEFINED
DICTRA_FCC_A1 REJECTED
SYS: go bin
Current database: Steels/Fe-Alloys v11.0

```

```

VA           /- DEFINED
DICTRA_FCC_A1 REJECTED
Simple binary phase diagram calculation module

```

```

Database: /TCBIN/: TCBIN
Current database: TC Binary Solutions v1.1

```

```

VA           /- DEFINED
BCC_B2      FCC_L12          FCC_L102
D021_HCP REJECTED
First element: al zn
Phase Diagram, Phase fraction (F), G- or A-curves (G/A): /Phase_Diagram/: A
Temperature (C): /1000/: 300
VA           /- DEFINED
BCC_B2      FCC_L12          FCC_L102
D021_HCP REJECTED
REINITIATING GES .....
AL           ZN DEFINED
GAS:G        LIQUID:L          IONIC_LIQUID:Y
FCC_A1       BCC_A2            A2_BCC
HCP_A3       HCP_ZN            DIAMOND_A4
BCT_A5       TETRAGONAL_A6    RHOMBHEDRAL_A7
CBCC_A12     CUB_A13           B32_ALLI
B3_ZINCBLENDE C14_LAVES       C15_LAVES
C16_AL2CU    C36_LAVES       D019_AL1M3
D513_AL3NI2  D82_FEZN_GAMMA  L10_ALTI
AGZN_ZETA    AL5FE4           ALCE_AMORPHOUS
ALCU_ETA     FEZN4            FEZN_DELTA
FEZN_ZETA   REJECTED
LIQUID:L    RESTORED
FCC_A1      RESTORED
HCP_A3      RESTORED
HCP_ZN      RESTORED
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ...

```

List of references for assessed data

```

'A T Dinsdale, SGTE Data for Pure Elements, Calphad 15(1991)4 p 317-425; '
'A T Dinsdale, SGTE Data for Pure Elements, update 2001'
'S an Mey, Z Metallkde 84(1993)7 p 451-455; Al-Zn'
-OK-
Creating a new composition set FCC_A1#2
The condition X(ZN)=.1234 created

```

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

```

Forcing automatic start values
Automatic start values will be set
No initial equilibrium, using default
Step will start from axis value 0.123400
....OK

```

```

Phase Region from 0.123400 for:
FCC_A1#
Global test at 3.23400E-01 ... Backtracking to find phase change for FCC_A1#2
Global test at 1.48400E-01 .... OK
Global check of adding phase at 1.70853E-01
Calculated 5 equilibria

```

```

Phase Region from 0.170853 for:
FCC_A1#
FCC_A1#
Global test at 3.48400E-01 .... OK
Global check of removing phase at 5.51861E-01

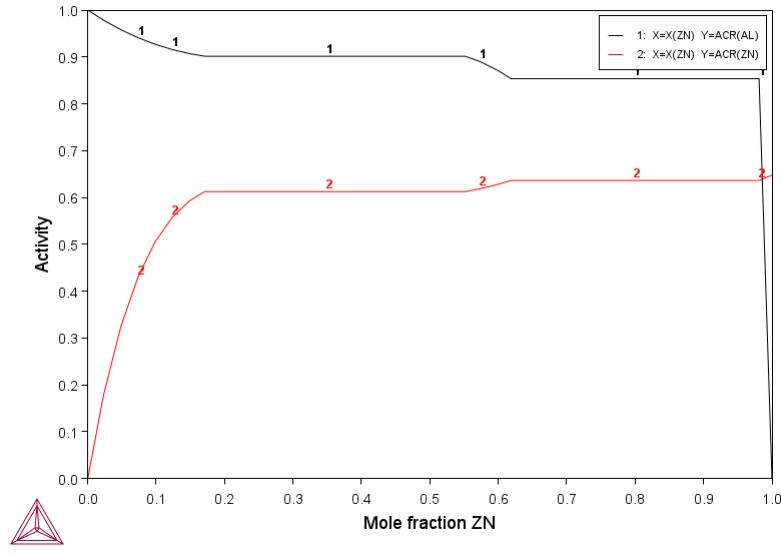
```

```

Calculated      19 equilibria
Phase Region from  0.551861      for:
  FCC_A1#2
Global check of adding phase at  6.18456E-01
Calculated      5 equilibria
Phase Region from  0.618456      for:
  FCC_A1#2
  HCP_ZN
Global test at  7.98400E-01 .... OK
Global check of removing phase at  9.81102E-01
Calculated      18 equilibria
Phase Region from  0.981102      for:
  HCP_ZN
Terminating at    1.00000
Calculated      4 equilibria
Phase Region from  0.123400      for:
  FCC_A1#1
Terminating at    0.100000E-11
Calculated      8 equilibria
*** Buffer saved on file: C:\Users\azureuser\AppData\Local\Temp\GCURVE_002.POLY3
POSTPROCESSOR VERSION 3.2

```

AL ZN

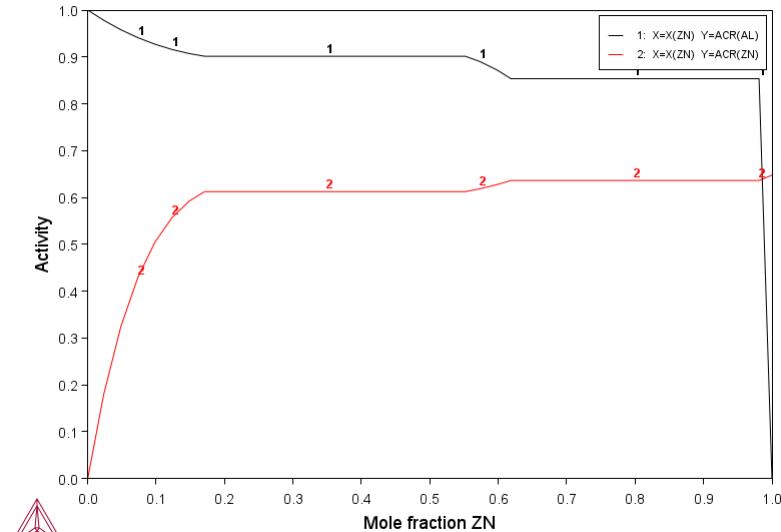


```

POST:
POST: set-title example 34c
POST:
POST: plot

```

example 34c



```

POST:
POST: Hit RETURN to continue
POST: @@ Now plot a Phase fraction (F) curve for
POST: @@ x(zn)=.5. The miscibility gap is found now
POST: back

```

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

SYS: go bin

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

Simple binary phase diagram calculation module

Database: /TCBIN/: TCBIN

Current database: TC Binary Solutions v1.1

```

VA          /- DEFINED
BCC_B2      FCC_L12           FCC_L102
D021_HCP REJECTED
First element: al zn
Phase Diagram, Phase fraction (F), G- or A-curves (G/A): /Phase_Diagram/: F
Fraction of: zn ./5/: .5
VA          /- DEFINED
BCC_B2      FCC_L12           FCC_L102
D021_HCP REJECTED
REINITIATING GES .....
AL          ZN DEFINED
GAS:G       LIQUID:L          IONIC_LIQUID:Y
FCC_A1      BCC_A2            A2_BCC
HCP_A3      HCP_ZN            DIAMOND_A4
BCT_A5      TETRAGONAL_A6    RHOMBOHEDRAL_A7
CBCC_A12    CUB_A13           B32_ALLI
B3_ZINCLENDE C14_LAVES        C15_LAVES
C16_AL2CU   C36_LAVES        D019_AL1M3
D513_AL3NI2 DB2_FEZN_GAMMA  L10_ALTI
AGZN_ZETA   AL5FE4           ALCE_AMORPHOUS
ALCU_ETA    FEZN4            FEZN_DELTA
FEZN_ZETA  REJECTED
LIQUID:L RESTORED
FCC_A1 RESTORED
HCP_A3 RESTORED
HCP_ZN RESTORED
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS .....

List of references for assessed data

'A T Dinsdale, SGTE Data for Pure Elements, Calphad 15(1991)4 p 317-425; '
'A T Dinsdale, SGTE Data for Pure Elements, update 2001'
'S an Mey, Z Metallkde 84(1993)7 p 451-455; Al-Zn'
-OK-
Creating a new composition set FCC_A1#2
Forcing automatic start values
Automatic start values will be set
No initial equilibrium, using default
Step will start from axis value 1000.00
...OK

Phase Region from 1000.00 for:
  LIQUID
Global test at 9.20000E+02 .... OK
Global test at 8.20000E+02 .... OK
Global check of adding phase at 7.88048E+02
Calculated 24 equilibria

Phase Region from 788.048 for:
  LIQUID
  FCC_A1#1
Global test at 7.26000E+02 .... OK
Global test at 7.06000E+02 .... OK
Global check of removing phase at 7.00299E+02
Calculated 23 equilibria

Phase Region from 700.299 for:
  FCC_A1#1
Global test at 6.28000E+02 .... OK
Global test at 5.28000E+02 .. Backtracking to find phase change for FCC_A1#2
Global test at 6.18000E+02 .... OK
Global test at 5.98000E+02 .... OK
Global check of adding phase at 5.96831E+02
Calculated 15 equilibria

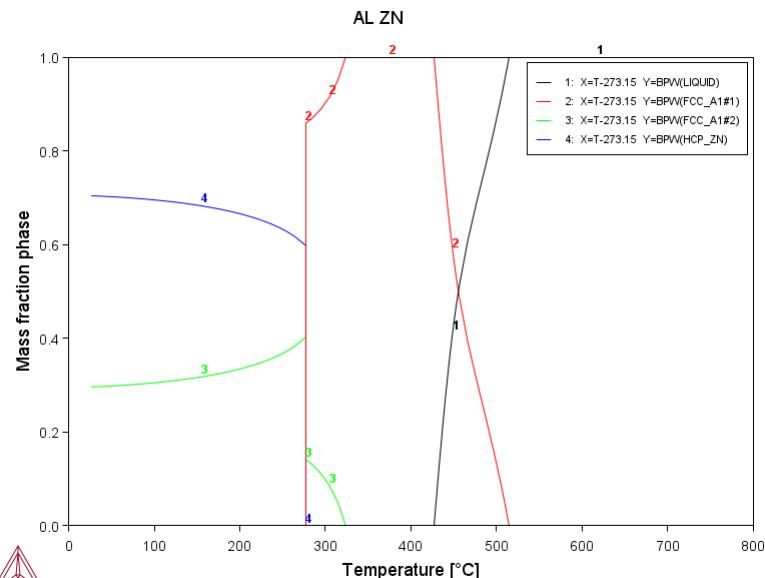
Phase Region from 596.831 for:
  FCC_A1#1
  FCC_A1#2
Global check of adding phase at 5.50386E+02
Calculated 7 equilibria

Phase Region from 550.386 for:
  FCC_A1#1
  FCC_A1#2
  HCP_ZN
Calculated 2 equilibria

Phase Region from 550.386 for:
  FCC_A1#2
  HCP_ZN
Global test at 4.78000E+02 .... OK
Global test at 3.78000E+02 .... OK
Terminating at 300.000
Calculated 29 equilibria
*** Buffer saved on file: C:\Users\azureuser\AppData\Local\Temp\PF CURVE_002.POLY3
POSTPROCESSOR VERSION 3.2

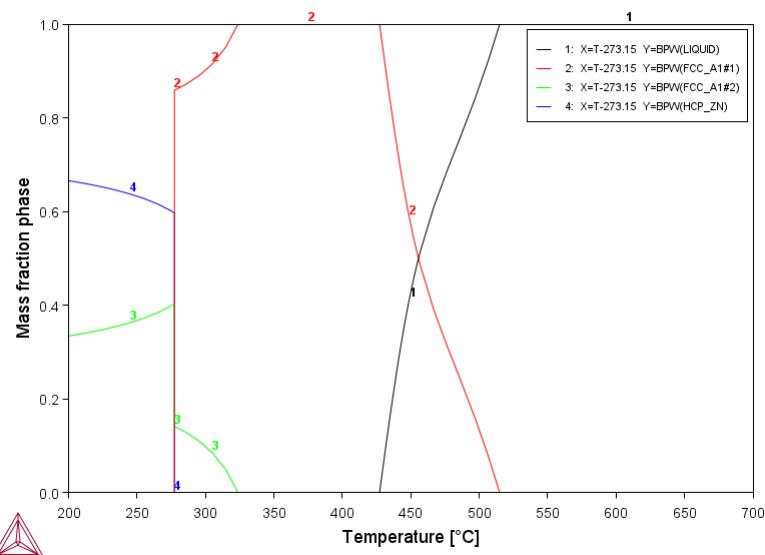
```

Setting automatic diagram axes



```
POST:
POST: s-s x n 200 700
POST: set-title example 34d
POST:
POST: plot
```

example 34d



POST:

SYS:About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

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Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

```
SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce35\tce35.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Calculating a potential diagram using
SYS: @@ the POTENTIAL module.
SYS:
SYS: @@ There are no commands for this module, you
SYS: @@ just follow the prompts.
SYS:
SYS: go pot

Simple potential phase diagram calculation module

Database: /POT/: SUBDEMO
THERMODYNAMIC DATABASE module
Database folder: C:\jenkins\workspace\generate_console_examples\databases\data
Current database: Substance Demo Database v1.0

VA           /* DEFINED
Matrix element: /FE/: FE
First potential species: /S1O2/: C1O1
Second potential species: /O2/: O2
Temperature: /1000/: 1000
VA           /* DEFINED
REINITIATING GES .....
FE          C          O
           DEFINED
16:23:04,872 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS .....

List of references for assessed data

'C1<G> T.C.R.A.S. Class: 1 C1<G> C<G>' 
'C1O1<G> JANAF THERMOCHEMICAL TABLES SGTE ** C1O1<G> CO<G> CARBON MONOXIDE
  <GAS> STANDARD STATE : CODATA KEY VALUE. /CP FROM JANAF PUB. 9/65'
'C1O2<G> T.C.R.A.S. Class: 2 C1O2<G> CO2<G> CARBON DIOXIDE <GAS>
'C2<G> T.C.R.A.S. Class: 2 C2<G> CARBON Diatomic Gas.'
'C2O1<G> T.C.R.A.S. Class: 5 C2O1<G> C2O<G>
'C3<G> T.C.R.A.S. Class: 6 C3<G> CARBON <TRIATOMIC GAS>
'C3O2<G> T.C.R.A.S. Class: 6 C3O2<G>
'C4<G> T.C.R.A.S. Class: 7 C4<G>
'C5<G> T.C.R.A.S. Class: 7 C5<G>
'C5FE105<G> JANAF 1982 SGTE C5FE105<G> Fe(CO)5<G> IRON PENTACARBONYL <GAS>
  ASSESSMENT DATED 3/78'
'C60<G> MHR-95 C60<G> Data processed from [94Kor/Sid] M.V. Korobov, L.N.
  sidorov, J. Chem. Thermo., 26, 61-73 (1994). Recalculated from the
  rotational data in [91McK] and vibration frequencies in [94Kor/Sid].
  Note that a frequency with degeneracy 5 is missing from list in
  [94Kor/Sid], taken to be 419 cm-1, which gives very good, though not
  exact, agreement with values quoted in [94Kor/Sid]. Note discrepancy
  between calculated DrS(298) = -8943.5 J mol K-1 for the reaction 60C<g>
  =>C60<g> and that given by [94Kor/Sid] in their Table 5, -8950 J mol K
  -1. Enthalpy of formation: DHf = 2588 kJ/mol from DsubH(298.15K) = 166
  +/- 11 kJ mol-1 [94Kor/Sid]. Vapour pressure values reproduced very
  well. [91McK] J.T. McKinnon, J. Phys. Chem. 95 8941(1993).'
'FE1<G> THERMODATA FE1<G> Fe<G> Data provided by T.C.R.A.S. October 1996
  Modified by ThermoData - new assessment'
'FE1O1<G> TCRAS 5-F FEO IRON OXIDE 23/11/06 FE1O1<G> FeO<G>'
'FE1O2<G> T.C.R.A.S Class: 6 FE1O2<G> FeO2<G> Data provided by TCRAS.
  October 1996. Error in version 1997. S298 corrected to 1bar 20080222
  AAZ TCRAS2006 : dH, S'
'FE2<G> THERMODATA FE2<G> Fe2<G> Data provided by T.C.R.A.S. October 1996
  Modified by ThermoData - new assessment. Typing error corrected 12/06'
'02<G> TCRAS 21/06/90 02<G> OXYGEN Gaseous Standard State.'
'03<G> TCRAS 02/06/80 03<G> OZONE Gaseous Standard State.'
'C1FE103 N.P.L. SGTE ** C1FE103 FeCo3 Siderite IRON<2> CARBONATE
  DECOMPOSES BEFORE FUSION.'
'C1FE3 N.P.L. SGTE ** C1FE3 Fe3C Cementite CEMENTITE'
'C5FE105<L> I. BARIN 3rd. Edition C5FE105 Liquid Fe(CO)5 Liquid IRON
  PENTACARBONYL (Liquid). Same as in previous versions. Rounding of H298.'
'C60 MHR-95 C60 Data processed from [94Kor/Sid] M.V. Korobov, L.N. sidorov,
  J. Chem. The Fitted to the data in [94Kor/Sid], who took the phase
  transition at 257K that [94Kor/Sid] do not give an explicit value for
  S(298.15K). S(298.15K) = 422.6 J mol K-1 was calculated from S(300) =
  425.8 and Cp e calculated from Drs(298) for 60C<graphite>=>C60 given by
  [94Kor/Sid] in their Table 5, which gives S(298.15K) = 425.4 J mol K
  -1. Enthalpy of formation : DHf = +2422 +/- 14 kJ/mol from [92Ste/Chi],
  the value preferred, if obliquely, by [94Kor/Sid]. [92Ste/Chi]W.V.
  Steele, R.D. Chirico, N.K. Smith, W.e. Billups, P.R. Elmore, A.E.
  Wheeler, J. Phys. Chem. 96 4731 (1993).'
'C1<DIAMOND> S.G.T.E. ** C_DIAMOND <DIAMOND> Data from SGTE Unary DB, data
  added by atd 7/9/95, H298-H0 taken from 1994 database (ex THERMODATA
  01/93)'
'FE1O1 T.C.R.A.S Class: 5 FE1O1 FeO FeO_Wustite IRON OXIDE. Data provided
  by T.C.R.A.S. in 2000'
'FE2O3<FE203_GAMMA> T.C.R.A.S Class: 5 FE2O3_GAMMA Fe2O3_Gamma Data
  provided by T.C.R.A.S. in 2000'
'FE1 S.G.T.E. ** FE1 Fe Data from SGTE Unary DB'
'C1<GRAPHITE> S.G.T.E. ** C_GRAPHITE Data from SGTE Unary DB, pressure
  dependent data added by atd 7/9/95'
'FE2O3<HEMATITE> T.C.R.A.S Class: 7 FE2O3 Fe2O3 Hematite Data provided by
  T.C.R.A.S. in 2000 with previous description of the magnetic
  transition fitted by IA. In version 2000 only H298 has been changed.'
'FE3O4<MAGNETITE> JANAF 4th Ed. FE3O4 Fe3O4 MAGNETITE Data refitted by IA
```

to reproduce the magnetic transition.'
 'FE0.94701<WUSTITE> T.C.R.A.S Class: 5 FE0.94701 Fe0.9470 WUSTITE WUSTITE.
 Data provided by T.C.R.A.S. in 2000 20080222 AAZ TCRAS2006 : dH, S'
 -OK-
 This command is DEPRECATED and to be removed in the future!
 Please use ADVANCED_OPTIONS instead of SPECIAL_OPTIONS
 The condition LNACR(C101,GAS)=-140.8589 created
 The condition LNACR(O2,GAS)=-140.8589 created
 Normal POLY minimization, not global
 Version S mapping is selected

Organizing start points
 Using ADDED start equilibria
 Working hard
 Generating start point 1
 Generating start point 2
 Generating start point 3
 Generating start point 4

Phase region boundary 1 at: -4.633E+01 -1.409E+02
 FE_S
 ** GRAPHITE
 Calculated.. 81 equilibria
 Terminating at axis limit.

Phase region boundary 2 at: -1.259E+02 -3.000E+02
 FE_S
 ** GRAPHITE
 Calculated.. 126 equilibria

Phase region boundary 3 at: -9.383E-01 -5.007E+01
 ** FE1O1_S
 FE_S
 ** GRAPHITE

Phase region boundary 4 at: -9.383E-01 -5.007E+01
 ** FE1O1_S
 FE_S
 Calculated.. 151 equilibria
 Terminating at axis limit.

Phase region boundary 5 at: -9.383E-01 -5.007E+01
 ** FE1O1_S
 GRAPHITE
 Calculated.. 2 equilibria

Phase region boundary 6 at: -3.398E-01 -4.887E+01
 ** GAS
 ** FE1O1_S
 GRAPHITE

Phase region boundary 7 at: -3.398E-01 -4.887E+01
 ** GAS
 GRAPHITE
 ++++++

Phase region boundary 8 at: -3.398E-01 -4.887E+01
 ** GAS
 FE1O1_S
 Calculated.. 7 equilibria

Phase region boundary 9 at: -3.272E+00 -4.059E+01
 ** GAS
 FE1O1_S
 ** MAGNETITE

Phase region boundary 10 at: -3.272E+00 -4.059E+01
 FE1O1_S
 ** MAGNETITE
 Calculated.. 150 equilibria
 Terminating at axis limit.

Phase region boundary 11 at: -3.272E+00 -4.059E+01
 GAS
 ** MAGNETITE
 Calculated.. 10 equilibria

Phase region boundary 12 at: -1.174E+01 -2.359E+01
 GAS
 ** HEMATITE
 ** MAGNETITE

Phase region boundary 13 at: -1.174E+01 -2.359E+01
 GAS
 ** HEMATITE
 Calculated.. 168 equilibria
 Terminating at axis limit.

Phase region boundary 14 at: -1.174E+01 -2.359E+01
 ** HEMATITE
 MAGNETITE
 Calculated.. 146 equilibria
 Terminating at axis limit.

Phase region boundary 15 at: -4.633E+01 -1.409E+02
 FE_S
 ** GRAPHITE
 Calculated.. 47 equilibria
 Terminating at known equilibrium

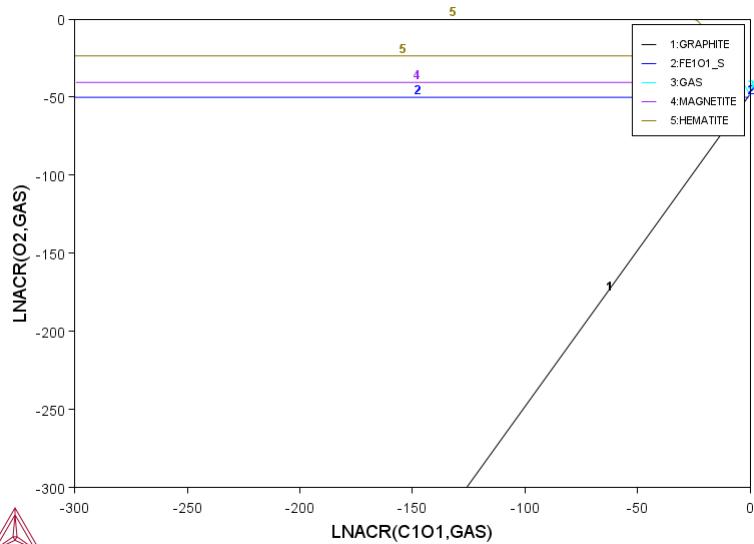
Phase region boundary 16 at: -1.409E+02 -5.007E+01
 ** FE1O1_S
 FE_S
 Calculated.. 81 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 17 at: -1.409E+02 -5.007E+01
 ** FE1O1_S
 FE_S
 Calculated.. 71 equilibria
 Terminating at known equilibrium
 *** BUFFER SAVED ON FILE: c:\jenkins\workspace\generate_console_examples\examples\tcex35\POT.POLY3
 CPU time for mapping 6 seconds

POSTPROCESSOR VERSION 3.2

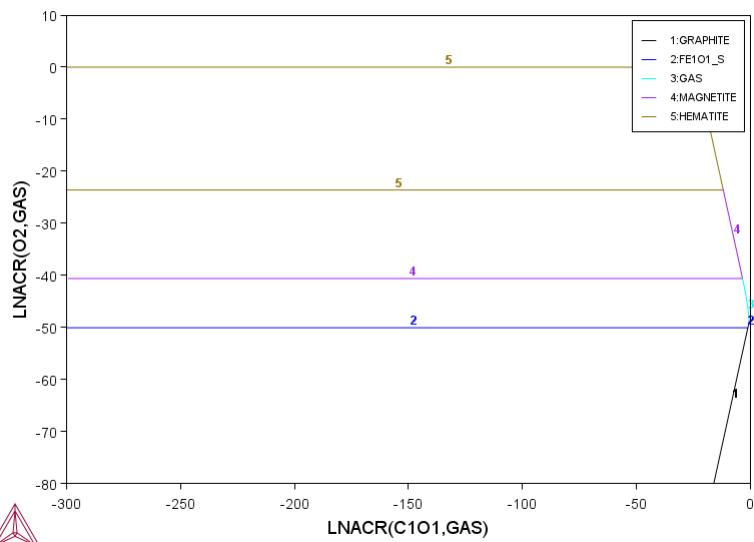
Setting automatic diagram axes

FE C1O1 O2; Database: SUBDEMO



POST: s-s y n -80 10
POST: set-title example 35a
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot

example 35a



POST:
POST: set-inter
POST:

tce36a**SYS:About**

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

```
SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce36a\tce36a.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Assessment. The use of the PARROT module
SYS:
SYS: @@ This is the setup file for Windows systems
SYS:
SYS: @@ First the elements and phases must be entered in G-E-S module
SYS: GO G
GIBBS ENERGY SYSTEM
16:24:47,731 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
GES6: ENTER-ELEMENT A B
THERMODYNAMIC DATABASE module
Database folder: C:\jenkins\workspace\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA          /- DEFINED
DICTRA_FCC_A1 REJECTED
GES6: AMEND-ELEMENT-DATA A BCC 20 0 0 1
GES6: AMEND-ELEMENT-DATA B BCC 50 0 0 1
GES6: ENTER-PHASE LIQUID L 1 A B; N N
GES6: ENTER-PHASE BCC,, 1 A B; N N
GES6: ENTER-PHASE FCC,, 1 A B; N N
GES6: ENTER-PHASE A2B,, 2 2 1 A; B; N N
CONSTITUENTS IN SUBLATTICE           1
CONSTITUENTS IN SUBLATTICE           2
GES6: @@ There is a miscibility gap in the bcc, this must be stated here
GES6: AMEND_PHASE BCC COMPOSITION_SETS 2 B
Creating a new composition set BCC#2
GES6: @@ We can also set the major constituent of the first composition set
GES6: AMEND_PHASE BCC MAJOR 1 A
GES6:
GES6: @@ The FCC phase is stable only for element B
GES6: AMEND_PHASE FCC MAJOR 1 B
GES6: @@ The parameters can be entered in the PARROT module
GES6: GO PAR

PARROT VERSION 5.3

Global minimization used as test only
PARROT: ENTER-PARAMETER G(BCC,A) 500 0; 2000 N
G(BCC,A;0)-G(BCC,A;0)
PARROT: ENTER-PARAMETER G(BCC,B) 500 0; 2000 N
G(BCC,B;0)-G(BCC,B;0)
PARROT: ENTER-PARAMETER G(LIQUID,A) 500 14000-10*T; 2000 N
G(LIQUID,A;0)-G(BCC,A;0)
PARROT: ENTER-PARAMETER G(LIQUID,B) 500 18000-12*T; 2000 N
G(LIQUID,B;0)-G(BCC,B;0)
PARROT: ENTER-PARAMETER G(FCC,B) 500 3300-3*T; 2000 N
G(FCC,B;0)-G(BCC,B;0)
PARROT: ENTER-PARAMETER G(FCC,A) 500 408; 2000 N
G(FCC,A;0)-G(BCC,A;0)
PARROT: ENTER-PARAMETER G(A2B) 500 V1+V2*T+V3*T*LOG(T); 2000 N
G(A2B,A;0) - 2 G(BCC,A;0)-G(BCC,B;0)
PARROT: ENTER-PARAMETER G(LIQUID,A,B;0) 500 V11+V12*T; 2000 N
G(LIQUID,A,B;0)
PARROT: ENTER-PARAMETER G(LIQUID,A,B;1) 500 V13+V14*T; 2000 N
G(LIQUID,A,B;1)
PARROT: ENTER-PARAMETER G(BCC,A,B;0) 500 V15+V16*T; 2000 N
G(BCC,A,B;0)
PARROT: ENTER-PARAMETER G(BCC,A,B;1) 500 V17+V18*T; 2000 N
G(BCC,A,B;1)
PARROT: ENTER-PARAMETER G(FCC,A,B;0) 500 V19+V20*T; 2000 N
G(FCC,A,B;0)
PARROT: ENTER-PARAMETER G(FCC,A,B;1) 500 V21+V22*T; 2000 N
G(FCC,A,B;1)
PARROT:
PARROT: @@ Everything is saved to an unformatted work file by the Create command
PARROT: CREATE tce36
PARROT:
PARROT: Hit RETURN to continue
PARROT:
PARROT: @@ The experimental data file is compiled to the work file.
PARROT: COMPILE tce36 screen Y exp36
POP files may include graphics information using the
GRAPHICS_PLOT command. A file name for generating an ".exp" file must be given.
$ 
$ POP file for assessment example
$ 
$ Enter some constants used later.
ENTER_SYMBOL CONSTANT DX=0.02,P0=101325,DH=500,DT=10
$ 
$ Eutectic point at A rich side from ref #2.
$ T=1193 K, 40.8 w/o B in liquid, 13 w/o B in bcc.
$ In a binary system one must have four conditions if P is not fixed.
$ We obtain this by fixing the pressure and that three phases must be stable.
$ The amount of the fixed phases is irrelevant here
CREATE_NEW_EQUILIBRIUM 1,1
CHANGE_STATUS PHASE LIQUID,BCC,A2B=FIX 1
SET-CONDITION P=P0
EXPERIMENT T=1193:DT,W(LIQ,B)=.408:DX,W(BCC,B)=.13:DX
GRAPHICS 1 .408 1193 MSS
GRAPHICS 1 .13 1193 DS5
GRAPHICS 1 .555 1193 DS5
LABEL AINV
SET-ALT X(A2B,A)=.6666667
```

```

SET_ALL_START 1193 Y
Automatic start values will be set
$
$ Congrent melting temperature for A2B 1341 K.
$ We will include the enthalpy of transformation also and this
$ requires a function.
ENTER_SYMBOL FUNCTION HTR=HM(LIQUID)-HM(A2B);
$
$ Note how one specifies that this is a congruent transformation!
CREATE_NEW_EQUILIBRIUM 2,1
CHANGE_STATUS PHASE LIQ,A2B=FIX 1
SET_CONDITION P=P0,X(LIQ,B)-X(A2B,B)=0
EXPERIMENT T=1341:DT
EXPERIMENT HTR=3727:500
GRAPHICS 1 .555 1341 MS7
LABEL AINV
SET_ALT X(A)=.6666667
SET_ALL_START 1341 Y
Automatic start values will be set
$
$ Eutectic point at B rich side.
$ T=1049 K, 27 w/o A in liquid, 9.3 w/o A in bcc.
CREATE_NEW_EQUILIBRIUM 3,1
CHANGE_STATUS PHASE LIQ,BCC,A2B=FIX 1
SET_CONDITION P=P0
EXPERIMENT T=1049:DT,W(LIQ,A)=.27:DX,W(BCC,A)=.093:DX
SET_ALT X(A2B,A)=.6666667
GRAPHICS 1 .907 1049 MS5
GRAPHICS 1 .73 1049 DS5
GRAPHICS 1 .555 1049 DS5
LABEL AINV
SET_ALL_START 1049 Y
Automatic start values will be set
$
$ Peritectic point. T=1203 K, 19 w/o A in liquid, 6.9 w/o A in bcc,
$ 6.0 w/o A in fcc.
CREATE_NEW_EQUILIBRIUM 4,1
CHANGE_STATUS PHASE LIQ,BCC,FCC=FIX 1
SET_CONDITION P=P0
EXPERIMENT T=1203:DT,W(LIQ,A)=.19:DX,W(BCC,A)=.069:DX,W(FCC,A)=.06:DX
GRAPHICS 1 .81 1203 MS5
GRAPHICS 1 .931 1203 DS5
GRAPHICS 1 .94 1203 DS5
LABEL AINV
SET_ALL_START 1203 Y
Automatic start values will be set
$
$ Eutectoid transformation of A2B -> BCC1 + BCC2, from ref #3
$ T=726, 3.7 at/o B in A, 11.4 at/o A in B
$ Note that miscibility gaps are indicated by using # after the phase
$ name and then give an integer.
CREATE_NEW_EQUILIBRIUM 5,1
CHANGE_STATUS PHASE BCC#1,BCC#2,A2B=FIX 1
SET_CONDITION P=P0
EXPERIMENT T=726:DT,X(BCC#1,B)=.037:DX,X(BCC#2,A)=.114:DX
SET_ALT X(A2B,A)=.6666667
GRAPHICS 1 0.09 726 MS5
GRAPHICS 1 0.95 726 DS5
LABEL AINV
SET_ALL_START 726 Y
Automatic start values will be set
$
$ It is sometimes useful to decribe an invariant equilibria as
$ three tie-lines between each pair of phases at the same temperature.
$ In this case it helps to add a tie-line across the miscibility gap
$ at the invariant temperature.
CREATE_NEW_EQUILIBRIUM 6,1
CHANGE_STATUS PHASE BCC#1,BCC#2=FIX 1
SET_CONDITION P=P0 T=726
EXPERIMENT X(BCC#1,B)=.037:DX,X(BCC#2,A)=.114:DX
LABEL AINV
SET_ALL_START Y
Automatic start values will be set
$
$ From ref #4 the liquidus at the B rich end:
$ The table values are referenced inside the table_head using @<column>
TABLE_HEAD 10
CREATE_NEW_EQUILIBRIUM 0010,1
CHANGE_STATUS PHASE LIQ,FCC=FIX 1
SET_CONDITION T=1594,P=P0
EXPERIMENT W(LIQ,A)=0.02:DX
LABEL ALF
GRAPHICS 1 .98 1594 MS5
SET_ALL_START Y
Automatic start values will be set
CREATE_NEW_EQUILIBRIUM 0011,1
CHANGE_STATUS PHASE LIQ,FCC=FIX 1
SET_CONDITION T=1548,P=P0
EXPERIMENT W(LIQ,A)=0.042:DX
LABEL ALF
GRAPHICS 1 .958 1548 MS5
SET_ALL_START Y
Automatic start values will be set
CREATE_NEW_EQUILIBRIUM 0012,1
CHANGE_STATUS PHASE LIQ,FCC=FIX 1
SET_CONDITION T=1499,P=P0
EXPERIMENT W(LIQ,A)=0.065:DX
LABEL ALF
GRAPHICS 1 .935 1499 MS5
SET_ALL_START Y
Automatic start values will be set
CREATE_NEW_EQUILIBRIUM 0013,1
CHANGE_STATUS PHASE LIQ,FCC=FIX 1
SET_CONDITION T=1438,P=P0
EXPERIMENT W(LIQ,A)=0.093:DX
LABEL ALF
GRAPHICS 1 .907 1438 MS5
SET_ALL_START Y
Automatic start values will be set
$
$ From ref #5 we have the following tie-lines
TABLE_HEAD 20
CREATE_NEW_EQUILIBRIUM 0020,1
CHANGE_STATUS PHASE LIQ,FCC=FIX 1
SET_CONDITION T=1413,P=P0

```

```

EXPERIMENT W(LIQ,A)=.104:DX,W(FCC,A)=.038:DX
GRAPHICS 1 .896 1413 MS9
GRAPHICS 1 .962 1413 DS9
LABEL ATIE
SET_ALL_START Y
Automatic start values will be set
SET_START_VALUE Y(LIQ,A)=.104,Y(FCC,A)=.038
CREATE_NEW_EQUILIBRIUM 0021,1
CHANGE_STATUS PHASE LIQ,FCC=FIX 1
SET_CONDITION T=1337,P=P0
EXPERIMENT W(LIQ,A)=.136:DX,W(FCC,A)=.047:DX
GRAPHICS 1 .864 1337 MS9
GRAPHICS 1 .953 1337 DS9
LABEL ATIE
SET_ALL_START Y
Automatic start values will be set
SET_START_VALUE Y(LIQ,A)=.136,Y(FCC,A)=.047
CREATE_NEW_EQUILIBRIUM 0022,1
CHANGE_STATUS PHASE LIQ,FCC=FIX 1
SET_CONDITION T=1213,P=P0
EXPERIMENT W(LIQ,A)=.187:DX,W(FCC,A)=.059:DX
GRAPHICS 1 .813 1213 MS9
GRAPHICS 1 .941 1213 DS9
LABEL ATIE
SET_ALL_START Y
Automatic start values will be set
SET_START_VALUE Y(LIQ,A)=.187,Y(FCC,A)=.059
CREATE_NEW_EQUILIBRIUM 0023,1
CHANGE_STATUS PHASE LIQ,BCC=FIX 1
SET_CONDITION T=1100,P=P0
EXPERIMENT W(LIQ,A)=.245:DX,W(BCC,A)=.085:DX
GRAPHICS 1 .755 1100 MS9
GRAPHICS 1 .915 1100 DS9
LABEL ATIE
SET_ALL_START Y
Automatic start values will be set
SET_START_VALUE Y(LIQ,A)=.245,Y(BCC,A)=.085

$ Thermochemical data
$ Activities of B in liquid (reference state fcc) at 1573 K.
$ The command SET_REFERENCE_STATE is used for this as the default
$ reference state for B is FCC.
$
$ Note that we have set an uncertainty on the fraction (condition) also.
TABLE_HEAD 100
CREATE_NEW_EQUILIBRIUM 0100,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET_CONDITION T=1573,P=P0,X(LIQ,B)=.90:DX
SET_REFERENCE_STATE B FCC,,,
16:24:49,455 [Thread-0] INFO Database: Preparing system for use: UNKNOWN_1682612687654
16:24:50,298 [Thread-0] INFO Phase: Preparing phase for use: FCC
EXPERIMENT ACR(B)=.94:DX
GRAPHICS 3 .90 .94 MS1
LABEL AA
CREATE_NEW_EQUILIBRIUM 0101,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET_CONDITION T=1573,P=P0,X(LIQ,B)=.80:DX
SET_REFERENCE_STATE B FCC,,,
EXPERIMENT ACR(B)=.84:DX
GRAPHICS 3 .80 .84 MS1
LABEL AA
CREATE_NEW_EQUILIBRIUM 0102,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET_CONDITION T=1573,P=P0,X(LIQ,B)=.70:DX
SET_REFERENCE_STATE B FCC,,,
EXPERIMENT ACR(B)=.74:DX
GRAPHICS 3 .70 .74 MS1
LABEL AA
CREATE_NEW_EQUILIBRIUM 0103,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET_CONDITION T=1573,P=P0,X(LIQ,B)=.60:DX
SET_REFERENCE_STATE B FCC,,,
EXPERIMENT ACR(B)=.64:DX
GRAPHICS 3 .60 .64 MS1
LABEL AA
CREATE_NEW_EQUILIBRIUM 0104,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET_CONDITION T=1573,P=P0,X(LIQ,B)=.50:DX
SET_REFERENCE_STATE B FCC,,,
EXPERIMENT ACR(B)=.54:DX
GRAPHICS 3 .50 .54 MS1
LABEL AA
CREATE_NEW_EQUILIBRIUM 0105,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET_CONDITION T=1573,P=P0,X(LIQ,B)=.40:DX
SET_REFERENCE_STATE B FCC,,,
EXPERIMENT ACR(B)=.44:DX
GRAPHICS 3 .40 .44 MS1
LABEL AA
CREATE_NEW_EQUILIBRIUM 0106,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET_CONDITION T=1573,P=P0,X(LIQ,B)=.30:DX
SET_REFERENCE_STATE B FCC,,,
EXPERIMENT ACR(B)=.34:DX
GRAPHICS 3 .30 .34 MS1
LABEL AA
CREATE_NEW_EQUILIBRIUM 0107,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET_CONDITION T=1573,P=P0,X(LIQ,B)=.20:DX
SET_REFERENCE_STATE B FCC,,,
EXPERIMENT ACR(B)=.23:DX
GRAPHICS 3 .20 .23 MS1
LABEL AA
CREATE_NEW_EQUILIBRIUM 0108,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET_CONDITION T=1573,P=P0,X(LIQ,B)=.10:DX
SET_REFERENCE_STATE B FCC,,,
EXPERIMENT ACR(B)=.12:DX
GRAPHICS 3 .10 .12 MS1
LABEL AA

$ Enthalpy of mixing at 1773 K (reference state: liquid)
TABLE_HEAD 110
CREATE_NEW_EQUILIBRIUM 0110,1

```

```

CHANGE_STATUS PHASE LIQ=FIX 1
SET_CONDITION T=1773,P=P0,X(LIQ,B)=.9
SET_REFERENCE_STATE A LIQ * 1E5
16:12:45:50,735 [Thread-0] INFO Phase: Preparing phase for use: LIQUID
SET_REFERENCE_STATE B LIQ * 1E5
EXPERIMENT HMR(LIQ)=-1964:DH
GRAPHICS 2 .9 -1964 MS2
LABEL AH
SET_ALL_START Y
Automatic start values will be set
CREATE_NEW_EQUILIBRIUM 0111,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET_CONDITION T=1773,P=P0,X(LIQ,B)=.8
SET_REFERENCE_STATE A LIQ * 1E5
SET_REFERENCE_STATE B LIQ * 1E5
EXPERIMENT HMR(LIQ)=-3500:DH
GRAPHICS 2 .8 -3500 MS2
LABEL AH
SET_ALL_START Y
Automatic start values will be set
CREATE_NEW_EQUILIBRIUM 0112,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET_CONDITION T=1773,P=P0,X(LIQ,B)=.7
SET_REFERENCE_STATE A LIQ * 1E5
SET_REFERENCE_STATE B LIQ * 1E5
EXPERIMENT HMR(LIQ)=-4588:DH
GRAPHICS 2 .7 -4588 MS2
LABEL AH
SET_ALL_START Y
Automatic start values will be set
CREATE_NEW_EQUILIBRIUM 0113,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET_CONDITION T=1773,P=P0,X(LIQ,B)=.6
SET_REFERENCE_STATE A LIQ * 1E5
SET_REFERENCE_STATE B LIQ * 1E5
EXPERIMENT HMR(LIQ)=-5239:DH
GRAPHICS 2 .6 -5239 MS2
LABEL AH
SET_ALL_START Y
Automatic start values will be set
CREATE_NEW_EQUILIBRIUM 0114,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET_CONDITION T=1773,P=P0,X(LIQ,B)=.5
SET_REFERENCE_STATE A LIQ * 1E5
SET_REFERENCE_STATE B LIQ * 1E5
EXPERIMENT HMR(LIQ)=-5454:DH
GRAPHICS 2 .5 -5454 MS2
LABEL AH
SET_ALL_START Y
Automatic start values will be set
CREATE_NEW_EQUILIBRIUM 0115,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET_CONDITION T=1773,P=P0,X(LIQ,B)=.4
SET_REFERENCE_STATE A LIQ * 1E5
SET_REFERENCE_STATE B LIQ * 1E5
EXPERIMENT HMR(LIQ)=-5233:DH
GRAPHICS 2 .4 -5233 MS2
LABEL AH
SET_ALL_START Y
Automatic start values will be set
CREATE_NEW_EQUILIBRIUM 0116,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET_CONDITION T=1773,P=P0,X(LIQ,B)=.3
SET_REFERENCE_STATE A LIQ * 1E5
SET_REFERENCE_STATE B LIQ * 1E5
EXPERIMENT HMR(LIQ)=-4575:DH
GRAPHICS 2 .3 -4575 MS2
LABEL AH
SET_ALL_START Y
Automatic start values will be set
CREATE_NEW_EQUILIBRIUM 0117,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET_CONDITION T=1773,P=P0,X(LIQ,B)=.2
SET_REFERENCE_STATE A LIQ * 1E5
SET_REFERENCE_STATE B LIQ * 1E5
EXPERIMENT HMR(LIQ)=-3481:DH
GRAPHICS 2 .2 -3481 MS2
LABEL AH
SET_ALL_START Y
Automatic start values will be set
CREATE_NEW_EQUILIBRIUM 0118,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET_CONDITION T=1773,P=P0,X(LIQ,B)=.1
SET_REFERENCE_STATE A LIQ * 1E5
SET_REFERENCE_STATE B LIQ * 1E5
EXPERIMENT HMR(LIQ)=-1950:DH
GRAPHICS 2 .1 -1950 MS2
LABEL AH
SET_ALL_START Y
Automatic start values will be set

$ Heat of melting for the compound. T=1341. H(liq)-H(A2B)=3727 J/mol.
$ This datum has already been used.
$
$ Do not forget the following line!
SAVE_WORKSPACES
PARROT:
PARROT: @@
PARROT: @@ Next file shows how to choose a rough start guess of the coefficients
PARROT: @@ and run the actual assessment. The values below are the final result.
PARROT: @@ S-O-V 1 20450,////
PARROT: @@ S-O-V 2 -30.386,////
PARROT: @@ S-O-V 3 0.131,////
PARROT: @@ S-O-V 11 -21817,////
PARROT: @@ S-O-V 12 15.34,////
PARROT: @@ S-O-V 15 24212,////
PARROT: @@ S-O-V 16 -8.328,////
PARROT: @@ S-O-V 17 3105,////
PARROT: @@ S-O-V 19 22030,////
PARROT: @@ S-O-V 20 -6.981,////
PARROT: @@ Save the start guess on the work file
PARROT: s-o-v 1 0
PARROT: s-o-v 2 0
PARROT: s-o-v 11 0

```

```

PARROT: s-o-v 12 0
PARROT: s-o-v 15 0
PARROT: s-o-v 16 0
PARROT: s-o-v 17 0
PARROT: s-o-v 19 0
PARROT: s-o-v 20 0
PARROT:
PARROT: save
PARROT: @@ Now execute tce36b.TCM to continue the assessment example
PARROT: Hit RETURN to continue
PARROT: mac tce36b.TCM
PARROT: s-s-f tce36
PARROT: @@ List parameters to be optimized, all zero initially
PARROT: l-a-v
OUTPUT TO SCREEN OR FILE /SCREEN/:

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO VOO

VAR.    VALUE      START VALUE      SCALING FACTOR      REL.STAND.DEV
V1      0.00000000E+00  0.00000000E+00  1.00000000E+03  0.00000000E+00
V2      0.00000000E+00  0.00000000E+00  1.00000000E+03  0.00000000E+00
V11     0.00000000E+00  0.00000000E+00  1.00000000E+03  0.00000000E+00
V12     0.00000000E+00  0.00000000E+00  1.00000000E+03  0.00000000E+00
V15     0.00000000E+00  0.00000000E+00  1.00000000E+03  0.00000000E+00
V16     0.00000000E+00  0.00000000E+00  1.00000000E+03  0.00000000E+00
V17     0.00000000E+00  0.00000000E+00  1.00000000E+03  0.00000000E+00
V19     0.00000000E+00  0.00000000E+00  1.00000000E+03  0.00000000E+00
V20     0.00000000E+00  0.00000000E+00  1.00000000E+03  0.00000000E+00

NUMBER OF OPTIMIZING VARIABLES : 9
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
PARROT: @@ Set alt mode to start
PARROT: s-alt Y
PARROT: @@ Check if all equilibria can be calculated
PARROT: ed
ED_EXP: read 1
ED_EXP: c-a
Eq Lab Iter Weight Temp Exp Fix phases or comments
16:24:51,251 [Thread-0] INFO Phase: Preparing phase for use: A2B
16:24:51,617 [Thread-0] INFO Phase: Preparing phase for use: BCC
 1 AINV *alt* 1.0 1193.0 LIQUID A2B BCC
 2 AINV *alt* 1.0 1341.0 LIQUID A2B
 3 AINV *alt* 1.0 1049.0 LIQUID A2B BCC
 4 AINV *alt* 1.0 1203.0 LIQUID BCC FCC
 5 AINV *alt* 1.0 726.0 A2B BCC BCC#2
 6 AINV *alt* 1.0 726.0 BCC BCC#2
Failed using alternate for FCC#1           setting weight to zero
 10 ALF *alt* 1.0 1594.0 LIQUID FCC
Failed using alternate for FCC#1           setting weight to zero
 11 ALF *alt* 1.0 1548.0 LIQUID FCC
Failed using alternate for FCC#1           setting weight to zero
 12 ALF *alt* 1.0 1499.0 LIQUID FCC
Failed using alternate for FCC#1           setting weight to zero
 13 ALF *alt* 1.0 1438.0 LIQUID FCC
 20 ATIE *alt* 1.0 1413.0 LIQUID FCC
 21 ATIE *alt* 1.0 1337.0 LIQUID FCC
 22 ATIE *alt* 1.0 1213.0 LIQUID FCC
 23 ATIE *alt* 1.0 1100.0 LIQUID BCC
100 AA   5 1. 1573.0 LIQUID
101 AA   4 1. 1573.0 LIQUID
102 AA   2 1. 1573.0 LIQUID
103 AA   3 1. 1573.0 LIQUID
104 AA   4 1. 1573.0 LIQUID
105 AA   6 1. 1573.0 LIQUID
106 AA   8 1. 1573.0 LIQUID
107 AA   9 1. 1573.0 LIQUID
108 AA  11 1. 1573.0 LIQUID
110 AH   8 1. 1773.0 LIQUID
111 AH   6 1. 1773.0 LIQUID
112 AH   5 1. 1773.0 LIQUID
113 AH   3 1. 1773.0 LIQUID
114 AH   2 1. 1773.0 LIQUID
115 AH   3 1. 1773.0 LIQUID
116 AH   5 1. 1773.0 LIQUID
117 AH   7 1. 1773.0 LIQUID
118 AH   8 1. 1773.0 LIQUID
Number of alternate equilibria          14
ED_EXP: @@ Equilibra with label ALF cannot use alt mode
ED_EXP: s-we 0 alf
Changed weight on                      4 equilibria.
ED_EXP: c-a
Eq Lab Iter Weight Temp Exp Fix phases or comments
 118 AH   2 1. 1773.0 LIQUID
ED_EXP: save
ED_EXP: @@ Save changes of weights before leaving the editor
ED_EXP: ba
PARROT: @@ Optimize zero times as a check
PARROT: opt 0
Alternate calculation is on
Use    47 experiments, maximum is      2000
Use    1082 real workspace, maximum is 50000
PARROT: l-r C SCREEN

=====
OUTPUT FROM P A R R O T . DATE 2023. 4.27 16:24:52

```

*** SUCCESSFUL OPTIMIZATION. ***
NUMBER OF ITERATIONS: 0

== OPTIMIZING CONDITIONS ==

```

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
  MAXFUN = 0 DMAX = 1.00000000E+02 H = 1.00000000E-04

```

```
ACC = (INITIAL SUM OF SQUARES) * 1.0000000E-03
```

```
-- OPTIMIZING VARIABLES ==
```

```
AVAILABLE VARIABLES ARE V1 TO VOO
```

| VAR. | VALUE | START VALUE | SCALING FACTOR | REL.STAND.DEV |
|------|----------------|----------------|----------------|----------------|
| V1 | 0.00000000E+00 | 0.00000000E+00 | 1.00000000E+03 | 0.00000000E+00 |
| V2 | 0.00000000E+00 | 0.00000000E+00 | 1.00000000E+03 | 0.00000000E+00 |
| V11 | 0.00000000E+00 | 0.00000000E+00 | 1.00000000E+03 | 0.00000000E+00 |
| V12 | 0.00000000E+00 | 0.00000000E+00 | 1.00000000E+03 | 0.00000000E+00 |
| V15 | 0.00000000E+00 | 0.00000000E+00 | 1.00000000E+03 | 0.00000000E+00 |
| V16 | 0.00000000E+00 | 0.00000000E+00 | 1.00000000E+03 | 0.00000000E+00 |
| V17 | 0.00000000E+00 | 0.00000000E+00 | 1.00000000E+03 | 0.00000000E+00 |
| V19 | 0.00000000E+00 | 0.00000000E+00 | 1.00000000E+03 | 0.00000000E+00 |
| V20 | 0.00000000E+00 | 0.00000000E+00 | 1.00000000E+03 | 0.00000000E+00 |

```
NUMBER OF OPTIMIZING VARIABLES : 9
```

```
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
```

```
THE SUM OF SQUARES HAS CHANGED FROM 0.00000000E+00 TO 1.22023362E+03
```

```
DEGREES OF FREEDOM 38. REDUCED SUM OF SQUARES 3.21114110E+01
```

```
Number of alternate equilibria 10
```

| SYMBOL | STATUS | VALUE/FUNCTION |
|------------|----------|-----------------------------------|
| FUNCTION R | 298.15 | 8.314510000000000 ; 6000 N REFO ! |
| 2 RTLNP | 20000000 | +R*T*LN(1E-05*P) |

```
LIQUID:L (A,B)1.0
```

| ===== [A] ===== | | |
|-----------------|---------------------|--------|
| G(LIQUID,A;0) | 298.15 +14000-10*T; | 6000 N |

| ===== [B] ===== | | |
|-----------------|---------------------|--------|
| G(LIQUID,B;0) | 298.15 +18000-12*T; | 6000 N |

| ===== [A, B] ===== | | |
|--------------------|--------------------|--------|
| G(LIQUID,A,B;0) | 298.15 +V11+V12*T; | 6000 N |
| G(LIQUID,A,B;1) | 298.15 +V13+V14*T; | 6000 N |

```
$ ===== BLOCK NUMBER 1
```

| DEFINED CONSTANTS | DX=2E-2, P0=101325, DH=500, DT=10 |
|----------------------------------|---|
| DEFINED FUNCTIONS AND VARIABLES% | HTR=HM(LIQUID)-HM(A2B) |
| 1 Alternate equilibrium calc | 1.81 |
| 2 Alternate equilibrium calc | 0.39 |
| 2 HTR=3727 | 1.5333E+04 5.00E+02 1.1606E+04 23.21 * |
| 3 Alternate equilibrium calc | 1.32 |
| 4 Alternate equilibrium calc | 1.56 |
| 5 Alternate equilibrium calc | 4.14 |
| 6 Alternate equilibrium calc | 3.83 |
| 20 Alternate equilibrium calc | 0.87 |
| 21 Alternate equilibrium calc | 0.97 |
| 22 Alternate equilibrium calc | 1.14 |
| 23 Alternate equilibrium calc | 1.20 |
| 100 ACR(B)=0.94 | 0.9382 2.89E-02 -1.8474E-03 -6.3948E-02 |
| 101 ACR(B)=0.84 | 0.8339 2.89E-02 -6.0866E-03 -0.2107 |
| 102 ACR(B)=0.74 | 0.7297 2.89E-02 -1.0326E-02 -0.3574 |
| 103 ACR(B)=0.64 | 0.6254 2.89E-02 -1.4565E-02 -0.5042 |
| 104 ACR(B)=0.54 | 0.5212 2.89E-02 -1.8804E-02 -0.6509 |
| 105 ACR(B)=0.44 | 0.4170 2.89E-02 -2.3043E-02 -0.7976 |
| 106 ACR(B)=0.34 | 0.3127 2.89E-02 -2.7282E-02 -0.9444 |
| 107 ACR(B)=0.23 | 0.2085 2.89E-02 -2.1522E-02 -0.7450 |
| 108 ACR(B)=0.12 | 0.1042 2.89E-02 -1.5761E-02 -0.5455 |
| 110 HMR(LIQUID)=-1964 | 0.000 5.00E+02 1964. 3.928 |
| 111 HMR(LIQUID)=-3500 | 3.6380E-12 5.00E+02 3500. 7.000 * |
| 112 HMR(LIQUID)=-4588 | 3.6380E-12 5.00E+02 4588. 9.176 * |
| 113 HMR(LIQUID)=-5239 | 0.000 5.00E+02 5239. 10.48 * |
| 114 HMR(LIQUID)=-5454 | 1.8190E-12 5.00E+02 5454. 10.91 * |
| 115 HMR(LIQUID)=-5233 | 5.4570E-12 5.00E+02 5233. 10.47 * |
| 116 HMR(LIQUID)=-4575 | 3.6380E-12 5.00E+02 4575. 9.150 * |
| 117 HMR(LIQUID)=-3481 | -3.6380E-12 5.00E+02 3481. 6.962 * |
| 118 HMR(LIQUID)=-1950 | 0.000 5.00E+02 1950. 3.900 |

```
PARROT:
```

```
PARROT:Hit RETURN to continue
```

```
PARROT: @@ Note only one error from alternate calculations.
```

```
PARROT: @@ This error represents the difference in chemical
```

```
PARROT: @@ potentials of the phases.
```

```
PARROT: @@ Experiments with just one phase is calculated as normal.
```

```
PARROT: @@ Next command supresses the listing of parameters.
```

```
PARROT: s-o-l 1 Y Y N n N
```

```
PARROT: l-r C SCREEN
```

```
=====
OUTPUT FROM P A R R O T . DATE 2023. 4.27 16:24:52
```

```
*** SUCCESSFUL OPTIMIZATION. ***
NUMBER OF ITERATIONS: 0
```

```
-- OPTIMIZING CONDITIONS ==
```

| RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N |
|---|
| MINIMUM SAVE ON FILE: Y |
| ERROR FOR INEQUALITIES = 1.00000000E+00 |
| RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04 |
| ARGUMENTS FOR SUBROUTINE VA05AD (HSL) |
| MAXFUN = 0 DMAX = 1.00000000E+02 H = 1.00000000E-04 |

```
ACC = (INITIAL SUM OF SQUARES) * 1.0000000E-03
```

```
-- OPTIMIZING VARIABLES ==
```

```
AVAILABLE VARIABLES ARE V1 TO VOO
```

| VAR. | VALUE | START VALUE | SCALING FACTOR | REL.STAND.DEV |
|------|----------------|----------------|----------------|----------------|
| V1 | 0.00000000E+00 | 0.00000000E+00 | 1.00000000E+03 | 0.00000000E+00 |
| V2 | 0.00000000E+00 | 0.00000000E+00 | 1.00000000E+03 | 0.00000000E+00 |
| V11 | 0.00000000E+00 | 0.00000000E+00 | 1.00000000E+03 | 0.00000000E+00 |
| V12 | 0.00000000E+00 | 0.00000000E+00 | 1.00000000E+03 | 0.00000000E+00 |
| V15 | 0.00000000E+00 | 0.00000000E+00 | 1.00000000E+03 | 0.00000000E+00 |
| V16 | 0.00000000E+00 | 0.00000000E+00 | 1.00000000E+03 | 0.00000000E+00 |
| V17 | 0.00000000E+00 | 0.00000000E+00 | 1.00000000E+03 | 0.00000000E+00 |
| V19 | 0.00000000E+00 | 0.00000000E+00 | 1.00000000E+03 | 0.00000000E+00 |
| V20 | 0.00000000E+00 | 0.00000000E+00 | 1.00000000E+03 | 0.00000000E+00 |

```
NUMBER OF OPTIMIZING VARIABLES : 9
```

```
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
```

```
THE SUM OF SQUARES HAS CHANGED FROM 0.00000000E+00 TO 1.22023362E+03
```

```
DEGREES OF FREEDOM 38. REDUCED SUM OF SQUARES 3.21114110E+01
```

```
Number of alternate equilibria 10
```

```
$ ====== BLOCK NUMBER 1
```

```
DEFINED CONSTANTS  
DX=2E-2, P0=101325, DH=500, DT=10
```

```
DEFINED FUNCTIONS AND VARIABLES%
```

| HTR=HM(LIQUID)-HM(A2B) | | | | |
|-------------------------------|-------------|----------|-------------|-------------|
| 1 Alternate equilibrium calc | | | 1.81 | |
| 2 Alternate equilibrium calc | | | 0.39 | |
| 2 HTR=3727 | 1.5333E+04 | 5.00E+02 | 1.1606E+04 | 23.21 * |
| 3 Alternate equilibrium calc | | | 1.32 | |
| 4 Alternate equilibrium calc | | | 1.56 | |
| 5 Alternate equilibrium calc | | | 4.14 | |
| 6 Alternate equilibrium calc | | | 3.83 | |
| 20 Alternate equilibrium calc | | | 0.87 | |
| 21 Alternate equilibrium calc | | | 0.97 | |
| 22 Alternate equilibrium calc | | | 1.14 | |
| 23 Alternate equilibrium calc | | | 1.20 | |
| 100 ACR(B)=0.94 | 0.9382 | 2.89E-02 | -1.8474E-03 | -6.3948E-02 |
| 101 ACR(B)=0.84 | 0.8339 | 2.89E-02 | -6.0866E-03 | -0.2107 |
| 102 ACR(B)=0.74 | 0.7297 | 2.89E-02 | -1.0326E-02 | -0.3574 |
| 103 ACR(B)=0.64 | 0.6254 | 2.89E-02 | -1.4565E-02 | -0.5042 |
| 104 ACR(B)=0.54 | 0.5212 | 2.89E-02 | -1.8804E-02 | -0.6509 |
| 105 ACR(B)=0.44 | 0.4170 | 2.89E-02 | -2.3043E-02 | -0.7976 |
| 106 ACR(B)=0.34 | 0.3127 | 2.89E-02 | -2.7282E-02 | -0.9444 |
| 107 ACR(B)=0.23 | 0.2085 | 2.89E-02 | -2.1522E-02 | -0.7450 |
| 108 ACR(B)=0.12 | 0.1042 | 2.89E-02 | -1.5761E-02 | -0.5455 |
| 110 HMR(LIQUID)=-1964 | 0.000 | 5.00E+02 | 1964. | 3.928 |
| 111 HMR(LIQUID)=-3500 | 3.6380E-12 | 5.00E+02 | 3500. | 7.000 * |
| 112 HMR(LIQUID)=-4588 | 3.6380E-12 | 5.00E+02 | 4588. | 9.176 * |
| 113 HMR(LIQUID)=-5239 | 0.000 | 5.00E+02 | 5239. | 10.48 * |
| 114 HMR(LIQUID)=-5454 | 1.8190E-12 | 5.00E+02 | 5454. | 10.91 * |
| 115 HMR(LIQUID)=-5233 | 5.4570E-12 | 5.00E+02 | 5233. | 10.47 * |
| 116 HMR(LIQUID)=-4575 | 3.6380E-12 | 5.00E+02 | 4575. | 9.150 * |
| 117 HMR(LIQUID)=-3481 | -3.6380E-12 | 5.00E+02 | 3481. | 6.962 * |
| 118 HMR(LIQUID)=-1950 | 0.000 | 5.00E+02 | 1950. | 3.900 |

```
PARROT:
```

```
PARROT: @@ Now optimize
```

```
PARROT: opt 30
```

```
Alternate calculation is on
```

```
Use 47 experiments, maximum is 2000
```

```
Use 1082 real workspace, maximum is 50000
```

```
The following output is provided by subroutine VA05A
```

| AT THE 0 TH ITERATION WE HAVE THE SUM OF SQUARES 1.22023362E+03 | | | | | | | | | |
|--|------------|---|-------------|---|-------------|---|------------|---|------------|
| 1 | 0.0000E+00 | 2 | 0.0000E+00 | 3 | 0.0000E+00 | 4 | 0.0000E+00 | 5 | 0.0000E+00 |
| 6 | 0.0000E+00 | 7 | 0.0000E+00 | 8 | 0.0000E+00 | 9 | 0.0000E+00 | | |
| AT THE 1 ST ITERATION WE HAVE THE SUM OF SQUARES 1.22023056E+03 | | | | | | | | | |
| 1 | 1.0000E-04 | 2 | 0.0000E+00 | 3 | 0.0000E+00 | 4 | 0.0000E+00 | 5 | 0.0000E+00 |
| 6 | 0.0000E+00 | 7 | 0.0000E+00 | 8 | 0.0000E+00 | 9 | 0.0000E+00 | | |
| AT THE 2 ND ITERATION WE HAVE THE SUM OF SQUARES 1.22026107E+03 | | | | | | | | | |
| 1 | 1.0000E-04 | 2 | 1.0000E-04 | 3 | 0.0000E+00 | 4 | 0.0000E+00 | 5 | 0.0000E+00 |
| 6 | 0.0000E+00 | 7 | 0.0000E+00 | 8 | 0.0000E+00 | 9 | 0.0000E+00 | | |
| AT THE 3 RD ITERATION WE HAVE THE SUM OF SQUARES 1.22023821E+03 | | | | | | | | | |
| 1 | 1.0000E-04 | 2 | 0.0000E+00 | 3 | 1.0000E-04 | 4 | 0.0000E+00 | 5 | 0.0000E+00 |
| 6 | 0.0000E+00 | 7 | 0.0000E+00 | 8 | 0.0000E+00 | 9 | 0.0000E+00 | | |
| AT THE 4 TH ITERATION WE HAVE THE SUM OF SQUARES 1.21985896E+03 | | | | | | | | | |
| 1 | 1.0000E-04 | 2 | 0.0000E+00 | 3 | 0.0000E+00 | 4 | 1.0000E-04 | 5 | 0.0000E+00 |
| 6 | 0.0000E+00 | 7 | 0.0000E+00 | 8 | 0.0000E+00 | 9 | 0.0000E+00 | | |
| AT THE 5 TH ITERATION WE HAVE THE SUM OF SQUARES 1.21985855E+03 | | | | | | | | | |
| 1 | 1.0000E-04 | 2 | 0.0000E+00 | 3 | 0.0000E+00 | 4 | 1.0000E-04 | 5 | 1.0000E-04 |
| 6 | 0.0000E+00 | 7 | 0.0000E+00 | 8 | 0.0000E+00 | 9 | 0.0000E+00 | | |
| AT THE 6 TH ITERATION WE HAVE THE SUM OF SQUARES 1.21952877E+03 | | | | | | | | | |
| 1 | 1.0000E-04 | 2 | 0.0000E+00 | 3 | 0.0000E+00 | 4 | 1.0000E-04 | 5 | 1.0000E-04 |
| 6 | 1.0000E-04 | 7 | 0.0000E+00 | 8 | 0.0000E+00 | 9 | 0.0000E+00 | | |
| AT THE 7 TH ITERATION WE HAVE THE SUM OF SQUARES 1.21952862E+03 | | | | | | | | | |
| 1 | 1.0000E-04 | 2 | 0.0000E+00 | 3 | 0.0000E+00 | 4 | 1.0000E-04 | 5 | 1.0000E-04 |
| 6 | 1.0000E-04 | 7 | 1.0000E-04 | 8 | 0.0000E+00 | 9 | 0.0000E+00 | | |
| AT THE 8 TH ITERATION WE HAVE THE SUM OF SQUARES 1.21952856E+03 | | | | | | | | | |
| 1 | 1.0000E-04 | 2 | 0.0000E+00 | 3 | 0.0000E+00 | 4 | 1.0000E-04 | 5 | 1.0000E-04 |
| 6 | 1.0000E-04 | 7 | 1.0000E-04 | 8 | 1.0000E-04 | 9 | 0.0000E+00 | | |
| AT THE 9 TH ITERATION WE HAVE THE SUM OF SQUARES 1.21945175E+03 | | | | | | | | | |
| 1 | 1.0000E-04 | 2 | 0.0000E+00 | 3 | 0.0000E+00 | 4 | 1.0000E-04 | 5 | 1.0000E-04 |
| 6 | 1.0000E-04 | 7 | 1.0000E-04 | 8 | 1.0000E-04 | 9 | 1.0000E-04 | | |
| AT THE 10 TH ITERATION WE HAVE THE SUM OF SQUARES 1.21347918E+03 | | | | | | | | | |
| 1 | 1.1575E-04 | 2 | -1.5562E-04 | 3 | -3.9485E-05 | 4 | 1.9219E-03 | 5 | 1.0209E-04 |

```

6 1.7933E-03 7 1.0073E-04 8 1.0031E-04 9 4.9349E-04

    AT THE 11 TH ITERATION WE HAVE THE SUM OF SQUARES 1.20857820E+03
1 5.7604E-04 2 -2.8000E-04 3 -5.5554E-04 4 2.9761E-04 5 1.0310E-03
6 3.2119E-03 7 1.5940E-04 8 5.6558E-04 9 8.6813E-04

    AT THE 12 TH ITERATION WE HAVE THE SUM OF SQUARES 1.20419111E+03
1 1.7516E-03 2 -4.0933E-04 3 -1.8427E-03 4 1.7341E-03 5 1.9072E-03
6 4.5182E-03 7 3.6464E-04 8 -3.6442E-03 9 1.2034E-03

    AT THE 13 TH ITERATION WE HAVE THE SUM OF SQUARES 1.20018978E+03
1 4.9648E-03 2 -5.3990E-04 3 -5.3422E-03 4 4.2170E-04 5 1.3347E-03
6 5.8647E-03 7 1.0916E-03 8 -1.0101E-02 9 1.5910E-03

    AT THE 14 TH ITERATION WE HAVE THE SUM OF SQUARES 1.19656103E+03
1 8.7053E-03 2 -6.5937E-04 3 -9.4047E-03 4 1.6713E-03 5 2.0974E-03
6 6.9625E-03 7 1.8270E-03 8 -2.5618E-02 9 1.9085E-03

    AT THE 15 TH ITERATION WE HAVE THE SUM OF SQUARES 1.19290094E+03
1 1.6702E-02 2 -7.8966E-04 3 -1.8062E-02 4 5.3932E-04 5 2.8046E-03
6 8.1461E-03 7 3.5323E-03 8 -5.6536E-02 9 2.2985E-03

    AT THE 16 TH ITERATION WE HAVE THE SUM OF SQUARES 1.18895830E+03
1 2.9858E-02 2 -9.1157E-04 3 -3.2288E-02 4 1.6316E-03 5 6.0823E-03
6 9.0741E-03 7 6.1592E-03 8 -1.1985E-01 9 2.6324E-03

    AT THE 17 TH ITERATION WE HAVE THE SUM OF SQUARES 1.18371837E+03
1 5.7117E-02 2 -1.0621E-03 3 -6.1738E-02 4 6.6639E-04 5 1.1595E-02
6 1.0112E-02 7 1.1749E-02 8 -2.4612E-01 9 3.0842E-03

    AT THE 18 TH ITERATION WE HAVE THE SUM OF SQUARES 1.17576312E+03
1 1.0981E-01 2 -1.2302E-03 3 -1.1865E-01 4 1.6444E-03 5 2.3333E-02
6 1.0904E-02 7 2.2419E-02 8 -4.9950E-01 9 3.5580E-03

    AT THE 19 TH ITERATION WE HAVE THE SUM OF SQUARES 1.17580513E+03
1 1.0990E-01 2 -1.2331E-03 3 -1.1866E-01 4 1.6767E-03 5 2.3329E-02
6 1.0908E-02 7 2.2420E-02 8 -4.9948E-01 9 3.5631E-03

    AT THE 20 TH ITERATION WE HAVE THE SUM OF SQUARES 1.17576903E+03
1 1.0981E-01 2 -1.1307E-03 3 -1.1865E-01 4 1.6454E-03 5 2.3333E-02
6 1.0913E-02 7 2.2419E-02 8 -4.9950E-01 9 3.5581E-03

    AT THE 21 TH ITERATION WE HAVE THE SUM OF SQUARES 1.17573283E+03
1 1.0983E-01 2 -1.2301E-03 3 -1.1856E-01 4 1.6164E-03 5 2.3336E-02
6 1.0901E-02 7 2.2419E-02 8 -4.9952E-01 9 3.5536E-03

    AT THE 22 TH ITERATION WE HAVE THE SUM OF SQUARES 1.15839218E+03
1 2.4518E-01 2 -1.5171E-03 3 -2.6482E-01 4 8.9861E-04 5 8.1369E-02
6 1.1834E-02 7 4.7658E-02 8 -9.8754E-01 9 4.3315E-03

    AT THE 23 TH ITERATION WE HAVE THE SUM OF SQUARES 1.15852299E+03
1 2.4519E-01 2 -1.5109E-03 3 -2.6483E-01 4 8.8627E-04 5 8.1438E-02
6 1.1766E-02 7 4.7658E-02 8 -9.8753E-01 9 4.3220E-03

    AT THE 24 TH ITERATION WE HAVE THE SUM OF SQUARES 1.12429813E+03
1 5.3084E-01 2 -1.9804E-03 3 -5.7319E-01 4 1.9224E-03 5 3.5638E-01
6 1.2271E-02 7 9.3910E-02 8 -1.9219E+00 9 5.3987E-03

    AT THE 25 TH ITERATION WE HAVE THE SUM OF SQUARES 1.12430373E+03
1 5.3084E-01 2 -1.9806E-03 3 -5.7319E-01 4 1.9278E-03 5 3.5639E-01
6 1.2272E-02 7 9.4010E-02 8 -1.9219E+00 9 5.3997E-03

    AT THE 26 TH ITERATION WE HAVE THE SUM OF SQUARES 1.05801741E+03
1 1.1108E+00 2 -2.8497E-03 3 -1.1990E+00 4 1.6568E-03 5 1.0413E+00
6 1.2349E-02 7 1.7987E-01 8 -3.7400E+00 9 7.2585E-03

    AT THE 27 TH ITERATION WE HAVE THE SUM OF SQUARES 1.05799591E+03
1 1.1108E+00 2 -2.8479E-03 3 -1.1990E+00 4 1.6562E-03 5 1.0413E+00
6 1.2329E-02 7 1.7987E-01 8 -3.7401E+00 9 7.3562E-03

    AT THE 28 TH ITERATION WE HAVE THE SUM OF SQUARES 9.32316154E+02
1 2.2754E+00 2 -4.5180E-03 3 -2.4557E+00 4 3.1330E-03 5 2.5155E+00
6 1.1608E-02 7 3.4709E-01 8 -7.3322E+00 9 1.0723E-02

    AT THE 29 TH ITERATION WE HAVE THE SUM OF SQUARES 9.32175313E+02
1 2.2754E+00 2 -4.5239E-03 3 -2.4557E+00 4 3.0908E-03 5 2.5156E+00
6 1.1674E-02 7 3.4709E-01 8 -7.3322E+00 9 1.0740E-02

    AT THE 30 TH ITERATION WE HAVE THE SUM OF SQUARES 9.32266255E+02
1 2.2754E+00 2 -4.5260E-03 3 -2.4557E+00 4 3.1696E-03 5 2.5156E+00
6 1.1696E-02 7 3.4708E-01 8 -7.3322E+00 9 1.0745E-02

*** ERROR RETURN FROM VA05A BECAUSE THERE HAVE BEEN 30 CALLS OF CALFUN

THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED 30 iterations
1 2.2754E+00 2 -4.5239E-03 3 -2.4557E+00 4 3.0908E-03 5 2.5156E+00
6 1.1674E-02 7 3.4709E-01 8 -7.3322E+00 9 1.0740E-02

1 2.7586E-01 2 2.7586E-01 3 -2.3479E-02 4 -2.9092E-01 5 -1.4825E-01
6 -2.4894E-01 7 2.0604E+01 8 1.1427E-01 9 1.1427E-01 10 -2.1551E-01
11 -1.4793E-01 12 6.1401E-02 13 -4.3625E-02 14 -7.7890E-01 15 -8.0449E-02
16 4.8856E-01 17 4.8856E-01 18 -7.3181E-01 19 1.4636E+00 20 -7.3181E-01
21 1.4636E+00 22 -4.1620E-01 23 -1.1022E-02 24 -5.4162E-01 25 -2.8760E-02
26 -7.6572E-01 27 -7.3156E-02 28 -1.2544E-01 29 -0.0373E-01 30 -4.2178E-03
31 2.5901E-03 32 6.6371E-02 33 1.4719E-01 34 2.0341E-01 35 1.9322E-01
36 7.6393E-02 37 1.5206E-01 38 3.2167E-02 39 3.4860E+00 40 6.2142E+00
41 8.1446E+00 42 9.2993E+00 43 9.6801E+00 44 9.2873E+00 45 8.1186E+00
46 6.1762E+00 47 3.4580E+00

    THE SUM OF SQUARES IS 9.32175313E+02
PARROT: cont 30
Alternate calculation is on
Use 47 experiments, maximum is 2000
Use 1082 real workspace, maximum is 50000
The following output is provided by subroutine VA05A
Optimization continuing with same Jacobian

    AT THE 0 TH ITERATION WE HAVE THE SUM OF SQUARES 6.42380150E+02
1 5.3285E+00 2 -8.7738E-03 3 -5.7408E+00 4 4.7675E-03 5 5.1386E+00
6 9.8927E-03 7 8.7845E-01 8 -1.4032E+01 9 1.6957E-02

    AT THE 1 ST ITERATION WE HAVE THE SUM OF SQUARES 3.93290146E+02
1 8.5797E+00 2 -1.3317E-02 3 -9.2391E+00 4 7.4937E-03 5 8.0040E+00
6 7.9956E-03 7 1.4404E+00 8 -2.1386E+01 9 2.3783E-02

```

```

AT THE 2 ND ITERATION WE HAVE THE SUM OF SQUARES 2.09584482E+02
1 1.1739E+01 2 -1.7636E-02 3 -1.2638E+01 4 9.3817E-03 5 1.0889E+01
6 5.4398E-03 7 1.9808E+00 8 -2.8820E+01 9 3.0390E-02

AT THE 3 RD ITERATION WE HAVE THE SUM OF SQUARES 1.80933267E+01
1 1.7814E+01 2 -2.5899E-02 3 -1.9174E+01 4 1.3734E-02 5 1.6703E+01
6 -6.1012E-06 7 3.0058E+00 8 -4.3892E+01 9 4.3587E-02

AT THE 4 TH ITERATION WE HAVE THE SUM OF SQUARES 9.80055457E-01
1 2.0269E+01 2 -2.9190E-02 3 -2.1813E+01 4 1.5556E-02 5 1.9856E+01
6 -3.2629E-03 7 3.3757E+00 8 -5.2038E+01 9 5.0440E-02

THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED 4 iterations
1 2.0269E+01 2 -2.9190E-02 3 -2.1813E+01 4 1.5556E-02 5 1.9856E+01
6 -3.2629E-03 7 3.3757E+00 8 -5.2038E+01 9 5.0440E-02

```

THE SUM OF SQUARES IS 9.80055457E-01

PARROT: l-r C SCREEN

```
=====
OUTPUT FROM P A R R O T . DATE 2023. 4.27 16:24:52
```

*** OPTIMIZATION ERROR. TOO MANY ITERATIONS ***
NUMBER OF ITERATIONS: 5

== OPTIMIZING CONDITIONS ==

```

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 30 DMAX = 1.00000000E+02 H = 1.00000000E-04
ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03

```

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

| VAR. | VALUE | START VALUE | SCALING FACTOR | REL.STAND.DEV |
|------|-----------------|----------------|----------------|----------------|
| V1 | 2.02691575E+04 | 0.00000000E+00 | 1.00000000E+03 | 1.60588758E+00 |
| V2 | -2.91902487E+01 | 0.00000000E+00 | 1.00000000E+03 | 1.00991504E-02 |
| V11 | -2.18127452E+04 | 0.00000000E+00 | 1.00000000E+03 | 8.65821610E-01 |
| V12 | 1.55559594E+01 | 0.00000000E+00 | 1.00000000E+03 | 2.63408119E-03 |
| V15 | 1.98563337E+04 | 0.00000000E+00 | 1.00000000E+03 | 1.43532259E+01 |
| V16 | -3.26288514E+00 | 0.00000000E+00 | 1.00000000E+03 | 1.71198600E-02 |
| V17 | 3.37569402E+03 | 0.00000000E+00 | 1.00000000E+03 | 4.53503069E+00 |
| V19 | -5.20384129E+04 | 0.00000000E+00 | 1.00000000E+03 | 3.15140236E+01 |
| V20 | 5.04396032E+01 | 0.00000000E+00 | 1.00000000E+03 | 2.47934071E-02 |

NUMBER OF OPTIMIZING VARIABLES : 9

ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO

THE SUM OF SQUARES HAS CHANGED FROM 1.22023362E+03 TO 9.80055457E-01

DEGREES OF FREEDOM 38. REDUCED SUM OF SQUARES 2.57909331E-02

Number of alternate equilibria 10

\$ ===== BLOCK NUMBER 1

```

DEFINED CONSTANTS
DX=2E-2, P0=101325, DH=500, DT=10
DEFINED FUNCTIONS AND VARIABLES%
  HTR=HM(LIQUID)-HM(A2B)
  1 Alternate equilibrium calc
  2 Alternate equilibrium calc
2 HTR=3727          3730.      5.00E+02   2.671      5.3418E-03
  3 Alternate equilibrium calc
  4 Alternate equilibrium calc
  5 Alternate equilibrium calc
  6 Alternate equilibrium calc
20 Alternate equilibrium calc
21 Alternate equilibrium calc
22 Alternate equilibrium calc
23 Alternate equilibrium calc
100 ACR(B)=0.94    0.9401     2.84E-02   6.0225E-05  2.1226E-03
101 ACR(B)=0.84    0.8407     2.80E-02   7.1693E-04  2.5569E-02
102 ACR(B)=0.74    0.7431     2.79E-02   3.1370E-03  0.1125
103 ACR(B)=0.64    0.6461     2.79E-02   6.0968E-03  0.2186
104 ACR(B)=0.54    0.5483     2.81E-02   8.3480E-03  0.2973
105 ACR(B)=0.44    0.4486     2.85E-02   8.5910E-03  0.3019
106 ACR(B)=0.34    0.3454     2.90E-02   5.4463E-03  0.1875
107 ACR(B)=0.23    0.2374     2.99E-02   7.4229E-03  0.2484
108 ACR(B)=0.12    0.1229     3.10E-02   2.8825E-03  9.3002E-02
110 HMR(LIQUID)=-1964 -1963.    5.00E+02   0.8529    1.7059E-03
111 HMR(LIQUID)=-3500 -3490.    5.00E+02   9.961     1.9922E-02
112 HMR(LIQUID)=-4588 -4581.    5.00E+02   7.324     1.4647E-02
113 HMR(LIQUID)=-5239 -5235.    5.00E+02   3.941     7.8823E-03
114 HMR(LIQUID)=-5454 -5453.    5.00E+02   0.8137   1.6274E-03
115 HMR(LIQUID)=-5233 -5235.    5.00E+02   -2.059   -4.1177E-03
116 HMR(LIQUID)=-4575 -4581.    5.00E+02   -5.676   -1.1353E-02
117 HMR(LIQUID)=-3481 -3490.    5.00E+02   -9.039   -1.8078E-02
118 HMR(LIQUID)=-1950 -1963.    5.00E+02   -13.15   -2.6294E-02

```

PARROT:

PARROT:Hit RETURN to continue

```

PARROT: @@ The liquid data fits reasonably. Simplify its parameters.
PARROT: l-p-d liq
Property type /ALL/: s-f-v 11-14
S-F-V is not a valid property type
11-14 is not a valid property type
Property type: @@ Rescale the start values of the parameters to current values
@@ is not a valid property type
RESCALE is not a valid property type
THE is not a valid property type
START is not a valid property type
VALUES is not a valid property type
OF is not a valid property type
THE is not a valid property type
PARAMETERS is not a valid property type
TO is not a valid property type
CURRENT is not a valid property type
VALUES is not a valid property type
Property type: resc
RESC is not a valid property type
Property type: l-a-v
L-A-V is not a valid property type
Property type:
LIQUID:L (A,B)1.0

===== [A] =====
G(LIQUID,A;0) 298.15 +14000-10*T; 6000 N

===== [B] =====
G(LIQUID,B;0) 298.15 +18000-12*T; 6000 N

===== [A, B] =====
G(LIQUID,A,B;0) 298.15 +V11+V12*T; 6000 N
G(LIQUID,A,B;1) 298.15 +V13+V14*T; 6000 N
PARROT: Hit RETURN to continue
PARROT: mac tcex36cpd
PARROT: set-echo
NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
POLY:
POLY: @@ In PARROT, the global minimization is turned off automatically.
POLY: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY: @@ message will be given.
POLY:
POLY: advanced-option global yes,
Settings for global minimization:
*** WARNING *** Global equilibrium calculation may create new composition sets
and this may corrupt your PARROT work file (.PAR file).
Do not go back to PARROT but exit from POLY after your POLY calculations.
POLY:
POLY: def-com,,,
POLY: s-a-v 1 w(b) 0 1,,,
The condition W(B)=.1234 created
POLY: s-a-v 2 t 300 1700,,,
The condition T=942.2 created
POLY: s-c t=500
POLY: l-c
W(B)=0.1234, T=500
DEGREES OF FREEDOM 2
POLY: c-e
Creating condition P=1E5
Creating condition N=1
Using global minimization procedure
Calculated 628 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY: save tcex36 y
POLY: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12
Organizing start points
Using ADDED start equilibria
Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21

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Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Generating start point 27
Generating start point 28

Phase region boundary 1 at: 8.907E-02 3.100E+02
    BCC#1
    ** FCC
Calculated..          2 equilibria
Terminating at axis limit.

Phase region boundary 2 at: 8.956E-02 3.000E+02
    BCC#1
    ** FCC
Calculated.           29 equilibria

Phase region boundary 3 at: 1.213E-01 1.253E+03
    ** LIQUID
    BCC#1
    ** FCC
Calculated.           21 equilibria

Phase region boundary 4 at: 2.038E-01 1.253E+03
    ** LIQUID
    BCC#1
    FCC
Calculated.           6 equilibria

Phase region boundary 5 at: 2.413E-01 1.253E+03
    ** LIQUID
    FCC
Calculated.           6 equilibria

Phase region boundary 6 at: 3.546E-01 1.219E+03
    ** LIQUID
    ** A2B
    FCC
Calculated.           24 equilibria

Phase region boundary 7 at: 4.342E-01 1.219E+03
    ** A2B
    FCC
Calculated.           24 equilibria

Phase region boundary 8 at: 6.572E-01 1.191E+03
    ** LIQUID
    ** A2B
    FCC
Calculated.           44 equilibria

Phase region boundary 9 at: 7.154E-01 1.191E+03
    ** LIQUID
    FCC
Calculated.           44 equilibria

Phase region boundary 10 at: 6.257E-01 1.191E+03
    ** LIQUID
    A2B
Calculated.           23 equilibria
Terminating at known equilibrium

Phase region boundary 11 at: 8.907E-02 3.100E+02
    BCC#1
    ** FCC
Calculated.           28 equilibria
Terminating at known equilibrium

Phase region boundary 12 at: 8.907E-02 3.100E+02
    BCC#1
    ** FCC
Calculated..          2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 13 at: 8.907E-02 3.100E+02
    BCC#1
    ** FCC
Calculated.           28 equilibria
Terminating at known equilibrium

Phase region boundary 14 at: 4.559E-01 1.196E+03
    ** A2B
    FCC
Calculated.           3 equilibria
Terminating at known equilibrium

Phase region boundary 15 at: 4.559E-01 1.196E+03
    ** A2B
    FCC
Calculated.           21 equilibria
Terminating at known equilibrium

Phase region boundary 16 at: 6.122E-01 1.168E+03
    ** A2B
    FCC
Calculated.           16 equilibria
Terminating at known equilibrium

Phase region boundary 17 at: 6.122E-01 1.168E+03
    ** A2B
    FCC
Calculated.           9 equilibria
Terminating at known equilibrium

Phase region boundary 18 at: 9.533E-01 3.100E+02
    BCC#1
    ** FCC
Calculated..          2 equilibria
Terminating at axis limit.

Phase region boundary 19 at: 9.530E-01 3.000E+02
    BCC#1
    ** FCC
Calculated.           31 equilibria

Phase region boundary 20 at: 9.533E-01 3.100E+02
    BCC#1

```

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** FCC
Calculated          29 equilibria
Phase region boundary 21 at:  9.533E-01  3.100E+02
    BCC#1
    ** FCC
Calculated..        2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 22 at:  9.533E-01  3.100E+02
    BCC#1
    ** FCC
Calculated          29 equilibria
Phase region boundary 23 at:  6.769E-02  7.700E+02
    BCC#1
    ** FCC
Calculated..        15 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 24 at:  6.769E-02  7.700E+02
    BCC#1
    ** FCC
Calculated..        15 equilibria
Terminating at known equilibrium
Phase region boundary 25 at:  9.745E-01  7.700E+02
    BCC#1
    ** FCC
Calculated..        15 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 26 at:  9.745E-01  7.700E+02
    BCC#1
    ** FCC
Calculated          18 equilibria
Phase region boundary 27 at:  1.086E-01  1.230E+03
    BCC#1
    ** FCC
Calculated..        28 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 28 at:  1.086E-01  1.230E+03
    BCC#1
    ** FCC
Calculated..        2 equilibria
Terminating at known equilibrium

Phase region boundary 29 at:  8.359E-01  1.230E+03
    ** LIQUID
    FCC
Calculated..        13 equilibria
Terminating at known equilibrium

Phase region boundary 30 at:  8.359E-01  1.230E+03
    ** LIQUID
    FCC
Calculated          37 equilibria
Phase region boundary 31 at:  6.124E-03  1.396E+03
    LIQUID
    ** BCC#1
Calculated..        11 equilibria
Phase region boundary 32 at:  6.124E-03  1.396E+03
    LIQUID
    ** BCC#1
Calculated..        9 equilibria
Terminating at known equilibrium

Phase region boundary 33 at:  2.658E-01  1.244E+03
    LIQUID
    ** FCC
Calculated..        2 equilibria
Terminating at known equilibrium

Phase region boundary 34 at:  2.658E-01  1.244E+03
    LIQUID
    ** FCC
Calculated..        5 equilibria
Terminating at known equilibrium

Phase region boundary 35 at:  6.122E-01  1.246E+03
    LIQUID
    ** A2B
Calculated..        13 equilibria
Terminating at known equilibrium

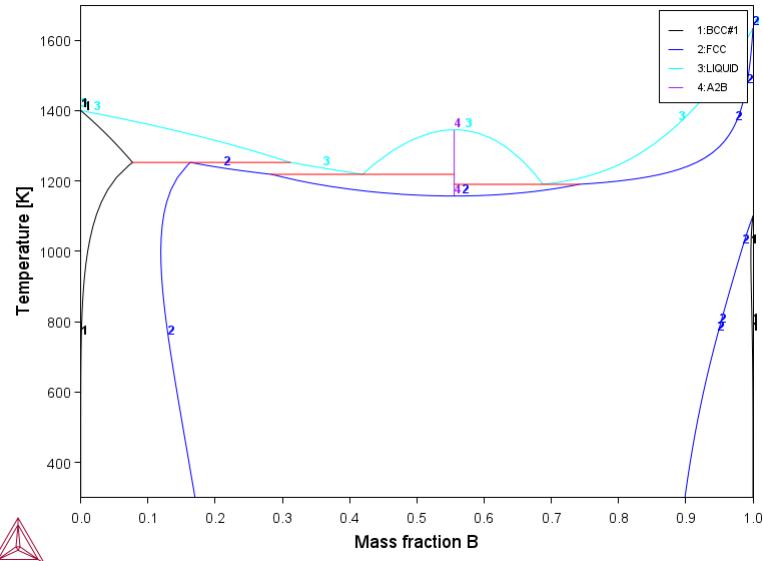
Phase region boundary 36 at:  6.122E-01  1.246E+03
    LIQUID
    ** A2B
Calculated..        4 equilibria
Terminating at known equilibrium

Phase region boundary 37 at:  9.944E-01  1.601E+03
    LIQUID
    ** FCC
Calculated..        33 equilibria
Terminating at known equilibrium

Phase region boundary 38 at:  9.944E-01  1.601E+03
    LIQUID
    ** FCC
Calculated..        12 equilibria
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\generate_console_examples\examples\tcex36a\tcex36.POLY3
CPU time for mapping      2 seconds
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2
Setting automatic diagram axes

```

POST: s-l d
POST: plot



POST:
POST: set-inter
POST: Hit RETURN to continue
POST: ba
POLY: ba

PARROT VERSION 5.3

Global minimization used as test only
PARROT: @@ This does not look very good, optimize more ...
PARROT: opt 30
Alternate calculation is on
Use 47 experiments, maximum is 2000
Use 1082 real workspace, maximum is 50000
The following output is provided by subroutine VA05A

AT THE 0 TH ITERATION WE HAVE THE SUM OF SQUARES 9.80055457E-01
1 2.0269E+01 2 -2.9190E-02 3 -2.1813E+01 4 1.5556E-02 5 1.9856E+01
6 -3.2629E-03 7 3.3757E+00 8 -5.2038E+01 9 5.0440E-02

AT THE 1 ST ITERATION WE HAVE THE SUM OF SQUARES 9.80055005E-01
1 2.0269E+01 2 -2.9190E-02 3 -2.1813E+01 4 1.5556E-02 5 1.9856E+01
6 -3.2629E-03 7 3.3757E+00 8 -5.2038E+01 9 5.0440E-02

AT THE 2 ND ITERATION WE HAVE THE SUM OF SQUARES 9.80160261E-01
1 2.0269E+01 2 -2.9090E-02 3 -2.1813E+01 4 1.5556E-02 5 1.9856E+01
6 -3.2629E-03 7 3.3757E+00 8 -5.2038E+01 9 5.0440E-02

AT THE 3 RD ITERATION WE HAVE THE SUM OF SQUARES 9.80157333E-01
1 2.0269E+01 2 -2.9190E-02 3 -2.1813E+01 4 1.5556E-02 5 1.9856E+01
6 -3.2629E-03 7 3.3757E+00 8 -5.2038E+01 9 5.0440E-02

AT THE 4 TH ITERATION WE HAVE THE SUM OF SQUARES 1.16296743E+00
1 2.0269E+01 2 -2.9190E-02 3 -2.1813E+01 4 1.5656E-02 5 1.9856E+01
6 -3.2629E-03 7 3.3757E+00 8 -5.2038E+01 9 5.0440E-02

AT THE 5 TH ITERATION WE HAVE THE SUM OF SQUARES 9.80051270E-01
1 2.0269E+01 2 -2.9190E-02 3 -2.1813E+01 4 1.5556E-02 5 1.9856E+01
6 -3.2629E-03 7 3.3757E+00 8 -5.2038E+01 9 5.0440E-02

AT THE 6 TH ITERATION WE HAVE THE SUM OF SQUARES 9.80813197E-01
1 2.0269E+01 2 -2.9190E-02 3 -2.1813E+01 4 1.5556E-02 5 1.9856E+01
6 -3.1629E-03 7 3.3757E+00 8 -5.2038E+01 9 5.0440E-02

AT THE 7 TH ITERATION WE HAVE THE SUM OF SQUARES 9.80051333E-01
1 2.0269E+01 2 -2.9190E-02 3 -2.1813E+01 4 1.5556E-02 5 1.9856E+01
6 -3.2629E-03 7 3.3758E+00 8 -5.2038E+01 9 5.0440E-02

AT THE 8 TH ITERATION WE HAVE THE SUM OF SQUARES 9.80049855E-01
1 2.0269E+01 2 -2.9190E-02 3 -2.1813E+01 4 1.5556E-02 5 1.9856E+01
6 -3.2629E-03 7 3.3757E+00 8 -5.2038E+01 9 5.0440E-02

AT THE 9 TH ITERATION WE HAVE THE SUM OF SQUARES 9.80401721E-01
1 2.0269E+01 2 -2.9190E-02 3 -2.1813E+01 4 1.5556E-02 5 1.9856E+01
6 -3.2629E-03 7 3.3757E+00 8 -5.2038E+01 9 5.0540E-02

AT THE 10 TH ITERATION WE HAVE THE SUM OF SQUARES 6.82789004E-01
1 2.0269E+01 2 -2.9190E-02 3 -2.1813E+01 4 1.5186E-02 5 1.9856E+01
6 -3.2629E-03 7 3.3757E+00 8 -5.2038E+01 9 5.0440E-02

AT THE 11 TH ITERATION WE HAVE THE SUM OF SQUARES 6.82577932E-01
1 2.0269E+01 2 -2.9192E-02 3 -2.1813E+01 4 1.5176E-02 5 1.9856E+01
6 -3.2705E-03 7 3.3757E+00 8 -5.2038E+01 9 5.0430E-02

AT THE 12 TH ITERATION WE HAVE THE SUM OF SQUARES 6.82336722E-01
1 2.0269E+01 2 -2.9194E-02 3 -2.1813E+01 4 1.5185E-02 5 1.9857E+01
6 -3.2761E-03 7 3.3757E+00 8 -5.2038E+01 9 5.0424E-02

AT THE 13 TH ITERATION WE HAVE THE SUM OF SQUARES 6.82128219E-01
1 2.0269E+01 2 -2.9196E-02 3 -2.1813E+01 4 1.5176E-02 5 1.9858E+01
6 -3.2836E-03 7 3.3756E+00 8 -5.2038E+01 9 5.0415E-02

AT THE 14 TH ITERATION WE HAVE THE SUM OF SQUARES 6.81884071E-01
1 2.0269E+01 2 -2.9198E-02 3 -2.1813E+01 4 1.5185E-02 5 1.9860E+01
6 -3.2898E-03 7 3.3755E+00 8 -5.2038E+01 9 5.0410E-02

AT THE 15 TH ITERATION WE HAVE THE SUM OF SQUARES 6.81663607E-01
1 2.0269E+01 2 -2.9200E-02 3 -2.1813E+01 4 1.5177E-02 5 1.9862E+01
6 -3.2978E-03 7 3.3754E+00 8 -5.2039E+01 9 5.0402E-02

AT THE 16 TH ITERATION WE HAVE THE SUM OF SQUARES 6.81381607E-01
 1 2.0269E+01 2 -2.9201E-02 3 -2.1813E+01 4 1.5184E-02 5 1.9866E+01
 6 -3.3059E-03 7 3.3752E+00 8 -5.2040E+01 9 5.0397E-02

AT THE 17 TH ITERATION WE HAVE THE SUM OF SQUARES 6.81129365E-01
 1 2.0269E+01 2 -2.9203E-02 3 -2.1813E+01 4 1.5177E-02 5 1.9870E+01
 6 -3.3149E-03 7 3.3750E+00 8 -5.2042E+01 9 5.0392E-02

AT THE 18 TH ITERATION WE HAVE THE SUM OF SQUARES 6.80795641E-01
 1 2.0269E+01 2 -2.9205E-02 3 -2.1813E+01 4 1.5184E-02 5 1.9876E+01
 6 -3.3262E-03 7 3.3746E+00 8 -5.2047E+01 9 5.0390E-02

AT THE 19 TH ITERATION WE HAVE THE SUM OF SQUARES 6.80795562E-01
 1 2.0269E+01 2 -2.9205E-02 3 -2.1813E+01 4 1.5184E-02 5 1.9876E+01
 6 -3.3262E-03 7 3.3746E+00 8 -5.2047E+01 9 5.0390E-02

AT THE 20 TH ITERATION WE HAVE THE SUM OF SQUARES 6.81280583E-01
 1 2.0269E+01 2 -2.9105E-02 3 -2.1813E+01 4 1.5184E-02 5 1.9876E+01
 6 -3.3262E-03 7 3.3746E+00 8 -5.2047E+01 9 5.0390E-02

AT THE 21 TH ITERATION WE HAVE THE SUM OF SQUARES 6.80795396E-01
 1 2.0269E+01 2 -2.9205E-02 3 -2.1813E+01 4 1.5184E-02 5 1.9876E+01
 6 -3.3262E-03 7 3.3746E+00 8 -5.2047E+01 9 5.0390E-02

AT THE 22 TH ITERATION WE HAVE THE SUM OF SQUARES 6.80507941E-01
 1 2.0269E+01 2 -2.9207E-02 3 -2.1813E+01 4 1.5178E-02 5 1.9883E+01
 6 -3.3371E-03 7 3.3742E+00 8 -5.2053E+01 9 5.0388E-02

AT THE 23 TH ITERATION WE HAVE THE SUM OF SQUARES 6.80149053E-01
 1 2.0269E+01 2 -2.9209E-02 3 -2.1813E+01 4 1.5184E-02 5 1.9893E+01
 6 -3.3520E-03 7 3.3737E+00 8 -5.2063E+01 9 5.0390E-02

AT THE 24 TH ITERATION WE HAVE THE SUM OF SQUARES 6.81521092E-01
 1 2.0269E+01 2 -2.9209E-02 3 -2.1813E+01 4 1.5184E-02 5 1.9893E+01
 6 -3.2520E-03 7 3.3737E+00 8 -5.2063E+01 9 5.0390E-02

AT THE 25 TH ITERATION WE HAVE THE SUM OF SQUARES 6.80148501E-01
 1 2.0269E+01 2 -2.9209E-02 3 -2.1813E+01 4 1.5184E-02 5 1.9893E+01
 6 -3.3520E-03 7 3.3738E+00 8 -5.2063E+01 9 5.0390E-02

AT THE 26 TH ITERATION WE HAVE THE SUM OF SQUARES 6.79848373E-01
 1 2.0269E+01 2 -2.9210E-02 3 -2.1813E+01 4 1.5178E-02 5 1.9902E+01
 6 -3.3650E-03 7 3.3733E+00 8 -5.2074E+01 9 5.0394E-02

AT THE 27 TH ITERATION WE HAVE THE SUM OF SQUARES 6.81329349E-01
 1 2.0269E+01 2 -2.9210E-02 3 -2.1813E+01 4 1.5178E-02 5 1.9902E+01
 6 -3.3651E-03 7 3.3733E+00 8 -5.2074E+01 9 5.0494E-02

AT THE 28 TH ITERATION WE HAVE THE SUM OF SQUARES 7.01631023E-01
 1 2.0269E+01 2 -2.9210E-02 3 -2.1813E+01 4 1.5078E-02 5 1.9902E+01
 6 -3.3650E-03 7 3.3733E+00 8 -5.2074E+01 9 5.0394E-02

AT THE 29 TH ITERATION WE HAVE THE SUM OF SQUARES 6.79391883E-01
 1 2.0269E+01 2 -2.9212E-02 3 -2.1813E+01 4 1.5185E-02 5 1.9903E+01
 6 -3.3700E-03 7 3.3732E+00 8 -5.2052E+01 9 5.0370E-02

AT THE 30 TH ITERATION WE HAVE THE SUM OF SQUARES 6.78927109E-01
 1 2.0269E+01 2 -2.9214E-02 3 -2.1813E+01 4 1.5178E-02 5 1.9905E+01
 6 -3.3737E-03 7 3.3732E+00 8 -5.2029E+01 9 5.0348E-02

*** ERROR RETURN FROM VA05A BECAUSE THERE HAVE BEEN 30 CALLS OF CALFUN

THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED 30 iterations

| | | | | | | | | | |
|---|-------------|---|-------------|---|-------------|---|------------|---|------------|
| 1 | 2.0269E+01 | 2 | -2.9214E-02 | 3 | -2.1813E+01 | 4 | 1.5178E-02 | 5 | 1.9905E+01 |
| 6 | -3.3737E-03 | 7 | 3.3732E+00 | 8 | -5.2029E+01 | 9 | 5.0348E-02 | | |

| | | | | | | | | | |
|----|-------------|----|-------------|----|-------------|----|-------------|----|-------------|
| 1 | 8.1479E-03 | 2 | 8.1479E-03 | 3 | 2.2738E-03 | 4 | 1.7472E-01 | 5 | 1.3209E-01 |
| 6 | -1.4013E-01 | 7 | 5.1900E-03 | 8 | 8.8089E-03 | 9 | 8.8089E-03 | 10 | 6.7254E-02 |
| 11 | 4.8765E-03 | 12 | 1.2124E-01 | 13 | 2.8616E-03 | 14 | -3.6817E-01 | 15 | -9.0760E-03 |
| 16 | 2.7022E-02 | 17 | 2.7022E-02 | 18 | -1.0865E-01 | 19 | 7.1701E-02 | 20 | -1.0865E-01 |
| 21 | 7.1701E-02 | 22 | 4.9475E-01 | 23 | 6.5317E-03 | 24 | 1.9521E-01 | 25 | 3.1164E-03 |
| 26 | -3.3004E-01 | 27 | -5.0147E-03 | 28 | 8.3162E-02 | 29 | 6.0590E-03 | 30 | -1.2865E-02 |
| 31 | -2.8643E-02 | 32 | 3.7909E-03 | 33 | 5.0512E-02 | 34 | 7.6377E-02 | 35 | 4.6150E-02 |
| 36 | -7.4224E-02 | 37 | 2.1008E-02 | 38 | -5.0984E-02 | 39 | 1.7198E-03 | 40 | 1.9946E-02 |
| 41 | 1.4679E-02 | 42 | 7.9194E-03 | 43 | 1.6661E-03 | 44 | -4.0806E-03 | 45 | -1.1321E-02 |
| 46 | -1.8054E-02 | 47 | -2.6280E-02 | | | | | | |

THE SUM OF SQUARES IS 6.78927109E-01

PARROT: resc
 PARROT: opt 30
 Alternate calculation is on
 Use 47 experiments, maximum is 2000
 Use 1082 real workspace, maximum is 50000
 The following output is provided by subroutine VA05A

AT THE 0 TH ITERATION WE HAVE THE SUM OF SQUARES 6.78927109E-01
 1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
 6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 1 ST ITERATION WE HAVE THE SUM OF SQUARES 6.78926993E-01
 1 1.0001E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
 6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 2 ND ITERATION WE HAVE THE SUM OF SQUARES 6.78916038E-01
 1 1.0001E+00 2 1.0001E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
 6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 3 RD ITERATION WE HAVE THE SUM OF SQUARES 6.78945788E-01
 1 1.0001E+00 2 1.0001E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
 6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 4 TH ITERATION WE HAVE THE SUM OF SQUARES 6.78906584E-01
 1 1.0001E+00 2 1.0001E+00 3 1.0000E+00 4 1.0001E+00 5 1.0000E+00
 6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 5 TH ITERATION WE HAVE THE SUM OF SQUARES 6.78837383E-01
 1 1.0001E+00 2 1.0001E+00 3 1.0000E+00 4 1.0001E+00 5 1.0001E+00
 6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 6 TH ITERATION WE HAVE THE SUM OF SQUARES 6.78835540E-01
 1 1.0001E+00 2 1.0001E+00 3 1.0000E+00 4 1.0001E+00 5 1.0001E+00
 6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 7 TH ITERATION WE HAVE THE SUM OF SQUARES 6.78835578E-01

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1 1.0001E+00 2 1.0001E+00 3 1.0000E+00 4 1.0001E+00 5 1.0001E+00
6 1.0001E+00 7 1.0001E+00 8 1.0000E+00 9 1.0000E+00

    AT THE 8 TH ITERATION WE HAVE THE SUM OF SQUARES 6.78868108E-01
1 1.0001E+00 2 1.0001E+00 3 1.0000E+00 4 1.0001E+00 5 1.0001E+00
6 1.0001E+00 7 1.0000E+00 8 1.0001E+00 9 1.0000E+00

    AT THE 9 TH ITERATION WE HAVE THE SUM OF SQUARES 6.78889246E-01
1 1.0001E+00 2 1.0001E+00 3 1.0000E+00 4 1.0001E+00 5 1.0001E+00
6 1.0001E+00 7 1.0000E+00 8 1.0000E+00 9 1.0001E+00

    AT THE 10 TH ITERATION WE HAVE THE SUM OF SQUARES 6.74450014E-01
1 9.9994E-01 2 1.0012E+00 3 9.9903E-01 4 1.0006E+00 5 1.0070E+00
6 1.0003E+00 7 1.0000E+00 8 9.9681E-01 9 9.9473E-01

    AT THE 11 TH ITERATION WE HAVE THE SUM OF SQUARES 6.68058362E-01
1 1.0001E+00 2 1.0012E+00 3 1.0000E+00 4 1.0001E+00 5 1.0078E+00
6 1.0062E+00 7 9.9971E-01 8 9.9116E-01 9 9.9045E-01

    AT THE 12 TH ITERATION WE HAVE THE SUM OF SQUARES 6.58643628E-01
1 1.0002E+00 2 1.0014E+00 3 9.9931E-01 4 1.0004E+00 5 1.0097E+00
6 1.0173E+00 7 9.9908E-01 8 9.7862E-01 9 9.8233E-01

    AT THE 13 TH ITERATION WE HAVE THE SUM OF SQUARES 6.39240498E-01
1 1.0003E+00 2 1.0014E+00 3 9.9998E-01 4 1.0000E+00 5 1.0132E+00
6 1.0415E+00 7 9.9792E-01 8 9.5651E-01 9 9.6461E-01

    AT THE 14 TH ITERATION WE HAVE THE SUM OF SQUARES 6.02850786E-01
1 1.0002E+00 2 1.0016E+00 3 9.9938E-01 4 1.0003E+00 5 1.0201E+00
6 1.0892E+00 7 9.9556E-01 8 9.1205E-01 9 9.2862E-01

    AT THE 15 TH ITERATION WE HAVE THE SUM OF SQUARES 5.32698582E-01
1 1.0003E+00 2 1.0015E+00 3 1.0000E+00 4 9.9995E-01 5 1.0338E+00
6 1.1863E+00 7 9.9094E-01 8 8.2377E-01 9 8.5798E-01

    AT THE 16 TH ITERATION WE HAVE THE SUM OF SQUARES 4.07951111E-01
1 1.0002E+00 2 1.0014E+00 3 9.9950E-01 4 1.0000E+00 5 1.0611E+00
6 1.3799E+00 7 9.8167E-01 8 6.4693E-01 9 7.1641E-01

    AT THE 17 TH ITERATION WE HAVE THE SUM OF SQUARES 2.15131231E-01
1 1.0003E+00 2 1.0010E+00 3 9.9999E-01 4 9.9951E-01 5 1.1159E+00
6 1.7687E+00 7 9.6322E-01 8 2.9420E-01 9 4.3403E-01

    AT THE 18 TH ITERATION WE HAVE THE SUM OF SQUARES 5.88510515E-02
1 1.0003E+00 2 1.0001E+00 3 1.0000E+00 4 9.9894E-01 5 1.2254E+00
6 2.5464E+00 7 9.2633E-01 8 -4.1115E-01 9 -1.3067E-01

1 8.7494E-03 2 8.7494E-03 3 1.5856E-03 4 2.6880E-03 5 1.3187E-01
6 -1.4046E-01 7 5.5953E-04 8 9.4827E-03 9 9.4827E-03 10 -5.3272E-04
11 3.2046E-03 12 1.2921E-03 13 1.9468E-04 14 -2.7835E-04 15 5.3573E-04
16 2.3622E-03 17 2.3622E-03 18 -1.5556E-04 19 -3.1254E-04 20 -1.5556E-04
21 -3.1254E-04 22 1.1733E-03 23 1.8044E-03 24 4.3832E-03 25 3.5408E-04
26 -5.5597E-03 27 3.1954E-03 28 -2.0086E-03 29 3.7500E-03 30 -1.3498E-02
31 -3.0927E-02 32 -7.7845E-04 33 4.3460E-02 34 6.7114E-02 35 3.5424E-02
36 -8.5221E-02 37 1.1421E-02 38 -5.7086E-02 39 1.7355E-03 40 1.9974E-02
41 1.4716E-02 42 7.9614E-03 43 1.7098E-03 44 -4.0386E-03 45 -1.1284E-02
46 -1.8026E-02 47 -2.6264E-02
```

THE SUM OF SQUARES IS 5.88510515E-02

```

PARROT: @@ No change in the parameters, check the diagram again
PARROT: mac tce36cpd
PARROT: set-echo
NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3

POLY:
POLY: @@ In PARROT, the global minimization is turned off automatically.
POLY: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY: @@ message will be given.
POLY:
POLY: advanced-option global yes,
Settings for global minimization:
*** WARNING *** Global equilibrium calculation may create new composition sets
and this may corrupt your PARROT work file (.PAR file).
Do not go back to PARROT but exit from POLY after your POLY calculations.

POLY:
POLY: def-com,,,
POLY: s-a-v 1 w(b) 0 1,,,
The condition W(B)=.1234 created
POLY: s-a-v 2 t 300 1700,,,
The condition T=942.2 created
POLY: s-c t=500
POLY: l-c
W(B)=0.1234, T=500
DEGREES OF FREEDOM 2
POLY: c-e
Creating condition P=1E5
Creating condition N=1
Using global minimization procedure
Calculated 628 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY: save tce36 y
```

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

```

POLY: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
```

```

Generating start equilibrium 11
Generating start equilibrium 12
Organizing start points
Using ADDED start equilibria
Generating start point  1
Generating start point  2
Generating start point  3
Generating start point  4
Generating start point  5
Generating start point  6
Generating start point  7
Generating start point  8
Generating start point  9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Generating start point 27
Generating start point 28

Phase region boundary 1 at: 7.140E-01 3.100E+02
   BCC#1
   ** BCC#2
Calculated..          2 equilibria
Terminating at axis limit.

Phase region boundary 2 at: 7.141E-01 3.000E+02
   BCC#1
   ** BCC#2
Calculated.          14 equilibria

Phase region boundary 3 at: 6.814E-01 7.280E+02
   ** A2B
   BCC#1
   ** BCC#2
Calculated.          14 equilibria

Phase region boundary 4 at: 3.627E-01 7.280E+02
   ** A2B
   BCC#1
Calculated.          14 equilibria

Phase region boundary 5 at: 3.781E-01 1.183E+03
   ** LIQUID
   ** A2B
   BCC#1
Calculated.          31 equilibria

Phase region boundary 6 at: 2.906E-01 1.183E+03
   ** LIQUID
   BCC#1
Calculated.          31 equilibria

Phase region boundary 7 at: 4.911E-01 1.183E+03
   ** LIQUID
   A2B
Calculated.          33 equilibria

Phase region boundary 8 at: 6.476E-01 1.037E+03
   ** LIQUID
   A2B
   ** BCC#1
Calculated.          10 equilibria
Terminating at known equilibrium

Phase region boundary 10 at: 8.252E-01 1.037E+03
   LIQUID
   ** BCC#1
Calculated.          8 equilibria

Phase region boundary 11 at: 8.754E-01 1.203E+03
   LIQUID
   ** BCC#1
   ** FCC
Calculated.          31 equilibria

Phase region boundary 12 at: 8.805E-01 1.203E+03
   LIQUID
   ** FCC
Calculated.          31 equilibria

Phase region boundary 13 at: 9.357E-01 1.203E+03
   BCC#1
   ** FCC
Calculated.          19 equilibria

Phase region boundary 14 at: 7.140E-01 3.100E+02
   BCC#1
   ** BCC#2
Calculated..          13 equilibria
Terminating at known equilibrium

Phase region boundary 15 at: 7.140E-01 3.100E+02
   BCC#1
   ** BCC#2
Calculated..          2 equilibria
Terminating at known equilibrium

```

Terminating at axis limit.

Phase region boundary 16 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 17 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 18 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 19 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 20 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2
 Calculated. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 21 at: 7.140E-01 3.100E+02
 BCC#1
 BCC#2
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 22 at: 7.140E-01 3.100E+02
 BCC#1
 BCC#2
 Calculated. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 23 at: 7.140E-01 3.100E+02
 BCC#1
 BCC#2
 Calculated.. 2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

Phase region boundary 24 at: 7.140E-01 3.100E+02
 BCC#1
 BCC#2
 Calculated. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 25 at: 3.648E-01 7.700E+02
 ** A2B
 BCC#1
 Calculated 10 equilibria

Phase region boundary 26 at: 3.648E-01 7.700E+02
 ** A2B
 BCC#1
 Calculated. 3 equilibria
 Terminating at known equilibrium

Phase region boundary 27 at: 3.648E-01 7.700E+02
 ** A2B
 BCC#1
 Calculated. 13 equilibria
 Terminating at known equilibrium

Phase region boundary 28 at: 7.907E-01 7.700E+02
 ** A2B
 BCC#1
 Calculated 10 equilibria

Phase region boundary 29 at: 7.907E-01 7.700E+02
 ** A2B
 BCC#1
 Calculated. 3 equilibria
 Terminating at known equilibrium

Phase region boundary 30 at: 7.907E-01 7.700E+02
 ** A2B
 BCC#1
 Calculated. 9 equilibria
 Terminating at known equilibrium

Phase region boundary 31 at: 2.435E-01 1.230E+03
 ** LIQUID
 BCC#1
 Calculated. 4 equilibria
 Terminating at known equilibrium

Phase region boundary 32 at: 2.435E-01 1.230E+03
 ** LIQUID
 BCC#1
 Calculated 26 equilibria

Phase region boundary 33 at: 8.864E-01 1.230E+03
 ** LIQUID
 FCC
 Calculated. 2 equilibria
 Terminating at known equilibrium

Phase region boundary 34 at: 8.864E-01 1.230E+03
 ** LIQUID
 FCC
 Calculated 29 equilibria

```

Phase region boundary 35 at: 6.404E-03 1.397E+03
    LIQUID
    ** BCC#1
Calculated                8 equilibria

Phase region boundary 36 at: 6.404E-03 1.397E+03
    LIQUID
    ** BCC#1
Calculated                13 equilibria
Terminating at known equilibrium

Phase region boundary 37 at: 2.295E-01 1.243E+03
    LIQUID
    ** BCC#1
Calculated                21 equilibria

Phase region boundary 38 at: 2.295E-01 1.243E+03
    LIQUID
    ** BCC#1
Calculated                4 equilibria
Terminating at known equilibrium

Phase region boundary 39 at: 6.122E-01 1.209E+03
    LIQUID
    ** A2B
Calculated                12 equilibria
Terminating at known equilibrium

Phase region boundary 40 at: 6.122E-01 1.209E+03
    LIQUID
    ** A2B
Calculated                8 equilibria
Terminating at known equilibrium

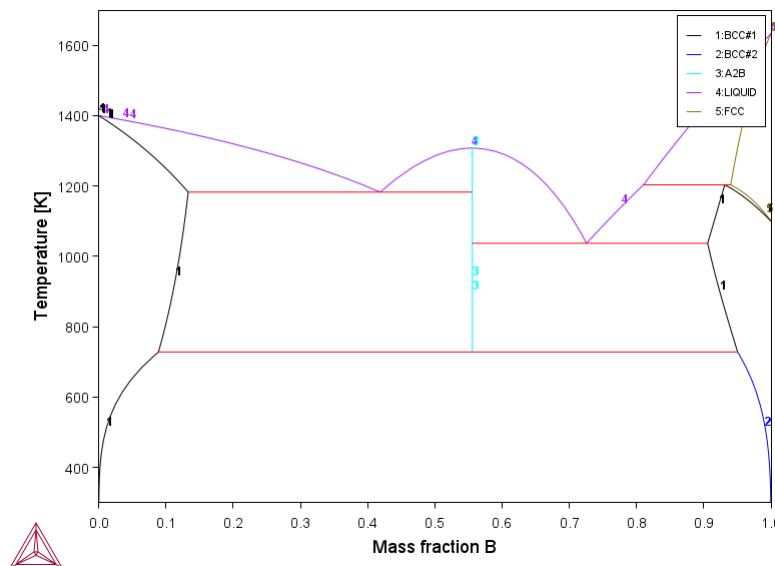
Phase region boundary 41 at: 9.928E-01 1.613E+03
    LIQUID
    ** FCC
Calculated                19 equilibria
Terminating at known equilibrium

Phase region boundary 42 at: 9.928E-01 1.613E+03
    LIQUID
    ** FCC
Calculated                8 equilibria
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\generate_console_examples\examples\tcex36a\tcex36.POLY3
CPU time for mapping      1 seconds
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: s-l d
POST: plot

```



```

POST:
POST: set-inter
POST: Hit RETURN to continue
POST: ba
POLY: ba

```

```

PARROT VERSION 5.3

```

```

Global minimization used as test only
PARROT: @@ Turn off alternate mode and try to calculate all equilibria
PARROT: s-salt Y
Alternate calculation is on
PARROT: ed
ED_EXP: read 1
ED_EXP: c-a
Eq Lab Iter Weight Temp Exp Fix phases or comments
 1 AINV 4 1. 1182.6 LIQUID A2B BCC
 2 AINV 2 1. 1307.4 LIQUID A2B
 3 AINV 3 1. 1037.1 LIQUID A2B BCC
 4 AINV 3 1. 1203.1 LIQUID BCC FCC
 5 AINV 3 1. 728.0 A2B BCC BCC#2
 6 AINV 2 1. 726.0 BCC BCC#2
10 ALF < unused > 1594.0 LIQUID FCC
11 ALF < unused > 1548.0 LIQUID FCC
12 ALF < unused > 1499.0 LIQUID FCC
13 ALF < unused > 1438.0 LIQUID FCC
20 ATIE 3 1. 1413.0 LIQUID FCC
21 ATIE 3 1. 1337.0 LIQUID FCC
22 ATIE 3 1. 1213.0 LIQUID FCC

```

```

23 ATIE 3 1. 1100.0 LIQUID BCC
100 AA 2 1. 1573.0 LIQUID
101 AA 2 1. 1573.0 LIQUID
102 AA 2 1. 1573.0 LIQUID
103 AA 2 1. 1573.0 LIQUID
104 AA 2 1. 1573.0 LIQUID
105 AA 2 1. 1573.0 LIQUID
106 AA 2 1. 1573.0 LIQUID
107 AA 2 1. 1573.0 LIQUID
108 AA 2 1. 1573.0 LIQUID
110 AH 2 1. 1773.0 LIQUID
111 AH 2 1. 1773.0 LIQUID
112 AH 2 1. 1773.0 LIQUID
113 AH 2 1. 1773.0 LIQUID
114 AH 2 1. 1773.0 LIQUID
115 AH 2 1. 1773.0 LIQUID
116 AH 2 1. 1773.0 LIQUID
117 AH 2 1. 1773.0 LIQUID
118 AH 2 1. 1773.0 LIQUID
ED_EXP: @@ Remove the equilibria with just liquid as we do not optimize
ED_EXP: @@ any liquid parameters and restore those with label ALF
ED_EXP: s-we 0 100-118
ED_EXP: s-we 1 alf
Changed weight on 4 equilibria.
ED_EXP: s-e 1
Equilibrium number 1, label AINV
ED_EXP: c-a
Eq Lab Iter Weight Temp Exp Fix phases or comments
 1 AINV 2 1. 1182.6 LIQUID A2B BCC
 2 AINV 2 1. 1307.4 LIQUID A2B
 3 AINV 2 1. 1037.1 LIQUID A2B BCC
 4 AINV 2 1. 1203.1 LIQUID BCC FCC
 5 AINV 2 1. 728.0 A2B BCC BCC#2
 6 AINV 2 1. 726.0 BCC BCC#2
10 ALF 6 1. 1594.0 LIQUID FCC
11 ALF 6 1. 1548.0 LIQUID FCC
12 ALF 7 1. 1499.0 LIQUID FCC
13 ALF 7 1. 1438.0 LIQUID FCC
20 ATIE 2 1. 1413.0 LIQUID FCC
21 ATIE 2 1. 1337.0 LIQUID FCC
22 ATIE 2 1. 1213.0 LIQUID FCC
23 ATIE 2 1. 1100.0 LIQUID BCC
100 AA < unused > 1573.0 LIQUID
101 AA < unused > 1573.0 LIQUID
102 AA < unused > 1573.0 LIQUID
103 AA < unused > 1573.0 LIQUID
104 AA < unused > 1573.0 LIQUID
105 AA < unused > 1573.0 LIQUID
106 AA < unused > 1573.0 LIQUID
107 AA < unused > 1573.0 LIQUID
108 AA < unused > 1573.0 LIQUID
110 AH < unused > 1773.0 LIQUID
111 AH < unused > 1773.0 LIQUID
112 AH < unused > 1773.0 LIQUID
113 AH < unused > 1773.0 LIQUID
114 AH < unused > 1773.0 LIQUID
115 AH < unused > 1773.0 LIQUID
116 AH < unused > 1773.0 LIQUID
117 AH < unused > 1773.0 LIQUID
118 AH < unused > 1773.0 LIQUID
ED_EXP: save
ED_EXP: @@ Save changes
ED_EXP: ba
PARROT: opt 0
Use      29 experiments, maximum is      2000
Use      740 real workspace, maximum is    50000
PARROT: l-r C SCREEN

```

```
=====
OUTPUT FROM P A R R O T . DATE 2023. 4.27 16:25:39
```

```
*** SUCCESSFUL OPTIMIZATION. ***
NUMBER OF ITERATIONS: 0
```

```
-- OPTIMIZING CONDITIONS --
```

```
RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.0000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 0 DMAX = 1.0000000E+02 H = 1.0000000E-04
ACC = (INITIAL SUM OF SQUARES) * 1.0000000E-03
```

```
-- OPTIMIZING VARIABLES --
```

```
AVAILABLE VARIABLES ARE V1 TO VOO
```

| VAR. | VALUE | START VALUE | SCALING FACTOR | REL.STAND.DEV |
|------|-----------------|-----------------|-----------------|----------------|
| V1 | 2.02764407E+04 | 2.02694367E+04 | 2.02694367E+04 | 7.92318772E-02 |
| V2 | -2.92160244E+01 | -2.92138211E+01 | -2.92138211E+01 | 3.43000985E-01 |
| V11 | -2.18125805E+04 | -2.18126679E+04 | -2.18126679E+04 | 3.96945631E-02 |
| V12 | 1.51623098E+01 | 1.51783975E+01 | 1.51783975E+01 | 5.85501240E-02 |
| V15 | 2.43913409E+04 | 1.99045950E+04 | 1.99045950E+04 | 7.47154887E-01 |
| V16 | -8.59082453E+00 | -3.37369312E+00 | -3.37369312E+00 | 5.21151940E+00 |
| V17 | 3.12468126E+03 | 3.37316715E+03 | 3.37316715E+03 | 1.34672167E+00 |
| V19 | 2.13918769E+04 | -5.20289889E+04 | -5.20289889E+04 | 1.95628101E+00 |
| V20 | -6.57912798E+00 | 5.03479181E+01 | 5.03479181E+01 | 1.56676312E+00 |

```
NUMBER OF OPTIMIZING VARIABLES : 9
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 6.78927109E-01 TO 1.42233582E+01
DEGREES OF FREEDOM 20. REDUCED SUM OF SQUARES 7.11167912E-01
```

```
$ ===== BLOCK NUMBER 1
```

```

DEFINED CONSTANTS
DX=2E-2, P0=101325, DH=500, DT=10
DEFINED FUNCTIONS AND VARIABLES%
HTR=HM(LIQUID)-HM(A2B)
1 T=1193 1183. 10. -10.44 -1.044
1 W(LIQUID,B)=0.408 0.4187 2.00E-02 1.0728E-02 0.5364
1 W(BCC#1,B)=0.13 0.1331 2.00E-02 3.1127E-03 0.1556
2 T=1341 1307. 10. -33.59 -3.359
2 HTR=3727 3727. 5.00E+02 0.2797 5.5932E-04
3 T=1049 1037. 10. -11.89 -1.189
3 W(LIQUID,A)=0.27 0.2745 2.00E-02 4.4553E-03 0.2228
3 W(BCC#1,A)=9.3E-2 9.4213E-02 2.00E-02 1.2128E-03 6.0639E-02
4 T=1203 1203. 10. 9.6295E-02 9.6295E-03
4 W(LIQUID,A)=0.19 0.1897 2.00E-02 -2.7851E-04 -1.3925E-02
4 W(BCC#1,A)=6.9E-2 6.8759E-02 2.00E-02 -2.4083E-04 -1.2042E-02
4 W(FCC,A)=6E-2 5.9907E-02 2.00E-02 -9.2714E-05 -4.6357E-03
5 T=726 728.0 10. 2.028 0.2028
5 X(BCC#1,B)=3.7E-2 3.7554E-02 2.00E-02 5.5382E-04 2.7691E-02
5 X(BCC#2,A)=0.114 0.1154 2.00E-02 1.4411E-03 7.2054E-02
6 X(BCC#1,B)=3.7E-2 3.6982E-02 2.00E-02 -1.8093E-05 -9.0466E-04
6 X(BCC#2,A)=0.114 0.1140 2.00E-02 3.0256E-05 1.5128E-03
10 W(LIQUID,B)=2E-2 1.9238E-02 2.00E-02 -7.6216E-04 -3.8108E-02
11 W(LIQUID,A)=4.2E-2 4.1239E-02 2.00E-02 -7.6122E-04 -3.8061E-02
12 W(LIQUID,A)=6.5E-2 6.4104E-02 2.00E-02 -8.9553E-04 -4.4777E-02
13 W(LIQUID,A)=9.3E-2 9.1746E-02 2.00E-02 -1.2536E-03 -6.2678E-02
20 W(LIQUID,A)=0.104 0.1028 2.00E-02 -1.1911E-03 -5.9554E-02
20 W(FCC,A)=3.8E-2 3.7461E-02 2.00E-02 -5.3913E-04 -2.6957E-02
21 W(LIQUID,A)=0.136 0.1355 2.00E-02 -5.1073E-04 -2.5536E-02
21 W(FCC,A)=4.7E-2 4.6507E-02 2.00E-02 -4.9321E-04 -2.4660E-02
22 W(LIQUID,A)=0.187 0.1858 2.00E-02 -1.1514E-03 -5.7572E-02
22 W(FCC,A)=5.9E-2 5.8999E-02 2.00E-02 -2.3513E-06 -1.1757E-04
23 W(LIQUID,A)=0.245 0.2435 2.00E-02 -1.4886E-03 -7.4431E-02
23 W(BCC#1,A)=8.5E-2 8.4494E-02 2.00E-02 -5.0596E-04 -2.5298E-02

```

```

PARROT:
PARROT:Hit RETURN to continue
PARROT: @@ When we optimize zero times we sometimes find an error for
PARROT: @@ equilibrium 4. It can be on the wrong side, at high A instead
PARROT: @@ of high B. Try to correct that in the Edit module.
PARROT: ed
ED_EXP: read 1
ED_EXP: s-e 4
Equilibrium number 4, label AINV
ED_EXP: s-a-s
T /1203.096295/: 1200
Automatic start values for phase constituents? /N/: N

Phase LIQUID
Major constituent(s) /*/: b

Phase BCC
Major constituent(s) /b/: b

Phase FCC
Major constituent(s) /b/: b
ED_EXP:
ED_EXP: c-e
Testing result with global minimization
13 ITS, CPU TIME USED 0 SECONDS
ED_EXP: l-e
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
Output from POLY-3, equilibrium = 4, label AINV, database:

Conditions:
P=101325
FIXED PHASES
LIQUID=1 BCC#1=1 FCC=1
DEGREES OF FREEDOM 0

Temperature 1203.10 K ( 929.95 C), Pressure 1.013250E+05
Number of moles of components 3.00000E+00, Mass in grams 1.30126E+02
Total Gibbs energy -9.82402E+03, Enthalpy 1.98069E+04, Volume 0.000000E+00

Component Moles W-Fraction Activity Potential Ref.stat
A 6.6247E-01 1.0182E-01 3.9003E-01 -9.4183E+03 SER
B 2.3375E+00 8.9818E-01 8.5787E-01 -1.5335E+03 SER

FCC Status FIXED Driving force 0.0000E+00
Moles 1.00000E+00, Mass 4.5877E+01, Volume fraction 0.0000E+00 Mass fractions:
B 9.40093E-01 A 5.99073E-02

BCC#1 Status FIXED Driving force 0.0000E+00
Moles 1.00000E+00, Mass 4.5325E+01, Volume fraction 0.0000E+00 Mass fractions:
B 9.31241E-01 A 6.87592E-02

LIQUID Status FIXED Driving force 0.0000E+00
Moles 1.00000E+00, Mass 3.8923E+01, Volume fraction 0.0000E+00 Mass fractions:
B 8.10279E-01 A 1.89721E-01
EXPERIMENT T=1203:DT $1203.1:10 NO=1
EXPERIMENT W(LIQUID,A)=0.19:DX $0.189721:2E-2 NO=2
EXPERIMENT W(BCC#1,A)=6.9E-2:DX $6.87592E-2:2E-2 NO=3
EXPERIMENT W(FCC,A)=6E-2:DX $5.99073E-2:2E-2 NO=4
ED_EXP: ba
PARROT: @@ The error is still there, calculate the phase diagram.
PARROT: mac tce36cpd
PARROT: set-echo
NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
POLY:
POLY: @@ In PARROT, the global minimization is turned off automatically.
POLY: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY: @@ message will be given.
POLY:
POLY: advanced-option global yes,
Settings for global minimization:
*** WARNING *** Global equilibrium calculation may create new composition sets
and this may corrupt your PARROT work file (.PAR file).
Do not go back to PARROT but exit from POLY after your POLY calculations.
POLY:

```

```
POLY: def-com,,,,
POLY: s-a-v 1 w(b) 0 1,,,,
The condition W(B)=.1234 created
POLY: s-a-v 2 t 300 1700,,,
The condition T=942.2 created
POLY: s-c t=500
POLY: l-c
W(B)=0.1234, T=500
DEGREES OF FREEDOM 2
POLY: c-e
Creating condition P=1E5
Creating condition N=1
Using global minimization procedure
Calculated          628 grid points in      0 s
Found the set of lowest grid points in      0 s
Calculated POLY solution      0 s, total time  0 s
POLY: save tcex36 y
```

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

```
POLY: map
Version S mapping is selected
Generating start equilibrium  1
Generating start equilibrium  2
Generating start equilibrium  3
Generating start equilibrium  4
Generating start equilibrium  5
Generating start equilibrium  6
Generating start equilibrium  7
Generating start equilibrium  8
Generating start equilibrium  9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12
```

Organizing start points

Using ADDED start equilibria

```
Generating start point   1
Generating start point   2
Generating start point   3
Generating start point   4
Generating start point   5
Generating start point   6
Generating start point   7
Generating start point   8
Generating start point   9
Generating start point  10
Working hard
Generating start point  11
Generating start point  12
Generating start point  13
Generating start point  14
Generating start point  15
Generating start point  16
Generating start point  17
Generating start point  18
Generating start point  19
Generating start point  20
Working hard
Generating start point  21
Generating start point  22
Generating start point  23
Generating start point  24
Generating start point  25
Generating start point  26
Generating start point  27
Generating start point  28
```

Phase region boundary 1 at: 7.140E-01 3.100E+02

BCC#1

** BCC#2

Calculated..

2 equilibria

Terminating at axis limit.

Phase region boundary 2 at: 7.141E-01 3.000E+02

BCC#1

** BCC#2

Calculated..

14 equilibria

Phase region boundary 3 at: 6.814E-01 7.280E+02

** A2B

BCC#1

** BCC#2

Calculated..

14 equilibria

Phase region boundary 4 at: 3.627E-01 7.280E+02

** A2B

BCC#1

** BCC#2

Calculated..

14 equilibria

Phase region boundary 5 at: 3.781E-01 1.183E+03

** LIQUID

** A2B

BCC#1

Calculated..

31 equilibria

Phase region boundary 6 at: 2.906E-01 1.183E+03

** LIQUID

BCC#1

Calculated..

31 equilibria

Phase region boundary 7 at: 4.911E-01 1.183E+03

** LIQUID

A2B

Calculated..

33 equilibria

Phase region boundary 8 at: 6.476E-01 1.037E+03

** LIQUID

A2B

** BCC#1

Phase region boundary 9 at: 7.634E-01 1.037E+03

A2B

```

** BCC#1
Calculated.          10 equilibria
Terminating at known equilibrium

Phase region boundary 10 at: 8.252E-01 1.037E+03
    LIQUID
** BCC#1
Calculated.          8 equilibria

Phase region boundary 11 at: 8.754E-01 1.203E+03
    LIQUID
** BCC#1
** FCC
Calculated.          31 equilibria

Phase region boundary 12 at: 8.805E-01 1.203E+03
    LIQUID
** FCC
Calculated.          19 equilibria

Phase region boundary 13 at: 9.357E-01 1.203E+03
    BCC#1
** FCC
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 14 at: 7.140E-01 3.100E+02
    BCC#1
** BCC#2
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 15 at: 7.140E-01 3.100E+02
    BCC#1
** BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 16 at: 7.140E-01 3.100E+02
    BCC#1
** BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 17 at: 7.140E-01 3.100E+02
    BCC#1
** BCC#2
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 18 at: 7.140E-01 3.100E+02
    BCC#1
** BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 19 at: 7.140E-01 3.100E+02
    BCC#1
** BCC#2
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 20 at: 7.140E-01 3.100E+02
    BCC#1
** BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 21 at: 7.140E-01 3.100E+02
    BCC#1
BCC#2
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 22 at: 7.140E-01 3.100E+02
    BCC#1
BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 23 at: 7.140E-01 3.100E+02
    BCC#1
BCC#2
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 24 at: 7.140E-01 3.100E+02
    BCC#1
BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 25 at: 3.648E-01 7.700E+02
    ** A2B
    BCC#1
Calculated.          10 equilibria

Phase region boundary 26 at: 3.648E-01 7.700E+02
    ** A2B
    BCC#1
Calculated.          3 equilibria
Terminating at known equilibrium

Phase region boundary 27 at: 3.648E-01 7.700E+02
    ** A2B
    BCC#1
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 28 at: 7.907E-01 7.700E+02
    ** A2B
    BCC#1
Calculated.          10 equilibria

```

```

Phase region boundary 29 at: 7.907E-01 7.700E+02
** A2B
BCC#1
Calculated.          3 equilibria
Terminating at known equilibrium

Phase region boundary 30 at: 7.907E-01 7.700E+02
** A2B
BCC#1
Calculated.          9 equilibria
Terminating at known equilibrium

Phase region boundary 31 at: 2.435E-01 1.230E+03
** LIQUID
BCC#1
Calculated.          4 equilibria
Terminating at known equilibrium

Phase region boundary 32 at: 2.435E-01 1.230E+03
** LIQUID
FCC
Calculated.          26 equilibria
Terminating at known equilibrium

Phase region boundary 33 at: 8.864E-01 1.230E+03
** LIQUID
FCC
Calculated.          2 equilibria
Terminating at known equilibrium

Phase region boundary 34 at: 8.864E-01 1.230E+03
** LIQUID
FCC
Calculated.          29 equilibria
Terminating at known equilibrium

Phase region boundary 35 at: 6.404E-03 1.397E+03
LIQUID
** BCC#1
Calculated.          8 equilibria
Terminating at known equilibrium

Phase region boundary 36 at: 6.404E-03 1.397E+03
LIQUID
** BCC#1
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 37 at: 2.295E-01 1.243E+03
LIQUID
** BCC#1
Calculated.          21 equilibria
Terminating at known equilibrium

Phase region boundary 38 at: 2.295E-01 1.243E+03
LIQUID
** BCC#1
Calculated.          4 equilibria
Terminating at known equilibrium

Phase region boundary 39 at: 6.122E-01 1.209E+03
LIQUID
** A2B
Calculated.          12 equilibria
Terminating at known equilibrium

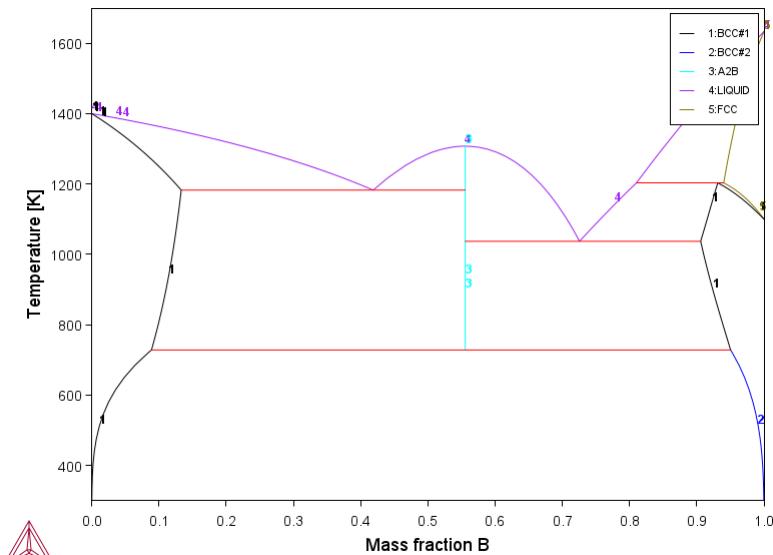
Phase region boundary 40 at: 6.122E-01 1.209E+03
LIQUID
** A2B
Calculated.          8 equilibria
Terminating at known equilibrium

Phase region boundary 41 at: 9.928E-01 1.613E+03
LIQUID
** FCC
Calculated.          19 equilibria
Terminating at known equilibrium

Phase region boundary 42 at: 9.928E-01 1.613E+03
LIQUID
** FCC
Calculated.          8 equilibria
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\generate_console_examples\examples\tcex36a\tcex36.POLY3
CPU time for mapping      1 seconds
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2
Setting automatic diagram axes

POST: s-l d
POST: plot

```



```

POST:
POST: set-inter
POST:Hit RETURN to continue
POST: @@ The phase diagram shows there is no equilibrium between liquid,
POST: @@ fcc and bcc at high B content. For the moment we better remove
POST: @@ equilibrium 4 from the optimization.
POST: ba
POLY: ba

```

PARROT VERSION 5.3

```

Global minimization used as test only
PARROT: ed
ED_EXP: read 1
ED_EXP: s-we 0 4
ED_EXP: save
ED_EXP: ba
PARROT: opt 0
Use      25 experiments, maximum is      2000
Use      664 real workspace, maximum is   50000
PARROT: l-r C SCREEN

```

```
=====
OUTPUT FROM P A R R O T . DATE 2023. 4.27 16:26: 3
```

```
*** SUCCESSFUL OPTIMIZATION. ***
NUMBER OF ITERATIONS: 0
```

```
== OPTIMIZING CONDITIONS ==
```

```

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.0000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 0 DMAX = 1.0000000E+02 H = 1.0000000E-04
ACC = (INITIAL SUM OF SQUARES) * 1.0000000E-03

```

```
== OPTIMIZING VARIABLES ==
```

```
AVAILABLE VARIABLES ARE V1 TO V00
```

| VAR. | VALUE | START VALUE | SCALING FACTOR | REL.STAND.DEV |
|------|-----------------|-----------------|-----------------|----------------|
| V1 | 2.02764407E+04 | 2.02694367E+04 | 2.02694367E+04 | 7.92318772E-02 |
| V2 | -2.92160244E+01 | -2.92138211E+01 | -2.92138211E+01 | 3.43000985E-01 |
| V11 | -2.18125805E+04 | -2.18126679E+04 | -2.18126679E+04 | 3.96945631E-02 |
| V12 | 1.51623098E+01 | 1.51783975E+01 | 1.51783975E+01 | 5.85501240E-02 |
| V15 | 2.43913409E+04 | 1.99045950E+04 | 1.99045950E+04 | 7.47154887E-01 |
| V16 | -8.59082453E+00 | -3.37369312E+00 | -3.37369312E+00 | 5.21151940E+00 |
| V17 | 3.12468126E+03 | 3.37316715E+03 | 3.37316715E+03 | 1.34672167E+00 |
| V19 | 2.13918769E+04 | -5.20289889E+04 | -5.20289889E+04 | 1.95628101E+00 |
| V20 | -6.57912798E+00 | 5.03479181E+01 | 5.03479181E+01 | 1.56676312E+00 |

```

NUMBER OF OPTIMIZING VARIABLES : 9
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 6.78927109E-01 TO 1.42229051E+01
DEGREES OF FREEDOM 16. REDUCED SUM OF SQUARES 8.88931568E-01

```

```
$ ===== BLOCK NUMBER 1
```

```

DEFINED CONSTANTS
DX=2E-2, P0=101325, DH=500, DT=10
DEFINED FUNCTIONS AND VARIABLES%
HTR=HM(LIQUID)-HM(A2B)
1 T=1193           1183.      10.     -10.44    -1.044
1 W(LIQUID,B)=0.408 0.4187    2.00E-02  1.0728E-02  0.5364
1 W(BCC#1,B)=0.13  0.1331    2.00E-02  3.1127E-03  0.1556
2 T=1341           1307.      10.     -33.59    -3.359
2 HTR=3727          3727.    5.00E+02  0.2797    5.5932E-04
3 T=1049           1037.      10.     -11.89    -1.189
3 W(LIQUID,A)=0.27 0.2745    2.00E-02  4.4553E-03  0.2228
3 W(BCC#1,A)=9.3E-2 9.4213E-02 2.00E-02  1.2128E-03  6.0639E-02

```

```

5 T=726          728.0      10.      2.028      0.2028
5 X(BCC#1,B)=3.7E-2   3.7554E-02  2.00E-02  5.5382E-04  2.7691E-02
5 X(BCC#2,A)=0.114    0.1154     2.00E-02  1.4411E-03  7.2054E-02
6 X(BCC#1,B)=3.7E-2   3.6982E-02  2.00E-02 -1.8093E-05 -9.0466E-04
6 X(BCC#2,A)=0.114    0.1140     2.00E-02  3.0256E-05  1.5128E-03
10 W(LIQUID,A)=2E-2   1.9238E-02  2.00E-02 -7.6216E-04 -3.8108E-02
11 W(LIQUID,A)=4.2E-2  4.1239E-02  2.00E-02 -7.6122E-04 -3.8061E-02
12 W(LIQUID,A)=6.5E-2  6.4104E-02  2.00E-02 -8.9553E-04 -4.4777E-02
13 W(LIQUID,A)=9.3E-2  9.1746E-02  2.00E-02 -1.2536E-03 -6.2678E-02
20 W(LIQUID,A)=0.104    0.1028     2.00E-02 -1.1911E-03 -5.9554E-02
20 W(FCC,A)=3.8E-2    3.7461E-02  2.00E-02 -5.3913E-04 -2.6957E-02
21 W(LIQUID,A)=0.136    0.1355     2.00E-02 -5.1073E-04 -2.5536E-02
21 W(FCC,A)=4.7E-2    4.6507E-02  2.00E-02 -4.9321E-04 -2.4660E-02
22 W(LIQUID,A)=0.187    0.1858     2.00E-02 -1.1514E-03 -5.7572E-02
22 W(FCC,A)=5.9E-2    5.8998E-02  2.00E-02 -2.3513E-06 -1.1757E-04
23 W(LIQUID,A)=0.245    0.2435     2.00E-02 -1.4886E-03 -7.4431E-02
23 W(BCC#1,A)=8.5E-2   8.4494E-02  2.00E-02 -5.0596E-04 -2.5298E-02

```

PARROT:
PARROT:Hit RETURN to continue

PARROT: opt 30
Use 25 experiments, maximum is 2000
Use 664 real workspace, maximum is 50000
The following output is provided by subroutine VA05A

```

        AT THE 0 TH ITERATION WE HAVE THE SUM OF SQUARES 1.42229051E+01
1 1.0003E+00 2 1.0001E+00 3 1.0000E+00 4 9.9894E-01 5 1.2254E+00
6 2.5464E+00 7 9.2633E-01 8 -4.1115E-01 9 -1.3067E-01

        AT THE 1 ST ITERATION WE HAVE THE SUM OF SQUARES 1.44292233E+01
1 1.0004E+00 2 1.0001E+00 3 1.0000E+00 4 9.9894E-01 5 1.2254E+00
6 2.5464E+00 7 9.2633E-01 8 -4.1115E-01 9 -1.3067E-01

        AT THE 2 ND ITERATION WE HAVE THE SUM OF SQUARES 1.38536356E+01
1 1.0003E+00 2 1.0002E+00 3 1.0000E+00 4 9.9894E-01 5 1.2254E+00
6 2.5464E+00 7 9.2633E-01 8 -4.1115E-01 9 -1.3067E-01

        AT THE 3 RD ITERATION WE HAVE THE SUM OF SQUARES 1.40117756E+01
1 1.0003E+00 2 1.0002E+00 3 1.0001E+00 4 9.9894E-01 5 1.2254E+00
6 2.5464E+00 7 9.2633E-01 8 -4.1115E-01 9 -1.3067E-01

        AT THE 4 TH ITERATION WE HAVE THE SUM OF SQUARES 1.37170710E+01
1 1.0003E+00 2 1.0002E+00 3 1.0000E+00 4 9.9904E-01 5 1.2254E+00
6 2.5464E+00 7 9.2633E-01 8 -4.1115E-01 9 -1.3067E-01

        AT THE 5 TH ITERATION WE HAVE THE SUM OF SQUARES 1.37228897E+01
1 1.0003E+00 2 1.0002E+00 3 1.0000E+00 4 9.9904E-01 5 1.2255E+00
6 2.5464E+00 7 9.2633E-01 8 -4.1115E-01 9 -1.3067E-01

        AT THE 6 TH ITERATION WE HAVE THE SUM OF SQUARES 1.37159752E+01
1 1.0003E+00 2 1.0002E+00 3 1.0000E+00 4 9.9904E-01 5 1.2254E+00
6 2.5465E+00 7 9.2633E-01 8 -4.1115E-01 9 -1.3067E-01

        AT THE 7 TH ITERATION WE HAVE THE SUM OF SQUARES 1.37155463E+01
1 1.0003E+00 2 1.0002E+00 3 1.0000E+00 4 9.9904E-01 5 1.2254E+00
6 2.5465E+00 7 9.2643E-01 8 -4.1115E-01 9 -1.3067E-01

        AT THE 8 TH ITERATION WE HAVE THE SUM OF SQUARES 1.37147159E+01
1 1.0003E+00 2 1.0002E+00 3 1.0000E+00 4 9.9904E-01 5 1.2254E+00
6 2.5465E+00 7 9.2643E-01 8 -4.1105E-01 9 -1.3067E-01

        AT THE 9 TH ITERATION WE HAVE THE SUM OF SQUARES 1.37158309E+01
1 1.0003E+00 2 1.0002E+00 3 1.0000E+00 4 9.9904E-01 5 1.2254E+00
6 2.5465E+00 7 9.2643E-01 8 -4.1105E-01 9 -1.3057E-01

        AT THE 10 TH ITERATION WE HAVE THE SUM OF SQUARES 2.64414110E-01
1 9.9785E-01 2 1.0047E+00 3 9.9805E-01 4 1.0007E+00 5 1.2253E+00
6 2.5465E+00 7 9.2644E-01 8 -4.1104E-01 9 -1.3069E-01

        AT THE 11 TH ITERATION WE HAVE THE SUM OF SQUARES 2.19706808E-01
1 9.9840E-01 2 1.0045E+00 3 9.9795E-01 4 1.0013E+00 5 1.2245E+00
6 2.5410E+00 7 9.2578E-01 8 -4.1189E-01 9 -1.3125E-01

        AT THE 12 TH ITERATION WE HAVE THE SUM OF SQUARES 1.52062252E-01
1 9.9920E-01 2 1.0048E+00 3 9.9766E-01 4 1.0020E+00 5 1.2230E+00
6 2.5300E+00 7 9.2430E-01 8 -4.1400E-01 9 -1.3270E-01

        AT THE 13 TH ITERATION WE HAVE THE SUM OF SQUARES 8.12099343E-02
1 1.0002E+00 2 1.0046E+00 3 9.9788E-01 4 1.0040E+00 5 1.2201E+00
6 2.5077E+00 7 9.2151E-01 8 -4.1714E-01 9 -1.3467E-01

        AT THE 14 TH ITERATION WE HAVE THE SUM OF SQUARES 9.74454544E-03
1 1.0021E+00 2 1.0046E+00 3 9.9832E-01 4 1.0077E+00 5 1.2144E+00
6 2.4631E+00 7 9.1620E-01 8 -4.2374E-01 9 -1.3891E-01

THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED 14 iterations
1 1.0021E+00 2 1.0046E+00 3 9.9832E-01 4 1.0077E+00 5 1.2144E+00
6 2.4631E+00 7 9.1620E-01 8 -4.2374E-01 9 -1.3891E-01

1 -3.4861E-02 2 -1.5514E-02 3 -2.4093E-03 4 -1.3972E-03 5 -6.4683E-03
6 1.2808E-02 7 1.2979E-02 8 8.8500E-03 9 -6.7916E-02 10 8.7946E-03
11 -2.8432E-02 12 1.8322E-02 13 -5.1193E-03 14 -2.2658E-02 15 -9.1289E-03
16 -5.7318E-03 17 -1.5840E-02 18 -1.0792E-02 19 8.8361E-03 20 2.5356E-02
21 5.2861E-03 22 -1.2624E-02 23 4.7238E-03 24 -3.2501E-03 25 5.4648E-03

```

THE SUM OF SQUARES IS 9.74454544E-03

PARROT: cont 30

It is safe to CONTINUE only after TOO MANY ITERATIONS
and no change in variables and experiments ...
Now anything can happen ...

PARROT: l-r C SCREEN

```
=====
OUTPUT FROM P A R R O T . DATE 2023. 4.27 16:26: 3
```

*** SUCCESSFUL OPTIMIZATION. ***
NUMBER OF ITERATIONS: 15

```

== OPTIMIZING CONDITIONS ==
RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 30 DMAX = 1.00000000E+02 H = 1.00000000E-04
ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03

```

```
-- OPTIMIZING VARIABLES --
```

```
AVAILABLE VARIABLES ARE V1 TO VOO
```

| VAR. | VALUE | START VALUE | SCALING FACTOR | REL.STAND.DEV |
|------|-----------------|-----------------|-----------------|----------------|
| V1 | 2.03113219E+04 | 2.02694367E+04 | 2.02694367E+04 | 1.11597087E-01 |
| V2 | -2.93492365E+01 | -2.92138211E+01 | -2.92138211E+01 | 1.03070625E-01 |
| V11 | -2.17760708E+04 | -2.18126679E+04 | -2.18126679E+04 | 2.13585334E-01 |
| V12 | 1.52955219E+01 | 1.51783975E+01 | 1.51783975E+01 | 3.57094533E-01 |
| V15 | 2.41721137E+04 | 1.99045950E+04 | 1.99045950E+04 | 1.91672505E-01 |
| V16 | -8.30983887E+00 | -3.37369312E+00 | -3.37369312E+00 | 1.38270139E+00 |
| V17 | 3.09048341E+03 | 3.37316715E+03 | 3.37316715E+03 | 2.44072470E-01 |
| V19 | 2.20465939E+04 | -5.20289889E+04 | -5.20289889E+04 | 3.12880572E-01 |
| V20 | -6.99361189E+00 | 5.03479181E+01 | 5.03479181E+01 | 2.63983824E-01 |

```
NUMBER OF OPTIMIZING VARIABLES : 9
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 1.42229051E+01 TO 9.74454544E-03
DEGREES OF FREEDOM 16. REDUCED SUM OF SQUARES 6.09034090E-04
```

```
$ ===== BLOCK NUMBER 1
```

```
DEFINED CONSTANTS
DX=2E-2, P0=101325, DH=500, DT=10
```

```
DEFINED FUNCTIONS AND VARIABLES%
```

```
HTR=HM(LIQUID)-HM(A2B)
1 T=1193.          1193.      10.      -0.3486   -3.4861E-02
1 W(LIQUID,B)=0.408 0.4077  2.00E-02 -3.1028E-04 -1.5514E-02
1 W(BCC#1,B)=0.13 0.1300  2.00E-02 -4.8185E-05 -2.4093E-03
2 T=1341.          1341.      10.      -1.3972E-02 -1.3972E-03
2 HTR=3727          3724.      5.00E+02 -3.234    -6.4683E-03
3 T=1049.          1049.      10.      0.1281    1.2808E-02
3 W(LIQUID,A)=0.27 0.2703  2.00E-02 2.5959E-04  1.2979E-02
3 W(BCC#1,A)=9.3E-2 9.3177E-02 2.00E-02 1.7700E-04  8.8500E-03
5 T=726.            725.3     10.      -0.6792   -6.7916E-02
5 X(BCC#1,B)=3.7E-2 3.7176E-02 2.00E-02 1.7589E-04  8.7946E-03
5 X(BCC#2,A)=0.114 0.1134  2.00E-02 -5.6864E-04 -2.8432E-02
6 X(BCC#1,B)=3.7E-2 3.7366E-02 2.00E-02 3.6644E-04  1.8322E-02
6 X(BCC#2,A)=0.114 0.1139  2.00E-02 -1.0239E-04 -5.1193E-03
10 W(LIQUID,W)=2E-2 1.9547E-02 2.00E-02 -4.5316E-04 -2.2658E-02
11 W(LIQUID,A)=4.2E-2 4.1817E-02 2.00E-02 -1.8258E-04 -9.1289E-03
12 W(LIQUID,A)=6.5E-2 6.4885E-02 2.00E-02 -1.1464E-04 -5.7318E-03
13 W(LIQUID,A)=9.3E-2 9.2683E-02 2.00E-02 -3.1679E-04 -1.5840E-02
20 W(LIQUID,A)=0.104 0.1038  2.00E-02 -2.1584E-04 -1.0792E-02
20 W(FCC,A)=3.8E-2 3.8177E-02 2.00E-02 1.7672E-04  8.8361E-03
21 W(LIQUID,A)=0.136 0.1365  2.00E-02 5.0713E-04  2.5356E-02
21 W(FCC,A)=4.7E-2 4.7106E-02 2.00E-02 1.0572E-04  5.2861E-03
22 W(LIQUID,A)=0.187 0.1867  2.00E-02 -2.5247E-04 -1.2624E-02
22 W(FCC,A)=5.9E-2 5.9094E-02 2.00E-02 9.4476E-05  4.7238E-03
23 W(LIQUID,A)=0.245 0.2449  2.00E-02 -6.5002E-05 -3.2501E-03
23 W(BCC#1,A)=8.5E-2 8.5109E-02 2.00E-02 1.0930E-04  5.4648E-03
```

```
PARROT:
```

```
PARROT:Hit RETURN to continue
```

```
PARROT: @@ Optimization converged, try to add equilibrium 4 again
```

```
PARROT: ed
```

```
ED_EXP: read 1
```

```
ED_EXP: s-e 4
```

```
Equilibrium number           4, label AINV
```

```
ED_EXP: s-a-s
```

```
T /1203.096295/: 1200
```

```
Automatic start values for phase constituents? /N/: N
```

```
Phase LIQUID
```

```
Major constituent(s) /b/: b
```

```
Phase BCC
```

```
Major constituent(s) /b/: b
```

```
Phase FCC
```

```
Major constituent(s) /b/: b
```

```
ED_EXP:
```

```
ED_EXP: c-e
```

```
Testing result with global minimization
```

```
13 ITS, CPU TIME USED 0 SECONDS
```

```
ED_EXP: 1-e
```

```
OUTPUT TO SCREEN OR FILE /SCREEN/:
```

```
Options /WVCS/: WVCS
```

```
Output from POLY-3, equilibrium =        4, label AINV, database:
```

```
Conditions:
```

```
P=101325
```

```
FIXED PHASES
```

```
LIQUID=1 BCC#1=1 FCC=1
```

```
DEGREES OF FREEDOM 0
```

```
Temperature 1203.85 K ( 930.70 C), Pressure 1.013250E+05
```

```
Number of moles of components 3.00000E+00, Mass in grams 1.30090E+02
```

```
Total Gibbs energy -9.76906E+03, Enthalpy 1.98639E+04, Volume 0.00000E+00
```

| Component | Moles | W-Fraction | Activity | Potential | Ref.stat |
|-----------|------------|------------|------------|-------------|----------|
| A | 6.6368E-01 | 1.0203E-01 | 3.9406E-01 | -9.3214E+03 | SER |
| B | 2.3363E+00 | 8.9797E-01 | 8.5796E-01 | -1.5334E+03 | SER |

| FCC | Status | FIXED | Driving force | 0.0000E+00 |
|-------|-------------|------------------|----------------------------|-----------------|
| Moles | 1.0000E+00, | Mass 4.5879E+01, | Volume fraction 0.0000E+00 | Mass fractions: |
| B | 9.40119E-01 | A 5.98805E-02 | | |

```

BCC#1          Status FIXED      Driving force 0.0000E+00
Moles 1.0000E+00, Mass 4.5314E+01, Volume fraction 0.0000E+00 Mass fractions:
B 9.31057E-01 A 6.89427E-02

LIQUID          Status FIXED      Driving force 0.0000E+00
Moles 1.0000E+00, Mass 3.8896E+01, Volume fraction 0.0000E+00 Mass fractions:
B 8.09691E-01 A 1.90309E-01
SET_WEIGHT 0,,,
EXPERIMENT T=1203:DT
EXPERIMENT W(LIQUID,A)=0.19:DX
EXPERIMENT W(BCC#1,A)=6.9E-2:DX
EXPERIMENT W(FCC,A)=6E-2:DX
ED EXP: ba
PARROT: @@ It still fails, try to calculate the phase diagram again.
PARROT: mac tcecx36cpd
PARROT: set-echo
NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
POLY:
POLY: @@ In PARROT, the global minimization is turned off automatically.
POLY: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY: @@ message will be given.
POLY:
POLY: advanced-option global yes,,
Settings for global minimization:
*** WARNING *** Global equilibrium calculation may create new composition sets
and this may corrupt your PARROT work file (.PAR file).
Do not go back to PARROT but exit from POLY after your POLY calculations.
POLY:
POLY: def-com,,,
POLY: s-a-v 1 w(b) 0 1,,,
The condition W(B)=.1234 created
POLY: s-a-v 2 t 300 1700,,,
The condition T=942.2 created
POLY: s-c t=500
POLY: l-c
W(B)=0.1234, T=500
DEGREES OF FREEDOM 2
POLY: c-e
Creating condition P=1E5
Creating condition N=1
Using global minimization procedure
Calculated       628 grid points in      0 s
Found the set of lowest grid points in      0 s
Calculated POLY solution      0 s, total time      0 s
POLY: save tcecx36 y

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

POLY: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Generating start point 27
Generating start point 28

Phase region boundary 1 at: 7.140E-01 3.100E+02
   BCC#1
   ** BCC#2
Calculated..           2 equilibria
Terminating at axis limit.

Phase region boundary 2 at: 7.141E-01 3.000E+02
   BCC#1
   ** BCC#2
Calculated..           14 equilibria

Phase region boundary 3 at: 6.821E-01 7.253E+02

```

```

** A2B
  BCC#1
** BCC#2

Phase region boundary  4 at:  3.624E-01  7.253E+02
** A2B
  BCC#1
Calculated.          15 equilibria

Phase region boundary  5 at:  3.770E-01  1.193E+03
** LIQUID
** A2B
  BCC#1
Calculated.          30 equilibria

Phase region boundary  6 at:  2.826E-01  1.193E+03
** LIQUID
  BCC#1
Calculated.          33 equilibria

Phase region boundary  7 at:  4.862E-01  1.193E+03
** LIQUID
  A2B
Calculated.          33 equilibria

Phase region boundary  8 at:  6.501E-01  1.049E+03
** LIQUID
  A2B
** BCC#1
Calculated.          11 equilibria
Terminating at known equilibrium

Phase region boundary 10 at:  8.275E-01  1.049E+03
  LIQUID
** BCC#1
Calculated.          8 equilibria

Phase region boundary 11 at:  8.750E-01  1.204E+03
  LIQUID
** BCC#1
** FCC
Calculated.          31 equilibria

Phase region boundary 12 at:  8.803E-01  1.204E+03
  LIQUID
** FCC
Calculated.          31 equilibria

Phase region boundary 13 at:  9.356E-01  1.204E+03
  BCC#1
** FCC
Calculated.          21 equilibria

Phase region boundary 14 at:  7.140E-01  3.100E+02
  BCC#1
** BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 15 at:  7.140E-01  3.100E+02
  BCC#1
** BCC#2
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 16 at:  7.140E-01  3.100E+02
  BCC#1
** BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 17 at:  7.140E-01  3.100E+02
  BCC#1
** BCC#2
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 18 at:  7.140E-01  3.100E+02
  BCC#1
** BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 19 at:  7.140E-01  3.100E+02
  BCC#1
** BCC#2
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 20 at:  7.140E-01  3.100E+02
  BCC#1
** BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 21 at:  7.140E-01  3.100E+02
  BCC#1
** BCC#2
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 22 at:  7.140E-01  3.100E+02
  BCC#1
** BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 23 at:  7.140E-01  3.100E+02
  BCC#1
** BCC#2

```

```

Calculated..                                2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 24 at:    7.140E-01  3.100E+02
** BCC#1
BCC#2
Calculated.                               13 equilibria
Terminating at known equilibrium

Phase region boundary 25 at:    3.645E-01  7.700E+02
** A2B
BCC#1
Calculated.                               10 equilibria

Phase region boundary 26 at:    3.645E-01  7.700E+02
** A2B
BCC#1
Calculated.                               3 equilibria
Terminating at known equilibrium

Phase region boundary 27 at:    3.645E-01  7.700E+02
** A2B
BCC#1
Calculated.                               14 equilibria
Terminating at known equilibrium

Phase region boundary 28 at:    7.913E-01  7.700E+02
** A2B
BCC#1
Calculated.                               10 equilibria

Phase region boundary 29 at:    7.913E-01  7.700E+02
** A2B
BCC#1
Calculated.                               3 equilibria
Terminating at known equilibrium

Phase region boundary 30 at:    7.913E-01  7.700E+02
** A2B
BCC#1
Calculated.                               9 equilibria
Terminating at known equilibrium

Phase region boundary 31 at:    2.448E-01  1.230E+03
** LIQUID
BCC#1
Calculated.                               4 equilibria
Terminating at known equilibrium

Phase region boundary 32 at:    2.448E-01  1.230E+03
** LIQUID
BCC#1
Calculated.                               26 equilibria

Phase region boundary 33 at:    8.859E-01  1.230E+03
** LIQUID
FCC
Calculated.                               2 equilibria
Terminating at known equilibrium

Phase region boundary 34 at:    8.859E-01  1.230E+03
** LIQUID
FCC
Calculated.                               29 equilibria

Phase region boundary 35 at:    6.414E-03  1.397E+03
** BCC#1
Calculated.                               11 equilibria

Phase region boundary 36 at:    6.414E-03  1.397E+03
** LIQUID
** BCC#1
Calculated.                               13 equilibria
Terminating at known equilibrium

Phase region boundary 37 at:    2.298E-01  1.244E+03
** LIQUID
** BCC#1
Calculated.                               22 equilibria

Phase region boundary 38 at:    2.298E-01  1.244E+03
** LIQUID
** BCC#1
Calculated.                               4 equilibria
Terminating at known equilibrium

Phase region boundary 39 at:    6.122E-01  1.240E+03
** LIQUID
** A2B
Calculated.                               14 equilibria
Terminating at known equilibrium

Phase region boundary 40 at:    6.122E-01  1.240E+03
** LIQUID
** A2B
Calculated.                               8 equilibria
Terminating at known equilibrium

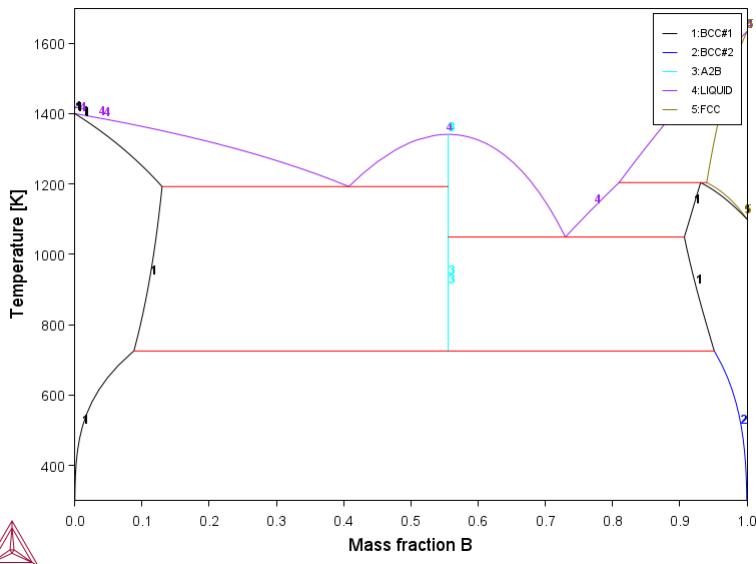
Phase region boundary 41 at:    9.927E-01  1.613E+03
** LIQUID
** FCC
Calculated.                               20 equilibria
Terminating at known equilibrium

Phase region boundary 42 at:    9.927E-01  1.613E+03
** LIQUID
** FCC
Calculated.                               13 equilibria
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\generate_console_examples\examples\tcex36a\tcex36.POLY3
CPU time for mapping                      1 seconds
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

```

```
POST: s-l d  
POST: plot
```



```
POST:  
POST: set-inter  
POST:Hit RETURN to continue  
POST: @@ Sometimes a very strange shape of the fcc phase here and no  
POST: @@ equilibrium between liq, fcc and bcc at high B content.  
POST: ba  
POLY: ba
```

```
PARROT VERSION 5.3  
Global minimization used as test only  
PARROT: l-r C SCREEN
```

```
=====  
OUTPUT FROM P A R R O T . DATE 2023. 4.27 16:26:27
```

```
*** SUCCESSFUL OPTIMIZATION. ***  
NUMBER OF ITERATIONS: 15
```

```
== OPTIMIZING CONDITIONS ==
```

```
RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N  
MINIMUM SAVE ON FILE: Y  
ERROR FOR INEQUALITIES = 1.00000000E+00  
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04  
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)  
MAXFUN = 30 DMAX = 1.00000000E+02 H = 1.00000000E-04  
ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03
```

```
== OPTIMIZING VARIABLES ==
```

```
AVAILABLE VARIABLES ARE V1 TO V00
```

| VAR. | VALUE | START VALUE | SCALING FACTOR | REL.STAND.DEV |
|------|-----------------|-----------------|-----------------|----------------|
| V1 | 2.03113219E+04 | 2.02694367E+04 | 2.02694367E+04 | 1.11597087E-01 |
| V2 | -2.93492365E+01 | -2.92138211E+01 | -2.92138211E+01 | 1.03070625E-01 |
| V11 | -2.17760708E+04 | -2.18126679E+04 | -2.18126679E+04 | 2.13585334E-01 |
| V12 | 1.52955219E+01 | 1.51783975E+01 | 1.51783975E+01 | 3.57094533E-01 |
| V15 | 2.41721137E+04 | 1.99045950E+04 | 1.99045950E+04 | 1.91672506E-01 |
| V16 | -8.30983887E+00 | -3.37369312E+00 | -3.37369312E+00 | 1.38270139E+00 |
| V17 | 3.09048341E+03 | 3.37316715E+03 | 3.37316715E+03 | 2.44072470E-01 |
| V19 | 2.20465939E+04 | -5.20289889E+04 | -5.20289889E+04 | 3.12880572E-01 |
| V20 | -6.99361189E+00 | 5.03479181E+01 | 5.03479181E+01 | 2.63983824E-01 |

```
NUMBER OF OPTIMIZING VARIABLES : 9  
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO  
THE SUM OF SQUARES HAS CHANGED FROM 1.42229051E+01 TO 9.74454544E-03  
DEGREES OF FREEDOM 16. REDUCED SUM OF SQUARES 6.09034090E-04
```

```
$ ===== BLOCK NUMBER 1
```

```
DEFINED CONSTANTS  
DX=2E-2, P0=101325, DH=500, DT=10  
DEFINED FUNCTIONS AND VARIABLES%  
HTR=HM(LIQUID)-HM(A2B)  
1 T=1193 1193. 10. -0.3486 -3.4861E-02  
1 W(LIQUID,B)=0.408 0.4077 2.00E-02 -3.1028E-04 -1.5514E-02  
1 W(BCC#1,B)=0.13 0.1300 2.00E-02 -4.8185E-05 -2.4093E-03  
2 T=1341 1341. 10. -1.3972E-02 -1.3972E-03  
2 HTR=3727 3724. 5.00E+02 -3.234 -6.4683E-03  
3 T=1049 1049. 10. 0.1281 1.2808E-02  
3 W(LIQUID,A)=0.27 0.2703 2.00E-02 2.5959E-04 1.2979E-02  
3 W(BCC#1,A)=9.3E-2 9.3177E-02 2.00E-02 1.7700E-04 8.8500E-03  
5 T=726 725.3 10. -0.6792 -6.7916E-02  
5 X(BCC#1,B)=3.7E-2 3.7176E-02 2.00E-02 1.7589E-04 8.7946E-03  
5 X(BCC#2,A)=0.114 0.1134 2.00E-02 -5.6864E-04 -2.8432E-02  
6 X(BCC#1,B)=3.7E-2 3.7366E-02 2.00E-02 3.6644E-04 1.8322E-02  
6 X(BCC#2,A)=0.114 0.1139 2.00E-02 -1.0239E-04 -5.1193E-03  
10 W(LIQUID,A)=2E-2 1.9547E-02 2.00E-02 -4.5316E-04 -2.2658E-02
```

```

11 W(LIQUID,A)=4.2E-2      4.1817E-02 2.00E-02 -1.8258E-04 -9.1289E-03
12 W(LIQUID,A)=6.5E-2      6.4885E-02 2.00E-02 -1.1464E-04 -5.7318E-03
13 W(LIQUID,A)=9.3E-2      9.2683E-02 2.00E-02 -3.1679E-04 -1.5840E-02
20 W(LIQUID,A)=0.104      0.1038 2.00E-02 -2.1584E-04 -1.0792E-02
20 W(FCC,A)=3.8E-2        3.8177E-02 2.00E-02 1.7672E-04 8.8361E-03
21 W(LIQUID,A)=0.136      0.1365 2.00E-02 5.0713E-04 2.5356E-02
21 W(FCC,A)=4.7E-2        4.7106E-02 2.00E-02 1.0572E-04 5.2861E-03
22 W(LIQUID,A)=0.187      0.1867 2.00E-02 -2.5247E-04 -1.2624E-02
22 W(FCC,A)=5.9E-2        5.9094E-02 2.00E-02 9.4476E-05 4.7238E-03
23 W(LIQUID,A)=0.245      0.2449 2.00E-02 -6.5002E-05 -3.2501E-03
23 W(BCC#1,A)=8.5E-2      8.5109E-02 2.00E-02 1.0930E-04 5.4648E-03

```

PARROT:
PARROT: @@ Note that all other experiments are well fitted.
PARROT: @@ Try to improve by optimizing a little more...
PARROT: resc
PARROT: opt 30
Use 25 experiments, maximum is 2000
Use 664 real workspace, maximum is 50000
The following output is provided by subroutine VA05A

```

AT THE 0 TH ITERATION WE HAVE THE SUM OF SQUARES 9.74454544E-03
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 1 ST ITERATION WE HAVE THE SUM OF SQUARES 9.46287292E-03
1 1.0001E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 2 ND ITERATION WE HAVE THE SUM OF SQUARES 1.01760795E-02
1 1.0001E+00 2 1.0001E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 3 RD ITERATION WE HAVE THE SUM OF SQUARES 1.12779746E-02
1 1.0001E+00 2 1.0000E+00 3 1.0001E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 4 TH ITERATION WE HAVE THE SUM OF SQUARES 8.64113625E-03
1 1.0001E+00 2 1.0000E+00 3 1.0000E+00 4 1.0001E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 5 TH ITERATION WE HAVE THE SUM OF SQUARES 8.98355304E-03
1 1.0001E+00 2 1.0000E+00 3 1.0000E+00 4 1.0001E+00 5 1.0001E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 6 TH ITERATION WE HAVE THE SUM OF SQUARES 8.57688356E-03
1 1.0001E+00 2 1.0000E+00 3 1.0000E+00 4 1.0001E+00 5 1.0000E+00
6 1.0001E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 7 TH ITERATION WE HAVE THE SUM OF SQUARES 8.57334286E-03
1 1.0001E+00 2 1.0000E+00 3 1.0000E+00 4 1.0001E+00 5 1.0000E+00
6 1.0001E+00 7 1.0001E+00 8 1.0000E+00 9 1.0000E+00

AT THE 8 TH ITERATION WE HAVE THE SUM OF SQUARES 8.56977404E-03
1 1.0001E+00 2 1.0000E+00 3 1.0000E+00 4 1.0001E+00 5 1.0000E+00
6 1.0001E+00 7 1.0001E+00 8 1.0001E+00 9 1.0000E+00

AT THE 9 TH ITERATION WE HAVE THE SUM OF SQUARES 8.56911730E-03
1 1.0001E+00 2 1.0000E+00 3 1.0000E+00 4 1.0001E+00 5 1.0000E+00
6 1.0001E+00 7 1.0001E+00 8 1.0001E+00 9 1.0001E+00

AT THE 10 TH ITERATION WE HAVE THE SUM OF SQUARES 7.44783934E-03
1 1.0003E+00 2 1.0000E+00 3 9.9986E-01 4 1.0002E+00 5 9.9991E-01
6 1.0001E+00 7 1.0001E+00 8 1.0001E+00 9 1.0001E+00

AT THE 11 TH ITERATION WE HAVE THE SUM OF SQUARES 7.00359799E-03
1 1.0003E+00 2 9.9999E-01 3 9.9987E-01 4 1.0002E+00 5 9.9989E-01
6 1.0000E+00 7 1.0001E+00 8 1.0002E+00 9 1.0003E+00

AT THE 12 TH ITERATION WE HAVE THE SUM OF SQUARES 6.60590931E-03
1 1.0004E+00 2 1.0001E+00 3 9.9985E-01 4 1.0003E+00 5 9.9985E-01
6 9.9976E-01 7 9.9998E-01 8 1.0004E+00 9 1.0007E+00

AT THE 13 TH ITERATION WE HAVE THE SUM OF SQUARES 6.17427348E-03
1 1.0004E+00 2 1.0000E+00 3 9.9988E-01 4 1.0004E+00 5 9.9974E-01
6 9.9929E-01 7 9.9982E-01 8 1.0008E+00 9 1.0016E+00

AT THE 14 TH ITERATION WE HAVE THE SUM OF SQUARES 5.66906876E-03
1 1.0005E+00 2 1.0001E+00 3 9.9991E-01 4 1.0006E+00 5 9.9953E-01
6 9.9831E-01 7 9.9949E-01 8 1.0017E+00 9 1.0033E+00

AT THE 15 TH ITERATION WE HAVE THE SUM OF SQUARES 5.09779201E-03
1 1.0006E+00 2 1.0000E+00 3 9.9999E-01 4 1.0008E+00 5 9.9905E-01
6 9.9637E-01 7 9.9884E-01 8 1.0034E+00 9 1.0067E+00

AT THE 16 TH ITERATION WE HAVE THE SUM OF SQUARES 4.81234015E-03
1 1.0006E+00 2 9.9994E-01 3 1.0001E+00 4 1.0012E+00 5 9.9829E-01
6 9.9334E-01 7 9.9782E-01 8 1.0060E+00 9 1.0120E+00

THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED 16 iterations
1 1.0006E+00 2 9.9994E-01 3 1.0001E+00 4 1.0012E+00 5 9.9829E-01
6 9.9334E-01 7 9.9782E-01 8 1.0060E+00 9 1.0120E+00

-3.1865E-02 2 -1.3193E-02 3 -4.4272E-03 4 1.7361E-03 5 -1.5956E-02
6 1.5790E-02 7 1.4972E-02 8 3.8578E-03 9 -3.8165E-03 10 2.0927E-02
11 -9.7839E-03 12 2.1463E-02 13 -8.4745E-03 14 -2.0909E-02 15 -6.0982E-03
16 -2.0333E-03 17 -1.2077E-02 18 -7.2009E-03 19 1.0768E-02 20 2.7874E-02
21 4.8281E-03 22 -1.3188E-02 23 -2.7045E-03 24 -1.7201E-03 25 1.8302E-05

```

THE SUM OF SQUARES IS 4.81234015E-03

PARROT: 1-r C SCREEN

```
=====
OUTPUT FROM P A R R O T . DATE 2023. 4.27 16:26:27
```

*** SUCCESSFUL OPTIMIZATION. ***
NUMBER OF ITERATIONS: 17

== OPTIMIZING CONDITIONS ==

```

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 30 DMAX = 1.00000000E+02 H = 1.00000000E-04
ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03

```

```
-- OPTIMIZING VARIABLES ==
```

```
AVAILABLE VARIABLES ARE V1 TO VOO
```

| VAR. | VALUE | START VALUE | SCALING FACTOR | REL.STAND.DEV |
|------|-----------------|-----------------|-----------------|----------------|
| V1 | 2.03241480E+04 | 2.03113219E+04 | 2.03113219E+04 | 1.07789751E-01 |
| V2 | -2.93474147E+01 | -2.93492365E+01 | -2.93492365E+01 | 9.90180593E-02 |
| V11 | -2.17781793E+04 | -2.17760708E+04 | -2.17760708E+04 | 2.12187949E-01 |
| V12 | 1.53144655E+01 | 1.52955219E+01 | 1.52955219E+01 | 3.48644514E-01 |
| V15 | 2.41307635E+04 | 2.41721137E+04 | 2.41721137E+04 | 1.52757863E-01 |
| V16 | -8.25451509E+00 | -8.30983887E+00 | -8.30983887E+00 | 5.44741433E-01 |
| V17 | 3.08373775E+03 | 3.09048341E+03 | 3.09048341E+03 | 2.65207592E-01 |
| V19 | 2.21799162E+04 | 2.20465939E+04 | 2.20465939E+04 | 7.22762929E-01 |
| V20 | -7.07722170E+00 | -6.99361189E+00 | -6.99361189E+00 | 1.85433581E+00 |

```
NUMBER OF OPTIMIZING VARIABLES : 9
```

```
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 9.74454544E-03 TO 4.81234015E-03
DEGREES OF FREEDOM 16. REDUCED SUM OF SQUARES 3.00771259E-04
```

```
$ ====== BLOCK NUMBER 1
```

```

DEFINED CONSTANTS
DX=2E-2, P0=101325, DH=500, DT=10
DEFINED FUNCTIONS AND VARIABLES%
HTR=HM(LIQUID)-HM(A2B)
1 T=1193. 1193. 10. -0.3187 -3.1865E-02
1 W(LIQUID,B)=0.408 0.4077 2.00E-02 -2.6385E-04 -1.3193E-02
1 W(BCC#1,B)=0.13 0.1299 2.00E-02 -8.8545E-05 -4.4272E-03
2 T=1341 1341. 10. 1.7361E-02 1.7361E-03
2 HTR=3727 3719. 5.00E+02 -7.978 -1.5956E-02
3 T=1049 1049. 10. 0.1579 1.5790E-02
3 W(LIQUID,A)=0.27 0.2703 2.00E-02 2.9945E-04 1.4972E-02
3 W(BCC#1,A)=9.3E-2 9.3077E-02 2.00E-02 7.7156E-05 3.8578E-03
5 T=726 726.0 10. -3.8165E-02 -3.8165E-03
5 X(BCC#1,B)=3.7E-2 3.7419E-02 2.00E-02 4.1853E-04 2.0927E-02
5 X(BCC#2,A)=0.114 0.1138 2.00E-02 -1.9568E-04 -9.7839E-03
6 X(BCC#1,B)=3.7E-2 3.7429E-02 2.00E-02 4.2926E-04 2.1463E-02
6 X(BCC#2,A)=0.114 0.1138 2.00E-02 -1.6949E-04 -8.4745E-03
10 W(LIQUID,A)=2E-2 1.9582E-02 2.00E-02 -4.1818E-04 -2.0909E-02
11 W(LIQUID,A)=4.2E-2 4.1878E-02 2.00E-02 -1.2196E-04 -6.0982E-03
12 W(LIQUID,A)=6.5E-2 6.4959E-02 2.00E-02 -4.0666E-05 -2.0333E-03
13 W(LIQUID,A)=9.3E-2 9.2758E-02 2.00E-02 -2.4154E-04 -1.2077E-02
20 W(LIQUID,A)=0.104 0.1039 2.00E-02 -1.4402E-04 -7.2009E-03
20 W(FCC,A)=3.8E-2 3.8215E-02 2.00E-02 2.1537E-04 1.0768E-02
21 W(LIQUID,A)=0.136 0.1366 2.00E-02 5.5747E-04 2.7874E-02
21 W(FCC,A)=4.7E-2 4.7097E-02 2.00E-02 9.6563E-05 4.8281E-03
22 W(LIQUID,A)=0.187 0.1867 2.00E-02 -2.6375E-04 -1.3188E-02
22 W(FCC,A)=5.9E-2 5.8946E-02 2.00E-02 -5.4090E-05 -2.7045E-03
23 W(LIQUID,A)=0.245 0.2450 2.00E-02 -3.4402E-05 -1.7201E-03
23 W(BCC#1,A)=8.5E-2 8.5000E-02 2.00E-02 3.6603E-07 1.8302E-05

```

```
PARROT:
```

```
PARROT: Hit RETURN to continue
```

```
PARROT: @@ Calculate the phase diagram again
```

```
PARROT: mac tce36cpd
```

```
PARROT: set-echo
```

```
NO SUCH COMMAND, USE HELP
```

```
PARROT: @@ Calculate the phase diagram
```

```
PARROT: @@ This TCM should be run in PARROT
```

```
PARROT: go p-3
```

```
POLY:
```

```
POLY: @@ In PARROT, the global minimization is turned off automatically.
```

```
POLY: @@ Back in POLY-3, one needs to turn it on manually, but a warning
```

```
POLY: @@ message will be given.
```

```
POLY:
```

```
POLY: advanced-option global yes,,
```

```
Settings for global minimization:
```

```
*** WARNING *** Global equilibrium calculation may create new composition sets
and this may corrupt your PARROT work file (.PAR file).
```

```
Do not go back to PARROT but exit from POLY after your POLY calculations.
```

```
POLY:
```

```
POLY: def-com,,,
```

```
POLY: s-a-v 1 w(b) 0 1,,,
```

```
The condition W(B)=.1234 created
```

```
POLY: s-a-v 2 t 300 1700,,,
```

```
The condition T=942.2 created
```

```
POLY: s-c t=500
```

```
POLY: l-c
```

```
W(B)=0.1234, T=500
```

```
DGREES OF FREEDOM 2
```

```
POLY: c-e
```

```
Creating condition P=1E5
```

```
Creating condition N=1
```

```
Using global minimization procedure
```

```
Calculated 628 grid points in 0 s
```

```
Found the set of lowest grid points in 0 s
```

```
Calculated POLY solution 0 s, total time 0 s
```

```
POLY: save tce36 y
```

```
This file contains results from a previous STEP or MAP command.
```

```
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.
```

```
POLY: map
```

```
Version S mapping is selected
```

```
Generating start equilibrium 1
```

```
Generating start equilibrium 2
```

```
Generating start equilibrium 3
```

```
Generating start equilibrium 4
```

```

Generating start equilibrium  5
Generating start equilibrium  6
Generating start equilibrium  7
Generating start equilibrium  8
Generating start equilibrium  9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Generating start point  1
Generating start point  2
Generating start point  3
Generating start point  4
Generating start point  5
Generating start point  6
Generating start point  7
Generating start point  8
Generating start point  9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Generating start point 27
Generating start point 28

Phase region boundary  1 at:  7.140E-01  3.100E+02
   BCC#1
   ** BCC#2
Calculated..          2 equilibria
Terminating at axis limit.

Phase region boundary  2 at:  7.141E-01  3.000E+02
   BCC#1
   ** BCC#2
Calculated.          14 equilibria

Phase region boundary  3 at:  6.821E-01  7.260E+02
   ** A2B
   BCC#1
   ** BCC#2
Calculated.          15 equilibria

Phase region boundary  4 at:  3.626E-01  7.260E+02
   ** A2B
   BCC#1
Calculated.          15 equilibria

Phase region boundary  5 at:  3.769E-01  1.193E+03
   ** LIQUID
   ** A2B
   BCC#1
Calculated.          26 equilibria

Phase region boundary  6 at:  2.826E-01  1.193E+03
   ** LIQUID
   BCC#1
Calculated.          26 equilibria

Phase region boundary  7 at:  4.863E-01  1.193E+03
   ** LIQUID
   A2B
Calculated.          33 equilibria

Phase region boundary  8 at:  6.500E-01  1.049E+03
   ** LIQUID
   A2B
   ** BCC#1
Calculated.          29 equilibria

Phase region boundary  9 at:  7.642E-01  1.049E+03
   A2B
   ** BCC#1
Calculated.          11 equilibria
Terminating at known equilibrium

Phase region boundary 10 at:  8.276E-01  1.049E+03
   LIQUID
   ** BCC#1
Calculated.          8 equilibria

Phase region boundary 11 at:  8.751E-01  1.204E+03
   LIQUID
   ** BCC#1
   ** FCC
Calculated.          29 equilibria

Phase region boundary 12 at:  8.804E-01  1.204E+03
   LIQUID
   ** FCC
Calculated.          29 equilibria

Phase region boundary 13 at:  9.358E-01  1.204E+03
   BCC#1
   ** FCC
Calculated.          18 equilibria

Phase region boundary 14 at:  7.140E-01  3.100E+02
   BCC#1
   ** BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

```

```

Phase region boundary 15 at: 7.140E-01 3.100E+02
    BCC#1
    ** BCC#2
Calculated..          2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 16 at: 7.140E-01 3.100E+02
    BCC#1
    ** BCC#2
Calculated..          13 equilibria
Terminating at known equilibrium

Phase region boundary 17 at: 7.140E-01 3.100E+02
    BCC#1
    ** BCC#2
Calculated..          2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 18 at: 7.140E-01 3.100E+02
    BCC#1
    ** BCC#2
Calculated..          13 equilibria
Terminating at known equilibrium

Phase region boundary 19 at: 7.140E-01 3.100E+02
    BCC#1
    ** BCC#2
Calculated..          2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 20 at: 7.140E-01 3.100E+02
    BCC#1
    ** BCC#2
Calculated..          13 equilibria
Terminating at known equilibrium

Phase region boundary 21 at: 7.140E-01 3.100E+02
    ** BCC#1
    BCC#2
Calculated..          2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 22 at: 7.140E-01 3.100E+02
    ** BCC#1
    BCC#2
Calculated..          13 equilibria
Terminating at known equilibrium

Phase region boundary 23 at: 7.140E-01 3.100E+02
    ** BCC#1
    BCC#2
Calculated..          2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 24 at: 7.140E-01 3.100E+02
    ** BCC#1
    BCC#2
Calculated..          13 equilibria
Terminating at known equilibrium

Phase region boundary 25 at: 3.646E-01 7.700E+02
    ** A2B
    BCC#1
Calculated..          10 equilibria

Phase region boundary 26 at: 3.646E-01 7.700E+02
    ** A2B
    BCC#1
Calculated..          3 equilibria
Terminating at known equilibrium

Phase region boundary 27 at: 3.646E-01 7.700E+02
    ** A2B
    BCC#1
Calculated..          14 equilibria
Terminating at known equilibrium

Phase region boundary 28 at: 7.912E-01 7.700E+02
    ** A2B
    BCC#1
Calculated..          10 equilibria

Phase region boundary 29 at: 7.912E-01 7.700E+02
    ** A2B
    BCC#1
Calculated..          3 equilibria
Terminating at known equilibrium

Phase region boundary 30 at: 7.912E-01 7.700E+02
    ** A2B
    BCC#1
Calculated..          9 equilibria
Terminating at known equilibrium

Phase region boundary 31 at: 2.448E-01 1.230E+03
    ** LIQUID
    BCC#1
Calculated..          4 equilibria
Terminating at known equilibrium

Phase region boundary 32 at: 2.448E-01 1.230E+03
    ** LIQUID
    BCC#1
Calculated..          26 equilibria

Phase region boundary 33 at: 8.860E-01 1.230E+03
    ** LIQUID
    FCC
Calculated..          2 equilibria
Terminating at known equilibrium

```

```

Phase region boundary 34 at: 8.860E-01 1.230E+03
** LIQUID
  FCC
Calculated           29 equilibria

Phase region boundary 35 at: 6.414E-03 1.397E+03
  LIQUID
** BCC#1
Calculated           12 equilibria

Phase region boundary 36 at: 6.414E-03 1.397E+03
  LIQUID
** BCC#1
Calculated           13 equilibria
Terminating at known equilibrium

Phase region boundary 37 at: 2.298E-01 1.244E+03
  LIQUID
** BCC#1
Calculated           19 equilibria
Terminating at known equilibrium

Phase region boundary 38 at: 2.298E-01 1.244E+03
  LIQUID
** BCC#1
Calculated           4 equilibria
Terminating at known equilibrium

Phase region boundary 39 at: 6.122E-01 1.240E+03
  LIQUID
** A2B
Calculated           14 equilibria
Terminating at known equilibrium

Phase region boundary 40 at: 6.122E-01 1.240E+03
  LIQUID
** A2B
Calculated           8 equilibria
Terminating at known equilibrium

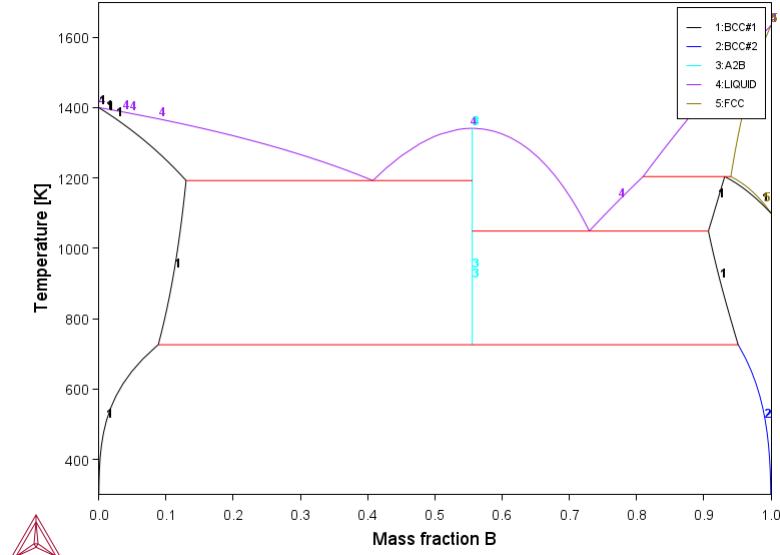
Phase region boundary 41 at: 9.927E-01 1.613E+03
  LIQUID
** FCC
Calculated           19 equilibria
Terminating at known equilibrium

Phase region boundary 42 at: 9.927E-01 1.613E+03
  LIQUID
** FCC
Calculated           10 equilibria
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\generate_console_examples\examples\tcex36a\tcex36.POLY3
CPU time for mapping      1 seconds
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

```

Setting automatic diagram axes

POST: s-l d
POST: plot



POST:
POST: set-inter
POST: Hit RETURN to continue
POST: ba
POLY: ba

PARROT VERSION 5.3

```

Global minimization used as test only
PARROT: @@ Now there is an equilibrium between fcc, bcc and liquid
PARROT: @@ at high B. Restore equilibrium 4 on the POP file
PARROT: ed
ED_EXP: read 1
ED_EXP: s-e 4
Equilibrium number          4, label AINV
ED_EXP: s-we 1
Equilibria (range) or label(s) /PRESENT/: PRESENT
ED_EXP: s-a-s
T /1203.096295/: 1200
Automatic start values for phase constituents? /N/: N

```

Phase LIQUID
Major constituent(s) /b/: b

Phase BCC
Major constituent(s) /b/: b
 Phase FCC
Major constituent(s) /b/: b
ED_EXP:
ED_EXP: c-e
 Testing result with global minimization
 13 ITS, CPU TIME USED 0 SECONDS
ED_EXP: l-e
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium = 4, label AINV, database:
 Conditions:
 P=101325
 FIXED PHASES
 LIQUID=1 BCC#1=1 FCC=1
 DEGREES OF FREEDOM 0
 Temperature 1203.86 K (930.71 C), Pressure 1.013250E+05
 Number of moles of components 3.00000E+00, Mass in grams 1.30108E+02
 Total Gibbs energy -9.75173E+03, Enthalpy 1.98662E+04, Volume 0.00000E+00
 Component Moles W-Fraction Activity Potential Ref.stat
 A 6.6307E-01 1.0193E-01 3.9435E-01 -9.3141E+03 SER
 B 2.3369E+00 8.9807E-01 8.5824E-01 -1.5302E+03 SER
 FCC Status FIXED Driving force 0.0000E+00
 Moles 1.0000E+00, Mass 4.5889E+01, Volume fraction 0.0000E+00 Mass fractions:
 B 9.40282E-01 A 5.97178E-02
 BCC#1 Status FIXED Driving force 0.0000E+00
 Moles 1.0000E+00, Mass 4.5321E+01, Volume fraction 0.0000E+00 Mass fractions:
 B 9.31176E-01 A 6.88242E-02
 LIQUID Status FIXED Driving force 0.0000E+00
 Moles 1.0000E+00, Mass 3.8897E+01, Volume fraction 0.0000E+00 Mass fractions:
 B 8.09709E-01 A 1.90291E-01
 EXPERIMENT T=1203:DT \$1203.86:10 NO=1
 EXPERIMENT W(LIQUID,A)=0.19:DX \$0.190291:2E-2 NO=2
 EXPERIMENT W(BCC#1,A)=6.9E-2:DX \$6.88242E-2:2E-2 NO=3
 EXPERIMENT W(FCC,A)=6E-2:DX \$5.97178E-2:2E-2 NO=4
ED_EXP: @@ Now equilibrium 4 is on the high B side
ED_EXP: save
ED_EXP: ba
PARROT: resc
PARROT: opt 0
 Use 29 experiments, maximum is 2000
 Use 740 real workspace, maximum is 50000
PARROT: l-r C SCREEN

```

=====
OUTPUT FROM P A R R O T . DATE 2023. 4.27 16:26:52

```

*** SUCCESSFUL OPTIMIZATION. ***
NUMBER OF ITERATIONS: 0

== OPTIMIZING CONDITIONS ==

```

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 0 DMAX = 1.00000000E+02 H = 1.00000000E-04
ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03

```

== OPTIMIZING VARIABLES ==

```

AVAILABLE VARIABLES ARE V1 TO V00

```

| VAR. | VALUE | START VALUE | SCALING FACTOR | REL.STAND.DEV |
|------|-----------------|-----------------|-----------------|----------------|
| V1 | 2.03241480E+04 | 2.03241480E+04 | 2.03241480E+04 | 0.00000000E+00 |
| V2 | -2.93474147E+01 | -2.93474147E+01 | -2.93474147E+01 | 0.00000000E+00 |
| V11 | -2.17781793E+04 | -2.17781793E+04 | -2.17781793E+04 | 0.00000000E+00 |
| V12 | 1.53144655E+01 | 1.53144655E+01 | 1.53144655E+01 | 0.00000000E+00 |
| V15 | 2.41307635E+04 | 2.41307635E+04 | 2.41307635E+04 | 0.00000000E+00 |
| V16 | -8.25451509E+00 | -8.25451509E+00 | -8.25451509E+00 | 0.00000000E+00 |
| V17 | 3.08373775E+03 | 3.08373775E+03 | 3.08373775E+03 | 0.00000000E+00 |
| V19 | 2.21799162E+04 | 2.21799162E+04 | 2.21799162E+04 | 0.00000000E+00 |
| V20 | -7.07722170E+00 | -7.07722170E+00 | -7.07722170E+00 | 0.00000000E+00 |

NUMBER OF OPTIMIZING VARIABLES : 9
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 0.00000000E+00 TO 1.26424758E-02
DEGREES OF FREEDOM 20. REDUCED SUM OF SQUARES 6.32123790E-04

\$ ===== BLOCK NUMBER 1

```

DEFINED CONSTANTS
DX=2E-2, P0=101325, DH=500, DT=10
DEFINED FUNCTIONS AND VARIABLES%
HTR=HM(LIQUID)-HM(A2B)
1 T=1193 1193. 10. -0.3187 -3.1865E-02
1 W(LIQUID,B)=0.408 0.4077 2.00E-02 -2.6385E-04 -1.3193E-02
1 W(BCC#1,B)=0.13 0.1299 2.00E-02 -8.8545E-05 -4.4272E-03
2 T=1341 1341. 10. 1.7361E-02 1.7361E-03
2 HTR=3727 3719. 5.00E+02 -7.978 -1.5956E-02
3 T=1049 1049. 10. 0.1579 1.5790E-02
3 W(LIQUID,A)=0.27 0.2703 2.00E-02 2.9945E-04 1.4972E-02
3 W(BCC#1,A)=9.3E-2 9.3077E-02 2.00E-02 7.7156E-05 3.8578E-03
4 T=1203 1204. 10. 0.8569 8.5689E-02
4 W(LIQUID,A)=0.19 0.1903 2.00E-02 2.9070E-04 1.4535E-02

```

```

4 W(BCC#1,A)=6.9E-2      6.8824E-02 2.00E-02 -1.7582E-04 -8.7909E-03
4 W(FCC,A)=6E-2          5.9718E-02 2.00E-02 -2.8217E-04 -1.4108E-02
5 T=726                   726.0       10.        -3.8165E-02 -3.8165E-03
5 X(BCC#1,B)=3.7E-2      3.7419E-02 2.00E-02 4.1853E-04 2.0927E-02
5 X(BCC#2,A)=0.114       0.1138      2.00E-02 -1.9568E-04 -9.7839E-03
6 X(BCC#1,B)=3.7E-2      3.7429E-02 2.00E-02 4.2926E-04 2.1463E-02
6 X(BCC#2,A)=0.114       0.1138      2.00E-02 -1.6949E-04 -8.4745E-03
10 W(LIQUID,A)=2E-2      1.9582E-02 2.00E-02 -4.1818E-04 -2.0909E-02
11 W(LIQUID,A)=4.2E-2     4.1878E-02 2.00E-02 -1.2196E-04 -6.0982E-03
12 W(LIQUID,A)=6.5E-2     6.4959E-02 2.00E-02 -4.0666E-05 -2.0333E-03
13 W(LIQUID,A)=9.3E-2     9.2758E-02 2.00E-02 -2.4154E-04 -1.2077E-02
20 W(LIQUID,A)=0.104      0.1039      2.00E-02 -1.4402E-04 -7.2009E-03
20 W(FCC,A)=3.8E-2       3.8215E-02 2.00E-02 2.1537E-04 1.0768E-02
21 W(LIQUID,A)=0.136      0.1366      2.00E-02 5.5747E-04 2.7874E-02
21 W(FCC,A)=4.7E-2       4.7097E-02 2.00E-02 9.6563E-05 4.8281E-03
22 W(LIQUID,A)=0.187      0.1867      2.00E-02 -2.6375E-04 -1.3188E-02
22 W(FCC,A)=5.9E-2       5.8946E-02 2.00E-02 -5.4090E-05 -2.7045E-03
23 W(LIQUID,A)=0.245      0.2450      2.00E-02 -3.4402E-05 -1.7201E-03
23 W(BCC#1,A)=8.5E-2     8.5000E-02 2.00E-02 3.6603E-07 1.8302E-05

```

PARROT:
PARROT: Hit RETURN to continue

PARROT: opt 30

Use 29 experiments, maximum is 2000

Use 740 real workspace, maximum is 50000

The following output is provided by subroutine VA05A

```

AT THE 0 TH ITERATION WE HAVE THE SUM OF SQUARES 1.26424758E-02
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 1 ST ITERATION WE HAVE THE SUM OF SQUARES 1.34796802E-02
1 1.0001E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 2 ND ITERATION WE HAVE THE SUM OF SQUARES 1.53664207E-02
1 1.0000E+00 2 1.0001E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 3 RD ITERATION WE HAVE THE SUM OF SQUARES 1.28798434E-02
1 1.0000E+00 2 1.0000E+00 3 1.0001E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 4 TH ITERATION WE HAVE THE SUM OF SQUARES 1.32465571E-02
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0001E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 5 TH ITERATION WE HAVE THE SUM OF SQUARES 1.08001950E-02
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0001E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 6 TH ITERATION WE HAVE THE SUM OF SQUARES 1.15155757E-02
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0001E+00
6 1.0001E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 7 TH ITERATION WE HAVE THE SUM OF SQUARES 1.09510442E-02
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0001E+00
6 1.0000E+00 7 1.0001E+00 8 1.0000E+00 9 1.0000E+00

AT THE 8 TH ITERATION WE HAVE THE SUM OF SQUARES 1.22381754E-02
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0001E+00
6 1.0000E+00 7 1.0000E+00 8 1.0001E+00 9 1.0000E+00

AT THE 9 TH ITERATION WE HAVE THE SUM OF SQUARES 1.03010801E-02
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0001E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 10 TH ITERATION WE HAVE THE SUM OF SQUARES 6.86871314E-03
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 9.9998E-01 5 1.0003E+00
6 9.9991E-01 7 9.9998E-01 8 9.9981E-01 9 1.0002E+00

AT THE 11 TH ITERATION WE HAVE THE SUM OF SQUARES 6.73254515E-03
1 1.0000E+00 2 1.0001E+00 3 9.9991E-01 4 9.9983E-01 5 1.0003E+00
6 1.0000E+00 7 9.9992E-01 8 9.9986E-01 9 1.0004E+00

AT THE 12 TH ITERATION WE HAVE THE SUM OF SQUARES 6.56656708E-03
1 1.0001E+00 2 1.0001E+00 3 9.9970E-01 4 9.9952E-01 5 1.0003E+00
6 1.0002E+00 7 9.9981E-01 8 9.9993E-01 9 1.0008E+00

AT THE 13 TH ITERATION WE HAVE THE SUM OF SQUARES 6.33995780E-03
1 1.0003E+00 2 1.0003E+00 3 9.9930E-01 4 9.9888E-01 5 1.0004E+00
6 1.0006E+00 7 9.9958E-01 8 1.0001E+00 9 1.0017E+00

AT THE 14 TH ITERATION WE HAVE THE SUM OF SQUARES 6.07822334E-03
1 1.0007E+00 2 1.0006E+00 3 9.9852E-01 4 9.9761E-01 5 1.0004E+00
6 1.0015E+00 7 9.9912E-01 8 1.0005E+00 9 1.0034E+00

AT THE 15 TH ITERATION WE HAVE THE SUM OF SQUARES 5.98271436E-03
1 1.0010E+00 2 1.0010E+00 3 9.9763E-01 4 9.9616E-01 5 1.0005E+00
6 1.0024E+00 7 9.9860E-01 8 1.0009E+00 9 1.0053E+00

THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED 15 iterations
1 1.0010E+00 2 1.0010E+00 3 9.9763E-01 4 9.9616E-01 5 1.0005E+00
6 1.0024E+00 7 9.9860E-01 8 1.0009E+00 9 1.0053E+00

1 -3.4110E-02 2 -1.6134E-02 3 -4.8976E-03 4 2.9028E-03 5 -7.2607E-03
6 1.1782E-02 7 1.1607E-02 8 3.8729E-03 9 7.2213E-03 10 2.9067E-02
11 -5.8157E-03 12 -5.4689E-03 13 -2.8369E-03 14 2.3683E-02 15 -9.7509E-03
16 2.4082E-02 17 -8.7767E-03 18 -2.1085E-02 19 -6.5180E-03 20 -2.7324E-03
21 -1.3089E-02 22 -8.3120E-03 23 1.2190E-02 24 2.6627E-02 25 7.4285E-03
26 -1.3946E-02 27 2.4126E-03 28 -7.2773E-03 29 -1.5808E-03

```

THE SUM OF SQUARES IS 5.98271436E-03

PARROT: 1-r C SCREEN

=====
OUTPUT FROM P A R R O T . DATE 2023. 4.27 16:26:52

*** SUCCESSFUL OPTIMIZATION. ***
NUMBER OF ITERATIONS: 16

```

== OPTIMIZING CONDITIONS ==
RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 30 DMAX = 1.00000000E+02 H = 1.00000000E-04
ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03

```

```

== OPTIMIZING VARIABLES ==

```

```

AVAILABLE VARIABLES ARE V1 TO V00

```

| VAR. | VALUE | START VALUE | SCALING FACTOR | REL.STAND.DEV |
|------|-----------------|-----------------|-----------------|----------------|
| V1 | 2.03454575E+04 | 2.03241480E+04 | 2.03241480E+04 | 1.02425063E-01 |
| V2 | -2.93769523E+01 | -2.93474147E+01 | -2.93474147E+01 | 9.37774032E-02 |
| V11 | -2.17266504E+04 | -2.17781793E+04 | -2.17781793E+04 | 2.00756550E-01 |
| V12 | 1.52556784E+01 | 1.53144655E+01 | 1.53144655E+01 | 3.29254808E-01 |
| V15 | 2.41427067E+04 | 2.41307635E+04 | 2.41307635E+04 | 1.34941848E-01 |
| V16 | -8.27426942E+00 | -8.25451509E+00 | -8.25451509E+00 | 4.84810452E-01 |
| V17 | 3.07943184E+03 | 3.08373775E+03 | 3.08373775E+03 | 2.31437249E-01 |
| V19 | 2.21987820E+04 | 2.21799162E+04 | 2.21799162E+04 | 5.66916492E-01 |
| V20 | -7.11452781E+00 | -7.07722170E+00 | -7.07722170E+00 | 1.53543798E+00 |

```

NUMBER OF OPTIMIZING VARIABLES : 9

```

```

ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 1.26424758E-02 TO 5.98271436E-03
DEGREES OF FREEDOM 20. REDUCED SUM OF SQUARES 2.99135718E-04

```

```

$ ====== BLOCK NUMBER 1

```

```

DEFINED CONSTANTS
DX=2E-2, PO=101325, DH=500, DT=10

```

```

DEFINED FUNCTIONS AND VARIABLES%

```

| HTR=HM(LIQUID)-HM(A2B) | T=1193 | 1193. | 10. | -0.3411 | -3.4110E-02 |
|------------------------|--------|------------|----------|-------------|-------------|
| 1 W(LIQUID,B)=0.408 | 1 | 0.4077 | 2.00E-02 | -3.2268E-04 | -1.6134E-02 |
| 1 W(BCC#1,B)=0.13 | 1 | 0.1299 | 2.00E-02 | -9.7952E-05 | -4.8976E-03 |
| 2 T=1341 | 2 | 1341. | 10. | 2.9028E-02 | 2.9028E-03 |
| 2 HTR=3727 | 2 | 3723. | 5.00E+02 | -3.630 | -7.2607E-03 |
| 3 T=1049 | 3 | 1049. | 10. | 0.1178 | 1.1782E-02 |
| 3 W(LIQUID,A)=0.27 | 3 | 0.2702 | 2.00E-02 | 2.3215E-04 | 1.1607E-02 |
| 3 W(BCC#1,A)=9.3E-2 | 3 | 9.3077E-02 | 2.00E-02 | 7.7458E-05 | 3.8729E-03 |
| 4 T=1203 | 4 | 1203. | 10. | 7.2213E-02 | 7.2213E-03 |
| 4 W(LIQUID,A)=0.19 | 4 | 0.1906 | 2.00E-02 | 5.8134E-04 | 2.9067E-02 |
| 4 W(BCC#1,A)=6.9E-2 | 4 | 6.8884E-02 | 2.00E-02 | -1.1631E-04 | -5.8157E-03 |
| 4 W(FCC,A)=6E-2 | 4 | 5.9891E-02 | 2.00E-02 | -1.0938E-04 | -5.4689E-03 |
| 5 T=726 | 5 | 726.0 | 10. | -2.8369E-02 | -2.8369E-03 |
| 5 X(BCC#1,B)=3.7E-2 | 5 | 3.7474E-02 | 2.00E-02 | 4.7365E-04 | 2.3683E-02 |
| 5 X(BCC#2,A)=0.114 | 5 | 0.1138 | 2.00E-02 | -1.9502E-04 | -9.7509E-03 |
| 6 X(BCC#1,B)=3.7E-2 | 6 | 3.7482E-02 | 2.00E-02 | 4.8165E-04 | 2.4082E-02 |
| 6 X(BCC#2,A)=0.114 | 6 | 0.1138 | 2.00E-02 | -1.7553E-04 | -8.7767E-03 |
| 10 W(LIQUID,A)=2E-2 | 10 | 1.9578E-02 | 2.00E-02 | -4.2170E-04 | -2.1085E-02 |
| 11 W(LIQUID,A)=4.2E-2 | 11 | 4.1870E-02 | 2.00E-02 | -1.3036E-04 | -6.5180E-03 |
| 12 W(LIQUID,A)=6.5E-2 | 12 | 6.4945E-02 | 2.00E-02 | -5.4648E-05 | -2.7324E-03 |
| 13 W(LIQUID,A)=9.3E-2 | 13 | 9.2738E-02 | 2.00E-02 | -2.6178E-04 | -1.3089E-02 |
| 20 W(LIQUID,A)=0.104 | 20 | 0.1038 | 2.00E-02 | -1.6624E-04 | -8.3120E-03 |
| 20 W(FCC,A)=3.8E-2 | 20 | 3.8244E-02 | 2.00E-02 | 2.4381E-04 | 1.2190E-02 |
| 21 W(LIQUID,A)=0.136 | 21 | 0.1365 | 2.00E-02 | 5.3254E-04 | 2.6627E-02 |
| 21 W(FCC,A)=4.7E-2 | 21 | 4.7149E-02 | 2.00E-02 | 1.4857E-04 | 7.4285E-03 |
| 22 W(LIQUID,A)=0.187 | 22 | 0.1867 | 2.00E-02 | -2.7892E-04 | -1.3946E-02 |
| 22 W(FCC,A)=5.9E-2 | 22 | 5.9048E-02 | 2.00E-02 | 4.8251E-05 | 2.4126E-03 |
| 23 W(LIQUID,A)=0.245 | 23 | 0.2449 | 2.00E-02 | -1.4555E-04 | -7.2773E-03 |
| 23 W(BCC#1,A)=8.5E-2 | 23 | 8.4968E-02 | 2.00E-02 | -3.1616E-05 | -1.5808E-03 |

```

PARROT:

```

```

PARROT:

```

```

PARROT:Hit RETURN to continue

```

```

PARROT: @@ Now optimize all parameters and all experiments

```

```

PARROT: l-a-v

```

```

OUTPUT TO SCREEN OR FILE /SCREEN/:

```

```

== OPTIMIZING VARIABLES ==

```

```

AVAILABLE VARIABLES ARE V1 TO V00

```

| VAR. | VALUE | START VALUE | SCALING FACTOR | REL.STAND.DEV |
|------|-----------------|-----------------|-----------------|----------------|
| V1 | 2.03454575E+04 | 2.03241480E+04 | 2.03241480E+04 | 1.02425063E-01 |
| V2 | -2.93769523E+01 | -2.93474147E+01 | -2.93474147E+01 | 9.37774032E-02 |
| V11 | -2.17266504E+04 | -2.17781793E+04 | -2.17781793E+04 | 2.00756550E-01 |
| V12 | 1.52556784E+01 | 1.53144655E+01 | 1.53144655E+01 | 3.29254808E-01 |
| V15 | 2.41427067E+04 | 2.41307635E+04 | 2.41307635E+04 | 1.34941848E-01 |
| V16 | -8.27426942E+00 | -8.25451509E+00 | -8.25451509E+00 | 4.84810452E-01 |
| V17 | 3.07943184E+03 | 3.08373775E+03 | 3.08373775E+03 | 2.31437249E-01 |
| V19 | 2.21987820E+04 | 2.21799162E+04 | 2.21799162E+04 | 5.66916492E-01 |
| V20 | -7.11452781E+00 | -7.07722170E+00 | -7.07722170E+00 | 1.53543798E+00 |

```

NUMBER OF OPTIMIZING VARIABLES : 9

```

```

ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 1.26424758E-02 TO 5.98271436E-03
DEGREES OF FREEDOM 20. REDUCED SUM OF SQUARES 2.99135718E-04

```

```

PARROT: s-o-v 11-12

```

```

PARROT: ed

```

```

ED_EXP: read 1

```

```

ED_EXP: c-a

```

| Eq | Lab | Iter | Weight | Temp | Exp | Fix phases or comments |
|----|------|------|--------|--------|-----|------------------------|
| 1 | AINV | 2 | 1. | 1192.7 | | LIQUID A2B BCC |
| 2 | AINV | 2 | 1. | 1341.0 | | LIQUID A2B |
| 3 | AINV | 2 | 1. | 1049.1 | | LIQUID A2B BCC |
| 4 | AINV | 2 | 1. | 1203.1 | | LIQUID BCC FCC |
| 5 | AINV | 2 | 1. | 726.0 | | A2B BCC BCC#2 |
| 6 | AINV | 2 | 1. | 726.0 | | BCC BCC#2 |
| 10 | ALF | 2 | 1. | 1594.0 | | LIQUID FCC |
| 11 | ALF | 2 | 1. | 1548.0 | | LIQUID FCC |
| 12 | ALF | 2 | 1. | 1499.0 | | LIQUID FCC |
| 13 | ALF | 2 | 1. | 1438.0 | | LIQUID FCC |

```

20 ATIE 2 1. 1413.0 LIQUID FCC
21 ATIE 2 1. 1337.0 LIQUID FCC
22 ATIE 2 1. 1213.0 LIQUID FCC
23 ATIE 2 1. 1100.0 LIQUID BCC
100 AA < unused > 1573.0 LIQUID
101 AA < unused > 1573.0 LIQUID
102 AA < unused > 1573.0 LIQUID
103 AA < unused > 1573.0 LIQUID
104 AA < unused > 1573.0 LIQUID
105 AA < unused > 1573.0 LIQUID
106 AA < unused > 1573.0 LIQUID
107 AA < unused > 1573.0 LIQUID
108 AA < unused > 1573.0 LIQUID
110 AH < unused > 1773.0 LIQUID
111 AH < unused > 1773.0 LIQUID
112 AH < unused > 1773.0 LIQUID
113 AH < unused > 1773.0 LIQUID
114 AH < unused > 1773.0 LIQUID
115 AH < unused > 1773.0 LIQUID
116 AH < unused > 1773.0 LIQUID
117 AH < unused > 1773.0 LIQUID
118 AH < unused > 1773.0 LIQUID
ED_EXP: s-we 1 100-118
ED_EXP: s-e 1
Equilibrium number 1, label AINV
ED_EXP: c-a
Eq Lab Iter Weight Temp Exp Fix phases or comments
 1 AINV 2 1. 1192.7 LIQUID A2B BCC
 2 AINV 2 1. 1341.0 LIQUID A2B
 3 AINV 2 1. 1049.1 LIQUID A2B BCC
 4 AINV 2 1. 1203.1 LIQUID BCC FCC
 5 AINV 2 1. 726.0 A2B BCC BCC#2
 6 AINV 2 1. 726.0 BCC BCC#2
 10 ALF 2 1. 1594.0 LIQUID FCC
 11 ALF 2 1. 1548.0 LIQUID FCC
 12 ALF 2 1. 1499.0 LIQUID FCC
 13 ALF 2 1. 1438.0 LIQUID FCC
 20 ATIE 2 1. 1413.0 LIQUID FCC
 21 ATIE 2 1. 1337.0 LIQUID FCC
 22 ATIE 2 1. 1213.0 LIQUID FCC
 23 ATIE 2 1. 1100.0 LIQUID BCC
100 AA 2 1. 1573.0 LIQUID
101 AA 2 1. 1573.0 LIQUID
102 AA 2 1. 1573.0 LIQUID
103 AA 2 1. 1573.0 LIQUID
104 AA 2 1. 1573.0 LIQUID
105 AA 2 1. 1573.0 LIQUID
106 AA 2 1. 1573.0 LIQUID
107 AA 2 1. 1573.0 LIQUID
108 AA 2 1. 1573.0 LIQUID
110 AH 2 1. 1773.0 LIQUID
111 AH 2 1. 1773.0 LIQUID
112 AH 2 1. 1773.0 LIQUID
113 AH 2 1. 1773.0 LIQUID
114 AH 2 1. 1773.0 LIQUID
115 AH 2 1. 1773.0 LIQUID
116 AH 2 1. 1773.0 LIQUID
117 AH 2 1. 1773.0 LIQUID
118 AH 2 1. 1773.0 LIQUID
ED_EXP: save
ED_EXP: ba
PARROT: opt 30
Use      47 experiments, maximum is      2000
Use      1082 real workspace, maximum is   50000
The following output is provided by subroutine VA05A

      AT THE 0 TH ITERATION WE HAVE THE SUM OF SQUARES 8.33570265E-02
1 1.0010E+00 2 1.0010E+00 3 1.0000E+00 4 1.0000E+00 5 1.0005E+00
6 1.0024E+00 7 9.9860E-01 8 1.0009E+00 9 1.0053E+00

      AT THE 1 ST ITERATION WE HAVE THE SUM OF SQUARES 8.41937045E-02
1 1.0011E+00 2 1.0010E+00 3 1.0000E+00 4 1.0000E+00 5 1.0005E+00
6 1.0024E+00 7 9.9860E-01 8 1.0009E+00 9 1.0053E+00

      AT THE 2 ND ITERATION WE HAVE THE SUM OF SQUARES 8.60717820E-02
1 1.0010E+00 2 1.0011E+00 3 1.0000E+00 4 1.0000E+00 5 1.0005E+00
6 1.0024E+00 7 9.9860E-01 8 1.0009E+00 9 1.0053E+00

      AT THE 3 RD ITERATION WE HAVE THE SUM OF SQUARES 8.25035987E-02
1 1.0010E+00 2 1.0010E+00 3 1.0001E+00 4 1.0000E+00 5 1.0005E+00
6 1.0024E+00 7 9.9860E-01 8 1.0009E+00 9 1.0053E+00

      AT THE 4 TH ITERATION WE HAVE THE SUM OF SQUARES 8.29656474E-02
1 1.0010E+00 2 1.0010E+00 3 1.0001E+00 4 1.0001E+00 5 1.0005E+00
6 1.0024E+00 7 9.9860E-01 8 1.0009E+00 9 1.0053E+00

      AT THE 5 TH ITERATION WE HAVE THE SUM OF SQUARES 8.28360165E-02
1 1.0010E+00 2 1.0010E+00 3 1.0001E+00 4 1.0000E+00 5 1.0006E+00
6 1.0024E+00 7 9.9860E-01 8 1.0009E+00 9 1.0053E+00

      AT THE 6 TH ITERATION WE HAVE THE SUM OF SQUARES 8.24869746E-02
1 1.0010E+00 2 1.0010E+00 3 1.0001E+00 4 1.0000E+00 5 1.0005E+00
6 1.0025E+00 7 9.9860E-01 8 1.0009E+00 9 1.0053E+00

      AT THE 7 TH ITERATION WE HAVE THE SUM OF SQUARES 8.24932705E-02
1 1.0010E+00 2 1.0010E+00 3 1.0001E+00 4 1.0000E+00 5 1.0005E+00
6 1.0025E+00 7 9.9870E-01 8 1.0009E+00 9 1.0053E+00

      AT THE 8 TH ITERATION WE HAVE THE SUM OF SQUARES 8.26745409E-02
1 1.0010E+00 2 1.0010E+00 3 1.0001E+00 4 1.0000E+00 5 1.0005E+00
6 1.0025E+00 7 9.9860E-01 8 1.0010E+00 9 1.0053E+00

      AT THE 9 TH ITERATION WE HAVE THE SUM OF SQUARES 8.24684053E-02
1 1.0010E+00 2 1.0010E+00 3 1.0001E+00 4 1.0000E+00 5 1.0005E+00
6 1.0025E+00 7 9.9860E-01 8 1.0009E+00 9 1.0054E+00

      AT THE 10 TH ITERATION WE HAVE THE SUM OF SQUARES 8.18224864E-02
1 1.0010E+00 2 1.0011E+00 3 1.0001E+00 4 9.9998E-01 5 1.0005E+00
6 1.0026E+00 7 9.9862E-01 8 1.0008E+00 9 1.0053E+00

      AT THE 11 TH ITERATION WE HAVE THE SUM OF SQUARES 8.12660409E-02
1 1.0010E+00 2 1.0010E+00 3 1.0002E+00 4 9.9994E-01 5 1.0005E+00
6 1.0026E+00 7 9.9863E-01 8 1.0008E+00 9 1.0053E+00

      AT THE 12 TH ITERATION WE HAVE THE SUM OF SQUARES 8.05808485E-02

```

```

1 1.0010E+00 2 1.0011E+00 3 1.0002E+00 4 9.9991E-01 5 1.0005E+00
6 1.0028E+00 7 9.9866E-01 8 1.0007E+00 9 1.0052E+00

    AT THE 13 TH ITERATION WE HAVE THE SUM OF SQUARES 7.96879372E-02
1 1.0011E+00 2 1.0011E+00 3 1.0002E+00 4 9.9982E-01 5 1.0006E+00
6 1.0030E+00 7 9.9872E-01 8 1.0006E+00 9 1.0050E+00

    AT THE 14 TH ITERATION WE HAVE THE SUM OF SQUARES 7.83108964E-02
1 1.0011E+00 2 1.0012E+00 3 1.0002E+00 4 9.9969E-01 5 1.0007E+00
6 1.0036E+00 7 9.9884E-01 8 1.0002E+00 9 1.0046E+00

    AT THE 15 TH ITERATION WE HAVE THE SUM OF SQUARES 7.61191324E-02
1 1.0012E+00 2 1.0014E+00 3 1.0002E+00 4 9.9942E-01 5 1.0009E+00
6 1.0048E+00 7 9.9909E-01 8 9.9962E-01 9 1.0039E+00

    AT THE 16 TH ITERATION WE HAVE THE SUM OF SQUARES 7.26636708E-02
1 1.0014E+00 2 1.0017E+00 3 1.0003E+00 4 9.9891E-01 5 1.0013E+00
6 1.0072E+00 7 9.9960E-01 8 9.9838E-01 9 1.0024E+00

    AT THE 17 TH ITERATION WE HAVE THE SUM OF SQUARES 6.84347888E-02
1 1.0019E+00 2 1.0023E+00 3 1.0003E+00 4 9.9787E-01 5 1.0022E+00
6 1.0120E+00 7 1.0006E+00 8 9.9591E-01 9 9.9958E-01

    AT THE 18 TH ITERATION WE HAVE THE SUM OF SQUARES 6.73854818E-02
1 1.0022E+00 2 1.0028E+00 3 1.0003E+00 4 9.9703E-01 5 1.0030E+00
6 1.0160E+00 7 1.0014E+00 8 9.9405E-01 9 9.9767E-01

THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED 18 iterations
1 1.0022E+00 2 1.0028E+00 3 1.0003E+00 4 9.9703E-01 5 1.0030E+00
6 1.0160E+00 7 1.0014E+00 8 9.9405E-01 9 9.9767E-01

1 -5.7840E-02 2 -9.3600E-03 3 1.4182E-02 4 2.0795E-02 5 -2.5749E-02
6 -5.2102E-02 7 1.9270E-02 8 2.6821E-02 9 1.3107E-02 10 2.7155E-02
11 8.7712E-03 12 1.3244E-02 13 -4.8660E-02 14 2.1787E-02 15 4.7259E-03
16 2.8667E-02 17 2.1548E-02 18 -2.2040E-02 19 -8.2405E-03 20 -4.9758E-03
21 -1.5646E-02 22 -1.0901E-02 23 1.5212E-02 24 2.4270E-02 25 1.4695E-02
26 -1.4884E-02 27 2.0284E-02 28 -1.2749E-02 29 1.5398E-02 30 -9.5907E-03
31 -1.6831E-02 32 2.7436E-02 33 8.7019E-02 34 1.2434E-01 35 1.0168E-01
36 -1.7318E-02 37 7.0579E-02 38 -1.9476E-02 39 1.6076E-02 40 4.5469E-02
41 4.8178E-02 42 4.6204E-02 43 4.1546E-02 44 3.4204E-02 45 2.2178E-02
46 7.4692E-03 47 -1.1924E-02
```

THE SUM OF SQUARES IS 6.73854818E-02

PARROT: l-r C SCREEN

```
=====
OUTPUT FROM P A R R O T . DATE 2023. 4.27 16:26:52
```

*** SUCCESSFUL OPTIMIZATION. ***
NUMBER OF ITERATIONS: 19

== OPTIMIZING CONDITIONS ==

```
RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 30 DMAX = 1.00000000E+02 H = 1.00000000E-04
ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03
```

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO VOO

| VAR. | VALUE | START VALUE | SCALING FACTOR | REL.STAND.DEV |
|------|-----------------|-----------------|-----------------|----------------|
| V1 | 2.03690179E+04 | 2.03241480E+04 | 2.03241480E+04 | 2.99180591E-02 |
| V2 | -2.94289024E+01 | -2.93474147E+01 | -2.93474147E+01 | 2.27345071E-02 |
| V11 | -2.17329087E+04 | -2.17266504E+04 | -2.17266504E+04 | 3.48585256E-02 |
| V12 | 1.52104360E+01 | 1.52556784E+01 | 1.52556784E+01 | 5.50983410E-02 |
| V15 | 2.42024574E+04 | 2.41307635E+04 | 2.41307635E+04 | 8.32025762E-02 |
| V16 | -8.38635734E+00 | -8.25451509E+00 | -8.25451509E+00 | 2.56507888E-01 |
| V17 | 3.08808414E+03 | 3.08373775E+03 | 3.08373775E+03 | 2.30206897E-01 |
| V19 | 2.20479620E+04 | 2.21799162E+04 | 2.21799162E+04 | 4.85909938E-01 |
| V20 | -7.06072567E+00 | -7.07722170E+00 | -7.07722170E+00 | 1.21873157E+00 |

NUMBER OF OPTIMIZING VARIABLES : 9
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 8.33570265E-02 TO 6.73854818E-02
DEGREES OF FREEDOM 38. REDUCED SUM OF SQUARES 1.77330215E-03

\$ ===== BLOCK NUMBER 1

DEFINED CONSTANTS
DX=2E-2, P0=101325, DH=500, DT=10

DEFINED FUNCTIONS AND VARIABLES%
HTR=HM(LIQUID)-HM(A2B)

| | | | | |
|-----------------------|------------|----------|-------------|-------------|
| 1 T=1193 | 1192. | 10. | -0.5784 | -5.7840E-02 |
| 1 W(LIQUID,B)=0.408 | 0.4078 | 2.00E-02 | -1.8720E-04 | -9.3600E-03 |
| 1 W(BCC#1,B)=0.13 | 0.1303 | 2.00E-02 | 2.8363E-04 | 1.4182E-02 |
| 2 T=1341 | 1341. | 10. | 0.2079 | 2.0795E-02 |
| 2 HTR=3727 | 3714. | 5.00E+02 | -12.87 | -2.5749E-02 |
| 3 T=1049 | 1048. | 10. | -0.5210 | -5.2102E-02 |
| 3 W(LIQUID,A)=0.27 | 0.2704 | 2.00E-02 | 3.8540E-04 | 1.9270E-02 |
| 3 W(BCC#1,A)=9.3E-2 | 9.3536E-02 | 2.00E-02 | 5.3643E-04 | 2.6821E-02 |
| 4 T=1203 | 1203. | 10. | 0.1311 | 1.3107E-02 |
| 4 W(LIQUID,A)=0.19 | 0.1905 | 2.00E-02 | 5.4310E-04 | 2.7155E-02 |
| 4 W(BCC#1,A)=6.9E-2 | 6.9175E-02 | 2.00E-02 | 1.7542E-04 | 8.7712E-03 |
| 4 W(FCC,A)=6E-2 | 6.0265E-02 | 2.00E-02 | 2.6489E-04 | 1.3244E-02 |
| 5 T=726 | 725.5 | 10. | -0.4866 | -4.8660E-02 |
| 5 X(BCC#1,B)=3.7E-2 | 3.7436E-02 | 2.00E-02 | 4.3575E-04 | 2.1787E-02 |
| 5 X(BCC#2,A)=0.114 | 0.1141 | 2.00E-02 | 9.4518E-05 | 4.7259E-03 |
| 6 X(BCC#1,B)=3.7E-2 | 3.7573E-02 | 2.00E-02 | 5.7335E-04 | 2.8667E-02 |
| 6 X(BCC#2,A)=0.114 | 0.1144 | 2.00E-02 | 4.3096E-04 | 2.1548E-02 |
| 10 W(LIQUID,A)=2E-2 | 1.9559E-02 | 2.00E-02 | -4.4080E-04 | -2.2040E-02 |
| 11 W(LIQUID,A)=4.2E-2 | 4.1835E-02 | 2.00E-02 | -1.6481E-04 | -8.2405E-03 |

```

12 W(LIQUID,A)=6.5E-2      6.4900E-02 2.00E-02 -9.9516E-05 -4.9758E-03
13 W(LIQUID,A)=9.3E-2      9.2687E-02 2.00E-02 -3.1292E-04 -1.5646E-02
20 W(LIQUID,A)=0.104       0.1038 2.00E-02 -2.1802E-04 -1.0901E-02
20 W(FCC,A)=3.8E-2        3.8304E-02 2.00E-02 3.0425E-04 1.5212E-02
21 W(LIQUID,A)=0.136       0.1365 2.00E-02 4.8540E-04 2.4270E-02
21 W(FCC,A)=4.7E-2        4.7294E-02 2.00E-02 2.9390E-04 1.4695E-02
22 W(LIQUID,A)=0.187       0.1867 2.00E-02 -2.9768E-04 -1.4884E-02
22 W(FCC,A)=5.9E-2        5.9406E-02 2.00E-02 4.0567E-04 2.0284E-02
23 W(BCC1,A)=8.5E-2       0.2447 2.00E-02 -2.5499E-04 -1.2749E-02
23 W(BCC1,A)=8.5E-2       8.5308E-02 2.00E-02 3.0796E-04 1.5398E-02
100 ACR(B)=0.94           0.9397 2.85E-02 -2.7298E-04 -9.5907E-03
101 ACR(B)=0.84           0.8395 2.82E-02 -4.7442E-04 -1.6831E-02
102 ACR(B)=0.74           0.7408 2.81E-02 7.6972E-04 2.7436E-02
103 ACR(B)=0.64           0.6424 2.81E-02 2.4423E-03 8.7019E-02
104 ACR(B)=0.54           0.5435 2.82E-02 3.5095E-03 0.1243
105 ACR(B)=0.44           0.4429 2.85E-02 2.9022E-03 0.1017
106 ACR(B)=0.34           0.3395 2.90E-02 -5.0270E-04 -1.7318E-02
107 ACR(B)=0.23           0.2321 2.97E-02 2.0966E-03 7.0579E-02
108 ACR(B)=0.12           0.1194 3.06E-02 -5.9597E-04 -1.9476E-02
110 HMR(LIQUID)=-1964     -1956. 5.00E+02 8.038 1.6076E-02
111 HMR(LIQUID)=-3500      -3477. 5.00E+02 22.73 4.5469E-02
112 HMR(LIQUID)=-4588      -4564. 5.00E+02 24.09 4.8178E-02
113 HMR(LIQUID)=-5239      -5216. 5.00E+02 23.10 4.6204E-02
114 HMR(LIQUID)=-5454      -5433. 5.00E+02 20.77 4.1546E-02
115 HMR(LIQUID)=-5233      -5216. 5.00E+02 17.10 3.4204E-02
116 HMR(LIQUID)=-4575      -4564. 5.00E+02 11.09 2.2178E-02
117 HMR(LIQUID)=-3481      -3477. 5.00E+02 3.735 7.4692E-03
118 HMR(LIQUID)=-1950      -1956. 5.00E+02 -5.962 -1.1924E-02

```

```

PARROT:
PARROT:
PARROT:Hit RETURN to continue
PARROT: @@ Calculate the phase diagram one last time.
PARROT: mac tce36cpd
PARROT: set-echo
NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
POLY:
POLY: @@ In PARROT, the global minimization is turned off automatically.
POLY: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY: @@ message will be given.
POLY:

```

```

POLY: advanced-option global yes,,,
Settings for global minimization:
*** WARNING *** Global equilibrium calculation may create new composition sets
and this may corrupt your PARROT work file (.PAR file).
Do not go back to PARROT but exit from POLY after your POLY calculations.
POLY:
POLY: def=con,,,,
POLY: s-a-v 1 w(b) 0 1,,,,
The condition W(B)=.1234 created
POLY: s-a-v 2 t 300 1700,,,,
The condition T=942.2 created
POLY: s-t=500
POLY: l-c
W(B)=0.1234, T=500
DEGREES OF FREEDOM 2
POLY: c-e
Creating condition P=1E5
Creating condition N=1
Using global minimization procedure
Calculated          628 grid points in          0 s
Found the set of lowest grid points in          0 s
Calculated POLY solution      0 s, total time    0 s
POLY: save tce36 y

```

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

```

POLY: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

```

Organizing start points

Using ADDED start equilibria

```

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21

```

```

Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Generating start point 27
Generating start point 28

Phase region boundary 1 at: 7.140E-01 3.100E+02
    BCC#1
    ** BCC#2
Calculated..          2 equilibria
Terminating at axis limit.

Phase region boundary 2 at: 7.141E-01 3.000E+02
    BCC#1
    ** BCC#2
Calculated.          14 equilibria

Phase region boundary 3 at: 6.819E-01 7.255E+02
    ** A2B
    BCC#1
    ** BCC#2

Phase region boundary 4 at: 3.626E-01 7.255E+02
    ** A2B
    BCC#1
Calculated.          15 equilibria

Phase region boundary 5 at: 3.771E-01 1.192E+03
    ** LIQUID
    ** A2B
    BCC#1

Phase region boundary 6 at: 2.828E-01 1.192E+03
    ** LIQUID
    BCC#1
Calculated.          28 equilibria

Phase region boundary 7 at: 4.863E-01 1.192E+03
    ** LIQUID
    A2B
Calculated.          28 equilibria

Phase region boundary 8 at: 6.500E-01 1.048E+03
    ** LIQUID
    A2B
    ** BCC#1

Phase region boundary 9 at: 7.639E-01 1.048E+03
    A2B
    ** BCC#1
Calculated.          11 equilibria
Terminating at known equilibrium

Phase region boundary 10 at: 8.273E-01 1.048E+03
    LIQUID
    ** BCC#1
Calculated.          8 equilibria

Phase region boundary 11 at: 8.748E-01 1.203E+03
    LIQUID
    ** BCC#1
    ** FCC

Phase region boundary 12 at: 8.800E-01 1.203E+03
    LIQUID
    ** FCC
Calculated.          33 equilibria

Phase region boundary 13 at: 9.353E-01 1.203E+03
    BCC#1
    ** FCC
Calculated.          20 equilibria

Phase region boundary 14 at: 7.140E-01 3.100E+02
    BCC#1
    ** BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 15 at: 7.140E-01 3.100E+02
    BCC#1
    ** BCC#2
Calculated..          2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 16 at: 7.140E-01 3.100E+02
    BCC#1
    ** BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 17 at: 7.140E-01 3.100E+02
    BCC#1
    ** BCC#2
Calculated..          2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 18 at: 7.140E-01 3.100E+02
    BCC#1
    ** BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 19 at: 7.140E-01 3.100E+02
    BCC#1
    ** BCC#2
Calculated..          2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 20 at: 7.140E-01 3.100E+02
    BCC#1

```

```

** BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 21 at: 7.140E-01 3.100E+02
** BCC#1
BCC#2
Calculated..        2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 22 at: 7.140E-01 3.100E+02
** BCC#1
BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 23 at: 7.140E-01 3.100E+02
** BCC#1
BCC#2
Calculated..        2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 24 at: 7.140E-01 3.100E+02
** BCC#1
BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 25 at: 3.647E-01 7.700E+02
** A2B
BCC#1
Calculated.          10 equilibria

Phase region boundary 26 at: 3.647E-01 7.700E+02
** A2B
BCC#1
Calculated.          3 equilibria
Terminating at known equilibrium

Phase region boundary 27 at: 3.647E-01 7.700E+02
** A2B
BCC#1
Calculated.          14 equilibria
Terminating at known equilibrium

Phase region boundary 28 at: 7.910E-01 7.700E+02
** A2B
BCC#1
Calculated.          10 equilibria

Phase region boundary 29 at: 7.910E-01 7.700E+02
** A2B
BCC#1
Calculated.          3 equilibria
Terminating at known equilibrium

Phase region boundary 30 at: 7.910E-01 7.700E+02
** A2B
BCC#1
Calculated.          9 equilibria
Terminating at known equilibrium

Phase region boundary 31 at: 2.448E-01 1.230E+03
** LIQUID
BCC#1
Calculated.          4 equilibria
Terminating at known equilibrium

Phase region boundary 32 at: 2.448E-01 1.230E+03
** LIQUID
BCC#1
Calculated.          26 equilibria

Phase region boundary 33 at: 8.858E-01 1.230E+03
** LIQUID
FCC
Calculated.          2 equilibria
Terminating at known equilibrium

Phase region boundary 34 at: 8.858E-01 1.230E+03
** LIQUID
FCC
Calculated.          29 equilibria

Phase region boundary 35 at: 6.415E-03 1.397E+03
LIQUID
** BCC#1
Calculated.          13 equilibria

Phase region boundary 36 at: 6.415E-03 1.397E+03
LIQUID
** BCC#1
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 37 at: 2.299E-01 1.244E+03
LIQUID
** BCC#1
Calculated.          20 equilibria

Phase region boundary 38 at: 2.299E-01 1.244E+03
LIQUID
** BCC#1
Calculated.          4 equilibria
Terminating at known equilibrium

Phase region boundary 39 at: 6.122E-01 1.240E+03
LIQUID
** A2B
Calculated.          14 equilibria
Terminating at known equilibrium

Phase region boundary 40 at: 6.122E-01 1.240E+03
LIQUID

```

```

** A2B
Calculated.          8 equilibria
Terminating at known equilibrium

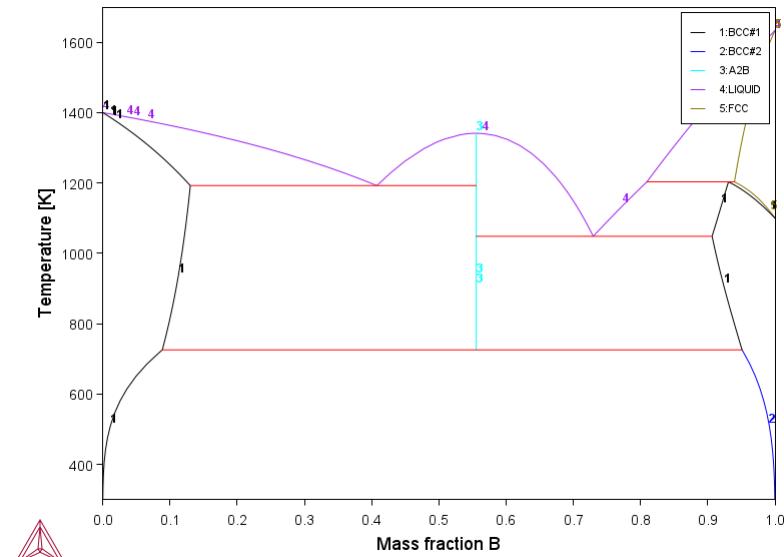
Phase region boundary 41 at: 9.927E-01 1.613E+03
    LIQUID
** FCC
Calculated.          20 equilibria
Terminating at known equilibrium

Phase region boundary 42 at: 9.927E-01 1.613E+03
    LIQUID
** FCC
Calculated.          8 equilibria
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\generate_console_examples\examples\tcex36a\tcex36.POLY3
CPU time for mapping      1 seconds
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: s-l d
POST: plot

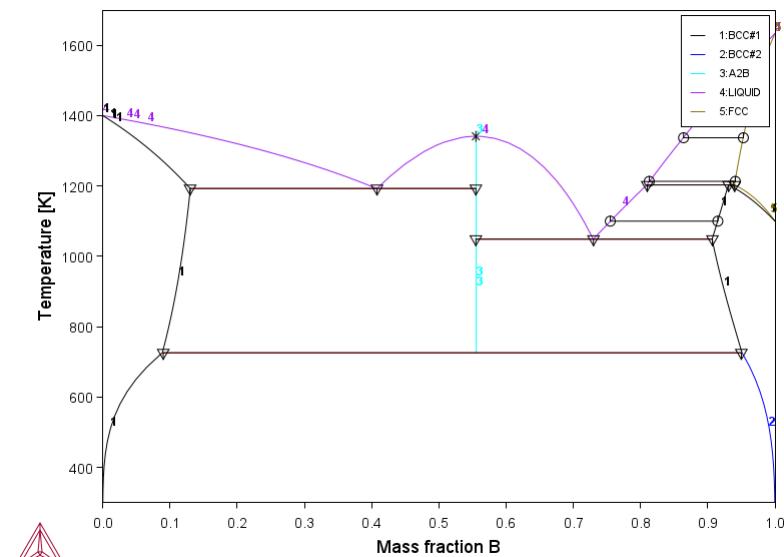
```



```

POST:
POST: set-inter
POST: Hit RETURN to continue
POST: @@ Add the experimental data
POST: a-e-d y exp36 0; 1
POST: plot

```



```

POST:
POST:
POST: Hit RETURN to continue
POST: @@ Also calculate the enthalpies in the liquid
POST: ba
POLY: read,,
POLY:
POLY:
POLY: s-a-v 2 none
POLY: s-c t=1773
POLY: c-e
Using global minimization procedure
Calculated          628 grid points in      0 s
Found the set of lowest grid points in      0 s
Calculated POLY solution      0 s, total time      0 s
POLY: sh hmr
HMR=13116.471
POLY: l-st c
*** STATUS FOR ALL COMPONENTS

```

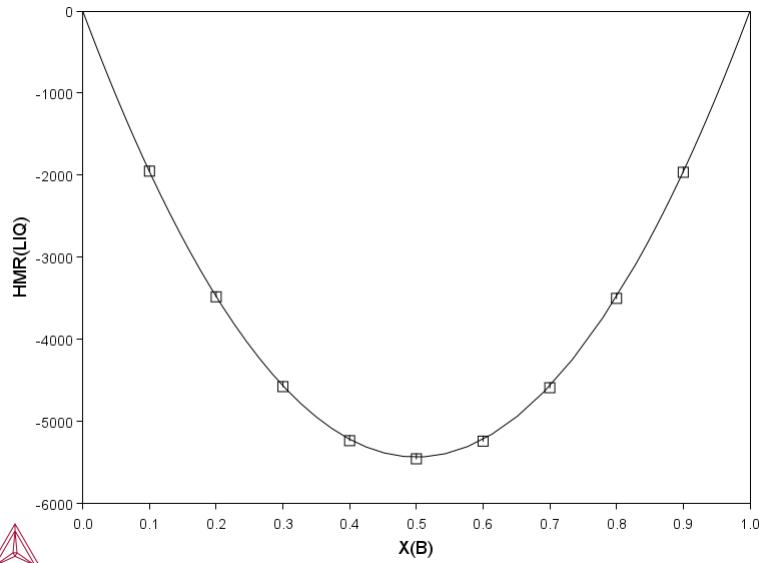
```

COMPONENT          STATUS    REF. STATE      T (K)      P (Pa)
A                 ENTERED   SER
B                 ENTERED   SER
POLY: s-r-s a liq * 1e5
POLY: s-r-s b liq * 1e5
POLY: save tce36h y
POLY: step normal
No initial equilibrium, using default
Step will start from axis value 0.123400
...OK

Phase Region from 0.123400 for:
LIQUID
Global test at 3.23400E-01 .... OK
Global test at 5.73400E-01 .... OK
Global test at 8.23400E-01 .... OK
Global test at 9.53400E-01 .... OK
Global test at 1.00000E+00 .... OK
Terminating at 1.00000
Calculated 51 equilibria

Phase Region from 0.123400 for:
LIQUID
Global test at 8.34000E-02 .... OK
Global test at 3.34000E-02 .... OK
Terminating at 0.250000E-11
Calculated 28 equilibria
*** Buffer saved on file: c:\jenkins\workspace\generate_console_examples\examples\tce36a\tce36h.POLY3
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2
POST: s-d-a x x(b)
POST: s-d-a y hmr(liq)
POST: a-e-d y exp36 0; 2
POST: plot

```



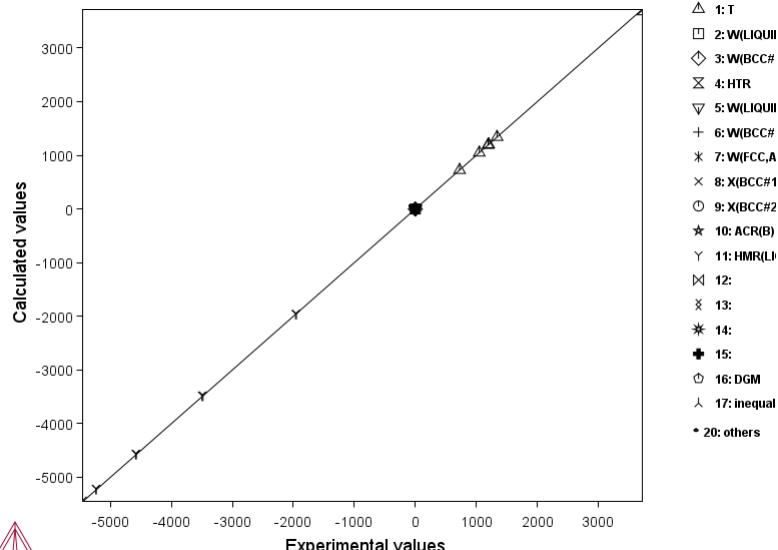
```

POST:
POST: Hit RETURN to continue
POST: @@ We can see the fitting results by the following method
POST: @@ Data points falling on the diagonal line indicates
POST: @@ perfect fitting.
POST: @@
POST: ba
POLY: ba

```

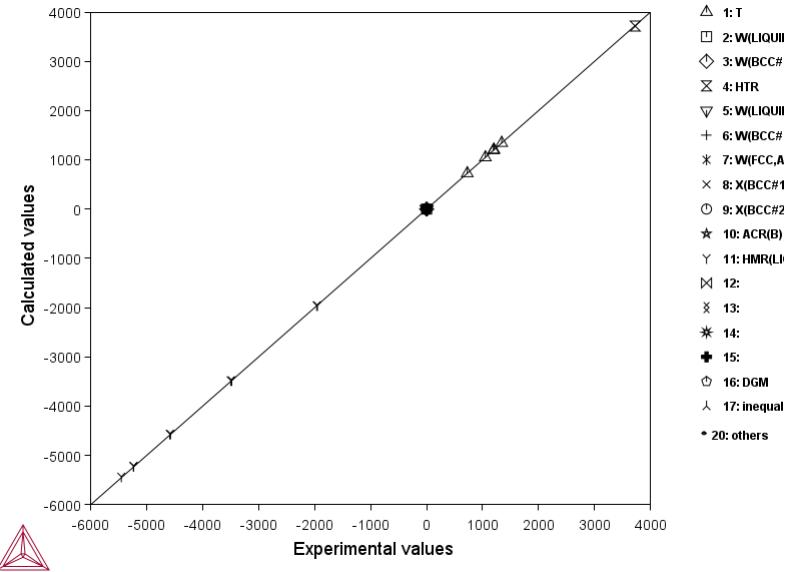
PARROT VERSION 5.3

Global minimization used as test only
PARROT: l-result gra pexp36 1,



POST: s-s-s y n -6000 4000

POST: s-s-s x n -6000 4000
POST: plot



POST: b
PARROT: set-inter
PARROT: set-inter
PARROT:

tce36a-tce36b

PARROT:About
NO SUCH COMMAND, USE HELP
PARROT:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce36a\tce36b.TCM.test"
PARROT: s-s-f tce36
PARROT: @@ List parameters to be optimized, all zero initially
PARROT: l-a-v
OUTPUT TO SCREEN OR FILE /SCREEN/:

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

| VAR. | VALUE | START VALUE | SCALING FACTOR | REL.STAND.DEV |
|------|-----------------|-----------------|-----------------|----------------|
| V1 | 2.03690179E+04 | 2.03241480E+04 | 2.03241480E+04 | 2.99180591E-02 |
| V2 | -2.94289024E+01 | -2.93474147E+01 | -2.93474147E+01 | 2.27345071E-02 |
| V11 | -2.17329087E+04 | -2.17266504E+04 | -2.17266504E+04 | 3.48585256E-02 |
| V12 | 1.52104360E+01 | 1.52556784E+01 | 1.52556784E+01 | 5.50983410E-02 |
| V15 | 2.42024574E+04 | 2.41307635E+04 | 2.41307635E+04 | 8.32025762E-02 |
| V16 | -8.38635734E+00 | -8.25451509E+00 | -8.25451509E+00 | 2.56507888E-01 |
| V17 | 3.08808414E+03 | 3.08373775E+03 | 3.08373775E+03 | 2.30206897E-01 |
| V19 | 2.20479620E+04 | 2.21799162E+04 | 2.21799162E+04 | 4.85909938E-01 |
| V20 | -7.06072567E+00 | -7.07722170E+00 | -7.07722170E+00 | 1.21873157E+00 |

NUMBER OF OPTIMIZING VARIABLES : 9
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 8.33570265E-02 TO 6.73854818E-02
DEGREES OF FREEDOM 38. REDUCED SUM OF SQUARES 1.77330215E-03

PARROT: @@ Set alt mode to start
PARROT: s-alt Y
PARROT: @@ Check if all equilibria can be calculated
PARROT: ed
ED_EXP: read 1
ED_EXP: c-a

| Eq | Lab | Iter | Weight | Temp | Exp | Fix phases or comments | |
|---|--|-------|--------|--------|-----|------------------------|--|
| 1 | AINV | *alt* | 1.0 | 1193.0 | | LIQUID A2B BCC | |
| 2 | AINV | *alt* | 1.0 | 1341.0 | | LIQUID A2B | |
| 3 | AINV | *alt* | 1.0 | 1049.0 | | LIQUID A2B BCC | |
| 4 | AINV | *alt* | 1.0 | 1203.0 | | LIQUID BCC FCC | |
| 5 | AINV | *alt* | 1.0 | 726.0 | | A2B BCC BCC#2 | |
| 6 | AINV | *alt* | 1.0 | 726.0 | | BCC BCC#2 | |
| Failed using alternate for FCC#1 setting weight to zero | | | | | | | |
| 10 | ALF | *alt* | 1.0 | 1594.0 | | LIQUID FCC | |
| Failed using alternate for FCC#1 setting weight to zero | | | | | | | |
| 11 | ALF | *alt* | 1.0 | 1548.0 | | LIQUID FCC | |
| Failed using alternate for FCC#1 setting weight to zero | | | | | | | |
| 12 | ALF | *alt* | 1.0 | 1499.0 | | LIQUID FCC | |
| Failed using alternate for FCC#1 setting weight to zero | | | | | | | |
| 13 | ALF | *alt* | 1.0 | 1438.0 | | LIQUID FCC | |
| 20 | ATIE | *alt* | 1.0 | 1413.0 | | LIQUID FCC | |
| 21 | ATIE | *alt* | 1.0 | 1337.0 | | LIQUID FCC | |
| 22 | ATIE | *alt* | 1.0 | 1213.0 | | LIQUID FCC | |
| 23 | ATIE | *alt* | 1.0 | 1100.0 | | LIQUID BCC | |
| 100 | AA | 2 | 1. | 1573.0 | | LIQUID | |
| 101 | AA | 2 | 1. | 1573.0 | | LIQUID | |
| 102 | AA | 2 | 1. | 1573.0 | | LIQUID | |
| 103 | AA | 2 | 1. | 1573.0 | | LIQUID | |
| 104 | AA | 2 | 1. | 1573.0 | | LIQUID | |
| 105 | AA | 2 | 1. | 1573.0 | | LIQUID | |
| 106 | AA | 2 | 1. | 1573.0 | | LIQUID | |
| 107 | AA | 2 | 1. | 1573.0 | | LIQUID | |
| 108 | AA | 2 | 1. | 1573.0 | | LIQUID | |
| 110 | AH | 2 | 1. | 1773.0 | | LIQUID | |
| 111 | AH | 2 | 1. | 1773.0 | | LIQUID | |
| 112 | AH | 2 | 1. | 1773.0 | | LIQUID | |
| 113 | AH | 2 | 1. | 1773.0 | | LIQUID | |
| 114 | AH | 2 | 1. | 1773.0 | | LIQUID | |
| 115 | AH | 2 | 1. | 1773.0 | | LIQUID | |
| 116 | AH | 2 | 1. | 1773.0 | | LIQUID | |
| 117 | AH | 2 | 1. | 1773.0 | | LIQUID | |
| 118 | AH | 2 | 1. | 1773.0 | | LIQUID | |
| Number of alternate equilibria 14 | | | | | | | |
| ED_EXP: | @@ Equilibria with label ALF cannot use alt mode | | | | | | |
| ED_EXP: | s-we 0 alf | | | | | | |
| Changed weight on 4 equilibria. | | | | | | | |
| ED_EXP: | c-a | | | | | | |
| Eq Lab Iter Weight Temp Exp Fix phases or comments | | | | | | | |
| 118 | AH | 2 | 1. | 1773.0 | | LIQUID | |
| ED_EXP: | save | | | | | | |
| ED_EXP: | @@ Save changes of weights before leaving the editor | | | | | | |
| ED_EXP: | ba | | | | | | |
| PARROT: | @@ Optimize zero times as a check | | | | | | |
| PARROT: | opt 0 | | | | | | |
| Alternate calculation is on | | | | | | | |
| Use | 47 experiments, maximum is | 2000 | | | | | |
| Use | 1082 real workspace, maximum is | 50000 | | | | | |
| PARROT: | l-r C SCREEN | | | | | | |

=====
OUTPUT FROM P A R R O T . DATE 2023. 4.27 16:29:41

*** SUCCESSFUL OPTIMIZATION. ***
NUMBER OF ITERATIONS: 0

== OPTIMIZING CONDITIONS ==

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 0 DMAX = 1.00000000E+02 H = 1.00000000E-04
ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

| VAR. | VALUE | START VALUE | SCALING FACTOR | REL.STAND.DEV |
|------|-----------------|-----------------|-----------------|----------------|
| V1 | 2.03690179E+04 | 2.03241480E+04 | 2.03241480E+04 | 2.99180591E-02 |
| V2 | -2.94289024E+01 | -2.93474147E+01 | -2.93474147E+01 | 2.27345071E-02 |
| V11 | -2.17329087E+04 | -2.17266504E+04 | -2.17266504E+04 | 3.48585256E-02 |
| V12 | 1.52104360E+01 | 1.52556784E+01 | 1.52556784E+01 | 5.50983410E-02 |
| V15 | 2.42024574E+04 | 2.41307635E+04 | 2.41307635E+04 | 8.32025762E-02 |
| V16 | -8.38635734E+00 | -8.25451509E+00 | -8.25451509E+00 | 2.56507888E-01 |
| V17 | 3.08808414E+03 | 3.08373775E+03 | 3.08373775E+03 | 2.30206897E-01 |
| V19 | 2.20479620E+04 | 2.21799162E+04 | 2.21799162E+04 | 4.85909938E-01 |
| V20 | -7.06072567E+00 | -7.07722170E+00 | -7.07722170E+00 | 1.21873157E+00 |

NUMBER OF OPTIMIZING VARIABLES : 9
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 8.33570265E-02 TO 8.89363154E-02
DEGREES OF FREEDOM 38. REDUCED SUM OF SQUARES 2.34042935E-03

Number of alternate equilibria 10

\$ ===== BLOCK NUMBER 1

| DEFINED CONSTANTS | DX=2E-2, P0=101325, DH=500, DT=10 |
|----------------------------------|---|
| DEFINED FUNCTIONS AND VARIABLES% | HTR=HM(LIQUID)-HM(A2B) |
| 1 Alternate equilibrium calc | 0.00 |
| 2 Alternate equilibrium calc | 0.19 |
| 2 HTR=3727 | 3714. 5.00E+02 -12.87 -2.5749E-02 |
| 3 Alternate equilibrium calc | 0.00 |
| 4 Alternate equilibrium calc | 0.00 |
| 5 Alternate equilibrium calc | 0.01 |
| 6 Alternate equilibrium calc | 0.01 |
| 20 Alternate equilibrium calc | 0.01 |
| 21 Alternate equilibrium calc | 0.00 |
| 22 Alternate equilibrium calc | 0.01 |
| 23 Alternate equilibrium calc | 0.00 |
| 100 ACR(B)=0.94 | 0.9397 2.85E-02 -2.7298E-04 -9.5907E-03 |
| 101 ACR(B)=0.84 | 0.8395 2.82E-02 -4.7442E-04 -1.6831E-02 |
| 102 ACR(B)=0.74 | 0.7408 2.81E-02 7.6972E-04 2.7436E-02 |
| 103 ACR(B)=0.64 | 0.6424 2.81E-02 2.4423E-03 8.7019E-02 |
| 104 ACR(B)=0.54 | 0.5435 2.82E-02 3.5095E-03 0.1243 |
| 105 ACR(B)=0.44 | 0.4429 2.85E-02 2.9022E-03 0.1017 |
| 106 ACR(B)=0.34 | 0.3395 2.90E-02 -5.0270E-04 -1.7318E-02 |
| 107 ACR(B)=0.23 | 0.2321 2.97E-02 2.0966E-03 7.0579E-02 |
| 108 ACR(B)=0.12 | 0.1194 3.06E-02 -5.9597E-04 -1.9476E-02 |
| 110 HMR(LIQUID)=-1964 | -1956. 5.00E+02 8.038 1.6076E-02 |
| 111 HMR(LIQUID)=-3500 | -3477. 5.00E+02 22.73 4.5469E-02 |
| 112 HMR(LIQUID)=-4588 | -4564. 5.00E+02 24.09 4.8178E-02 |
| 113 HMR(LIQUID)=-5239 | -5216. 5.00E+02 23.10 4.6204E-02 |
| 114 HMR(LIQUID)=-5454 | -5433. 5.00E+02 20.77 4.1546E-02 |
| 115 HMR(LIQUID)=-5233 | -5216. 5.00E+02 17.10 3.4204E-02 |
| 116 HMR(LIQUID)=-4575 | -4564. 5.00E+02 11.09 2.2178E-02 |
| 117 HMR(LIQUID)=-3481 | -3477. 5.00E+02 3.735 7.4692E-03 |
| 118 HMR(LIQUID)=-1950 | -1956. 5.00E+02 -5.962 -1.1924E-02 |

PARROT:

PARROT: Hit RETURN to continue

PARROT: @@ Note only one error from alternate calculations.

PARROT: @@ This error represents the difference in chemical

PARROT: @@ potentials of the phases.

PARROT: @@ Experiments with just one phase is calculated as normal.

PARROT: @@ Next command supresses the listing of parameters.

PARROT: s-o-l 1 Y Y N n N

PARROT: l-r C SCREEN

=====
OUTPUT FROM P A R R O T . DATE 2023. 4.27 16:29:41

*** SUCCESSFUL OPTIMIZATION. ***

NUMBER OF ITERATIONS: 0

== OPTIMIZING CONDITIONS ==

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 0 DMAX = 1.00000000E+02 H = 1.00000000E-04
ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

| VAR. | VALUE | START VALUE | SCALING FACTOR | REL.STAND.DEV |
|------|-----------------|-----------------|-----------------|----------------|
| V1 | 2.03690179E+04 | 2.03241480E+04 | 2.03241480E+04 | 2.99180591E-02 |
| V2 | -2.94289024E+01 | -2.93474147E+01 | -2.93474147E+01 | 2.27345071E-02 |
| V11 | -2.17329087E+04 | -2.17266504E+04 | -2.17266504E+04 | 3.48585256E-02 |
| V12 | 1.52104360E+01 | 1.52556784E+01 | 1.52556784E+01 | 5.50983410E-02 |
| V15 | 2.42024574E+04 | 2.41307635E+04 | 2.41307635E+04 | 8.32025762E-02 |
| V16 | -8.38635734E+00 | -8.25451509E+00 | -8.25451509E+00 | 2.56507888E-01 |
| V17 | 3.08808414E+03 | 3.08373775E+03 | 3.08373775E+03 | 2.30206897E-01 |
| V19 | 2.20479620E+04 | 2.21799162E+04 | 2.21799162E+04 | 4.85909938E-01 |
| V20 | -7.06072567E+00 | -7.07722170E+00 | -7.07722170E+00 | 1.21873157E+00 |

NUMBER OF OPTIMIZING VARIABLES : 9
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 8.33570265E-02 TO 8.89363154E-02
DEGREES OF FREEDOM 38. REDUCED SUM OF SQUARES 2.34042935E-03

Number of alternate equilibria 10

```

SYMBOL      STATUS   VALUE/FUNCTION
FUNCTION R      298.15    8.314510000000000 ; 6000 N REFO !
2 RTLNP 20000000 +R*T*LN(1E-05*P)
FUNCTION V1      298.15    20369.0178675949 ; 6000 N REFO !
FUNCTION V2      298.15    -29.4289023907393 ; 6000 N REFO !
FUNCTION V11     298.15    -21732.9087358100 ; 6000 N REFO !
FUNCTION V12     298.15    15.2104360332482 ; 6000 N REFO !
FUNCTION V15     298.15    24202.4574075405 ; 6000 N REFO !
FUNCTION V16     298.15    -8.38635733841773 ; 6000 N REFO !
FUNCTION V17     298.15    3088.08413618746 ; 6000 N REFO !
FUNCTION V19     298.15    22047.9619915124 ; 6000 N REFO !
FUNCTION V20     298.15    -7.06072566566526 ; 6000 N REFO !

LIQUID:L (A,B)1.0

===== [A] =====
G(LIQUID,A;0)          298.15 +14000-10*T;           6000 N

===== [B] =====
G(LIQUID,B;0)          298.15 +18000-12*T;           6000 N

===== [A, B] =====
G(LIQUID,A,B;0)          298.15 +V11+V12*T;           6000 N
G(LIQUID,A,B;1)          298.15 +V13+V14*T;           6000 N

$ ====== BLOCK NUMBER 1

DEFINED CONSTANTS
DX=2E-2, P0=101325, DH=500, DT=10
DEFINED FUNCTIONS AND VARIABLES%
HTR=HM(LIQUID)-HM(A2B)
1 Alternate equilibrium calc          0.00
2 Alternate equilibrium calc          0.19
2 HTR=3727          3714.      5.00E+02 -12.87      -2.5749E-02
3 Alternate equilibrium calc          0.00
4 Alternate equilibrium calc          0.00
5 Alternate equilibrium calc          0.01
6 Alternate equilibrium calc          0.01
20 Alternate equilibrium calc          0.01
21 Alternate equilibrium calc          0.00
22 Alternate equilibrium calc          0.01
23 Alternate equilibrium calc          0.00
100 ACR(B)=0.94          0.9397    2.85E-02 -2.7298E-04 -9.5907E-03
101 ACR(B)=0.84          0.8395    2.82E-02 -4.7442E-04 -1.6831E-02
102 ACR(B)=0.74          0.7408    2.81E-02 7.6972E-04 2.7436E-02
103 ACR(B)=0.64          0.6424    2.81E-02 2.4423E-03 8.7019E-02
104 ACR(B)=0.54          0.5435    2.82E-02 3.5095E-03 0.1243
105 ACR(B)=0.44          0.4429    2.85E-02 2.9022E-03 0.1017
106 ACR(B)=0.34          0.3395    2.90E-02 -5.0270E-04 -1.7318E-02
107 ACR(B)=0.23          0.2321    2.97E-02 2.0966E-03 7.0579E-02
108 ACR(B)=0.12          0.1194    3.06E-02 -5.9597E-04 -1.9476E-02
110 HMR(LIQUID)=-1964    -1956.    5.00E+02 8.038 1.6076E-02
111 HMR(LIQUID)=-3500    -3477.    5.00E+02 22.73 4.5469E-02
112 HMR(LIQUID)=-4588    -4564.    5.00E+02 24.09 4.8178E-02
113 HMR(LIQUID)=-5239    -5216.    5.00E+02 23.10 4.6204E-02
114 HMR(LIQUID)=-5454    -5433.    5.00E+02 20.77 4.1546E-02
115 HMR(LIQUID)=-5233    -5216.    5.00E+02 17.10 3.4204E-02
116 HMR(LIQUID)=-4575    -4564.    5.00E+02 11.09 2.2178E-02
117 HMR(LIQUID)=-3481    -3477.    5.00E+02 3.735 7.4692E-03
118 HMR(LIQUID)=-1950    -1956.    5.00E+02 -5.962 -1.1924E-02

PARROT:
PARROT: @@ Now optimize
PARROT: opt 30
Alternate calculation is on
Use      47 experiments, maximum is      2000
Use      1082 real workspace, maximum is 50000
The following output is provided by subroutine VA05A

      AT THE 0 TH ITERATION WE HAVE THE SUM OF SQUARES 8.89363154E-02
1 1.0022E+00 2 1.0028E+00 3 1.0003E+00 4 9.9703E-01 5 1.0030E+00
6 1.0160E+00 7 1.0014E+00 8 9.9405E-01 9 9.9767E-01

      AT THE 1 ST ITERATION WE HAVE THE SUM OF SQUARES 8.90038393E-02
1 1.0023E+00 2 1.0028E+00 3 1.0003E+00 4 9.9703E-01 5 1.0030E+00
6 1.0160E+00 7 1.0014E+00 8 9.9405E-01 9 9.9767E-01

      AT THE 2 ND ITERATION WE HAVE THE SUM OF SQUARES 8.89455551E-02
1 1.0022E+00 2 1.0029E+00 3 1.0003E+00 4 9.9703E-01 5 1.0030E+00
6 1.0160E+00 7 1.0014E+00 8 9.9405E-01 9 9.9767E-01

      AT THE 3 RD ITERATION WE HAVE THE SUM OF SQUARES 8.79612375E-02
1 1.0022E+00 2 1.0028E+00 3 1.0004E+00 4 9.9703E-01 5 1.0030E+00
6 1.0160E+00 7 1.0014E+00 8 9.9405E-01 9 9.9767E-01

      AT THE 4 TH ITERATION WE HAVE THE SUM OF SQUARES 8.85897174E-02
1 1.0022E+00 2 1.0028E+00 3 1.0004E+00 4 9.9713E-01 5 1.0030E+00
6 1.0160E+00 7 1.0014E+00 8 9.9405E-01 9 9.9767E-01

      AT THE 5 TH ITERATION WE HAVE THE SUM OF SQUARES 8.79383634E-02
1 1.0022E+00 2 1.0028E+00 3 1.0004E+00 4 9.9703E-01 5 1.0031E+00
6 1.0160E+00 7 1.0014E+00 8 9.9405E-01 9 9.9767E-01

      AT THE 6 TH ITERATION WE HAVE THE SUM OF SQUARES 8.79442924E-02
1 1.0022E+00 2 1.0028E+00 3 1.0004E+00 4 9.9703E-01 5 1.0031E+00
6 1.0161E+00 7 1.0014E+00 8 9.9405E-01 9 9.9767E-01

      AT THE 7 TH ITERATION WE HAVE THE SUM OF SQUARES 8.79365897E-02
1 1.0022E+00 2 1.0028E+00 3 1.0004E+00 4 9.9703E-01 5 1.0031E+00
6 1.0160E+00 7 1.0015E+00 8 9.9405E-01 9 9.9767E-01

      AT THE 8 TH ITERATION WE HAVE THE SUM OF SQUARES 8.79319355E-02
1 1.0022E+00 2 1.0028E+00 3 1.0004E+00 4 9.9703E-01 5 1.0031E+00
6 1.0160E+00 7 1.0015E+00 8 9.9415E-01 9 9.9777E-01

      AT THE 9 TH ITERATION WE HAVE THE SUM OF SQUARES 8.79338852E-02
1 1.0022E+00 2 1.0028E+00 3 1.0004E+00 4 9.9703E-01 5 1.0031E+00
6 1.0160E+00 7 1.0015E+00 8 9.9415E-01 9 9.9777E-01

```

```

AT THE 10 TH ITERATION WE HAVE THE SUM OF SQUARES 6.30390236E-02
1 1.0020E+00 2 1.0027E+00 3 1.0040E+00 4 9.9469E-01 5 1.0032E+00
6 1.0160E+00 7 1.0015E+00 8 9.9417E-01 9 9.9766E-01

AT THE 11 TH ITERATION WE HAVE THE SUM OF SQUARES 5.99860627E-02
1 9.9912E-01 2 1.0021E+00 3 1.0031E+00 4 9.9346E-01 5 1.0040E+00
6 1.0181E+00 7 1.0024E+00 8 9.9347E-01 9 9.9640E-01

AT THE 12 TH ITERATION WE HAVE THE SUM OF SQUARES 5.92638696E-02
1 9.9863E-01 2 1.0002E+00 3 1.0037E+00 4 9.9347E-01 5 1.0062E+00
6 1.0253E+00 7 1.0053E+00 8 9.9226E-01 9 9.9450E-01

AT THE 13 TH ITERATION WE HAVE THE SUM OF SQUARES 5.88513858E-02
1 9.9780E-01 2 9.9671E-01 3 1.0039E+00 4 9.9383E-01 5 1.0104E+00
6 1.0395E+00 7 1.0108E+00 8 9.8922E-01 9 9.8910E-01

THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED 13 iterations
1 7.4326E-03 2 7.4326E-03 3 1.5765E-03 4 2.3877E-03 5 1.3275E-01
6 -1.4001E-01 7 -7.2748E-04 8 1.1726E-03 9 8.1726E-03 10 -3.4807E-04
11 3.2690E-03 12 1.6869E-03 13 2.3657E-04 14 2.8647E-03 15 6.0691E-04
16 1.5562E-03 17 1.5562E-03 18 1.4162E-04 19 1.0022E-03 20 1.4162E-04
21 1.0022E-03 22 -2.0799E-03 23 1.7706E-03 24 3.3746E-03 25 3.3485E-04
26 -2.7392E-03 27 3.2562E-03 28 -1.7543E-03 29 3.8068E-03 30 -1.3488E-02
31 -3.0889E-02 32 -7.0118E-04 33 4.3579E-02 34 6.7271E-02 35 3.5606E-02
36 -8.5035E-02 37 1.1584E-02 38 -5.6982E-02 39 2.0218E-03 40 2.0483E-02
41 1.5384E-02 42 8.7248E-03 43 2.5050E-03 44 -3.2752E-03 45 -1.0616E-02
46 -1.7517E-02 47 -2.5978E-02

```

THE SUM OF SQUARES IS 5.88513858E-02

PARROT: cont 30

It is safe to CONTINUE only after TOO MANY ITERATIONS
and no change in variables and experiments ...
Now anything can happen ...

PARROT: l-r C SCREEN

```
=====
OUTPUT FROM P A R R O T . DATE 2023. 4.27 16:29:41
```

*** SUCCESSFUL OPTIMIZATION. ***
NUMBER OF ITERATIONS: 14

-- OPTIMIZING CONDITIONS --

```

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 30 DMAX = 1.00000000E+02 H = 1.00000000E-04
ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03

```

-- OPTIMIZING VARIABLES --

AVAILABLE VARIABLES ARE V1 TO VOO

| VAR. | VALUE | START VALUE | SCALING FACTOR | REL.STAND.DEV |
|------|-----------------|-----------------|-----------------|----------------|
| V1 | 2.02794315E+04 | 2.03241480E+04 | 2.03241480E+04 | 7.90185123E-02 |
| V2 | -2.92509568E+01 | -2.93474147E+01 | -2.93474147E+01 | 3.41436176E-01 |
| V11 | -2.18109901E+04 | -2.17266504E+04 | -2.17266504E+04 | 3.98516861E-02 |
| V12 | 1.51615699E+01 | 1.52556784E+01 | 1.52556784E+01 | 5.81303100E-02 |
| V15 | 2.43818988E+04 | 2.41307635E+04 | 2.41307635E+04 | 6.16271652E-01 |
| V16 | -8.58039496E+00 | -8.25451509E+00 | -8.25451509E+00 | 2.12986151E+00 |
| V17 | 3.11711755E+03 | 3.08373775E+03 | 3.08373775E+03 | 1.47312536E+00 |
| V19 | 2.19408897E+04 | 2.21799162E+04 | 2.21799162E+04 | 4.58864967E+00 |
| V20 | -7.00004752E+00 | -7.07722170E+00 | -7.07722170E+00 | 1.11448303E+01 |

NUMBER OF OPTIMIZING VARIABLES : 9

ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO

THE SUM OF SQUARES HAS CHANGED FROM 8.89363154E-02 TO 5.88513858E-02

DEGREES OF FREEDOM 38. REDUCED SUM OF SQUARES 1.54872068E-03

Number of alternate equilibria 10

| SYMBOL | STATUS | VALUE/FUNCTION | |
|--------------|----------|-------------------|-----------------|
| FUNCTION R | 298.15 | 8.31451000000000 | ; 6000 N REFO ! |
| 2 RTLNP | 20000000 | +R*T*LN(1E-05*P) | |
| FUNCTION V1 | 298.15 | 20279.4314990643 | ; 6000 N REFO ! |
| FUNCTION V2 | 298.15 | -29.2509568040070 | ; 6000 N REFO ! |
| FUNCTION V11 | 298.15 | -21810.9900742145 | ; 6000 N REFO ! |
| FUNCTION V12 | 298.15 | 15.1615699397423 | ; 6000 N REFO ! |
| FUNCTION V15 | 298.15 | 24381.8988000705 | ; 6000 N REFO ! |
| FUNCTION V16 | 298.15 | -8.58039495967295 | ; 6000 N REFO ! |
| FUNCTION V17 | 298.15 | 3117.11754857285 | ; 6000 N REFO ! |
| FUNCTION V19 | 298.15 | 21940.8896847721 | ; 6000 N REFO ! |
| FUNCTION V20 | 298.15 | -7.00004752115290 | ; 6000 N REFO ! |

LIQUID:L (A,B)1.0

==== [A] ====
G(LIQUID,A;0) 298.15 +14000-10*T; 6000 N

==== [B] ====
G(LIQUID,B;0) 298.15 +18000-12*T; 6000 N

==== [A, B] ====
G(LIQUID,A,B;0) 298.15 +V11+V12*T; 6000 N
G(LIQUID,A,B;1) 298.15 +V13+V14*T; 6000 N

```

$ ====== BLOCK NUMBER 1

DEFINED CONSTANTS
  DX=2E-2, P0=101325, DH=500, DT=10
DEFINED FUNCTIONS AND VARIABLES%
  HTR=HM(LIQUID)-HM(A2B)
  1 Alternate equilibrium calc          0.01
  2 Alternate equilibrium calc          0.19
2 HTR=3727.      3727.      5.00E+02 -0.3637    -7.2748E-04
  3 Alternate equilibrium calc          0.01
  4 Alternate equilibrium calc          0.00
  5 Alternate equilibrium calc          0.00
  6 Alternate equilibrium calc          0.00
20 Alternate equilibrium calc          0.00
21 Alternate equilibrium calc          0.00
22 Alternate equilibrium calc          0.00
23 Alternate equilibrium calc          0.00
100 ACR(B)=0.94        0.9396    2.85E-02 -3.8431E-04 -1.3488E-02
101 ACR(B)=0.84        0.8391    2.82E-02 -8.7217E-04 -3.0889E-02
102 ACR(B)=0.74        0.7400    2.81E-02 -1.9713E-05 -7.0118E-04
103 ACR(B)=0.64        0.6412    2.81E-02 1.2257E-03  4.3579E-02
104 ACR(B)=0.54        0.5419    2.83E-02 1.9021E-03  6.7271E-02
105 ACR(B)=0.44        0.4410    2.86E-02 1.0172E-03  3.5606E-02
106 ACR(B)=0.34        0.3375    2.90E-02 -2.4678E-03 -8.5035E-02
107 ACR(B)=0.23        0.2303    2.96E-02 3.4343E-04  1.1584E-02
108 ACR(B)=0.12        0.1183    3.05E-02 -1.7363E-03 -5.6982E-02
110 HMR(LIQUID)==-1964   -1963.   5.00E+02  1.011   2.0218E-03
111 HMR(LIQUID)==-3500   -3490.   5.00E+02 10.24   2.0483E-02
112 HMR(LIQUID)==-4588   -4580.   5.00E+02 7.692   1.5384E-02
113 HMR(LIQUID)==-5239   -5235.   5.00E+02 4.362   8.7248E-03
114 HMR(LIQUID)==-5454   -5453.   5.00E+02 1.252   2.5050E-03
115 HMR(LIQUID)==-5233   -5235.   5.00E+02 -1.638   -3.2752E-03
116 HMR(LIQUID)==-4575   -4580.   5.00E+02 -5.308   -1.0616E-02
117 HMR(LIQUID)==-3481   -3490.   5.00E+02 -8.758   -1.7517E-02
118 HMR(LIQUID)==-1950   -1963.   5.00E+02 -12.99  -2.5978E-02

```

```

PARROT:
PARROT:Hit RETURN to continue
PARROT: @@ The liquid data fits reasonably. Simplify its parameters.
PARROT: l-p-d liq
Property type /ALL/: s-f-v 11-14
S-F-V is not a valid property type
11-14 is not a valid property type
Property type: @@ Rescale the start values of the parameters to current values
@@ is not a valid property type
RESCALE is not a valid property type
THE is not a valid property type
START is not a valid property type
VALUES is not a valid property type
OF is not a valid property type
THE is not a valid property type
PARAMETERS is not a valid property type
TO is not a valid property type
CURRENT is not a valid property type
VALUES is not a valid property type
Property type: resc
RESC is not a valid property type
Property type: l-a-v
L-A-V is not a valid property type
Property type:
LIQUID:L (A,B)1.0

```

```

===== [A] =====
G(LIQUID,A;0)           298.15 +14000-10*T;           6000 N

===== [B] =====
G(LIQUID,B;0)           298.15 +18000-12*T;           6000 N

===== [A, B] =====
G(LIQUID,A,B;0)          298.15 +V11+V12*T;           6000 N
G(LIQUID,A,B;1)          298.15 +V13+V14*T;           6000 N

```

```

PARROT:Hit RETURN to continue
PARROT: mac tce36cpd
PARROT: set-echo
NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
POLY:
POLY: @@ In PARROT, the global minimization is turned off automatically.
POLY: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY: @@ message will be given.
POLY:
POLY: advanced-option global yes.,
Settings for global minimization:
*** WARNING *** Global equilibrium calculation may create new composition sets
and this may corrupt your PARROT work file (.PAR file).
Do not go back to PARROT but exit from POLY after your POLY calculations.
POLY:
POLY: def-com,,
POLY: s-a-v 1 w(b) 0 1,,
The condition W(B)=.1234 created
POLY: s-a-v 2 t 300 1700,,
The condition T=942.2 created
POLY: s-c t=500
POLY: l-c
W(B)=0.1234, T=500
DEGREES OF FREEDOM 2
POLY: c-e
Creating condition P=1E5
Creating condition N=1
Using global minimization procedure
Calculated       628 grid points in      0 s
Found the set of lowest grid points in      0 s
Calculated POLY solution      0 s, total time      0 s
POLY: save tce36 y

```

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

POLY: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Generating start point 27
Generating start point 28

Phase region boundary 1 at: 7.140E-01 3.100E+02
 BCC#1
 ** BCC#2

Calculated.. 2 equilibria
Terminating at axis limit.

Phase region boundary 2 at: 7.141E-01 3.000E+02
 BCC#1
 ** BCC#2

Calculated.. 14 equilibria

Phase region boundary 3 at: 6.816E-01 7.270E+02
 ** A2B
 BCC#1
 ** BCC#2

Phase region boundary 4 at: 3.626E-01 7.270E+02
 ** A2B
 BCC#1
Calculated.. 15 equilibria

Phase region boundary 5 at: 3.779E-01 1.184E+03
 ** LIQUID
 ** A2B
 BCC#1

Phase region boundary 6 at: 2.893E-01 1.184E+03
 ** LIQUID
 BCC#1
Calculated.. 26 equilibria

Phase region boundary 7 at: 4.903E-01 1.184E+03
 ** LIQUID
 A2B
Calculated.. 33 equilibria

Phase region boundary 8 at: 6.480E-01 1.038E+03
 ** LIQUID
 A2B
 ** BCC#1

Phase region boundary 9 at: 7.636E-01 1.038E+03
 A2B
 ** BCC#1
Calculated.. 10 equilibria
Terminating at known equilibrium

Phase region boundary 10 at: 8.257E-01 1.038E+03
 LIQUID
 ** BCC#1
Calculated.. 8 equilibria

Phase region boundary 11 at: 8.759E-01 1.204E+03
 LIQUID
 ** BCC#1
 ** FCC

Phase region boundary 12 at: 8.812E-01 1.204E+03
 LIQUID
 ** FCC
Calculated.. 28 equilibria

```

Phase region boundary 13 at: 9.361E-01 1.204E+03
  BCC#1
  ** FCC
Calculated           18 equilibria

Phase region boundary 14 at: 7.140E-01 3.100E+02
  BCC#1
  ** BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 15 at: 7.140E-01 3.100E+02
  BCC#1
  ** BCC#2
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 16 at: 7.140E-01 3.100E+02
  BCC#1
  ** BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 17 at: 7.140E-01 3.100E+02
  BCC#1
  ** BCC#2
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 18 at: 7.140E-01 3.100E+02
  BCC#1
  ** BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 19 at: 7.140E-01 3.100E+02
  BCC#1
  ** BCC#2
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 20 at: 7.140E-01 3.100E+02
  BCC#1
  ** BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 21 at: 7.140E-01 3.100E+02
  BCC#1
  ** BCC#2
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 22 at: 7.140E-01 3.100E+02
  BCC#1
  ** BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 23 at: 7.140E-01 3.100E+02
  BCC#1
  ** BCC#2
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 24 at: 7.140E-01 3.100E+02
  BCC#1
  ** BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 25 at: 3.646E-01 7.700E+02
  ** A2B
  BCC#1
Calculated.          10 equilibria

Phase region boundary 26 at: 3.646E-01 7.700E+02
  ** A2B
  BCC#1
Calculated.          3 equilibria
Terminating at known equilibrium

Phase region boundary 27 at: 3.646E-01 7.700E+02
  ** A2B
  BCC#1
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 28 at: 7.909E-01 7.700E+02
  ** A2B
  BCC#1
Calculated.          10 equilibria

Phase region boundary 29 at: 7.909E-01 7.700E+02
  ** A2B
  BCC#1
Calculated.          3 equilibria
Terminating at known equilibrium

Phase region boundary 30 at: 7.909E-01 7.700E+02
  ** A2B
  BCC#1
Calculated.          9 equilibria
Terminating at known equilibrium

Phase region boundary 31 at: 2.436E-01 1.230E+03
  ** LIQUID
  BCC#1
Calculated.          4 equilibria
Terminating at known equilibrium

```

```

Phase region boundary 32 at: 2.436E-01 1.230E+03
** LIQUID
BCC#1
Calculated 26 equilibria

Phase region boundary 33 at: 8.867E-01 1.230E+03
** LIQUID
FCC
Calculated. 2 equilibria
Terminating at known equilibrium

Phase region boundary 34 at: 8.867E-01 1.230E+03
** LIQUID
FCC
Calculated 29 equilibria

Phase region boundary 35 at: 6.405E-03 1.397E+03
LIQUID
** BCC#1
Calculated 9 equilibria

Phase region boundary 36 at: 6.405E-03 1.397E+03
LIQUID
** BCC#1
Calculated. 13 equilibria
Terminating at known equilibrium

Phase region boundary 37 at: 2.296E-01 1.243E+03
LIQUID
** BCC#1
Calculated 20 equilibria

Phase region boundary 38 at: 2.296E-01 1.243E+03
LIQUID
** BCC#1
Calculated. 4 equilibria
Terminating at known equilibrium

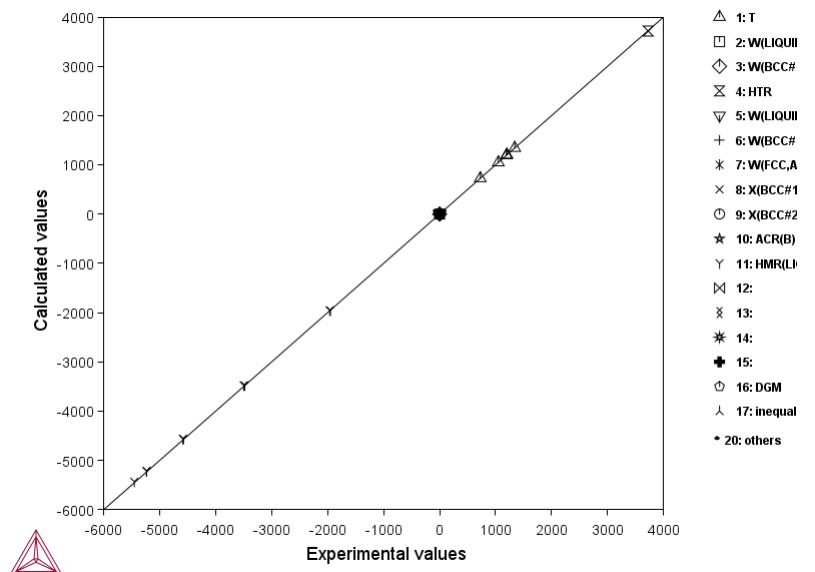
Phase region boundary 39 at: 6.122E-01 1.213E+03
LIQUID
** A2B
Calculated. 12 equilibria
Terminating at known equilibrium

Phase region boundary 40 at: 6.122E-01 1.213E+03
LIQUID
** A2B
Calculated. 8 equilibria
Terminating at known equilibrium

Phase region boundary 41 at: 9.927E-01 1.613E+03
LIQUID
** FCC
Calculated. 19 equilibria
Terminating at known equilibrium

Phase region boundary 42 at: 9.927E-01 1.613E+03
LIQUID
** FCC
Calculated 14 equilibria
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\generate_console_examples\examples\tcex36a\tcex36.POLY3
CPU time for mapping 1 seconds
POLY: post
POST: s-l d
POST: plot

```



```

POST:
POST: set-inter
POST: Hit RETURN to continue
POST: ba
POLY: ba

PARROT VERSION 5.3

Global minimization used as test only
PARROT: @@ This does not look very good, optimize more ...
PARROT: opt 30
Alternate calculation is on
Use    47 experiments, maximum is      2000
Use   1082 real workspace, maximum is  50000
The following output is provided by subroutine VA05A

```

AT THE 0 TH ITERATION WE HAVE THE SUM OF SQUARES 5.88513858E-02
1 9.9780E-01 2 9.9671E-01 3 1.0039E+00 4 9.9383E-01 5 1.0104E+00
6 1.0395E+00 7 1.0108E+00 8 9.8922E-01 9 9.8910E-01

AT THE 1 ST ITERATION WE HAVE THE SUM OF SQUARES 5.88554272E-02
1 9.9790E-01 2 9.9671E-01 3 1.0039E+00 4 9.9383E-01 5 1.0104E+00
6 1.0395E+00 7 1.0108E+00 8 9.8922E-01 9 9.8910E-01

AT THE 2 ND ITERATION WE HAVE THE SUM OF SQUARES 5.88532425E-02
1 9.9780E-01 2 9.9681E-01 3 1.0039E+00 4 9.9383E-01 5 1.0104E+00
6 1.0395E+00 7 1.0108E+00 8 9.8922E-01 9 9.8910E-01

AT THE 3 RD ITERATION WE HAVE THE SUM OF SQUARES 5.88529276E-02
1 9.9780E-01 2 9.9671E-01 3 1.0040E+00 4 9.9383E-01 5 1.0104E+00
6 1.0395E+00 7 1.0108E+00 8 9.8922E-01 9 9.8910E-01

AT THE 4 TH ITERATION WE HAVE THE SUM OF SQUARES 5.88588701E-02
1 9.9780E-01 2 9.9671E-01 3 1.0039E+00 4 9.9383E-01 5 1.0104E+00
6 1.0395E+00 7 1.0108E+00 8 9.8922E-01 9 9.8910E-01

AT THE 5 TH ITERATION WE HAVE THE SUM OF SQUARES 5.88509921E-02
1 9.9780E-01 2 9.9671E-01 3 1.0039E+00 4 9.9383E-01 5 1.0105E+00
6 1.0395E+00 7 1.0108E+00 8 9.8922E-01 9 9.8910E-01

AT THE 6 TH ITERATION WE HAVE THE SUM OF SQUARES 5.88507588E-02
1 9.9780E-01 2 9.9671E-01 3 1.0039E+00 4 9.9383E-01 5 1.0105E+00
6 1.0396E+00 7 1.0108E+00 8 9.8922E-01 9 9.8910E-01

AT THE 7 TH ITERATION WE HAVE THE SUM OF SQUARES 5.88505860E-02
1 9.9780E-01 2 9.9671E-01 3 1.0039E+00 4 9.9383E-01 5 1.0105E+00
6 1.0396E+00 7 1.0109E+00 8 9.8922E-01 9 9.8910E-01

AT THE 8 TH ITERATION WE HAVE THE SUM OF SQUARES 5.88511893E-02
1 9.9780E-01 2 9.9671E-01 3 1.0039E+00 4 9.9383E-01 5 1.0105E+00
6 1.0396E+00 7 1.0109E+00 8 9.8932E-01 9 9.8910E-01

AT THE 9 TH ITERATION WE HAVE THE SUM OF SQUARES 5.88504121E-02
1 9.9780E-01 2 9.9671E-01 3 1.0039E+00 4 9.9383E-01 5 1.0105E+00
6 1.0396E+00 7 1.0109E+00 8 9.8922E-01 9 9.8920E-01

THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED 9 iterations
1 9.9780E-01 2 9.9671E-01 3 1.0039E+00 4 9.9383E-01 5 1.0105E+00
6 1.0396E+00 7 1.0109E+00 8 9.8922E-01 9 9.8920E-01

1 7.4326E-03 2 7.4326E-03 3 1.5772E-03 4 2.5373E-03 5 1.3275E-01
6 -1.4001E-01 7 -7.2748E-04 8 8.1726E-03 9 8.1726E-03 10 -2.3980E-04
11 3.2732E-03 12 1.7797E-03 13 2.3825E-04 14 2.8014E-03 15 6.0530E-04
16 1.4495E-03 17 1.4495E-03 18 3.5507E-04 19 6.8544E-04 20 3.5507E-04
21 6.8544E-04 22 -2.1504E-03 23 1.7700E-03 24 3.3071E-03 25 3.3383E-04
26 -2.8028E-03 27 3.2547E-03 28 -1.6514E-03 29 3.8100E-03 30 -1.3488E-02
31 -3.0889E-02 32 -7.0118E-04 33 4.3579E-02 34 6.7271E-02 35 3.5606E-02
36 -8.5035E-02 37 1.1584E-02 38 -5.6982E-02 39 2.0218E-03 40 2.0483E-02
41 1.5384E-02 42 8.7248E-03 43 2.5050E-03 44 -3.2752E-03 45 -1.0616E-02
46 -1.7517E-02 47 -2.5978E-02

THE SUM OF SQUARES IS 5.88504121E-02

PARROT: resc
PARROT: opt 30
Alternate calculation is on
Use 47 experiments, maximum is 2000
Use 1082 real workspace, maximum is 50000
The following output is provided by subroutine VA05A

AT THE 0 TH ITERATION WE HAVE THE SUM OF SQUARES 5.88504121E-02
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 1 ST ITERATION WE HAVE THE SUM OF SQUARES 5.88543926E-02
1 1.0001E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 2 ND ITERATION WE HAVE THE SUM OF SQUARES 5.88523124E-02
1 1.0000E+00 2 1.0001E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 3 RD ITERATION WE HAVE THE SUM OF SQUARES 5.88520390E-02
1 1.0000E+00 2 1.0000E+00 3 1.0001E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 4 TH ITERATION WE HAVE THE SUM OF SQUARES 5.88577975E-02
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0001E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 5 TH ITERATION WE HAVE THE SUM OF SQUARES 5.88509852E-02
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 6 TH ITERATION WE HAVE THE SUM OF SQUARES 5.88502669E-02
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0001E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 7 TH ITERATION WE HAVE THE SUM OF SQUARES 5.88500914E-02
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0001E+00 7 1.0001E+00 8 1.0000E+00 9 1.0000E+00

AT THE 8 TH ITERATION WE HAVE THE SUM OF SQUARES 5.88506027E-02
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0001E+00 7 1.0001E+00 8 1.0001E+00 9 1.0000E+00

AT THE 9 TH ITERATION WE HAVE THE SUM OF SQUARES 5.88499540E-02
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0001E+00 7 1.0001E+00 8 1.0000E+00 9 1.0000E+00

THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED 9 iterations
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0001E+00 7 1.0001E+00 8 1.0000E+00 9 1.0000E+00

1 7.4326E-03 2 7.4326E-03 3 1.5772E-03 4 2.4671E-03 5 1.3275E-01
6 -1.4001E-01 7 -7.2748E-04 8 8.1726E-03 9 8.1726E-03 10 -3.0935E-04
11 3.2656E-03 12 1.6979E-03 13 2.3392E-04 14 2.7388E-03 15 6.0370E-04
16 1.4677E-03 17 1.4677E-03 18 2.5194E-04 19 7.3729E-04 20 2.5194E-04
21 7.3729E-04 22 -2.2202E-03 23 1.7693E-03 24 3.2404E-03 25 3.3281E-04
26 -2.8657E-03 27 3.2531E-03 28 -1.7249E-03 29 3.8036E-03 30 -1.3488E-02
31 -3.0889E-02 32 -7.0118E-04 33 4.3579E-02 34 6.7271E-02 35 3.5606E-02
36 -8.5035E-02 37 1.1584E-02 38 -5.6982E-02 39 2.0218E-03 40 2.0483E-02

```
41 1.5384E-02 42 8.7248E-03 43 2.5050E-03 44 -3.2752E-03 45 -1.0616E-02
46 -1.7517E-02 47 -2.5978E-02
```

```
THE SUM OF SQUARES IS 5.88499540E-02
PARROT: @@ No change in the parameters, check the diagram again
PARROT: mac tcecx36cpd
PARROT: set-echo
NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
POLY:
POLY: @@ In PARROT, the global minimization is turned off automatically.
POLY: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY: @@ message will be given.
POLY:
POLY: advanced-option global yes,
Settings for global minimization:
*** WARNING *** Global equilibrium calculation may create new composition sets
and this may corrupt your PARROT work file (.PAR file).
Do not go back to PARROT but exit from POLY after your POLY calculations.
```

```
POLY:
POLY: def-com,,,
POLY: s-a+v 1 w(b) 0 1,,,
The condition W(B)=.1234' created
POLY: s-a+v 2 t 300 1700,,,
The condition T=942.2' created
POLY: s-c t=500
POLY: l-c
W(B)=0.1234, T=500
DEGREES OF FREEDOM 2
POLY: c-e
Creating condition P=1E5
Creating condition N=1
Using global minimization procedure
Calculated 628 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY: save tcecx36 y
```

```
This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.
```

```
POLY: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12
```

```
Organizing start points
```

```
Using ADDED start equilibria
```

```
Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Generating start point 27
Generating start point 28
```

```
Phase region boundary 1 at: 7.140E-01 3.100E+02
  BCC#1
  ** BCC#2
```

```
Calculated.. 2 equilibria
```

```
Terminating at axis limit.
```

```
Phase region boundary 2 at: 7.141E-01 3.000E+02
  BCC#1
  ** BCC#2
```

```
Calculated. 14 equilibria
```

```
Phase region boundary 3 at: 6.816E-01 7.270E+02
  ** A2B
  BCC#1
  ** BCC#2
```

```
Phase region boundary 4 at: 3.625E-01 7.270E+02
  ** A2B
  BCC#1
```

```
Calculated. 15 equilibria
```

```

Phase region boundary  5 at:  3.779E-01  1.184E+03
  ** LIQUID
  ** A2B
  BCC#1

Phase region boundary  6 at:  2.893E-01  1.184E+03
  ** LIQUID
  BCC#1
Calculated.          27 equilibria

Phase region boundary  7 at:  4.903E-01  1.184E+03
  ** LIQUID
  A2B
Calculated.          33 equilibria

Phase region boundary  8 at:  6.480E-01  1.038E+03
  ** LIQUID
  A2B
  ** BCC#1

Phase region boundary  9 at:  7.636E-01  1.038E+03
  A2B
  ** BCC#1
Calculated.          10 equilibria
Terminating at known equilibrium

Phase region boundary 10 at:  8.257E-01  1.038E+03
  LIQUID
  ** BCC#1
Calculated.          8 equilibria

Phase region boundary 11 at:  8.758E-01  1.204E+03
  LIQUID
  ** BCC#1
  ** FCC

Phase region boundary 12 at:  8.811E-01  1.204E+03
  LIQUID
  ** FCC
Calculated.          31 equilibria

Phase region boundary 13 at:  9.361E-01  1.204E+03
  BCC#1
  ** FCC
Calculated.          21 equilibria

Phase region boundary 14 at:  7.140E-01  3.100E+02
  BCC#1
  ** BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 15 at:  7.140E-01  3.100E+02
  BCC#1
  ** BCC#2
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 16 at:  7.140E-01  3.100E+02
  BCC#1
  ** BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 17 at:  7.140E-01  3.100E+02
  BCC#1
  ** BCC#2
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 18 at:  7.140E-01  3.100E+02
  BCC#1
  ** BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 19 at:  7.140E-01  3.100E+02
  BCC#1
  ** BCC#2
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 20 at:  7.140E-01  3.100E+02
  BCC#1
  ** BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 21 at:  7.140E-01  3.100E+02
  ** BCC#1
  BCC#2
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 22 at:  7.140E-01  3.100E+02
  ** BCC#1
  BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 23 at:  7.140E-01  3.100E+02
  ** BCC#1
  BCC#2
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 24 at:  7.140E-01  3.100E+02
  ** BCC#1
  BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

```

```

Phase region boundary 25 at: 3.646E-01 7.700E+02
** A2B
BCC#1
Calculated.          10 equilibria

Phase region boundary 26 at: 3.646E-01 7.700E+02
** A2B
BCC#1
Calculated.          3 equilibria
Terminating at known equilibrium

Phase region boundary 27 at: 3.646E-01 7.700E+02
** A2B
BCC#1
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 28 at: 7.909E-01 7.700E+02
** A2B
BCC#1
Calculated.          10 equilibria

Phase region boundary 29 at: 7.909E-01 7.700E+02
** A2B
BCC#1
Calculated.          3 equilibria
Terminating at known equilibrium

Phase region boundary 30 at: 7.909E-01 7.700E+02
** A2B
BCC#1
Calculated.          9 equilibria
Terminating at known equilibrium

Phase region boundary 31 at: 2.436E-01 1.230E+03
** LIQUID
BCC#1
Calculated.          4 equilibria
Terminating at known equilibrium

Phase region boundary 32 at: 2.436E-01 1.230E+03
** LIQUID
BCC#1
Calculated.          26 equilibria

Phase region boundary 33 at: 8.867E-01 1.230E+03
** LIQUID
FCC
Calculated.          2 equilibria
Terminating at known equilibrium

Phase region boundary 34 at: 8.867E-01 1.230E+03
** LIQUID
FCC
Calculated.          29 equilibria

Phase region boundary 35 at: 6.405E-03 1.397E+03
LIQUID
** BCC#1
Calculated.          10 equilibria

Phase region boundary 36 at: 6.405E-03 1.397E+03
LIQUID
** BCC#1
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 37 at: 2.296E-01 1.243E+03
LIQUID
** BCC#1
Calculated.          23 equilibria

Phase region boundary 38 at: 2.296E-01 1.243E+03
LIQUID
** BCC#1
Calculated.          4 equilibria
Terminating at known equilibrium

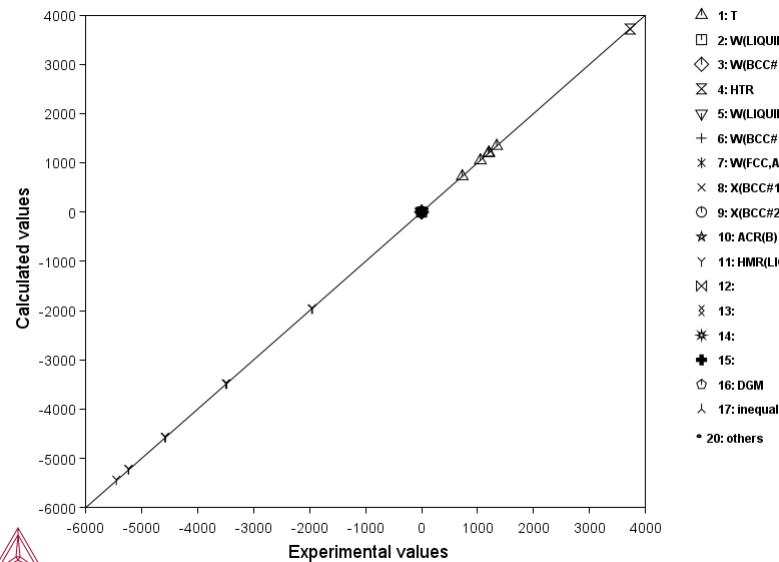
Phase region boundary 39 at: 6.122E-01 1.213E+03
LIQUID
** A2B
Calculated.          12 equilibria
Terminating at known equilibrium

Phase region boundary 40 at: 6.122E-01 1.213E+03
LIQUID
** A2B
Calculated.          8 equilibria
Terminating at known equilibrium

Phase region boundary 41 at: 9.927E-01 1.613E+03
LIQUID
** FCC
Calculated.          19 equilibria
Terminating at known equilibrium

Phase region boundary 42 at: 9.927E-01 1.613E+03
LIQUID
** FCC
Calculated.          14 equilibria
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\generate_console_examples\examples\tcex36a\tcex36.POLY3
CPU time for mapping      1 seconds
POLY: post
POST: s-l d
POST: plot

```



```
POST:  
POST: set-inter  
POST:Hit RETURN to continue  
POST: ba  
POLY: ba
```

PARROT VERSION 5.3

```
Global minimization used as test only  
PARROT: @@ Turn off alternate mode and try to calculate all equilibria  
PARROT: s-alt Y
```

Alternate calculation is on

```
PARROT: ed  
ED_EXP: read 1  
ED_EXP: c-a
```

| Eq | Lab | Iter | Weight | Temp | Exp | Fix phases or comments |
|-----|------|------------|--------|--------|-----|------------------------|
| 1 | AINV | 4 | 1. | 1184.0 | | LIQUID A2B BCC |
| 2 | AINV | 2 | 1. | 1312.5 | | LIQUID A2B |
| 3 | AINV | 3 | 1. | 1038.5 | | LIQUID A2B BCC |
| 4 | AINV | 3 | 1. | 1204.4 | | LIQUID BCC FCC |
| 5 | AINV | 3 | 1. | 727.0 | | A2B BCC BCC#2 |
| 6 | AINV | 2 | 1. | 726.0 | | BCC BCC#2 |
| 10 | ALF | < unused > | | 1594.0 | | LIQUID FCC |
| 11 | ALF | < unused > | | 1548.0 | | LIQUID FCC |
| 12 | ALF | < unused > | | 1499.0 | | LIQUID FCC |
| 13 | ALF | < unused > | | 1438.0 | | LIQUID FCC |
| 20 | ATIE | 3 | 1. | 1413.0 | | LIQUID FCC |
| 21 | ATIE | 3 | 1. | 1337.0 | | LIQUID FCC |
| 22 | ATIE | 3 | 1. | 1213.0 | | LIQUID FCC |
| 23 | ATIE | 3 | 1. | 1100.0 | | LIQUID BCC |
| 100 | AA | 2 | 1. | 1573.0 | | LIQUID |
| 101 | AA | 2 | 1. | 1573.0 | | LIQUID |
| 102 | AA | 2 | 1. | 1573.0 | | LIQUID |
| 103 | AA | 2 | 1. | 1573.0 | | LIQUID |
| 104 | AA | 2 | 1. | 1573.0 | | LIQUID |
| 105 | AA | 2 | 1. | 1573.0 | | LIQUID |
| 106 | AA | 2 | 1. | 1573.0 | | LIQUID |
| 107 | AA | 2 | 1. | 1573.0 | | LIQUID |
| 108 | AA | 2 | 1. | 1573.0 | | LIQUID |
| 110 | AH | 2 | 1. | 1773.0 | | LIQUID |
| 111 | AH | 2 | 1. | 1773.0 | | LIQUID |
| 112 | AH | 2 | 1. | 1773.0 | | LIQUID |
| 113 | AH | 2 | 1. | 1773.0 | | LIQUID |
| 114 | AH | 2 | 1. | 1773.0 | | LIQUID |
| 115 | AH | 2 | 1. | 1773.0 | | LIQUID |
| 116 | AH | 2 | 1. | 1773.0 | | LIQUID |
| 117 | AH | 2 | 1. | 1773.0 | | LIQUID |
| 118 | AH | 2 | 1. | 1773.0 | | LIQUID |

```
ED_EXP: @@ Remove the equilibria with just liquid as we do not optimize
```

```
ED_EXP: @@ any liquid parameters and restore those with label ALF
```

```
ED_EXP: s-we 0 100-118
```

```
ED_EXP: s-we 1 alf
```

```
Changed weight on 4 equilibria.
```

```
ED_EXP: s-e 1
```

```
Equilibrium number 1, label AINV
```

```
ED_EXP: c-a
```

| Eq | Lab | Iter | Weight | Temp | Exp | Fix phases or comments |
|-----|------|------------|--------|--------|-----|------------------------|
| 1 | AINV | 2 | 1. | 1184.0 | | LIQUID A2B BCC |
| 2 | AINV | 2 | 1. | 1312.5 | | LIQUID A2B |
| 3 | AINV | 2 | 1. | 1038.5 | | LIQUID A2B BCC |
| 4 | AINV | 2 | 1. | 1204.4 | | LIQUID BCC FCC |
| 5 | AINV | 2 | 1. | 727.0 | | A2B BCC BCC#2 |
| 6 | AINV | 2 | 1. | 726.0 | | BCC BCC#2 |
| 10 | ALF | 3 | 1. | 1594.0 | | LIQUID FCC |
| 11 | ALF | 3 | 1. | 1548.0 | | LIQUID FCC |
| 12 | ALF | 3 | 1. | 1499.0 | | LIQUID FCC |
| 13 | ALF | 3 | 1. | 1438.0 | | LIQUID FCC |
| 20 | ATIE | 2 | 1. | 1413.0 | | LIQUID FCC |
| 21 | ATIE | 2 | 1. | 1337.0 | | LIQUID FCC |
| 22 | ATIE | 2 | 1. | 1213.0 | | LIQUID FCC |
| 23 | ATIE | 2 | 1. | 1100.0 | | LIQUID BCC |
| 100 | AA | < unused > | | 1573.0 | | LIQUID |
| 101 | AA | < unused > | | 1573.0 | | LIQUID |
| 102 | AA | < unused > | | 1573.0 | | LIQUID |
| 103 | AA | < unused > | | 1573.0 | | LIQUID |
| 104 | AA | < unused > | | 1573.0 | | LIQUID |
| 105 | AA | < unused > | | 1573.0 | | LIQUID |
| 106 | AA | < unused > | | 1573.0 | | LIQUID |
| 107 | AA | < unused > | | 1573.0 | | LIQUID |
| 108 | AA | < unused > | | 1573.0 | | LIQUID |
| 110 | AH | < unused > | | 1773.0 | | LIQUID |
| 111 | AH | < unused > | | 1773.0 | | LIQUID |

```

112 AH < unused > 1773.0 LIQUID
113 AH < unused > 1773.0 LIQUID
114 AH < unused > 1773.0 LIQUID
115 AH < unused > 1773.0 LIQUID
116 AH < unused > 1773.0 LIQUID
117 AH < unused > 1773.0 LIQUID
118 AH < unused > 1773.0 LIQUID
ED_EXP: save
ED_EXP: @@ Save changes
ED_EXP: ba
PARROT: opt 0
Use      29 experiments, maximum is      2000
Use    740 real workspace, maximum is   50000
PARROT: l-r C SCREEN

=====
OUTPUT FROM P A R R O T . DATE 2023. 4.27 16:30:32

*** SUCCESSFUL OPTIMIZATION. ***
NUMBER OF ITERATIONS: 0

== OPTIMIZING CONDITIONS ==
RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 0 DMAX = 1.00000000E+02 H = 1.00000000E-04
ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03

== OPTIMIZING VARIABLES ==
AVAILABLE VARIABLES ARE V1 TO VOO



| VAR. | VALUE           | START VALUE     | SCALING FACTOR  | REL.STAND.DEV  |
|------|-----------------|-----------------|-----------------|----------------|
| V1   | 2.02794315E+04  | 2.02794315E+04  | 2.02794315E+04  | 7.91928257E-02 |
| V2   | -2.92509568E+01 | -2.92509568E+01 | -2.92509568E+01 | 3.42563286E-01 |
| V11  | -2.18109901E+04 | -2.18109901E+04 | -2.18109901E+04 | 3.96976145E-02 |
| V12  | 1.51615699E+01  | 1.51615699E+01  | 1.51615699E+01  | 5.86492608E-02 |
| V15  | 2.43843119E+04  | 2.43843119E+04  | 2.43843119E+04  | 6.09982804E-01 |
| V16  | -8.58207853E+00 | -8.58122041E+00 | -8.58122041E+00 | 2.04927288E+00 |
| V17  | 3.11773766E+03  | 3.11742592E+03  | 3.11742592E+03  | 1.45720326E+00 |
| V19  | 2.19408897E+04  | 2.19408897E+04  | 2.19408897E+04  | 4.63892033E+00 |
| V20  | -7.00145532E+00 | -7.00075524E+00 | -7.00075524E+00 | 1.12676047E+01 |



NUMBER OF OPTIMIZING VARIABLES : 9
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 5.88504121E-02 TO 1.03756241E+01
DEGREES OF FREEDOM 20. REDUCED SUM OF SQUARES 5.18781206E-01



| SYMBOL       | STATUS                    | VALUE/FUNCTION                    |
|--------------|---------------------------|-----------------------------------|
| FUNCTION R   | 298.15                    | 8.314510000000000 ; 6000 N REFO ! |
| 2 RTLNP      | 20000000 +R*T*LN(1E-05*p) |                                   |
| FUNCTION V1  | 298.15                    | 20279.4314990643 ; 6000 N REFO !  |
| FUNCTION V2  | 298.15                    | -29.2509568040070 ; 6000 N REFO ! |
| FUNCTION V11 | 298.15                    | -21810.990742145 ; 6000 N REFO !  |
| FUNCTION V12 | 298.15                    | 15.1615699397423 ; 6000 N REFO !  |
| FUNCTION V15 | 298.15                    | 24384.3118764252 ; 6000 N REFO !  |
| FUNCTION V16 | 298.15                    | -8.58207853322303 ; 6000 N REFO ! |
| FUNCTION V17 | 298.15                    | 3117.73766494043 ; 6000 N REFO !  |
| FUNCTION V19 | 298.15                    | 21940.8896847721 ; 6000 N REFO !  |
| FUNCTION V20 | 298.15                    | -7.00145531884739 ; 6000 N REFO ! |



LIQUID:L (A,B)1.0

==== [A] ====
G(LIQUID,A;0) 298.15 +14000-10*T; 6000 N

==== [B] ====
G(LIQUID,B;0) 298.15 +18000-12*T; 6000 N

==== [A, B] ====
G(LIQUID,A,B;0) 298.15 +V11+V12*T; 6000 N
G(LIQUID,A,B;1) 298.15 +V13+V14*T; 6000 N

$ ===== BLOCK NUMBER 1

DEFINED CONSTANTS
DX=2E-2, PO=101325, DH=500, DT=10
DEFINED FUNCTIONS AND VARIABLES%
HTR=HM(LIQUID)-HM(A2B)
1 T=1193 1184. 10. -9.002 -0.9002
1 W(LIQUID,B)=0.408 0.4170 2.00E-02 9.0023E-03 0.4501
1 W(BCC#1,B)=0.13 0.1325 2.00E-02 2.5110E-03 0.1256
2 T=1341 1312. 10. -28.53 -2.853
2 HTR=3727 3727. 5.00E+02 -0.3638 -7.2770E-04
3 T=1049 1038. 10. -10.54 -1.054
3 W(LIQUID,A)=0.27 0.2738 2.00E-02 3.7580E-03 0.1879
3 W(BCC#1,A)=9.3E-2 9.3931E-02 2.00E-02 9.3112E-04 4.6556E-02
4 T=1203 1204. 10. 1.425 0.1425
4 W(LIQUID,A)=0.19 0.1889 2.00E-02 -1.0604E-03 -5.3019E-02
4 W(BCC#1,A)=6.9E-2 6.8483E-02 2.00E-02 -5.1666E-04 -2.5833E-02
4 W(FCC,A)=6E-2 5.9382E-02 2.00E-02 -6.1767E-04 -3.0884E-02
5 T=726 727. 0 10. 1.009 0.1009
5 X(BCC#1,B)=3.7E-2 3.7326E-02 2.00E-02 3.2606E-04 1.6303E-02
5 X(BCC#2,A)=0.114 0.1146 2.00E-02 6.4970E-04 3.2485E-02
6 X(BCC#1,B)=3.7E-2 3.7042E-02 2.00E-02 4.1911E-05 2.0956E-03
6 X(BCC#2,A)=0.114 0.1139 2.00E-02 -5.0621E-05 -2.5310E-03
10 W(LIQUID,A)=2E-2 1.9382E-02 2.00E-02 -6.1755E-04 -3.0878E-02
11 W(LIQUID,A)=4.2E-2 4.1481E-02 2.00E-02 -5.1853E-04 -2.5926E-02

```

```

12 W(LIQUID,A)=6.5E-2      6.4385E-02  2.00E-02 -6.1455E-04 -3.0728E-02
13 W(LIQUID,A)=9.3E-2      9.2002E-02  2.00E-02 -9.9753E-04 -4.9876E-02
20 W(LIQUID,A)=0.104       0.1030     2.00E-02 -9.6353E-04 -4.8176E-02
20 W(FCC,A)=3.8E-2        3.7715E-02  2.00E-02 -2.8484E-04 -1.4242E-02
21 W(LIQUID,A)=0.136       0.1356     2.00E-02 -4.1873E-04 -2.0936E-02
21 W(FCC,A)=4.7E-2        4.6618E-02  2.00E-02 -3.8208E-04 -1.9104E-02
22 W(LIQUID,A)=0.187       0.1856     2.00E-02 -1.3888E-03 -6.9440E-02
22 W(FCC,A)=5.9E-2        5.8640E-02  2.00E-02 -3.6037E-04 -1.8018E-02
23 W(LIQUID,A)=0.245       0.2435     2.00E-02 -1.5426E-03 -7.7132E-02
23 W(BCC#1,A)=8.5E-2      8.4427E-02  2.00E-02 -5.7339E-04 -2.8669E-02

```

```

PARROT:
PARROT: Hit RETURN to continue
PARROT: @@ When we optimize zero times we sometimes find an error for
PARROT: @@ equilibrium 4. It can be on the wrong side, at high A instead
PARROT: @@ of high B. Try to correct that in the Edit module.
PARROT: ed
ED_EXP: read 1
ED_EXP: s-e 4
Equilibrium number           4, label AINV
ED_EXP: s-a-s
T /1204.424718/: 1200
Automatic start values for phase constituents? /N/: N

```

```

Phase LIQUID
Major constituent(s) /b/: b

Phase BCC
Major constituent(s) /b/: b

Phase FCC
Major constituent(s) /b/: b
ED_EXP:
ED_EXP: c-e
Testing result with global minimization
 13 ITS, CPU TIME USED   0 SECONDS
ED_EXP: l-e
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
Output from POLY-3, equilibrium =      4, label AINV, database:

Conditions:
P=101325
FIXED PHASES
LIQUID=1 BCC#1=1 FCC=1
DEGREES OF FREEDOM 0

```

```

Temperature 1204.42 K ( 931.27 C), Pressure 1.013250E+05
Number of moles of components 3.00000E+00, Mass in grams 1.30212E+02
Total Gibbs energy -9.82809E+03, Enthalpy 1.98600E+04, Volume 0.00000E+00

```

```

Component          Moles      W-Fraction    Activity    Potential  Ref.stat
A                 6.5962E-01  1.0131E-01  3.8835E-01 -9.4718E+03 SER
B                 2.3404E+00  8.9869E-01  8.5833E-01 -1.5298E+03 SER

FCC                Status FIXED      Driving force 0.0000E+00
Moles 1.00000E+00, Mass 4.5911E+01, Volume fraction 0.0000E+00 Mass fractions:
B 9.40618E-01  A 5.93823E-02

BCC#1              Status FIXED      Driving force 0.0000E+00
Moles 1.00000E+00, Mass 4.5342E+01, Volume fraction 0.0000E+00 Mass fractions:
B 9.31517E-01  A 6.84833E-02

```

```

LIQUID              Status FIXED      Driving force 0.0000E+00
Moles 1.00000E+00, Mass 3.8959E+01, Volume fraction 0.0000E+00 Mass fractions:
B 8.11060E-01  A 1.88940E-01
EXPERIMENT T=1203:DT $1204.42:10 NO=1
EXPERIMENT W(LIQUID,A)=0.19:DX $0.18894:2E-2 NO=2
EXPERIMENT W(BCC#1,A)=6.9E-2:DX $6.84833E-2:2E-2 NO=3
EXPERIMENT W(FCC,A)=6E-2:DX $5.93823E-2:2E-2 NO=4

```

```

ED_EXP: ba
PARROT: @@ The error is still there, calculate the phase diagram.
PARROT: mac tcex36cpd
PARROT: set-echo

```

```

NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3

```

```
POLY:
```

```
POLY: @@ In PARROT, the global minimization is turned off automatically.
POLY: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY: @@ message will be given.
```

```
POLY:
```

```
POLY: advanced-option global yes,,,
Settings for global minimization:
*** WARNING *** Global equilibrium calculation may create new composition sets
and this may corrupt your PARROT work file (.PAR file).
Do not go back to PARROT but exit from POLY after your POLY calculations.
```

```
POLY:
```

```
POLY: def-com,,,
POLY: s-a-v 1 w(b) 0 1,,,
The condition W(B)=.1234 created
```

```
POLY: s-a-v 2 t 300 1700,,,
The condition T=942.2 created
```

```
POLY: s-c t=500
```

```
POLY: l-c
```

```
W(B)=0.1234, T=500
```

```
DEGREES OF FREEDOM 2
```

```
POLY: c-e
```

```
Creating condition P=1E5
```

```
Creating condition N=1
```

```
Using global minimization procedure
```

```
Calculated      628 grid points in      0 s
```

```
Found the set of lowest grid points in      0 s
```

```
Calculated POLY solution      0 s, total time      0 s
```

```
POLY: save tcex36 y
```

```
This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.
```

```
POLY: map
```

```
Version S mapping is selected
```

```

Generating start equilibrium  1
Generating start equilibrium  2
Generating start equilibrium  3
Generating start equilibrium  4
Generating start equilibrium  5
Generating start equilibrium  6
Generating start equilibrium  7
Generating start equilibrium  8
Generating start equilibrium  9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Generating start point  1
Generating start point  2
Generating start point  3
Generating start point  4
Generating start point  5
Generating start point  6
Generating start point  7
Generating start point  8
Generating start point  9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Generating start point 27
Generating start point 28

Phase region boundary  1 at:  7.140E-01  3.100E+02
   BCC#1
   ** BCC#2
Calculated..           2 equilibria
Terminating at axis limit.

Phase region boundary  2 at:  7.141E-01  3.000E+02
   BCC#1
   ** BCC#2
Calculated.           14 equilibria

Phase region boundary  3 at:  6.816E-01  7.270E+02
   ** A2B
   BCC#1
   ** BCC#2
Calculated.           15 equilibria

Phase region boundary  4 at:  3.625E-01  7.270E+02
   ** A2B
   BCC#1
Calculated.           15 equilibria

Phase region boundary  5 at:  3.779E-01  1.184E+03
   ** LIQUID
   ** A2B
   BCC#1
Calculated.           27 equilibria

Phase region boundary  6 at:  2.893E-01  1.184E+03
   ** LIQUID
   BCC#1
Calculated.           27 equilibria

Phase region boundary  7 at:  4.903E-01  1.184E+03
   ** LIQUID
   A2B
Calculated.           33 equilibria

Phase region boundary  8 at:  6.480E-01  1.038E+03
   ** LIQUID
   A2B
   ** BCC#1
Calculated.           8 equilibria

Phase region boundary  9 at:  7.636E-01  1.038E+03
   A2B
   ** BCC#1
Calculated.           10 equilibria
Terminating at known equilibrium

Phase region boundary 10 at:  8.257E-01  1.038E+03
   LIQUID
   ** BCC#1
Calculated.           8 equilibria

Phase region boundary 11 at:  8.758E-01  1.204E+03
   LIQUID
   ** BCC#1
   ** FCC
Calculated.           31 equilibria

Phase region boundary 12 at:  8.811E-01  1.204E+03
   LIQUID
   ** FCC
Calculated.           31 equilibria

Phase region boundary 13 at:  9.361E-01  1.204E+03
   BCC#1
   ** FCC
Calculated.           21 equilibria

Phase region boundary 14 at:  7.140E-01  3.100E+02

```

```

BCC#1
** BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 15 at: 7.140E-01 3.100E+02
    BCC#1
    ** BCC#2
Calculated..          2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 16 at: 7.140E-01 3.100E+02
    BCC#1
    ** BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 17 at: 7.140E-01 3.100E+02
    BCC#1
    ** BCC#2
Calculated..          2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 18 at: 7.140E-01 3.100E+02
    BCC#1
    ** BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 19 at: 7.140E-01 3.100E+02
    BCC#1
    ** BCC#2
Calculated..          2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 20 at: 7.140E-01 3.100E+02
    BCC#1
    ** BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 21 at: 7.140E-01 3.100E+02
    BCC#1
    BCC#2
Calculated..          2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 22 at: 7.140E-01 3.100E+02
    * * BCC#1
    BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 23 at: 7.140E-01 3.100E+02
    * * BCC#1
    BCC#2
Calculated..          2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 24 at: 7.140E-01 3.100E+02
    * * BCC#1
    BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 25 at: 3.646E-01 7.700E+02
    * * A2B
    BCC#1
Calculated.          10 equilibria

Phase region boundary 26 at: 3.646E-01 7.700E+02
    * * A2B
    BCC#1
Calculated.          3 equilibria
Terminating at known equilibrium

Phase region boundary 27 at: 3.646E-01 7.700E+02
    * * A2B
    BCC#1
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 28 at: 7.909E-01 7.700E+02
    * * A2B
    BCC#1
Calculated.          10 equilibria

Phase region boundary 29 at: 7.909E-01 7.700E+02
    * * A2B
    BCC#1
Calculated.          3 equilibria
Terminating at known equilibrium

Phase region boundary 30 at: 7.909E-01 7.700E+02
    * * A2B
    BCC#1
Calculated.          9 equilibria
Terminating at known equilibrium

Phase region boundary 31 at: 2.436E-01 1.230E+03
    * * LIQUID
    BCC#1
Calculated.          4 equilibria
Terminating at known equilibrium

Phase region boundary 32 at: 2.436E-01 1.230E+03
    * * LIQUID
    BCC#1
Calculated.          26 equilibria

Phase region boundary 33 at: 8.867E-01 1.230E+03

```

```

** LIQUID
FCC
Calculated.          2 equilibria
Terminating at known equilibrium

Phase region boundary 34 at:   8.867E-01  1.230E+03
** LIQUID
FCC
Calculated           29 equilibria

Phase region boundary 35 at:   6.405E-03  1.397E+03
LIQUID
** BCC#1
Calculated           10 equilibria

Phase region boundary 36 at:   6.405E-03  1.397E+03
LIQUID
** BCC#1
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 37 at:   2.296E-01  1.243E+03
LIQUID
** BCC#1
Calculated           23 equilibria

Phase region boundary 38 at:   2.296E-01  1.243E+03
LIQUID
** BCC#1
Calculated.          4 equilibria
Terminating at known equilibrium

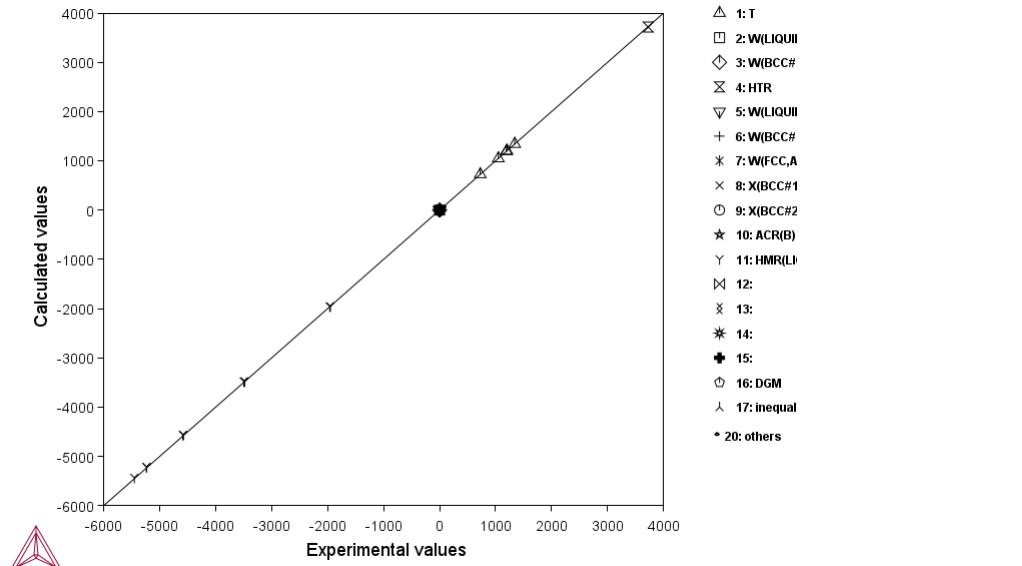
Phase region boundary 39 at:   6.122E-01  1.213E+03
LIQUID
** A2B
Calculated.          12 equilibria
Terminating at known equilibrium

Phase region boundary 40 at:   6.122E-01  1.213E+03
LIQUID
** A2B
Calculated.          8 equilibria
Terminating at known equilibrium

Phase region boundary 41 at:   9.927E-01  1.613E+03
LIQUID
** FCC
Calculated.          19 equilibria
Terminating at known equilibrium

Phase region boundary 42 at:   9.927E-01  1.613E+03
LIQUID
** FCC
Calculated.          14 equilibria
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\generate_console_examples\examples\tcex36a\tcex36.POLY3
CPU time for mapping      2 seconds
POLY: post
POST: s-l d
POST: plot

```



```

POST:
POST: set-inter
POST: Hit RETURN to continue
POST: @@ The phase diagram shows there is no equilibrium between liquid,
POST: @@ fcc and bcc at high B content. For the moment we better remove
POST: @@ equilibrium 4 from the optimization.
POST: ba
POLY: ba

```

```

PARROT VERSION 5.3

Global minimization used as test only
PARROT: ed
ED_EXP: read 1
ED_EXP: s-we 0 4
ED_EXP: save
ED_EXP: ba
PARROT: opt 0
Use      25 experiments, maximum is      2000
Use      664 real workspace, maximum is    50000
PARROT: l-r C SCREEN

```

```
=====  
OUTPUT FROM P A R R O T . DATE 2023. 4.27 16:30:56
```

```
*** SUCCESSFUL OPTIMIZATION. ***  
NUMBER OF ITERATIONS: 0
```

```
== OPTIMIZING CONDITIONS ==
```

```
RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N  
MINIMUM SAVE ON FILE: Y  
ERROR FOR INEQUALITIES = 1.00000000E+00  
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04  
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)  
MAXFUN = 0 DMAX = 1.00000000E+02 H = 1.00000000E-04  
ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03
```

```
== OPTIMIZING VARIABLES ==
```

```
AVAILABLE VARIABLES ARE V1 TO VOO
```

| VAR. | VALUE | START VALUE | SCALING FACTOR | REL. STAND. DEV |
|------|-----------------|-----------------|-----------------|-----------------|
| V1 | 2.02794315E+04 | 2.02794315E+04 | 2.02794315E+04 | 7.91928257E-02 |
| V2 | -2.92509568E+01 | -2.92509568E+01 | -2.92509568E+01 | 3.42563286E-01 |
| V11 | -2.18109901E+04 | -2.18109901E+04 | -2.18109901E+04 | 3.96976145E-02 |
| V12 | 1.51615699E+01 | 1.51615699E+01 | 1.51615699E+01 | 5.86492608E-02 |
| V15 | 2.43843119E+04 | 2.43843119E+04 | 2.43843119E+04 | 6.09982804E-01 |
| V16 | -8.58207853E+00 | -8.58122041E+00 | -8.58122041E+00 | 2.04927288E+00 |
| V17 | 3.11773766E+03 | 3.11742592E+03 | 3.11742592E+03 | 1.45720326E+00 |
| V19 | 2.19408897E+04 | 2.19408897E+04 | 2.19408897E+04 | 4.63892033E+00 |
| V20 | -7.00145532E+00 | -7.00075524E+00 | -7.00075524E+00 | 1.12676047E+01 |

```
NUMBER OF OPTIMIZING VARIABLES : 9
```

```
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO  
THE SUM OF SQUARES HAS CHANGED FROM 5.88504121E-02 TO 1.03508938E+01  
DEGREES OF FREEDOM 16. REDUCED SUM OF SQUARES 6.46930861E-01
```

| SYMBOL | STATUS | VALUE/FUNCTION |
|--------------|---------------------------|-----------------------------------|
| FUNCTION R | 298.15 | 8.31451000000000 ; 6000 N REFO ! |
| 2 RTLNP | 20000000 +R*T*LN(1E-05*P) | |
| FUNCTION V1 | 298.15 | 20279.4314990643 ; 6000 N REFO ! |
| FUNCTION V2 | 298.15 | -29.2509568040070 ; 6000 N REFO ! |
| FUNCTION V11 | 298.15 | -21810.990142145 ; 6000 N REFO ! |
| FUNCTION V12 | 298.15 | 15.1615699397423 ; 6000 N REFO ! |
| FUNCTION V15 | 298.15 | 24384.3118764252 ; 6000 N REFO ! |
| FUNCTION V16 | 298.15 | -8.58207853322303 ; 6000 N REFO ! |
| FUNCTION V17 | 298.15 | 3117.73766494043 ; 6000 N REFO ! |
| FUNCTION V19 | 298.15 | 21940.8896847721 ; 6000 N REFO ! |
| FUNCTION V20 | 298.15 | -7.00145531884739 ; 6000 N REFO ! |

```
LIQUID:L (A,B)1.0
```

| ===== [A] ===== | | |
|--------------------|---------------------|--------|
| G(LIQUID,A;0) | 298.15 +14000-10*T; | 6000 N |
| ===== [B] ===== | | |
| G(LIQUID,B;0) | 298.15 +18000-12*T; | 6000 N |
| ===== [A, B] ===== | | |
| G(LIQUID,A,B;0) | 298.15 +V11+V12*T; | 6000 N |
| G(LIQUID,A,B;1) | 298.15 +V13+V14*T; | 6000 N |

```
$ ===== BLOCK NUMBER 1
```

| DEFINED CONSTANTS | | |
|-----------------------------------|------------|----------------------------------|
| DX=2E-2, PO=101325, DH=500, DT=10 | | |
| DEFINED FUNCTIONS AND VARIABLES% | | |
| HTR=HM(LIQUID)-HM(A2B) | | |
| 1 T=1193 | 1184. | 10. -9.002 -0.9002 |
| 1 W(LIQUID,B)=0.408 | 0.4170 | 2.00E-02 9.0023E-03 0.4501 |
| 1 W(BCC#1,B)=0.13 | 0.1325 | 2.00E-02 2.5110E-03 0.1256 |
| 2 T=1341 | 1312. | 10. -28.53 -2.853 |
| 2 HTR=3727 | 3727. | 5.00E+02 -0.3638 -7.2770E-04 |
| 3 T=1049 | 1038. | 10. -10.54 -1.054 |
| 3 W(LIQUID,A)=0.27 | 0.2738 | 2.00E-02 3.7580E-03 0.1879 |
| 3 W(BCC#1,A)=9.3E-2 | 9.3931E-02 | 2.00E-02 9.3112E-04 4.6556E-02 |
| 5 T=726 | 727.0 | 10. 1.009 0.1009 |
| 5 X(BCC#1,B)=3.7E-2 | 3.7326E-02 | 2.00E-02 3.2606E-04 1.6303E-02 |
| 5 X(BCC#2,A)=0.114 | 0.1146 | 2.00E-02 6.4970E-04 3.2485E-02 |
| 6 X(BCC#1,B)=3.7E-2 | 3.7042E-02 | 2.00E-02 4.1911E-05 2.0956E-03 |
| 6 X(BCC#2,A)=0.114 | 0.1139 | 2.00E-02 -5.0621E-05 -2.5310E-03 |
| 10 W(LIQUID,A)=2E-2 | 1.9382E-02 | 2.00E-02 -6.1755E-04 -3.0878E-02 |
| 11 W(LIQUID,A)=4.2E-2 | 4.1481E-02 | 2.00E-02 -5.1853E-04 -2.5926E-02 |
| 12 W(LIQUID,A)=6.5E-2 | 6.4385E-02 | 2.00E-02 -6.1455E-04 -3.0728E-02 |
| 13 W(LIQUID,A)=9.3E-2 | 9.2002E-02 | 2.00E-02 -9.9753E-04 -4.9876E-02 |
| 20 W(LIQUID,A)=0.104 | 0.1030 | 2.00E-02 -9.6353E-04 -4.8176E-02 |
| 20 W(FCC,A)=3.8E-2 | 3.7715E-02 | 2.00E-02 -2.8484E-04 -1.4242E-02 |
| 21 W(LIQUID,A)=0.136 | 0.1356 | 2.00E-02 -4.1873E-04 -2.0936E-02 |
| 21 W(FCC,A)=4.7E-2 | 4.6618E-02 | 2.00E-02 -3.8208E-04 -1.9104E-02 |
| 22 W(LIQUID,A)=0.187 | 0.1856 | 2.00E-02 -1.3888E-03 -6.9440E-02 |
| 22 W(FCC,A)=5.9E-2 | 5.8640E-02 | 2.00E-02 -3.6037E-04 -1.8018E-02 |
| 23 W(LIQUID,A)=0.245 | 0.2435 | 2.00E-02 -1.5426E-03 -7.7132E-02 |
| 23 W(BCC#1,A)=8.5E-2 | 8.4427E-02 | 2.00E-02 -5.7339E-04 -2.8669E-02 |

```
PARROT:
```

```
PARROT:Hit RETURN to continue
```

```
PARROT: opt 30
```

```
Use 25 experiments, maximum is 2000
```

```
Use 664 real workspace, maximum is 50000
```

```
The following output is provided by subroutine VA05A
```

```

AT THE 0 TH ITERATION WE HAVE THE SUM OF SQUARES 1.03508938E+01
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0001E+00 7 1.0001E+00 8 1.0000E+00 9 1.0001E+00

AT THE 1 ST ITERATION WE HAVE THE SUM OF SQUARES 1.05260129E+01
1 1.0001E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0001E+00 7 1.0001E+00 8 1.0000E+00 9 1.0001E+00

AT THE 2 ND ITERATION WE HAVE THE SUM OF SQUARES 1.00358079E+01
1 1.0000E+00 2 1.0001E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0001E+00 7 1.0001E+00 8 1.0000E+00 9 1.0001E+00

AT THE 3 RD ITERATION WE HAVE THE SUM OF SQUARES 1.01714045E+01
1 1.0000E+00 2 1.0001E+00 3 1.0001E+00 4 1.0000E+00 5 1.0000E+00
6 1.0001E+00 7 1.0001E+00 8 1.0000E+00 9 1.0001E+00

AT THE 4 TH ITERATION WE HAVE THE SUM OF SQUARES 9.91871683E+00
1 1.0000E+00 2 1.0001E+00 3 1.0000E+00 4 1.0001E+00 5 1.0000E+00
6 1.0001E+00 7 1.0001E+00 8 1.0000E+00 9 1.0001E+00

AT THE 5 TH ITERATION WE HAVE THE SUM OF SQUARES 9.92573051E+00
1 1.0000E+00 2 1.0001E+00 3 1.0000E+00 4 1.0001E+00 5 1.0001E+00
6 1.0001E+00 7 1.0001E+00 8 1.0000E+00 9 1.0001E+00

AT THE 6 TH ITERATION WE HAVE THE SUM OF SQUARES 9.91605701E+00
1 1.0000E+00 2 1.0001E+00 3 1.0000E+00 4 1.0001E+00 5 1.0000E+00
6 1.0002E+00 7 1.0001E+00 8 1.0000E+00 9 1.0001E+00

AT THE 7 TH ITERATION WE HAVE THE SUM OF SQUARES 9.91568464E+00
1 1.0000E+00 2 1.0001E+00 3 1.0000E+00 4 1.0001E+00 5 1.0000E+00
6 1.0002E+00 7 1.0002E+00 8 1.0000E+00 9 1.0001E+00

AT THE 8 TH ITERATION WE HAVE THE SUM OF SQUARES 9.91603391E+00
1 1.0000E+00 2 1.0001E+00 3 1.0000E+00 4 1.0001E+00 5 1.0000E+00
6 1.0002E+00 7 1.0002E+00 8 1.0001E+00 9 1.0001E+00

AT THE 9 TH ITERATION WE HAVE THE SUM OF SQUARES 9.91553746E+00
1 1.0000E+00 2 1.0001E+00 3 1.0000E+00 4 1.0001E+00 5 1.0000E+00
6 1.0002E+00 7 1.0002E+00 8 1.0000E+00 9 1.0002E+00

AT THE 10 TH ITERATION WE HAVE THE SUM OF SQUARES 2.62188304E-01
1 9.9791E-01 2 1.0039E+00 3 9.9835E-01 4 1.0015E+00 5 9.9992E-01
6 1.0002E+00 7 1.0002E+00 8 1.0000E+00 9 1.0002E+00

AT THE 11 TH ITERATION WE HAVE THE SUM OF SQUARES 1.84424024E-01
1 9.9876E-01 2 1.0036E+00 3 9.9813E-01 4 1.0027E+00 5 9.9858E-01
6 9.9624E-01 7 9.9908E-01 8 1.0011E+00 9 1.0013E+00

AT THE 12 TH ITERATION WE HAVE THE SUM OF SQUARES 9.30581656E-02
1 9.9982E-01 2 1.0039E+00 3 9.9787E-01 4 1.0041E+00 5 9.9651E-01
6 9.8851E-01 7 9.9668E-01 8 1.0039E+00 9 1.0050E+00

AT THE 13 TH ITERATION WE HAVE THE SUM OF SQUARES 1.62061450E-02
1 1.0012E+00 2 1.0033E+00 3 9.9860E-01 4 1.0085E+00 5 9.9194E-01
6 9.7109E-01 7 9.9185E-01 8 1.0062E+00 9 1.0032E+00

AT THE 14 TH ITERATION WE HAVE THE SUM OF SQUARES 4.83083490E-03
1 1.0020E+00 2 1.0031E+00 3 9.9903E-01 4 1.0110E+00 5 9.8937E-01
6 9.6104E-01 7 9.8922E-01 8 1.0081E+00 9 1.0035E+00

THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED 14 iterations
1 1.0020E+00 2 1.0031E+00 3 9.9903E-01 4 1.0110E+00 5 9.8937E-01
6 9.6104E-01 7 9.8922E-01 8 1.0081E+00 9 1.0035E+00

1 -3.1045E-02 2 -1.2730E-02 3 -4.4920E-03 4 2.6758E-03 5 -1.7908E-02
6 1.5844E-02 7 1.5494E-02 8 3.3258E-03 9 -3.9381E-03 10 2.0912E-02
11 -9.6601E-03 12 2.1466E-02 13 -8.3094E-03 14 -2.1576E-02 15 -7.1595E-03
16 -3.1652E-03 17 -1.2932E-02 18 -7.8557E-03 19 9.4297E-03 20 2.8031E-02
21 4.0812E-03 22 -1.1349E-02 23 -1.3920E-03 24 -9.7046E-04 25 -2.6692E-04

```

THE SUM OF SQUARES IS 4.83083490E-03

PARROT: cont 30

It is safe to CONTINUE only after TOO MANY ITERATIONS
and no change in variables and experiments ...
Now anything can happen ...

PARROT: l-r C SCREEN

```
=====
OUTPUT FROM P A R R O T . DATE 2023. 4.27 16:30:56
```

*** SUCCESSFUL OPTIMIZATION. ***
NUMBER OF ITERATIONS: 15

== OPTIMIZING CONDITIONS ==

```
RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 30 DMAX = 1.00000000E+02 H = 1.00000000E-04
ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03
```

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO VOO

| VAR. | VALUE | START VALUE | SCALING FACTOR | REL.STAND.DEV |
|------|-----------------|-----------------|-----------------|----------------|
| V1 | 2.03192526E+04 | 2.02794315E+04 | 2.02794315E+04 | 1.03256129E-01 |
| V2 | -2.93407339E+01 | -2.92509568E+01 | -2.92509568E+01 | 9.50349210E-02 |
| V11 | -2.17899144E+04 | -2.18109901E+04 | -2.18109901E+04 | 2.03679598E-01 |
| V12 | 1.53278493E+01 | 1.51615699E+01 | 1.51615699E+01 | 3.38209139E-01 |
| V15 | 2.41251226E+04 | 2.43843119E+04 | 2.43843119E+04 | 1.49764018E-01 |
| V16 | -8.24687780E+00 | -8.58122041E+00 | -8.58122041E+00 | 5.17740140E-01 |
| V17 | 3.08382018E+03 | 3.11742592E+03 | 3.11742592E+03 | 2.63521177E-01 |
| V19 | 2.21176852E+04 | 2.19408897E+04 | 2.19408897E+04 | 6.93239683E-01 |

V20 -7.02506636E+00 -7.00075524E+00 -7.00075524E+00 1.73851269E+00

NUMBER OF OPTIMIZING VARIABLES : 9
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 1.03508938E+01 TO 4.83083490E-03
DEGREES OF FREEDOM 16. REDUCED SUM OF SQUARES 3.01927181E-04

| SYMBOL | STATUS | VALUE/FUNCTION |
|--------------|----------|-----------------------------------|
| FUNCTION R | 298.15 | 8.314510000000000 ; 6000 N REFO ! |
| 2 RTLNP | 20000000 | +R*T*LN(1B-05*P) |
| FUNCTION V1 | 298.15 | 20319.2526367168 ; 6000 N REFO ! |
| FUNCTION V2 | 298.15 | -29.3407338796858 ; 6000 N REFO ! |
| FUNCTION V11 | 298.15 | -21789.9143983616 ; 6000 N REFO ! |
| FUNCTION V12 | 298.15 | 15.3278493485650 ; 6000 N REFO ! |
| FUNCTION V15 | 298.15 | 24125.1226142511 ; 6000 N REFO ! |
| FUNCTION V16 | 298.15 | -8.24687780176102 ; 6000 N REFO ! |
| FUNCTION V17 | 298.15 | 3083.82017668620 ; 6000 N REFO ! |
| FUNCTION V19 | 298.15 | 22117.6851953482 ; 6000 N REFO ! |
| FUNCTION V20 | 298.15 | -7.02506635732492 ; 6000 N REFO ! |

LIQUID:L (A,B)1.0

==== [A] ====
G(LIQUID,A;0) 298.15 +14000-10*T; 6000 N

==== [B] ====
G(LIQUID,B;0) 298.15 +18000-12*T; 6000 N

==== [A, B] ====
G(LIQUID,A,B;0) 298.15 +V11+V12*T; 6000 N
G(LIQUID,A,B;1) 298.15 +V13+V14*T; 6000 N

\$ ===== BLOCK NUMBER 1

DEFINED CONSTANTS
DX=2E-2, P0=101325, DH=500, DT=10
DEFINED FUNCTIONS AND VARIABLES%
HTR=HM(LIQUID)-HM(A2B)
1 T=1193 1193. 10. -0.3105 -3.1045E-02
1 W(LIQUID,B)=0.408 0.4077 2.00E-02 -2.5459E-04 -1.2730E-02
1 W(BCC#1,B)=0.13 0.1299 2.00E-02 -8.9839E-05 -4.4920E-03
2 T=1341 1341. 10. 2.6758E-02 2.6758E-03
2 HTR=3727 3718. 5.00E+02 -8.954 -1.7908E-02
3 T=1049 1049. 10. 0.1584 1.5844E-02
3 W(LIQUID,A)=0.27 0.2703 2.00E-02 3.0989E-04 1.5494E-02
3 W(BCC#1,A)=9.3E-2 9.3067E-02 2.00E-02 6.6517E-05 3.3258E-03
5 T=726 726.0 10. -3.9381E-02 -3.9381E-03
5 X(BCC#1,B)=3.7E-2 3.7418E-02 2.00E-02 4.1825E-04 2.0912E-02
5 X(BCC#2,A)=0.114 0.1138 2.00E-02 -1.9320E-04 -9.6601E-03
6 X(BCC#1,B)=3.7E-2 3.7429E-02 2.00E-02 4.2932E-04 2.1466E-02
6 X(BCC#2,A)=0.114 0.1138 2.00E-02 -1.6619E-04 -8.3094E-03
10 W(LIQUID,B)=2E-2 1.9568E-02 2.00E-02 -4.3151E-04 -2.1576E-02
11 W(LIQUID,A)=4.2E-2 4.1857E-02 2.00E-02 -1.4319E-04 -7.1595E-03
12 W(LIQUID,A)=6.5E-2 6.4937E-02 2.00E-02 -6.3303E-05 -3.1652E-03
13 W(LIQUID,A)=9.3E-2 9.2741E-02 2.00E-02 -2.5863E-04 -1.2932E-02
20 W(LIQUID,A)=0.104 0.1038 2.00E-02 -1.5711E-04 -7.8557E-03
20 W(FCC,A)=3.8E-2 3.8189E-02 2.00E-02 1.8859E-04 9.4297E-03
21 W(LIQUID,A)=0.136 0.1366 2.00E-02 5.6062E-04 2.8031E-02
21 W(FCC,A)=4.7E-2 4.7082E-02 2.00E-02 8.1625E-05 4.0812E-03
22 W(LIQUID,A)=0.187 0.1868 2.00E-02 -2.2697E-04 -1.1349E-02
22 W(FCC,A)=5.9E-2 5.8972E-02 2.00E-02 -2.7840E-05 -1.3920E-03
23 W(LIQUID,A)=0.245 0.2450 2.00E-02 -1.9409E-05 -9.7046E-04
23 W(BCC#1,A)=8.5E-2 8.4995E-02 2.00E-02 -5.3384E-06 -2.6692E-04

PARROT:
PARROT:Hit RETURN to continue
PARROT: @@ Optimization converged, try to add equilibrium 4 again
PARROT: ed
ED_EXP: read 1
ED_EXP: s-e 4
Equilibrium number 4, label AINV
ED_EXP: s-a-s
T /1204.424718/: 1200
Automatic start values for phase constituents? /N/: N

Phase LIQUID
Major constituent(s) /b/: b

Phase BCC
Major constituent(s) /b/: b

Phase FCC
Major constituent(s) /b/: b
ED_EXP:
ED_EXP: c-e
Testing result with global minimization
13 ITS, CPU TIME USED 0 SECONDS
ED_EXP: l-e
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /WVCS/: VWCS
Output from POLY-3, equilibrium = 4, label AINV, database:

Conditions:
P=101325
FIXED PHASES
LIQUID=1 BCC#1=1 FCC=1
DEGREES OF FREEDOM 0

Temperature 1203.73 K (930.58 C), Pressure 1.013250E+05
Number of moles of components 3.00000E+00, Mass in grams 1.30100E+02
Total Gibbs energy -9.74919E+03, Enthalpy 1.98559E+04, Volume 0.00000E+00

| Component | Moles | W-Fraction | Activity | Potential | Ref.stat |
|-----------|------------|------------|------------|-------------|----------|
| A | 6.6333E-01 | 1.0197E-01 | 3.9460E-01 | -9.3067E+03 | SER |
| B | 2.3367E+00 | 8.9803E-01 | 8.5822E-01 | -1.5303E+03 | SER |

FCC Status FIXED Driving force 0.0000E+00

```

Moles 1.0000E+00, Mass 4.5887E+01, Volume fraction 0.0000E+00 Mass fractions:
B 9.40241E-01 A 5.97588E-02

BCC#1           Status FIXED      Driving force 0.0000E+00
Moles 1.0000E+00, Mass 4.5320E+01, Volume fraction 0.0000E+00 Mass fractions:
B 9.31155E-01 A 6.88454E-02

LIQUID          Status FIXED      Driving force 0.0000E+00
Moles 1.0000E+00, Mass 3.8893E+01, Volume fraction 0.0000E+00 Mass fractions:
B 8.09622E-01 A 1.90378E-01
SET WEIGHT 0,,
EXPERIMENT T=1203:DT
EXPERIMENT W(LIQUID,A)=0.19:DX
EXPERIMENT W(BCC#1,A)=6.98E-2:DX
EXPERIMENT W(FCC,A)=6E-2:DX
ED EXP: ba
PARROT: @@ It still fails, try to calculate the phase diagram again.
PARROT: mac tcex36cpd
PARROT: set-echo
NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
POLY:
POLY: @@ In PARROT, the global minimization is turned off automatically.
POLY: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY: @@ message will be given.
POLY:
POLY: advanced-option global yes,,
Settings for global minimization:
*** WARNING *** Global equilibrium calculation may create new composition sets
and this may corrupt your PARROT work file (.PAR file).
Do not go back to PARROT but exit from POLY after your POLY calculations.
POLY:
POLY: def-com,,
POLY: s-a-v 1 w(b) 0 1,,
The condition W(B)=.1234 created
POLY: s-a-v 2 t 300 1700,,
The condition T=942.2 created
POLY: s-c t=500
POLY: 1-c
W(B)=0.1234, T=500
DEGREES OF FREEDOM 2
POLY: c-e
Creating condition P=1E5
Creating condition N=1
Using global minimization procedure
Calculated       628 grid points in      0 s
Found the set of lowest grid points in      0 s
Calculated POLY solution      0 s, total time      0 s
POLY: save tcex36 y

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

POLY: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Generating start point 27
Generating start point 28

Phase region boundary 1 at: 7.140E-01 3.100E+02
  BCC#1
  ** BCC#2
Calculated..          2 equilibria
Terminating at axis limit.

Phase region boundary 2 at: 7.141E-01 3.000E+02
  BCC#1
  ** BCC#2

```

```

Calculated.          14 equilibria

Phase region boundary 3 at:  6.821E-01  7.260E+02
** A2B
  BCC#1
** BCC#2

Phase region boundary 4 at:  3.626E-01  7.260E+02
** A2B
  BCC#1
Calculated.          15 equilibria

Phase region boundary 5 at:  3.769E-01  1.193E+03
** LIQUID
** A2B
  BCC#1
Calculated.          28 equilibria

Phase region boundary 6 at:  2.826E-01  1.193E+03
** LIQUID
  BCC#1
Calculated.          33 equilibria

Phase region boundary 7 at:  4.863E-01  1.193E+03
** LIQUID
  A2B
Calculated.          33 equilibria

Phase region boundary 8 at:  6.500E-01  1.049E+03
** LIQUID
  A2B
** BCC#1
Calculated.          11 equilibria
Terminating at known equilibrium

Phase region boundary 10 at:  8.276E-01  1.049E+03
  LIQUID
** BCC#1
Calculated.          8 equilibria

Phase region boundary 11 at:  8.750E-01  1.204E+03
  LIQUID
** BCC#1
** FCC
Calculated.          32 equilibria

Phase region boundary 12 at:  8.803E-01  1.204E+03
  LIQUID
** FCC
Calculated.          23 equilibria

Phase region boundary 13 at:  9.357E-01  1.204E+03
  BCC#1
** FCC
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 14 at:  7.140E-01  3.100E+02
  BCC#1
** BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 15 at:  7.140E-01  3.100E+02
  BCC#1
** BCC#2
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 16 at:  7.140E-01  3.100E+02
  BCC#1
** BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 17 at:  7.140E-01  3.100E+02
  BCC#1
** BCC#2
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 18 at:  7.140E-01  3.100E+02
  BCC#1
** BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 19 at:  7.140E-01  3.100E+02
  BCC#1
** BCC#2
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 20 at:  7.140E-01  3.100E+02
  BCC#1
** BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 21 at:  7.140E-01  3.100E+02
  ** BCC#1
  BCC#2
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 22 at:  7.140E-01  3.100E+02
  ** BCC#1
  BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

```

```

Phase region boundary 23 at: 7.140E-01 3.100E+02
** BCC#1
BCC#2
Calculated..          2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 24 at: 7.140E-01 3.100E+02
** BCC#1
BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 25 at: 3.646E-01 7.700E+02
** A2B
BCC#1
Calculated.          10 equilibria

Phase region boundary 26 at: 3.646E-01 7.700E+02
** A2B
BCC#1
Calculated.          3 equilibria
Terminating at known equilibrium

Phase region boundary 27 at: 3.646E-01 7.700E+02
** A2B
BCC#1
Calculated.          14 equilibria
Terminating at known equilibrium

Phase region boundary 28 at: 7.912E-01 7.700E+02
** A2B
BCC#1
Calculated.          10 equilibria

Phase region boundary 29 at: 7.912E-01 7.700E+02
** A2B
BCC#1
Calculated.          3 equilibria
Terminating at known equilibrium

Phase region boundary 30 at: 7.912E-01 7.700E+02
** A2B
BCC#1
Calculated.          9 equilibria
Terminating at known equilibrium

Phase region boundary 31 at: 2.448E-01 1.230E+03
** LIQUID
BCC#1
Calculated.          4 equilibria
Terminating at known equilibrium

Phase region boundary 32 at: 2.448E-01 1.230E+03
** LIQUID
BCC#1
Calculated.          26 equilibria

Phase region boundary 33 at: 8.860E-01 1.230E+03
** LIQUID
FCC
Calculated.          2 equilibria
Terminating at known equilibrium

Phase region boundary 34 at: 8.860E-01 1.230E+03
** LIQUID
FCC
Calculated.          29 equilibria

Phase region boundary 35 at: 6.414E-03 1.397E+03
LIQUID
** BCC#1
Calculated.          11 equilibria

Phase region boundary 36 at: 6.414E-03 1.397E+03
LIQUID
** BCC#1
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 37 at: 2.298E-01 1.244E+03
LIQUID
** BCC#1
Calculated.          18 equilibria

Phase region boundary 38 at: 2.298E-01 1.244E+03
LIQUID
** BCC#1
Calculated.          4 equilibria
Terminating at known equilibrium

Phase region boundary 39 at: 6.122E-01 1.240E+03
LIQUID
** A2B
Calculated.          14 equilibria
Terminating at known equilibrium

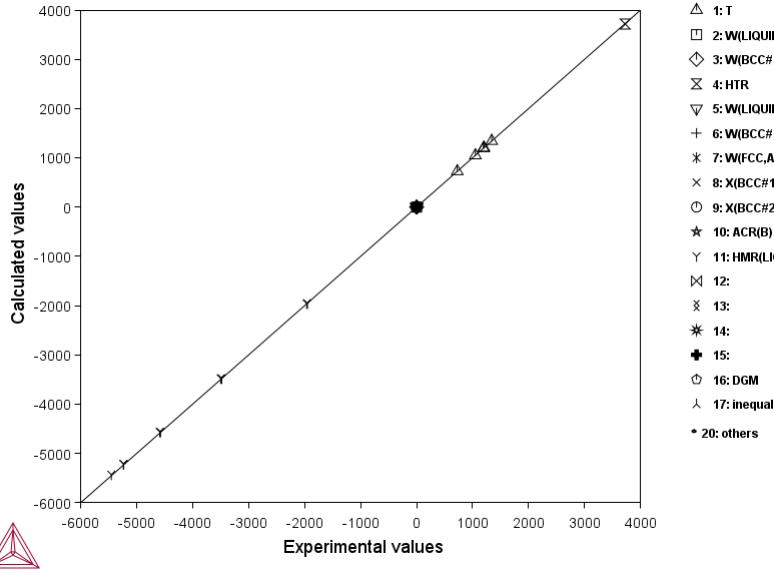
Phase region boundary 40 at: 6.122E-01 1.240E+03
LIQUID
** A2B
Calculated.          8 equilibria
Terminating at known equilibrium

Phase region boundary 41 at: 9.927E-01 1.613E+03
LIQUID
** FCC
Calculated.          19 equilibria
Terminating at known equilibrium

Phase region boundary 42 at: 9.927E-01 1.613E+03
LIQUID
** FCC
Calculated.          9 equilibria
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\generate_console_examples\examples\tcex36a\tcex36.POLY3
CPU time for mapping      1 seconds
POLY: post

```

POST: s-l d
POST: plot



POST:

POST: set-inter

POST: Hit RETURN to continue

POST: @@ Sometimes a very strange shape of the fcc phase here and no equilibrium between liq, fcc and bcc at high B content.

POST: ba

POLY: ba

PARROT VERSION 5.3

Global minimization used as test only
PARROT: l-r C SCREEN

=====
OUTPUT FROM P A R R O T . DATE 2023. 4.27 16:31:20

*** SUCCESSFUL OPTIMIZATION. ***
NUMBER OF ITERATIONS: 15

== OPTIMIZING CONDITIONS ==

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 30 DMAX = 1.00000000E+02 H = 1.00000000E-04
ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO VOO

| VAR. | VALUE | START VALUE | SCALING FACTOR | REL. STAND. DEV |
|------|-----------------|-----------------|-----------------|-----------------|
| V1 | 2.03192526E+04 | 2.02794315E+04 | 2.02794315E+04 | 1.03256129E-01 |
| V2 | -2.93407339E+01 | -2.92509568E+01 | -2.92509568E+01 | 9.50349210E-02 |
| V11 | -2.17899144E+04 | -2.18109901E+04 | -2.18109901E+04 | 2.03679598E-01 |
| V12 | 1.53278493E+01 | 1.51615699E+01 | 1.51615699E+01 | 3.38209139E-01 |
| V15 | 2.41251226E+04 | 2.43843119E+04 | 2.43843119E+04 | 1.49764018E-01 |
| V16 | -8.24687780E+00 | -8.58122041E+00 | -8.58122041E+00 | 5.17740140E-01 |
| V17 | 3.08382018E+03 | 3.11742592E+03 | 3.11742592E+03 | 2.63521177E-01 |
| V19 | 2.21176852E+04 | 2.19408897E+04 | 2.19408897E+04 | 6.93239683E-01 |
| V20 | -7.02506636E+00 | -7.00075524E+00 | -7.00075524E+00 | 1.73851269E+00 |

NUMBER OF OPTIMIZING VARIABLES : 9
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 1.03508938E+01 TO 4.83083490E-03
DEGREES OF FREEDOM 16. REDUCED SUM OF SQUARES 3.01927181E-04

| SYMBOL | STATUS | VALUE/FUNCTION |
|--------------|---------------------------|-----------------------------------|
| FUNCTION R | 298.15 | 8.31451000000000 ; 6000 N REFO ! |
| 2 RTLNP | 20000000 +R*T*LN(1E-05*P) | |
| FUNCTION V1 | 298.15 | 20319.2526367168 ; 6000 N REFO ! |
| FUNCTION V2 | 298.15 | -29.3407338796858 ; 6000 N REFO ! |
| FUNCTION V11 | 298.15 | -21789.9143983616 ; 6000 N REFO ! |
| FUNCTION V12 | 298.15 | 15.3278493485650 ; 6000 N REFO ! |
| FUNCTION V15 | 298.15 | 24125.1226142511 ; 6000 N REFO ! |
| FUNCTION V16 | 298.15 | -8.24687780176102 ; 6000 N REFO ! |
| FUNCTION V17 | 298.15 | 3083.82017668620 ; 6000 N REFO ! |
| FUNCTION V19 | 298.15 | 22117.6851953482 ; 6000 N REFO ! |
| FUNCTION V20 | 298.15 | -7.02506635732492 ; 6000 N REFO ! |

LIQUID:L (A,B)1.0

==== [A] ====
G(LIQUID,A;0) 298.15 +14000-10*T; 6000 N

==== [B] ====

```

G(LIQUID,B;0)          298.15 +18000-12*T;           6000 N
G(LIQUID,A,B;0)          298.15 +V11+V12*T;           6000 N
G(LIQUID,A,B;1)          298.15 +V13+V14*T;           6000 N

$ ====== BLOCK NUMBER 1

DEFINED CONSTANTS
DX=2E-2, P0=101325, DH=500, DT=10
DEFINED FUNCTIONS AND VARIABLES%
HTR=HM(LIQUID)-HM(A2B)
1 T=1193                 1193.      10.     -0.3105    -3.1045E-02
1 W(LIQUID,B)=0.408       0.4077    2.00E-02  -2.5459E-04  -1.2730E-02
1 W(BCC#1,B)=0.13         0.1299    2.00E-02  -8.9839E-05  -4.4920E-03
2 T=1341                 1341.      10.     2.6758E-02   2.6758E-03
2 HTR=3727                3718.     5.00E+02  -8.954     -1.7908E-02
3 T=1049                 1049.      10.     0.1584     1.5844E-02
3 W(LIQUID,A)=0.27        0.2703    2.00E-02  3.0989E-04   1.5494E-02
3 W(BCC#1,A)=9.3E-2       9.3067E-02 2.00E-02  6.6517E-05   3.3258E-03
5 T=726                  726.0     10.     -3.9381E-02  -3.9381E-03
5 X(BCC#1,B)=3.7E-2       3.7418E-02 2.00E-02  4.1825E-04   2.0912E-02
5 X(BCC#2,A)=0.114        0.1138    2.00E-02  -1.9320E-04  -9.6601E-03
6 X(BCC#1,B)=3.7E-2       3.7429E-02 2.00E-02  4.2932E-04   2.1466E-02
6 X(BCC#2,A)=0.114        0.1138    2.00E-02  -1.6619E-04  -8.3094E-03
10 W(LIQUID,A)=2E-2        1.9568E-02 2.00E-02  -4.3151E-04  -2.1576E-02
11 W(LIQUID,A)=4.2E-2       4.1857E-02 2.00E-02  -1.4319E-04  -7.1595E-03
12 W(LIQUID,A)=6.5E-2       6.4937E-02 2.00E-02  -6.3303E-05  -3.1652E-03
13 W(LIQUID,A)=9.3E-2       9.2741E-02 2.00E-02  -2.5863E-04  -1.2932E-02
20 W(LIQUID,A)=0.104        0.1038    2.00E-02  -1.5711E-04  -7.8557E-03
20 W(FCC,A)=3.8E-2        3.8189E-02 2.00E-02  1.8859E-04   9.4297E-03
21 W(LIQUID,A)=0.136        0.1366    2.00E-02  5.6062E-04   2.8031E-02
21 W(FCC,A)=4.7E-2        4.7082E-02 2.00E-02  8.1625E-05   4.0812E-03
22 W(LIQUID,A)=0.187        0.1868    2.00E-02  -2.2697E-04  -1.1349E-02
22 W(FCC,A)=5.9E-2        5.8972E-02 2.00E-02  -2.7840E-05  -1.3920E-03
23 W(LIQUID,A)=0.245        0.2450    2.00E-02  -1.9409E-05  -9.7046E-04
23 W(BCC#1,A)=8.5E-2       8.4995E-02 2.00E-02  -5.3384E-06  -2.6692E-04

PARROT:
PARROT: @@ Note that all other experiments are well fitted.
PARROT: @@ Try to improve by optimizing a little more...
PARROT: resc
PARROT: opt 30
Use      25 experiments, maximum is      2000
Use      664 real workspace, maximum is    50000
The following output is provided by subroutine VA05A

      AT THE 0 TH ITERATION WE HAVE THE SUM OF SQUARES 4.83083490E-03
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

      AT THE 1 ST ITERATION WE HAVE THE SUM OF SQUARES 5.61883845E-03
1 1.0001E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

      AT THE 2 ND ITERATION WE HAVE THE SUM OF SQUARES 7.65789784E-03
1 1.0000E+00 2 1.0001E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

      AT THE 3 RD ITERATION WE HAVE THE SUM OF SQUARES 5.28376337E-03
1 1.0000E+00 2 1.0000E+00 3 1.0001E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

      AT THE 4 TH ITERATION WE HAVE THE SUM OF SQUARES 5.25226723E-03
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0001E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

      AT THE 5 TH ITERATION WE HAVE THE SUM OF SQUARES 4.87673682E-03
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0001E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

      AT THE 6 TH ITERATION WE HAVE THE SUM OF SQUARES 4.83638847E-03
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0001E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

      AT THE 7 TH ITERATION WE HAVE THE SUM OF SQUARES 4.83105767E-03
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0001E+00 8 1.0000E+00 9 1.0000E+00

      AT THE 8 TH ITERATION WE HAVE THE SUM OF SQUARES 4.83475968E-03
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0001E+00 9 1.0000E+00

      AT THE 9 TH ITERATION WE HAVE THE SUM OF SQUARES 4.83108484E-03
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0001E+00 9 1.0000E+00

      AT THE 10 TH ITERATION WE HAVE THE SUM OF SQUARES 4.82945245E-03
1 1.0000E+00 2 1.0000E+00 3 9.9999E-01 4 9.9999E-01 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0001E+00

      AT THE 11 TH ITERATION WE HAVE THE SUM OF SQUARES 4.82870201E-03
1 1.0000E+00 2 1.0000E+00 3 9.9998E-01 4 9.9998E-01 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0001E+00 9 1.0002E+00

      AT THE 12 TH ITERATION WE HAVE THE SUM OF SQUARES 4.82775823E-03
1 1.0000E+00 2 1.0000E+00 3 9.9997E-01 4 9.9996E-01 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0001E+00 9 1.0004E+00

      AT THE 13 TH ITERATION WE HAVE THE SUM OF SQUARES 4.82617766E-03
1 1.0000E+00 2 1.0000E+00 3 9.9995E-01 4 9.9991E-01 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0003E+00 9 1.0007E+00

      AT THE 14 TH ITERATION WE HAVE THE SUM OF SQUARES 4.82385422E-03
1 1.0000E+00 2 1.0000E+00 3 9.9990E-01 4 9.9985E-01 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0005E+00 9 1.0013E+00

      AT THE 15 TH ITERATION WE HAVE THE SUM OF SQUARES 4.81986290E-03
1 1.0001E+00 2 1.0001E+00 3 9.9982E-01 4 9.9971E-01 5 1.0001E+00
6 1.0003E+00 7 1.0000E+00 8 1.0010E+00 9 1.0025E+00

```

AT THE 16 TH ITERATION WE HAVE THE SUM OF SQUARES 4.81442134E-03
 1 1.0001E+00 2 1.0001E+00 3 9.9966E-01 4 9.9944E-01 5 1.0002E+00
 6 1.0006E+00 7 9.9999E-01 8 1.0019E+00 9 1.0049E+00

THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED 16 iterations
 1 1.0001E+00 2 1.0001E+00 3 9.9966E-01 4 9.9944E-01 5 1.0002E+00
 6 1.0006E+00 7 9.9999E-01 8 1.0019E+00 9 1.0049E+00

1 -3.1647E-02 2 -1.2983E-02 3 -4.4578E-03 4 1.6762E-03 5 -1.6612E-02
 6 1.5808E-02 7 1.5173E-02 8 3.6678E-03 9 -3.9296E-03 10 2.0887E-02
 11 -9.7709E-03 12 2.1440E-02 13 -8.4228E-03 14 -2.1134E-02 15 -6.4546E-03
 16 -2.4107E-03 17 -1.2357E-02 18 -7.4116E-03 19 1.0311E-02 20 2.7942E-02
 21 4.5683E-03 22 -1.2547E-02 23 -2.2732E-03 24 -1.4363E-03 25 -7.9612E-05

THE SUM OF SQUARES IS 4.81442134E-03

PARROT: 1-r C SCREEN

=====
 OUTPUT FROM P A R R O T . DATE 2023. 4.27 16:31:20

*** SUCCESSFUL OPTIMIZATION. ***
 NUMBER OF ITERATIONS: 17

== OPTIMIZING CONDITIONS ==

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
 MINIMUM SAVE ON FILE: Y
 ERROR FOR INEQUALITIES = 1.00000000E+00
 RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
 MAXFUN = 30 DMAX = 1.0000000E+02 H = 1.0000000E-04
 ACC = (INITIAL SUM OF SQUARES) * 1.0000000E-03

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO VOO

| VAR. | VALUE | START VALUE | SCALING FACTOR | REL_STAND_DEV |
|------|-----------------|-----------------|-----------------|----------------|
| V1 | 2.03222963E+04 | 2.03192526E+04 | 2.03192526E+04 | 1.07718654E-01 |
| V2 | -2.93449017E+01 | -2.93407339E+01 | -2.93407339E+01 | 9.89624550E-02 |
| V11 | -2.17824323E+04 | -2.17899144E+04 | -2.17899144E+04 | 2.12028670E-01 |
| V12 | 1.53193300E+01 | 1.53278493E+01 | 1.53278493E+01 | 3.47657571E-01 |
| V15 | 2.41287698E+04 | 2.41251226E+04 | 2.41251226E+04 | 1.52846789E-01 |
| V16 | -8.25177741E+00 | -8.24687780E+00 | -8.24687780E+00 | 5.48129903E-01 |
| V17 | 3.08380218E+03 | 3.08382018E+03 | 3.08382018E+03 | 2.65350523E-01 |
| V19 | 2.21586154E+04 | 2.21176852E+04 | 2.21176852E+04 | 7.19986933E-01 |
| V20 | -7.05926808E+00 | -7.02506636E+00 | -7.02506636E+00 | 1.84443655E+00 |

NUMBER OF OPTIMIZING VARIABLES : 9
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM 4.83083490E-03 TO 4.81442134E-03
 DEGREES OF FREEDOM 16. REDUCED SUM OF SQUARES 3.00901333E-04

| SYMBOL | STATUS | VALUE/FUNCTION | |
|--------------|---------------------------|-------------------|-----------------|
| FUNCTION R | 298.15 | 8.31451000000000 | ; 6000 N REFO ! |
| 2 RTLNP | 20000000 +R*T*LN(1E-05*P) | | |
| FUNCTION V1 | 298.15 | 20322.2963348921 | ; 6000 N REFO ! |
| FUNCTION V2 | 298.15 | -29.3449016776570 | ; 6000 N REFO ! |
| FUNCTION V11 | 298.15 | -21782.4326003615 | ; 6000 N REFO ! |
| FUNCTION V12 | 298.15 | 15.3193299910642 | ; 6000 N REFO ! |
| FUNCTION V15 | 298.15 | 24128.7697675338 | ; 6000 N REFO ! |
| FUNCTION V16 | 298.15 | -8.25177741207503 | ; 6000 N REFO ! |
| FUNCTION V17 | 298.15 | 3083.80218472902 | ; 6000 N REFO ! |
| FUNCTION V19 | 298.15 | 22158.6154152669 | ; 6000 N REFO ! |
| FUNCTION V20 | 298.15 | -7.05926807679739 | ; 6000 N REFO ! |

LIQUID:L (A,B)1.0

| ===== [A] ===== | | |
|--------------------|---------------------|--------|
| G(LIQUID,A;0) | 298.15 +14000-10*T; | 6000 N |
| ===== [B] ===== | | |
| G(LIQUID,B;0) | 298.15 +18000-12*T; | 6000 N |
| ===== [A, B] ===== | | |
| G(LIQUID,A,B;0) | 298.15 +V11+V12*T; | 6000 N |
| G(LIQUID,A,B;1) | 298.15 +V13+V14*T; | 6000 N |

\$ ===== BLOCK NUMBER 1

DEFINED CONSTANTS
 DX=2E-2, PO=101325, DH=500, DT=10
 DEFINED FUNCTIONS AND VARIABLES%
 HTR=HM(LIQUID)-HM(A2B)

| | | | | |
|-----------------------|------------|----------|-------------|-------------|
| 1 T=1193 | 1193. | 10. | -0.3165 | -3.1647E-02 |
| 1 W(LIQUID,B)=0.408 | 0.4077 | 2.00E-02 | -2.5966E-04 | -1.2983E-02 |
| 1 W(BCC#1,B)=0.13 | 0.1299 | 2.00E-02 | -8.9156E-05 | -4.4578E-03 |
| 2 T=1341 | 1341. | 10. | 1.6762E-02 | 1.6762E-03 |
| 2 HTR=3727 | 3719. | 5.00E+02 | -8.306 | -1.6612E-02 |
| 3 T=1049 | 1049. | 10. | 0.1581 | 1.5808E-02 |
| 3 W(LIQUID,A)=0.27 | 0.2703 | 2.00E-02 | 3.0346E-04 | 1.5173E-02 |
| 3 W(BCC#1,A)=9.3E-2 | 9.3073E-02 | 2.00E-02 | 7.3357E-05 | 3.6678E-03 |
| 5 T=726 | 726.0 | 10. | -3.9296E-02 | -3.9296E-03 |
| 5 X(BCC#1,B)=3.7E-2 | 3.7418E-02 | 2.00E-02 | 4.1775E-04 | 2.0887E-02 |
| 5 X(BCC#2,A)=0.114 | 0.1138 | 2.00E-02 | -1.9542E-04 | -9.7709E-03 |
| 6 X(BCC#1,B)=3.7E-2 | 3.7429E-02 | 2.00E-02 | 4.2879E-04 | 2.1440E-02 |
| 6 X(BCC#2,A)=0.114 | 0.1138 | 2.00E-02 | -1.6846E-04 | -8.4228E-03 |
| 10 W(LIQUID,A)=2E-2 | 1.9577E-02 | 2.00E-02 | -4.2268E-04 | -2.1134E-02 |
| 11 W(LIQUID,A)=4.2E-2 | 4.1871E-02 | 2.00E-02 | -1.2909E-04 | -6.4546E-03 |
| 12 W(LIQUID,A)=6.5E-2 | 6.4952E-02 | 2.00E-02 | -4.8215E-05 | -2.4107E-03 |
| 13 W(LIQUID,A)=9.3E-2 | 9.2753E-02 | 2.00E-02 | -2.4714E-04 | -1.2357E-02 |

```

20 W(LIQUID,A)=0.104      0.1039    2.00E-02 -1.4823E-04 -7.4116E-03
20 W(FCC,A)=3.8E-2        3.8206E-02 2.00E-02 2.0623E-04 1.0311E-02
21 W(LIQUID,A)=0.136      0.1366    2.00E-02 5.5883E-04 2.7942E-02
21 W(FCC,A)=4.7E-2        4.7091E-02 2.00E-02 9.1366E-05 4.5683E-03
22 W(LIQUID,A)=0.187      0.1867    2.00E-02 -2.5095E-04 -1.2547E-02
22 W(FCC,A)=5.9E-2        5.8955E-02 2.00E-02 -4.5465E-05 -2.2732E-03
23 W(LIQUID,A)=0.245      0.2450    2.00E-02 -2.8725E-05 -1.4363E-03
23 W(BCC#1,A)=8.5E-2     8.4998E-02 2.00E-02 -1.5922E-06 -7.9612E-05

```

```

PARROT:
PARROT:Hit RETURN to continue
PARROT: @@ Calculate the phase diagram again
PARROT: mac tce36cpd
PARROT: set-echo
NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
POLY:
POLY: @@ In PARROT, the global minimization is turned off automatically.
POLY: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY: @@ message will be given.
POLY:
POLY: advanced-option global yes.,
Settings for global minimization:
*** WARNING *** Global equilibrium calculation may create new composition sets
and this may corrupt your PARROT work file (.PAR file).
Do not go back to PARROT but exit from POLY after your POLY calculations.
POLY:
POLY: def-com,,,
POLY: s-a-v 1 w(b) 0 1,,,
The condition W(B)=.1234 created
POLY: s-a-v 2 t 300 1700,,,
The condition T=942.2 created
POLY: s- t=t500
POLY: l-c
W(B)=0.1234, T=500
DEGREES OF FREEDOM 2
POLY: c-e
Creating condition P=1E5
Creating condition N=1
Using global minimization procedure
Calculated          628 grid points in      0 s
Found the set of lowest grid points in      0 s
Calculated POLY solution      0 s, total time  0 s
POLY: save tce36 y

```

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

```

POLY: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

```

Organizing start points

Using ADDED start equilibria

```

Generating start point  1
Generating start point  2
Generating start point  3
Generating start point  4
Generating start point  5
Generating start point  6
Generating start point  7
Generating start point  8
Generating start point  9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Generating start point 27
Generating start point 28

```

```

Phase region boundary 1 at: 7.140E-01 3.100E+02
  BCC#1
  ** BCC#2
Calculated..           2 equilibria
Terminating at axis limit.

```

```

Phase region boundary 2 at: 7.141E-01 3.000E+02
  BCC#1
  ** BCC#2
Calculated..           14 equilibria

```

```

Phase region boundary 3 at: 6.821E-01 7.260E+02
  ** A2B

```

```

      BCC#1
** BCC#2

Phase region boundary  4 at:  3.626E-01  7.260E+02
** A2B
BCC#1
Calculated.          15 equilibria

Phase region boundary  5 at:  3.769E-01  1.193E+03
** LIQUID
** A2B
BCC#1

Phase region boundary  6 at:  2.826E-01  1.193E+03
** LIQUID
BCC#1
Calculated.          26 equilibria

Phase region boundary  7 at:  4.863E-01  1.193E+03
** LIQUID
A2B
Calculated.          33 equilibria

Phase region boundary  8 at:  6.500E-01  1.049E+03
** LIQUID
A2B
** BCC#1

Phase region boundary  9 at:  7.642E-01  1.049E+03
A2B
** BCC#1
Calculated.          11 equilibria
Terminating at known equilibrium

Phase region boundary 10 at:  8.276E-01  1.049E+03
LIQUID
** BCC#1
Calculated.          8 equilibria

Phase region boundary 11 at:  8.751E-01  1.204E+03
LIQUID
** BCC#1
** FCC

Phase region boundary 12 at:  8.804E-01  1.204E+03
LIQUID
** FCC
Calculated.          32 equilibria

Phase region boundary 13 at:  9.357E-01  1.204E+03
BCC#1
** FCC
Calculated.          24 equilibria

Phase region boundary 14 at:  7.140E-01  3.100E+02
BCC#1
** BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 15 at:  7.140E-01  3.100E+02
BCC#1
** BCC#2
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 16 at:  7.140E-01  3.100E+02
BCC#1
** BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 17 at:  7.140E-01  3.100E+02
BCC#1
** BCC#2
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 18 at:  7.140E-01  3.100E+02
BCC#1
** BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 19 at:  7.140E-01  3.100E+02
BCC#1
** BCC#2
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 20 at:  7.140E-01  3.100E+02
BCC#1
** BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 21 at:  7.140E-01  3.100E+02
** BCC#1
BCC#2
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 22 at:  7.140E-01  3.100E+02
** BCC#1
BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 23 at:  7.140E-01  3.100E+02
** BCC#1
BCC#2
Calculated..         2 equilibria

```

```

Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 24 at: 7.140E-01 3.100E+02
  ** BCC#1
  BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 25 at: 3.646E-01 7.700E+02
  ** A2B
  BCC#1
Calculated.          10 equilibria

Phase region boundary 26 at: 3.646E-01 7.700E+02
  ** A2B
  BCC#1
Calculated.          3 equilibria
Terminating at known equilibrium

Phase region boundary 27 at: 3.646E-01 7.700E+02
  ** A2B
  BCC#1
Calculated.          14 equilibria
Terminating at known equilibrium

Phase region boundary 28 at: 7.912E-01 7.700E+02
  ** A2B
  BCC#1
Calculated.          10 equilibria

Phase region boundary 29 at: 7.912E-01 7.700E+02
  ** A2B
  BCC#1
Calculated.          3 equilibria
Terminating at known equilibrium

Phase region boundary 30 at: 7.912E-01 7.700E+02
  ** A2B
  BCC#1
Calculated.          9 equilibria
Terminating at known equilibrium

Phase region boundary 31 at: 2.448E-01 1.230E+03
  ** LIQUID
  BCC#1
Calculated.          4 equilibria
Terminating at known equilibrium

Phase region boundary 32 at: 2.448E-01 1.230E+03
  ** LIQUID
  BCC#1
Calculated.          26 equilibria

Phase region boundary 33 at: 8.860E-01 1.230E+03
  ** LIQUID
  FCC
Calculated.          2 equilibria
Terminating at known equilibrium

Phase region boundary 34 at: 8.860E-01 1.230E+03
  ** LIQUID
  FCC
Calculated.          29 equilibria

Phase region boundary 35 at: 6.414E-03 1.397E+03
  ** BCC#1
Calculated.          12 equilibria

Phase region boundary 36 at: 6.414E-03 1.397E+03
  ** LIQUID
  BCC#1
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 37 at: 2.298E-01 1.244E+03
  ** LIQUID
  BCC#1
Calculated.          18 equilibria

Phase region boundary 38 at: 2.298E-01 1.244E+03
  ** LIQUID
  BCC#1
Calculated.          4 equilibria
Terminating at known equilibrium

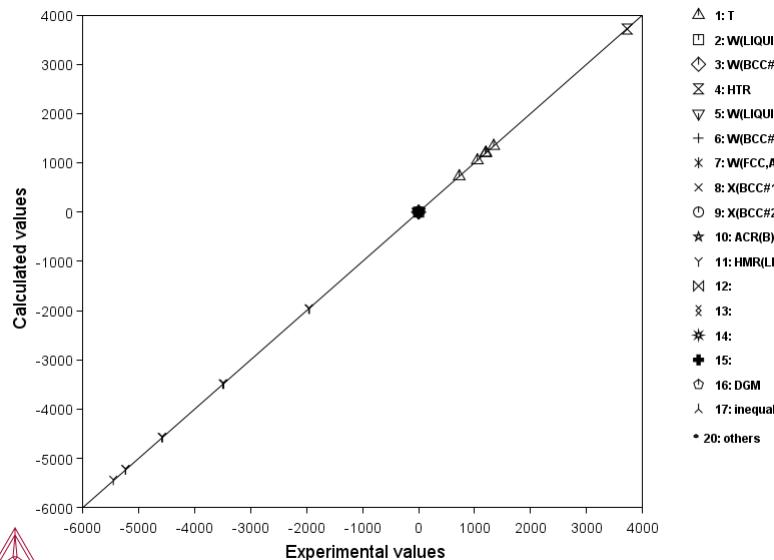
Phase region boundary 39 at: 6.122E-01 1.240E+03
  ** LIQUID
  A2B
Calculated.          14 equilibria
Terminating at known equilibrium

Phase region boundary 40 at: 6.122E-01 1.240E+03
  ** LIQUID
  A2B
Calculated.          8 equilibria
Terminating at known equilibrium

Phase region boundary 41 at: 9.927E-01 1.613E+03
  ** LIQUID
  FCC
Calculated.          19 equilibria
Terminating at known equilibrium

Phase region boundary 42 at: 9.927E-01 1.613E+03
  ** LIQUID
  FCC
Calculated.          10 equilibria
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\generate_console_examples\examples\tcex36a\tcex36.POLY3
CPU time for mapping      1 seconds
POLY: post
POST: s-l d
POST: plot

```



```

POST:
POST: set-inter
POST:Hit RETURN to continue
POST: ba
POLY: ba

```

PARROT VERSION 5.3

```

Global minimization used as test only
PARROT: @@ Now there is an equilibrium between fcc, bcc and liquid
PARROT: @@ at high B. Restore equilibrium 4 on the POP file
PARROT: ed
ED_EXP: read 1
ED_EXP: s-e 4
Equilibrium number           4, label AINV
ED_EXP: s-we 1
Equilibria (range) or label(s) /PRESENT/: PRESENT
ED_EXP: s-a-s
T /1204.424718/: 1200
Automatic start values for phase constituents? /N/: N

```

```

Phase LIQUID
Major constituent(s) /b/: b

```

```

Phase BCC
Major constituent(s) /b/: b

```

```

Phase FCC
Major constituent(s) /b/: b

```

```

ED_EXP:

```

```

ED_EXP: c-e

```

```

Testing result with global minimization
13 ITS, CPU TIME USED 0 SECONDS

```

```

ED_EXP: l-e

```

```

OUTPUT TO SCREEN OR FILE /SCREEN/:

```

```

Options /VWCS/: VWCS

```

```

Output from POLY-3, equilibrium =      4, label AINV, database:

```

Conditions:

P=101325

FIXED PHASES

LIQUID=1 BCC#1=1 FCC=1

DEGREES OF FREEDOM 0

Temperature 1203.82 K (930.67 C), Pressure 1.013250E+05
 Number of moles of components 3.00000E+00, Mass in grams 1.30105E+02
 Total Gibbs energy -9.75086E+03, Enthalpy 1.98626E+04, Volume 0.00000E+00

| Component | Moles | W-Fraction | Activity | Potential | Ref.stat |
|-----------|------------|------------|------------|-------------|----------|
| A | 6.6316E-01 | 1.0194E-01 | 3.9443E-01 | -9.3116E+03 | SER |
| B | 2.3368E+00 | 8.9806E-01 | 8.5823E-01 | -1.5302E+03 | SER |

FCC Status FIXED Driving force 0.0000E+00
 Moles 1.0000E+00, Mass 4.5889E+01, Volume fraction 0.0000E+00 Mass fractions:
 B 9.40269E-01 A 5.97312E-02

BCC#1 Status FIXED Driving force 0.0000E+00
 Moles 1.0000E+00, Mass 4.5321E+01, Volume fraction 0.0000E+00 Mass fractions:
 B 9.31169E-01 A 6.88312E-02

LIQUID Status FIXED Driving force 0.0000E+00
 Moles 1.0000E+00, Mass 3.8896E+01, Volume fraction 0.0000E+00 Mass fractions:

B 8.09680E-01 A 1.90320E-01

EXPERIMENT T=1203:DT \$1203.82:10 NO=1

EXPERIMENT W(LIQUID,A)=0.19:DX \$0.19032:2E-2 NO=2

EXPERIMENT W(BCC#1,A)=6.9E-2:DX \$6.88312E-2:2E-2 NO=3

EXPERIMENT W(FCC,A)=6E-2:DX \$5.97312E-2:2E-2 NO=4

ED_EXP: @@ Now equilibrium 4 is on the high B side

ED_EXP: save

ED_EXP: ba

PARROT: resc

PARROT: opt 0

Use 29 experiments, maximum is 2000

Use 740 real workspace, maximum is 50000

PARROT: l-r C SCREEN

```

=====
OUTPUT FROM P A R R O T . DATE 2023. 4.27 16:31:43

```

```
*** SUCCESSFUL OPTIMIZATION. ***
NUMBER OF ITERATIONS: 0

== OPTIMIZING CONDITIONS ==

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 0 DMAX = 1.00000000E+02 H = 1.00000000E-04
ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03
```

```
-- OPTIMIZING VARIABLES ==
```

```
AVAILABLE VARIABLES ARE V1 TO VOO
```

| VAR. | VALUE | START VALUE | SCALING FACTOR | REL.STAND.DEV |
|------|-----------------|-----------------|-----------------|----------------|
| V1 | .03222963E+04 | .03222963E+04 | .03222963E+04 | 0.00000000E+00 |
| V2 | -2.93449017E+01 | -2.93449017E+01 | -2.93449017E+01 | 0.00000000E+00 |
| V11 | -2.17824326E+04 | -2.17824326E+04 | -2.17824326E+04 | 0.00000000E+00 |
| V12 | 1.53193300E+01 | 1.53193300E+01 | 1.53193300E+01 | 0.00000000E+00 |
| V15 | 2.41287698E+04 | 2.41287698E+04 | 2.41287698E+04 | 0.00000000E+00 |
| V16 | -8.25177741E+00 | -8.25177741E+00 | -8.25177741E+00 | 0.00000000E+00 |
| V17 | 3.08380218E+03 | 3.08380218E+03 | 3.08380218E+03 | 0.00000000E+00 |
| V19 | 2.21586154E+04 | 2.21586154E+04 | 2.21586154E+04 | 0.00000000E+00 |
| V20 | -7.05926808E+00 | -7.05926808E+00 | -7.05926808E+00 | 0.00000000E+00 |

```
NUMBER OF OPTIMIZING VARIABLES : 9
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 0.00000000E+00 TO 1.20076306E-02
DEGREES OF FREEDOM 20. REDUCED SUM OF SQUARES 6.00381531E-04
```

| SYMBOL | STATUS | VALUE/FUNCTION |
|--------------|---------------------------|-----------------------------------|
| FUNCTION R | 298.15 | 8.314510000000000 ; 6000 N REFO ! |
| 2 RTLNP | 20000000 +R*T*LN(1E-05*p) | |
| FUNCTION V1 | 298.15 | 20322.2963348921 ; 6000 N REFO ! |
| FUNCTION V2 | 298.15 | -29.3449016776570 ; 6000 N REFO ! |
| FUNCTION V11 | 298.15 | -21782.4326003615 ; 6000 N REFO ! |
| FUNCTION V12 | 298.15 | 15.3193299910642 ; 6000 N REFO ! |
| FUNCTION V15 | 298.15 | 24128.7697675338 ; 6000 N REFO ! |
| FUNCTION V16 | 298.15 | -8.25177741207503 ; 6000 N REFO ! |
| FUNCTION V17 | 298.15 | 3083.80218472902 ; 6000 N REFO ! |
| FUNCTION V19 | 298.15 | 22158.6154152669 ; 6000 N REFO ! |
| FUNCTION V20 | 298.15 | -7.05926807679739 ; 6000 N REFO ! |

```
LIQUID:L (A,B)1.0
```

```
===== [A] =====
G(LIQUID,A;0) 298.15 +14000-10*T; 6000 N
```

```
===== [B] =====
G(LIQUID,B;0) 298.15 +18000-12*T; 6000 N
```

```
===== [A, B] =====
G(LIQUID,A,B;0) 298.15 +V11+V12*T; 6000 N
G(LIQUID,A,B;1) 298.15 +V13+V14*T; 6000 N
```

```
$ ===== BLOCK NUMBER 1
```

| DEFINED CONSTANTS | DX=2E-2, P0=101325, DH=500, DT=10 |
|----------------------------------|---|
| DEFINED FUNCTIONS AND VARIABLES% | HTR=HM(LIQUID)-HM(A2B) |
| 1 T=1193 | 1193. 10. -0.3165 -3.1647E-02 |
| 1 W(LIQUID,B)=0.408 | 0.4077 2.00E-02 -2.5966E-04 -1.2983E-02 |
| 1 W(BCC#1,B)=0.13 | 0.1299 2.00E-02 -8.9156E-05 -4.4578E-03 |
| 2 T=1341 | 1341. 10. 1.6762E-02 1.6762E-03 |
| 2 HTR=3727 | 3719. 5.00E+02 -8.306 -1.6612E-02 |
| 3 T=1049 | 1049. 10. 0.1581 1.5808E-02 |
| 3 W(LIQUID,A)=0.27 | 0.2703 2.00E-02 3.0346E-04 1.5173E-02 |
| 3 W(BCC#1,A)=9.3E-2 | 9.3073E-02 2.00E-02 7.3357E-05 3.6678E-03 |
| 4 T=1203 | 1204. 10. 0.8177 8.1768E-02 |
| 4 W(LIQUID,A)=0.19 | 0.1903 2.00E-02 3.1961E-04 1.5980E-02 |
| 4 W(BCC#1,A)=6.9E-2 | 6.8831E-02 2.00E-02 -1.6881E-04 -8.4404E-03 |
| 4 W(FCC,A)=6E-2 | 5.9731E-02 2.00E-02 -2.6879E-04 -1.3440E-02 |
| 5 T=726 | 726.0 10. -3.9296E-02 -3.9296E-03 |
| 5 X(BCC#1,B)=3.7E-2 | 3.7418E-02 2.00E-02 4.1775E-04 2.0887E-02 |
| 5 X(BCC#2,A)=0.114 | 0.1138 2.00E-02 -1.9542E-04 -9.7709E-03 |
| 6 X(BCC#1,B)=3.7E-2 | 3.7429E-02 2.00E-02 4.2879E-04 2.1440E-02 |
| 6 X(BCC#2,A)=0.114 | 0.1138 2.00E-02 -1.6846E-04 -8.4228E-03 |
| 10 W(LIQUID,A)=2E-2 | 1.9577E-02 2.00E-02 -4.2268E-04 -2.1134E-02 |
| 11 W(LIQUID,A)=4.2E-2 | 4.1871E-02 2.00E-02 -1.2909E-04 -6.4546E-03 |
| 12 W(LIQUID,A)=6.5E-2 | 6.4952E-02 2.00E-02 -4.8215E-05 -2.4107E-03 |
| 13 W(LIQUID,A)=9.3E-2 | 9.2753E-02 2.00E-02 -2.4714E-04 -1.2357E-02 |
| 20 W(LIQUID,A)=0.104 | 0.1039 2.00E-02 -1.4823E-04 -7.4116E-03 |
| 20 W(FCC,A)=3.8E-2 | 3.8206E-02 2.00E-02 2.0623E-04 1.0311E-02 |
| 21 W(LIQUID,A)=0.136 | 0.1366 2.00E-02 5.5883E-04 2.7942E-02 |
| 21 W(FCC,A)=4.7E-2 | 4.7091E-02 2.00E-02 9.1366E-05 4.5683E-03 |
| 22 W(LIQUID,A)=0.187 | 0.1867 2.00E-02 -2.5095E-04 -1.2547E-02 |
| 22 W(FCC,A)=5.9E-2 | 5.8955E-02 2.00E-02 -4.5465E-05 -2.2732E-03 |
| 23 W(LIQUID,A)=0.245 | 0.2450 2.00E-02 -2.8725E-05 -1.4363E-03 |
| 23 W(BCC#1,A)=8.5E-2 | 8.4998E-02 2.00E-02 -1.5922E-06 -7.9612E-03 |

```
PARROT:
```

```
PARROT:Hit RETURN to continue
```

```
PARROT: opt 30
```

```
Use 29 experiments, maximum is 2000
```

```
Use 740 real workspace, maximum is 50000
```

```
The following output is provided by subroutine VA05A
```

AT THE 0 TH ITERATION WE HAVE THE SUM OF SQUARES 1.20076306E-02
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 1 ST ITERATION WE HAVE THE SUM OF SQUARES 1.28463852E-02
1 1.0001E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 2 ND ITERATION WE HAVE THE SUM OF SQUARES 1.47299889E-02
1 1.0000E+00 2 1.0001E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 3 RD ITERATION WE HAVE THE SUM OF SQUARES 1.22550436E-02
1 1.0000E+00 2 1.0000E+00 3 1.0001E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 4 TH ITERATION WE HAVE THE SUM OF SQUARES 1.26043232E-02
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0001E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 5 TH ITERATION WE HAVE THE SUM OF SQUARES 1.02678642E-02
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0001E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 6 TH ITERATION WE HAVE THE SUM OF SQUARES 1.09408185E-02
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0001E+00
6 1.0001E+00 7 1.0000E+00 8 1.0000E+00 9 1.0000E+00

AT THE 7 TH ITERATION WE HAVE THE SUM OF SQUARES 1.04096810E-02
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0001E+00
6 1.0000E+00 7 1.0001E+00 8 1.0000E+00 9 1.0000E+00

AT THE 8 TH ITERATION WE HAVE THE SUM OF SQUARES 1.16225973E-02
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0001E+00
6 1.0000E+00 7 1.0000E+00 8 1.0001E+00 9 1.0000E+00

AT THE 9 TH ITERATION WE HAVE THE SUM OF SQUARES 9.80133230E-03
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0001E+00
6 1.0000E+00 7 1.0000E+00 8 1.0000E+00 9 1.0001E+00

AT THE 10 TH ITERATION WE HAVE THE SUM OF SQUARES 6.80666370E-03
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 9.9998E-01 5 1.0003E+00
6 9.9991E-01 7 9.9998E-01 8 9.9983E-01 9 1.0002E+00

AT THE 11 TH ITERATION WE HAVE THE SUM OF SQUARES 6.70491045E-03
1 1.0000E+00 2 1.0000E+00 3 9.9993E-01 4 9.9987E-01 5 1.0003E+00
6 1.0000E+00 7 9.9994E-01 8 9.9988E-01 9 1.0004E+00

AT THE 12 TH ITERATION WE HAVE THE SUM OF SQUARES 6.58115401E-03
1 1.0001E+00 2 1.0001E+00 3 9.9977E-01 4 9.9963E-01 5 1.0003E+00
6 1.0002E+00 7 9.9986E-01 8 9.9999E-01 9 1.0009E+00

AT THE 13 TH ITERATION WE HAVE THE SUM OF SQUARES 6.40883693E-03
1 1.0002E+00 2 1.0002E+00 3 9.9946E-01 4 9.9913E-01 5 1.0004E+00
6 1.0005E+00 7 9.9969E-01 8 1.0002E+00 9 1.0018E+00

AT THE 14 TH ITERATION WE HAVE THE SUM OF SQUARES 6.18132314E-03
1 1.0005E+00 2 1.0005E+00 3 9.9985E-01 4 9.9915E-01 5 1.0004E+00
6 1.0012E+00 7 9.9936E-01 8 1.0007E+00 9 1.0036E+00

AT THE 15 TH ITERATION WE HAVE THE SUM OF SQUARES 5.98609640E-03
1 1.0011E+00 2 1.0010E+00 3 9.9763E-01 4 9.9616E-01 5 1.0006E+00
6 1.0025E+00 7 9.9869E-01 8 1.0017E+00 9 1.0072E+00

THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED 15 iterations
1 1.0011E+00 2 1.0010E+00 3 9.9763E-01 4 9.9616E-01 5 1.0006E+00
6 1.0025E+00 7 9.9869E-01 8 1.0017E+00 9 1.0072E+00

1 -3.4102E-02 2 -1.5978E-02 3 -5.3322E-03 4 2.9266E-03 5 -7.9586E-03
6 1.1424E-02 7 1.1769E-02 8 3.4025E-03 9 7.8404E-03 10 2.9223E-02
11 -5.9126E-03 12 -5.6075E-03 13 -3.2816E-03 14 2.3212E-02 15 -1.0523E-02
16 2.3674E-02 17 -9.3960E-03 18 -2.1057E-02 19 -6.4509E-03 20 -2.6191E-03
21 -1.2918E-02 22 -8.1196E-03 23 1.2186E-02 24 2.6873E-02 25 7.3890E-03
26 -1.3669E-02 27 2.3056E-03 28 -7.0927E-03 29 -1.8888E-03

THE SUM OF SQUARES IS 5.98609640E-03

PARROT: l-r C SCREEN

=====
OUTPUT FROM P A R R O T . DATE 2023. 4.27 16:31:43

*** SUCCESSFUL OPTIMIZATION. ***
NUMBER OF ITERATIONS: 16

== OPTIMIZING CONDITIONS ==

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 30 DMAX = 1.00000000E+02 H = 1.00000000E-04
ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

| VAR. | VALUE | START VALUE | SCALING FACTOR | REL.STAND.DEV |
|------|-----------------|-----------------|-----------------|----------------|
| V1 | 2.03437449E+04 | 2.03222963E+04 | 2.03222963E+04 | 1.02353982E-01 |
| V2 | -2.93745547E+01 | -2.93449017E+01 | -2.93449017E+01 | 9.37147973E-02 |
| V11 | -2.17307895E+04 | -2.17824326E+04 | -2.17824326E+04 | 2.00613324E-01 |
| V12 | 1.52604480E+01 | 1.53193300E+01 | 1.53193300E+01 | 3.28967109E-01 |
| V15 | 2.41421947E+04 | 2.41287698E+04 | 2.41287698E+04 | 1.34897021E-01 |
| V16 | -8.27252982E+00 | -8.25177741E+00 | -8.25177741E+00 | 4.84759643E-01 |
| V17 | 3.07975220E+03 | 3.08380218E+03 | 3.08380218E+03 | 2.31442373E-01 |
| V19 | 2.21953895E+04 | 2.21586154E+04 | 2.21586154E+04 | 5.66892734E-01 |
| V20 | -7.11044761E+00 | -7.05926808E+00 | -7.05926808E+00 | 1.53808339E+00 |

NUMBER OF OPTIMIZING VARIABLES : 9
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM 1.20076306E-02 TO 5.98609640E-03
 DEGREES OF FREEDOM 20. REDUCED SUM OF SQUARES 2.99304820E-04

| SYMBOL | STATUS | VALUE/FUNCTION |
|--------------|----------|-----------------------------------|
| FUNCTION R | 298.15 | 8.314510000000000 ; 6000 N REFO ! |
| 2 RTLNP | 20000000 | +RT*T*LN(1E-05*P) |
| FUNCTION V1 | 298.15 | 20343.7448819327 ; 6000 N REFO ! |
| FUNCTION V2 | 298.15 | -29.3745546720144 ; 6000 N REFO ! |
| FUNCTION V11 | 298.15 | -21730.7895141686 ; 6000 N REFO ! |
| FUNCTION V12 | 298.15 | 15.2604479553599 ; 6000 N REFO ! |
| FUNCTION V15 | 298.15 | 24142.1946587226 ; 6000 N REFO ! |
| FUNCTION V16 | 298.15 | -8.27252981535250 ; 6000 N REFO ! |
| FUNCTION V17 | 298.15 | 3079.75220049574 ; 6000 N REFO ! |
| FUNCTION V19 | 298.15 | 22195.3894552626 ; 6000 N REFO ! |
| FUNCTION V20 | 298.15 | -7.11044760781585 ; 6000 N REFO ! |

LIQUID:L (A,B)1.0

| ===== [A] ===== | | |
|--------------------|---------------------|--------|
| G(LIQUID,A;0) | 298.15 +14000-10*T; | 6000 N |
| ===== [B] ===== | | |
| G(LIQUID,B;0) | 298.15 +18000-12*T; | 6000 N |
| ===== [A, B] ===== | | |
| G(LIQUID,A,B;0) | 298.15 +V11+V12*T; | 6000 N |
| G(LIQUID,A,B;1) | 298.15 +V13+V14*T; | 6000 N |

\$ ===== BLOCK NUMBER 1

DEFINED CONSTANTS
 DX=2E-2, P0=101325, DH=500, DT=10

DEFINED FUNCTIONS AND VARIABLES%

| HTR=HM(LIQUID)-HM(A2B) | | | | |
|------------------------|------------|----------|-------------|-------------|
| 1 T=1193 | 1193. | 10. | -0.3410 | -3.4102E-02 |
| 1 W(LIQUID,B)=0.408 | 0.4077 | 2.00E-02 | -3.1957E-04 | -1.5978E-02 |
| 1 W(BCC#1,B)=0.13 | 0.1299 | 2.00E-02 | -1.0664E-04 | -5.3322E-03 |
| 2 T=1341 | 1341. | 10. | 2.9266E-02 | 2.9266E-03 |
| 2 HTR=3727 | 3723. | 5.00E+02 | -3.979 | -7.9586E-03 |
| 3 T=1049 | 1049. | 10. | 0.1142 | 1.1424E-02 |
| 3 W(LIQUID,A)=0.27 | 0.2702 | 2.00E-02 | 2.3539E-04 | 1.1769E-02 |
| 3 W(BCC#1,A)=9.3E-2 | 9.3068E-02 | 2.00E-02 | 6.8050E-05 | 3.4025E-03 |
| 4 T=1203 | 1203. | 10. | 7.8404E-02 | 7.8404E-03 |
| 4 W(LIQUID,A)=0.19 | 0.1906 | 2.00E-02 | 5.8446E-04 | 2.9223E-02 |
| 4 W(BCC#1,A)=6.9E-2 | 6.8882E-02 | 2.00E-02 | -1.1825E-04 | -5.9126E-03 |
| 4 W(FCC,A)=6E-2 | 5.9888E-02 | 2.00E-02 | -1.1215E-04 | -5.6075E-03 |
| 5 T=726 | 726.0 | 10. | -3.2816E-02 | -3.2816E-03 |
| 5 X(BCC#1,B)=3.7E-2 | 3.7464E-02 | 2.00E-02 | 4.6424E-04 | 2.3212E-02 |
| 5 X(BCC#2,A)=0.114 | 0.1138 | 2.00E-02 | -2.1045E-04 | -1.0523E-02 |
| 6 X(BCC#1,B)=3.7E-2 | 3.7473E-02 | 2.00E-02 | 4.7348E-04 | 2.3674E-02 |
| 6 X(BCC#2,A)=0.114 | 0.1138 | 2.00E-02 | -1.8792E-04 | -9.3960E-03 |
| 10 W(LIQUID,A)=2B-2 | 1.9579E-02 | 2.00E-02 | -4.2115E-04 | -2.1057E-02 |
| 11 W(LIQUID,A)=4.2E-2 | 4.1871E-02 | 2.00E-02 | -1.2902E-04 | -6.4509E-03 |
| 12 W(LIQUID,A)=6.5E-2 | 6.4948E-02 | 2.00E-02 | -5.2382E-05 | -2.6191E-03 |
| 13 W(LIQUID,A)=9.3E-2 | 9.2742E-02 | 2.00E-02 | -2.5837E-04 | -1.2918E-02 |
| 20 W(LIQUID,A)=0.104 | 0.1038 | 2.00E-02 | -1.6239E-04 | -8.1196E-03 |
| 20 W(FCC,A)=3.8E-2 | 3.8244E-02 | 2.00E-02 | 2.4372E-04 | 1.2186E-02 |
| 21 W(LIQUID,A)=0.136 | 0.1365 | 2.00E-02 | 5.3747E-04 | 2.6873E-02 |
| 21 W(FCC,A)=4.7E-2 | 4.7148E-02 | 2.00E-02 | 1.4778E-04 | 7.3890E-03 |
| 22 W(LIQUID,A)=0.187 | 0.1867 | 2.00E-02 | -2.7338E-04 | -1.3669E-02 |
| 22 W(FCC,A)=5.9E-2 | 5.9046E-02 | 2.00E-02 | 4.6111E-05 | 2.3056E-03 |
| 23 W(LIQUID,A)=0.245 | 0.2449 | 2.00E-02 | -1.4185E-04 | -7.0927E-03 |
| 23 W(BCC#1,A)=8.5E-2 | 8.4962E-02 | 2.00E-02 | -3.7776E-05 | -1.8888E-03 |

PARROT:

PARROT:

PARROT: Hit RETURN to continue

PARROT: @@ Now optimize all parameters and all experiments

PARROT: l-a-v

OUTPUT TO SCREEN OR FILE /SCREEN/:

-- OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO VOO

| VAR. | VALUE | START VALUE | SCALING FACTOR | REL.STAND.DEV |
|------|-----------------|-----------------|-----------------|----------------|
| V1 | 2.03437449E+04 | 2.03222963E+04 | 2.03222963E+04 | 1.02353982E-01 |
| V2 | -2.93745547E+01 | -2.93449017E+01 | -2.93449017E+01 | 9.37147973E-02 |
| V11 | -2.17307895E+04 | -2.17824326E+04 | -2.17824326E+04 | 2.00613324E-01 |
| V12 | 1.52604480E+01 | 1.53193300E+01 | 1.53193300E+01 | 3.28967109E-01 |
| V15 | 2.41421947E+04 | 2.41287698E+04 | 2.41287698E+04 | 1.34897021E-01 |
| V16 | -8.27252982E+00 | -8.25177741E+00 | -8.25177741E+00 | 4.84759643E-01 |
| V17 | 3.07975220E+03 | 3.08380218E+03 | 3.08380218E+03 | 2.31442373E-01 |
| V19 | 2.21953895E+04 | 2.21586154E+04 | 2.21586154E+04 | 5.66892734E-01 |
| V20 | -7.11044761E+00 | -7.05926808E+00 | -7.05926808E+00 | 1.53808339E+00 |

NUMBER OF OPTIMIZING VARIABLES : 9

ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO

THE SUM OF SQUARES HAS CHANGED FROM 1.20076306E-02 TO 5.98609640E-03
 DEGREES OF FREEDOM 20. REDUCED SUM OF SQUARES 2.99304820E-04

PARROT: s-o-v 11-12

PARROT: ed

ED_EXP: read 1

ED_EXP: c-a

| Eq | Lab | Iter | Weight | Temp | Exp | Fix phases or comments |
|----|------|------|--------|--------|-----|------------------------|
| 1 | AINV | 2 | 1. | 1192.7 | | LIQUID A2B BCC |
| 2 | AINV | 2 | 1. | 1341.0 | | LIQUID A2B |
| 3 | AINV | 2 | 1. | 1049.1 | | LIQUID A2B BCC |
| 4 | AINV | 2 | 1. | 1203.1 | | LIQUID BCC FCC |
| 5 | AINV | 2 | 1. | 726.0 | | A2B BCC BCC#2 |
| 6 | AINV | 2 | 1. | 726.0 | | BCC BCC#2 |
| 10 | ALF | 2 | 1. | 1594.0 | | LIQUID FCC |
| 11 | ALF | 2 | 1. | 1548.0 | | LIQUID FCC |
| 12 | ALF | 2 | 1. | 1499.0 | | LIQUID FCC |

```

13 ALF    2   1.    1438.0    LIQUID FCC
20 ATIE   2   1.    1413.0    LIQUID FCC
21 ATIE   2   1.    1337.0    LIQUID FCC
22 ATIE   2   1.    1213.0    LIQUID FCC
23 ATIE   2   1.    1100.0    LIQUID BCC
100 AA < unused > 1573.0    LIQUID
101 AA < unused > 1573.0    LIQUID
102 AA < unused > 1573.0    LIQUID
103 AA < unused > 1573.0    LIQUID
104 AA < unused > 1573.0    LIQUID
105 AA < unused > 1573.0    LIQUID
106 AA < unused > 1573.0    LIQUID
107 AA < unused > 1573.0    LIQUID
108 AA < unused > 1573.0    LIQUID
110 AH < unused > 1773.0    LIQUID
111 AH < unused > 1773.0    LIQUID
112 AH < unused > 1773.0    LIQUID
113 AH < unused > 1773.0    LIQUID
114 AH < unused > 1773.0    LIQUID
115 AH < unused > 1773.0    LIQUID
116 AH < unused > 1773.0    LIQUID
117 AH < unused > 1773.0    LIQUID
118 AH < unused > 1773.0    LIQUID
ED_EXP: s-we 1 100-118
ED_EXP: s-e 1
Equilibrium number           1, label AINV
ED_EXP: c-a
Eq  Lab Iter Weight Temp   Exp Fix phases or comments
  1 AINV  2   1.    1192.7    LIQUID A2B BCC
  2 AINV  2   1.    1341.0    LIQUID A2B
  3 AINV  2   1.    1049.1    LIQUID A2B BCC FCC
  4 AINV  2   1.    1203.1    LIQUID BCC FCC
  5 AINV  2   1.    726.0     A2B BCC BCC#2
  6 AINV  2   1.    726.0     BCC BCC#2
100 ALF   2   1.    1594.0    LIQUID FCC
101 ALF   2   1.    1548.0    LIQUID FCC
102 ALF   2   1.    1499.0    LIQUID FCC
103 ALF   2   1.    1438.0    LIQUID FCC
20 ATIE   2   1.    1413.0    LIQUID FCC
21 ATIE   2   1.    1337.0    LIQUID FCC
22 ATIE   2   1.    1213.0    LIQUID FCC
23 ATIE   2   1.    1100.0    LIQUID BCC
100 AA < unused > 1573.0    LIQUID
101 AA < unused > 1573.0    LIQUID
102 AA < unused > 1573.0    LIQUID
103 AA < unused > 1573.0    LIQUID
104 AA < unused > 1573.0    LIQUID
105 AA < unused > 1573.0    LIQUID
106 AA < unused > 1573.0    LIQUID
107 AA < unused > 1573.0    LIQUID
108 AA < unused > 1573.0    LIQUID
110 AH < unused > 1773.0    LIQUID
111 AH < unused > 1773.0    LIQUID
112 AH < unused > 1773.0    LIQUID
113 AH < unused > 1773.0    LIQUID
114 AH < unused > 1773.0    LIQUID
115 AH < unused > 1773.0    LIQUID
116 AH < unused > 1773.0    LIQUID
117 AH < unused > 1773.0    LIQUID
118 AH < unused > 1773.0    LIQUID
ED_EXP: save
ED_EXP: ba
PARROT: opt 30
Use      47 experiments, maximum is      2000
Use      1082 real workspace, maximum is  50000
The following output is provided by subroutine VA05A

      AT THE  0 TH ITERATION WE HAVE THE SUM OF SQUARES  8.37676666E-02
1  1.0011E+00  2  1.0010E+00  3  1.0000E+00  4  1.0000E+00  5  1.0006E+00
6  1.0025E+00  7  9.9869E-01  8  1.0017E+00  9  1.0072E+00

      AT THE  1 ST ITERATION WE HAVE THE SUM OF SQUARES  8.45966510E-02
1  1.0012E+00  2  1.0010E+00  3  1.0000E+00  4  1.0000E+00  5  1.0006E+00
6  1.0025E+00  7  9.9869E-01  8  1.0017E+00  9  1.0072E+00

      AT THE  2 ND ITERATION WE HAVE THE SUM OF SQUARES  8.64908738E-02
1  1.0011E+00  2  1.0011E+00  3  1.0000E+00  4  1.0000E+00  5  1.0006E+00
6  1.0025E+00  7  9.9869E-01  8  1.0017E+00  9  1.0072E+00

      AT THE  3 RD ITERATION WE HAVE THE SUM OF SQUARES  8.29333236E-02
1  1.0011E+00  2  1.0010E+00  3  1.0001E+00  4  1.0000E+00  5  1.0006E+00
6  1.0025E+00  7  9.9869E-01  8  1.0017E+00  9  1.0072E+00

      AT THE  4 TH ITERATION WE HAVE THE SUM OF SQUARES  8.34050981E-02
1  1.0011E+00  2  1.0010E+00  3  1.0001E+00  4  1.0001E+00  5  1.0006E+00
6  1.0025E+00  7  9.9869E-01  8  1.0017E+00  9  1.0072E+00

      AT THE  5 TH ITERATION WE HAVE THE SUM OF SQUARES  8.32695445E-02
1  1.0011E+00  2  1.0010E+00  3  1.0001E+00  4  1.0000E+00  5  1.0007E+00
6  1.0025E+00  7  9.9869E-01  8  1.0017E+00  9  1.0072E+00

      AT THE  6 TH ITERATION WE HAVE THE SUM OF SQUARES  8.29173322E-02
1  1.0011E+00  2  1.0010E+00  3  1.0001E+00  4  1.0000E+00  5  1.0006E+00
6  1.0026E+00  7  9.9869E-01  8  1.0017E+00  9  1.0072E+00

      AT THE  7 TH ITERATION WE HAVE THE SUM OF SQUARES  8.29244170E-02
1  1.0011E+00  2  1.0010E+00  3  1.0001E+00  4  1.0000E+00  5  1.0006E+00
6  1.0026E+00  7  9.9879E-01  8  1.0017E+00  9  1.0072E+00

      AT THE  8 TH ITERATION WE HAVE THE SUM OF SQUARES  8.31150247E-02
1  1.0011E+00  2  1.0010E+00  3  1.0001E+00  4  1.0000E+00  5  1.0006E+00
6  1.0026E+00  7  9.9869E-01  8  1.0018E+00  9  1.0072E+00

      AT THE  9 TH ITERATION WE HAVE THE SUM OF SQUARES  8.28948396E-02
1  1.0011E+00  2  1.0010E+00  3  1.0001E+00  4  1.0000E+00  5  1.0006E+00
6  1.0026E+00  7  9.9869E-01  8  1.0017E+00  9  1.0073E+00

      AT THE 10 TH ITERATION WE HAVE THE SUM OF SQUARES  8.22511567E-02
1  1.0010E+00  2  1.0011E+00  3  1.0001E+00  4  9.9998E-01  5  1.0006E+00
6  1.0027E+00  7  9.9870E-01  8  1.0016E+00  9  1.0073E+00

      AT THE 11 TH ITERATION WE HAVE THE SUM OF SQUARES  8.16968288E-02
1  1.0011E+00  2  1.0011E+00  3  1.0002E+00  4  9.9994E-01  5  1.0006E+00
6  1.0027E+00  7  9.9871E-01  8  1.0016E+00  9  1.0073E+00

```

```

AT THE 12 TH ITERATION WE HAVE THE SUM OF SQUARES 8.10067067E-02
1 1.0010E+00 2 1.0011E+00 3 1.0002E+00 4 9.9990E-01 5 1.0006E+00
6 1.0029E+00 7 9.9874E-01 8 1.0015E+00 9 1.0072E+00

AT THE 13 TH ITERATION WE HAVE THE SUM OF SQUARES 8.00971091E-02
1 1.0011E+00 2 1.0011E+00 3 1.0002E+00 4 9.9981E-01 5 1.0006E+00
6 1.0032E+00 7 9.9880E-01 8 1.0014E+00 9 1.0070E+00

AT THE 14 TH ITERATION WE HAVE THE SUM OF SQUARES 7.86821321E-02
1 1.0011E+00 2 1.0012E+00 3 1.0002E+00 4 9.9966E-01 5 1.0008E+00
6 1.0038E+00 7 9.9892E-01 8 1.0011E+00 9 1.0067E+00

AT THE 15 TH ITERATION WE HAVE THE SUM OF SQUARES 7.64149946E-02
1 1.0012E+00 2 1.0014E+00 3 1.0002E+00 4 9.9936E-01 5 1.0010E+00
6 1.0050E+00 7 9.9916E-01 8 1.0004E+00 9 1.0060E+00

AT THE 16 TH ITERATION WE HAVE THE SUM OF SQUARES 7.28311497E-02
1 1.0015E+00 2 1.0017E+00 3 1.0002E+00 4 9.9879E-01 5 1.0014E+00
6 1.0074E+00 7 9.9965E-01 8 9.9923E-01 9 1.0046E+00

AT THE 17 TH ITERATION WE HAVE THE SUM OF SQUARES 6.84499664E-02
1 1.0019E+00 2 1.0024E+00 3 1.0002E+00 4 9.9764E-01 5 1.0023E+00
6 1.0124E+00 7 1.0006E+00 8 9.9680E-01 9 1.0019E+00

AT THE 18 TH ITERATION WE HAVE THE SUM OF SQUARES 6.73854820E-02
1 1.0023E+00 2 1.0029E+00 3 1.0001E+00 4 9.9672E-01 5 1.0031E+00
6 1.0163E+00 7 1.0014E+00 8 9.9501E-01 9 1.0002E+00

THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED 18 iterations
1 1.0023E+00 2 1.0029E+00 3 1.0001E+00 4 9.9672E-01 5 1.0031E+00
6 1.0163E+00 7 1.0014E+00 8 9.9501E-01 9 1.0002E+00

1 -5.7838E-02 2 -9.3605E-03 3 1.4183E-02 4 2.0794E-02 5 -2.5747E-02
6 -5.2100E-02 7 1.9269E-02 8 2.6822E-02 9 1.3105E-02 10 2.7154E-02
11 8.7707E-03 12 1.3244E-02 13 -4.8660E-02 14 2.1790E-02 15 4.7290E-03
16 2.8670E-02 17 2.1551E-02 18 -2.2040E-02 19 -8.2402E-03 20 -4.9755E-03
21 -1.5646E-02 22 -1.0901E-02 23 1.5213E-02 24 2.4270E-02 25 1.4695E-02
26 -1.4885E-02 27 2.0283E-02 28 -1.2750E-02 29 1.5398E-02 30 -9.5909E-03
31 -1.6832E-02 32 2.7435E-02 33 8.7018E-02 34 1.2433E-01 35 1.0168E-01
36 -1.7320E-02 37 7.0577E-02 38 -1.9477E-02 39 1.6078E-02 40 4.5471E-02
41 4.8181E-02 42 4.6207E-02 43 4.1549E-02 44 3.4207E-02 45 2.2181E-02
46 7.4714E-03 47 -1.1922E-02

```

THE SUM OF SQUARES IS 6.73854820E-02

PARROT: l-r C SCREEN

```
=====
OUTPUT FROM P A R R O T . DATE 2023. 4.27 16:31:44
```

```
*** SUCCESSFUL OPTIMIZATION. ***
NUMBER OF ITERATIONS: 19
```

```
-- OPTIMIZING CONDITIONS --
```

```
RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 30 DMAX = 1.00000000E+02 H = 1.00000000E-04
ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03
```

```
-- OPTIMIZING VARIABLES --
```

```
AVAILABLE VARIABLES ARE V1 TO V00
```

| VAR. | VALUE | START VALUE | SCALING FACTOR | REL.STAND.DEV |
|------|-----------------|-----------------|-----------------|----------------|
| V1 | 2.03690187E+04 | 2.03222963E+04 | 2.03222963E+04 | 2.99244801E-02 |
| V2 | -2.94289046E+01 | -2.93449017E+01 | -2.93449017E+01 | 2.27402481E-02 |
| V11 | -2.17329018E+04 | -2.17307895E+04 | -2.17307895E+04 | 3.48515529E-02 |
| V12 | 1.52104284E+01 | 1.52604480E+01 | 1.52604480E+01 | 5.50818499E-02 |
| V15 | 2.42024493E+04 | 2.41287698E+04 | 2.41287698E+04 | 8.32414603E-02 |
| V16 | -8.38635212E+00 | -8.25177741E+00 | -8.25177741E+00 | 2.56685138E-01 |
| V17 | 3.08808170E+03 | 3.08380218E+03 | 3.08380218E+03 | 2.30230261E-01 |
| V19 | 2.20479876E+04 | 2.21586154E+04 | 2.21586154E+04 | 4.86430739E-01 |
| V20 | -7.06074720E+00 | -7.05926808E+00 | -7.05926808E+00 | 1.22189066E+00 |

```
NUMBER OF OPTIMIZING VARIABLES : 9
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 8.37676666E-02 TO 6.73854820E-02
DEGREES OF FREEDOM 38. REDUCED SUM OF SQUARES 1.77330216E-03
```

| SYMBOL | STATUS | VALUE/FUNCTION |
|--------------|----------|-----------------------------------|
| FUNCTION R | 298.15 | 8.31451000000000 ; 6000 N REFO ! |
| 2 RTLNP | 20000000 | +RT*T*LN(1E-05*T) |
| FUNCTION V1 | 298.15 | 20369.0186606815 ; 6000 N REFO ! |
| FUNCTION V2 | 298.15 | -29.4289045584415 ; 6000 N REFO ! |
| FUNCTION V11 | 298.15 | -21732.9018447203 ; 6000 N REFO ! |
| FUNCTION V12 | 298.15 | 15.2104284489495 ; 6000 N REFO ! |
| FUNCTION V15 | 298.15 | 24202.4492818878 ; 6000 N REFO ! |
| FUNCTION V16 | 298.15 | -8.38635212256223 ; 6000 N REFO ! |
| FUNCTION V17 | 298.15 | 3088.08169693190 ; 6000 N REFO ! |
| FUNCTION V19 | 298.15 | 22047.9876432569 ; 6000 N REFO ! |
| FUNCTION V20 | 298.15 | -7.06074720080492 ; 6000 N REFO ! |

LIQUID:L (A,B)1.0

```
==== [A] ====
G(LIQUID,A;0) 298.15 +14000-10*T; 6000 N
```

```
==== [B] ====
G(LIQUID,B;0) 298.15 +18000-12*T; 6000 N
```

```

==== [A, B] ====
G(LIQUID,A,B;0)          298.15 +V11+V12*T;           6000 N
G(LIQUID,A,B;1)          298.15 +V13+V14*T;           6000 N

$ ====== BLOCK NUMBER 1

DEFINED CONSTANTS
DX=2E-2, P0=101325, DH=500, DT=10
DEFINED FUNCTIONS AND VARIABLES%
HTR=HM(LIQUID)-HM(A2B)
1 T=1193                  1192.      10.      -0.5784     -5.7838E-02
1 W(LIQUID,B)=0.408       0.4078    2.00E-02   -1.8721E-04   -9.3605E-03
1 W(BCC#1,B)=0.13         0.1303    2.00E-02   2.8366E-04    1.4183E-02
2 T=1341                  1341.      10.      0.2079     2.0794E-02
2 HTR=3727                 3714.      5.00E+02   -12.87     -2.5747E-02
3 T=1049                  1048.      10.      -0.5210     -5.2100E-02
3 W(LIQUID,A)=0.27        0.2704    2.00E-02   3.8539E-04    1.9269E-02
3 W(BCC#1,A)=9.3E-2       9.3536E-02  2.00E-02   5.3645E-04    2.6822E-02
4 T=1203                  1203.      10.      0.1311     1.3105E-02
4 W(LIQUID,A)=0.19        0.1905    2.00E-02   5.4309E-04    2.7154E-02
4 W(BCC#1,A)=6.9E-2       6.9175E-02  2.00E-02   1.7541E-04    8.7707E-03
4 W(FCC,A)=6E-2           6.0265E-02  2.00E-02   2.6487E-04    1.3244E-02
5 T=726                   725.5      10.      -0.4866     -4.8660E-02
5 X(BCC#1,B)=3.7E-2       3.7436E-02  2.00E-02   4.3580E-04    2.1790E-02
5 X(BCC#2,A)=0.114        0.1141    2.00E-02   9.4580E-05    4.7290E-03
6 X(BCC#1,B)=3.7E-2       3.7573E-02  2.00E-02   5.7340E-04    2.8670E-02
6 X(BCC#2,A)=0.114        0.1144    2.00E-02   4.3102E-04    2.1551E-02
10 W(LIQUID,A)=2E-2        1.9559E-02  2.00E-02   -4.4080E-04   -2.2040E-02
11 W(LIQUID,A)=4.2E-2       4.1835E-02  2.00E-02   -1.6480E-04   -8.2402E-03
12 W(LIQUID,A)=6.5E-2       6.4900E-02  2.00E-02   -9.9511E-05   -4.9755E-03
13 W(LIQUID,A)=9.3E-2       9.2687E-02  2.00E-02   -3.1291E-04   -1.5646E-02
20 W(LIQUID,A)=0.104       0.1038    2.00E-02   -2.1801E-04   -1.0901E-02
20 W(FCC,A)=3.8E-2         3.8304E-02  2.00E-02   3.0425E-04    1.5213E-02
21 W(LIQUID,A)=0.136       0.1365    2.00E-02   4.8540E-04    2.4270E-02
21 W(FCC,A)=4.7E-2         4.7294E-02  2.00E-02   2.9390E-04    1.4695E-02
22 W(LIQUID,A)=0.187       0.1867    2.00E-02   -2.9770E-04   -1.4885E-02
22 W(FCC,A)=5.9E-2         5.9406E-02  2.00E-02   4.0566E-04    2.0283E-02
23 W(LIQUID,A)=0.245       0.2447    2.00E-02   -2.5500E-04   -1.2750E-02
23 W(BCC#1,A)=8.5E-2       8.5308E-02  2.00E-02   3.0796E-04    1.5398E-02
100 ACR(B)=0.94            0.9397    2.85E-02   -2.7299E-04   -9.5909E-03
101 ACR(B)=0.84            0.8395    2.82E-02   -4.7444E-04   -1.6832E-02
102 ACR(B)=0.74            0.7408    2.81E-02   7.6969E-04    2.7435E-02
103 ACR(B)=0.64            0.6424    2.81E-02   2.4423E-03    8.7018E-02
104 ACR(B)=0.54            0.5435    2.82E-02   3.5094E-03    0.1243
105 ACR(B)=0.44            0.4429    2.85E-02   2.9021E-03    0.1017
106 ACR(B)=0.34            0.3395    2.90E-02   -5.0277E-04   -1.7320E-02
107 ACR(B)=0.23            0.2321    2.97E-02   2.0965E-03    7.0577E-02
108 ACR(B)=0.12            0.1194    3.06E-02   -5.9601E-04   -1.9477E-02
110 HMR(LIQUID)==-1964      -1956.    5.00E+02   8.039      1.6078E-02
111 HMR(LIQUID)==-3500      -3477.    5.00E+02   22.74      4.5471E-02
112 HMR(LIQUID)==-4588      -4564.    5.00E+02   24.09      4.8181E-02
113 HMR(LIQUID)==-5239      -5216.    5.00E+02   23.10      4.6207E-02
114 HMR(LIQUID)==-5454      -5433.    5.00E+02   20.77      4.1549E-02
115 HMR(LIQUID)==-5233      -5216.    5.00E+02   17.10      3.4207E-02
116 HMR(LIQUID)==-4575      -4564.    5.00E+02   11.09      2.2181E-02
117 HMR(LIQUID)==-3481      -3477.    5.00E+02   3.736      7.4714E-03
118 HMR(LIQUID)==-1950      -1956.    5.00E+02   -5.961     -1.1922E-02

```

```

PARROT:
PARROT:
PARROT: Hit RETURN to continue
PARROT: @@ Calculate the phase diagram one last time.
PARROT: mac tcex36cpd
PARROT: set-echo
NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
POLY:
POLY: @@ In PARROT, the global minimization is turned off automatically.
POLY: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY: @@ message will be given.
POLY:
POLY: advanced-option global yes,
Settings for global minimization:
*** WARNING *** Global equilibrium calculation may create new composition sets
and this may corrupt your PARROT work file (.PAR file).
Do not go back to PARROT but exit from POLY after your POLY calculations.
POLY:
POLY: def-com,,
POLY: s-a-v 1 w(b) 0 1,,,'
The condition W(B)=.1234 created
POLY: s-a-v 2 t 300 1700,,''
The condition T=942.2 created
POLY: s-c t=500
POLY: 1-c
W(B)=0.1234, T=500
DEGREES OF FREEDOM 2
POLY: c-e
Creating condition P=1E5
Creating condition N=1
Using global minimization procedure
Calculated          628 grid points in          0 s
Found the set of lowest grid points in          0 s
Calculated POLY solution      0 s, total time      0 s
POLY: save tcex36 y

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

```

```

POLY: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9

```

```

Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12
Organizing start points
Using ADDED start equilibria
Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Generating start point 27
Generating start point 28
Phase region boundary 1 at: 7.140E-01 3.100E+02
  BCC#1
  ** BCC#2
Calculated.. 2 equilibria
Terminating at axis limit.

Phase region boundary 2 at: 7.141E-01 3.000E+02
  BCC#1
  ** BCC#2
Calculated. 14 equilibria

Phase region boundary 3 at: 6.819E-01 7.255E+02
  ** A2B
  BCC#1
  ** BCC#2

Phase region boundary 4 at: 3.626E-01 7.255E+02
  ** A2B
  BCC#1
Calculated. 15 equilibria

Phase region boundary 5 at: 3.771E-01 1.192E+03
  ** LIQUID
  ** A2B
  BCC#1

Phase region boundary 6 at: 2.828E-01 1.192E+03
  ** LIQUID
  BCC#1
Calculated. 27 equilibria

Phase region boundary 7 at: 4.863E-01 1.192E+03
  ** LIQUID
  A2B
Calculated. 28 equilibria

Phase region boundary 8 at: 6.500E-01 1.048E+03
  ** LIQUID
  A2B
  ** BCC#1

Phase region boundary 9 at: 7.639E-01 1.048E+03
  A2B
  ** BCC#1
Calculated. 11 equilibria
Terminating at known equilibrium

Phase region boundary 10 at: 8.273E-01 1.048E+03
  LIQUID
  ** BCC#1
Calculated. 8 equilibria

Phase region boundary 11 at: 8.748E-01 1.203E+03
  LIQUID
  ** BCC#1
  ** FCC

Phase region boundary 12 at: 8.800E-01 1.203E+03
  LIQUID
  ** FCC
Calculated. 33 equilibria

Phase region boundary 13 at: 9.353E-01 1.203E+03
  BCC#1
  ** FCC
Calculated. 20 equilibria

Phase region boundary 14 at: 7.140E-01 3.100E+02
  BCC#1
  ** BCC#2
Calculated.. 13 equilibria
Terminating at known equilibrium

Phase region boundary 15 at: 7.140E-01 3.100E+02
  BCC#1
  ** BCC#2
Calculated.. 2 equilibria

```

```

Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 16 at: 7.140E-01 3.100E+02
  ** BCC#1
  ** BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 17 at: 7.140E-01 3.100E+02
  ** BCC#1
  ** BCC#2
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 18 at: 7.140E-01 3.100E+02
  ** BCC#1
  ** BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 19 at: 7.140E-01 3.100E+02
  ** BCC#1
  ** BCC#2
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 20 at: 7.140E-01 3.100E+02
  ** BCC#1
  ** BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 21 at: 7.140E-01 3.100E+02
  ** BCC#1
  ** BCC#2
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 22 at: 7.140E-01 3.100E+02
  ** BCC#1
  ** BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 23 at: 7.140E-01 3.100E+02
  ** BCC#1
  ** BCC#2
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 24 at: 7.140E-01 3.100E+02
  ** BCC#1
  ** BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 25 at: 3.647E-01 7.700E+02
  ** A2B
  ** BCC#1
Calculated.          10 equilibria

Phase region boundary 26 at: 3.647E-01 7.700E+02
  ** A2B
  ** BCC#1
Calculated.          3 equilibria
Terminating at known equilibrium

Phase region boundary 27 at: 3.647E-01 7.700E+02
  ** A2B
  ** BCC#1
Calculated.          14 equilibria
Terminating at known equilibrium

Phase region boundary 28 at: 7.910E-01 7.700E+02
  ** A2B
  ** BCC#1
Calculated.          10 equilibria

Phase region boundary 29 at: 7.910E-01 7.700E+02
  ** A2B
  ** BCC#1
Calculated.          3 equilibria
Terminating at known equilibrium

Phase region boundary 30 at: 7.910E-01 7.700E+02
  ** A2B
  ** BCC#1
Calculated.          9 equilibria
Terminating at known equilibrium

Phase region boundary 31 at: 2.448E-01 1.230E+03
  ** LIQUID
  ** BCC#1
Calculated.          4 equilibria
Terminating at known equilibrium

Phase region boundary 32 at: 2.448E-01 1.230E+03
  ** LIQUID
  ** FCC
Calculated.          26 equilibria

Phase region boundary 33 at: 8.858E-01 1.230E+03
  ** LIQUID
  ** FCC
Calculated.          2 equilibria
Terminating at known equilibrium

Phase region boundary 34 at: 8.858E-01 1.230E+03
  ** LIQUID
  ** FCC
Calculated.          29 equilibria

```

```

Phase region boundary 35 at: 6.415E-03 1.397E+03
    LIQUID
    ** BCC#1
Calculated.          13 equilibria

Phase region boundary 36 at: 6.415E-03 1.397E+03
    LIQUID
    ** BCC#1
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 37 at: 2.299E-01 1.244E+03
    LIQUID
    ** BCC#1
Calculated.          20 equilibria

Phase region boundary 38 at: 2.299E-01 1.244E+03
    LIQUID
    ** BCC#1
Calculated.          4 equilibria
Terminating at known equilibrium

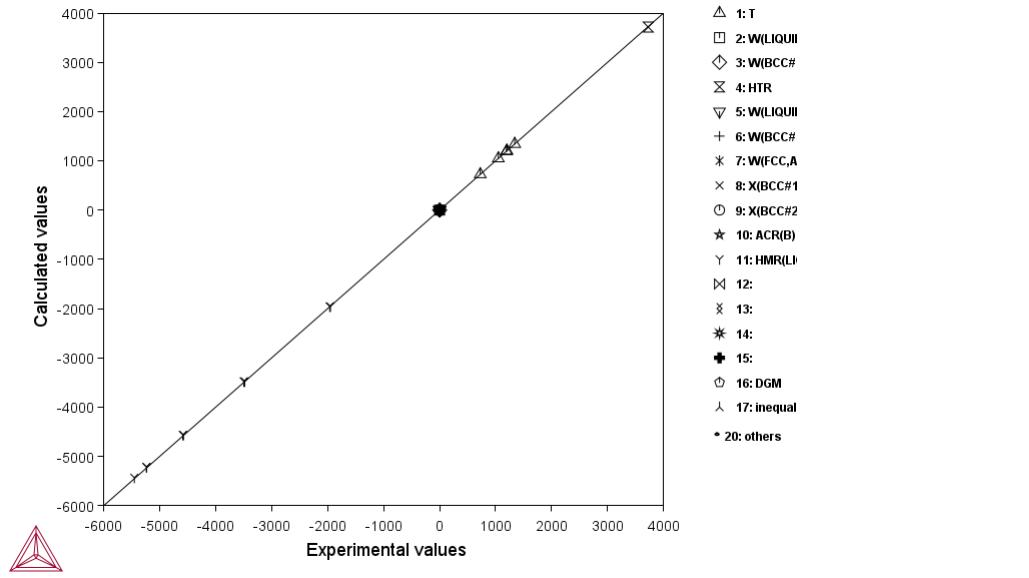
Phase region boundary 39 at: 6.122E-01 1.240E+03
    LIQUID
    ** A2B
Calculated.          14 equilibria
Terminating at known equilibrium

Phase region boundary 40 at: 6.122E-01 1.240E+03
    LIQUID
    ** A2B
Calculated.          8 equilibria
Terminating at known equilibrium

Phase region boundary 41 at: 9.927E-01 1.613E+03
    LIQUID
    ** FCC
Calculated.          20 equilibria
Terminating at known equilibrium

Phase region boundary 42 at: 9.927E-01 1.613E+03
    LIQUID
    ** FCC
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\generate_console_examples\examples\tcex36a\tcex36.POLY3
CPU time for mapping      1 seconds
POLY: post
POST: s-l d
POST: plot

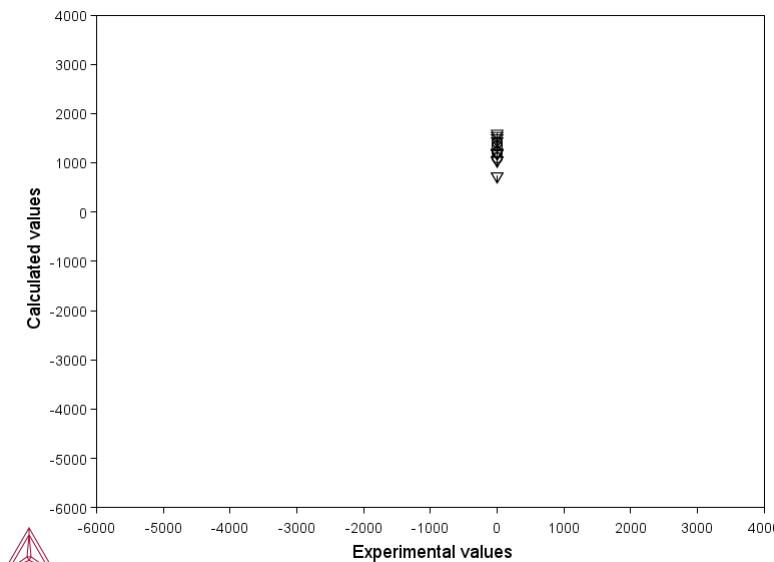
```



```

POST:
POST: set-inter
POST:Hit RETURN to continue
POST:@@ Add the experimental data
POST: a-e-d y exp36 0; 1
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
*** ERROR 3004 IN LPOSTP: NO AXIS DEFINED
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot

```



```

POST:
POST:
POST:Hit RETURN to continue
POST: @@ Also calculate the enthalpies in the liquid
POST: ba
POLY: read,,
POLY:
POLY:
POLY: s-a-v 2 none
POLY: s-c t=1773
POLY: c-e
Using global minimization procedure
Calculated          628 grid points in      0 s
Found the set of lowest grid points in      0 s
Calculated POLY solution      0 s, total time      0 s
POLY: sh hmr
HMR=13116.472
POLY: l-st c
*** STATUS FOR ALL COMPONENTS
COMPONENT           STATUS   REF. STATE      T (K)      P (Pa)
A                  ENTERED  SER
B                  ENTERED  SER
POLY: s-r-s a liq * 1e5
POLY: s-r-s b liq * 1e5
POLY: save tcex36h y

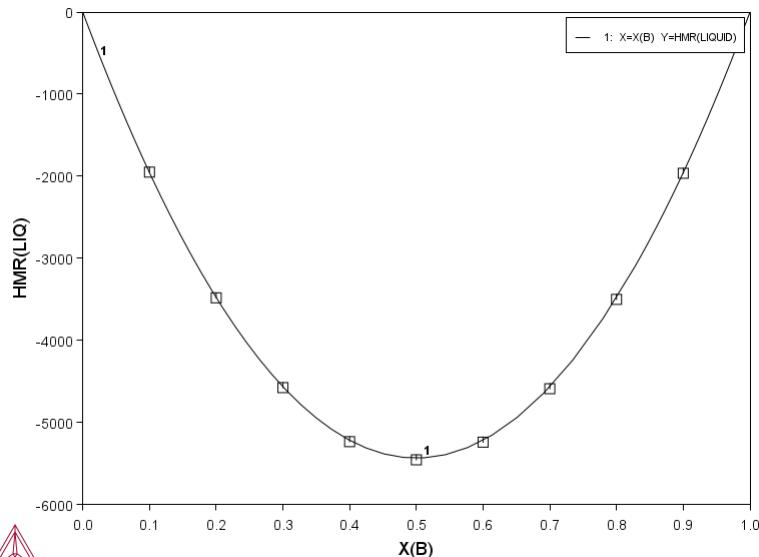
This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

POLY: step normal
No initial equilibrium, using default
Step will start from axis value  0.123400
...OK

Phase Region from  0.123400      for:
    LIQUID
Global test at  3.23400E-01 .... OK
Global test at  5.73400E-01 .... OK
Global test at  8.23400E-01 .... OK
Global test at  9.53400E-01 .... OK
Global test at  1.00000E+00 .... OK
Terminating at  1.00000
Calculated      51 equilibria

Phase Region from  0.123400      for:
    LIQUID
Global test at  8.34000E-02 .... OK
Global test at  3.34000E-02 .... OK
Terminating at  0.250000E-11
Calculated      28 equilibria
*** Buffer saved on file: c:\jenkins\workspace\generate_console_examples\examples\tcex36a\tcex36h.POLY3
POLY: post
POST: s-d-a x x(b)
POST: s-d-a y hmr(liq)
POST: a-e-d y exp36 0; 2
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot

```



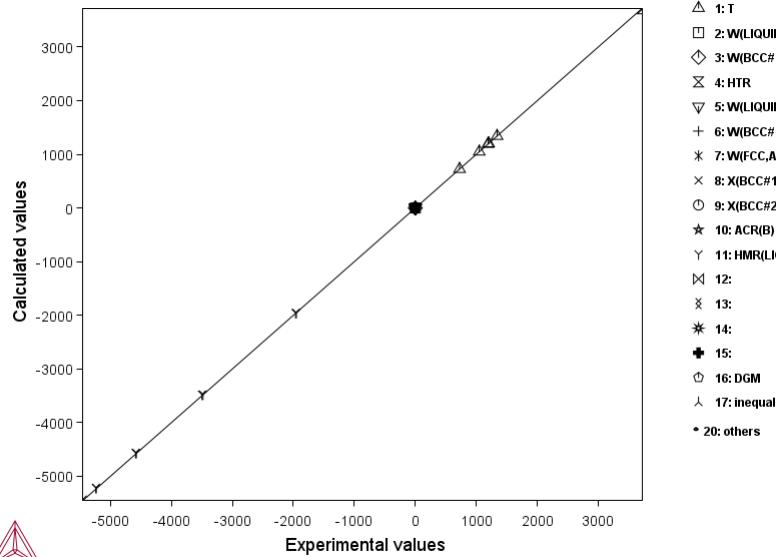
```

POST:
POST:Hit RETURN to continue
POST: @@ We can see the fitting results by the following method
POST: @@ Data points falling on the diagonal line indicates
POST: @@ perfect fitting.
POST: @@
POST: ba
POLY: ba

```

PARROT VERSION 5.3

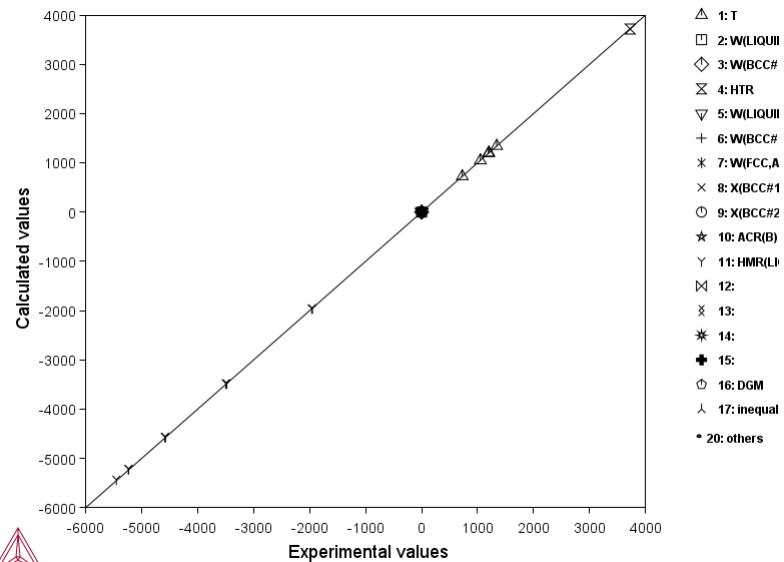
Global minimization used as test only
PARROT: l-result gra pexp36 1,



```

POST: s-s-s y n -6000 4000
POST: s-s-s x n -6000 4000
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
*** ERROR 3004 IN LPOSTP: NO AXIS DEFINED
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot

```



POST: b
PARROT: set-inter
PARROT:

tce36a-tce36cpd

```
PARROT:About
NO SUCH COMMAND, USE HELP
PARROT:PARROT:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce36a\tce36cpd.TCM.test"
PARROT: set-echo
NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
POLY:
POLY: @@ In PARROT, the global minimization is turned off automatically.
POLY: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY: @@ message will be given.
POLY:
POLY: advanced-option global yes.,
Settings for global minimization:
*** WARNING *** Global equilibrium calculation may create new composition sets
and this may corrupt your PARROT work file (.PAR file).
Do not go back to PARROT but exit from POLY after your POLY calculations.
POLY:
POLY: def-com,,,,
POLY: s-a-v 1 w(b) 0 1,,,,
The condition W(B)=.1234 created
POLY: s-a-v 2 t 300 1700,,,
The condition T=942.2 created
POLY: s-c t=500
POLY: l-c
W(B)=0.1234, T=500
DEGREES OF FREEDOM 2
POLY: c-e
Creating condition P=1E5
Creating condition N=1
Using global minimization procedure
Calculated          628 grid points in           0 s
Found the set of lowest grid points in           0 s
Calculated POLY solution      0 s, total time   0 s
POLY: save tce36 y
```

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

```
POLY: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12
```

Organizing start points

Using ADDED start equilibria

```
Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Generating start point 27
Generating start point 28
```

```
Phase region boundary 1 at: 7.140E-01 3.100E+02
  BCC#1
  ** BCC#2
```

```
Calculated..          2 equilibria
Terminating at axis limit.
```

```
Phase region boundary 2 at: 7.141E-01 3.000E+02
  BCC#1
  ** BCC#2
```

```
Calculated..          14 equilibria
```

```
Phase region boundary 3 at: 6.819E-01 7.255E+02
  ** A2B
  BCC#1
  ** BCC#2
```

```
Phase region boundary 4 at: 3.626E-01 7.255E+02
  ** A2B
  BCC#1
Calculated..          15 equilibria
```

```

Phase region boundary  5 at:  3.771E-01  1.192E+03
  ** LIQUID
  ** A2B
  BCC#1

Phase region boundary  6 at:  2.828E-01  1.192E+03
  ** LIQUID
  BCC#1
Calculated.          27 equilibria

Phase region boundary  7 at:  4.863E-01  1.192E+03
  ** LIQUID
  A2B
Calculated.          28 equilibria

Phase region boundary  8 at:  6.500E-01  1.048E+03
  ** LIQUID
  A2B
  ** BCC#1

Phase region boundary  9 at:  7.639E-01  1.048E+03
  A2B
  ** BCC#1
Calculated.          11 equilibria
Terminating at known equilibrium

Phase region boundary 10 at:  8.273E-01  1.048E+03
  LIQUID
  ** BCC#1
Calculated.          8 equilibria

Phase region boundary 11 at:  8.748E-01  1.203E+03
  LIQUID
  ** BCC#1
  ** FCC

Phase region boundary 12 at:  8.800E-01  1.203E+03
  LIQUID
  ** FCC
Calculated.          33 equilibria

Phase region boundary 13 at:  9.353E-01  1.203E+03
  BCC#1
  ** FCC
Calculated.          20 equilibria

Phase region boundary 14 at:  7.140E-01  3.100E+02
  BCC#1
  ** BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 15 at:  7.140E-01  3.100E+02
  BCC#1
  ** BCC#2
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 16 at:  7.140E-01  3.100E+02
  BCC#1
  ** BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 17 at:  7.140E-01  3.100E+02
  BCC#1
  ** BCC#2
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 18 at:  7.140E-01  3.100E+02
  BCC#1
  ** BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 19 at:  7.140E-01  3.100E+02
  BCC#1
  ** BCC#2
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 20 at:  7.140E-01  3.100E+02
  BCC#1
  ** BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 21 at:  7.140E-01  3.100E+02
  ** BCC#1
  BCC#2
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 22 at:  7.140E-01  3.100E+02
  ** BCC#1
  BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 23 at:  7.140E-01  3.100E+02
  ** BCC#1
  BCC#2
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 24 at:  7.140E-01  3.100E+02
  ** BCC#1
  BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

```

```

Phase region boundary 25 at: 3.647E-01 7.700E+02
** A2B
BCC#1
Calculated.          10 equilibria

Phase region boundary 26 at: 3.647E-01 7.700E+02
** A2B
BCC#1
Calculated.          3 equilibria
Terminating at known equilibrium

Phase region boundary 27 at: 3.647E-01 7.700E+02
** A2B
BCC#1
Calculated.          14 equilibria
Terminating at known equilibrium

Phase region boundary 28 at: 7.910E-01 7.700E+02
** A2B
BCC#1
Calculated.          10 equilibria

Phase region boundary 29 at: 7.910E-01 7.700E+02
** A2B
BCC#1
Calculated.          3 equilibria
Terminating at known equilibrium

Phase region boundary 30 at: 7.910E-01 7.700E+02
** A2B
BCC#1
Calculated.          9 equilibria
Terminating at known equilibrium

Phase region boundary 31 at: 2.448E-01 1.230E+03
** LIQUID
BCC#1
Calculated.          4 equilibria
Terminating at known equilibrium

Phase region boundary 32 at: 2.448E-01 1.230E+03
** LIQUID
BCC#1
Calculated.          26 equilibria

Phase region boundary 33 at: 8.858E-01 1.230E+03
** LIQUID
FCC
Calculated.          2 equilibria
Terminating at known equilibrium

Phase region boundary 34 at: 8.858E-01 1.230E+03
** LIQUID
FCC
Calculated.          29 equilibria

Phase region boundary 35 at: 6.415E-03 1.397E+03
LIQUID
** BCC#1
Calculated.          13 equilibria

Phase region boundary 36 at: 6.415E-03 1.397E+03
LIQUID
** BCC#1
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 37 at: 2.299E-01 1.244E+03
LIQUID
** BCC#1
Calculated.          20 equilibria

Phase region boundary 38 at: 2.299E-01 1.244E+03
LIQUID
** BCC#1
Calculated.          4 equilibria
Terminating at known equilibrium

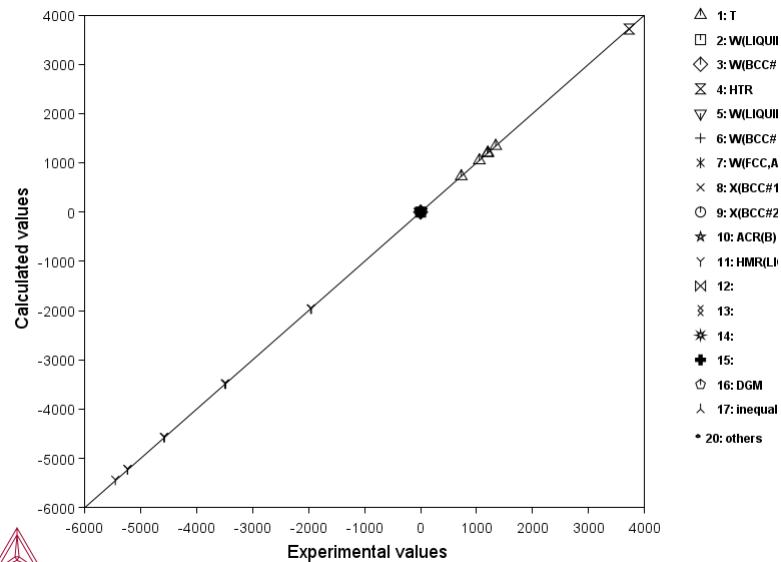
Phase region boundary 39 at: 6.122E-01 1.240E+03
LIQUID
** A2B
Calculated.          14 equilibria
Terminating at known equilibrium

Phase region boundary 40 at: 6.122E-01 1.240E+03
LIQUID
** A2B
Calculated.          8 equilibria
Terminating at known equilibrium

Phase region boundary 41 at: 9.927E-01 1.613E+03
LIQUID
** FCC
Calculated.          20 equilibria
Terminating at known equilibrium

Phase region boundary 42 at: 9.927E-01 1.613E+03
LIQUID
** FCC
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\generate_console_examples\examples\tcex36a\tcex36.POLY3
CPU time for mapping      1 seconds
POLY: post
POST: s-l d
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
*** ERROR 3004 IN LPOSTP: NO AXIS DEFINED
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot

```



POST:
POST: set-inter
POST:

SYS:About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

```

SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce37\tce37.TCM.test"
SYS: @@ Calculating an Isothermal Section
SYS:
SYS: @@ This example shows how to use command
SYS: @@ lines to enter and calculate an isothermal
SYS: @@ section using the POLY3 module.
SYS:
SYS: go data
THERMODYNAMIC DATABASE module
Database folder: C:\jenkins\workspace\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA           /*- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE11: sw fedemo
Current database: Iron Demo Database v4.0

VA           /*- DEFINED
TDB_FEDEMO: def-sys
ELEMENTS: fe cr ni
  FE          CR          NI
  DEFINED
TDB_FEDEMO: l-s c
LIQUID:L   :CR FE NI:
BCC_A2     :CR FE NI:VA:
LAVES_PHASE_C14 :CR FE NI:CR FE NI:
CBCC_A12   :CR FE NI:VA:
CHI_A12    :CR FE NI:CR:CR FE NI:
CUB_A13    :CR FE NI:VA:
FCC_A1     :CR FE NI:VA:
HCP_A3     :CR FE NI:VA:
SIGMA      :CR FE NI:CR:CR FE NI:
TDB_FEDEMO: Hit RETURN to continue
TDB_FEDEMO: get
16:35:54,645 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ...

List of references for assessed data

'A.T. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
'M. Ghasemi, Thermo-Calc Software AB, Sweden, 2020; Unifying liquid volume
database'
'M. Ghasemi, Thermo-Calc Software AB, Sweden, 2019; Viscosity of metallic
liquid'
'M Ghasemi, Thermo-Calc Software AB: assessing the surface tension of
metallic liquid'
'Y. Tang, in TCCU2, Thermo-Calc Software AB, Stockholm, Sweden'
'M. J. Assael, J. Phys. Chem. Ref. Data 35 (2006) 285; Fe, Al'
'M. J. Assael, High Temp. High Press., 41 (2012); Sb, Pb, Bi, Ni, Ag'
'B.J. Lee, CALPHAD, 17 (1993) 251-268; revision of Fe-Cr and Fe -Ni liquid'
'B.J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
'X.G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
volumes'
'X.G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270
(1986); CR-FE'
'A.T. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); CR -NI'
'A.T. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); FE-NI'
'N. Saunders, COST 507 Report (1998); Cr-Ti'
'B.J. Lee, unpublished work at KTH (1999); update of steel database'
'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; C14_LAVES'
'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equilib., 19
(1998) 441-448; Fe-Ti'
'R. Naraghi, Thermo-Calc Software AB, Sweden, 2019; Cr-Fe-Nb'
'R. Naraghi, Thermo-Calc Software AB, Sweden, Volume data updated for
TCFE9 database (TCFE v9.0, Jan, 2017).'
'Unassessed parameter; Linear combination of unary data'
'P. Gustafson, TRITA-MAC 354 (1987); C-Cr-Fe-Mo-W'
'J-O. Andersson, Metall. Trans. A, 19A (1988) 1385-1394; TRITA 0322 (1986);
CR-FE-MO'
'L.J. Zhang, Int.J. Mater. Res.,100(2) 160-175 (2009),Fe-Mn-Ni'
'K. Frisk, Metall. Trans. A, 21A (1990) 2477-2488; TRITA 0409 (1989); CR
-FE-N'
'L.L. Zhu, H.Y. Qi, L. Jiang, Z.P. Jin, J.C. Zhao, Intermetallics. 64
(2015) 86-95; Cr-Ru and Cr-Ni-Ru'
'B. Sundman et al., Report EUR 20315, Contract No 7210-PR/050, 2002; New
Sigma model'
'R. Naraghi, Thermo-Calc Software AB, Sweden (2015); FROST project'
-OK-
TDB_FEDEMO: go p-3

POLY version 3.32
POLY: l-st
Option /CPS/: cps
*** STATUS FOR ALL COMPONENTS
COMPONENT      STATUS      REF. STATE      T (K)      P (Pa)
VA            ENTERED    SER
CR            ENTERED    SER
FE            ENTERED    SER
NI            ENTERED    SER
*** STATUS FOR ALL PHASES
PHASE        STATUS      DRIVING FORCE    MOLES
SIGMA       ENTERED    0.000000E+00  0.000000E+00

```

```

LAVES_PHASE_C14      ENTERED      0.000000E+00  0.000000E+00
HCP_A3               ENTERED      0.000000E+00  0.000000E+00
FCC_A1               ENTERED      0.000000E+00  0.000000E+00
CUB_A13              ENTERED      0.000000E+00  0.000000E+00
CHI_A12              ENTERED      0.000000E+00  0.000000E+00
CBCC_A12             ENTERED      0.000000E+00  0.000000E+00
BCC_A2               ENTERED      0.000000E+00  0.000000E+00
LIQUID               ENTERED      0.000000E+00  0.000000E+00
*** STATUS FOR ALL SPECIES
CR ENTERED   FE ENTERED   NI ENTERED   VA ENTERED
POLY: @@ Set conditions for a point inside the diagram

POLY: s-c x(cr)=0.2 x(ni)=0.4
POLY: s-c t=1673 p=1e5 n=1
POLY: l-c
X(CR)=0.2, X(NI)=0.4, T=1673, P=100000, N=1
DEGREES OF FREEDOM 0
POLY: c-e
Using global minimization procedure
Calculated          15786 grid points in      3 s
Found the set of lowest grid points in      0 s
Calculated POLY solution      0 s, total time      3 s
POLY: l-e
OUTPUT TO SCREEN OR FILE /SCREEN/: SCREEN
Options /WVCS/: WVCS
Output from POLY-3, equilibrium =      1, label A0 , database: FEDEMO

Conditions:
X(CR)=0.2, X(NI)=0.4, T=1673, P=100000, N=1
DEGREES OF FREEDOM 0

Temperature 1673.00 K ( 1399.85 C), Pressure 1.000000E+05
Number of moles of components 1.000000E00, Mass in grams 5.62140E+01
Total Gibbs energy -1.08423E+05, Enthalpy 4.89973E+04, Volume 7.34210E-06

Component      Moles      W-Fraction Activity Potential Ref.stat
CR            2.0000E-01  1.8499E-01 7.8623E-04 -9.9434E+04 SER
FE            4.0000E-01  3.9739E-01 4.0953E-04 -1.0851E+05 SER
NI            4.0000E-01  4.1762E-01 3.0004E-04 -1.1283E+05 SER

FCC_A1           Status ENTERED      Driving force 0.0000E+00
Moles 1.0000E+00, Mass 5.6214E+01, Volume fraction 1.0000E+00 Mass fractions:
NI 4.17618E-01 FE 3.97389E-01 CR 1.84993E-01
POLY: s-a-v
Axis number: /1/: 1
Condition /NONE/: x(ni)
Min value /0/: 0
Max value /1/: 1
Increment /.025/: .025
POLY: s-a-v 2
Condition /NONE/: x(cr)
Min value /0/: 0
Max value /1/: 1
Increment /.025/: .025
POLY: save tce37 y
POLY:
POLY: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Organizing start points
Using ADDED start equilibria
Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Phase region boundary 1 at: 9.201E-03 4.019E-02
** BCC_A2
  FCC_A1
Calculated          14 equilibria
Phase region boundary 2 at: 9.201E-03 4.019E-02
** BCC_A2
  FCC_A1
Calculated.        31 equilibria
Phase region boundary 3 at: 1.950E-01 3.373E-01
** LIQUID
** BCC_A2
  FCC_A1
Calculated          53 equilibria
Phase region boundary 4 at: 2.267E-01 3.103E-01
** LIQUID
  FCC_A1
Calculated          53 equilibria
Phase region boundary 5 at: 1.883E-01 3.539E-01
** LIQUID
  BCC_A2
Calculated          49 equilibria

```

```

Phase region boundary 6 at: 1.950E-01 3.373E-01
** BCC_A2
  FCC_A1
Calculated           51 equilibria

Phase region boundary 7 at: 3.334E-01 3.082E-01
** LIQUID
  FCC_A1
Calculated           10 equilibria
Terminating at known equilibrium

Phase region boundary 8 at: 3.334E-01 3.082E-01
** LIQUID
  FCC_A1
Calculated           39 equilibria

Phase region boundary 9 at: 6.543E-01 3.046E-01
** LIQUID
  FCC_A1
Calculated           35 equilibria
Terminating at known equilibrium

Phase region boundary 10 at: 6.543E-01 3.046E-01
** LIQUID
  FCC_A1
Calculated           23 equilibria

Phase region boundary 11 at: 1.678E-01 3.000E-01
  BCC_A2
** FCC_A1
Calculated           34 equilibria

Phase region boundary 12 at: 1.678E-01 3.000E-01
  BCC_A2
** FCC_A1
Calculated           4 equilibria
Terminating at known equilibrium

Phase region boundary 13 at: 3.086E-01 5.984E-01
** LIQUID
  BCC_A2
Calculated           21 equilibria
Terminating at known equilibrium

Phase region boundary 14 at: 3.086E-01 5.984E-01
** LIQUID
  BCC_A2
Calculated           25 equilibria

Phase region boundary 15 at: 1.097E-02 4.525E-02
  BCC_A2
** FCC_A1
Calculated           15 equilibria

Phase region boundary 16 at: 1.097E-02 4.525E-02
  BCC_A2
** FCC_A1
Calculated           31 equilibria
Terminating at known equilibrium

Phase region boundary 17 at: 3.342E-01 6.558E-01
  LIQUID
** BCC_A2
Calculated           26 equilibria
Terminating at known equilibrium

Phase region boundary 18 at: 3.342E-01 6.558E-01
  LIQUID
** BCC_A2
Calculated           13 equilibria

Phase region boundary 19 at: 6.736E-01 3.160E-01
  LIQUID
** FCC_A1
Calculated           37 equilibria
Terminating at known equilibrium

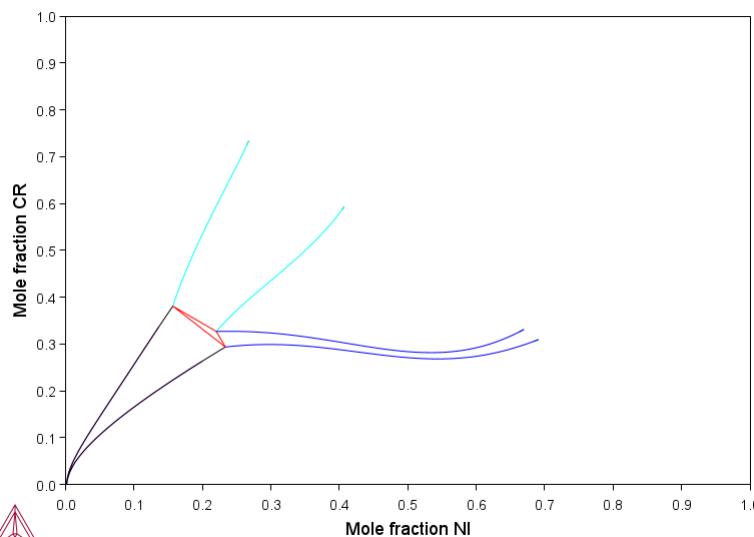
Phase region boundary 20 at: 6.736E-01 3.160E-01
  LIQUID
** FCC_A1
Calculated           18 equilibria
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\generate_console_examples\examples\tcex37\tcex37.POLY3
CPU time for mapping          6 seconds
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: @@ Use default axis on the diagram
POST:
POST: set-title example 37a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot

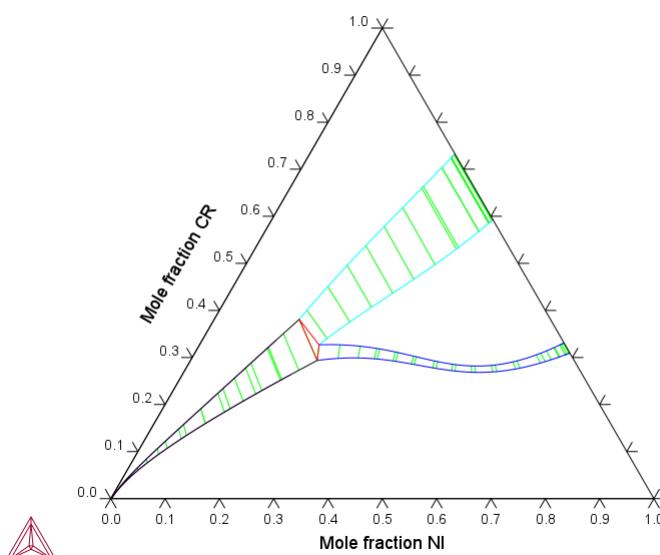
```

example 37a



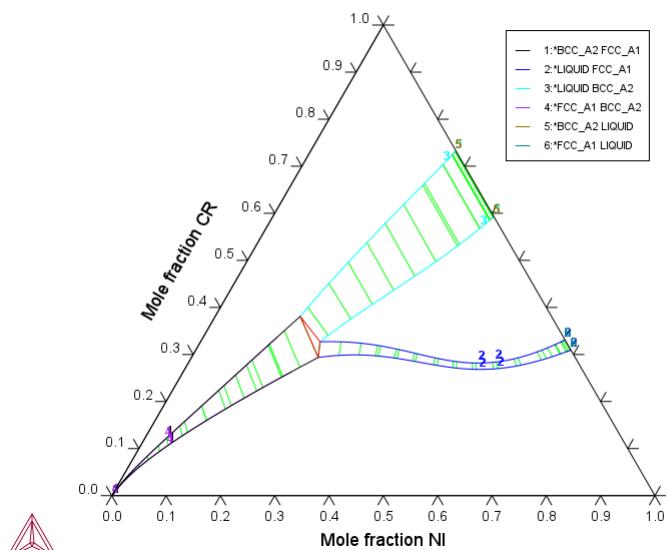
```
POST:  
POST:  
POST:Hit RETURN to continue  
POST: @@ By default a diagram is always square. set it triangular,  
POST: @@ add tie-lines and set scaling on the axis  
POST: s-d-t  
TRIANGULAR DIAGRAM (Y OR N) /N/: y  
POST: s-t-s  
PLOTTING EVERY TIE-LINE NO /0/: 3  
POST: s-sc  
AXIS (X, Y OR Z) : x  
AUTOMATIC SCALING (Y OR N) /N/: n  
MIN VALUE : 0  
MAX VALUE : 1  
POST: s-s y n 0 1  
POST: set-title example 37b  
POST:  
POST:  
POST: SET_EXP_FILE_FORMAT 5  
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y  
POST: SET_EXP_FILE_FORMAT 10  
POST:  
POST: plot
```

example 37b



```
POST:  
POST:  
POST:Hit RETURN to continue  
POST: @@ To identify the phases also set labels  
POST: @@ To add text in phase regions use a dataplot file  
POST: set-lab b  
POST: set-title example 37c  
POST:  
POST:  
POST: SET_EXP_FILE_FORMAT 5  
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y  
POST: SET_EXP_FILE_FORMAT 10  
POST:  
POST: plot
```

example 37c



POST:
POST: set-inter
POST:

tce38

SYS:About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce38\tce38.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Calculating the Morral *rose*
SYS:
SYS: @@ This example uses the Gibbs energy system
SYS: @@ (GES) module to calculate the Morral rose,
SYS: @@ which are miscibility gaps.
SYS:
SYS: set-log ex38,,,
SYS: go g
... the command in full is GOTO_MODULE
GIBBS ENERGY SYSTEM
16:37:16,079 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
GES6: reinitiate,,,
GES6:
GES6: @@ Enter a phase with just a ternary interaction parameter
GES6: e-e a b c
... the command in full is ENTER_ELEMENT
THERMODYNAMIC DATABASE module
Database folder: C:\jenkins\workspace\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0
VA /- DEFINED
DICTRA_FCC_A1 REJECTED
GES6: a-e-d a fcc_a1 10,,,
... the command in full is AMEND_ELEMENT_DATA
GES6: a-e-d b fcc_a1 10,,,
... the command in full is AMEND_ELEMENT_DATA
GES6: a-e-d c fcc_a1 10,,,
... the command in full is AMEND_ELEMENT_DATA
GES6:
GES6:
GES6: e-ph fcc_a1,,1 A B C;,,,
... the command in full is ENTER_PHASE
GES6:
GES6:
GES6: e-par l(fcc_a1,a,b,c),,50000;,,,
... the command in full is ENTER_PARAMETER
L(FCC_A1,A,B,C;0)
GES6: l-d
... the command in full is LIST_DATA
OUTPUT TO SCREEN OR FILE /SCREEN/: SCREEN
OPTIONS?:
Property type /ALL/: ALL
Element Stable Element Reference Mass H298-H0 S298
VA UNKNOWN 0.0000E+00 0.0000E+00 0.0000E+00
A FCC_A1 1.0000E+01 0.0000E+00 0.0000E+00
B FCC_A1 1.0000E+01 1.2220E+03 5.9000E+00
C FCC_A1 1.0000E+01 1.0540E+03 5.7400E+00
FCC_A1 (A,B,C)1.0

==== [A, B, C] ====
L(FCC_A1,A,B,C;0) 298.15 +50000; 6000 N
GES6:
GES6:
GES6: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY:

POLY: s-c t=600 p=1e5 n=1 x(b)=.3 x(c)=.1
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
16:37:17,801 [Thread-0] INFO Database: Preparing system for use: UNKNOWN_1682613436112
16:37:18,588 [Thread-0] INFO Phase: Preparing phase for use: FCC_A1
Calculated 1965 grid points in 4 s
Found the set of lowest grid points in 0 s
Creating a new composition set FCC_A1#2
Calculated POLY solution 0 s, total time 4 s
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
Output from POLY-3, equilibrium = 1, label A0 , database: User dat

Conditions:
T=600, P=100000, N=1, X(B)=0.3, X(C)=0.1
DEGREES OF FREEDOM 0

Temperature 600.00 K (326.85 C), Pressure 1.000000E+05
Number of moles of components 1.000000E+00, Mass in grams 1.000000E+01
Total Gibbs energy -3.58989E+03, Enthalpy 6.74567E+02, Volume 0.000000E+00

Component Moles W-Fraction Activity Potential Ref.stat
A 6.0000E-01 6.0000E-01 5.7356E-01 -2.7732E+03 SER
B 3.0000E-01 3.0000E-01 3.8092E-01 -4.8149E+03 SER
C 1.0000E-01 1.0000E-01 3.8092E-01 -4.8149E+03 SER

FCC_A1#1 Status ENTERED Driving force 0.0000E+00
Moles 8.7781E-01, Mass 8.7781E+00, Volume fraction 0.0000E+00 Mass fractions:

```

A 6.00000E-01 B 3.32342E-01 C 6.76579E-02

FCC_A1#2 Status ENTERED Driving force 0.0000E+00
Moles 1.2219E-01, Mass 1.2219E+00, Volume fraction 0.0000E+00 Mass fractions:
A 6.00000E-01 C 3.32342E-01 B 6.76579E-02
POLY:Hit RETURN to continue
POLY:
POLY: s-a-v 1 x(b) 0 1 0.01
... the command in full is SET_AXIS_VARIABLE
POLY: s-a-v 2 x(c) 0 1 0.01
... the command in full is SET_AXIS_VARIABLE
POLY:
POLY: save tce38 y
... the command in full is SAVE_WORKSPACES
POLY:
POLY: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9

Organizing start points

Using ADDED start equilibria

Trying global minimization! 3
Generating start point 1
Generating start point 2
Trying global minimization! 3
Generating start point 3
Generating start point 4
Trying global minimization! 3
Generating start point 5
Generating start point 6
Trying global minimization! 3
Generating start point 7
Generating start point 8
Trying global minimization! 3
Generating start point 9
Generating start point 10
Working hard
Trying global minimization! 3
Generating start point 11
Generating start point 12

Phase region boundary 1 at: 2.333E-01 2.333E-01
  FCC_A1#1
  ** FCC_A1#2
Calculated                      31 equilibria

Phase region boundary 2 at: 2.333E-01 2.333E-01
  FCC_A1#1
  ** FCC_A1#2
Creating a new composition set FCC_A1#3
Calculated                      10 equilibria

Phase region boundary 3 at: 2.333E-01 2.333E-01
  FCC_A1#1
  ** FCC_A1#2
Calculated                      5 equilibria

Phase region boundary 4 at: 2.699E-01 2.699E-01
  FCC_A1#1
  ** FCC_A1#2
  ** FCC_A1#3
Calculated                      41 equilibria

Phase region boundary 5 at: 4.603E-01 2.699E-01
  FCC_A1#1
  ** FCC_A1#3
Calculated                      47 equilibria

Phase region boundary 6 at: 2.699E-01 4.603E-01
  FCC_A1#2
  ** FCC_A1#3
Calculated                      47 equilibria

Phase region boundary 7 at: 2.699E-01 2.699E-01
  FCC_A1#1
  ** FCC_A1#2
Calculated                      34 equilibria

Phase region boundary 8 at: 6.633E-01 1.683E-01
  FCC_A1#1
  ** FCC_A1#2
Calculated                      26 equilibria

Phase region boundary 9 at: 6.633E-01 1.683E-01
  FCC_A1#1
  ** FCC_A1#2
Calculated                      33 equilibria

Phase region boundary 10 at: 6.633E-01 1.683E-01
  FCC_A1#1
  ** FCC_A1#2
Calculated                      22 equilibria
Terminating at known equilibrium

Phase region boundary 11 at: 2.333E-01 2.333E-01
  FCC_A1#1
  ** FCC_A1#2
Calculated                      34 equilibria

Phase region boundary 12 at: 2.333E-01 2.333E-01
  FCC_A1#1
  ** FCC_A1#2
Calculated                      10 equilibria

Phase region boundary 13 at: 2.333E-01 2.333E-01
  FCC_A1#1

```

```

** FCC_A1#2
Calculated.          5 equilibria
Terminating at known equilibrium

Phase region boundary 14 at: 1.683E-01 6.633E-01
  FCC_A1#1
** FCC_A1#2
Calculated.          32 equilibria

Phase region boundary 15 at: 1.683E-01 6.633E-01
  FCC_A1#1
** FCC_A1#2
Calculated.          22 equilibria
Terminating at known equilibrium

Phase region boundary 16 at: 1.683E-01 6.633E-01
  FCC_A1#1
** FCC_A1#2
Calculated.          30 equilibria

Phase region boundary 17 at: 2.333E-01 5.333E-01
  FCC_A1#1
** FCC_A1#2
Calculated.          19 equilibria
Terminating at known equilibrium

Phase region boundary 18 at: 2.333E-01 5.333E-01
  FCC_A1#1
** FCC_A1#2
Calculated.          43 equilibria

Phase region boundary 19 at: 2.333E-01 5.333E-01
  FCC_A1#1
** FCC_A1#2
Calculated.          43 equilibria

Phase region boundary 20 at: 6.633E-01 1.683E-01
  FCC_A1#1
** FCC_A1#2
Calculated.          26 equilibria

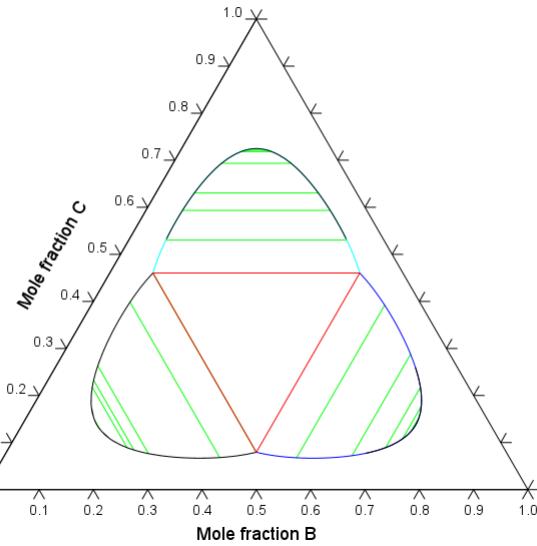
Phase region boundary 21 at: 6.633E-01 1.683E-01
  FCC_A1#1
** FCC_A1#2
Calculated.          33 equilibria
Terminating at known equilibrium
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\generate_console_examples\examples\tcex38\tcex38.POLY3
CPU time for mapping      3 seconds
POLY:
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST:
POST: s-d-a x m-f b
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y m-f c
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-t y ....
... the command in full is SET_DIAGRAM_TYPE
POST: s-s x n 0 1
... the command in full is SET_SCALING_STATUS
POST: s-s y n 0 1
... the command in full is SET_SCALING_STATUS
POST: s-t-s 10
... the command in full is SET_TIELINE_STATUS
POST: set-title example 38a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
The composition set FCC_A1#3 created from the store file
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 38a



```

POST:
POST:Hit RETURN to continue
POST:
POST: back
POLY: read,
... the command in full is READ_WORKSPACES
POLY:
POLY: @@ We will calculate at a higher temperature
POLY: @@ with a stable phase in the middle.
POLY: s-c t=696
... the command in full is SET_CONDITION
POLY: s-c x(b)=.44 x(c)=.28
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated          1965 grid points in      0 s
Found the set of lowest grid points in      0 s
Creating a new composition set FCC_A1#3
Calculated POLY solution      0 s, total time      0 s
POLY:
POLY: save tce38b y
... the command in full is SAVE_WORKSPACES
POLY:
POLY:
POLY: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9

Organizing start points

Using ADDED start equilibria

Working hard
Trying global minimization! 3
Generating start point 1
Generating start point 2
Trying global minimization! 3
Generating start point 3
Generating start point 4
Trying global minimization! 3
Generating start point 5
Generating start point 6

Phase region boundary 1 at: 2.683E-01 2.683E-01
  FCC_A1#1
  ** FCC_A1#2
Calculated           37 equilibria

Phase region boundary 2 at: 2.683E-01 2.683E-01
  FCC_A1#1
  ** FCC_A1#2
Calculated           6 equilibria

Phase region boundary 3 at: 2.683E-01 2.683E-01
  FCC_A1#1
  ** FCC_A1#2
Calculated           6 equilibria

Phase region boundary 4 at: 2.683E-01 2.683E-01
  FCC_A1#1
  ** FCC_A1#2
Calculated           6 equilibria

Phase region boundary 5 at: 2.683E-01 2.683E-01
  FCC_A1#1
  ** FCC_A1#2
Calculated           6 equilibria

Phase region boundary 6 at: 2.683E-01 2.683E-01
  FCC_A1#1
  ** FCC_A1#2
Calculated           6 equilibria

Phase region boundary 7 at: 2.683E-01 2.683E-01
  FCC_A1#1
  ** FCC_A1#2
Calculated           6 equilibria

Phase region boundary 8 at: 2.998E-01 2.998E-01
  FCC_A1#1
  ** FCC_A1#2
  ** FCC_A1#3

Phase region boundary 9 at: 3.618E-01 2.650E-01
  FCC_A1#1
  ** FCC_A1#3
Calculated           7 equilibria

Phase region boundary 10 at: 3.618E-01 2.650E-01
  FCC_A1#1
  ** FCC_A1#3
Calculated           5 equilibria

Phase region boundary 11 at: 3.732E-01 2.650E-01
  FCC_A1#1
  ** FCC_A1#2
  ** FCC_A1#3

Phase region boundary 12 at: 4.004E-01 2.998E-01
  FCC_A1#1
  ** FCC_A1#2
Calculated           43 equilibria

Phase region boundary 13 at: 3.732E-01 3.618E-01
  ** FCC_A1#2
  FCC_A1#3

```

```

Calculated           4 equilibria
Phase region boundary 14 at: 3.732E-01 3.618E-01
** FCC_A1#2
** FCC_A1#3
Calculated.          3 equilibria
Phase region boundary 15 at: 3.618E-01 3.732E-01
** FCC_A1#1
** FCC_A1#2
FCC_A1#3
Calculated           9 equilibria
Phase region boundary 16 at: 2.650E-01 3.732E-01
** FCC_A1#1
FCC_A1#3
Calculated           7 equilibria
Terminating at known equilibrium
Phase region boundary 17 at: 2.650E-01 3.732E-01
** FCC_A1#1
FCC_A1#3
Calculated           7 equilibria
Phase region boundary 18 at: 2.998E-01 4.004E-01
** FCC_A1#1
** FCC_A1#2
Calculated           68 equilibria
Phase region boundary 19 at: 2.998E-01 2.998E-01
FCC_A1#1
** FCC_A1#2
Calculated           28 equilibria
Phase region boundary 20 at: 2.683E-01 2.683E-01
FCC_A1#1
** FCC_A1#2
Calculated           35 equilibria
Phase region boundary 21 at: 2.683E-01 2.683E-01
FCC_A1#1
** FCC_A1#2
Calculated           6 equilibria
Phase region boundary 22 at: 2.683E-01 2.683E-01
FCC_A1#1
** FCC_A1#2
Calculated           6 equilibria
Phase region boundary 23 at: 2.683E-01 2.683E-01
FCC_A1#1
** FCC_A1#2
Calculated           6 equilibria
Phase region boundary 24 at: 2.683E-01 2.683E-01
FCC_A1#1
** FCC_A1#2
Calculated           6 equilibria
Phase region boundary 25 at: 2.683E-01 2.683E-01
FCC_A1#1
** FCC_A1#2
Calculated           6 equilibria
Phase region boundary 26 at: 2.683E-01 2.683E-01
FCC_A1#1
** FCC_A1#2
Calculated           6 equilibria
Terminating at known equilibrium
Phase region boundary 27 at: 2.683E-01 4.633E-01
FCC_A1#1
** FCC_A1#2
Calculated           9 equilibria
Phase region boundary 28 at: 2.683E-01 4.633E-01
FCC_A1#1
** FCC_A1#2
Calculated           9 equilibria
Phase region boundary 29 at: 2.683E-01 4.633E-01
FCC_A1#1
** FCC_A1#2
Calculated           9 equilibria
Phase region boundary 30 at: 2.683E-01 4.633E-01
FCC_A1#1
** FCC_A1#2
Calculated           9 equilibria
Phase region boundary 31 at: 2.683E-01 4.633E-01
FCC_A1#1
** FCC_A1#2
Calculated           9 equilibria
Phase region boundary 32 at: 2.683E-01 4.633E-01
FCC_A1#1
** FCC_A1#2
Calculated           9 equilibria
Terminating at known equilibrium
Phase region boundary 33 at: 2.683E-01 4.633E-01
FCC_A1#1
** FCC_A1#2
Calculated           40 equilibria
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\generate_console_examples\examples\tcex38\tcex38b.POLY3
CPU time for mapping      2 seconds
POLY:
POLY:
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2
Setting automatic diagram axes
POST:
POST:
POST: set-title example 38b

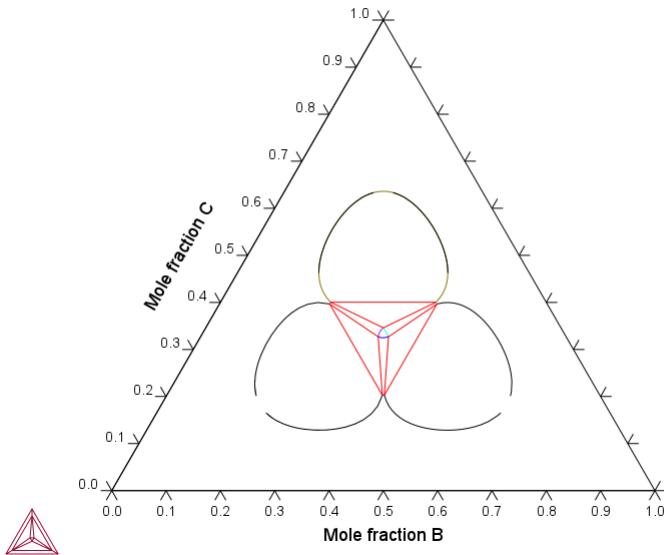
```

```

POST: s-d-t y,,,
... the command in full is SET_DIAGRAM_TYPE
POST: s-s x n 0 1
... the command in full is SET_SCALING_STATUS
POST: s-s y n 0 1
... the command in full is SET_SCALING_STATUS
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 38b



```

POST:
POST:Hit RETURN to continue
POST:
POST: back
POLY: @@ =====
POLY: @@ Now a quaternary.
POLY: @@
POLY: @@ Square rose by John Morral
POLY: @@
POLY: go g
... the command in full is GOTO_MODULE
GIBBS ENERGY SYSTEM
GES6: reinitiate,,,
GES6: e-e a b c d
... the command in full is ENTER_ELEMENT
GES6: a-e-d a liquid 10,,,
... the command in full is AMEND_ELEMENT_DATA
GES6: a-e-d b liquid 10,,,
... the command in full is AMEND_ELEMENT_DATA
GES6: a-e-d c liquid 10,,,
... the command in full is AMEND_ELEMENT_DATA
GES6: a-e-d d liquid 10,,,
... the command in full is AMEND_ELEMENT_DATA
GES6: e-ph liquid
... the command in full is ENTER_PHASE
TYPE CODE:
NUMBER OF SUBLATTICES /1/: 1
NAME OF CONSTITUENT: A B C D
NAME OF CONSTITUENT:
WILL YOU ADD CONSTITUENTS LATER /NO/: NO
DO YOU WANT A LIST OF POSSIBLE PARAMETERS /NO/: NO
GES6: e-par g(liquid,a,b,c,d)
... the command in full is ENTER_PARAMETER
G(LIQUID,A,B,C,D;0)
LOW TEMPERATURE LIMIT /298.15/: 298.15
FUNCTION: 100000
&
HIGH TEMPERATURE LIMIT /6000/: 6000
ANY MORE RANGES /N/: N
GES6:
GES6: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY: reinitiate,,,
... the command in full is REINITIATE_MODULE
POLY: s-c t=170 p=1e5 n=1 x(d)=.25 x(a)=.3 x(a)+x(c)=.5
... the command in full is SET_CONDITION
POLY: l-c
... the command in full is LIST_CONDITIONS
T=170, P=100000, N=1, X(D)=0.25, X(A)=0.3, X(A)+X(C)=0.5
DEGREES OF FREEDOM 0
POLY:
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
16:37:23,263 [Thread-0] INFO Database: Preparing system for use: UNKNOWN_1682613443146
16:37:23,639 [Thread-0] INFO Phase: Preparing phase for use: LIQUID
Testing POLY result by global minimization procedure
Calculated 1787 grid points in 0 s
Creating a new composition set LIQUID#2
32 ITS, CPU TIME USED 2 SECONDS
POLY: l-e
... the command in full is LIST_EQUIlibRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:

```

```

Options /VWCS/: VXCS
Output from POLY-3, equilibrium =      1, label A0 , database: User dat

Conditions:
T=170, P=100000, N=1, X(D)=0.25, X(A)=0.3, X(A)+X(C)=0.5
DEGREES OF FREEDOM 0

Temperature    170.00 K ( -103.15 C), Pressure 1.00000E+05
Number of moles of components 1.00000E+00, Mass in grams 1.00000E+01
Total Gibbs energy -1.58399E+03, Enthalpy 2.18612E+02, Volume 0.00000E+00

Component      Moles      M-Fraction Activity Potential Ref.stat
A            3.0000E-01  3.0000E-01 3.1587E-01 -1.6289E+03 SER
B            2.5000E-01  2.5000E-01 2.9182E-01 -1.7409E+03 SER
C            2.0000E-01  2.0000E-01 3.5423E-01 -1.4669E+03 SER
D            2.5000E-01  2.5000E-01 3.5423E-01 -1.4669E+03 SER

LIQUID#1          Status ENTERED     Driving force 0.0000E+00
Moles 5.8530E-01, Mass 5.8530E+00, Volume fraction 0.0000E+00 Mole fractions:
D 3.71549E-01 A 3.00000E-01 B 2.50000E-01 C 7.84507E-02

LIQUID#2          Status ENTERED     Driving force 0.0000E+00
Moles 4.1470E-01, Mass 4.1470E+00, Volume fraction 0.0000E+00 Mole fractions:
C 3.71549E-01 A 3.00000E-01 B 2.50000E-01 D 7.84507E-02

POLY: s-a-v 1 x(a)
... the command in full is SET_AXIS_VARIABLE
Min value /0/: 0
Max value /1/: .5
Increment /.0125/: .01
POLY: s-a-v 2 x(d)
... the command in full is SET_AXIS_VARIABLE
Min value /0/: 0
Max value /1/: .5
Increment /.0125/: .01
POLY:
POLY: add +1
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY:
POLY: save tcex38c y
... the command in full is SAVE_WORKSPACES
POLY: map
Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Tie-lines not in the plane of calculation
Generating start point 1
Generating start point 2

Phase region boundary 1 at: 4.478E-01 2.500E-01
LIQUID#1
** LIQUID#2
Creating a new composition set LIQUID#3
Calculated.           45 equilibria

Phase region boundary 2 at: 4.478E-01 2.500E-01
LIQUID#1
** LIQUID#2
Calculated.           41 equilibria

Phase region boundary 3 at: 2.500E-01 5.217E-02
LIQUID#1
** LIQUID#2
** LIQUID#3
Creating a new composition set LIQUID#4
Calculated.           31 equilibria

Phase region boundary 4 at: 2.500E-01 5.217E-02
LIQUID#1
** LIQUID#2
** LIQUID#3
Calculated.           15 equilibria

Phase region boundary 5 at: 1.816E-01 1.816E-01
LIQUID#1
** LIQUID#2
LIQUID#3
** LIQUID#4
Calculated.           15 equilibria
Terminating at known equilibrium

Phase region boundary 6 at: 3.184E-01 1.816E-01
LIQUID#1
LIQUID#2
** LIQUID#3
Calculated.           15 equilibria
Terminating at known equilibrium

Phase region boundary 7 at: 3.184E-01 1.816E-01
LIQUID#1
LIQUID#2
** LIQUID#4
Calculated.           14 equilibria

Phase region boundary 8 at: 4.478E-01 2.500E-01
** LIQUID#1
LIQUID#2
** LIQUID#4
Calculated.           14 equilibria

Phase region boundary 9 at: 4.478E-01 2.500E-01
** LIQUID#1
LIQUID#2
** LIQUID#4
Calculated.           43 equilibria

Phase region boundary 10 at: 4.478E-01 2.500E-01
LIQUID#2
** LIQUID#4
Calculated.           43 equilibria

Phase region boundary 11 at: 2.500E-01 4.478E-01
LIQUID#2
** LIQUID#3
** LIQUID#4

Phase region boundary 12 at: 2.500E-01 4.478E-01

```

```

LIQUID#2
LIQUID#3
** LIQUID#4
Calculated                      20 equilibria

Phase region boundary 13 at: 2.500E-01 4.478E-01
LIQUID#2
LIQUID#3
** LIQUID#4
Calculated.                     15 equilibria
Terminating at known equilibrium

Phase region boundary 14 at: 2.500E-01 4.478E-01
LIQUID#2
** LIQUID#3
Calculated.                     41 equilibria

Phase region boundary 15 at: 5.217E-02 2.500E-01
LIQUID#2
** LIQUID#3
** LIQUID#4
Calculated.                     20 equilibria

Phase region boundary 16 at: 5.217E-02 2.500E-01
LIQUID#2
** LIQUID#3
LIQUID#4
Calculated.                     15 equilibria
Terminating at known equilibrium

Phase region boundary 17 at: 5.217E-02 2.500E-01
LIQUID#2
** LIQUID#3
LIQUID#4
Calculated.                     41 equilibria
Terminating at known equilibrium

Phase region boundary 18 at: 5.217E-02 2.500E-01
LIQUID#2
** LIQUID#4
Calculated.                     15 equilibria
Terminating at known equilibrium

Phase region boundary 19 at: 5.217E-02 2.500E-01
LIQUID#2
LIQUID#3
** LIQUID#4
Calculated.                     15 equilibria
Terminating at known equilibrium

Phase region boundary 20 at: 2.500E-01 4.478E-01
LIQUID#2
** LIQUID#3
LIQUID#4
Calculated.                     20 equilibria

Phase region boundary 21 at: 2.500E-01 4.478E-01
LIQUID#2
** LIQUID#3
LIQUID#4
Calculated.                     15 equilibria
Terminating at known equilibrium

Phase region boundary 22 at: 4.478E-01 2.500E-01
** LIQUID#1
LIQUID#2
Calculated.                     43 equilibria
Terminating at known equilibrium

Phase region boundary 23 at: 4.478E-01 2.500E-01
** LIQUID#1
LIQUID#2
LIQUID#4
Calculated.                     15 equilibria
Terminating at known equilibrium

Phase region boundary 24 at: 4.478E-01 2.500E-01
LIQUID#1
** LIQUID#2
Calculated.                     6 equilibria

Phase region boundary 25 at: 4.478E-01 2.500E-01
LIQUID#1
** LIQUID#2
Calculated.                     2 equilibria

Phase region boundary 26 at: 4.478E-01 2.500E-01
LIQUID#1
** LIQUID#2
Calculated.                     2 equilibria

Phase region boundary 27 at: 4.478E-01 2.500E-01
LIQUID#1
** LIQUID#2
Calculated.                     2 equilibria

Phase region boundary 28 at: 4.478E-01 2.500E-01
LIQUID#1
** LIQUID#2
Calculated.                     2 equilibria

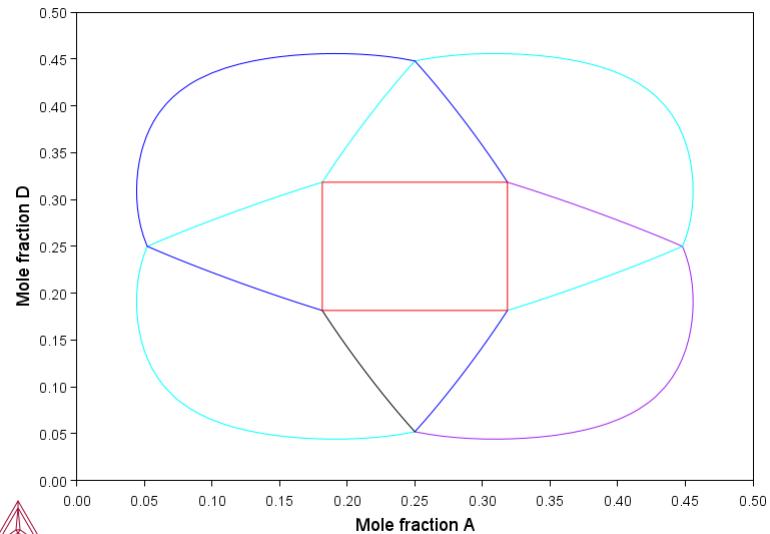
Phase region boundary 29 at: 4.478E-01 2.500E-01
LIQUID#1
** LIQUID#2
Calculated.                     2 equilibria
Calculated.                     2 equilibria
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\generate_console_examples\examples\tcex38\tcex38c.POLY3
CPU time for mapping           2 seconds
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2
Setting automatic diagram axes

POST:
POST:
POST: set-title example 38c
POST:
POST:

```

```
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
The composition set LIQUID#3 created from the store file
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
```

example 38c



```
POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:
```

tce39

SYS:About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce39\tce39.TCM.test"

SYS: set-echo

SYS:
SYS: @@ Calculating reversible Carnot cycles of a heat engine
SYS:
SYS: @@ This example shows how to calculate the reversible
SYS: @@ Carnot cycle of a heat engine using one mole of an ideal
SYS: @@ gas with two fictitious species A and A2. The GES, POLY3
SYS: @@ and POST modules are used.

SYS:
SYS: @@ One application of the Second Law is to the efficiencies
SYS: @@ of heat engines, pumps and refrigerators. Whenever there
SYS: @@ is a difference of temperature, work can be produced -
SYS: @@ the principle of heat engines. The Gibbs energy also
SYS: @@ enables the prediction of the maximum work that a process
SYS: @@ may achieve. The goal of this example is to help relate
SYS: @@ the results to different thermodynamic quantities.

SYS:
SYS: set-log ex39,,,

SYS:
SYS: go g

... the command in full is GOTO_MODULE
GIBBS ENERGY SYSTEM
16:38:41,324 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
GES6: rei,,,,

... the command in full is REINITIATE

GES6: e-e a
... the command in full is ENTER_ELEMENT
THERMODYNAMIC DATABASE module
Database folder: C:\jenkins\workspace\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED
DICTRA_FCC_A1 REJECTED
GES6: a-e-d a gas 10,,,
... the command in full is AMEND_ELEMENT_DATA
GES6: e-sp A2 A2
... the command in full is ENTER_SPECIES
GES6: e-ph gas g 1 A A2; N N
... the command in full is ENTER_PHASE
GES6: @@ The Gibbs free energy for these species could be described
GES6: @@ by the general formula: $G_m = a + bT + cT \ln T + dT^2 + \dots + RT \ln(P)$
GES6:
GES6: @@ To calculate the Carnot cycle you have to give some numerical
GES6: @@ values to the a, b, c, etc. constants of the G_m expression.
GES6: @@ It is important to understand that the coefficients cannot
GES6: @@ be chosen arbitrarily, for example c should be negative as
GES6: @@ the heat capacity at constant pressure, $C_p = - T \frac{d^2G}{dT^2}$
GES6: @@ and thus $C_p = - c - 2dT$, must always be > 0
GES6:
GES6: e-par g(gas,a) 298.15 6960-51*T-17*T*LN(T)+R*T*LN(1e-05*P),,,,
... the command in full is ENTER_PARAMETER
G(GAS,A;0)-G(GAS,A;0)
GES6: e-par g(gas,a2) 298.15 130670-38*T-17*T*LN(T)+R*T*LN(1e-05*P),,,,
... the command in full is ENTER_PARAMETER
G(GAS,A2;0)-2 G(GAS,A;0)

GES6: l-d,,,
... the command in full is LIST_DATA
Property type /ALL/:Hit RETURN to continue
Property type /ALL:
Element Stable Element Reference Mass H298-H0 S298
VA UNKNOWN 0.0000E+00 0.0000E+00 0.0000E+00
A GAS 1.0000E+01 0.0000E+00 0.0000E+00

Species Stoichiometry
A2 A2

GAS:G (A,A2)1.0

==== [A] ====
G(GAS,A2;0) 298.15 +130670-38*T-17*T*LN(T) 6000 N
+R*T*LN(1.0E-5*P);
G(GAS,A;0) 298.15 +6960-51*T-17*T*LN(T) 6000 N
+R*T*LN(1.0E-5*P);
GES6: @@ The Carnot cycle diagram gives the pressure and volume for
GES6: @@ the working media of a heat engine that operates between
GES6: @@ two temperatures T1 and T2, T1>T2.
GES6:
GES6: go p-3

... the command in full is GOTO_MODULE

POLY version 3.32
POLY: @@ The Carnot cycle is calculated for T1=500 K (the

POLY: @@ temperature of the hot reservoir) and T2=400 K
POLY: @@ (the temperature of the cold reservoir)
POLY: ent var t1=500;
... the command in full is ENTER_SYMBOL
POLY: ent var t2=400;
... the command in full is ENTER_SYMBOL
POLY:
POLY: @@ A Carnot cycle consists of four reversible stages:
POLY:
POLY: @@ Stage 1. Isothermal expansion at T1; the entropy change

```

POLY: @@ of the system is Q1/T1, where Q1 is the heat taken from
POLY: @@ the hot reservoir.
POLY:
POLY: s-c t=t1 p=1e7 n=1
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
16:38:43,000 [Thread-0] INFO Database: Preparing system for use: UNKNOWN_1682613521357
16:38:43,842 [Thread-0] INFO Phase: Preparing phase for use: GAS
Using global minimization procedure
Calculated 209 grid points in 1 s
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: xn
Output from POLY-3, equilibrium = 1, label A0 , database: User dat

Conditions:
T=T1, P=10000000, N=1
DEGREES OF FREEDOM 0

Temperature 500.00 K ( 226.85 C), Pressure 1.000000E+07
Number of moles of components 1.000000E+00, Mass in grams 1.000000E+01
Total Gibbs energy -5.22193E+04, Enthalpy 1.54600E+04, Volume 4.15726E-04

Component Moles M-Fraction Activity Potential Ref.stat
A 1.000000E+00 1.000000E+00 3.5061E-06 -5.2219E+04 SER

GAS Status ENTERED Driving force 0.0000E+00
Moles 1.000000E+00, Mass 1.000000E+01, Volume fraction 1.000000E+00 Mole fractions:
A 1.000000E+00
Constitution:
A 1.000000E+00 A2 8.75433E-20
POLY:Hit RETURN to continue
POLY:
POLY: @@ Set volume to 1 m3
POLY: s-c v
... the command in full is SET_CONDITION
Value /4.157255E-04/: 1
POLY: s-c n
... the command in full is SET_CONDITION
Value /1/: none
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Using already calculated grid
6 ITS, CPU TIME USED 0 SECONDS
POLY: l-e,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: User dat

Conditions:
T=T1, P=10000000, V=1
DEGREES OF FREEDOM 0

Temperature 500.00 K ( 226.85 C), Pressure 1.000000E+07
Number of moles of components 2.40543E+03, Mass in grams 2.40543E+04
Total Gibbs energy -1.25610E+08, Enthalpy 3.71880E+07, Volume 1.000000E+00

Component Moles M-Fraction Activity Potential Ref.stat
A 2.4054E+03 1.000000E+00 3.5061E-06 -5.2219E+04 SER

GAS Status ENTERED Driving force 0.0000E+00
Moles 2.4054E+03, Mass 2.4054E+04, Volume fraction 1.000000E+00 Mole fractions:
A 1.000000E+00
Constitution:
A 1.000000E+00 A2 8.75433E-20
POLY: s-c n
... the command in full is SET_CONDITION
Value /2405.433393/: 
POLY: s-c p
... the command in full is SET_CONDITION
Value /10000000/: none
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Using already calculated grid
6 ITS, CPU TIME USED 0 SECONDS
POLY: l-e,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: User dat

Conditions:
T=T1, N=2405.433393, V=1
DEGREES OF FREEDOM 0

Temperature 500.00 K ( 226.85 C), Pressure 1.000000E+07
Number of moles of components 2.40543E+03, Mass in grams 2.40543E+04
Total Gibbs energy -1.25610E+08, Enthalpy 3.71880E+07, Volume 1.000000E+00

Component Moles M-Fraction Activity Potential Ref.stat
A 2.4054E+03 1.000000E+00 3.5061E-06 -5.2219E+04 SER

GAS Status ENTERED Driving force 0.0000E+00
Moles 2.4054E+03, Mass 2.4054E+04, Volume fraction 1.000000E+00 Mole fractions:
A 1.000000E+00
Constitution:
A 1.000000E+00 A2 8.75433E-20
POLY: enter var ha=h;
... the command in full is ENTER_SYMBOL
POLY: enter var sa=s;
... the command in full is ENTER_SYMBOL
POLY: s-c s
... the command in full is SET_CONDITION
Value /325596.1064/: sa
POLY: s-c v=none
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Using already calculated grid

```

```

    6 ITS, CPU TIME USED 0 SECONDS
POLY: l-e.,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: User dat

Conditions:
T=T1, N=2405.433393, S=SA
DEGREES OF FREEDOM 0

Temperature 500.00 K ( 226.85 C), Pressure 1.000000E+07
Number of moles of components 2.40543E+03, Mass in grams 2.40543E+04
Total Gibbs energy -1.25610E+08, Enthalpy 3.71880E+07, Volume 1.00000E+00

Component Moles M-Fraction Activity Potential Ref.stat
A 2.4054E+03 1.0000E+00 3.5061E-06 -5.2219E+04 SER

GAS Status ENTERED Driving force 0.0000E+00
Moles 2.4054E+03, Mass 2.4054E+04, Volume fraction 1.0000E+00 Mole fractions:
A 1.00000E+00
Constitution:
A 1.00000E+00 A2 8.75433E-20
POLY:Hit RETURN to continue
POLY:
POLY: show t,p,v,g,n,h,s
... the command in full is SHOW_VALUE
T=500
P=1E7
V=1.
G=-1.2561005E8
N=2405.4334
H=3.7188E7
S=325596.11
POLY:Hit RETURN to continue
POLY:
POLY: ent var ga=g;
... the command in full is ENTER_SYMBOL
POLY: ent var pa=p;
... the command in full is ENTER_SYMBOL
POLY: ent var va=v;
... the command in full is ENTER_SYMBOL
POLY: @@ @@
POLY: save tcex39a y
... the command in full is SAVE_WORKSPACES
POLY: s-c t=500
... the command in full is SET_CONDITION
POLY: s-c s=204200
... the command in full is SET_CONDITION
POLY: s-a-v 1 s 204000 205000,,,
... the command in full is SET_AXIS_VARIABLE
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated 209 grid points in 0 s
17 ITS, CPU TIME USED 0 SECONDS
POLY: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 204200.
...OK

Phase Region from 204200. for:
GAS
Global test at 2.04400E+05 .... OK
Global test at 2.04650E+05 .... OK
Global test at 2.04900E+05 .... OK
Terminating at 205000.
Calculated 35 equilibria

Phase Region from 204200. for:
GAS
Global test at 2.04000E+05 .... OK
Terminating at 204000.
Calculated 11 equilibria
*** Buffer saved on file: c:\jenkins\workspace\generate_console_examples\examples\tcex39\tcex39a.POLY3
POLY:
POLY: @@ Stage 2. Adiabatic expansion. No heat leaves the system,
POLY: @@ so the change in its entropy is zero. In the course of
POLY: @@ this expansion the temperature falls from T1 to T2, the
POLY: @@ temperature of cold reservoir.
POLY:
POLY: s-c s=205000
... the command in full is SET_CONDITION
POLY: s-c t=450
... the command in full is SET_CONDITION
POLY: s-a-v 1 t 400 500,,,
... the command in full is SET_AXIS_VARIABLE
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated 209 grid points in 0 s
12 ITS, CPU TIME USED 0 SECONDS
POLY: step norm
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 450.000
...OK

Phase Region from 450.000 for:
GAS
Global test at 4.70000E+02 .... OK
Global test at 4.95000E+02 .... OK
Terminating at 500.000
Calculated 23 equilibria

Phase Region from 450.000 for:
GAS
Global test at 4.30000E+02 .... OK
Global test at 4.05000E+02 .... OK
Terminating at 400.000
Calculated 23 equilibria
*** Buffer saved on file: c:\jenkins\workspace\generate_console_examples\examples\tcex39\tcex39a.POLY3

```

```

POLY:
POLY: @@ Stage 3. Isothermal compression at T2. The heat Q2 is
POLY: @@ released to the cold reservoir, so the change in
POLY: @@ entropy of the system is -Q2/T2.
POLY:
POLY: s-c t=400
    ... the command in full is SET_CONDITION
POLY: s-c s=204200
    ... the command in full is SET_CONDITION
POLY: s-a-v 1 s 204000 205000,,
    ... the command in full is SET_AXIS_VARIABLE
POLY: c-e
    ... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated      209 grid points in          0 s
    8 ITS, CPU TIME USED   0 SECONDS
POLY: step norm
    ... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value     204200.
...OK

Phase Region from     204200.      for:
    GAS
Global test at  2.04400E+05 .... OK
Global test at  2.04650E+05 .... OK
Global test at  2.04900E+05 .... OK
Terminating at    205000.
Calculated      35 equilibria

Phase Region from     204200.      for:
    GAS
Global test at  2.04000E+05 .... OK
Terminating at    204000.
Calculated      11 equilibria
*** Buffer saved on file: c:\jenkins\workspace\generate_console_examples\examples\tcex39\tcex39a.POLY3
POLY:
POLY: @@ Stage 4. Adiabatic compression. No heat enters the system,
POLY: @@ so the change in entropy is zero. The temperature rises
POLY: @@ from T2 to T1.
POLY:
POLY: s-c s=204000
    ... the command in full is SET_CONDITION
POLY: s-c t=450
    ... the command in full is SET_CONDITION
POLY: s-a-v 1 t 400 500,,
    ... the command in full is SET_AXIS_VARIABLE
POLY: c-e
    ... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated      209 grid points in          0 s
    10 ITS, CPU TIME USED   0 SECONDS
POLY: step norm
    ... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value     450.000
...OK

Phase Region from     450.000      for:
    GAS
Global test at  4.70000E+02 .... OK
Global test at  4.95000E+02 .... OK
Terminating at    500.000
Calculated      23 equilibria

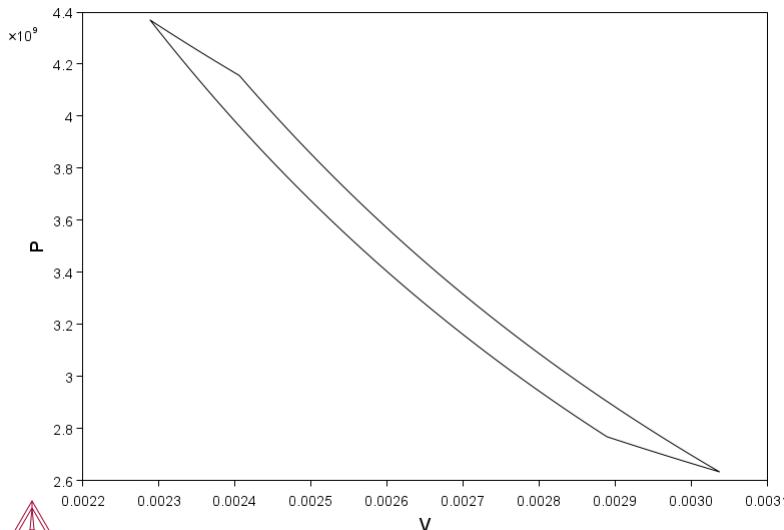
Phase Region from     450.000      for:
    GAS
Global test at  4.30000E+02 .... OK
Global test at  4.05000E+02 .... OK
Terminating at    400.000
Calculated      23 equilibria
*** Buffer saved on file: c:\jenkins\workspace\generate_console_examples\examples\tcex39\tcex39a.POLY3
POLY:
POLY: post
    POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST:
POST: s-d-a x v
    ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y p
    ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 39a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
    ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
    ... the command in full is PLOT_DIAGRAM

```

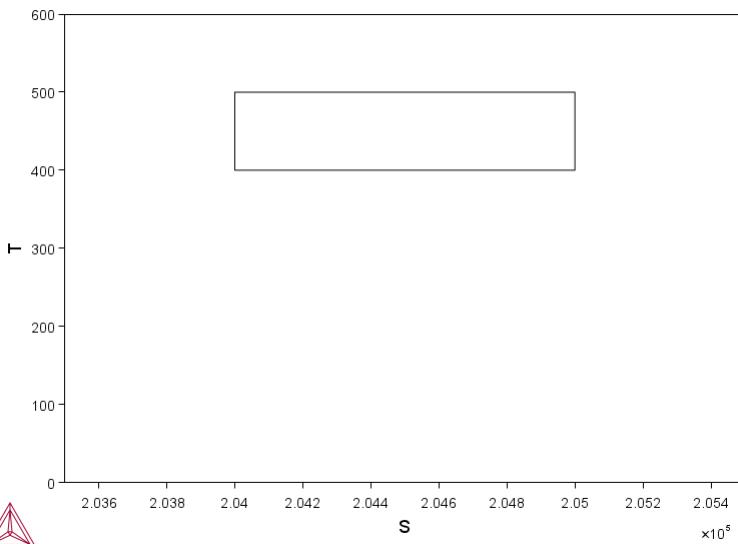
example 39a



```

POST:
POST:Hit RETURN to continue
POST:
POST: @@ The efficiency E of an engine which uses a Carnot
POST: @@ cycle is:
POST: @@ E=work performed/heat absorbed = W/Q1
POST: @@ If you plot the entropy versus temperature, you can
POST: @@ calculate the work performed just by calculating the
POST: @@ area of the surface depicted by the two squares and
POST: @@ by making the difference between them.
POST:
POST: s-d-a x s
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t
... the command in full is SET_DIAGRAM_AXIS
POST: s-s y n 0 600
... the command in full is SET_SCALING_STATUS
POST: s-s x n 203500 205500
... the command in full is SET_SCALING_STATUS
POST: set-title example 39b
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
example 39b

```



```

POST:
POST:Hit RETURN to continue
POST:
POST: @@ The influence of the value of the temperature T1 (the
POST: @@ temperature of the hot reservoir) on the efficiency of the
POST: @@ Carnot cycle is important. Therefore we will make another
POST: @@ calculation for T1=800 K and compare with the one for
POST: @@ T1=500 K (example 39a and b). T2=400 K in both cases.
POST:
POST: ba
... the command in full is BACK
POLY: read,,
... the command in full is READ_WORKSPACES
POLY: l-c
... the command in full is LIST_CONDITIONS
T=T1, N=2405.433393, S=SA
DEGREES OF FREEDOM 0
POLY: s-c s=none
... the command in full is SET_CONDITION

```

```

POLY: s-c t=800 p=1e7 n=1
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 209 grid points in 0 s
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VXNS/: xn
Output from POLY-3, equilibrium = 1, label A0 , database: User dat

Conditions:
T=800, P=10000000, N=1
DEGREES OF FREEDOM 0

Temperature 800.00 K ( 526.85 C), Pressure 1.000000E+07
Number of moles of components 1.00000E+00, Mass in grams 1.00000E+01
Total Gibbs energy -9.4119E+04, Enthalpy 2.05600E+04, Volume 6.65161E-04

Component Moles M-Fraction Activity Potential Ref.stat
A 1.00000E+00 1.00000E+00 7.1585E-07 -9.4119E+04 SER

GAS Status ENTERED Driving force 0.0000E+00
Moles 1.00000E+00, Mass 1.00000E+01, Volume fraction 1.00000E+00 Mole fractions:
A 1.00000E+00
Constitution:
A 1.00000E+00 A2 1.27812E-15
POLY: @@ Set volume to 1 m3
POLY: s-c v
... the command in full is SET_CONDITION
Value /6.651608E-04/: 1
POLY: s-c n
... the command in full is SET_CONDITION
Value /1/: none
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Using already calculated grid
7 ITS, CPU TIME USED 0 SECONDS
POLY: s-c n
... the command in full is SET_CONDITION
Value /1503.395871/:
POLY: s-c p
... the command in full is SET_CONDITION
Value /1000000/: none
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Using already calculated grid
6 ITS, CPU TIME USED 0 SECONDS
POLY: enter var ha=h;
... the command in full is ENTER_SYMBOL
POLY: enter var sa=s;
... the command in full is ENTER_SYMBOL
POLY: s-c s
... the command in full is SET_CONDITION
Value /215509.7923/: sa
POLY: s-c v=none
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Using already calculated grid
6 ITS, CPU TIME USED 0 SECONDS
POLY: show t,p,v,g,n,h,s
... the command in full is SHOW_VALUE
T=800
P=1E7
V=1.
G=-1.4149801E8
N=1503.3959
H=3.0909819E7
S=215509.79
POLY: Hit RETURN to continue
POLY:
POLY: save tcex39b y
... the command in full is SAVE_WORKSPACES
POLY: s-c s=272000
... the command in full is SET_CONDITION
POLY: s-a-v 1 s 270200 276200,,
... the command in full is SET_AXIS_VARIABLE
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated 209 grid points in 0 s
53 ITS, CPU TIME USED 0 SECONDS
POLY: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 272000.
...OK

Phase Region from 272000. for:
  GAS
Global test at 2.73200E+05 .... OK
Global test at 2.74700E+05 .... OK
Global test at 2.76200E+05 .... OK
Terminating at 276200.
Calculated 31 equilibria

Phase Region from 272000. for:
  GAS
Global test at 2.70800E+05 .... OK
Terminating at 270200.
Calculated 15 equilibria
*** Buffer saved on file: c:\jenkins\workspace\generate_console_examples\examples\tcex39\tcex39b.POLY3
POLY: s-c s=276200
... the command in full is SET_CONDITION
POLY: s-c t=750

```

```

... the command in full is SET_CONDITION
POLY: s-a-v 1 t 400 800,,
... the command in full is SET_AXIS_VARIABLE
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated          209 grid points in           0 s
 13 ITS, CPU TIME USED   0 SECONDS
POLY: step norm
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value    750.000
...OK

Phase Region from    750.000      for:
  GAS
Terminating at     800.000
Calculated       8 equilibria

Phase Region from    750.000      for:
  GAS
Global test at  6.70000E+02 .... OK
Global test at  5.70000E+02 .... OK
Global test at  4.70000E+02 .... OK
Terminating at    400.000
Calculated      38 equilibria
*** Buffer saved on file: c:\jenkins\workspace\generate_console_examples\examples\tcex39\tcex39b.POLY3
POLY: s-c t=400
... the command in full is SET_CONDITION
POLY: s-c s=270250
... the command in full is SET_CONDITION
POLY: s-a-v 1 s 270200 276200,,
... the command in full is SET_AXIS_VARIABLE
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated          209 grid points in           0 s
 9 ITS, CPU TIME USED   0 SECONDS
POLY: step norm
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value    270250.
...OK

Phase Region from    270250.      for:
  GAS
Global test at  2.71450E+05 .... OK
Global test at  2.72950E+05 .... OK
Global test at  2.74450E+05 .... OK
Global test at  2.75950E+05 .... OK
Terminating at    276200.
Calculated      43 equilibria

Phase Region from    270250.      for:
  GAS
Terminating at    270200.
Calculated      4 equilibria
*** Buffer saved on file: c:\jenkins\workspace\generate_console_examples\examples\tcex39\tcex39b.POLY3
POLY: s-c s=270200
... the command in full is SET_CONDITION
POLY: s-c t=750
... the command in full is SET_CONDITION
POLY: s-a-v 1 t 400 800,,
... the command in full is SET_AXIS_VARIABLE
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated          209 grid points in           0 s
 24 ITS, CPU TIME USED   0 SECONDS
POLY: step norm
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value    750.000
...OK

Phase Region from    750.000      for:
  GAS
Terminating at     800.000
Calculated       8 equilibria

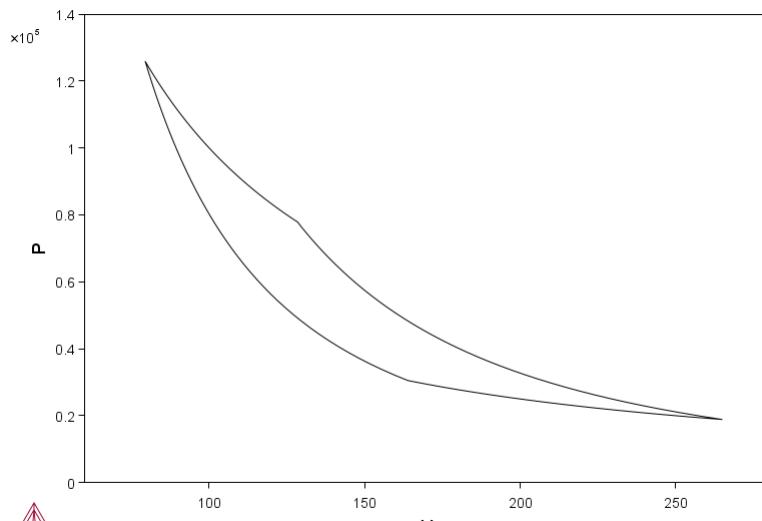
Phase Region from    750.000      for:
  GAS
Global test at  6.70000E+02 .... OK
Global test at  5.70000E+02 .... OK
Global test at  4.70000E+02 .... OK
Terminating at    400.000
Calculated      38 equilibria
*** Buffer saved on file: c:\jenkins\workspace\generate_console_examples\examples\tcex39\tcex39b.POLY3
POLY:
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST:
POST: s-d-a x v
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y p
... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 39c
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

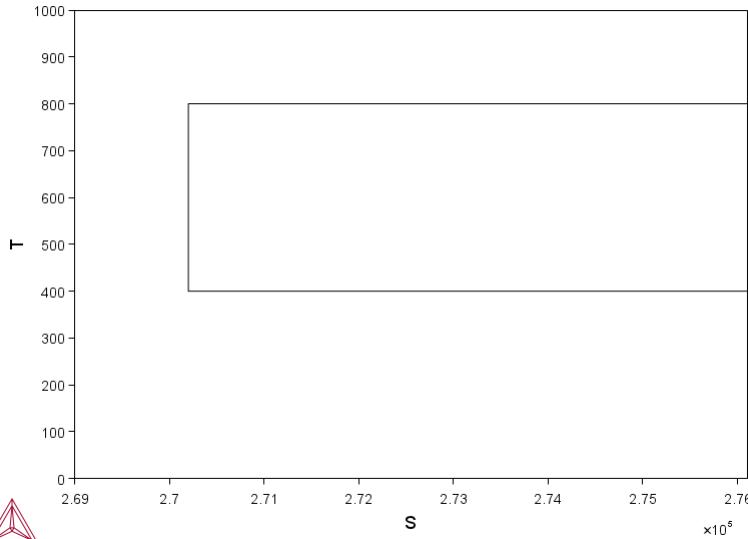
```

example 39c



```
POST:  
POST:Hit RETURN to continue  
POST:  
POST: s-d-a x s  
... the command in full is SET_DIAGRAM_AXIS  
POST: s-d-a y t  
... the command in full is SET_DIAGRAM_AXIS  
POST: s-s x n 269000 276100  
... the command in full is SET_SCALING_STATUS  
POST: s-s y n 0 1000  
... the command in full is SET_SCALING_STATUS  
POST: set-title example 39d  
POST:  
POST: SET_EXP_FILE_FORMAT 5  
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y  
... the command in full is MAKE_EXPERIMENTAL_DATAFI  
POST: SET_EXP_FILE_FORMAT 10  
POST:  
POST: plot  
... the command in full is PLOT_DIAGRAM
```

example 39d



```
POST:  
POST:Hit RETURN to continue  
POST:  
POST: @@ The efficiency for high value of T1 temperature is almost  
POST: @@ double compared with that one for low value of T1  
POST: @@ temperature (compare plot examples 39b with example 39d).  
POST:  
POST: @@ Now we will calculate the Carnot cycle for some real systems.  
POST: @@ The most well known engine is the steam engine.  
POST:  
POST: @@ The Carnot cycle for steam engine  
POST:  
POST: ba  
... the command in full is BACK  
POLY: go da  
... the command in full is GOTO_MODULE  
TDB_TCFE11: rej sys  
... the command in full is REJECT  
VA  
DICTRA_FCC_A1 REJECTED  
REINITIATING GES .....  
TDB_TCFE11: sw subdemo  
... the command in full is SWITCH_DATABASE  
Current database: Substance Demo Database v1.0  
VA  
TDB_SUBDEMO: def-sp h2o1  
... the command in full is DEFINE_SPECIES
```

```

H2O1 DEFINED
TDB_SUBDEMO: l-sys
... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/: CONSTITUENTS
GAS:G :H2O1:
H2O1_L :H2O1:
TDB_SUBDEMO: get
... the command in full is GET_DATA
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS .....
FUNCTIONS .....

List of references for assessed data

'H2O1<G> T.C.R.A.S. Class: 1 H2O1<G> H2O<G> WATER <GAS>, STEAM'
'H2O1<L> T.C.R.A.S. Class: 4 H2O1_Liquid H2O_Liquid Pure_Water WATER
T.C.R.A.S. Class: 4 cp modified by atd 12/9/94 and 5/7/2002'
-OK-
TDB_SUBDEMO: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY: l-st
... the command in full is LIST_STATUS
Option /CPS/: CPS
*** STATUS FOR ALL COMPONENTS
COMPONENT STATUS REF. STATE T(K) P(Pa)
VA ENTERED SER
H ENTERED SER
O ENTERED SER
*** STATUS FOR ALL PHASES
PHASE STATUS DRIVING FORCE MOLES
H2O1_L ENTERED 0.000000E+00 0.000000E+00
GAS ENTERED 0.000000E+00 0.000000E+00
*** STATUS FOR ALL SPECIES
H ENTERED H2O1 ENTERED O ENTERED VA ENTERED
POLY: c-st p h2o_l=sus
... the command in full is CHANGE_STATUS
POLY: l-st
... the command in full is LIST_STATUS
Option /CPS/: CPS
*** STATUS FOR ALL COMPONENTS
COMPONENT STATUS REF. STATE T(K) P(Pa)
VA ENTERED SER
H ENTERED SER
O ENTERED SER
*** STATUS FOR ALL PHASES
PHASE STATUS DRIVING FORCE MOLES
GAS ENTERED 0.000000E+00 0.000000E+00
SUSPENDED PHASES:
H2O1_L
*** STATUS FOR ALL SPECIES
H ENTERED H2O1 ENTERED O ENTERED VA ENTERED
POLY: @@ The Carnot cycle will be calculated for T1=350 K and T2=450 K
POLY:
POLY: s-c t=380 p=1e5 n=100 ac(o)=1
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated 1 grid points in 0 s
6 ITS, CPU TIME USED 0 SECONDS
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VXNS/: xn
Output from POLY-3, equilibrium = 1, label A0 , database: SUBDEMO

Conditions:
T=380, P=100000, N=100, AC(O)=1
DEGREES OF FREEDOM 0

Temperature 380.00 K ( 106.85 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+02, Mass in grams 6.00493E+02
Total Gibbs energy -1.04643E+07, Enthalpy -7.96861E+06, Volume 1.05317E+00

Component Moles M-Fraction Activity Potential Ref.stat
H 6.6667E+01 6.6667E-01 2.6556E-22 -1.5697E+05 SER
O 3.3333E+01 3.3333E-01 1.0000E+00 0.0000E+00 SER

GAS Status ENTERED Driving force 0.0000E+00
Moles 1.0000E+02, Mass 6.0049E+02, Volume fraction 1.0000E+00 Mole fractions:
H 6.66667E-01 O 3.33333E-01

Constitution:
H2O1 1.00000E+00
POLY: s-c p=None
... the command in full is SET_CONDITION
POLY: s-c s
... the command in full is SET_CONDITION
Value /6567.729231/: 6100
POLY: s-c t=350
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated 1 grid points in 0 s
11 ITS, CPU TIME USED 0 SECONDS
POLY: l-e,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: SUBDEMO

Conditions:
T=350, N=100, AC(O)=1, S=6100
DEGREES OF FREEDOM 0

Temperature 350.00 K ( 76.85 C), Pressure 3.863619E+05
Number of moles of components 1.00000E+02, Mass in grams 6.00493E+02
Total Gibbs energy -1.01376E+07, Enthalpy -8.00259E+06, Volume 2.51067E-01

Component Moles M-Fraction Activity Potential Ref.stat

```

```

H           6.6667E+01  6.6667E-01 2.0244E-23 -1.5206E+05 SER
O           3.3333E+01  3.3333E-01 1.0000E+00  0.0000E+00 SER

GAS          Status ENTERED      Driving force  0.0000E+00
Moles 1.0000E+02, Mass 6.0049E+02, Volume fraction 1.0000E+00 Mole fractions:
H 6.66667E-01  O 3.33333E-01
Constitution:
H2O1 1.00000E+00
POLY: @@ step in S with t=350
POLY: s-a-v 1 s 6000 7000,,,
... the command in full is SET_AXIS_VARIABLE
POLY: save tcex39c.y
... the command in full is SAVE_WORKSPACES
POLY: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value   6100.00
...OK

Phase Region from 6100.00 for:
  GAS
Global test at 6.30000E+03 .... OK
Global test at 6.55000E+03 .... OK
Global test at 6.80000E+03 .... OK
Terminating at 7000.00
Calculated 39 equilibria

Phase Region from 6100.00 for:
  GAS
Terminating at 6000.00
Calculated 7 equilibria
*** Buffer saved on file: c:\jenkins\workspace\generate_console_examples\examples\tcex39\tcex39c.POLY3
POLY:
POLY: read,,,
... the command in full is READ_WORKSPACES
POLY: s-c s=6000
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated 1 grid points in 0 s
  8 ITS, CPU TIME USED 1 SECONDS
POLY: @@ step in T with S=6000
POLY: s-a-v 1 t 350 450,,,
... the command in full is SET_AXIS_VARIABLE
POLY: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 350.000
...OK

Phase Region from 350.000 for:
  GAS
Global test at 3.70000E+02 .... OK
Global test at 3.95000E+02 .... OK
Global test at 4.20000E+02 .... OK
Global test at 4.45000E+02 .... OK
Terminating at 450.000
Calculated 43 equilibria
*** Buffer saved on file: c:\jenkins\workspace\generate_console_examples\examples\tcex39\tcex39c.POLY3
POLY:
POLY: read,,,
... the command in full is READ_WORKSPACES
POLY: s-c t=450
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated 1 grid points in 0 s
  9 ITS, CPU TIME USED 0 SECONDS
POLY: @@ Step in S with t=450
POLY: s-a-v 1 s 6000 7000,,,
... the command in full is SET_AXIS_VARIABLE
POLY: step norm
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 6100.00
...OK

Phase Region from 6100.00 for:
  GAS
Global test at 6.30000E+03 .... OK
Global test at 6.55000E+03 .... OK
Global test at 6.80000E+03 .... OK
Terminating at 7000.00
Calculated 39 equilibria

Phase Region from 6100.00 for:
  GAS
Terminating at 6000.00
Calculated 7 equilibria
*** Buffer saved on file: c:\jenkins\workspace\generate_console_examples\examples\tcex39\tcex39c.POLY3
POLY:
POLY: s-c s=7000
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated 1 grid points in 0 s
  41 ITS, CPU TIME USED 0 SECONDS
POLY: @@ Step in T with S=7000
POLY: s-a-v 1 t 350 450,,,
... the command in full is SET_AXIS_VARIABLE
POLY: step norm
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 450.000
...OK

Phase Region from 450.000 for:

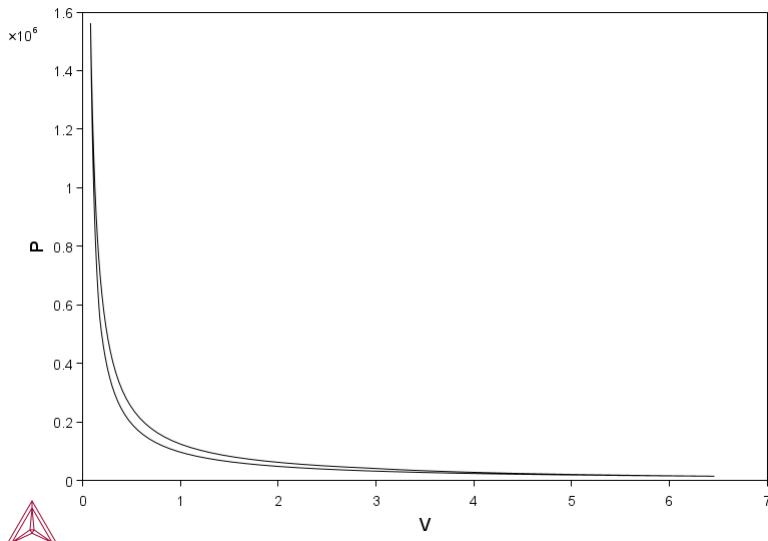
```

```

GAS
Global test at 4.30000E+02 .... OK
Global test at 4.05000E+02 .... OK
Global test at 3.80000E+02 .... OK
Global test at 3.55000E+02 .... OK
Terminating at 350.000
Calculated 43 equilibria
*** Buffer saved on file: c:\jenkins\workspace\generate_console_examples\examples\tcex39\tcex39c.POLY3
POLY:
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

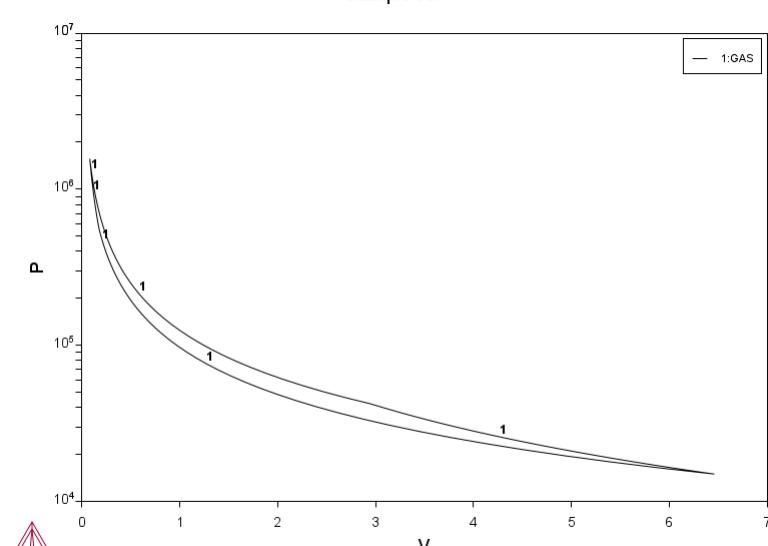
Setting automatic diagram axes

POST: s-p-f ##1,,,
... the command in full is SET_PLOT_FORMAT
CURRENT DEVICE: TC-UNITE Driver
POST:
POST: s-d-a x v
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y p
... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 39e
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFILE
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
example 39e
```



```

POST:
POST:Hit RETURN to continue
POST:
POST: s-a-ty y log
... the command in full is SET_AXIS_TYPE
POST: s-lab b
... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 39f
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFILE
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
example 39f
```

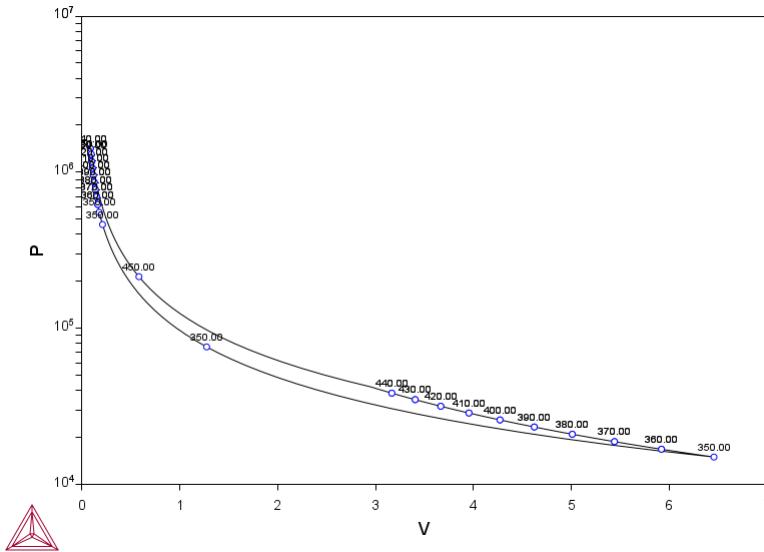


```
POST:
```

```

POST:Hit RETURN to continue
POST:
POST: @@ It is a bit difficult to distinguish from the calculated
POST: @@ diagram, example 39e, where the adiabatic expansion and
POST: @@ compression start. Therefore it is good to plot temperature
POST: @@ on the same diagram.
POST:
POST: s-d-a z t
    ... the command in full is SET_DIAGRAM_AXIS
POST: s-lab none
    ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 39g
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
    ... the command in full is MAKE_EXPERIMENTAL_DATAFILE
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
    ... the command in full is PLOT_DIAGRAM
example 39g

```



```

POST:
POST:Hit RETURN to continue
POST:
POST: @@ With Thermo-Calc you can also calculate the Carnot cycle
POST: @@ for real systems and include phase transformations.
POST:
POST: @@ Trying a Carnot cycle for water - it shows the case with
POST: @@ H2O_liquid to gas phase transformation. In the calculations
POST: @@ the volume of the liquid water is ignored.
POST:
POST: ba
    ... the command in full is BACK
POLY: go da
    ... the command in full is GOTO_MODULE
TDB_SUBDEMO: rej sys
    ... the command in full is REJECT
VA                                /- DEFINED
REINITIATING GES .....
TDB_SUBDEMO: sw subdemo
    ... the command in full is SWITCH_DATABASE
TDB_SUBDEMO: def-sp h2o1
    ... the command in full is DEFINE_SPECIES
H2O1 DEFINED
TDB_SUBDEMO: l-sys
    ... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENTS/: CONSTITUENTS
GAS:G      :H2O1:
H2O1_L    :H2O1:
TDB_SUBDEMO: get
    ... the command in full is GET_DATA
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS .....
FUNCTIONS .....

List of references for assessed data

'H2O1<G> T.C.R.A.S. Class: 1 H2O1<G> H2O<G> WATER <GAS>, STEAM'
'H2O1<L> T.C.R.A.S. Class: 4 H2O1_Liquid H2O_Liquid Pure_Water WATER
    T.C.R.A.S. Class: 4 cp modified by atd 12/9/94 and 5/7/2002'
-OK-
TDB_SUBDEMO: @@ patch
TDB_SUBDEMO: go g-e-s
    ... the command in full is GOTO_MODULE
GIBBS ENERGY SYSTEM
GES6: li-st,....
    ... the command in full is LIST_STATUS
GAS CONSTANT IN USER ENERGY UNITS:          8.31451000E+00
1 BAR IN USER PRESSURE UNITS:               1.00000000E+05
CURRENT VALUE OF TEMPERATURE (KELVIN):       298.15
CURRENT VALUE OF PRESSURE (PASCAL):          1.00000000E+05

CURRENT NUMBER OF ELEMENT      4

ELEMENT STABLE ELEMENT REFERENCE MASS      H298-H0      S298
-1 /- ELECTRON_GAS            0.0000E+00  0.0000E+00  0.0000E+00  80000000
0 VA VACUUM                  0.0000E+00  0.0000E+00  0.0000E+00  80000000
1 H 1/2 MOLE_H2(GAS)         1.0079E+00  4.2340E+03  6.5285E+01  08000000
2 O 1/2 MOLE_O2(GAS)         1.5999E+01  4.3410E+03  1.0252E+02  08000000

```

CURRENT NUMBER OF PHASE 2

| | | |
|----------|----------|-------------|
| PHASE | STATUS | SUBLATTICES |
| 1 GAS | 88200000 | 1 |
| 2 H2O1_L | 82200000 | 1 |

CURRENT NUMBER OF SPECIES 4

| | | | |
|---------|---------------|------|--|
| SPECIES | STOICHIOMETRY | | |
| 1 H | 80800000 | H | |
| 2 H2O1 | 00000000 | H2O1 | |
| 3 O | 80800000 | O | |
| 4 VA | 81800000 | VA | |

GES6: @@ patch
GES6: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY: l-st
... the command in full is LIST_STATUS
Option /CPS/: CPS
*** STATUS FOR ALL COMPONENTS

| | | | | | |
|-----------|---------|------|-------|-------|--------|
| COMPONENT | STATUS | REF. | STATE | T (K) | P (Pa) |
| VA | ENTERED | SER | | | |
| H | ENTERED | SER | | | |
| O | ENTERED | SER | | | |

*** STATUS FOR ALL PHASES

| | | | |
|--------|---------|---------------|--------------|
| PHASE | STATUS | DRIVING FORCE | MOLES |
| H2O1_L | ENTERED | 0.000000E+00 | 0.000000E+00 |
| GAS | ENTERED | 0.000000E+00 | 0.000000E+00 |

*** STATUS FOR ALL SPECIES

| | | | | | | | |
|---|---------|------|---------|---|---------|----|---------|
| H | ENTERED | H2O1 | ENTERED | O | ENTERED | VA | ENTERED |
|---|---------|------|---------|---|---------|----|---------|

POLY: c-st p h2o1=e 0
... the command in full is CHANGE_STATUS
POLY: l-st
... the command in full is LIST_STATUS
Option /CPS/: CPS
*** STATUS FOR ALL COMPONENTS

| | | | | | |
|-----------|---------|------|-------|-------|--------|
| COMPONENT | STATUS | REF. | STATE | T (K) | P (Pa) |
| VA | ENTERED | SER | | | |
| H | ENTERED | SER | | | |
| O | ENTERED | SER | | | |

*** STATUS FOR ALL PHASES

| | | | |
|--------|---------|---------------|--------------|
| PHASE | STATUS | DRIVING FORCE | MOLES |
| H2O1_L | ENTERED | 0.000000E+00 | 0.000000E+00 |
| GAS | ENTERED | 0.000000E+00 | 0.000000E+00 |

*** STATUS FOR ALL SPECIES

| | | | | | | | |
|---|---------|------|---------|---|---------|----|---------|
| H | ENTERED | H2O1 | ENTERED | O | ENTERED | VA | ENTERED |
|---|---------|------|---------|---|---------|----|---------|

POLY: s-c t=380 p=1e5 n=100 ac(o)=1
... the command in full is SET_CONDITION
POLY: l-c
... the command in full is LIST_CONDITIONS
T=380, P=100000, N=100, AC(O)=1
DEGREES OF FREEDOM 0
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated 2 grid points in 0 s
6 ITS, CPU TIME USED 0 SECONDS
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VXNS/: xn
Output from POLY-3, equilibrium = 1, label A0 , database: SUBDEMO
Conditions:
T=380, P=100000, N=100, AC(O)=1
DEGREES OF FREEDOM 0
Temperature 380.00 K (106.85 C), Pressure 1.000000E+05
Number of moles of components 1.000000E+02, Mass in grams 6.00493E+02
Total Gibbs energy -1.04643E+07, Enthalpy -7.96861E+06, Volume 1.05317E+00

| | | | | | |
|-----------|------------|------------|------------|-------------|----------|
| Component | Moles | M-Fraction | Activity | Potential | Ref.stat |
| H | 6.6667E+01 | 6.6667E-01 | 2.6556E-22 | -1.5697E+05 | SER |
| O | 3.3333E+01 | 3.3333E-01 | 1.0000E+00 | 0.0000E+00 | SER |

GAS Status ENTERED Driving force 0.0000E+00
Moles 1.0000E+02, Mass 6.0049E+02, Volume fraction 1.0000E+00 Mole fractions:
H 6.66667E-01 O 3.33333E-01
Constitution:
H2O1 1.00000E+00
POLY: s-c p=none
... the command in full is SET_CONDITION
POLY: s-c s
... the command in full is SET_CONDITION
Value /6567.729231/: 6100
POLY: s-c t=350
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated 2 grid points in 0 s
36 ITS, CPU TIME USED 0 SECONDS
POLY: l-e,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: SUBDEMO
Conditions:
T=350, N=100, AC(O)=1, S=6100
DEGREES OF FREEDOM 0
Temperature 350.00 K (76.85 C), Pressure 4.130269E+04
Number of moles of components 1.000000E+02, Mass in grams 6.00493E+02
Total Gibbs energy -1.03545E+07, Enthalpy -8.21947E+06, Volume 1.98337E+00

| | | | | | |
|-----------|------------|------------|------------|-------------|----------|
| Component | Moles | M-Fraction | Activity | Potential | Ref.stat |
| H | 6.6667E+01 | 6.6667E-01 | 6.6188E-24 | -1.5532E+05 | SER |
| O | 3.3333E+01 | 3.3333E-01 | 1.0000E+00 | 0.0000E+00 | SER |

GAS Status ENTERED Driving force 0.0000E+00

```

Moles 8.4450E+01, Mass 5.0711E+02, Volume fraction 1.0000E+00 Mole fractions:
H 6.66667E-01 O 3.33333E-01
Constitution:
H2O1 1.00000E+00

H2O1_L Status ENTERED Driving force 0.0000E+00
Moles 1.5550E+01, Mass 9.3379E+01, Volume fraction 0.0000E+00 Mole fractions:
H 6.66667E-01 O 3.33333E-01
Constitution:
H2O1 1.00000E+00
POLY: @@ step in S with t=350
POLY: s-a-v 1 s 6000 7000,,,
... the command in full is SET_AXIS_VARIABLE
POLY: save tcex39d y
... the command in full is SAVE_WORKSPACES
POLY: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 6100.00
...OK

Phase Region from 6100.00 for:
GAS
H2O1_L
Global test at 6.30000E+03 .... OK
Global test at 6.55000E+03 .... OK
Global check of removing phase at 6.71967E+03
Calculated 27 equilibria

Phase Region from 6719.67 for:
GAS
Global test at 6.90000E+03 .... OK
Terminating at 7000.00
Calculated 15 equilibria

Phase Region from 6100.00 for:
GAS
H2O1_L
Terminating at 6000.00
Calculated 7 equilibria
*** Buffer saved on file: c:\jenkins\workspace\generate_console_examples\examples\tcex39\tcex39d.POLY3
POLY:
POLY: read,,,
... the command in full is READ_WORKSPACES
POLY: s-c s=6000
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated 2 grid points in 0 s
6 ITS, CPU TIME USED 0 SECONDS
POLY: @@ step in T with S=6000
POLY: s-a-v 1 t 350 450,,,
... the command in full is SET_AXIS_VARIABLE
POLY: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 350.000
...OK

Phase Region from 350.000 for:
GAS
H2O1_L
Global test at 3.70000E+02 .... OK
Global test at 3.95000E+02 .... OK
Global test at 4.20000E+02 .... OK
Global test at 4.45000E+02 .... OK
Terminating at 450.000
Calculated 43 equilibria
*** Buffer saved on file: c:\jenkins\workspace\generate_console_examples\examples\tcex39\tcex39d.POLY3
POLY:
POLY: read,,,
... the command in full is READ_WORKSPACES
POLY: s-c t=450
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated 2 grid points in 0 s
12 ITS, CPU TIME USED 0 SECONDS
POLY: @@ Step in S with t=450
POLY: @@
POLY: s-a-v 1 s 6000 7000,,,
... the command in full is SET_AXIS_VARIABLE
POLY: step norm
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 6100.00
...OK

Phase Region from 6100.00 for:
GAS
H2O1_L
Global check of removing phase at 6.16203E+03
Calculated 5 equilibria

Phase Region from 6162.03 for:
GAS
Global test at 6.35000E+03 .... OK
Global test at 6.60000E+03 .... OK
Global test at 6.85000E+03 .... OK
Terminating at 7000.00
Calculated 37 equilibria

Phase Region from 6100.00 for:
GAS
H2O1_L
Terminating at 6000.00
Calculated 7 equilibria
*** Buffer saved on file: c:\jenkins\workspace\generate_console_examples\examples\tcex39\tcex39d.POLY3
POLY:
POLY: s-c s=7000
... the command in full is SET_CONDITION

```

```

POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated          2 grid points in          0 s
 40 ITS, CPU TIME USED 0 SECONDS
POLY: @@ Step in T with S=7000
POLY: s-a-v 1 t 350 450,,,,
... the command in full is SET_AXIS_VARIABLE
POLY: step norm
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 450.000
...OK

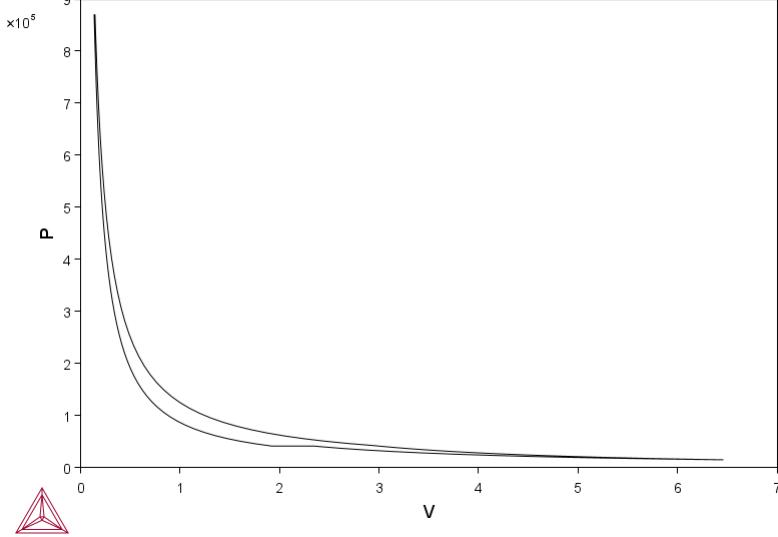
Phase Region from 450.000 for:
  GAS
Global test at 4.30000E+02 .... OK
Global test at 4.05000E+02 .... OK
Global test at 3.80000E+02 .... OK
Global test at 3.55000E+02 .... OK
Terminating at 350.000
Calculated 43 equilibria
*** Buffer saved on file: c:\jenkins\workspace\generate_console_examples\examples\tcex39\tcex39d.POLY3
POLY:
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: @@ The cycle shows the constant pressure at phase transformation.
POST: s-p-f #1,,,,,,,
... the command in full is SET_PLOT_FORMAT
CURRENT DEVICE: TC-UNITE Driver
POST:
POST: @@ To get a better understanding of this process it is possible
POST: @@ to plot the cycle using any set of thermodynamic state
POST: @@ variables. From the pressure-volume-temperature diagram,
POST: @@ example 39g, you can see the temperature variation on the
POST: @@ two adiabatical stages of the Carnot cycle.
POST: @@ The cycle shows the constant pressure at phase
POST: @@ transformation.
POST:
POST: s-d-a x v
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y p
... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 39h
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 39h

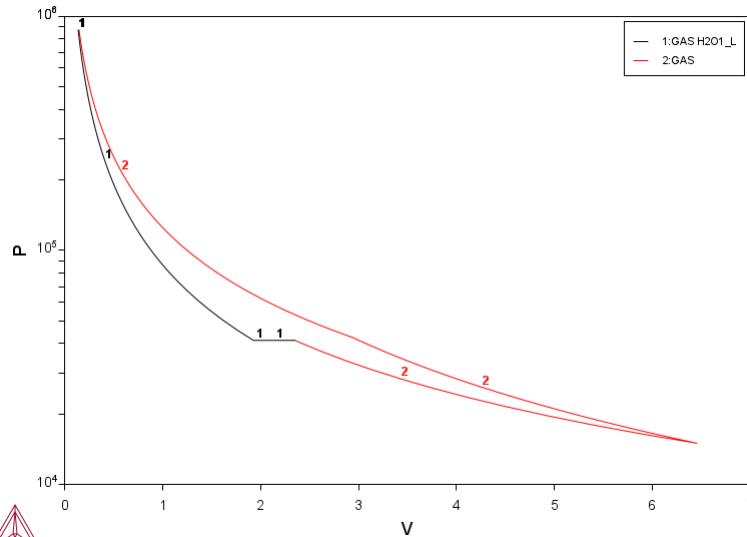


```

POST:
POST: Hit RETURN to continue
POST:
POST: s-a-t y log
... the command in full is SET_AXIS_TYPE
POST: s-lab b
... the command in full is SET_LABEL_CURVE_OPTION
POST: s-tit example 39i
... the command in full is SET_TITLE
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 39i

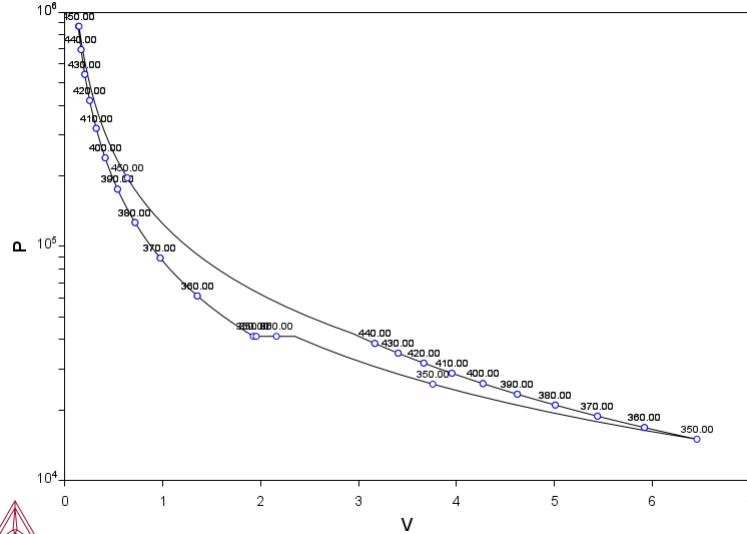


```

POST:
POST:Hit RETURN to continue
POST:
POST: s-d-a z t
... the command in full is SET_DIAGRAM_AXIS
POST: s-lab none
... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 39j
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 39j

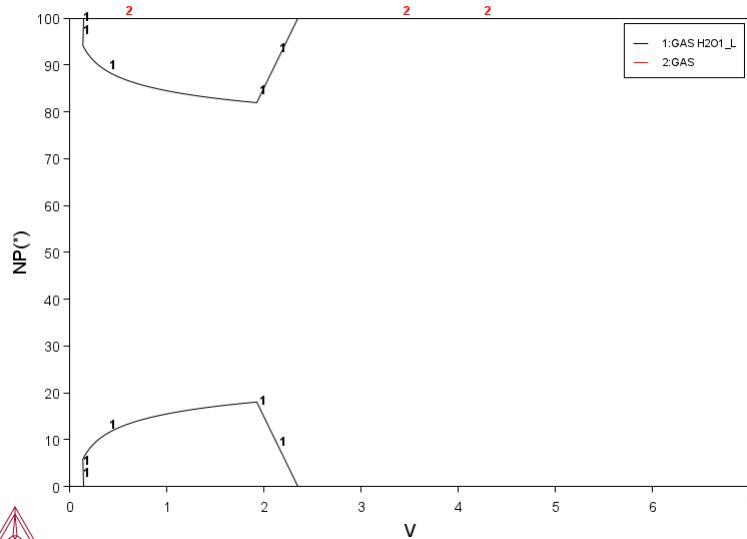


```

POST:
POST:Hit RETURN to continue
POST:
POST: @@ Another interesting aspect is it plots the amount of phases
POST: @@ versus volume. You can get information about both the kind
POST: @@ and amount of phases that fill up a certain volume.
POST:
POST: s-d-a z none
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y np(*),,
... the command in full is SET_DIAGRAM_AXIS
POST: s-a-ty y...
... the command in full is SET_AXIS_TYPE
POST: s-lab b
... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 39k
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

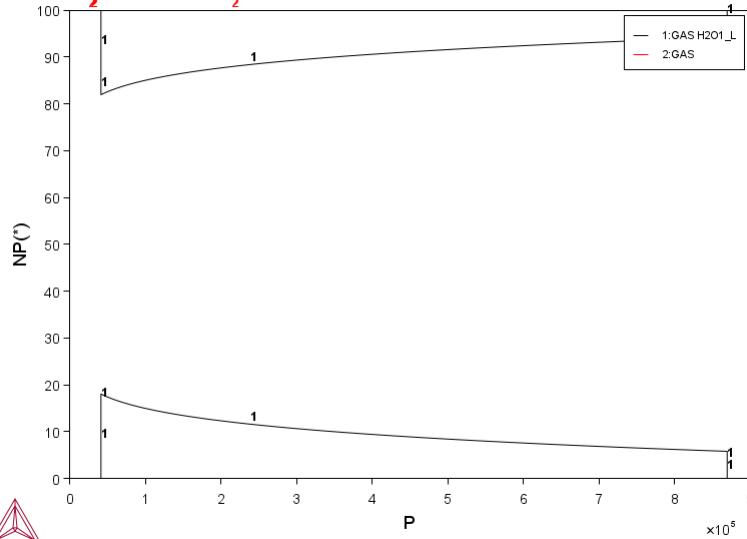
```

example 39k



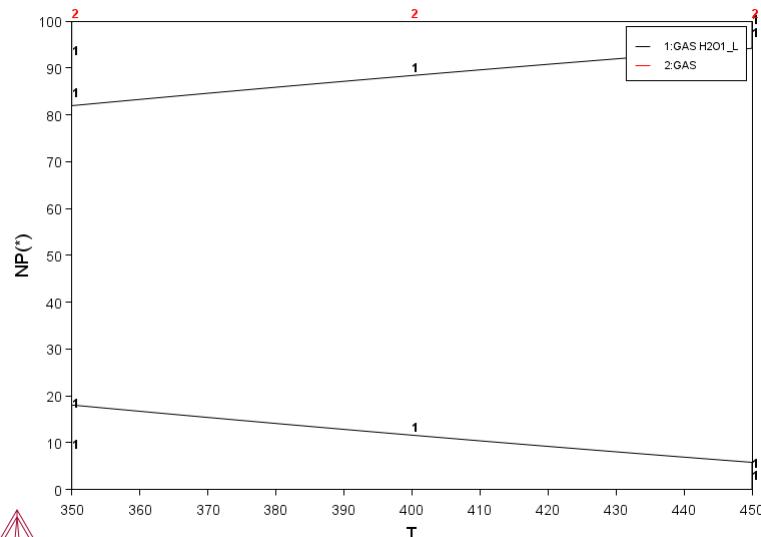
```
POST:  
POST:Hit RETURN to continue  
POST:  
POST: @@ The next plot shows the amount of phases versus pressure. It  
POST: @@ gives important information on the phase transformation  
POST: @@ pressure and on the ratio between the two phases in  
POST: @@ equilibrium at a certain pressure.  
POST:  
POST: s-d-a x p  
... the command in full is SET_DIAGRAM_AXIS  
POST: set-title example 391  
POST:  
POST: SET_EXP_FILE_FORMAT 5  
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y  
... the command in full is MAKE_EXPERIMENTAL_DATAFI  
POST: SET_EXP_FILE_FORMAT 10  
POST:  
POST: plot  
... the command in full is PLOT_DIAGRAM
```

example 39l



```
POST:  
POST:Hit RETURN to continue  
POST:  
POST: @@ By plotting the amount of phases versus temperature,  
POST: @@ example 39k, it is possible to know the phase transformation  
POST: @@ temperature and the ratio between the two phases in  
POST: @@ equilibrium at a certain temperature.  
POST:  
POST: s-d-a x t  
... the command in full is SET_DIAGRAM_AXIS  
POST: set-title example 39m  
POST:  
POST: SET_EXP_FILE_FORMAT 5  
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y  
... the command in full is MAKE_EXPERIMENTAL_DATAFI  
POST: SET_EXP_FILE_FORMAT 10  
POST:  
POST: plot  
... the command in full is PLOT_DIAGRAM
```

example 39m

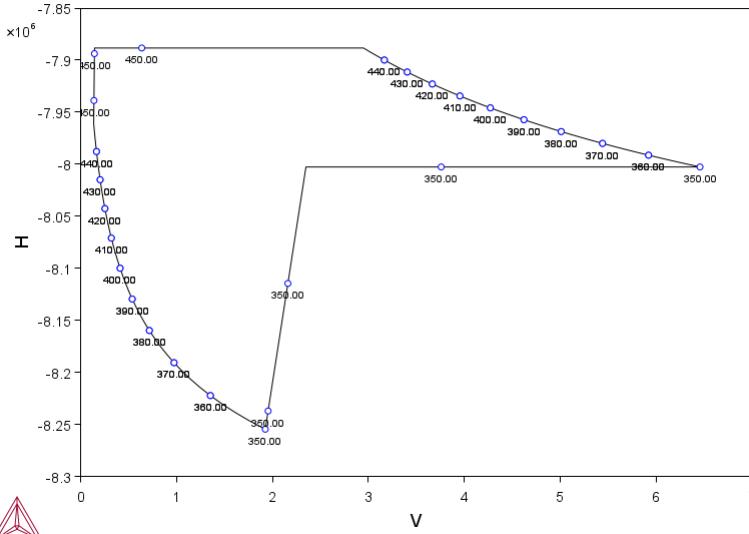


```

POST:
POST:Hit RETURN to continue
POST:
POST: @@ The enthalpy and Gibbs energy for the Carnot cycle could
POST: @@ also be plotted using the same calculation but a different
POST: @@ set for diagram axis. Note the important drop of the
POST: @@ enthalpy at the phase transformation point, example 39L.
POST:
POST: s-lab none
... the command in full is SET_LABEL_CURVE_OPTION
POST: s-d-a x v
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y h
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a z t
... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 39n
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 39n

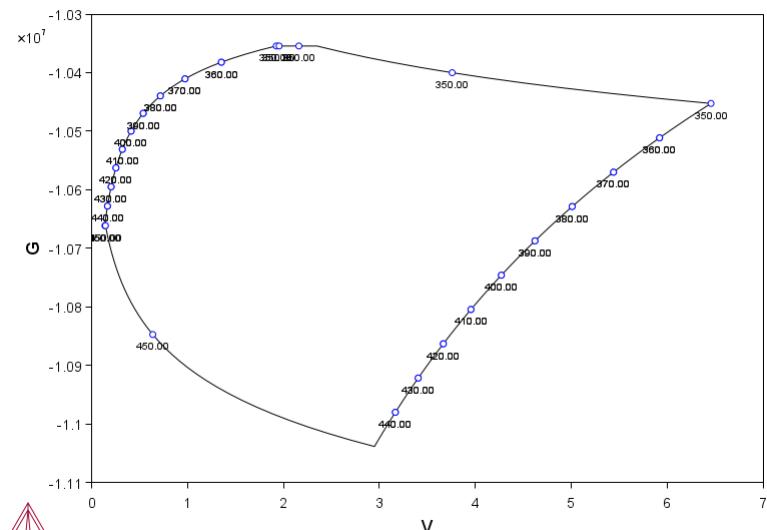


```

POST:
POST:Hit RETURN to continue
POST:
POST: s-d-a x v
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y g
... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 39o
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 39o



POST:
POST:Hit RETURN to continue
POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:

tce40-TCEX40

SYS:About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

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Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

```
SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce40\TCEX40.TCM.test"
SYS: @@ Working with the POURBAIX module.
SYS: go sys
SYS: set-echo
SYS:
SYS: set-log TCEX40.LOG
Heading: Part 1 - Pourbaix Diagram Calculations with the advanced POURBAIX module
SYS: set-ges 5
... the command in full is SET_GES_VERSION
SYS:
SYS: @@ Part 1 - Pourbaix Diagram Calculations with the advanced POURBAIX module
SYS:
SYS:
SYS: @@ Delete both for Windows and Linux to be able to run macro twice without stumbling on existing EXP file
SYS:
SYS: @@ TCEX40: Thermo-Calc (Console Mode) Standard Example No 40
SYS: @@ =====
SYS: @@ Copyright: Thermo-Calc Software AB, Stockholm, Sweden
SYS: @@ Developer: Dr. Pingfang Shi, Thermo-Calc Software AB
SYS: @@ Date: 2014-05-18 (revision)
SYS: @@ Text updated July 2021 (AJW)
SYS:
SYS: @@ =====
SYS: @@ Example description:
SYS: @@ =====
SYS: @@ TCEX40 is the first in a series of examples to demonstrate
SYS: @@ the POURBAIX module calculations and plotting.
SYS: @@ - Uses Option 1: Start a new Pourbaix diagram calculation
SYS: @@ - Part 1 of a 5 part example.
SYS: @@ - Note that example 40D is deprecated as of version 2022a.
SYS: @@ - Uses the TCS Public Aqueous Solution Database (PAQ2);
SYS: @@ - For the Fe-H2O-NaCl heterogeneous interaction system
SYS:
SYS: @@ The example automatically calculates and plots a Pourbaix
SYS: @@ diagram for 0.001 m Fe in a 0.1 m NaCl aqueous solution at
SYS: @@ 25 C and 1 bar. Other diagrams, along various phase
SYS: @@ boundaries for the same interactions resulting from the
SYS: @@ same Pourbaix module calculation, are also plotted.
SYS:
SYS: @@ =====
SYS: @@ Notes about the examples and the PAQ2 database:
SYS: @@ =====
SYS: @@ The so-called Pourbaix diagram is actually a phase diagram
SYS: @@ with independently-varied electropotential (Eh) and
SYS: @@ acidity (pH), for an heterogeneous interaction system at a
SYS: @@ certain bulk composition (that is by default always set as
SYS: @@ 1 kg of water solving a specified amount of metals and
SYS: @@ other solutes), under defined temperature and pressure
SYS: @@ conditions.
SYS:
SYS: @@ This example uses Option 1 followed by a choice of a
SYS: @@ single database, i.e., retrieving data from the PAQ2
SYS: @@ database. For this and other Thermo-Calc simulations,
SYS: @@ it can also be done with the TDB-GES-POLY-POST routine,
SYS: @@ which is used in example TCEX53.
SYS:
SYS: @@ The PAQ2 database is specially designed for Pourbaix
SYS: @@ diagram calculations (i.e., Eh-pH plots). It contains an
SYS: @@ AQUEOUS solution phase and REF_ELECTRODE phase (as a
SYS: @@ reference for electron in aqueous electrolyte systems),
SYS: @@ as well as some data for various solid phases (solution
SYS: @@ or stoichiometric) and a gaseous mixture phase.
SYS:
SYS: @@ A POLY3 file (POURBAIX.POLY3) is automatically saved at the
SYS: @@ end of the calculation. The POURBAIX.POLY3 file can be used
SYS: @@ with the other options and examples:
SYS: @@ Option 2: to plot other property diagrams of the calculated
SYS: @@ interaction system. See TCEX40B.
SYS: @@ Option 3: to make another Pourbaix calculation of the same
SYS: @@ chemical system but under different P-T-X
SYS: @@ conditions. See TCEX40C.
SYS:
SYS: @@ ** If you use the POLY3 file with the other examples it is
SYS: @@ important to make copies and rename these (for example
SYS: @@ TCEX40A.POLY3, TCEX40B.POLY3, etc.). This must be done
SYS: @@ outside of the Thermo-Calc software and after the TCEX40
SYS: @@ calculation and plotting is complete. This is so that the
SYS: @@ required POLY3 file structure is not lost.
SYS:
SYS: @@ ** A more advanced version of 40 and 40A can be found in
SYS: @@ TCEX40E, which also uses Option 1 but with multiple
SYS: @@ databases. However, licenses are required for three
SYS: @@ commercial Thermo-Calc databases. See the online help
SYS: @@ and the 40E macro text.
SYS: @@ -----
SYS:
SYS: @@... Now, let's start using the advanced POURBAIX module:
SYS: @@
SYS: go pour
... the command in full is GOTO_MODULE
```

WELCOME TO THE POURBAIX MODULE

!!!!!!!!!!!!!!

for Quick Calculations of Pourbaix Diagrams

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(Version 7.0, Mar. 2014)

Need any instruction on the POURBAIX module? /N/: ?

IMPORTANT NOTES for Calculating a POURBAIX Diagram:

- 1) The so-called Pourbaix diagram is actually a calculated equilibrium phase diagram mapped and plotted with the independently-varied electropotential (E_h , as defined with regard to the standard hydrogen electrode as its reference) and acidity (pH), that represents all the equilibrated phase boundaries among aqueous solution, gaseous mixture, and various primary and secondary solids (modelled as either complex solution or simple stoichiometric phases) in a certain multicomponent heterogeneous interaction system, under a defined T-P condition and a specific initial bulk composition (which is, by default, always set as 1 kg of water dissolving a specified amount of metals/alloys and other acids/alkalines/salts).
- 2) One must have at least a database containing an AQUEOUS solution phase (with thermodynamic data for water and various aqueous solutes), that shall be selected from TCAQ (PAQ) or AQS (PAQS) [which use the SIT Model or the Complete Revised HKF Model, respectively] within the Thermo-Calc database spectrum, or be chosen from an appropriate USER-specified database (it must be in the Thermo-Calc TDB format).
- 3) Due to the restrictions of aqueous solution model used within Thermo-Calc, such a database must be designed in the same format as in the default TCAQ (PAQ) or AQS (PAQS) for AQUEOUS solution phase. Among others, one should keep in mind the following regulations:
 - * The ELECTRON is defined as an special element (ZE) and as the only constituent in its reference phase REFERENCE_ELECTRODE (for determining the electropotential that is defined as E_h with the standard hydrogen electrode as the reference), but it is not defined as an aqueous species;
 - * The vacancy (VA) is unnecessary for AQUEOUS solution phase and it should be avoided in the definition of phase-constituents in the AQUEOUS phase;
 - * The AQUEOUS solution phase should always be defined as a constitutional solution phase, implying that all the aqueous solution species must be included in a single site, rather than in two or multiple sublattices.
- 4) Beside the AQUEOUS solution phase, there shall exist a GAS mixture phase containing at least H2O1, O2 and H2; and for multicomponent systems, normally there shall also contain some solid (stoichiometric or solution) phases. Of course, if desired, you could also choose to calculate and generate a Pourbaix diagram without considering the GAS mixture phase entirely; however, such a plot is not really a complete Pourbaix diagram, due to the fact that thermodynamically-stable phase boundaries between the AQUEOUS solution phase and GAS mixture phase will then not be calculated at all!
- 5) All the required thermodynamic data for calculations of Pourbaix diagrams or other diagrams must be retrieved either from one (Single) database which consists of an AQUEOUS solution phase, a GASEous mixture phase, a REF_ELECTRODE phase, and some SOLID phases (being solutions and/or stoichiometric compounds; for primary metals/alloys and for secondary products formed from heterogeneous chemical/electrochemical interactions, or from several (Multiple) databases that respectively contain various solutions/compounds (as listed above). Such databases suitable for calculations of aqueous-bearing heterogeneous interaction systems can be those default-prompted ones [i.e., in the Single-Database case, the PAQ or PAQS; and in the Multiple-Database case, the TCAQ or AQS as primarily-switched database, plus the SSUBx as firstly-appended one and the SSOLx as secondly-appended one if it is necessary; even more databases can be appended]. Of course, you could also choose to append required data from other appropriate databases (such as TCFE, TCSLD, TCNI/TTNi, TCAL/TTAL, TCMG/TTMg, TTZr, TCMP, SLAG, etc.) for GASEous mixture phase and for various solid solution and stoichiometric compound phases. Furthermore, an experienced user can also utilize his/her own USER-specified databases in various cases.
- 6) The current advanced POURBAIX-Module has been designed and developed in an efficient and effective way that it only requires the user to just answer some simple and necessary questions, rather than to go through basic modules (i.e., TDB, GES5, POLY3 and POST) and type the ordinary command-lines. Beside the default plotted Pourbaix diagram, it also allows the user to easily and quickly plot many different properties of the system, stable phases and aqueous species, varied along the calculated phase boundaries for the same defined heterogeneous interaction system. Moreover, it permits the user to directly change some plotting settings and manipulate all kinds of plotted diagrams.
- 7) The current advanced POURBAIX-Module has been extended so that it is additionally able to directly perform a normal STEPPING calculation (varied with a specified independent variable) and to easily generate various types of property diagrams, for the same heterogeneous interaction system that has been defined in a previous POURBAIX or TDB-GES5-PLOY3-POST calculation.

Enforce a PAUSE after plotting when running a MACRO? /N/: ?

Whenever running a Thermo-Calc MACRO (TCM) file, you may prefer to have a PAUSE after a specific diagram has been

plotted on SCREEN, for the multiple purposes of efficiently and easily manipulating the plotted diagram directly on the traditional TC-Graph window or Java-based TC-UNITE window, such as:

- * Printing it (of EMF/PS format) on connected printer(s);
- * Converting it (of EMF format) to (PDF) graphical files;
- * Saving it as an EMF graphical file;
- * Dumping it as a PNG or BMP graphical file;
- * Setting background colour for the current diagram and for all the sequential plots;
- * Setting default font/size for all the sequential plots;
- * Changing plotting Layers for all the sequential plots.

If no PAUSE is enforced, the POURBAIX Module will be going through all the sequential command-lines (answers) in the same POURBAIX session or till the SET_INTERACTIVE_MODE line in the MACRO file has been reached.

** By Y(y), a PAUSE is always enforced after each diagram;
** By N(n), no PAUSE will be enforced at any point at all.

Please then press <RETURN> at the PAUSE for continuation!

Enforce a PAUSE after plotting when running a MACRO? /N/: y

| 1. Start a completely new POURBAIX diagram calculation |
| 2. Open an old file & plot other property diagrams |
| 3. Open an old file & make another POURBAIX calculation |
| 4. Open an old file & make another STEPPING calculation |
|-----

Select option /1/: ?

One of the four options (1/2/3/4) should be entered here:

- 1 -- Make a completely new POURBAIX diagram calculation and automatically plot a pH-Eh diagram.
i.e., define a new chemical system;
specify the T-P-X conditions;
calculate the initial equilibria;
perform the pH-Eh mapping calculation;
plot pH-Eh & various property diagrams.
- 2 -- Open an existing POLY3 file created by POURBAIX Module (from a previous POURBAIX calculation Option 1 or 3 or a previous STEPPING calculation Option 4), and just selectively plot other property diagrams.
i.e., open the old GES and POLY3 workspaces;
plot pH-Eh or various property diagrams.
- 3 -- Open an existing POLY3 file created by POURBAIX Module and make another POURBAIX diagram calculation.
i.e., open the old GES and POLY3 workspaces;
adopt the defined chemical system;
modify the T-P-X conditions;
calculate the initial equilibria;
perform the pH-Eh mapping calculation;
plot pH-Eh & various property diagrams.
- 4 -- Open an existing POLY3 file created by POURBAIX Module (from a previous POURBAIX calculation Option 1 or 3 or a previous STEPPING calculation Option 4), and make a normal STEPPING calculation.
i.e., open the old GES and POLY3 workspaces;
adopt the defined chemical system;
specify one of the T-P-X conditions
as the stepping variable;
calculate the initial equilibria;
perform the stepping calculation;
plot various property diagrams.

Select option /1/: 1

- 1 -- Make a completely new POURBAIX diagram calculation and automatically plot a pH-Eh diagram.
i.e., define a new chemical system;
specify the T-P-X conditions;
calculate the initial equilibria;
perform the pH-Eh mapping calculation;
plot pH-Eh & various property diagrams.

Consider the GAS phase in calculating a Pourbaix diagram? /Y/: ?

You may optionally choose to ignore the GAS mixture phase on a calculated/plotted Pourbaix diagram. However, such a plot is actually not a complete Pourbaix diagram, due to that the thermodynamically-stable phase boundaries between the AQUEOUS solution phase and GAS mixture phase will not be calculated at all.

** By Y(y), GAS mixture phase shall be always considered;
** By N(n), GAS mixture phase will be completely ignored.

Consider the GAS phase in calculating a Pourbaix diagram? /Y/: Y

Use single database? /Y/: Y
Combined Database: /PAQ2/: PAQ2
THERMODYNAMIC DATABASE module
Database folder: C:\jenkins\workspace\generate_console_examples\databases\data
Current database: Public Aqueous Solution (SIT) v2.5

| | | |
|------------|------------|-----------------|
| H | O | ZE |
| VA_DEFINED | | |
| LIQUID:L | REJECTED | |
| GRAPHITE | DIAMOND_A4 | FC_ORTHORHOMBIC |
| MONOCLINIC | REJECTED | |
| CBCC_A12 | CUB_A13 | CHI_A12 |
| FE4N | FECN_CHI | REJECTED |
| CEMENTITE | M23C6 | M7C3 |

```

M5C2          M3C2          KSI_CARBIDE
PI REJECTED
FE3C          NI3C          CR3C2
CR7C3          CR23C6 REJECTED
COCO3          FECO3          NAHCO3
NA2CO3_S1      NA2CO3_S2      NICO3
CRC606 REJECTED
CO3N          CRN           CR2N
FE2N          NI3N REJECTED
NANO2_S1      NANO2_S2      NANO3
REJECTED
REJECTED
COCL2          CRCL2          CRCL3
FECL2          FECL3          NICL2
REJECTED
REJECTED
FECLO         NACLO4_S1      NACLO4_S2
REJECTED

```

DEFINE A CHEMICAL SYSTEM AND ITS INITIAL BULK COMPOSITION:
=====

Normally a POURBAIX diagram and related equilibrium property in a heterogeneous interaction system are calculated under a certain bulk composition which is usually 1 kg of water with defined amounts of dissolving solute substances. The solutes may either be completely dissolved into the aqueous solution, or be partially dissolved and simultaneously form some solid phases.

CHEMICAL SYSTEM (ELEMENTS):
Default defined elements (solvent H2O): H & O
and specially assigned ZE(electron) & VA(vacancy).

Prompt specified elements (solutes ELEM):
Fe Ni Co Cr C N S Na Cl

INITIAL BULK COMPOSITION:
Default defined composition (solvent): 1.0 kg of H2O
Prompt specified composition (solutes): x mole of ELEM

Notes: For accepting a default value, just RETURN at prompt;
For changing to a specific value, enter it at prompt.

=====

IMPORTANT NOTE for Entering Solutes in Chemical Formulas:
First element letter in UPPER case, and second lower case!
such as NaCl CO2 Cocl3 Fe0.93S NaSO4-1 H2SO4

Mass of Water (weight) = 1 kg

First solute: Fe
Molality of Fe [mol/kg] /.001/: .001
Second solute: NaCl .1
Next solute:

Defined chemical system and initial bulk composition:
Note: Solutes have been split up into chemical elements
and their mole numbers. If confirmed, the POURBAIX
Module will, in further steps, count the initial
bulk composition in terms of chemical elements.

```

H2O          1.0000000    kg
ZE          (specially assigned)
FE          0.100000000E-02   mole
CL          0.100000000E+00   mole
NA          0.100000000E+00   mole

```

Confirm defined system and initial bulk composition? /Y/: Y

RETRIEVE THERMODYNAMIC DATA FROM THE DATABASE: PAQ2

```

H          O          ZE
VA DEFINED
LIQUID:L REJECTED
GRAPHITE          DIAMOND_A4          FC_ORTHORHOMBIC
MONOCLINIC REJECTED
CBCC_A12          CUB_A13          CHI_A12
FE4N          FECN_CHI REJECTED
CEMENTITE          M23C6          M7C3
M5C2          M3C2          KSI_CARBIDE
PI REJECTED
FE3C          NI3C          CR3C2
CR7C3          CR23C6 REJECTED
COCO3          FECO3          NAHCO3
NA2CO3_S1      NA2CO3_S2      NICO3
CRC606 REJECTED
CO3N          CRN           CR2N
FE2N          NI3N REJECTED
NANO2_S1      NANO2_S2      NANO3
REJECTED
REJECTED
COCL2          CRCL2          CRCL3
FECL2          FECL3          NICL2
REJECTED
REJECTED
FECLO         NACLO4_S1      NACLO4_S2
REJECTED
REINITIATING GES .....
FE DEFINED
CL DEFINED
NA DEFINED
/- DEFINED

```

This database has following phases for the defined system

| | | |
|-----------|---------------|-----------|
| AQUEOUS:A | REF_ELECTRODE | GAS:G |
| FCC_A1 | BCC_A2 | HCP_A3 |
| HALITE | WUSTITE | MAGNETITE |
| HEMATITE | FE2O3_GAMMA | FE02H2 |
| FE03H3 | FEOOH | FE2O20H2 |
| NAO2 | NA2O_S1 | NA2O_S2 |
| NA2O_S3 | NA2O_S1 | NA2O_S2 |
| NAOH_S1 | NAOH_S2 | NA2FEO2 |

Reject phase(s) /NONE/: HCP_A3
HCP_A3 REJECTED
Reject phase(s) /NONE/: NONE
Restore phase(s): /NONE/: NONE

The following phases are retained in this system:

| | | |
|-------------|---------------|----------|
| AQUEOUS:A | REF_ELECTRODE | GAS:G |
| FCC_A1 | BCC_A2 | HALITE |
| WUSTITE | MAGNETITE | HEMATITE |
| FE2O3_GAMMA | FE02H2 | FE03H3 |
| FEOOH | FE2O2O2H2 | NAO2 |
| NA2O_S1 | NA2O_S2 | NA2O_S3 |
| NA2O2_S1 | NA2O2_S2 | NAOH_S1 |
| NAOH_S2 | NA2FEO2 | |

OK? /Y/: Y
ELEMENTS
SPECIES
PHASES
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS

List of references for assessed data

'TCS public data set for gaseous mixture in the Fe-Co-Cr-Na-Ni-C-H-O-N-S-Cl system.'
'TCS public data set for liquid mixture and alloy solutions in the Fe-Co-Cr-Na-Ni-C-H-O-N-S-Cl system.'
'TCS public data set for stoichiometric solids and liquids in the Fe-Co-Cr-Na-Ni-C-H-O-N-S-Cl system.'
'TCS Aqueous Solution Database, TCAQ2, v2.0 (2002/2003). Extracted data only for Fe-Co-Cr-Na-Ni-C-H-O-N-S-Cl bearing aqueous solution species from TCAQ2 which covers totally 83 elements and contains many more aqueous solution species.'

-OK-
Should any phase have a miscibility gap check? /N/: N

..... Reinitializing POLY3 workspaces

Enforce Global Minimization Technique in calculations? /N/: N

Save all functions, variables and tables in POLY3 file? /Y/: Y

Set numerical limits? /N/: N

SET CALCULATING PARAMETERS:

List of Default and Pre-defined Calculation Conditions:

Units: T in K, P in Pascal, B(H2O) in gram, N(ELEM) in mole

T=298.15, P=100000, B(H2O)=1000, N(H+1)=0, N(ZE)=0, N(CL)=0.1, N(FE)=1E-3,
N(NA)=0.1
DEGREES OF FREEDOM 0

Confirm defined conditions? /Y/: Y

Calculating start points; please be patient!

LIST THE FIRST DEFAULT STARTING EQUILIBRIUM POINT:

Output from POLY-3, equilibrium = 1, label A0 , database: PAQ2

Conditions:
T=298.15, P=100000, B(H2O)=1000, N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-16.11809565, MUR(ZE)=100
DEGREES OF FREEDOM 0

Temperature 298.15 K (25.00 C), Pressure 1.000000E+05
Number of moles of components 5.57094E+01, Mass in grams 1.00590E+03
Total Gibbs energy -1.70696E+07, Enthalpy -1.59069E+07, Volume 0.00000E+00

| Component | Moles | M-Fraction | Activity | Potential | Ref.stat |
|-----------|-------------|-------------|------------|-------------|----------|
| CL | 1.0000E-01 | 1.7950E-03 | 1.4499E-30 | -1.7032E+05 | SER |
| FE | 1.0000E-03 | 1.7950E-05 | 4.6321E-26 | -1.4461E+05 | SER |
| H+1 | -3.0000E-03 | -5.3851E-05 | 1.0000E-07 | -3.9956E+04 | SER |
| NA | 1.0000E-01 | 1.7950E-03 | 1.7205E-50 | -2.8406E+05 | SER |
| H2O | 5.5508E+01 | 9.9639E-01 | 9.9593E-01 | -1.0110E+01 | AQUEOUS |
| ZE | 3.0000E-03 | 5.3851E-05 | 1.0412E+00 | 1.0000E+02 | REF_ELEC |

| AQUEOUS | Status | ENTERED | Driving force | 0.0000E+00 |
|---|--------------|-------------|---------------|-----------------|
| Moles 5.5707E+01, Mass 1.0058E+03, Volume fraction 0.0000E+00 | | | | Mole fractions: |
| H2O 9.96410E-01 NA 1.79511E-03 FE 1.08146E-11 | | | | |
| CL 1.79511E-03 ZE 2.03382E-11 H+1 -1.36468E-11 | | | | |
| Constitution: | SiteFraction | Molality | Activity | log10Act |
| H2O | 9.96410E-01 | 5.55084E+01 | 9.96012E-01 | -0.0017 |
| CL-1 | 1.79511E-03 | 1.00003E-01 | 7.76756E-02 | -1.1097 |
| NA+1 | 1.79511E-03 | 1.00003E-01 | 7.76756E-02 | -1.1097 |
| OH-1 | 2.31689E-09 | 1.29070E-07 | 1.00218E-07 | -6.9991 |
| H+1 | 2.30788E-09 | 1.28568E-07 | 1.00000E-07 | -7.0000 |
| FE+2 | 6.21477E-12 | 3.46215E-10 | 1.26203E-10 | -9.8989 |
| FE0H+1 | 4.59380E-12 | 2.55913E-10 | 1.99003E-10 | -9.7011 |
| O3 | 1.00000E-15 | 0.00000E+00 | 2.6033E-113 | -112.5845 |
| H2O2 | 1.00000E-15 | 0.00000E+00 | 3.63324E-46 | -45.4397 |
| HCLO | 1.00000E-15 | 0.00000E+00 | 3.55905E-45 | -44.4487 |
| H2 | 1.00000E-15 | 0.00000E+00 | 5.46000E-18 | -17.2628 |
| HCLO2 | 1.00000E-15 | 0.00000E+00 | 1.38939E-87 | -86.8572 |
| FE0H+2 | 1.00000E-15 | 0.00000E+00 | 9.27035E-19 | -18.0329 |
| H02-1 | 1.00000E-15 | 0.00000E+00 | 7.68880E-51 | -50.1141 |
| FE03H3-1 | 1.00000E-15 | 0.00000E+00 | 1.69673E-51 | -50.7704 |
| FECL+2 | 1.00000E-15 | 0.00000E+00 | 3.39801E-23 | -22.4688 |
| FE2O2H2+4 | 1.00000E-15 | 0.00000E+00 | 3.71405E-35 | -34.4302 |
| FE+3 | 1.00000E-15 | 0.00000E+00 | 1.53892E-23 | -22.8128 |
| O2 | 1.00000E-15 | 0.00000E+00 | 2.54948E-58 | -57.5935 |
| CLO4-1 | 1.00000E-15 | 0.00000E+00 | 8.8489E-133 | -132.0531 |
| CLO3-1 | 1.00000E-15 | 0.00000E+00 | 1.5694E-105 | -104.8043 |
| CLO2-1 | 1.00000E-15 | 0.00000E+00 | 1.45414E-82 | -81.8374 |

```

CLO2           1.00000E-15   0.00000E+00   1.6417E-100   -99.7847
CLO-1          1.00000E-15   0.00000E+00   7.71560E-46    -45.1126
CL2            1.00000E-15   0.00000E+00   5.82418E-50    -49.2348
Solution Properties: pH = 7.0000 Eh = 0.0010 V I = 0.1000
pe = 0.0175 Ah = 0.1000 kJ m* = 0.2000
Aw = 0.9960 Os = 1.1089 pKw = 13.9973
At1= 1.00000E-15 At2= 1.2907E-07 (equiv_mol/kg_H2O)

```

```

HEMATITE      Status ENTERED     Driving force 0.0000E+00
Moles 2.5000E-03, Mass 7.9846E-02, Volume fraction 0.0000E+00 Mole fractions:
ZE 1.20000E+00 FE 4.00000E-01 NA 0.00000E+00
H2O 6.00000E-01 CL 0.00000E+00 H+1 -1.20000E+00
Constitution:
FE2O3 1.00000E+00

```

LIST THE DEFINED SYMBOLS:

```

DEFINED CONSTANTS
TSLIMIT0=99, AH2O=55.508435, WH2O=1.80152E-2, RNL=2.3025851, R=8.31451,
RNF=96485.309
DEFINED FUNCTIONS AND VARIABLES%
TC%=-T-273.15
PBAR%={P*1E-05
PKB%={P*1E-08
RT%={R*T
EH=MUR(ZE)/RNF
PH=- LOG10(ACR(H+1,AQUEOUS)*AH2O )
YH2O=Y(AQUEOUS,H2O)
ACRH2O=ACR(H2O,AQUEOUS)
RCH2O=ACR(H2O,AQUEOUS)
MLH2O=AH2O
ACTW=ACRH2O
OSMC=-YH2O/ (1-YH2O ) * LOG(ACRH2O )
TMI= (1-YH2O ) *AH2O/YH2O
AHZE=MUR(ZE)/1000
PEZE=MUR(ZE)/ (RNL*RT )
AI1=ACR(CL-1,AQUEOUS)*AH2O
RC1=ACR(CL-1,AQUEOUS)*YH2O/Y(AQUEOUS,CL-1)
ML1=Y(AQUEOUS,CL-1)*AH2O/YH2O
AI2=ACR(CL2,AQUEOUS)*AH2O
RC2=ACR(CL2,AQUEOUS)*YH2O/Y(AQUEOUS,CL2)
ML2=Y(AQUEOUS,CL2)*AH2O/YH2O
AI3=ACR(CL-1,AQUEOUS)*AH2O
RC3=ACR(CL-1,AQUEOUS)*YH2O/Y(AQUEOUS,CLO-1)
ML3=Y(AQUEOUS,CLO-1)*AH2O/YH2O
AI4=ACR(CLO2,AQUEOUS)*AH2O
RC4=ACR(CLO2,AQUEOUS)*YH2O/Y(AQUEOUS,CLO2)
ML4=Y(AQUEOUS,CLO2)*AH2O/YH2O
AI5=ACR(CLO2-1,AQUEOUS)*AH2O
RC5=ACR(CLO2-1,AQUEOUS)*YH2O/Y(AQUEOUS,CLO2-1)
ML5=Y(AQUEOUS,CLO2-1)*AH2O/YH2O
AI6=ACR(CLO3-1,AQUEOUS)*AH2O
RC6=ACR(CLO3-1,AQUEOUS)*YH2O/Y(AQUEOUS,CLO3-1)
ML6=Y(AQUEOUS,CLO3-1)*AH2O/YH2O
AI7=ACR(CLO4-1,AQUEOUS)*AH2O
RC7=ACR(CLO4-1,AQUEOUS)*YH2O/Y(AQUEOUS,CLO4-1)
ML7=Y(AQUEOUS,CLO4-1)*AH2O/YH2O
AI8=ACR(FE+2,AQUEOUS)*AH2O
RC8=ACR(FE+2,AQUEOUS)*YH2O/Y(AQUEOUS,FE+2)
ML8=Y(AQUEOUS,FE+2)*AH2O/YH2O
AI9=ACR(FE+3,AQUEOUS)*AH2O
RC9=ACR(FE+3,AQUEOUS)*YH2O/Y(AQUEOUS,FE+3)
ML9=Y(AQUEOUS,FE+3)*AH2O/YH2O
AI10=ACR(FE2O2H2+4,AQUEOUS)*AH2O
RC10=ACR(FE2O2H2+4,AQUEOUS)*YH2O/Y(AQUEOUS,FE2O2H2+4)
ML10=Y(AQUEOUS,FE2O2H2+4)*AH2O/YH2O
AI11=ACR(FECL+2,AQUEOUS)*AH2O
RC11=ACR(FECL+2,AQUEOUS)*YH2O/Y(AQUEOUS,FECL+2)
ML11=Y(AQUEOUS,FECL+2)*AH2O/YH2O
AI12=ACR(FEO3H3-1,AQUEOUS)*AH2O
RC12=ACR(FEO3H3-1,AQUEOUS)*YH2O/Y(AQUEOUS,FEO3H3-1)
ML12=Y(AQUEOUS,FEO3H3-1)*AH2O/YH2O
AI13=ACR(FEOH+1,AQUEOUS)*AH2O
RC13=ACR(FEOH+1,AQUEOUS)*YH2O/Y(AQUEOUS,FEOH+1)
ML13=Y(AQUEOUS,FEOH+1)*AH2O/YH2O
AI14=ACR(FEOH+2,AQUEOUS)*AH2O
RC14=ACR(FEOH+2,AQUEOUS)*YH2O/Y(AQUEOUS,FEOH+2)
ML14=Y(AQUEOUS,FEOH+2)*AH2O/YH2O
AI15=ACR(H+1,AQUEOUS)*AH2O
RC15=ACR(H+1,AQUEOUS)*YH2O/Y(AQUEOUS,H+1)
ML15=Y(AQUEOUS,H+1)*AH2O/YH2O
AI16=ACR(H2,AQUEOUS)*AH2O
RC16=ACR(H2,AQUEOUS)*YH2O/Y(AQUEOUS,H2)
ML16=Y(AQUEOUS,H2)*AH2O/YH2O
AI17=ACR(H2O,AQUEOUS)
RC17=ACR(H2O,AQUEOUS)/Y(AQUEOUS,H2O)
ML17=Y(AQUEOUS,H2O)*AH2O/YH2O
AI18=ACR(H2O2,AQUEOUS)*AH2O
RC18=ACR(H2O2,AQUEOUS)*YH2O/Y(AQUEOUS,H2O2)
ML18=Y(AQUEOUS,H2O2)*AH2O/YH2O
AI19=ACR(HClO,AQUEOUS)*AH2O
RC19=ACR(HClO,AQUEOUS)*YH2O/Y(AQUEOUS,HClO)
ML19=Y(AQUEOUS,HClO)*AH2O/YH2O
AI20=ACR(HClO2,AQUEOUS)*AH2O
RC20=ACR(HClO2,AQUEOUS)*YH2O/Y(AQUEOUS,HClO2)
ML20=Y(AQUEOUS,HClO2)*AH2O/YH2O
AI21=ACR(HO2-1,AQUEOUS)*AH2O
RC21=ACR(HO2-1,AQUEOUS)*YH2O/Y(AQUEOUS,HO2-1)
ML21=Y(AQUEOUS,HO2-1)*AH2O/YH2O
AI22=ACR(NA+1,AQUEOUS)*AH2O
RC22=ACR(NA+1,AQUEOUS)*YH2O/Y(AQUEOUS,NA+1)
ML22=Y(AQUEOUS,NA+1)*AH2O/YH2O
AI23=ACR(O2,AQUEOUS)*AH2O
RC23=ACR(O2,AQUEOUS)*YH2O/Y(AQUEOUS,O2)
ML23=Y(AQUEOUS,O2)*AH2O/YH2O
AI24=ACR(O3,AQUEOUS)*AH2O
RC24=ACR(O3,AQUEOUS)*YH2O/Y(AQUEOUS,O3)
ML24=Y(AQUEOUS,O3)*AH2O/YH2O
AI25=ACR(OH-1,AQUEOUS)*AH2O
RC25=ACR(OH-1,AQUEOUS)*YH2O/Y(AQUEOUS,OH-1)
ML25=Y(AQUEOUS,OH-1)*AH2O/YH2O
IS1=.5*ML1+.5*ML3+.5*ML5
IS2=.5*ML6+.5*ML7+.5*ML8*2**2
IS3=.5*ML9*3**2+.5*ML10*4**2+.5*ML11*2**2
IS4=.5*ML12+.5*ML13+.5*ML14*2**2
IS5=.5*ML15+.5*ML21+.5*ML22
ISTR=1*IS1+1*IS2+1*IS3+1*IS4+1*IS5

```

```

RLOGH= LOG10(ACR(H+1,AQUEOUS)*AH2O )
RLOGOH= LOG10(ACR(OH-1,AQUEOUS)*AH2O )
RLOGH2O= LOG10(ACRH2O )

DEFINED TABLES
GPT=T, P, PH, EH, ISTR
SFT=Y(AQUEOUS,CL-1), Y(AQUEOUS,CL2), Y(AQUEOUS,CLO-1), Y(AQUEOUS,CLO2),
Y(AQUEOUS,CLO2-1), Y(AQUEOUS,CLO3-1), Y(AQUEOUS,CLO4-1),
Y(AQUEOUS,FE+2), Y(AQUEOUS,FE+3), Y(AQUEOUS,FE2O2H2+4),
Y(AQUEOUS,FECL+2), Y(AQUEOUS,FEOH+1), Y(AQUEOUS,FEOH+2),
Y(AQUEOUS,H+1), Y(AQUEOUS,H2), Y(AQUEOUS,H2O),
Y(AQUEOUS,H2O2), Y(AQUEOUS,HCLO), Y(AQUEOUS,HClO2), Y(AQUEOUS,H2O-1),
Y(AQUEOUS,NA+1), Y(AQUEOUS,O2), Y(AQUEOUS,OH-1), PH, EH
AYT=AC(CL-1,AQUEOUS), AC(CL2,AQUEOUS), AC(CLO-1,AQUEOUS),
AC(CL2,AQUEOUS), AC(CL2-1,AQUEOUS), AC(CLO3-1,AQUEOUS),
AC(CL04-1,AQUEOUS), AC(FE+2,AQUEOUS), AC(FE+3,AQUEOUS),
AC(FE2O2H2+4,AQUEOUS), AC(FECL+2,AQUEOUS), AC(FEO3H3-1,AQUEOUS),
AC(FEOH+1,AQUEOUS), AC(FEOH+2,AQUEOUS), AC(H+1,AQUEOUS),
AC(H2,AQUEOUS), AC(H2O,AQUEOUS), AC(H2O2,AQUEOUS), AC(HClO,AQUEOUS),
AC(HClO2,AQUEOUS), AC(HO2-1,AQUEOUS), AC(NA+1,AQUEOUS), AC(O2,AQUEOUS),
AC(O3,AQUEOUS), AC(OH-1,AQUEOUS), PH, EH
ART=ACR(CL-1,AQUEOUS), ACR(CL2,AQUEOUS), ACR(CLO-1,AQUEOUS),
ACR(CL2,AQUEOUS), ACR(CL2-1,AQUEOUS), ACR(CLO3-1,AQUEOUS),
ACR(CL04-1,AQUEOUS), ACR(FE+2,AQUEOUS), ACR(FE+3,AQUEOUS),
ACR(FE2O2H2+4,AQUEOUS), ACR(FECL+2,AQUEOUS), ACR(FEO3H3-1,AQUEOUS),
ACR(FEOH+1,AQUEOUS), ACR(FEOH+2,AQUEOUS), ACR(H+1,AQUEOUS),
ACR(H2,AQUEOUS), ACR(H2O,AQUEOUS), ACR(H2O2,AQUEOUS),
ACR(HClO,AQUEOUS), ACR(HClO2,AQUEOUS), ACR(HO2-1,AQUEOUS),
ACR(NA+1,AQUEOUS), ACR(O2,AQUEOUS), ACR(O3,AQUEOUS), ACR(OH-1,AQUEOUS),
PH, EH
AIT=A11, A12, A13, A14, A15, A16, A17, A18, A19, A110, A111, A112, A113,
A114, A115, A116, A117, A118, A119, A120, A121, A122, A123, A124, A125,
PH, EH
RCT=RC1, RC2, RC3, RC4, RC5, RC6, RC7, RC8, RC9, RC10, RC11, RC12, RC13,
RC14, RC15, RC16, RC17, RC18, RC19, RC20, RC21, RC22, RC23, RC24, RC25,
PH, EH
MLT=ML1, ML2, ML3, ML4, ML5, ML6, ML7, ML8, ML9, ML10, ML11, ML12, ML13,
ML14, ML15, ML16, ML18, ML19, ML20, ML21, ML22, ML23, ML24, ML25, ISTR,
PH, EH

```

IMPORTANT FACTS:

The default definitions of the Eh and pH quantities in the advanced POURBAIX-Module (and in the ordinary TDB-GES-POLY calculation routines) should ALWAYS be as below:

$$\begin{aligned} \text{Eh} &= \text{MUR(ZE)}/\text{RNF} \\ \text{pH} &= -\log_{10}[\text{AI}(\text{H+1,AQUEOUS})] \\ &= -\log_{10}[\text{ACR}(\text{H+1,AQUEOUS})*\text{AH2O}] \end{aligned}$$

where RNF is the Faraday constant (96485.309 C/mol), and AH2O is the molecular weight of H2O (55.508435 g). MUR(ZE) is the electrochemical potential (ECP; in the unit of J/mol; w.r.t. the standard hydrogen electrode). ACR(H+1,AQUEOUS) is the site-fraction-based activity of the H+1 aqueous species in AQUEOUS solution phase, but AI(H+1,AQUEOUS) [that equals ACR(H+1,AQUEOUS)*AH2O] is the molality-based activity of the H+1 aqueous species that should be used for defining the pH quantity.

Within an aqueous-bearing heterogeneous interaction system, the fundamental system-components must be H2O, H+1 and ZE, which are corresponding to the basic elements O & H and the hypothetical electron (ZE) in the aqueous solution phase. For the additional chemical elements in the system, their corresponding system-components shall be defined as in their element forms (such as Fe, Cr, Mn, Ni, Na, Cl, S) or (for some) in their molecular forms (e.g., NaCl, H2S). The reference state for the H2O component must always be defined as the solvent species H2O in the AQUEOUS solution phase under the current temperature (*) and 100000 Pascal (i.e., 1 bar). The reference states for the H+1 and ZE components are by default set as their SER.

Various conventional properties of aqueous solute species I are converted in the following manners:

$$\begin{aligned} \text{ML} &= Y(\text{AQUEOUS,I})*\text{AH2O}/Y(\text{H2O}) \\ \text{RC} &= \text{ACR(I,AQUEOUS)}*\text{YH2O}/Y(\text{AQUEOUS,I}) \\ \text{AI} &= \text{RC}*\text{ML} \\ &= \text{ACR(I,AQUEOUS)}*\text{AH2O} \end{aligned}$$

where YH2O [i.e., Y(AQUEOUS,H2O)] and Y(AQUEOUS,I) are the site-fractions of solvent H2O and solute species I.

LIST THE DEFINED AXIS-VARIABLES:

| | | | |
|-----------------------|-----------------|----------------|--------------|
| Axis No 1: LNACR(H+1) | Min: -34.532608 | Max: 2.3025851 | Inc: 0.8 |
| Axis No 2: MUR(ZE) | Min: -150000 | Max: 200000 | Inc: 7718.85 |

NOTE: The default settings (listed above) for two mapping variables [in terms of lnACR(H+1) and MUR(ZE), and their minimum/maximum values and increment steps] are covering the following pH-Eh ranges/steps:

$$\begin{aligned} \text{pH: } 0.00 &\rightarrow 14.00, \text{ at a step of } 0.35 \\ \text{Eh: } -1.55 &\rightarrow 2.07, \text{ at a step of } 0.08 [\text{V}] \end{aligned}$$

The maximum pH limit has been calculated precisely and determined automatically by the POURBAIX-Module, as a function of the temperature-pressure conditions and initial bulk compositions of the current defined interaction system.

Accept the default settings for two mapping variables? /Y/: Y

LIST ALL THE INITIAL EQUILIBRIA FOR MAPPING:

```

No 1 +2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-16.118096, MUR(ZE)=100.
No 2 -2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-16.118096, MUR(ZE)=100.
No 3 +1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-16.118096, MUR(ZE)=100.
No 4 -1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-16.118096, MUR(ZE)=100.
No 5 +2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-16.118096, MUR(ZE)=-28400
No 6 -2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-16.118096, MUR(ZE)=-28400
No 7 +1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-16.118096, MUR(ZE)=-28400

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No 8 -1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-16.118096, MUR(ZE)=-28400
No 9 +2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-9.2103404, MUR(ZE)=-13000
No 10 -2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-9.2103404, MUR(ZE)=-13000
No 11 +1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-9.2103404, MUR(ZE)=-13000
No 12 -1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-9.2103404, MUR(ZE)=-13000
No 13 +2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-9.2103404, MUR(ZE)=86837
No 14 -2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-9.2103404, MUR(ZE)=86837
No 15 +1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-9.2103404, MUR(ZE)=86837
No 16 -1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-9.2103404, MUR(ZE)=86837
No 17 +2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-16.118096, MUR(ZE)=66000.
No 18 -2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-16.118096, MUR(ZE)=66000.
No 19 +1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-16.118096, MUR(ZE)=66000.
No 20 -1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-16.118096, MUR(ZE)=66000.

```

MAP THE FOURBAIX DIAGRAM:
Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Tie-lines not in the plane of calculation

```

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Generating start point 27
Generating start point 28
Generating start point 29
Generating start point 30
Working hard
Generating start point 31
Generating start point 32
Generating start point 33
Generating start point 34
Generating start point 35
Generating start point 36
Generating start point 37
Generating start point 38
Generating start point 39
Generating start point 40
Working hard
Working hard
Generating start point 41
Generating start point 42
Generating start point 43
Generating start point 44
Generating start point 45
Generating start point 46
Generating start point 47
Generating start point 48

```

Phase region boundary 1 at: -1.612E+01 7.911E+04

GAS
AQUEOUS

** HALITE
HEMATITE

Calculated.. 25 equilibria

Terminating at axis limit.

Phase region boundary 2 at: -3.453E+01 3.383E+04

GAS
AQUEOUS

** HALITE
HEMATITE

Calculated. 42 equilibria

Phase region boundary 3 at: -2.296E+00 1.134E+05

GAS
AQUEOUS

** HALITE
HEMATITE

Calculated.. 33 equilibria

```

Phase region boundary  5 at: -2.296E+00  1.134E+05
  GAS
  AQUEOUS
 ** HEMATITE
Calculated              5 equilibria

Phase region boundary  6 at: -2.296E+00  1.134E+05
  GAS
  AQUEOUS
  HALITE
 ** HEMATITE
Calculated              31 equilibria

Phase region boundary  7 at: -1.612E+01  7.911E+04
  GAS
  AQUEOUS
 ** HALITE
  HEMATITE
Calculated.           19 equilibria
Terminating at known equilibrium

Phase region boundary  8 at: -1.612E+01  7.817E+04
 ** GAS
  AQUEOUS
  HEMATITE
Calculated..          26 equilibria
Terminating at axis limit.

Phase region boundary  9 at: -3.453E+01  3.296E+04
 ** GAS
  AQUEOUS
  HEMATITE
Calculated.           43 equilibria

Phase region boundary 10 at: -1.975E+00  1.132E+05
 ** GAS
  AQUEOUS
 ** HEMATITE
Calculated..          9 equilibria
Terminating at axis limit.

Phase region boundary 11 at: -1.975E+00  1.132E+05
 ** GAS
  AQUEOUS
Calculated..          9 equilibria
Terminating at axis limit.

Phase region boundary 12 at: -1.975E+00  1.132E+05
  AQUEOUS
 ** HEMATITE
Calculated..          30 equilibria

Phase region boundary 13 at: -1.420E+01 -2.225E+04
  AQUEOUS
 ** HEMATITE
 ** MAGNETITE
Calculated..          30 equilibria
Terminating at axis limit.

Phase region boundary 14 at: -1.420E+01 -2.225E+04
  AQUEOUS
 ** HEMATITE
  MAGNETITE
Calculated..          30 equilibria
Terminating at axis limit.

Phase region boundary 15 at: -1.420E+01 -2.225E+04
  AQUEOUS
 ** MAGNETITE
Calculated..          4 equilibria

Phase region boundary 16 at: -1.625E+01 -4.067E+04
 ** GAS
  AQUEOUS
 ** MAGNETITE
Calculated..          4 equilibria

Phase region boundary 17 at: -1.625E+01 -4.067E+04
  GAS
  AQUEOUS
 ** MAGNETITE
Calculated..          33 equilibria

Phase region boundary 18 at: -1.625E+01 -4.067E+04
 ** GAS
  AQUEOUS
Calculated..          28 equilibria
Terminating at axis limit.

Phase region boundary 19 at: -1.625E+01 -4.067E+04
 ** GAS
  AQUEOUS
  MAGNETITE
Calculated..          27 equilibria
Terminating at axis limit.

Phase region boundary 20 at: -1.420E+01 -2.225E+04
  AQUEOUS
  HEMATITE
 ** MAGNETITE
Calculated..          30 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 21 at: -1.975E+00  1.132E+05
  GAS
  AQUEOUS
 ** HEMATITE
Calculated..          13 equilibria

Phase region boundary 22 at: -1.612E+01  7.817E+04
 ** GAS
  AQUEOUS
  HEMATITE
Calculated..          19 equilibria
Terminating at known equilibrium

Phase region boundary 23 at: -1.612E+01 -2.701E+04
  AQUEOUS
  HEMATITE

```

```

** MAGNETITE
Calculated.. 26 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 24 at: -1.612E+01 -2.701E+04
    AQUEOUS
    HEMATITE
    ** MAGNETITE
Calculated. 4 equilibria
Terminating at known equilibrium

Phase region boundary 25 at: -1.116E+01 1.000E+02
    AQUEOUS
    ** HEMATITE
Calculated. 7 equilibria
Terminating at known equilibrium

Phase region boundary 26 at: -1.116E+01 1.000E+02
    AQUEOUS
    ** HEMATITE
Calculated. 24 equilibria
Terminating at known equilibrium

Phase region boundary 27 at: -1.612E+01 -2.701E+04
    AQUEOUS
    ** HEMATITE
    MAGNETITE
Calculated.. 26 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 28 at: -1.612E+01 -2.701E+04
    AQUEOUS
    ** HEMATITE
    MAGNETITE
Calculated. 4 equilibria
Terminating at known equilibrium

Phase region boundary 29 at: -1.612E+01 -3.959E+04
    AQUEOUS
    ** MAGNETITE
Calculated. 2 equilibria
Terminating at known equilibrium

Phase region boundary 30 at: -1.612E+01 -3.959E+04
    AQUEOUS
    ** MAGNETITE
Calculated. 4 equilibria
Terminating at known equilibrium

Phase region boundary 31 at: -1.485E+01 -2.840E+04
    AQUEOUS
    ** MAGNETITE
Calculated. 3 equilibria
Terminating at known equilibrium

Phase region boundary 32 at: -1.485E+01 -2.840E+04
    AQUEOUS
    ** MAGNETITE
Calculated. 2 equilibria
Terminating at known equilibrium

Phase region boundary 33 at: -1.668E+01 -2.840E+04
    AQUEOUS
    ** HEMATITE
    MAGNETITE
Calculated.. 26 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 34 at: -1.668E+01 -2.840E+04
    AQUEOUS
    ** HEMATITE
    MAGNETITE
Calculated. 5 equilibria
Terminating at known equilibrium

Phase region boundary 35 at: -9.172E+00 9.539E+04
    ** GAS
    AQUEOUS
    HEMATITE
Calculated.. 35 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 36 at: -9.172E+00 9.539E+04
    ** GAS
    AQUEOUS
    HEMATITE
Calculated. 11 equilibria
Terminating at known equilibrium

Phase region boundary 37 at: -9.210E+00 9.529E+04
    ** GAS
    AQUEOUS
    HEMATITE
Calculated.. 35 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 38 at: -9.210E+00 9.529E+04
    ** GAS
    AQUEOUS
    HEMATITE
Calculated. 11 equilibria
Terminating at known equilibrium

Phase region boundary 39 at: -9.210E+00 1.461E+04
    AQUEOUS
    ** HEMATITE
Calculated. 8 equilibria
Terminating at known equilibrium

Phase region boundary 40 at: -9.210E+00 1.461E+04
    AQUEOUS

```

```

** HEMATITE
Calculated.          25 equilibria
Terminating at known equilibrium

Phase region boundary 41 at: -9.210E+00 -2.323E+04
** GAS
AQUEOUS
Calculated.          10 equilibria
Terminating at known equilibrium

Phase region boundary 42 at: -9.210E+00 -2.323E+04
** GAS
AQUEOUS
Calculated..         18 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 43 at: -5.086E+00 -1.300E+04
** GAS
AQUEOUS
Calculated.          16 equilibria
Terminating at known equilibrium

Phase region boundary 44 at: -5.086E+00 -1.300E+04
** GAS
AQUEOUS
Calculated..         13 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 45 at: -1.293E+01 -1.300E+04
AQUEOUS
** HEMATITE
Calculated.          3 equilibria
Terminating at known equilibrium

Phase region boundary 46 at: -1.293E+01 -1.300E+04
AQUEOUS
** HEMATITE
Calculated.          27 equilibria
Terminating at known equilibrium

Phase region boundary 47 at: -9.210E+00 9.623E+04
GAS
AQUEOUS
** HALITE
HEMATITE
Calculated..         33 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 48 at: -9.210E+00 9.623E+04
GAS
AQUEOUS
** HALITE
HEMATITE
Calculated.          10 equilibria
Terminating at known equilibrium

Phase region boundary 49 at: -9.210E+00 9.529E+04
** GAS
AQUEOUS
HEMATITE
Calculated..         35 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 50 at: -9.210E+00 9.529E+04
** GAS
AQUEOUS
HEMATITE
Calculated.          11 equilibria
Terminating at known equilibrium

Phase region boundary 51 at: -9.210E+00 -2.323E+04
** GAS
AQUEOUS
Calculated.          10 equilibria
Terminating at known equilibrium

Phase region boundary 52 at: -9.210E+00 -2.323E+04
** GAS
AQUEOUS
Calculated..         18 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 53 at: -9.210E+00 1.461E+04
AQUEOUS
** HEMATITE
Calculated.          8 equilibria
Terminating at known equilibrium

Phase region boundary 54 at: -9.210E+00 1.461E+04
AQUEOUS
** HEMATITE
Calculated.          23 equilibria
Terminating at known equilibrium

Phase region boundary 55 at: -1.975E+00 8.684E+04
AQUEOUS
** HEMATITE
Calculated.          26 equilibria
Terminating at known equilibrium

Phase region boundary 56 at: -1.975E+00 8.684E+04
AQUEOUS
** HEMATITE
Calculated..         5 equilibria
Terminating at known equilibrium

Phase region boundary 57 at: -1.262E+01 8.684E+04
** GAS
AQUEOUS
HEMATITE
Calculated..         31 equilibria

```

```

Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 58 at: -1.262E+01 8.684E+04
** GAS
AQUEOUS
HEMATITE
Calculated. 15 equilibria
Terminating at known equilibrium

Phase region boundary 59 at: -1.612E+01 7.817E+04
** GAS
AQUEOUS
HEMATITE
Calculated.. 26 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 60 at: -1.612E+01 7.817E+04
** GAS
AQUEOUS
HEMATITE
Calculated. 19 equilibria
Terminating at known equilibrium

Phase region boundary 61 at: -1.612E+01 -2.701E+04
AQUEOUS
HEMATITE
** MAGNETITE
Calculated.. 26 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 62 at: -1.612E+01 -2.701E+04
AQUEOUS
HEMATITE
** MAGNETITE
Calculated. 4 equilibria
Terminating at known equilibrium

Phase region boundary 63 at: -2.438E+00 6.600E+04
AQUEOUS
** HEMATITE
Calculated. 24 equilibria
Terminating at known equilibrium

Phase region boundary 64 at: -2.438E+00 6.600E+04
AQUEOUS
** HEMATITE
Calculated. 9 equilibria
Terminating at known equilibrium

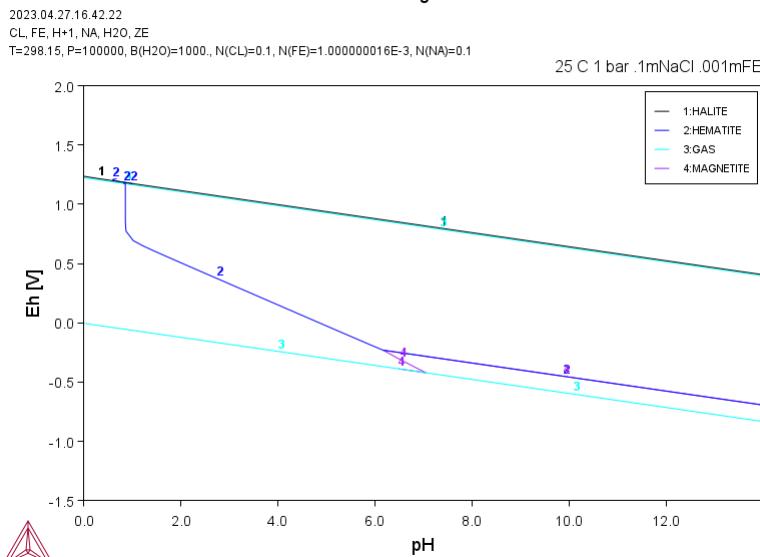
Phase region boundary 65 at: -2.103E+01 6.600E+04
** GAS
AQUEOUS
HEMATITE
Calculated.. 20 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 66 at: -2.103E+01 6.600E+04
** GAS
AQUEOUS
HEMATITE
Calculated. 26 equilibria
Terminating at known equilibrium
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\generate_console_examples\examples\tcex40\POURBAIX.POLY3
CPU time for mapping 133 seconds
POSTPROCESSOR VERSION 3.2

```

Setting automatic diagram axes
CURRENT DEVICE: TC-UNITE Driver
Plotting the diagram; please be patient!

Pourbaix Diagram



Hit RETURN to continue

Any missing phase boundary you could possibly think of? /N/: N

Change the pH/Eh steps for smoother curves? /N/: N

```

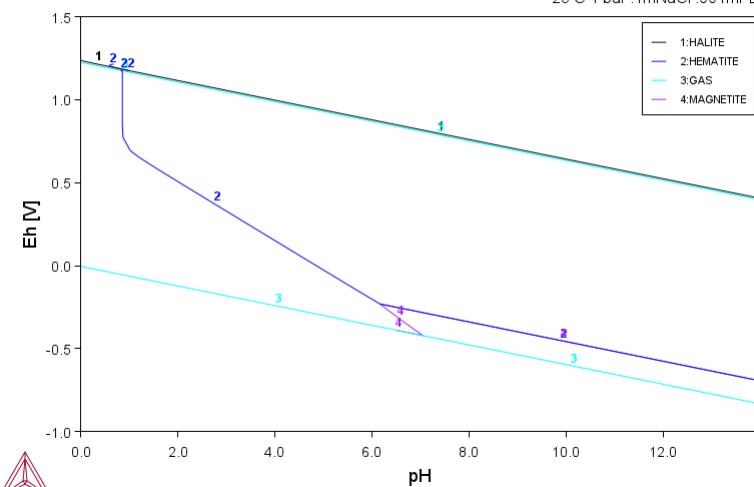
Zoom in? /N/: Y
Change scaling of X-axis? /N/: N
Change scaling of Y-axis? /N/: Y
Minimum /-1.2/: -1.0
Maximum /1.5/: 1.5
COMMAND NOT SUPPORTED IN THIS PLOT DRIVER
COMMAND NOT SUPPORTED IN THIS PLOT DRIVER
CURRENT DEVICE: TC-UNITE Driver
Plotting the diagram; please be patient!

```

Pourbaix Diagram

2023.04.27.16.42.45
 CL, FE, H+1, NA, H2O, ZE
 $T=298.15, P=100000, B(H2O)=1000, N(CL)=0.1, N(FE)=1.000000016E-3, N(NA)=0.1$

25 C 1 bar .1mNaCl .001mFE



Hit RETURN to continue

```

Another zoom? /N/: N
Change Curve-Label Option for the diagram? /N/: N
Add Label-Texts onto the Pourbaix diagram? /N/: N
Change the Subtitle of the diagram? /N/: N
Change Axis-Texts? /N/: N
Further Refine the diagram in POST Module? /N/: n
Hard copy of the diagram? /N/: n
Save X-Y coordinates of curve on text file? /N/: y
File name /POURBAIX/: TCEX40-1.EXP
FILE EXISTS, OVERWRITE (Y OR N) /N/: y

```

Modify the diagram? /N/: n

Any more diagram? /N/: N

```

SYS: y
NO SUCH COMMAND, USE HELP
SYS: 1.2
NO SUCH COMMAND, USE HELP
SYS: 0.25
NO SUCH COMMAND, USE HELP
SYS: N
NO SUCH COMMAND, USE HELP
SYS: Ags
NO SUCH COMMAND, USE HELP
SYS: 0.5
NO SUCH COMMAND, USE HELP
SYS: y
NO SUCH COMMAND, USE HELP
SYS: 8
NO SUCH COMMAND, USE HELP
SYS: 0.25
NO SUCH COMMAND, USE HELP
SYS: N
NO SUCH COMMAND, USE HELP
SYS: Aqs+Hm
NO SUCH COMMAND, USE HELP
SYS: 0.5
NO SUCH COMMAND, USE HELP
SYS: y
NO SUCH COMMAND, USE HELP
SYS: 8
NO SUCH COMMAND, USE HELP
SYS: -0.3
NO SUCH COMMAND, USE HELP
SYS: N
NO SUCH COMMAND, USE HELP
SYS: Aqs+Mt
NO SUCH COMMAND, USE HELP
SYS: 0.5
NO SUCH COMMAND, USE HELP
SYS: y
NO SUCH COMMAND, USE HELP
SYS: 6
NO SUCH COMMAND, USE HELP
SYS: 1.1
NO SUCH COMMAND, USE HELP
SYS: N
NO SUCH COMMAND, USE HELP
SYS: Gas (O2-dominant)
NO SUCH COMMAND, USE HELP
SYS: 0.5

```

NO SUCH COMMAND, USE HELP
SYS: y
NO SUCH COMMAND, USE HELP
SYS: 6
NO SUCH COMMAND, USE HELP
SYS: -0.8
NO SUCH COMMAND, USE HELP
SYS: N
NO SUCH COMMAND, USE HELP
SYS: Gas (H2-dominant)
NO SUCH COMMAND, USE HELP
SYS: 0.5
NO SUCH COMMAND, USE HELP
SYS: N
NO SUCH COMMAND, USE HELP
SYS: y
NO SUCH COMMAND, USE HELP
SYS: 3
NO SUCH COMMAND, USE HELP
SYS: 8
NO SUCH COMMAND, USE HELP
SYS: -0.45
NO SUCH COMMAND, USE HELP
SYS: Aqs+Mt
NO SUCH COMMAND, USE HELP
SYS: N
NO SUCH COMMAND, USE HELP
SYS: y
NO SUCH COMMAND, USE HELP
SYS: ?
... the command in full is HELP
ABOUT HP_CALCULATOR SET_INTERACTIVE_MODE
BACK INFORMATION SET_LOG_FILE
CLOSE_FILE MACRO_FILE_OPEN SET_PLOT_ENVIRONMENT
DISPLAY_LICENSE_INFO OPEN_FILE SET_TC_OPTIONS
EXIT SET_COMMAND_UNITS SET_TERMINAL
GOTO_MODULE SET_ECHO STOP_ON_ERROR
HELP SET_GES_VERSION
SYS: n
NO SUCH COMMAND, USE HELP
SYS: ph
NO SUCH COMMAND, USE HELP
SYS: ml(fe+2)
NO SUCH COMMAND, USE HELP
SYS: N
NO SUCH COMMAND, USE HELP
SYS: y
NO SUCH COMMAND, USE HELP
SYS: y
NO SUCH COMMAND, USE HELP
SYS: 0
NO SUCH COMMAND, USE HELP
SYS: 14
NO SUCH COMMAND, USE HELP
SYS: y
NO SUCH COMMAND, USE HELP
SYS: 1e-12
NO SUCH COMMAND, USE HELP
SYS: 1e-2
NO SUCH COMMAND, USE HELP
SYS: N
NO SUCH COMMAND, USE HELP
SYS: eh
NO SUCH COMMAND, USE HELP
SYS: tm
NO SUCH COMMAND, USE HELP
SYS: N
NO SUCH COMMAND, USE HELP
SYS: y
NO SUCH COMMAND, USE HELP
SYS: y
NO SUCH COMMAND, USE HELP
SYS: -1.0

```
NO SUCH COMMAND, USE HELP
SYS: 1.5
NO SUCH COMMAND, USE HELP
SYS: y
NO SUCH COMMAND, USE HELP
SYS: 0.1
NO SUCH COMMAND, USE HELP
SYS: 1
NO SUCH COMMAND, USE HELP
SYS: N
NO SUCH COMMAND, USE HELP
SYS: @@... Up to this point, the POURBAIX module run is complete.
SYS:
SYS: SET_INTERACTIVE
... the command in full is SET_INTERACTIVE_MODE
SYS:
```

tce41

SYS:About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

```
SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce41\tce41.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Calculation of a solubility product
SYS:
SYS: @@ Note that a TCFE database license is required
SYS: @@ to run the example.
SYS:
SYS: set-log ex41,,
SYS: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY: def-mat
... the command in full is DEFINE_MATERIAL
THERMODYNAMIC DATABASE module
Database folder: C:\jenkins\workspace\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA           /- DEFINED
DICTRA_FCC_A1 REJECTED
Database /TCFE11/: tcfe11
Major element or alloy: fe
Composition input in mass (weight) percent? /Y/:
1st alloying element: c .19
2nd alloying element: mn 1.16
Next alloying element: si .2
Next alloying element: cr .72
Next alloying element: ni .2
Next alloying element: mo .08
Next alloying element: cu .26
Next alloying element: al .027
Next alloying element: n .0089
Next alloying element:
Temperature (C) /1000/: 1056
VA           /- DEFINED
DICTRA_FCC_A1 REJECTED
REINITIATING GES .....
... the command in full is DEFINE_ELEMENTS
FE DEFINED
... the command in full is DEFINE_ELEMENTS
C DEFINED
... the command in full is DEFINE_ELEMENTS
MN DEFINED
... the command in full is DEFINE_ELEMENTS
SI DEFINED
... the command in full is DEFINE_ELEMENTS
CR DEFINED
... the command in full is DEFINE_ELEMENTS
NI DEFINED
... the command in full is DEFINE_ELEMENTS
MO DEFINED
... the command in full is DEFINE_ELEMENTS
CU DEFINED
... the command in full is DEFINE_ELEMENTS
AL DEFINED
... the command in full is DEFINE_ELEMENTS
N DEFINED
```

This database has following phases for the defined system

| | | |
|---------------|----------------|-------------|
| GAS:G | LIQUID:L | BCC_A2 |
| A2_BCC | BCC_B2 | FCC_A1 |
| A1_FCC | FCC_L12 | HCP_A3 |
| CBCC_A12 | CUB_A13 | DIAMOND_A4 |
| GRAPHITE_A9 | CEMENTITE_D011 | M23C6_D84 |
| M7C3_D101 | M6C_E93 | M5C2 |
| M3C2_D510 | MC_ETA | MC_SHP |
| KSI_CARBIDE | Z_PHASE | FE4N_LP1 |
| PI_A13 | SIGMA_D8B | HIGH_SIGMA |
| MU_D85 | P_PHASE | R_PHASE |
| CHI_A12 | C14_LAVES | C15_LAVES |
| M3SI | MN9Si2 | MN11Si19 |
| MN6Si | G_PHASE | ETA_M5SiN |
| CR3Si_A15 | FESI2_H | FESI2_L |
| MSI_B20 | M5Si3_D88 | NBNi3_D0A |
| NI3Ti_D024 | CU6Y | MOSi2_C11B |
| Mo5Si3_D8M | AL8Mn5_D810 | NB5Si3_D8L |
| MSI2_C40 | M11Si8 | M6Si5 |
| KAPPA_E21 | AL4C3_D71 | FE8Si2C |
| SIC_B3 | MN5SiC | CRZN17 |
| FEZN13 | CUZN_EPSILON | NIZN_B2 |
| NIZN_L10 | NI2ZN11_D82 | AL2FE |
| AL5Fe4 | AL5Fe2 | AL13Fe4 |
| AL7Cr | AL2Cr3 | ALN_B4 |
| Si3N4 | MN3N2 | MN6N5 |
| MnP_B31 | M2P_C22 | MULLITE:I |
| FLUORITE_C1:I | ZRO2_TETR:I | M2O3C_D53:I |
| M2O3H_D52:I | M4Si1_G3 | NI3Si12 |
| CO2Si_C37 | M2Si_TETA | NISI_B31 |
| NI3Si2 | CR5Si3_D8M | |

Reject phase(s) /NONE/: NONE
Restore phase(s) : /NONE/: NONE

.....

The following phases are retained in this system:

| | | |
|---------------|----------------|-------------|
| GAS:G | LIQUID:L | BCC_A2 |
| A2_BCC | BCC_B2 | FCC_A1 |
| A1_FCC | FCC_L12 | HCP_A3 |
| CBCC_A12 | CUB_A13 | DIAMOND_A4 |
| GRAPHITE_A9 | CEMENTITE_D011 | M23C6_D84 |
| M7C3_D101 | M6C_E93 | M5C2 |
| M3C2_D510 | MC_ETA | MC_SHP |
| KSI_CARBIDE | Z_PHASE | FE4N_LP1 |
| PI_A13 | SIGMA_D8B | HIGH_SIGMA |
| MU_D85 | P_PHASE | R_PHASE |
| CHI_A12 | C14_LAVES | C15_LAVES |
| M3SI | MN9Si2 | MN11Si19 |
| MN6Si | G_PHASE | ETA_M5SiN |
| CR3Si_A15 | FESI2_H | FEST2_L |
| MSI_B20 | M5Si3_D88 | NBNi3_D0A |
| NI3Ti_D024 | CU6Y | MOSi2_C11B |
| Mo5Si3_D8M | AL8Mn5_D810 | NB5Si3_D8L |
| MSi2_C40 | M11Si8 | M6Si5 |
| KAPPA_E21 | AL4C3_D71 | FE8Si2C |
| SIC_B3 | MN5SiC | CRZN17 |
| FEZNi3 | CUZN_EPSILON | NIZN_B2 |
| NIZN_L10 | NI2ZN11_D82 | AL2FE |
| Al5Fe4 | AL5Fe2 | AL13Fe4 |
| Al7Cr | AL2Cr3 | ALN_B4 |
| Si3N4 | MN3N2 | MN6N5 |
| MnP_B31 | M2P_C22 | MULLITE:I |
| FLUORITE_C1:I | ZRO2_TETR:I | M2O3C_D53:I |
| M2O3H_D52:I | M4Si1_G3 | NI3Si12 |
| CO2Si_C37 | M2Si1_TETA | NiSi_B31 |
| NI3Si2 | CR5Si3_D8M | |

OK? /Y/: Y
16:44:25,073 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
ELEMENTS
SPECIES
PHASES
... the command in full is AMEND_PHASE_DESCRIPTION
Creating a new composition set FCC_A1#2
... the command in full is AMEND_PHASE_DESCRIPTION
Creating a new composition set HCP_A3#2
... the command in full is AMEND_PHASE_DESCRIPTION
Suspending FLUORITE_C1 as it has net charge
Suspending M2O3C_D53 as it has net charge
Suspending M2O3H_D52 as it has net charge
Suspending MULLITE as it has net charge
Suspending ZRO2_TETR as it has net charge
PARAMETERS ...
FUNCTIONS

List of references for assessed data

'A.T. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
'Y. Tang, in TCCU2, Thermo-Calc Software AB, Stockholm, Sweden'
'X.G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar volumes'
'X.G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
'M.H.G. Jacobs, P.J. Spencer, CALPHAD, 20 (1996) 307-320; Si-Zn and Al-Si -Zn'
'N. Saunders, COST 507 Report (1998); Al-Cu'
'R. Naraghi, Thermo-Calc Software AB, Sweden, Volume data updated for TCFE9 database (TCFE v9.0, Jan, 2017).'
'S.H. Liu, Y. Du, H.L. Chen, CALPHAD, 30 (2006) 334-340; Al-Y'
'Unassessed parameter; Linear combination of unary data'
'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121-127; Molar volumes'
'M. Ghasemi, Thermo-Calc Software AB, Sweden, 2020; Unifying liquid volume database'
'B. Sundman et al., Report EUR 20315, Contract No 7210-PR/050, 2002; New Sigma model'
'P. Gustafson, TRITA-MAC 354 (1987); C-Cr-Fe-Mo-W'
'N. Saunders, COST 507 Report (1998); Cr-Ti'
'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; C15_LAVES'
'N. Dupin, Private communication, (2008); Volume data'
'B.J. Lee, KRISS, unpublished research, during 1993-1995'
'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; FE4N'
'L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2012; Molar volumes'
'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equilib., 19 (1998) 441-448; Fe-Ti'
'N. Dupin, introduction of Nb to NI15VA-4SL'
'H. Gohring, O. Fabrichnaya, A. Leineweber, E.J. Mittemeijer, Metall. Mater. Trans. A, 47A, 6173-86(2016); Fe-N, and Fe-C-N'
'N. Saunders, COST 507 Report (1998); Mn-Ti'
'W. Zheng, J. Alloys Compd., 632 (2015) 661-675'
'J-O. Andersson, CALPHAD, 12 (1988) 9-23; TRITA 0321 (1986); C-FE-MO'
'A.F. Guillermet, Z. Metallkd., 79 (1988) 524-536, TRITA-MAC 362 (1988); C -CO-NI AND C-CO-FE-NI'
'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; C14_LAVES'
'J. De Keyzer, G. Cacciamani, N. Dupin, P. Wollants, Calphad, 33, 109 -23(2009).'
'Thermo-Calc Software, Sweden, 2008: Volume data updated for \$TCFE6 database (TCFE v6, April, 2008).'
'A. Bolcavage and U.R. Kattner, J. Phase Equilib., 2, (1996); Nb-Ni'
'W. Xiong, Y. Du, X. Lu, J.C. Schuster, H. Chen, Intermetallics. 15 (2007) 1401-1408.'
'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
'I. Ansara, unpublished work (1991); Cr-Si'
'J. Grobner, H.L. Lukas, F. Aldinger, J. Alloys Comp., 220, 8-14 (1995); C -Y, Y-Al-C'
'D. Connable, J. Lacaze, P. Maugis and B. Sundman, CALPHAD, 32 (2008) 361-370; Al-C-Fe'
'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; Cementite'
'R. Naraghi, Thermo-Calc Software AB, Volume data updated for TCFE9'

database (TCFE v9.1, June, 2019).'
 'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; SIGMA and M7C3'
 'J. Grobner, H.L. Lukas, F. AlDinger, Calphad, 1996, 20 (2), 247-254; Al-C,
 Si-C, Al-Si-C'
 'N. Subasic, Licentiate Thesis, KTH, Sweden, (2000)'
 'COST2 database 1997'
 'N. Dupin, Private communication'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, Volume data updated for
 TCFE8 database (TCFE v8, May, 2015).'
 'L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2010; Molar volumes'
 'M. Seiersten, Unpublished work (1989); Al-Fe'
 'I. Ohnuma, unpublished work on B2 ordering (2001) Al-Fe'
 'B. Sundman, I. Ohnuma, N. Dupin, U.R. Kattner, S.G. Fries, Acta Mater. 57
 (2009) 2896-2908; Al-Fe'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; Molar volume Fe-Mn-Si
 and Al-Fe-Mn'
 'B.B. Lindahl, M. Selleby, CALPHAD, 43, 86-93(2013); Al-Fe-Mn'
 'C. Guo et al., Calphad 32 (2008) 637-649; Al-Fe-Zr'
 'L. Kjellqvist, Thermo-Calc Software AB, Stockholm, 2010; Unassessed
 parameter, linear combination of unary volume data'
 'B. Sundman, Modified for wrong stoichiometry (2004) Al-Fe'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2014; Al-Cr-Zn'
 'K.G. Chin, H.J. Lee, J.H. Kwak, J.Y. Kang, B.J. Lee, J. Alloys Compd.,
 505, 217-23 (2010); Al-Mn-C, Al-Fe-Mn-C'
 'Y. Du, J.C. Schuster, Z.K. Liu, R. Hu, P. Nash, W. Sun, et al.,
 Intermetallics. 16 (2008) 554-570.'
 'Y. Du, J. Wang, J. Zhao, J.C. Schuster, F. Weitzer, R. Schmid-Fetzer, M.
 Ohno, H. Xu, Z.K. Liu, S. Shang, W. Zhang, Int. J. Mater. Res., 98,
 855-71(2007); Al-Mn'
 'M.S. Kim, Y.B. Kang, J. Phase Equilib. Diffus. 36 (2015) 453-470.'
 'A. Jansson, PhD Thesis, Stockholm 1997; Al-Fe-Mn'
 'N. Saunders, COST 507 Report (1998); Al-Mo'
 'J. Miettinen, V. V. Visuri, and T. Fabritius, Acta Universitatis
 Ouluensis C Technica 758 (2020).'
 'M. Hillert and S. Jonsson, Metall. Trans. A, 23A (1992) 3141-3149; Al-Fe-N'
 'Q. Chen and B. Sundman, J. of Phase Equilibria, 19, (2), (1998), 146-160'
 'H.L. Lukas, COST 507 Report (1998); Al-N'
 'B.J. Lee, Private communication, (1999); Estimated parameter; Al-N'
 'N. Dupin, Thesis, LTPCM, France, 1995; Al-Ni, also in I. Ansara, N. Dupin,
 H.L. Lukas, B. Sundman J. Alloys Compds, 247 (1-2), 20-30 (1997)'
 'N. Dupin, I. Ansara, B. Sundman; CALPHAD, 25 (2), 279-298 (2001); Al-Cr-Ni'
 'N. Dupin, Thesis, LTPCM, France, 1995; Al-Ni-Ta'
 'N. Dupin, Private communication, (2003); AD/SN'
 'L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2013; Reassessed
 solubility of Al, Cr, Fe, Ni in Mn203. When Mn203 is modelled as the
 same phase as cubic Y2O3 (M203C).'
 'H. Mao, M Selleby and B Sundman, J. Am. Cera. Soc., 88 (2005) 2544-2551;
 Al203-SiO2'
 'TCS, TCMP2 - TCS MateriAL2S3 Processing Database v2 (2004)'
 'A.V. Khvan, B. Hallstedt, K. Chang, CALPHAD, 39, 54-61(2012); C-Cr-Nb'
 'J-O. Andersson, CALPHAD, 11 (1987) 271-276; TRITA 0314; C-CR'
 'J. Bratberg, Z. Metallkd., 96 (2005) 335-344; Fe-Cr-Mo-C'
 'B.J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
 'C. Qui, ISIJ International, 32 (1992), 1117-1127; Trita-MAC 482 (1992)
 Revision; C-Cr-Fe-Mo'
 'P. Gustafson, Metall. Trans. A, 19A (1988) 2547-2554; TRITA-MAC 348,
 (1987); C-CR-FE-W'
 'P. Villars, L.D. Calvert. Pearson's handbook of crystallographic data for
 intermetallic phases, Metals park, Ohio 1985: American society for
 metals'
 'B.J. Lee, Metall. Trans. A, 24A (1993) 1017-1025; Fe-Cr-Mn-C'
 'P. Gustafson, Inst. Met. Res. (IM-2549, 1990); C-CU-Fe'
 'Chandrakasekan et al., (1987) provisional; CU-Fe-P-C'
 'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
 'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
 'B. Hallstedt, D. Djurovic, J. von Appen, R. Dronskowski, A. Dick, F.
 Koermann, T. Hickel, J. Neugebauer, CALPHAD, 34, 129-33(2010); Fe-C'
 'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, Calphad 35.4
 (2011) 479-491; Fe-Mn-C'
 'W. Huang, Metall. Trans. A, 21A (1990) 2115-2123; TRITA-MAC 411 (Rev
 1989); C-FE-MN'
 'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, CALPHAD, 34, 279
 -85(2010); Mn-C'
 'J.H. Shim, C.S. Oh, D.N. Lee, Metall. Mater. Trans. B. 27 (1996) 955-966;
 Ti-Mo-C'
 'A. Gabriel, C. Chatillon, and I. Ansara, published in High Temp. Sci.
 (Parameters listed in CALPHAD, 11 (1987) 203-218); C-NI'
 'A. Gabriel, P. Gustafson, and I. Ansara, CALPHAD, 11 (1987) 203-218;
 TRITA-MAC 285 (1986); C-FE-NI'
 'A.F. Guillermet and G. Grimvall, J. Phys. Chem. Solids, 1992, 53, 105-125;
 Molar volumes'
 'P. Franke; revision of C-Si, Fe-Si and C-Fe-Si'
 'J. Lacaze and B. Sundman, Metall. Mater. Trans. A, 22A (1991) 2211-2223;
 Fe-Si and Fe-Si-C'
 'NPL, Unpublished work (1989); C-Mn-Si'
 'K. Zeng and M. Hamalainen, CALPHAD, 19 (1995) 93-104; Cr-Cu'
 'B. Sundman, Private communication, 2(1999); Estimated parameter'
 'W.H. Sun, S.H. Liu, added to make this phase less stable, 2010'
 'B.J. Lee, CALPHAD, 17 (1993) 251-268; revision of Fe-Cr and Fe-Ni liquid'
 'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270
 (1986); CR-FE'
 'K. Frisk, Metall. Trans. A, 21A (1990) 2477-2488; TRITA 0409 (1989); CR
 -FE-N'
 'J-O. Andersson, Metall. Trans. A, 19A (1988) 1385-1394; TRITA 0322 (1986);
 CR-FE-MO'
 'B.J. Lee, unpublished work at KTH (1999); update of steel database'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2019; Cr-Fe-Nb'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2014; Cr-Fe-Zn'
 'B.J. Lee, Metall. Trans. A, 24A (1993) 1919-1933; Cr-Mn, Fe-Cr-Mn'
 'K. Frisk, CALPHAD, 17 (1993) 335-349; Cr-Mn-N'
 'SGTE (2008): SSOL4-SGTE Substance Database V4.1, provided by Thermo-Calc
 Software'
 'K. Frisk, KTH Report D 60 (1984); CR-MO'
 'B. Sundman, Private communication; FCC parameter same as BCC; Cr-Mo'
 'J-O. Andersson, TRITA-MAC 323 (1986); C-CR-FE-MO'
 'K. Frisk, TRITA-MAC 429 (1990); CR-MO-NI'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2015; C14_LAVES'
 'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; Z_PHASE'
 'K. Frisk, CALPHAD, 15 (1991) 79-106; TRITA-MAC 393 (1989); CR-N, FE-N, MO
 -N, CR-MO-N'
 'Estimated parameter for solubility of N in cementite, 1999'
 'A.T. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); CR-NI'
 'L.L. Zhu, H.Y. Qi, L. Jiang, Z.P. Jin, J.C. Zhao, Intermetallics. 64
 (2015) 86-95; Cr-Ru and Cr-Ni-Ru'
 'Y.Du and J.C.Schuster, J. Phase Equilibria, 21(3) 281-86(2000); Cr-Si'
 'N. Dupin, Private communication; Si systems'

'A. Jacob, E. Povoden-Karadeniz, E. Kozeschnik, Calphad, 56 (2017) 80-91.
 'I. Ansara and A. Jansson, TRITA-MAC 533 (1993); Cu-Fe'
 'N. Zou et al., Calphad 64 (2019) 175-184'
 'C.Y. He, J. Alloys Compd., 457, 233-238 (2008); Cu-Mn'
 'C.P. Wang et al., J. Phase Equil. 21 (2000) 54-62; Cu-Fe-Mo and Cu-Fe-Nb'
 'Same or similar interaction as in the corresponding stable phase'
 'K. Frisk, IM-2929, Swedish Inst. Met. Res., (1992); Cu-N, Fe-Cu-N'
 'L. Kjellqvist, Thermo-Calc Software AB (2014); FROST project'
 'S. an Mey, CALPHAD, 16 (1992) 255-260; Cu-Ni'
 'A. Jansson, TRITA-MAC 340 (1987); CU-Fe-Ni'
 'M. Jacobs (1991), Revised by T. Buehler (1997), COST 507 Report; Cu-Si'
 'S.G. Fries, H.L. Lukas, R. Konetzki, R. Schmid-Fetzer, J. Phase Equil., 15(1994) 606-614; Cu-Y'
 'H. Mao, Thermo-Calc Software AB, Sweden, 2013; Molar volumes'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2014; Unifying HCP_ZN with HCP_A3'
 'W. Huang, CALPHAD, 13 (1989) 243-252; TRITA-MAC 388 (rev 1989); FE-MN'
 'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
 'S. Liu, B. Hallstedt, D. Music, Y. Du, CALPHAD, 38 (2012) 43-58; Mn-Nb and Fe-Mn-Nb'
 'A. Markstrom, Thermo-Calc software AB, Sweden, 2011'
 'A.F. Guillermet, CALPHAD, 6 (1982) 127-140; (sigma phase revised 1986); TRITA-MAC 200 (1982); FE-MO'
 'K. Frisk, TRITA-MAC 428 (1990); FE-MO-NI'
 'H.K. Danielsen and J. Hald, CALPHAD, 31 (2007) 505-514; Z-PHASE'
 'H. Du, J. Phase Equil., 14, 682-93(1993); Fe-N, Fe-C-N'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; MSC2'
 'C. Qiu, Metall. Trans. A, 24A (1993) 629-645; Fe-Mn-N'
 'A.T. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); FE-NI'
 'L. Zhang, J. Wang, Y. Du, R. Hu, P. Nash, X.G. Lu, et al., Acta Mater. 57 (2009) 5324-5341; Al-Fe-Ni'
 'L.J. Zhang, Int.J. Mater. Res., 100(2) 160-175 (2009), Fe-Mn-Ni'
 'S. Cotes, A.F. Guillermet, M. Sade, J. Alloys Compd., 208(1998) 168-177'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2019; Cr-Fe-Nb-Si'
 'A. Forsberg and J. Agren, J. Phase Equil., 14 (1993) 354-363; Fe-Mn-Si'
 'R. Naraghi, Thermo-Calc Software AB, Sweden (2019); Fe-Ni-Si'
 'J. Miettinen, G. Vassilev, J. Phase Equil. Diffus., 37(5) 2016, 283-290; Fe-P-Si'
 'C. Qiu and A.F. Guillermet, Z. Metallkd., 84 (1993) 11-12; Mn-N'
 'A. Markstrom, Thermo-Calc Software AB, Sweden, 2010; Molar volumes'
 'Shuhong Liu, unpublished work (2010), Mn-Ni, Al-Mn-Ni, Mn-Ni-Zn, Al-Cu-Fe-Mg -Mn-Si'
 'C.P. Guo, Intermetallics, 13(5), 525-534, (2005), Mn-Ni'
 'M. Chen, B. Hallstedt, L. J. Gauckler, J. Alloys Compd., 393 (2005) 114 -21; Mn-Y-O'
 'M. Chen, B. Hallstedt, L.J. Gauckler, Solid State Ionics, 176 (2005) 1457 -64; Mn-Zr-O, Mn-Y-Zr-O'
 'J. Miettinen, CALPHAD, 28 (2004) 313-320; Mn-Zn'
 'K. Frisk and B. Uhrenius, Metall. Mater. Trans. A, 27A (1996) 2869-2880; Mo-C-N, Fe-Mo-C-N'
 'K. Frisk, CALPHAD, 14 (1990) 311-320; MO-NI'
 'R. Naraghi, Thermo-Calc Software AB, Sweden (2018); Fe-Mo-Ni, Mo-Ni-Si, C14'
 'Y. Liu, G. Shao, P. Tsakiroopoulos, Intermatallitics 8 (2000) 953-962; Mo-Si, Al-Mo-Si'
 'A. Kusoffsky et al., Work within CCT-Applied Stainless steels, 2004; IM -2004-549; Fe-Cr-Si, Fe-N-Ni, Fe-Ni-Si, Fe-Cr-Cu, Fe-Cu-Mo, Cr-Mo-N-Ni, Fe-Cr-N-Ni, Fe-Al-Cr-Ni'
 'R. Naraghi, Thermo-Calc Software AB, Sweden (2015); FROST project'
 'K. Frisk, Z. Metallkd., 82 (1991) 59-66; TRITA-MAC 414 (1989); Fe-Ni-N'
 'K. Frisk, Int. J. Thermophys., 12 (1990) 417-431; TRITA-MAC 419 (1990); N -NI'
 'X. Ma, C. Li, F. Wang, W. Zhang, CALPHAD, 27 (2003) 383-388; N-Si'
 'Thermo-Calc Software, Sweden, 2009; Volume data updated for \$TCFE6 database (TCFE v6, November, 2009).'
 'L. Kjellqvist, Thermo-Calc Software AB (2013) estimated parameter; Ni-Zr-O'
 'T. Tokunaga, K. Nishio, H. Ohtani, M. Hasebe, Calphad, 27 (2003), 161-168; Ni-Si'
 'N. Dupin; L12 general relations, equivalence of 2 sublattice formalism with four sublattice formalism'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; Checking ternary P systems'
 'B. Sundman, Private communication (2003-4); Refitted Fe-Ni-Si'
 'W.W. Zhang, unpublished (2010), Fe-Ni-Si'
 'R. Naraghi, Thermo-Calc Software AB, Sweden (2019); M4Si1_G3'
 'J. Miettinen, CALPHAD, 27 (2003) 263-274; Cu-Ni-Zn'
 'H. Liang, Y.A.Chang, J. Phase Equil. 19 (1998) 25-37'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2016; Fe-Al-Cr-Ni'
 'H-L Chen, J. Mater. Res., 24(10) 3154-3164 (2009); Al-Cu-Fe'
 'C.Y. He, unpublished work (2008), Al-Cu-Mn'
 'H.L. Chen, unpublished work (2007), Al-Cu-Ni'
 'N. Dupin 2008, revision of mu and sigma in many systems'
 'L. Kjellqvist and M. Selleby, Unpublished research (2013); Al-Fe-Si-O'
 'A. Walnsch et al., Calphad 64 (2019) 78-89; Al-Mn-Ni'
 'A.V. Khvan, B. Hallstedt, C. Broeckmann, CALPHAD, 46, 24-33(2014); Cr-Fe-C'
 'J-O. Andersson, Metall. Trans. A, 19A (1988) 627-636 TRITA 0207 (1986); C -CR-FE'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2016; FCC Fe-Cr-C and C-Cr-Ni'
 'J. Bratberg, Thermo-Calc Software AB, Sweden, 2008; Fe-Cr-Mo-V-W-C'
 'P. Gustafsson, Inst. Met. Res. (Sweden) (1990); Estimations of C-CR-FE-V, C-CR-FE-MO-V-W, FE-N-W, FE-MN-N, FE-N-SI, CR-N-V, C-CR-N, FE-MO-N, CR -N-W, CR-TI-N'
 'NPL, unpublished work (1989); C-Cr-Ni'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; C-Cr-Si'
 'Y.Du, J.C.Schuster, J.Am.Ceram.Soc., 83 (8) 2067-73 (2000); C-Cr-Si'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; Adjusting hcp'
 'S. Nagakura, Transactions of the Iron and Steel Institute of Japan, 8 (1968) 265-294; Molar volumes'
 'I.K. Kupalova, V.I. Pavlova, High Speed Steels: Physical Properties, Prop. Data Updat. 2 (1988) 67-78; Molar volumes'
 'H. Du and M. Hillert, TRITA-MAC 435 (1990); C-Fe-N'
 'J. Miettinen and B. Hallstedt, CALPHAD, 22 (1998) 231-256; Fe-Si and Fe -Si-C'
 'W. Zheng et al., J. Iron Steel Res. Int. 24(2) (2017) 190-197'
 'C.P. Wang, D.X. Huang, J.J. Zhu, S.Y. Yang, X.J. Liu, J. Phase Equilib. Diffus. 35 (2014) 314-325; Cr-Cu-Mo and Cr-Cu-W'
 'T. Ikoma, M. Kajihara, Mater. Sci. Eng. A, 437 (2006) 293-300; Cr-Cu-Ni'
 'C. Qiu, Metall. Trans. A, 24A (1993) 2393-2409; Cr-Fe-Mn-N'
 'A. Markstrom, Thermo-Calc Software AB (2013), Extrapolations, assumptions adjustment'
 'B. Sundman, estimated parameter (2000); Cr-Ni-Mo'
 'B.J. Lee, Private communication, (2000); Estimated parameter'
 'A. Kusoffsky, Work within CCT-Applied Stainless steels, 2003; IM-2003-532; Fe-Cr-N, Fe-C-Cr-N, Fe-Cr-Mo-N, Fe-Cr-Mn-N'
 'A. Markstrom, Thermo-Calc Software AB, Sweden, 2017; FROST'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; Cr-Fe-Si'

'M. Lindholm, J. Phase Equilib., 18.5 (1997) 432; Cr-Fe-Si'
 'J. Kunze, P. Broz,
 I. Stloukal, Steel Research 67(1996) 279-284.'
 'K. Frisk, TRITA-MAC 422 (1990); CR-FE-N-NI'
 'J.C. Schuster and Y.Du, Metall. Mater. Trans.A, 31A(7) 1795-803(2000); Cr
 -Ni-Si.'
 'R. Naraghi, Thermo-Calc Software AB, Sweden (2019); Cr-Ni-Si'
 'L. Zhang, Y. Du, Q. Chen, H. Xu, F. Zheng, C. Tang, H. Chen, Int. J.
 Mater. Res. 99 (2008) 1306-1318; Cu-Fe-Mn'
 'J. Miettinen, CALPHAD, 27 (2003) 389-394, Cu-Fe-Si'
 'W.H. Sun, CALPHAD, 33, 642-649(2009),Cu-Mn-Ni'
 'K. Frisk, TRITA-MAC 433 (1990); FE-CR-MO-NI-N'
 'J. Miettinen, CALPHAD, 22 (1998) 275-300; Fe-Mo-Si'
 'B. Hu, Unpublished (2010); Mn-Ni-Si,Al-Cu-Fe-Ni'
 'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; Carbonitrides and
 M23C6'
 'J. Bratberg, Thermo-Calc Software AB, Sweden, 2008; Solubilities in M6C'
 'R. Naraghi, Thermo-Calc Software AB, Sweden (2019); Cheking the binaries.'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2019; ETA_M5SIN'
 'M. J. Assael, High Temp. High Press., 41 (2012); Sb, Pb, Bi, Ni, Ag'
 'M. Ghasemi, Thermo-Calc Software AB, Sweden, 2019; Viscosity of metallic
 liquid'
 'M. J. Assael, J. Phys. Chem. Ref. Data 39 (2010) 033105; Cu, Sn'
 'M. J. Assael, J. Phys. Chem. Ref. Data 35 (2006) 285; Fe, Al'
 'M. J. Assael, J. Phys. Chem. Ref. Data 41 (2012) 033101; Cd, Co, Ga, In,
 Hg, Si, Tl, Zn'
 'Q. Chen, Thermo-Calc Software AB (2014), L12 constraints'
 'M Ghasemi, Thermo-Calc Software AB: assessing the surface tension of
 metallic liquid'

-OK-

Should any phase have a miscibility gap check? /N/: N

Using global minimization procedure
 Calculated 60421 grid points in 17 s
 Found the set of lowest grid points in 0 s
 Calculated POLY solution 3 s, total time 20 s

POLY:

POLY: l-e,,

... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium = 1, label A0 , database: TCFE11

Conditions:

T=1329.15, W(C)=1.9E-3, W(MN)=1.16E-2, W(SI)=2E-3, W(CR)=7.2E-3, W(NI)=2E-3,
 W(MO)=8E-4, W(CU)=2.6E-3, W(AL)=2.7E-4, W(N)=8.9E-5, P=100000, N=1
 DEGREES OF FREEDOM 0

Temperature 1329.15 K (1056.00 C), Pressure 1.000000E+05
 Number of moles of components 1.000000E+00, Mass in grams 5.53245E+01
 Total Gibbs energy -6.89246E+04, Enthalpy 3.91344E+04, Volume 7.33623E-06

| Component | Moles | W-Fraction | Activity | Potential | Ref.stat |
|-----------|------------|------------|------------|-------------|----------|
| AL | 5.5361E-04 | 2.7000E-04 | 1.6366E-09 | -2.2357E+05 | SER |
| C | 8.7517E-03 | 1.9000E-03 | 8.6866E-03 | -5.2449E+04 | SER |
| CR | 7.6609E-03 | 7.2000E-03 | 7.7406E-05 | -1.0462E+05 | SER |
| CU | 2.2636E-03 | 2.6000E-03 | 1.0186E-04 | -1.0158E+05 | SER |
| FE | 9.6245E-01 | 9.7154E-01 | 2.2977E-03 | -6.7145E+04 | SER |
| MN | 1.1682E-02 | 1.1600E-02 | 1.1151E-05 | -1.2603E+05 | SER |
| MO | 4.6133E-04 | 8.0000E-04 | 1.0256E-05 | -1.2695E+05 | SER |
| N | 3.5153E-04 | 8.9000E-05 | 5.1866E-07 | -1.5993E+05 | SER |
| NI | 1.8853E-03 | 2.0000E-03 | 2.6599E-06 | -1.4187E+05 | SER |
| SI | 3.9398E-03 | 2.0000E-03 | 5.0540E-09 | -2.1111E+05 | SER |

FCC_A1#1 Status ENTERED Driving force 0.0000E+00
 Moles 9.9975E-01, Mass 5.5319E+01, Volume fraction 9.9978E-01 Mass fractions:
 FE 9.71631E-01 CR 7.20067E-03 NI 2.00019E-03 C 1.90018E-03 AL 2.09122E-04
 MN 1.16011E-02 CU 2.60024E-03 SI 2.00019E-03 MO 8.00074E-04 N 5.73920E-05

ALN_B4 Status ENTERED Driving force 0.0000E+00
 Moles 2.4973E-04, Mass 5.1181E-03, Volume fraction 2.1734E-04 Mass fractions:
 AL 6.58274E-01 SI 0.000000E+00 MO 0.000000E+00 FE 0.000000E+00 CR 0.000000E+00
 N 3.41726E-01 NI 0.000000E+00 MN 0.000000E+00 CU 0.000000E+00 C 0.000000E+00

POLY:Hit RETURN to continue

POLY:

POLY: def-dia

... the command in full is DEFINE_DIAGRAM

Same elements as before? /Y/: Y

For binary or ternary diagrams you may prefer the special modules

You must specify a value for all compositions and the temperature even if you want to use it as axis.

Mass (weight) percent of AL / .027/: .027
Mass (weight) percent of C / .19/: .19
Mass (weight) percent of CR / .72/: .72
Mass (weight) percent of CU / .26/: .26
Mass (weight) percent of MN / 1.16/: 1.16
Mass (weight) percent of MO / .08/: .08
Mass (weight) percent of N / .0089/: .0089
Mass (weight) percent of NI / .2/: .2
Mass (weight) percent of SI / .2/: .2

Temperature (C) /1056/: 1056

Using global minimization procedure

Using already calculated grid

Found the set of lowest grid points in 0 s

Calculated POLY solution 1 s, total time 1 s

You must now set an independent axis for your diagram as one of the following conditions:

Condition 1 is temperature (Celsius)
 Condition 2 is mass percent of C
 Condition 3 is mass percent of MN
 Condition 4 is mass percent of SI
 Condition 5 is mass percent of CR
 Condition 6 is mass percent of NI
 Condition 7 is mass percent of MO
 Condition 8 is mass percent of CU
 Condition 9 is mass percent of AL
 Condition 10 is mass percent of N

Give the number of the condition to vary /1/: 1

Minimum value (C) /800/: 650

Maximum value (C) /1800/: 1200

The second axis can be another of the conditions above and you will then calculate a phase diagram.

Or you may want to plot how some other quantities depend on the selected condition and you will then calculate a "property" diagram.

In addition to the conditions above you may use these selected dependent quantities on the vertical axis:
Dependent 11 is mass fraction of all phases
Dependent 12 is composition of a phase
Dependent 13 is the fraction of a component in all phases
(In the post processor you may select many other quantities)
Give the number of the quantity on second axis /11/: 11 tcex41
No initial equilibrium, using default
Step will start from axis value 1329.15
...OK

Phase Region from 1329.15 for:
ALN_B4
FCC_A1#1
Global check of removing phase at 1.38213E+03
Calculated 8 equilibria
Phase Region from 1382.13 for:
FCC_A1#1
Global test at 1.45915E+03 OK
Terminating at 1473.15
Calculated 13 equilibria
Phase Region from 1329.15 for:
ALN_B4
FCC_A1#1
Global test at 1.24915E+03 OK
Global test at 1.14915E+03 OK
Global check of adding phase at 1.07187E+03
Calculated 28 equilibria
Phase Region from 1071.87 for:
ALN_B4
BCC_A2
FCC_A1#1
Global test at 9.99150E+02 OK
Global check of adding phase at 9.95086E+02
Calculated 11 equilibria
Phase Region from 995.086 for:
ALN_B4
BCC_A2
CEMENTITE_D011
FCC_A1#1
Global check of removing phase at 9.68450E+02
Calculated 6 equilibria
Phase Region from 968.450 for:
ALN_B4
BCC_A2
CEMENTITE_D011
Terminating at 923.150
Calculated 8 equilibria
*** Buffer saved on file: c:\jenkins\workspace\generate_console_examples\examples\tcex41\tcex41.POLY3
POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

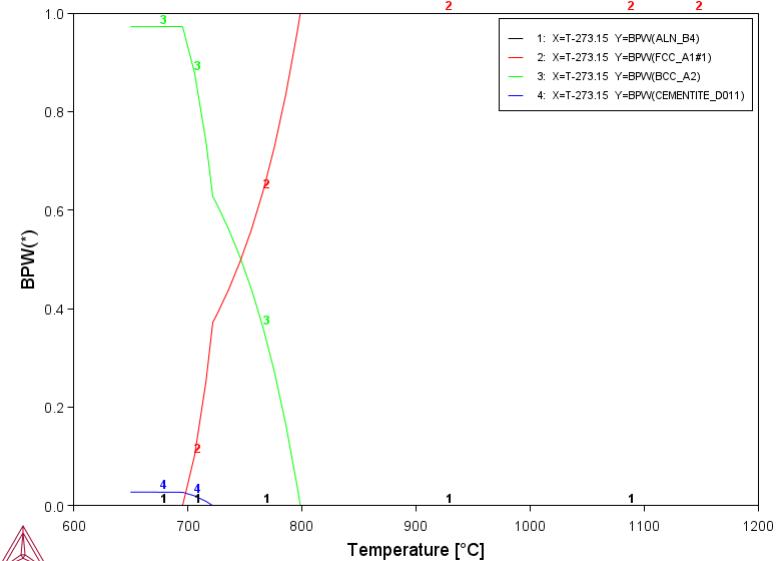
... the command in full is REINITIATE_PLOT_SETTINGS
POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

... the command in full is SET_AUTOMATIC_DIAGRAM_A

Setting automatic diagram axes

... the command in full is PLOT_DIAGRAM



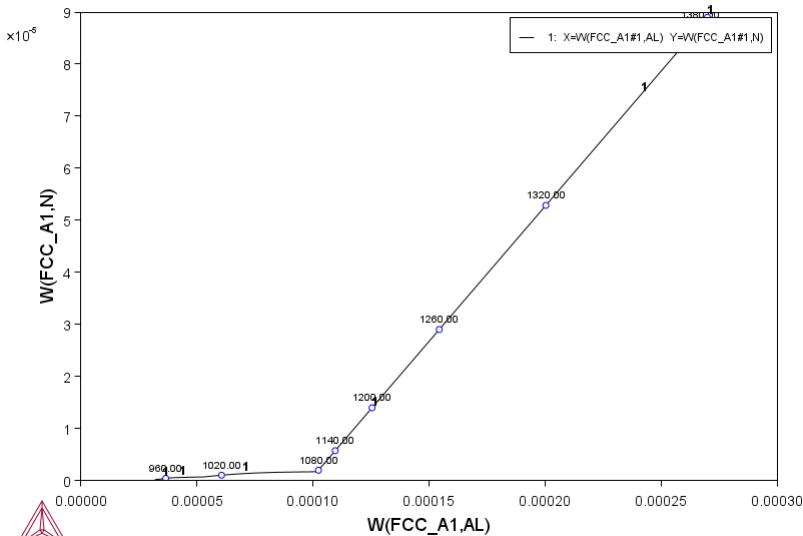
POST:
POST:Hit RETURN to continue
POST:
POST: s-d-a x w(fcc_a1,a1)
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y w(fcc_a1,n)
... the command in full is SET_DIAGRAM_AXIS
POST:
POST: s-d-a z t
... the command in full is SET_DIAGRAM_AXIS
POST:
POST:
POST: set-title example 41a
POST:

```

POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAIFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

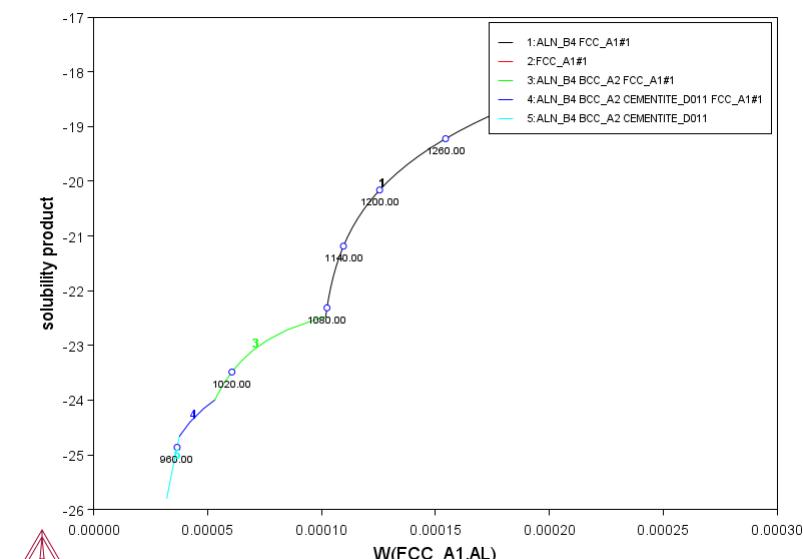
example 41a



```

POST:
POST:
POST: Hit RETURN to continue
POST: @@ Now let's go back to POLY3 and enter a function
POST: @@ corresponding to the solubility product
POST:
POST: back
POLY: enter fun
... the command in full is ENTER_SYMBOL
Name: sp
Function: log(w(fcc_a1,al)*w(fcc_a1,n));
POLY:
POLY: @@ Now go back to POST and plot the entered function
POLY: post
POST:
POST: s-d-a y sp
... the command in full is SET_DIAGRAM_AXIS
POST: s-lab b
... the command in full is SET_LABEL_CURVE_OPTION
POST: s-a-t-s y n solubility product
... the command in full is SET_AXIS_TEXT_STATUS
POST:
POST: set-title example 41b
POST:
POST: sel-plot new
... the command in full is SELECT_PLOT
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAIFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```



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POST:
POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:

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-85(2010); Mn-C'
 'W. Huang, CALPHAD, 13 (1989) 243-252; TRITA-MAC 388 (rev 1989); FE-MN'
 'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
 'S. Liu, B. Hallstedt, D. Music, Y. Du, CALPHAD, 38 (2012) 43-58; Mn-Nb
 and Fe-Mn-Nb'
 'A. Markstrom, Thermo-Calc software AB, Sweden, 2011'
 'L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2013; Reassessed
 solubility of Al, Cr, Fe, Ni in Mn₂O₃. When Mn₂O₃ is modelled as the
 same phase as cubic Y₂O₃ (M2O3C).'
 'M. Chen, B. Hallstedt, L. J. Gauckler, J. Alloys Compd., 393 (2005) 114
 -21; Mn-Y-O'
 'M. Chen, B. Hallstedt, L.J. Gauckler, Solid State Ionics, 176 (2005) 1457
 -64; Mn-Zr-O, Mn-Y-Zr-O'
 'J. Miettinen, CALPHAD, 28 (2004) 313-320; Mn-Zn'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, Volume data updated for
 TCFE8 database (TCFE v8, May, 2015).'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; Adjusting hcp'
 'M. Ghasemi, Thermo-Calc Software AB, Sweden, 2019; Viscosity of metallic
 liquid'
 'M. J. Assael, J. Phys. Chem. Ref. Data 35 (2006) 285; Fe, Al'
 'M Ghasemi, Thermo-Calc Software AB: assessing the surface tension of
 metallic liquid'
 -OK-

TDB_TCFE11: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32

POLY:

POLY: @@ To work with u-fractions, just set the status of component C to SPECIAL

POLY:

POLY: c-s com c

... the command in full is CHANGE_STATUS

Status: /ENTERED/: special

POLY: l-st

... the command in full is LIST_STATUS

Option /CPS/:

*** STATUS FOR ALL COMPONENTS

| COMPONENT | STATUS | REF. STATE | T (K) | P (Pa) |
|-----------|---------|------------|-------|--------|
| VA | ENTERED | SER | | |
| C | SPECIAL | SER | | |
| FE | ENTERED | SER | | |
| MN | ENTERED | SER | | |

*** STATUS FOR ALL PHASES

| PHASE | STATUS | DRIVING FORCE | MOLES |
|----------------|---------|---------------|--------------|
| NBNi3_D0A | ENTERED | 0.000000E+00 | 0.000000E+00 |
| M7C3_D101 | ENTERED | 0.000000E+00 | 0.000000E+00 |
| M23C6_D84 | ENTERED | 0.000000E+00 | 0.000000E+00 |
| KSI_CARBIDE | ENTERED | 0.000000E+00 | 0.000000E+00 |
| HCP_A3 | ENTERED | 0.000000E+00 | 0.000000E+00 |
| G_PHASE | ENTERED | 0.000000E+00 | 0.000000E+00 |
| FE4N_LP1 | ENTERED | 0.000000E+00 | 0.000000E+00 |
| FCC_L12 | ENTERED | 0.000000E+00 | 0.000000E+00 |
| FCC_A1 | ENTERED | 0.000000E+00 | 0.000000E+00 |
| DIAMOND_A4 | ENTERED | 0.000000E+00 | 0.000000E+00 |
| CUZN_EPSILON | ENTERED | 0.000000E+00 | 0.000000E+00 |
| CUB_A13 | ENTERED | 0.000000E+00 | 0.000000E+00 |
| CEMENTITE_D011 | ENTERED | 0.000000E+00 | 0.000000E+00 |
| CBCC_A12 | ENTERED | 0.000000E+00 | 0.000000E+00 |
| C15_LAVES | ENTERED | 0.000000E+00 | 0.000000E+00 |
| C14_LAVES | ENTERED | 0.000000E+00 | 0.000000E+00 |
| BCC_B2 | ENTERED | 0.000000E+00 | 0.000000E+00 |
| BCC_A2 | ENTERED | 0.000000E+00 | 0.000000E+00 |
| AL5FE4 | ENTERED | 0.000000E+00 | 0.000000E+00 |
| LIQUID | ENTERED | 0.000000E+00 | 0.000000E+00 |
| GAS | ENTERED | 0.000000E+00 | 0.000000E+00 |

*** STATUS FOR ALL SPECIES

| C | ENTERED | C4 | ENTERED | FE | ENTERED | FE+4 | ENTERED | MN+3 | ENTERED |
|----|---------|-----|---------|------|---------|------|---------|------|---------|
| C2 | ENTERED | C5 | ENTERED | FE+2 | ENTERED | MN | ENTERED | MN+4 | ENTERED |
| C3 | ENTERED | C60 | ENTERED | FE+3 | ENTERED | MN+2 | ENTERED | VA | ENTERED |

POLY:

POLY: Hit RETURN to continue

POLY: s-c t=900 p=1e5 n=1 w(c)=0.002 w(mn)=0.025

... the command in full is SET_CONDITION

POLY: c-e

... the command in full is COMPUTE_EQUILIBRIUM

Using global minimization procedure

Calculated 23045 grid points in 13 s
 Found the set of lowest grid points in 0 s
 Calculated POLY solution 1 s, total time 14 s

POLY: l-e

... the command in full is LIST_EQUILIBRIUM

OUTPUT TO SCREEN OR FILE /SCREEN/:

Options /WVCS/: WVCS

Output from POLY-3, equilibrium = 1, label A0 , database: TCFE11

Conditions:

T=900, P=100000, N=1, W(C)=2E-3, W(MN)=2.5E-2

DEGREES OF FREEDOM 0

Temperature 900.00 K (626.85 C), Pressure 1.000000E+05
 Number of moles of components 1.00000E+00, Mass in grams 5.54204E+01
 Total Gibbs energy -3.64344E+04, Enthalpy 2.02443E+04, Volume 7.24781E-06

| Component | Moles | W-Fraction | Activity | Potential | Ref.stat |
|-----------|------------|------------|------------|-------------|----------|
| C | 9.2099E-03 | 2.0000E-03 | 1.6686E-01 | -1.3399E+04 | SER |
| FE | 9.6562E-01 | 9.7500E-01 | 8.1714E-03 | -3.5972E+04 | SER |
| MN | 2.5169E-02 | 2.5000E-02 | 2.3252E-04 | -6.2607E+04 | SER |

| BCC_A2 | Status | ENTERED | Driving force | 0.0000E+00 |
|---|--------|---------|-----------------|------------|
| Moles 9.6367E-01, Mass 5.3797E+01, Volume fraction 9.6992E-01 | | | Mass fractions: | |
| FE 9.81934E-01 MN 1.80378E-02 C 2.86448E-05 | | | | |

| CEMENTITE_D011 | Status | ENTERED | Driving force | 0.0000E+00 |
|---|--------|---------|-----------------|------------|
| Moles 3.6326E-02, Mass 1.6238E+00, Volume fraction 3.0085E-02 | | | Mass fractions: | |
| FE 6.78866E-01 MN 2.53958E-01 C 6.71754E-02 | | | | |

POLY: s-a-v 1 w(c) 0 0.02

... the command in full is SET_AXIS_VARIABLE

Increment /5B-04/: 2.5E-04

POLY: s-a-v 2 t 800 1200 10

... the command in full is SET_AXIS_VARIABLE

POLY: sa tcez42a y

... the command in full is SAVE_WORKSPACES

POLY: map

Version S mapping is selected

```

Generating start equilibrium  1
Generating start equilibrium  2
Generating start equilibrium  3
Generating start equilibrium  4
Generating start equilibrium  5
Generating start equilibrium  6
Generating start equilibrium  7
Generating start equilibrium  8
Generating start equilibrium  9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Tie-lines not in the plane of calculation
Generating start point  1
Generating start point  2
Generating start point  3
Generating start point  4
Generating start point  5
Generating start point  6
Generating start point  7
Generating start point  8
Generating start point  9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Generating start point 27
Generating start point 28
Generating start point 29
Generating start point 30
Working hard
Generating start point 31
Generating start point 32

Phase region boundary  1 at:  1.965E-02  8.100E+02
  BCC_A2
  CEMENTITE_D011
  ** DIAMOND_A4
Calculated..          15 equilibria
Terminating at axis limit.

Phase region boundary  2 at:  1.632E-02  8.000E+02
  BCC_A2
  CEMENTITE_D011
  ** DIAMOND_A4
Calculated..          17 equilibria
Terminating at axis limit.

Phase region boundary  3 at:  1.965E-02  8.100E+02
  BCC_A2
  CEMENTITE_D011
  ** DIAMOND_A4
Calculated..          3 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  4 at:  2.500E-04  8.899E+02
  BCC_A2
  CEMENTITE_D011
  ** FCC_A1
Calculated..          3 equilibria

Phase region boundary  5 at:  1.687E-05  8.830E+02
  BCC_A2
  ** CEMENTITE_D011
  ** FCC_A1
Calculated..          22 equilibria

Phase region boundary  6 at:  1.687E-05  8.830E+02
  BCC_A2
  ** FCC_A1
Calculated..          22 equilibria

Phase region boundary  7 at:  1.687E-05  8.830E+02
  BCC_A2
  ** CEMENTITE_D011
Calculated..          10 equilibria
Terminating at axis limit.

Phase region boundary  8 at:  1.687E-05  8.830E+02
  BCC_A2
  ** CEMENTITE_D011
  FCC_A1
Calculated..          33 equilibria

Phase region boundary  9 at:  6.844E-03  9.776E+02
  ** BCC_A2
  ** CEMENTITE_D011
  FCC_A1
Calculated..          38 equilibria
Terminating at axis limit.

Phase region boundary 11 at:  6.844E-03  9.776E+02

```

```

** BCC_A2
  FCC_A1
Calculated                      45 equilibria

Phase region boundary 12 at:   6.844E-03  9.776E+02
** BCC_A2
  CEMENTITE_D011
  FCC_A1
Calculated..                  54 equilibria
Terminating at axis limit.

Phase region boundary 13 at:   1.687E-05  8.830E+02
  BCC_A2
  CEMENTITE_D011
** FCC_A1
Calculated..                  85 equilibria
Terminating at axis limit.

Phase region boundary 14 at:   2.500E-04  8.899E+02
  BCC_A2
  CEMENTITE_D011
** FCC_A1
Calculated..                  81 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 15 at:   6.750E-03  9.542E+02
  BCC_A2
  CEMENTITE_D011
** FCC_A1
Calculated..                  31 equilibria
Terminating at known equilibrium

Phase region boundary 16 at:   6.750E-03  9.542E+02
  BCC_A2
  CEMENTITE_D011
** FCC_A1
Calculated..                  55 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 17 at:   1.325E-02  9.705E+02
  BCC_A2
  CEMENTITE_D011
** FCC_A1
Calculated..                  57 equilibria
Terminating at known equilibrium

Phase region boundary 18 at:   1.325E-02  9.705E+02
  BCC_A2
  CEMENTITE_D011
** FCC_A1
Calculated..                  29 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 19 at:   1.965E-02  8.100E+02
  BCC_A2
  CEMENTITE_D011
** DIAMOND_A4
Calculated..                  15 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 20 at:   1.965E-02  8.100E+02
  BCC_A2
  CEMENTITE_D011
** DIAMOND_A4
Calculated..                  3 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 21 at:   1.975E-02  8.103E+02
  BCC_A2
  CEMENTITE_D011
** DIAMOND_A4
Calculated..                  15 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 22 at:   1.975E-02  8.103E+02
  BCC_A2
  CEMENTITE_D011
** DIAMOND_A4
Calculated..                  3 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 23 at:   1.009E-03  9.367E+02
  BCC_A2
  CEMENTITE_D011
  FCC_A1
Calculated..                  8 equilibria
Terminating at known equilibrium

Phase region boundary 24 at:   1.009E-03  9.367E+02
  BCC_A2
  CEMENTITE_D011
  FCC_A1
Calculated..                  28 equilibria
Terminating at known equilibrium

Phase region boundary 25 at:   3.542E-03  9.367E+02
  BCC_A2
  CEMENTITE_D011
** FCC_A1
Calculated..                  16 equilibria
Terminating at known equilibrium

Phase region boundary 26 at:   3.542E-03  9.367E+02
  BCC_A2
  CEMENTITE_D011
** FCC_A1
Calculated..                  68 equilibria
Terminating at known equilibrium
Terminating at axis limit.

```

```

Phase region boundary 27 at: 1.020E-03 1.063E+03
** BCC_A2
  FCC_A1
Calculated.          32 equilibria
Terminating at known equilibrium

Phase region boundary 28 at: 1.020E-03 1.063E+03
** BCC_A2
  FCC_A1
Calculated.          22 equilibria

Phase region boundary 29 at: 9.115E-03 1.063E+03
** CEMENTITE_D011
  FCC_A1
Calculated.          11 equilibria
Terminating at known equilibrium

Phase region boundary 30 at: 9.115E-03 1.063E+03
** CEMENTITE_D011
  FCC_A1
Calculated..         29 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 31 at: 1.287E-02 1.190E+03
** CEMENTITE_D011
  FCC_A1
Calculated.          36 equilibria
Terminating at known equilibrium

Phase region boundary 32 at: 1.287E-02 1.190E+03
** CEMENTITE_D011
  FCC_A1
Calculated..         4 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 33 at: 2.500E-04 1.081E+03
** BCC_A2
  FCC_A1
Calculated.          4 equilibria

Phase region boundary 34 at: 2.500E-04 1.081E+03
** BCC_A2
  FCC_A1
Calculated.          28 equilibria
Terminating at known equilibrium

Phase region boundary 35 at: 6.750E-03 9.786E+02
** BCC_A2
  FCC_A1
Calculated.          48 equilibria

Phase region boundary 36 at: 6.750E-03 9.786E+02
** BCC_A2
  FCC_A1
Calculated.          2 equilibria
Terminating at known equilibrium

Phase region boundary 37 at: 1.325E-02 9.814E+02
** BCC_A2
  CEMENTITE_D011
  FCC_A1
Calculated..         27 equilibria
Terminating at known equilibrium

Phase region boundary 38 at: 1.325E-02 9.814E+02
** BCC_A2
  CEMENTITE_D011
  FCC_A1
Calculated..         29 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 39 at: 1.287E-02 1.190E+03
** CEMENTITE_D011
  FCC_A1
Calculated.          36 equilibria
Terminating at known equilibrium

Phase region boundary 40 at: 1.287E-02 1.190E+03
** CEMENTITE_D011
  FCC_A1
Calculated..         4 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 41 at: 1.975E-02 9.841E+02
** BCC_A2
  CEMENTITE_D011
  FCC_A1
Calculated..         53 equilibria
Terminating at known equilibrium

Phase region boundary 42 at: 1.975E-02 9.841E+02
** BCC_A2
  CEMENTITE_D011
  FCC_A1
Calculated..         3 equilibria
Terminating at known equilibrium
Terminating at axis limit.
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\generate_console_examples\examples\tcex42\tcex42a.POLY3
CPU time for mapping      20 seconds
POLY: po
... the command in full is POST
POST-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

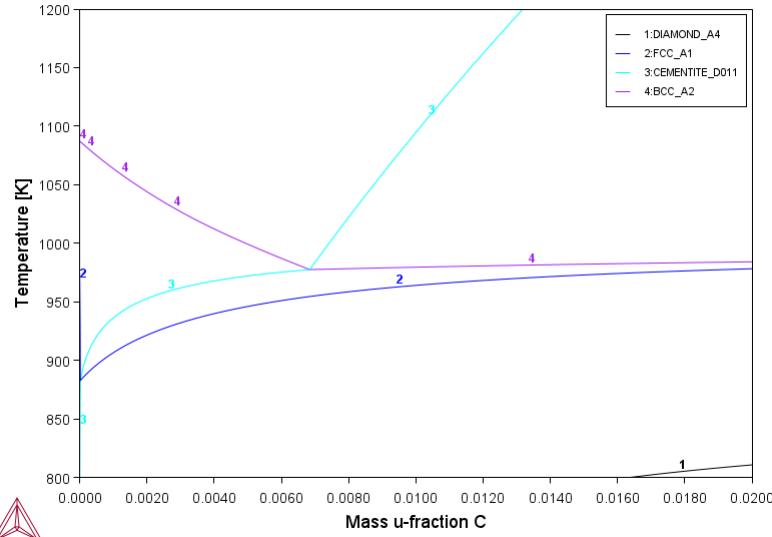
POST: s-lab e
... the command in full is SET_LABEL_CURVE_OPTION
POST: s-a-text x n Mass u-fraction C
... the command in full is SET_AXIS_TEXT_STATUS
POST: set-title example 42a
POST:

```

```

POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
example 42a

```



```

POST:
POST: Hit RETURN to continue
POST:
POST: make tcex42 y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST:
POST: back
POLY: read tcex42a
... the command in full is READ_WORKSPACES
POLY: s-a-v 1 t 800 1200 10
... the command in full is SET_AXIS_VARIABLE
POLY: s-a-v 2 none
... the command in full is SET_AXIS_VARIABLE
POLY: sa tcex42b y
... the command in full is SAVE_WORKSPACES
POLY: step
... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/: para

```

This command calculates a paraequilibrium between two phases.
You must calculate an equilibrium with the overall composition first.
Name of first phase: fcc_a1
Name of second phase: bcc_a2
Fast diffusing component: /C/: C
Fast diffusing component: /NONE/:
Output during stepping is:
axis value, phase amounts, u-fractions of interstitial(s) in phase 1 and 2,
and LNACR value(s) of interstitial(s)

| Phase Region from | 900.000 | for: | | | |
|-------------------|---------|-------|--------------|--------------|---------------|
| BCC_A2 | | | | | |
| FCC_A1 | | | | | |
| 9.000000E+02 | 0.176 | 0.824 | 4.978820E-02 | 6.632554E-04 | -2.411191E-01 |
| 8.900000E+02 | 0.161 | 0.839 | 5.422637E-02 | 6.913419E-04 | -2.814989E-02 |
| 8.800000E+02 | 0.148 | 0.852 | 5.873850E-02 | 7.164862E-04 | 1.826378E-01 |
| 8.700000E+02 | 0.137 | 0.863 | 6.331514E-02 | 7.386191E-04 | 3.918139E-01 |
| 8.600000E+02 | 0.127 | 0.873 | 6.794785E-02 | 7.576965E-04 | 5.998836E-01 |
| 8.500000E+02 | 0.119 | 0.881 | 7.262910E-02 | 7.736968E-04 | 8.072994E-01 |
| 8.400000E+02 | 0.111 | 0.889 | 7.735219E-02 | 7.866192E-04 | 1.014471E+00 |
| 8.300000E+02 | 0.105 | 0.895 | 8.211115E-02 | 7.964818E-04 | 1.221773E+00 |
| 8.200000E+02 | 0.099 | 0.901 | 8.690064E-02 | 8.033198E-04 | 1.429553E+00 |
| 8.100000E+02 | 0.093 | 0.907 | 9.171593E-02 | 8.071848E-04 | 1.638132E+00 |
| 8.000000E+02 | 0.089 | 0.911 | 9.655277E-02 | 8.081431E-04 | 1.847816E+00 |

| Phase Region from | 900.000 | for: | | | |
|-------------------|---------|--------|--------------|--------------|---------------|
| BCC_A2 | | | | | |
| FCC_A1 | | | | | |
| 9.000000E+02 | 0.176 | 0.824 | 4.978820E-02 | 6.632554E-04 | -2.411191E-01 |
| 9.100000E+02 | 0.193 | 0.807 | 4.543455E-02 | 6.323238E-04 | -4.569199E-01 |
| 9.200000E+02 | 0.214 | 0.786 | 4.117723E-02 | 5.986755E-04 | -6.763019E-01 |
| 9.300000E+02 | 0.239 | 0.761 | 3.702936E-02 | 5.624744E-04 | -9.001396E-01 |
| 9.400000E+02 | 0.270 | 0.730 | 3.300554E-02 | 5.239251E-04 | -1.129464E+00 |
| 9.500000E+02 | 0.308 | 0.692 | 2.912186E-02 | 4.832788E-04 | -1.365508E+00 |
| 9.600000E+02 | 0.355 | 0.645 | 2.539605E-02 | 4.408411E-04 | -1.609759E+00 |
| 9.700000E+02 | 0.415 | 0.585 | 2.184745E-02 | 3.969810E-04 | -1.864037E+00 |
| 9.800000E+02 | 0.493 | 0.507 | 1.849705E-02 | 3.521428E-04 | -2.130596E+00 |
| 9.900000E+02 | 0.597 | 0.403 | 1.536739E-02 | 3.068594E-04 | -2.412255E+00 |
| 1.000000E+03 | 0.739 | 0.261 | 1.248241E-02 | 2.617708E-04 | -2.712568E+00 |
| 1.010000E+03 | 0.942 | 0.058 | 9.854299E-03 | 2.173378E-04 | -3.037453E+00 |
| 1.020000E+03 | 1.258 | -0.258 | 7.421605E-03 | 1.722830E-04 | -3.406198E+00 |
| 1.030000E+03 | 1.821 | -0.821 | 5.162033E-03 | 1.261960E-04 | -3.851549E+00 |
| 1.040000E+03 | 3.087 | -2.087 | 3.064308E-03 | 7.892826E-05 | -4.452579E+00 |
| 1.050000E+03 | 8.516 | -7.516 | 1.118312E-03 | 3.035919E-05 | -5.537500E+00 |

*** Buffer saved on file c:\jenkins\WORKSP-1\GENERA~1\examples\tcex42\TCEX42~2.POL
*** ERROR 3 IN NS01AD: Numerical error

```

POLY:
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

```

Setting automatic diagram axes

```

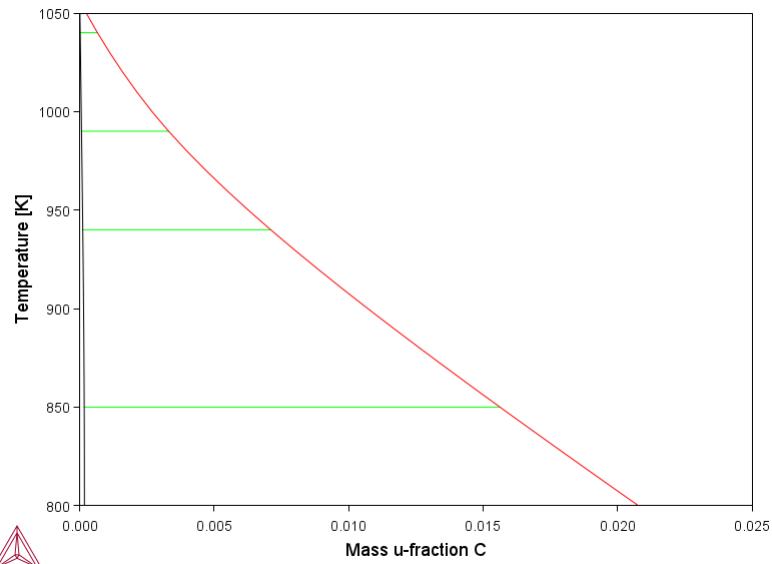
POST: s-d-a x w(*,c)
... the command in full is SET_DIAGRAM_AXIS

```

```

COLUMN NUMBER /*/: *
POST: s-d-a y t-k
... the command in full is SET_DIAGRAM_AXIS
POST: s-a-text x n Mass u-fraction C
... the command in full is SET_AXIS_TEXT_STATUS
POST: set-tie 5
... the command in full is SET_TIELINE_STATUS
POST: set-title example 42b
POST: sel-plot new
... the command in full is SELECT_PLOT
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

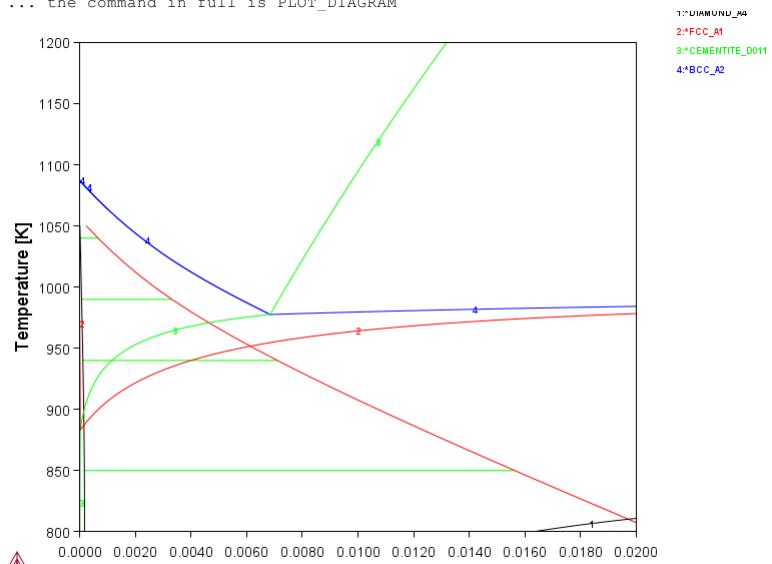




```

POST:
POST:Hit RETURN to continue
POST:
POST: ap-e y tcex42
... the command in full is APPEND EXPERIMENTAL DATA
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 1
POST: s-s x n 0 0.02
... the command in full is SET_SCALING_STATUS
POST: s-s y n 800 1200
... the command in full is SET_SCALING_STATUS
POST: set-title example 42c
POST: sel-plot new
... the command in full is SELECT_PLOT
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```





```

POST:Hit RETURN to continue
POST:
POST: back
POLY: read tcex42b
... the command in full is READ_WORKSPACES

```

```

POLY: s-c w(c)=0.01
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 23045 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
Output from POLY-3, equilibrium = 1, label A0 , database: TCFE11

Conditions:
T=900, P=100000, N=1, W(C)=1E-2, W(MN)=2.5E-2
DEGREES OF FREEDOM 0

Temperature 900.00 K ( 626.85 C), Pressure 1.000000E+05
Number of moles of components 1.000000E+00, Mass in grams 5.38780E+01
Total Gibbs energy -3.55310E+04, Enthalpy 2.03102E+04, Volume 7.05497E-06

Component Moles W-Fraction Activity Potential Ref.stat
C 4.4413E-02 1.0000E-02 2.8388E-01 -9.4226E+03 SER
FE 9.3131E-01 9.7500E-01 8.2599E-03 -3.5891E+04 SER
MN 2.4275E-02 2.5000E-02 9.2895E-05 -6.9473E+04 SER

BCC_A2 Status ENTERED Driving force 0.0000E+00
Moles 8.2303E-01, Mass 4.5951E+01, Volume fraction 8.4971E-01 Mass fractions:
FE 9.93109E-01 MN 6.84649E-03 C 4.43634E-05

CEMENTITE_D011 Status ENTERED Driving force 0.0000E+00
Moles 1.7697E-01, Mass 7.9271E+00, Volume fraction 1.5029E-01 Mass fractions:
FE 8.04416E-01 MN 1.28547E-01 C 6.70366E-02

POLY: step
... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/: para

This command calculates a paraequilibrium between two phases.
You must calculate an equilibrium with the overall composition first.
Name of first phase: fcc_a1
Name of second phase: cementite
Fast diffusing component: /C/: C
Fast diffusing component: /NONE/:
Output during stepping is:
axis value, phase amounts, u-fractions of interstitial(s) in phase 1 and 2,
and LNACR value(s) of interstitial(s)

Phase Region from 900.000 for:
CEMENTITE_D011
FCC_A1
9.000000E+02 0.932 0.068 2.565452E-02 3.333333E-01 -1.153986E+00
9.800000E+02 0.929 0.071 2.464593E-02 3.333333E-01 -1.126044E+00
8.800000E+02 0.926 0.074 2.365344E-02 3.333333E-01 -1.097675E+00
8.700000E+02 0.923 0.077 2.267732E-02 3.333333E-01 -1.068873E+00
8.600000E+02 0.921 0.079 2.171789E-02 3.333333E-01 -1.039635E+00
8.500000E+02 0.918 0.082 2.077544E-02 3.333333E-01 -1.009954E+00
8.400000E+02 0.915 0.085 1.985030E-02 3.333333E-01 -9.798261E-01
8.300000E+02 0.912 0.088 1.894282E-02 3.333333E-01 -9.492462E-01
8.200000E+02 0.910 0.090 1.805335E-02 3.333333E-01 -9.182089E-01
8.100000E+02 0.907 0.093 1.718224E-02 3.333333E-01 -8.867094E-01
8.000000E+02 0.905 0.095 1.632989E-02 3.333333E-01 -8.547425E-01

Phase Region from 900.000 for:
CEMENTITE_D011
FCC_A1
9.000000E+02 0.932 0.068 2.565452E-02 3.333333E-01 -1.153986E+00
9.100000E+02 0.935 0.065 2.667894E-02 3.333333E-01 -1.181505E+00
9.200000E+02 0.939 0.061 2.771894E-02 3.333333E-01 -1.208606E+00
9.300000E+02 0.942 0.058 2.877430E-02 3.333333E-01 -1.235294E+00
9.400000E+02 0.945 0.055 2.984478E-02 3.333333E-01 -1.261573E+00
9.500000E+02 0.949 0.051 3.093020E-02 3.333333E-01 -1.287447E+00
9.600000E+02 0.952 0.048 3.203036E-02 3.333333E-01 -1.312922E+00
9.700000E+02 0.956 0.044 3.314510E-02 3.333333E-01 -1.338000E+00
9.800000E+02 0.959 0.041 3.427427E-02 3.333333E-01 -1.362687E+00
9.900000E+02 0.963 0.037 3.541772E-02 3.333333E-01 -1.386986E+00
1.000000E+03 0.967 0.033 3.657534E-02 3.333333E-01 -1.410901E+00
1.010000E+03 0.970 0.030 3.774702E-02 3.333333E-01 -1.434437E+00
1.020000E+03 0.974 0.026 3.893267E-02 3.333333E-01 -1.457595E+00
1.030000E+03 0.978 0.022 4.013222E-02 3.333333E-01 -1.480381E+00
1.040000E+03 0.982 0.018 4.134560E-02 3.333333E-01 -1.502798E+00
1.050000E+03 0.987 0.013 4.257278E-02 3.333333E-01 -1.524849E+00
1.060000E+03 0.991 0.009 4.381372E-02 3.333333E-01 -1.546537E+00
1.070000E+03 0.995 0.005 4.506840E-02 3.333333E-01 -1.567865E+00
1.080000E+03 1.000 0.000 4.633683E-02 3.333333E-01 -1.588837E+00
1.090000E+03 1.004 -0.004 4.761902E-02 3.333333E-01 -1.609455E+00
1.100000E+03 1.009 -0.009 4.891500E-02 3.333333E-01 -1.629722E+00
1.110000E+03 1.013 -0.013 5.022480E-02 3.333333E-01 -1.649641E+00
1.120000E+03 1.018 -0.018 5.154847E-02 3.333333E-01 -1.669214E+00
1.130000E+03 1.023 -0.023 5.288611E-02 3.333333E-01 -1.688443E+00
1.140000E+03 1.028 -0.028 5.423778E-02 3.333333E-01 -1.707332E+00
1.150000E+03 1.033 -0.033 5.560358E-02 3.333333E-01 -1.725881E+00
1.160000E+03 1.038 -0.038 5.698363E-02 3.333333E-01 -1.744093E+00
1.170000E+03 1.043 -0.043 5.837804E-02 3.333333E-01 -1.761970E+00
1.180000E+03 1.049 -0.049 5.978696E-02 3.333333E-01 -1.779514E+00
1.190000E+03 1.054 -0.054 6.121053E-02 3.333333E-01 -1.796726E+00
1.200000E+03 1.060 -0.060 6.264893E-02 3.333333E-01 -1.813608E+00
*** Buffer saved on file c:\jenkins\WORKSP~1\GENERA~1\examples\tcex42\tcex42~2.POL

POLY:
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

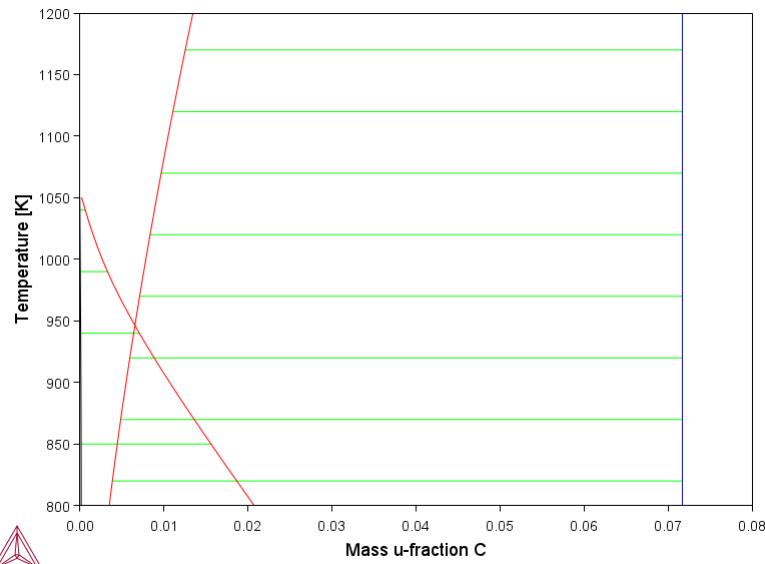
POST: s-d-a x w(*,c)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: s-d-a y t-k
... the command in full is SET_DIAGRAM_AXIS
POST: s-a-text x n Mass u-fraction C
... the command in full is SET_AXIS_TEXT_STATUS
POST: set-tie 5
... the command in full is SET_TIELINE_STATUS
POST: set-tit example 42d
... the command in full is SET_TITLE

```

```

POST: app-e n
... the command in full is APPEND_EXPERIMENTAL_DATA
POST: sel=plot new
... the command in full is SELECT_PLOT
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

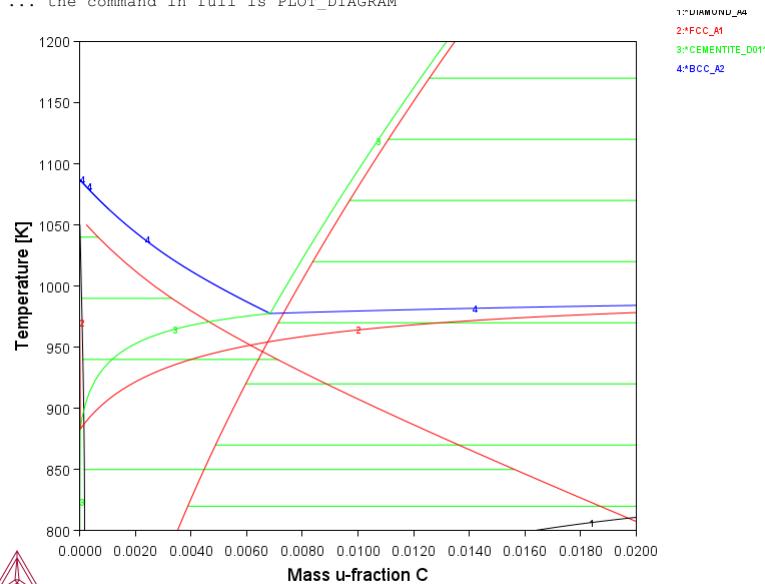
```



```

POST:
POST:Hit RETURN to continue
POST:
POST: app-e y tcex42
... the command in full is APPEND_EXPERIMENTAL_DATA
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 1
POST: s-s x n 0 0.02
... the command in full is SET_SCALING_STATUS
POST: set-title example 42e
POST: sel=plot new
... the command in full is SELECT_PLOT
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```



```

POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:

```

tce43**SYS:About**

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce43\tce43.TCM.test"

SYS: set-echo

SYS:

SYS: @@ Paraequilibrium calculation - Formation of

SYS: @@ Para-pearlite - Isothermal

SYS:

SYS: @@ This example uses an Fe-Mn-C system at 700 C to show a paraequilibrium calculation where there is formation of para-pearlite. It is an isothermal calculation and shows

SYS: the Step_with_Options command.

SYS:

SYS: @@ Note that a TCFE database license is required to run

SYS: the example.

SYS:

SYS: set-log ex43,,,

SYS: go p-3

... the command in full is GOTO_MODULE

POLY version 3.32

POLY: def-mater

... the command in full is DEFINE_MATERIAL

THERMODYNAMIC DATABASE module

Database folder: C:\jenkins\workspace\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

Database /TCFE11:/: tcfel1

Major element or alloy: fe

Composition input in mass (weight) percent? /Y/: Y

1st alloying element: c 0.1

2nd alloying element: mn 2

Next alloying element:

Temperature (C) /1000/: 700

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

REINITIATING GES

... the command in full is DEFINE_ELEMENTS

FE DEFINED

... the command in full is DEFINE_ELEMENTS

C DEFINED

... the command in full is DEFINE_ELEMENTS

MN DEFINED

This database has following phases for the defined system

| | | |
|-------------|----------------|--------------|
| GAS:G | LIQUID:L | BCC_A2 |
| A2_BCC | BCC_B2 | FCC_A1 |
| A1_FCC | FCC_L12 | HCP_A3 |
| CBCC_A12 | CUB_A13 | DIAMOND_A4 |
| GRAPHITE_A9 | CEMENTITE_D011 | M23C6_D84 |
| M7C3_D101 | M5C2 | KSI_CARBIDE |
| FE4N_LP1 | C14_LAVES | C15_LAVES |
| G_PHASE | NBNi3_D0A | CUZN_EPSILON |
| AL5FE4 | FLUORITE_C1:I | ZRO2_TETR:I |
| M2O3C_D53:I | M2O3H_D52:I | |

Reject phase(s) /NONE/: graphite m5c2

GRAPHITE_A9 MSC2 REJECTED

Reject phase(s) /NONE/: NONE

Restore phase(s) /NONE/: NONE

.....
The following phases are retained in this system:

| | | |
|----------------|-------------|---------------|
| GAS:G | LIQUID:L | BCC_A2 |
| A2_BCC | BCC_B2 | FCC_A1 |
| A1_FCC | FCC_L12 | HCP_A3 |
| CBCC_A12 | CUB_A13 | DIAMOND_A4 |
| CEMENTITE_D011 | M23C6_D84 | M7C3_D101 |
| KSI_CARBIDE | FE4N_LP1 | C14_LAVES |
| C15_LAVES | G_PHASE | NBNi3_D0A |
| CUZN_EPSILON | AL5FE4 | FLUORITE_C1:I |
| ZRO2_TETR:I | M2O3C_D53:I | M2O3H_D52:I |

.....

OK? /Y/: Y

16:48:14,681 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

ELEMENTS

SPECIES

PHASES

... the command in full is AMEND_PHASE_DESCRIPTION

Suspending FLUORITE_C1 as it has net charge

Suspending M2O3C_D53 as it has net charge
 Suspending M2O3H_D52 as it has net charge
 Suspending ZRO2_TETR as it has net charge
 PARAMETERS ...
 FUNCTIONS

List of references for assessed data

'A.T. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
 'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121-127; Molar volumes'
 'X.G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
 'Y. Tang, in TCCU2, Thermo-Calc Software AB, Stockholm, Sweden'
 'X.G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar volumes'
 'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equilib., 19 (1998) 441-448; Fe-Ti'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; C15_LAVES'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, Volume data updated for TCFE9 database (TCFE v9.0, Jan, 2017).'
 'N. Dupin, introduction of Nb to NI15VA-4SL'
 'N. Dupin, Private communication, (2008); Volume data'
 'H. Gohring, O. Fabrichnaya, A. Leineweber, E.J. Mittemeijer, Metall. Mater. Trans. A, 47A, 6173-86(2016); Fe-N, and Fe-C-N'
 'Unassessed parameter; Linear combination of unary data'
 'N. Saunders, COST 507 Report (1998); Mn-Ti'
 'W. Zheng, J. Alloys Compd., 632 (2015) 661-675'
 'L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2012; Molar volumes'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; FE4N'
 'M. Seiersten, Unpublished work (1989); Al-Fe'
 'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
 'M. Ghasemi, Thermo-Calc Software AB, Sweden, 2020; Unifying liquid volume database'
 'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
 'J-O. Andersson, CALPHAD, 12 (1988) 9-23; TRITA 0321 (1986); C-Fe-MO'
 'B. Hallstedt, D. Djurovic, J. von Appen, R. Dronskowsk, A. Dick, F. Koermann, T. Hickel, J. Neugebauer, CALPHAD, 34, 129-33(2010); Fe-C'
 'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowsk, Calphad 35.4 (2011) 479-491; Fe-Mn-C'
 'P. Villars, L.D. Calvert. Pearson's handbook of crystallographic data for intermetallic phases, Metals park, Ohio 1985: American society for metals'
 'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
 'W. Huang, Metall. Trans. A, 21A (1990) 2115-2123; TRITA-MAC 411 (Rev 1989); C-FE-MN'
 'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowsk, CALPHAD, 34, 279-85(2010); Mn-C'
 'W. Huang, CALPHAD, 13 (1989) 243-252; TRITA-MAC 388 (rev 1989); FE-MN'
 'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
 'S. Liu, B. Hallstedt, D. Music, Y. Du, CALPHAD, 38 (2012) 43-58; Mn-Nb and Fe-Mn-Nb'
 'A. Markstrom, Thermo-Calc software AB, Sweden, 2011'
 'L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2013; Reassessed solubility of Al, Cr, Fe, Ni in Mn2O3. When Mn2O3 is modelled as the same phase as cubic Y2O3 (M2O3C).'
 'M. Chen, B. Hallstedt, L. J. Gauckler, J. Alloys Compd., 393 (2005) 114-21; Mn-Y-O'
 'M. Chen, B. Hallstedt, L.J. Gauckler, Solid State Ionics, 176 (2005) 1457-64; Mn-Zr-O, Mn-Y-Zr-O'
 'J. Miettinen, CALPHAD, 28 (2004) 313-320; Mn-Zn'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, Volume data updated for TCFE8 database (TCFE v8, May, 2015).'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; Adjusting hcp'
 'M. Ghasemi, Thermo-Calc Software AB, Sweden, 2019; Viscosity of metallic liquid'
 'M. J. Assael, J. Phys. Chem. Ref. Data 35 (2006) 285; Fe, Al'
 'M Ghasemi, Thermo-Calc Software AB: assessing the surface tension of metallic liquid'

-OK-

Should any phase have a miscibility gap check? /N/: N

Using global minimization procedure

Calculated 23045 grid points in 12 s
 Found the set of lowest grid points in 0 s
 Calculated POLY solution 1 s, total time 13 s

POLY: 1-e
 ... the command in full is LIST_EQUIlibrium

OUTPUT TO SCREEN OR FILE /SCREEN/:

Options /VWCs/: VWCs
 Output from POLY-3, equilibrium = 1, label A0 , database: TCFE11

Conditions:
 T=973.15, W(C)=1E-3, W(MN)=2E-2, P=100000, N=1
 DEGREES OF FREEDOM 0

Temperature 973.15 K (700.00 C), Pressure 1.000000E+05
 Number of moles of components 1.000000E+00, Mass in grams 5.56256E+01
 Total Gibbs energy -4.11743E+04, Enthalpy 2.45990E+04, Volume 7.28130E-06

| Component | Moles | W-Fraction | Activity | Potential | Ref.stat |
|-----------|------------|------------|------------|-------------|----------|
| C | 4.6312E-03 | 1.0000E-03 | 1.2685E-01 | -1.6706E+04 | SER |
| FE | 9.7512E-01 | 9.7900E-01 | 6.6201E-03 | -4.0599E+04 | SER |
| MN | 2.0250E-02 | 2.0000E-02 | 1.0065E-04 | -7.4471E+04 | SER |

BCC_A2 Status ENTERED Driving force 0.0000E+00
 Moles 7.8411E-01, Mass 4.3770E+01, Volume fraction 7.8786E-01 Mass fractions:
 FE 9.87020E-01 MN 1.29127E-02 C 6.70791E-05

FCC_A1 Status ENTERED Driving force 0.0000E+00
 Moles 2.1589E-01, Mass 1.1855E+01, Volume fraction 2.1214E-01 Mass fractions:
 FE 9.49389E-01 MN 4.61663E-02 C 4.44436E-03

POLY:

POLY: @@ Change the status of component C to SPECIAL and work
POLY: @@ with u-fractions
POLY: c-s comp c
 ... the command in full is CHANGE_STATUS

Status: /ENTERED/: spec

POLY: c-e
 ... the command in full is COMPUTE_EQUIlibrium

Using global minimization procedure

Found the set of lowest grid points in 0 s
 Calculated POLY solution 0 s, total time 0 s

POLY:

POLY: s-a-v 1 w(c) 0 0.08
 ... the command in full is SET_AXIS_VARIABLE

```

Increment /.002/: 2.5E-04
POLY: s-a-v 2 w(mn) 0 0.1
... the command in full is SET_AXIS_VARIABLE
Increment /.0025/: .0025
POLY: l-a-v
... the command in full is LIST_AXIS_VARIABLE
Axis No 1: W(C) Min: 0 Max: 8E-2 Inc: 2.5E-4
Axis No 2: W(MN) Min: 0 Max: 0.1 Inc: 2.5E-3
POLY: save tceex43a y
... the command in full is SAVE_WORKSPACES
POLY: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Working hard
Working hard
Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard

Phase region boundary 1 at: 3.082E-02 1.597E-02
    BCC_A2
    ** CEMENTITE_D011
Calculated.          17 equilibria

Phase region boundary 2 at: 3.082E-02 1.597E-02
    BCC_A2
    ** CEMENTITE_D011
Calculated.          12 equilibria

Phase region boundary 3 at: 3.082E-02 4.346E-02
    BCC_A2
    ** CEMENTITE_D011
    ** FCC_A1
Calculated.          33 equilibria

Phase region boundary 4 at: 3.349E-03 1.844E-02
    BCC_A2
    ** FCC_A1
Calculated.          33 equilibria

Phase region boundary 5 at: 3.506E-02 5.674E-02
    CEMENTITE_D011
    ** FCC_A1
Calculated..         48 equilibria
Terminating at axis limit.

Phase region boundary 6 at: 3.082E-02 4.346E-02
    BCC_A2
    ** CEMENTITE_D011
Calculated.          31 equilibria

Phase region boundary 7 at: 3.082E-02 1.597E-02
    BCC_A2
    ** CEMENTITE_D011
Calculated.          17 equilibria

Phase region boundary 8 at: 3.082E-02 1.597E-02
    BCC_A2
    ** CEMENTITE_D011
Calculated.          12 equilibria
Terminating at known equilibrium

Phase region boundary 9 at: 3.082E-02 2.819E-03
    BCC_A2
    ** CEMENTITE_D011
Calculated.          12 equilibria

Phase region boundary 10 at: 3.082E-02 2.819E-03
    BCC_A2
    ** CEMENTITE_D011
Calculated.          18 equilibria
Terminating at known equilibrium

Phase region boundary 11 at: 3.082E-02 1.539E-03
    BCC_A2
    ** CEMENTITE_D011
Calculated.          13 equilibria

Phase region boundary 12 at: 3.082E-02 1.539E-03
    BCC_A2
    ** CEMENTITE_D011

```

```

Calculated.          18 equilibria
Terminating at known equilibrium

Phase region boundary 13 at:  4.555E-04  4.440E-02
  ** BCC_A2
  ** FCC_A1
Calculated.          18 equilibria
Terminating at known equilibrium

Phase region boundary 14 at:  4.555E-04  4.440E-02
  ** BCC_A2
  ** FCC_A1
Calculated.          15 equilibria

Phase region boundary 15 at:  1.376E-04  4.678E-02
  ** BCC_A2
  FCC_A1
Calculated.          19 equilibria
Terminating at known equilibrium

Phase region boundary 16 at:  1.376E-04  4.678E-02
  ** BCC_A2
  FCC_A1
Calculated.          16 equilibria

Phase region boundary 17 at:  3.479E-02  1.686E-01
  ** CEMENTITE_D011
  FCC_A1
Calculated.          46 equilibria
Terminating at known equilibrium

Phase region boundary 18 at:  3.479E-02  1.686E-01
  ** CEMENTITE_D011
  FCC_A1
Calculated..         3 equilibria
Terminating at axis limit.

Phase region boundary 19 at:  3.478E-02  1.711E-01
  ** CEMENTITE_D011
  FCC_A1
Calculated.          47 equilibria
Terminating at known equilibrium

Phase region boundary 20 at:  1.264E-04  4.686E-02
  ** BCC_A2
  FCC_A1
Calculated.          9 equilibria

Phase region boundary 21 at:  1.264E-04  4.686E-02
  ** BCC_A2
  FCC_A1
Calculated.          14 equilibria
Terminating at known equilibrium

Phase region boundary 22 at:  3.491E-02  1.118E-01
  ** CEMENTITE_D011
  FCC_A1
Calculated.          24 equilibria
Terminating at known equilibrium

Phase region boundary 23 at:  3.491E-02  1.118E-01
  ** CEMENTITE_D011
  FCC_A1
Calculated..         26 equilibria
Terminating at axis limit.

Phase region boundary 24 at:  3.478E-02  1.718E-01
  ** CEMENTITE_D011
  FCC_A1
Calculated.          48 equilibria
Terminating at known equilibrium

Phase region boundary 25 at:  3.501E-02  7.506E-02
  ** CEMENTITE_D011
  FCC_A1
Calculated.          9 equilibria
Terminating at known equilibrium

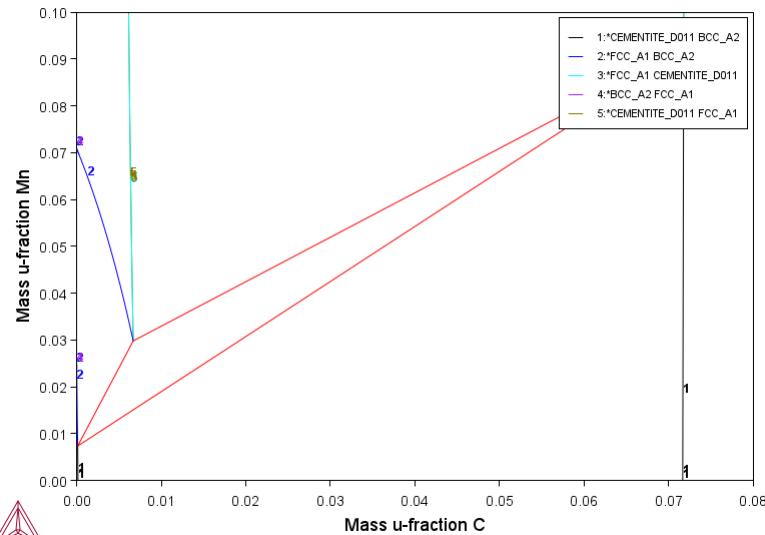
Phase region boundary 26 at:  3.501E-02  7.506E-02
  ** CEMENTITE_D011
  FCC_A1
Calculated..         40 equilibria
Terminating at axis limit.

Phase region boundary 27 at:  3.478E-02  1.701E-01
  ** CEMENTITE_D011
  FCC_A1
Calculated.          47 equilibria
Terminating at known equilibrium
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\generate_console_examples\examples\tcex43\tcex43a.POLY3
CPU time for mapping           9 seconds
POLY:
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2
Setting automatic diagram axes

POST: s-lab e
... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 43a
POST: s-ax-text x N Mass u-fraction C
... the command in full is SET_AXIS_TEXT_STATUS
POST: s-ax-text y N Mass u-fraction Mn
... the command in full is SET_AXIS_TEXT_STATUS
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 43a



POST:
POST: Hit RETURN to continue
POST:

POST: make tce43 y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: b
... the command in full is BACK
POLY: read tce43a
... the command in full is READ_WORKSPACES
POLY: s-a-v 1 w(mn) 0 0.1
... the command in full is SET_AXIS_VARIABLE
Increment / .0025 : .0025
POLY: s-a-v 2 none
... the command in full is SET_AXIS_VARIABLE
POLY: save tce43b y
... the command in full is SAVE_WORKSPACES
POLY: step
... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/: para

This command calculates a paraequilibrium between two phases.
You must calculate an equilibrium with the overall composition first.

Name of first phase: fcc_a1
Name of second phase: bcc_a2
Fast diffusing component: /C/: C
Fast diffusing component: /NONE/:

Output during stepping is:
axis value, phase amounts, u-fractions of interstitial(s) in phase 1 and 2,
and LNACR value(s) of interstitial(s)

| Phase Region from 0.200000E-01 for: | | | | | | |
|-------------------------------------|--------|--------|--------------|--------------|---------------|--|
| | BCC_A2 | FCC_A1 | | | | |
| 2.000000E-02 | 0.165 | 0.835 | 2.571891E-02 | 4.926050E-04 | -1.658137E+00 | |
| 1.750000E-02 | 0.148 | 0.852 | 2.818409E-02 | 5.501102E-04 | -1.529404E+00 | |
| 1.500000E-02 | 0.134 | 0.866 | 3.064279E-02 | 6.094293E-04 | -1.408661E+00 | |
| 1.250000E-02 | 0.123 | 0.877 | 3.309442E-02 | 6.705749E-04 | -1.294692E+00 | |
| 1.000000E-02 | 0.112 | 0.888 | 3.553901E-02 | 7.335731E-04 | -1.186526E+00 | |
| 7.500000E-03 | 0.104 | 0.896 | 3.797641E-02 | 7.984452E-04 | -1.083396E+00 | |
| 5.000000E-03 | 0.096 | 0.904 | 4.040649E-02 | 8.652122E-04 | -9.846802E-01 | |
| 2.500000E-03 | 0.089 | 0.911 | 4.282917E-02 | 9.338953E-04 | -8.898660E-01 | |
| 2.500000E-09 | 0.082 | 0.918 | 4.524437E-02 | 1.004515E-03 | -7.985285E-01 | |

| Phase Region from 0.200000E-01 for: | | | | | | |
|-------------------------------------|--------|--------|--------------|--------------|---------------|--|
| | BCC_A2 | FCC_A1 | | | | |
| 2.000000E-02 | 0.165 | 0.835 | 2.571891E-02 | 4.926050E-04 | -1.658137E+00 | |
| 2.250000E-02 | 0.185 | 0.815 | 2.324733E-02 | 4.368885E-04 | -1.796470E+00 | |
| 2.500000E-02 | 0.209 | 0.791 | 2.076966E-02 | 3.829392E-04 | -1.946558E+00 | |
| 2.750000E-02 | 0.240 | 0.760 | 1.828626E-02 | 3.307359E-04 | -2.111382E+00 | |
| 3.000000E-02 | 0.281 | 0.719 | 1.579754E-02 | 2.802573E-04 | -2.295244E+00 | |
| 3.250000E-02 | 0.338 | 0.662 | 1.330400E-02 | 2.314820E-04 | -2.504681E+00 | |
| 3.500000E-02 | 0.420 | 0.580 | 1.080620E-02 | 1.843887E-04 | -2.750349E+00 | |
| 3.750000E-02 | 0.552 | 0.448 | 8.304797E-03 | 1.389562E-04 | -3.051429E+00 | |
| 4.000000E-02 | 0.798 | 0.202 | 5.800548E-03 | 9.516350E-05 | -3.448165E+00 | |
| 4.250000E-02 | 1.418 | -0.418 | 3.294329E-03 | 5.298938E-05 | -4.051824E+00 | |
| 4.500000E-02 | 5.984 | -4.984 | 7.871532E-04 | 1.241291E-05 | -5.521312E+00 | |

*** Buffer saved on file c:\jenkins\WORKSP~1\GENERA~1\examples\tce43\tCEX43~2.POL

*** ERROR 7 IN NSO1AD: Numerical error

POLY: po
... the command in full is POST
POLY-3 POSTPROCESSOR VERSION 3.2

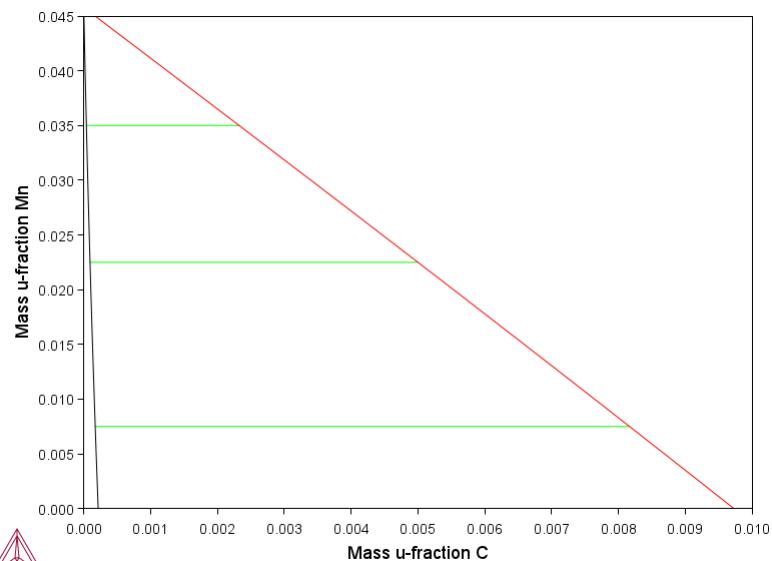
Setting automatic diagram axes

POST: s-d-a x w(*,c)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER */: *
POST: s-d-a y w(*,mn)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER */: *
POST: set-tie 5
... the command in full is SET_TIELINE_STATUS
POST: set-title example 43b
POST: s=ax-text x N Mass u-fraction C
... the command in full is SET_AXIS_TEXT_STATUS
POST: s=ax-text y N Mass u-fraction Mn
... the command in full is SET_AXIS_TEXT_STATUS
POST: sel=plot new
... the command in full is SELECT_PLOT
POST:

```

POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

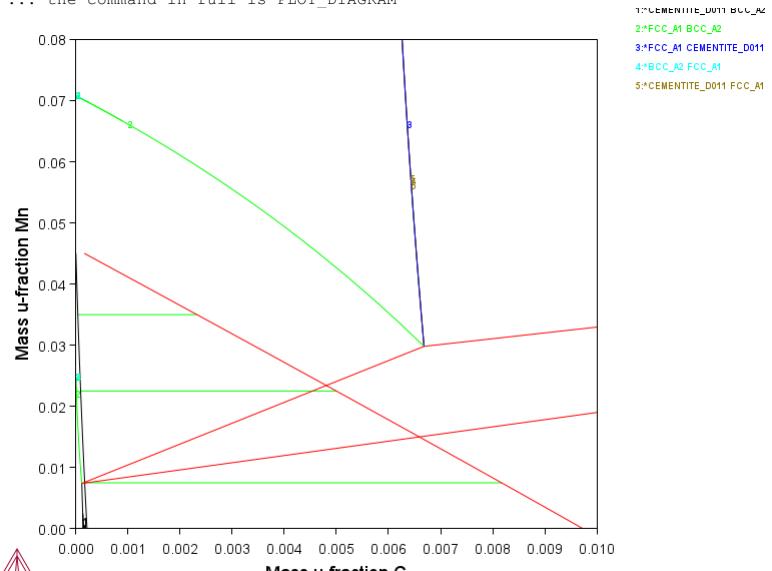
```



```

POST:
POST: Hit RETURN to continue
POST:
POST: app y tcex43
... the command in full is APPEND_EXPERIMENTAL_DATA
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 1
POST: s-s x n 0 0.01
... the command in full is SET_SCALING_STATUS
POST: s-s y n 0 0.08
... the command in full is SET_SCALING_STATUS
POST: set-title example 43c
POST: sel-plot new
... the command in full is SELECT_PLOT
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```



```

POST:
POST: Hit RETURN to continue
POST:
POST: b
... the command in full is BACK
POLY: read tcex43b
... the command in full is READ_WORKSPACES
POLY: l-c
... the command in full is LIST_CONDITIONS
T=973.15, W(C)=1E-3, W(MN)=2E-2, F=100000, N=1
DEGREES OF FREEDOM 0
POLY: s-c w(c)=0.008 w(mn)=0.07
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 23045 grid points in 0 s

```

```

Found the set of lowest grid points in          0 s
Calculated POLY solution      0 s, total time   0 s
POLY: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /WVCS/: WVCS
Output from POLY-3, equilibrium =      1, label A0 , database: TCFE11

Conditions:
T=973.15, W(C)=8E-3, W(MN)=7E-2, P=100000, N=1
DEGREES OF FREEDOM 0

Temperature    973.15 K ( 700.00 C), Pressure 1.000000E+05
Number of moles of components 1.000000E+00, Mass in grams 5.42144E+01
Total Gibbs energy -4.19930E+04, Enthalpy 2.75209E+04, Volume 7.10745E-06

Component       Moles     W-Fraction Activity Potential Ref.stat
C             3.5823E-02  8.0000E-03 1.7546E-01 -1.4082E+04 SER
FE            8.9565E-01  9.3000E-01 6.4327E-03 -4.0831E+04 SER
MN            6.8530E-02  7.0000E-02 1.4062E-04 -7.1765E+04 SER

FCC_A1           Status ENTERED Driving force 0.0000E+00
Moles 9.6765E-01, Mass 5.2767E+01, Volume fraction 9.7259E-01 Mass fractions:
FE 9.27196E-01 MN 6.64901E-02 C 6.31349E-03

CEMENTITE_D011    Status ENTERED Driving force 0.0000E+00
Moles 3.2348E-02, Mass 1.4478E+00, Volume fraction 2.7412E-02 Mass fractions:
FE 7.55790E-01 MN 1.77119E-01 C 6.70903E-02

POLY: advanced
... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: para

This command calculates a paraequilibrium between two phases.
You must calculate an equilibrium with the overall composition first.
Name of first phase: fcc_a1
Name of second phase: cementite
Fast diffusing component: /C/: C
Fast diffusing component: /NONE/:
NP(FCC_A1) = 0.9930 with U-fractions C = 3.50635E-02
NP(CEMENTITE) = 0.0070 with U-fractions C = 3.33333E-01
All other compositions the same in both phases
Note: LIST-EQUILIBRIUM is not relevant

POLY: step
... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/: para

This command calculates a paraequilibrium between two phases.
You must calculate an equilibrium with the overall composition first.
Name of first phase: fcc_a1
Name of second phase: cementite
Fast diffusing component: /C/: C
Fast diffusing component: /NONE/:
Output during stepping is:
axis value, phase amounts, u-fractions of interstitial(s) in phase 1 and 2,
and LNACK value(s) of interstitial(s)

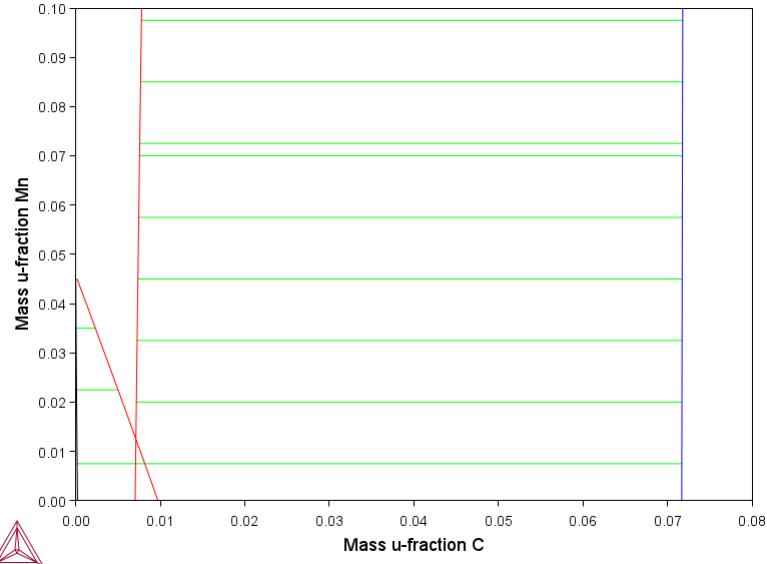
Phase Region from 0.700000E-01 for:
  CEMENTITE_D011
  FCC_A1
  7.000000E-02  0.993  0.007  3.506346E-02  3.333333E-01  -1.531026E+00
  6.750000E-02  0.993  0.007  3.497293E-02  3.333333E-01  -1.520657E+00
  6.500000E-02  0.992  0.008  3.488283E-02  3.333333E-01  -1.510297E+00
  6.250000E-02  0.992  0.008  3.479317E-02  3.333333E-01  -1.499947E+00
  6.000000E-02  0.992  0.008  3.470394E-02  3.333333E-01  -1.489605E+00
  5.750000E-02  0.992  0.008  3.461515E-02  3.333333E-01  -1.479273E+00
  5.500000E-02  0.991  0.009  3.452678E-02  3.333333E-01  -1.468950E+00
  5.250000E-02  0.991  0.009  3.443884E-02  3.333333E-01  -1.458637E+00
  5.000000E-02  0.991  0.009  3.435133E-02  3.333333E-01  -1.448333E+00
  4.750000E-02  0.990  0.010  3.426425E-02  3.333333E-01  -1.438038E+00
  4.500000E-02  0.990  0.010  3.417758E-02  3.333333E-01  -1.427753E+00
  4.250000E-02  0.990  0.010  3.409134E-02  3.333333E-01  -1.417478E+00
  4.000000E-02  0.989  0.011  3.400552E-02  3.333333E-01  -1.407212E+00
  3.750000E-02  0.989  0.011  3.392011E-02  3.333333E-01  -1.396955E+00
  3.500000E-02  0.989  0.011  3.383511E-02  3.333333E-01  -1.386709E+00
  3.250000E-02  0.989  0.011  3.375053E-02  3.333333E-01  -1.376471E+00
  3.000000E-02  0.988  0.012  3.366636E-02  3.333333E-01  -1.366244E+00
  2.750000E-02  0.988  0.012  3.358260E-02  3.333333E-01  -1.356026E+00
  2.500000E-02  0.988  0.012  3.349924E-02  3.333333E-01  -1.345819E+00
  2.250000E-02  0.988  0.012  3.341629E-02  3.333333E-01  -1.335621E+00
  2.000000E-02  0.987  0.013  3.333374E-02  3.333333E-01  -1.325433E+00
  1.750000E-02  0.987  0.013  3.325159E-02  3.333333E-01  -1.315254E+00
  1.500000E-02  0.987  0.013  3.316983E-02  3.333333E-01  -1.305087E+00
  1.250000E-02  0.986  0.014  3.308848E-02  3.333333E-01  -1.294928E+00
  1.000000E-02  0.986  0.014  3.300753E-02  3.333333E-01  -1.284780E+00
  7.500000E-03  0.986  0.014  3.292696E-02  3.333333E-01  -1.274642E+00
  5.000000E-03  0.986  0.014  3.284679E-02  3.333333E-01  -1.264514E+00
  2.500000E-03  0.985  0.015  3.276701E-02  3.333333E-01  -1.254396E+00
  2.500000E-09  0.985  0.015  3.268761E-02  3.333333E-01  -1.244288E+00

Phase Region from 0.700000E-01 for:
  CEMENTITE_D011
  FCC_A1
  7.000000E-02  0.993  0.007  3.506346E-02  3.333333E-01  -1.531026E+00
  7.250000E-02  0.993  0.007  3.515444E-02  3.333333E-01  -1.541404E+00
  7.500000E-02  0.994  0.006  3.524586E-02  3.333333E-01  -1.551791E+00
  7.750000E-02  0.994  0.006  3.533773E-02  3.333333E-01  -1.562187E+00
  8.000000E-02  0.994  0.006  3.543004E-02  3.333333E-01  -1.572592E+00
  8.250000E-02  0.995  0.005  3.552280E-02  3.333333E-01  -1.583006E+00
  8.500000E-02  0.995  0.005  3.561601E-02  3.333333E-01  -1.593429E+00
  8.750000E-02  0.995  0.005  3.570967E-02  3.333333E-01  -1.603861E+00
  9.000000E-02  0.995  0.005  3.580380E-02  3.333333E-01  -1.614302E+00
  9.250000E-02  0.996  0.004  3.589837E-02  3.333333E-01  -1.624751E+00
  9.500000E-02  0.996  0.004  3.599341E-02  3.333333E-01  -1.635209E+00
  9.750000E-02  0.996  0.004  3.608891E-02  3.333333E-01  -1.645676E+00
  1.000000E-01  0.997  0.003  3.618487E-02  3.333333E-01  -1.656152E+00
*** Buffer saved on file c:\jenkins\WORKSP-1\GENERA~1\examples\tcex43\tceX43~2.POL
POLY: po
... the command in full is POST
  POLY-3 POSTPROCESSOR VERSION 3.2
POST: s-d-a x w(*,c)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*:/ *
POST: s-d-a y w(*,mn)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*:/ *
```

```

POST: set-tie 5
... the command in full is SET_TIELINE_STATUS
POST: set-title example 43d
POST: s-ax-text x N Mass u-fraction C
... the command in full is SET_AXIS_TEXT_STATUS
POST: s-ax-text y N Mass u-fraction Mn
... the command in full is SET_AXIS_TEXT_STATUS
POST: app-e n
... the command in full is APPEND_EXPERIMENTAL_DATA
POST: sel-plot new
... the command in full is SELECT_PLOT
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

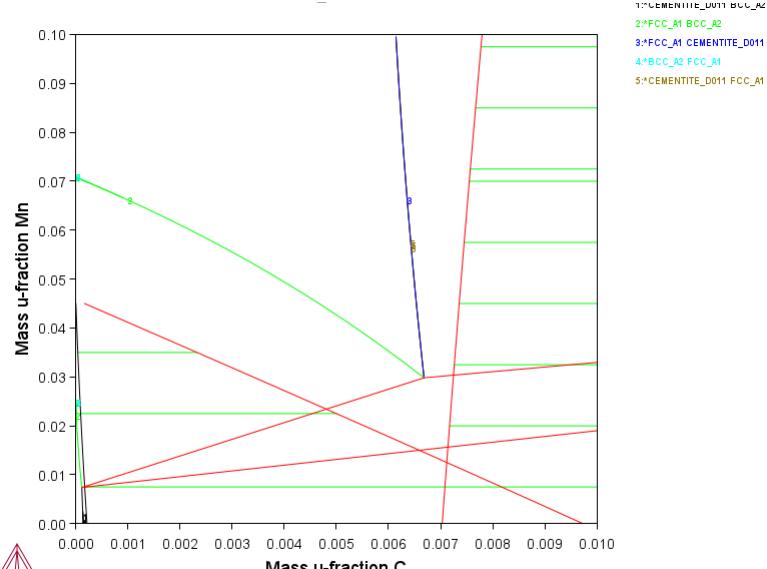




```

POST:
POST:
POST:Hit RETURN to continue
POST:
POST: s-s x n 0 0.01
... the command in full is SET_SCALING_STATUS
POST: s-s y n 0 0.10
... the command in full is SET_SCALING_STATUS
POST: app-e y tcex43
... the command in full is APPEND_EXPERIMENTAL_DATA
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-/: 1
POST: set-title example 43e
POST: sel-plot new
... the command in full is SELECT_PLOT
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```





```

POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE

```

POST:

SYS:About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

```
SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce44\tce44.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Exploring variables and functions.
SYS:
SYS: @@ This example uses variables and functions to predict
SYS: @@ properties e.g. proof strength for an austenitic
SYS: @@ stainless steel at elevated temperatures (20-550 C).
SYS: @@ The example was created using an expression from
SYS: @@ Eliasson, J., and Sandström, R. (2000). 'Proof
SYS: @@ strength values for austenitic stainless steels at
SYS: @@ elevated temperatures', Steel Research, 71(6-7), 249-254.
SYS: @@ Note that a TCFE database license is required to run
SYS: @@ the example.
SYS:
SYS: @@ Note that in Graphical Mode there is a Yield Strength
SYS: @@ Property Model that does not require user input of
SYS: @@ empirical functions.
SYS:
SYS: go da
THERMODYNAMIC DATABASE module
Database folder: C:\jenkins\workspace\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA           /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE11: sw tcfe11
TDE_TCFE11: def-sys
ELEMENTS: fe c si mn cr ni mo cu n
          C           SI
          MN          NI
          MO          N
DEFINED
TDB_TCFE11: get
16:49:51,725 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
Creating a new composition set FCC_A1#2
Creating a new composition set HCP_A3#2
Suspending FLUORITE_C1 as it has net charge
Suspending M203C_D53 as it has net charge
Suspending M203H_D52 as it has net charge
Suspending ZRO2_TETR as it has net charge
PARAMETERS ...
FUNCTIONS .....

List of references for assessed data

'A.T. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121-127; Molar
  volumes'
'X.G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
'M. Ghasemi, Thermo-Calc Software AB, Sweden, 2020; Unifying liquid volume
  database'
'X.G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
  volumes'
'B. Sundman et al., Report EUR 20315, Contract No 7210-PR/050, 2002; New
  Sigma model'
'P. Gustafson, TRITA-MAC 354 (1987); C-Cr-Fe-Mo-W'
'N. Saunders, COST 507 Report (1998); Cr-Ti'
'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; C15_LAVES'
'N. Dupin, Private communication, (2008); Volume data'
'B.J. Lee, KRISS, unpublished research, during 1993-1995'
'R. Naraghi, Thermo-Calc Software AB, Sweden, Volume data updated for
  TCFE9 database (TCFE v9.0, Jan, 2017).'
'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; FE4N'
'Unassessed parameter; Linear combination of unary data'
'Y. Tang, in TCCU2, Thermo-Calc Software AB, Stockholm, Sweden'
'N. Saunders, COST 507 Report (1998); Al-Cu'
'L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2012; Molar volumes'
'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equilib., 19
  (1998) 441-448; Fe-Ti'
'N. Dupin, introduction of Nb to NII15VA-4SL'
'H. Gohring, O. Fabrichnaya, A. Leineweber, E.J. Mittemeijer, Metall.
  Mater. Trans. A, 47A, 6173-86 (2016); Fe-N, and Fe-C-N'
'N. Saunders, COST 507 Report (1998); Mn-Ti'
'W. Zheng, J. Alloys Compd., 632 (2015) 661-675'
'J-O. Andersson, CALPHAD, 12 (1988) 9-23; TRITA 0321 (1986); C-FE-MO'
'A.F. Guillermet, Z. Metallkd., 79 (1988) 524-536, TRITA-MAC 362 (1988); C
  -CO-NI AND C-CO-FE-NI'
'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; C14_LAVES'
'J. De Keyzer, G. Cacciamani, N. Dupin, P. Wollants, Calphad, 33, 109
  -23 (2009).'
'Thermo-Calc Software, Sweden, 2008; Volume data updated for $TCFE6
  database (TCFE v6, April, 2008).'
'A. Bolcavage and U.R. Kattner, J. Phase Equilib., 2, (1996); Nb-Ni'
'W. Xiong, Y. Du, X. Lu, J.C. Schuster, H. Chen, Intermetallics. 15 (2007)
  1401-1408.'
'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
'I. Ansara, unpublished work (1991); Cr-Si'
'M. Seiersten, Unpublished work (1989); Al-Fe'
'A.V. Khvan, B. Hallstedt, K. Chang, CALPHAD, 39, 54-61(2012); C-Cr-Nb'
'J-O. Andersson, CALPHAD, 11 (1987) 271-276; TRITA 0314; C-CR'
'J. Bratberg, Z. Metallkd., 96 (2005) 335-344; Fe-Cr-Mo-C'
'B.J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
```

'C. Qui, ISIJ International, 32 (1992), 1117-1127; TRITA-MAC 482 (1992)
 Revision; C-Cr-Fe-Mo'
 'P. Gustafson, Metall. Trans. A, 19A (1988) 2547-2554; TRITA-MAC 348,
 (1987); C-CR-FE-W'
 'P. Villars, L.D. Calvert. Pearson's handbook of crystallographic data for
 intermetallic phases, Metals park, Ohio 1985: American society for
 metals'
 'B.J. Lee, Metall. Trans. A, 24A (1993) 1017-1025; Fe-Cr-Mn-C'
 'P. Gustafson, Inst. Met. Res. (IM-2549, 1990); C-CU-FE'
 'Chandrasekaran et al., (1987) provisional; CU-FE-P-C'
 'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
 'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
 'B. Hallstedt, D. Djurovic, J. von Appen, R. Dronskowski, A. Dick, F.
 Koermann, T. Hickel, J. Neugebauer, CALPHAD, 34, 129-33(2010); Fe-C'
 'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, Calphad 35.4
 (2011) 479-491; Fe-Mn-C'
 'W. Huang, Metall. Trans. A, 21A (1990) 2115-2123; TRITA-MAC 411 (Rev
 1989); C-FE-MN'
 'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, CALPHAD, 34, 279
 -85(2010); Mn-C'
 'J.H. Shim, C.S. Oh, D.N. Lee, Metall. Mater. Trans. B, 27 (1996) 955-966;
 Ti-Mo-C'
 'R. Naraghi, Thermo-Calc Software AB, Volume data updated for TCFE9
 database (TCFE v9.1, June, 2019).'
 'A. Gabriel, C. Chatillon, and I. Ansara, published in High Temp. Sci.
 (Parameters listed in CALPHAD, 11 (1987) 203-218); C-NI'
 'A. Gabriel, P. Gustafson, and I. Ansara, CALPHAD, 11 (1987) 203-218;
 TRITA-MAC 285 (1986); C-FE-NI'
 'A.F. Guillermet and G. Grimvall, J. Phys. Chem. Solids, 1992, 53, 105-125;
 Molar volumes'
 'J. Grobner, H.L. Lukas, F. Aldinger, Calphad, 1996, 20 (2), 247-254; Al-C,
 Si-C, Al-Si-C'
 'P. Franke; revision of C-Si, Fe-Si and C-Fe-Si'
 'J. Lacaze and B. Sundman, Metall. Mater. Trans. A, 22A (1991) 2211-2223;
 Fe-Si and Fe-Si-C'
 'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; Cementite'
 'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; SIGMA and M7C3'
 'NPL, Unpublished work (1989); C-Mn-Si'
 'K. Zeng and M. Hamalainen, CALPHAD, 19 (1995) 93-104; Cr-Cu'
 'B. Sundman, Private communication, 2(1999); Estimated parameter'
 'COST2 database 1997'
 'W.H. Sun, S.H. Liu, added to make this phase less stable, 2010'
 'B.J. Lee, CALPHAD, 17 (1993) 251-268; revision of Fe-Cr and Fe-Ni liquid'
 'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270
 (1986); CR-FE'
 'K. Frisk, Metall. Trans. A, 21A (1990) 2477-2488; TRITA 0409 (1989); CR
 -FE-N'
 'J-O. Andersson, Metall. Trans. A, 19A (1988) 1385-1394; TRITA 0322 (1986);
 CR-FE-MO'
 'B.J. Lee, unpublished work at KTH (1999); update of steel database'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2019; Cr-Fe-Nb'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2014; Cr-Fe-Zn'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, Volume data updated for
 TCFE8 database (TCFE v8, May, 2015).'
 'B.J. Lee, Metall. Trans. A, 24A (1993) 1919-1933; Cr-Mn, Fe-Cr-Mn'
 'K. Frisk, CALPHAD, 17 (1993) 335-349; Cr-Mn-N'
 'SGTE (2008): SSOL4-SGTE Substance Database V4.1, provided by Thermo-Calc
 Software'
 'K. Frisk, KTH Report D 60 (1984); CR-MO'
 'B. Sundman, Private communication; FCC parameter same as BCC; Cr-Mo'
 'J-O. Andersson, TRITA-MAC 323 (1986); C-CR-FE-MO'
 'K. Frisk, TRITA-MAC 429 (1990); CR-MO-NI'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2015; C14_LAVES'
 'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; Z_PHASE'
 'K. Frisk, CALPHAD, 15 (1991) 79-106; TRITA-MAC 393 (1989); CR-N, FE-N, MO
 -N, CR-MO-N'
 'Estimated parameter for solubility of N in cementite, 1999'
 'A.T. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); CR-NI'
 'N. Dupin, I. Ansara, B. Sundman, CALPHAD, 25 (2), 279-298 (2001); Al-Cr-Ni'
 'L.L. Zhu, H.Y. Qi, L. Jiang, Z.P. Jin, J.C. Zhao, Intermetallics. 64
 (2015) 86-95; Cr-Ru and Cr-Ni-Ru'
 'L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2010; Molar volumes'
 'L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2013; Reassessed
 solubility of Al, Cr, Fe, Ni in Mn2O3. When Mn2O3 is modelled as the
 same phase as cubic Y2O3 (M2O3C).'
 'Y. Du and J.C. Schuster, J. Phase Equilibria, 21(3) 281-86(2000); Cr-Si'
 'N. Dupin, Private communication; Si systems'
 'L. Kjellqvist, Thermo-Calc Software AB, Stockholm, 2010; Unassessed
 parameter, linear combination of unary volume data'
 'A. Jacob, E. Povoden-Karadeniz, E. Kozeschnik, Calphad, 56 (2017) 80-91.'
 'I. Ansara and A. Jansson, TRITA-MAC 533 (1993); Cu-Fe'
 'N. Zou et al., Calphad 64 (2019) 175-184'.
 'C.Y. He, J. Alloys Compd., 457, 233-238 (2008); Cu-Mn'
 'C.P. Wang et al., J. Phase Equil. 21 (2000) 54-62; Cu-Fe-Mo and Cu-Fe-Nb'
 'Same or similar interaction as in the corresponding stable phase'
 'K. Frisk, IM-2929, Swedish Inst. Met. Res., (1992); Cu-N, Fe-Cu-N'
 'L. Kjellqvist, Thermo-Calc Software AB (2014); FROST project'
 'S. an Mey, CALPHAD, 16 (1992) 255-260; Cu-Ni'
 'A. Jansson, TRITA-MAC 340 (1987); CU-FE-NI'
 'M. Jacobs (1991), Revised by T. Buehler (1997), COST 507 Report; Cu-Si'
 'S.G. Fries, H.L. Lukas, R. Konetzki, R. Schmid-Fetzer, J. Phase Equil.,
 15(1994) 606-614; Cu-Y'
 'H. Mao, Thermo-Calc Software AB, Sweden, 2013; Molar volumes'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2014; Unifying HCP_ZN with
 HCP_A3'
 'W. Huang, CALPHAD, 13 (1989) 243-252; TRITA-MAC 388 (rev 1999); FE-MN'
 'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
 'S. Liu, B. Hallstedt, D. Music, Y. Du, CALPHAD, 38 (2012) 43-58; Mn-Nb
 and Fe-Mn-Nb'
 'A. Markstrom, Thermo-Calc software AB, Sweden, 2011'
 'A.F. Guillermet, CALPHAD, 6 (1982) 127-140; (sigma phase revised 1986);
 TRITA-MAC 200 (1982); FE-MO'
 'K. Frisk, TRITA-MAC 428 (1990); FE-MO-NI'
 'H.K. Danielsen and J. Hald, CALPHAD, 31 (2007) 505-514; Z-PHASE'
 'H. Du, J. Phase Equil., 14, 682-93(1993); Fe-N, Fe-C-N'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; M5C2'
 'C. Qiu, Metall. Trans. A, 24A (1993) 629-645; Fe-Mn-N'
 'A.T. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); FE-NI'
 'L. Zhang, J. Wang, Y. Du, R. Hu, P. Nash, X.G. Lu, et al., Acta Mater. 57
 (2009) 5324-5341; Al-Fe-Ni'
 'L.J. Zhang, Int. J. Mater. Res., 100(2) 160-175 (2009), Fe-Mn-Ni'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; Molar volume Fe-Mn-Si
 and Al-Fe-Mn '
 'S. Cotes, A.F. Guillermet, M. Sade, J. Alloys Compd., 208(1998) 168-177'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2019; Cr-Fe-Nb-Si'
 'A. Forsberg and J. Agren, J. Phase Equil., 14 (1993) 354-363; Fe-Mn-Si'

'R. Naraghi, Thermo-Calc Software AB, Sweden (2019); Fe-Ni-Si'
 'J. Miettinen, G. Vassilev, J. Phase Equilib. Diffus, 37(5) 2016, 283-290;
 'Fe-P-Si'
 'C. Qiu and A.F. Guillermet, Z. Metallkd., 84 (1993) 11-12; Mn-N'
 'A. Markstrom, Thermo-Calc Software AB, Sweden, 2010; Molar volumes'
 'Shuhong Liu, unpublished work (2010), Mn-Ni, Al-Mn-Ni, Mn-Ni-Zn, Al-Cu-Fe-Mg
 -Mn-Si'
 'C.P. Guo, Intermetallics, 13(5), 525-534, (2005), Mn-Ni'
 'M. Chen, B. Hallstedt, L.J. Gauckler, J. Alloys Compd., 393 (2005) 114
 -21; Mn-Y-O'
 'M. Chen, B. Hallstedt, L.J. Gauckler, Solid State Ionics, 176 (2005) 1457
 -64; Mn-Zr-O, Mn-Y-Zr-O'
 'J. Miettinen, CALPHAD, 28 (2004) 313-320; Mn-Zn'
 'K. Frisk and B. Uhrenius, Metall. Mater. Trans. A, 27A (1996) 2869-2880;
 Mo-C-N, Fe-Mo-C-N'
 'K. Frisk, CALPHAD, 14 (1990) 311-320; MO-NI'
 'R. Naraghi, Thermo-Calc Software AB, Sweden (2018); Fe-Mo-Ni, Mo-Ni-Si,
 C14'
 'Y. Liu, G. Shao, P. Tsakiroopoulos, Intermatallics 8 (200) 953-962; Mo-Si,
 Al-Mo-Si'
 'A. Kusoffsky et al., Work within CCT-Applied Stainless steels, 2004; IM
 -2004-549; Fe-Cr-Si, Fe-Ni-Si, Fe-Cr-Cu, Fe-Cu-Mo, Cr-Mo-N-Ni,
 Fe-Cr-N-Ni, Fe-Al-Cr-Ni'
 'R. Naraghi, Thermo-Calc Software AB, Sweden (2015); FROST project'
 'K. Frisk, Z. Metallkd., 82 (1991) 59-66; TRITA-MAC 414 (1989); Fe-Ni-N'
 'K. Frisk, Int. J. Thermophys., 12 (1990) 417-431; TRITA-MAC 419 (1990); N
 -NI'
 'X. Ma, C. Li, F. Wang, W. Zhang, CALPHAD, 27 (2003) 383-388; N-Si'
 'Thermo-Calc Software, Sweden, 2009; Volume data updated for \$TCFE6
 database (TCFE v6, November, 2009).'
 'L. Kjellqvist, Thermo-Calc Software AB (2013) estimated parameter; Ni-Zr-O'
 'T. Tokunaga, K. Nishio, H. Ohtani, M. Hasebe, Calphad, 27 (2003), 161-168;
 Ni-Si'
 'N. Dupin; L12 general relations, equivalence of 2 sublattice formalism
 with four sublattice formalism'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; Checking ternary P
 systems'
 'B. Sundman, Private communication (2003-4); Refitted Fe-Ni-Si'
 'W.W. Zhang, unpublished (2010), Fe-Ni-Si'
 'R. Naraghi, Thermo-Calc Software AB, Sweden (2019); M4S11_G3'
 'J. Miettinen, CALPHAD, 27 (2003) 263-274; Cu-Ni-Zn'
 'H. Liang, Y.A.Chang, J. Phase Equilib. 19 (1998) 25-37'
 'A.V. Khvan, B. Hallstedt, C. Broeckmann, CALPHAD, 46, 24-33(2014); Cr-Fe-C'
 'J-O. Andersson, Metall. Trans. A, 19A (1988) 627-636 TRITA 0207 (1986); C
 -CR-FE'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2016; FCC Fe-Cr-C and C-Cr-Ni'
 'J. Bratberg, Thermo-Calc Software AB, Sweden, 2008; Fe-Cr-Mo-V-W-C'
 'P. Gustafsson, Inst. Met. Res. (Sweden) (1990); Estimations of C-CR-FE-V,
 C-CR-FE-MO-V-W, FE-N-W, FE-MN-N, FE-N-SI, CR-N-V, C-CR-N, FE-MO-N, CR
 -N-W, CR-TI-N'
 'NPL, unpublished work (1989); C-Cr-Ni'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; C-Cr-Si'
 'Y.Du, J.C.Schuster, J.Am.Ceram.Soc., 83 (8) 2067-73 (2000); C-Cr-Si'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; Adjusting hcp'
 'S. Nagakura, Transactions of the Iron and Steel Institute of Japan, 8
 (1968) 265-294; Molar volumes'
 'I.K. Kupalova, V.I. Pavlova, High Speed Steels: Physical Properties,
 Prop. Data Updat. 2 (1988) 67-78; Molar volumes'
 'H. Du and M. Hillert, TRITA-MAC 435 (1990); C-Fe-N'
 'J. Miettinen and B. Hallstedt, CALPHAD, 22 (1998) 231-256; Fe-Si and Fe
 -Si-C'
 'W. Zheng et al., J. Iron Steel Res. Int. 24(2)(2017) 190-197'
 'C.P. Wang, D.X. Huang, J.J. Zhu, S.Y. Yang, X.J. Liu, J. Phase Equilib.
 Diffus. 35 (2014) 314-325; Cr-Cu-Mo and Cr-Cu-W'
 'T. Ikoma, M. Kajihara, Mater. Sci. Eng. A, 437 (2006) 293-300; Cr-Cu-Ni'
 'C. Qiu, Metall. Trans. A, 24A (1993) 2393-2409; Cr-Fe-Mn-N'
 'A. Markstrom, Thermo-Calc Software AB (2013), Extrapolations, assumptions
 adjustment'
 'B. Sundman, estimated parameter (2000); Cr-Ni-Mo'
 'B.J. Lee, Private communication, (2000); Estimated parameter'
 'A. Kusoffsky, Work within CCT-Applied Stainless steels, 2003; IM-2003-532;
 Fe-Cr-N, Fe-C-Cr-N, Fe-Cr-Mo-N, Fe-Cr-Mn-N'
 'A. Markstrom, Thermo-Calc Software AB, Sweden, 2017; FROST'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2020; Cr-Fe-Si'
 'M. Lindholm, J. Phase Equilib., 18.5 (1997) 432; Cr-Fe-Si'
 'J. Kunze, P. Broz,
 I. Stloukal, Steel Research 67(1996) 279-284.'
 'K. Frisk, TRITA-MAC 422 (1990); CR-FE-N-NI'
 'J.C. Schuster and Y.Du, Metall. Mater. Trans.A, 31A(7) 1795-803(2000); Cr
 -Ni-Si.'
 'R. Naraghi, Thermo-Calc Software AB, Sweden (2019); Cr-Ni-Si'
 'L. Zhang, Y. Du, Q. Chen, H. Xu, F. Zheng, C. Tang, H. Chen, Int. J.
 Mater. Res. 99 (2008) 1306-1318; Cu-Fe-Mn'
 'J. Miettinen, CALPHAD, 27 (2003) 389-394; Cu-Fe-Si'
 'W.H. Sun, CALPHAD, 33, 642-649(2009), Cu-Mn-Ni'
 'K. Frisk, TRITA-MAC 433 (1990); FE-CR-MO-NI-N'
 'J. Miettinen, CALPHAD, 22 (1998) 275-300; Fe-Mo-Si'
 'B. Hu, Unpublished (2010); Mn-Ni-Si, Al-Cu-Fe-Ni'
 'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; Carbonitrides and
 M23C6'
 'J. Bratberg, Thermo-Calc Software AB, Sweden, 2008; Solubilities in M6C'
 'R. Naraghi, Thermo-Calc Software AB, Sweden (2019); Cheking the binaries.'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2019; ETA_M5SIN'
 'M. Ghasemi, Thermo-Calc Software AB, Sweden, 2019; Viscosity of metallic
 liquid'
 'M. J. Assael, J. Phys. Chem. Ref. Data 39 (2010) 033105; Cu, Sn'
 'M. J. Assael, J. Phys. Chem. Ref. Data 35 (2006) 285; Fe, Al'
 'M. J. Assael, High Temp. High Press., 41 (2012); Sb, Pb, Bi, Ni, Ag'
 'M. J. Assael, J. Phys. Chem. Ref. Data 41 (2012) 033101; Cd, Co, Ga, In,
 Hg, Si, Tl, Zn'
 'Q. Chen, Thermo-Calc Software AB (2014), L12 constraints'
 'M. Ghasemi, Thermo-Calc Software AB; assessing the surface tension of
 metallic liquid'
 -OK-
TDB_TCFE11:
TDE_TCFE11: go p-3

POLY version 3.32

POLY:

```

POLY: s-c p=1e5,n=1,t=1353
POLY: s-c w(c)=0.0009,w(n)=0.0007,w(cr)=.246,w(ni)=0.2,w(mn)=0.013
POLY: s-c w(si)=0.013,w(cu)=0.0024,w(mo)=0.003
POLY: l-c
P=100000, N=1, T=1353, W(C)=9E-4, W(N)=7E-4, W(CR)=0.246, W(NI)=0.2,

```

W(MN)=1.3E-2, W(SI)=1.3E-2, W(CU)=2.4E-3, W(MO)=3E-3
 DEGREES OF FREEDOM 0
POLY: c-e
 Using global minimization procedure
 Calculated 51488 grid points in 14 s
 Found the set of lowest grid points in 0 s
 Calculated POLY solution 1 s, total time 15 s
POLY: l-e
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium = 1, label A0 , database: TCFE11

Conditions:
 P=100000, N=1, T=1353, W(C)=9E-4, W(N)=7E-4, W(CR)=0.246, W(NI)=0.2,
 W(MN)=1.3E-2, W(SI)=1.3E-2, W(CU)=2.4E-3, W(MO)=3E-3
 DEGREES OF FREEDOM 0

Temperature 1353.00 K (1079.85 C), Pressure 1.000000E+05
 Number of moles of components 1.000000E+00, Mass in grams 5.44621E+01
 Total Gibbs energy -8.15441E+04, Enthalpy 3.59780E+04, Volume 7.33732E-06

| Component | Moles | W-Fraction | Activity | Potential | Ref.stat |
|-----------|------------|------------|------------|-------------|----------|
| C | 4.0809E-03 | 9.0000E-04 | 1.0130E-03 | -7.7563E+04 | SER |
| CR | 2.5767E-01 | 2.4600E-01 | 2.9911E-03 | -6.5384E+04 | SER |
| CU | 2.0569E-03 | 2.4000E-03 | 7.8672E-05 | -1.0631E+05 | SER |
| FE | 5.0808E-01 | 5.2100E-01 | 1.1694E-03 | -7.5948E+04 | SER |
| MN | 1.2887E-02 | 1.3000E-02 | 8.8491E-06 | -1.3089E+05 | SER |
| MO | 1.7030E-03 | 3.0000E-03 | 6.5792E-05 | -1.0832E+05 | SER |
| N | 2.7217E-03 | 7.0000E-04 | 1.4555E-07 | -1.7710E+05 | SER |
| NI | 1.8559E-01 | 2.0000E-01 | 1.8375E-04 | -9.6768E+04 | SER |
| SI | 2.5209E-02 | 1.3000E-02 | 8.7752E-09 | -2.0869E+05 | SER |

FCC_A1#1 Status ENTERED Driving force 0.0000E+00
 Moles 9.8834E-01, Mass 5.3940E+01, Volume fraction 9.8975E-01 Mass fractions:
 FE 5.24602E-01 NI 2.01793E-01 MN 1.30628E-02 CU 2.42325E-03 C 3.71539E-04
 CR 2.41136E-01 SI 1.31259E-02 MO 2.77863E-03 N 7.06780E-04

M23C6_D84 Status ENTERED Driving force 0.0000E+00
 Moles 1.1660E-02, Mass 5.2244E-01, Volume fraction 1.0249E-02 Mass fractions:
 CR 7.49151E-01 C 5.54617E-02 NI 1.48568E-02 N 0.00000E+00 SI 0.00000E+00
 FE 1.49155E-01 MO 2.58555E-02 MN 6.52026E-03 CU 0.00000E+00

POLY:
POLY: @@ Define some variables
POLY: enter-symb
Constant, variable, function or table? /FUNCTION/: variable
Name: cc
Function: 100*w(fcc_a1,c)
&
POLY: ent var csi=100*w(fcc_a1,si);
POLY: ent var cmn=100*w(fcc_a1,mn);
POLY: ent var ccr=100*w(fcc_a1,cr);
POLY: ent var cni=100*w(fcc_a1,ni);
POLY: ent var cmo=100*w(fcc_a1,mo);
POLY: ent var ccu=100*w(fcc_a1,cu);
POLY: ent var cn=100*w(fcc_a1,n);
POLY: ent var cfe=100*w(fcc_a1,fe);
POLY: ent var cm23=100*bpw(m23c6);
POLY:
POLY: li-sy
DEFINED FUNCTIONS AND VARIABLES%
 CC%=100*W(FCC_A1#1,C)
 CSI%=100*W(FCC_A1#1,SI)
 CMN%=100*W(FCC_A1#1,MN)
 CCR%=100*W(FCC_A1#1,CR)
 CNI%=100*W(FCC_A1#1,NI)
 CMO%=100*W(FCC_A1#1,MO)
 CCU%=100*W(FCC_A1#1,CU)
 CN%=100*W(FCC_A1#1,N)
 CFE%=100*W(FCC_A1#1,FE)
 CM23%=100*BPW(M23C6_D84)

POLY:
POLY: eval
Name(s): *
 CC=3.7153906E-2
 CSI=1.3125912
 CMN=1.306276
 CCR=24.113639
 CNI=20.179322
 CMO=0.27786319
 CCU=0.24232453
 CN=7.0677989E-2
 CFE=52.460153
 CM23=0.95926481

POLY:
POLY: enter-symb
Constant, variable, function or table? /FUNCTION/: FUNCTION
Name: tcst-273.15;
POLY:
POLY: @@ Enter empirical parameters as function of temperature
POLY: ent func bc=575-0.3686*tc;
POLY: ent func bsi=24.76+1.129e-4*tc*tc-0.09*tc;
POLY: ent func bmn=-1.4-0.007*tc;
POLY: ent func bcr=0.3-tc*7e-4;
POLY: ent func bni=5.3-tc*3.3e-3;
POLY: ent func bmo=6-tc*3.3e-3;
POLY: ent func bcu=-14+0.0116*tc;
POLY: ent func bn=937-2.74e-6*tc*tc*tc+5.24e-3*tc*tc-3.08*tc;
POLY: ent func bm23=48+0.0135*tc;
POLY: ent func at=1.68+4.248e-6*tc*tc-4.33e-3*tc;
POLY:
POLY: li-symb *

DEFINED FUNCTIONS AND VARIABLES%
 CC%=100*W(FCC_A1#1,C)
 CSI%=100*W(FCC_A1#1,SI)
 CMN%=100*W(FCC_A1#1,MN)
 CCR%=100*W(FCC_A1#1,CR)
 CNI%=100*W(FCC_A1#1,NI)
 CMO%=100*W(FCC_A1#1,MO)
 CCU%=100*W(FCC_A1#1,CU)
 CN%=100*W(FCC_A1#1,N)
 CFE%=100*W(FCC_A1#1,FE)
 CM23%=100*BPW(M23C6_D84)
 TC=T-273.15

```

BC=575-.3686*TC
BSI=24.76+1.129E-04*TC*TC-.09*TC
BMN=-1.4-.007*TC
BCR=.3-TC*7E-04
BNI=5.3-TC*.0033
BMO=6-TC*.0033
BCU=-14+.0116*TC
BN=937-2.74E-06*TC*TC*TC+.00524*TC*TC-3.08*TC
BM23=48+.0135*TC
AT=1.68+4.248E-06*TC*TC-.00433*TC
POLY:
POLY: eval
Name(s): *
CC=3.7153906E-2
CSI=1.3125912
CMN=1.306276
CCR=24.113639
CNI=20.179322
CMO=0.27786319
CCU=0.24232453
CN=7.0677989E-2
CFE=52.460153
CM23=0.95926481
BN=271.12745
BM23=62.577975
AT=1.9577404
POLY:
POLY: @@ Enter an empirical expression for the proof strength
POLY: @@ combining the variables and function parameters
POLY: @@ previously entered.
POLY: ent
Constant, variable, function or table? /FUNCTION/: FUNCTION
Name: rp1
Function: at+bc*cc+bsi*csi+bmtn*cmn+bni*cni;
POLY:
POLY: ent
Constant, variable, function or table? /FUNCTION/: FUNCTION
Name: rp2
Function: bcr*ccr+bmo*cmo+bcu*ccu+bn*cn+bm23*cm23;
POLY:
POLY: ent func rp02=rp1+rp2;
POLY:
POLY: eval
Name(s): *
CC=3.7153906E-2
CSI=1.3125912
CMN=1.306276
CCR=24.113639
CNI=20.179322
CMO=0.27786319
CCU=0.24232453
CN=7.0677989E-2
CFE=52.460153
CM23=0.95926481
TC=1079.85
BC=176.96729
BSI=59.223483
BMN=-8.95895
BCR=-0.455895
BNI=1.736495
BMO=2.436495
BCU=-1.47374
BN=271.12745
BM23=62.577975
AT=1.9577404
RP1=109.60742
RP2=68.518193
RP02=178.12561
POLY:
POLY: @@ Turn off the global minimization calculation and suspend
POLY: @@ all phases except fcc_a1#1. This speeds up the calculation,
POLY: @@ and allows us to consider only single-phase FCC at all T.
POLY:
POLY: advanced
Which option? /STEP_AND_MAP/: glo
Settings for global minimization:
Use global minimization as much as possible /Y/: n,,,
POLY:
POLY: c-s phase
Phase name(s): *
Status: /ENTERED/: sus
POLY:
POLY: ch-st phase fcc_a1#1=enter 1
POLY:
POLY: s-c t=500
POLY: c-e
Global equilibrium calculation turned off, you can turn it on with
ADVANCED_OPTIONS GLOBAL MINIMIZATION Y,,,
7 ITS, CPU TIME USED 0 SECONDS
POLY: l-e,,,
Output from POLY-3, equilibrium = 1, label A0 , database: TCFE11

Conditions:
P=100000, N=1, T=500, W(C)=9E-4, W(N)=7E-4, W(CR)=0.246, W(NI)=0.2,
W(MN)=1.3E-2, W(SI)=1.3E-2, W(CU)=2.4E-3, W(MO)=3E-3
DEGREES OF FREEDOM 0

Temperature 500.00 K ( 226.85 C), Pressure 1.000000E+05
Number of moles of components 1.000000E+00, Mass in grams 5.44621E+01
Total Gibbs energy -1.87392E+04, Enthalpy 9.55257E+03, Volume 7.01404E-06

Component Moles W-Fraction Activity Potential Ref.stat
C 4.0809E-03 9.0000E-04 1.2030E-01 -8.8042E+03 SER
CR 2.5767E-01 2.4600E-01 2.8885E-01 -5.1626E+03 SER
CU 2.0569E-03 2.4000E-03 3.5447E-01 -4.3117E+03 SER
FE 5.0808E-01 5.2100E-01 3.4197E-02 -1.4033E+04 SER

```

```

MN          1.2887E-02  1.3000E-02 3.8948E-05 -4.2210E+04 SER
MO          1.7030E-03  3.0000E-03 7.9503E-02 -1.0526E+04 SER
N          2.7217E-03  7.0000E-04 8.1730E-14 -1.2528E+05 SER
NI          1.8559E-01  2.0000E-01 6.7678E-04 -3.0340E+04 SER
SI          2.5209E-02  1.3000E-02 4.6361E-16 -1.4678E+05 SER

FCC_A1#1      Status ENTERED     Driving force 0.0000E+00
Moles 1.0000E+00, Mass 5.4462E+01, Volume fraction 1.0000E+00 Mass fractions:
FE 5.2100E-01 NI 2.0000E-01 SI 1.3000E-02 CU 2.4000E-03 N 7.0000E-04
CR 2.4600E-01 MN 1.3000E-02 MO 3.0000E-03 C 9.0000E-04
POLY: l-st
Option /CPS/:
*** STATUS FOR ALL COMPONENTS
COMPONENT      STATUS      REF. STATE      T (K)      P (Pa)
VA            ENTERED    SER
C             ENTERED    SER
CR            ENTERED    SER
CU            ENTERED    SER
FE            ENTERED    SER
MN            ENTERED    SER
MO            ENTERED    SER
N             ENTERED    SER
NI            ENTERED    SER
SI            ENTERED    SER
*** STATUS FOR ALL PHASES
PHASE          STATUS      DRIVING FORCE      MOLES
FCC_A1#1      ENTERED    0.000000E+00 1.000000E+00
SUSPENDED PHASES:
Z_PHASE SIGMA_D6B SIC_B3 SI3N4 R_PHASE P_PHASE PI_A13 NIZN_L10 NIZN_B2
NISI_B31 NISTI_D024 NI3Si2 NI3Si12 NI2ZN11 D82 NBNI13_D0A NB5Si3_D8L MU_D85
MSI_B20 MSI2_C40 MOSI2_C11B M05Si3_D8M MNP_B31 MN9Si2' MN6Si1 MN6N5 MNSSiC
MN3N2 MN11Si19 MC_SHP MC_ETA M7C3_D101 M6Si5 M6C_E93 M5Si3_D88 M5C2 M4Si1_G3
M3Si1 M3C2_D510 M2Si1_TETA M2P_C22 M23C6_D84 M11Si18 KSi_CARBIDE HIGH_SIGMA
HCP_A3#2 HCP_A3#1 G_PHASE GRAPHITE_A9 FESI2_L FESI2_H FE8Si2C FE4N_LP1
FCC_L12 FCC_A1#2 ETA_M5SiN DIAMOND_A4 CUZN_EPSILON_CUB A13 CU6Y CR2Ni17
CR5Si3_D8M CR3Si_A15 CO2Si_C37 CHI_A12 CEMENTITE_D011 CBCC_A12 C15_LAVES
C14_LAVES BCC_B2 BCC_A2 Al5Fe4 Al4C3_D71 LIQUID GAS
*** STATUS FOR ALL SPECIES
C      ENTERED    C5      ENTERED    CU2      ENTERED    N2      ENTERED
C1N1   ENTERED    CSN1    ENTERED    FE       ENTERED    N3      ENTERED
C1N2_CNN ENTERED    C60     ENTERED    FE+2    ENTERED    NI      ENTERED
C1N2_NCN ENTERED    C6N1    ENTERED    FE+3    ENTERED    NI+2    ENTERED
C2      ENTERED    C6N2    ENTERED    FE+4    ENTERED    NI+3    ENTERED
C2N1_CCN ENTERED    C9N1    ENTERED    MN      ENTERED    SI      ENTERED
C2N1_CNC ENTERED    CR      ENTERED    MN+2    ENTERED    SI+4    ENTERED
C2N2    ENTERED    CR+2    ENTERED    MN+3    ENTERED    SI3N4   ENTERED
C3      ENTERED    CR+3    ENTERED    MN+4    ENTERED    SI4/3   ENTERED
C3N1   ENTERED    CU      ENTERED    MO      ENTERED    VA      ENTERED
C4      ENTERED    CU+1    ENTERED    MO+2    ENTERED
C4N1   ENTERED    CU+2    ENTERED    N       ENTERED
C4N2   ENTERED    CU+3    ENTERED    N-3     ENTERED
POLY:Hit RETURN to continue
POLY: s-a-v 1 t
Min value /0/: 200
Max value /1/: 1000
Increment /20/: 10
POLY:
POLY: save tcex44 y
POLY:
POLY: @@ Step in temperature in order to evaluate proof strength
POLY: @@ as a function of temperature.
POLY:
POLY: step normal
No initial equilibrium, using default
Step will start from axis value 500.000
POLY has calculated initial equilibrium

Phase Region from 500.000 for:
  FCC_A1#1
Terminating at 1000.00
Calculated 53 equilibria

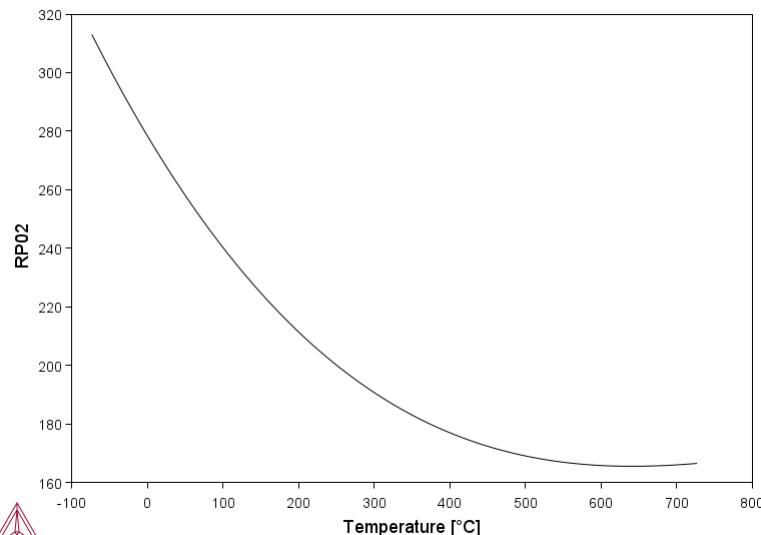
Phase Region from 500.000 for:
  FCC_A1#1
Terminating at 200.000
Calculated 33 equilibria
*** Buffer saved on file: c:\jenkins\workspace\generate_console_examples\examples\tcex44\tcex44.POLY3
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: s-d-a y rp02
POST: s-d-a x t-c
POST:
POST: set-title example 44a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot

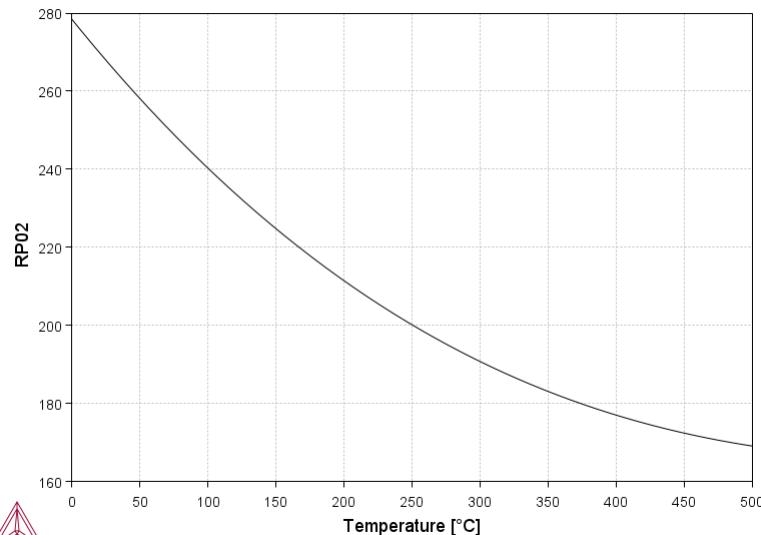
```

example 44a



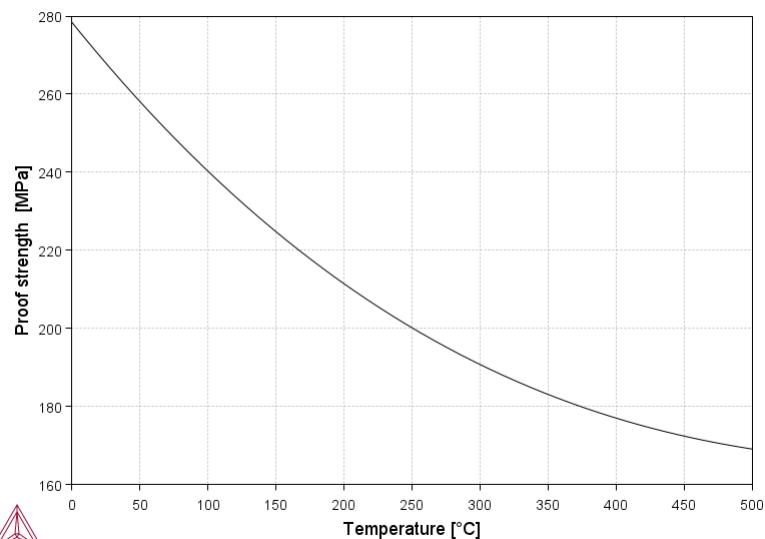
```
POST:  
POST:Hit RETURN to continue  
POST:  
POST: s-s-s x n 0 500  
POST:  
POST: set-ras y  
POST:  
POST: set-title example 44b  
POST:  
POST:  
POST: SET_EXP_FILE_FORMAT 5  
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y  
POST: SET_EXP_FILE_FORMAT 10  
POST:  
POST: plot
```

example 44b



```
POST:  
POST:Hit RETURN to continue  
POST:  
POST: set-axis-text-status  
POST: (X, Y OR Z) : y  
AUTOMATIC AXIS TEXT (Y OR N) /N/: n  
AXIS TEXT : Proof strength [MPa]  
POST:  
POST: set-title example 44c  
POST:  
POST:  
POST: SET_EXP_FILE_FORMAT 5  
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y  
POST: SET_EXP_FILE_FORMAT 10  
POST:  
POST: plot
```

example 44c



POST:
POST: set-inter
POST:

tce48

SYS:About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce48\tce48.TCM.test"

SYS: set-echo

SYS:

SYS: @@ Scheil solidification with C "back diffusion"

SYS:

SYS: @@ This is an example of Scheil solidification with
SYS: @@ simulated back diffusion of carbon in solid phases.

SYS: @@ The results are compared between a simple Scheil and
SYS: @@ equilibrium calculation.

SYS:

SYS: @@ First perform a Partial Equilibrium Scheil by assigning
SYS: @@ carbon as a fast diffusing element.

SYS: @@ Plot solidification curve and a microsegregation

SYS: @@ diagram and save to file (so called .exp files).

SYS:

SYS: @@ The "back diffusion" of C in solid phases is not from
SYS: @@ any calculation involving kinetics, but comes from the
SYS: @@ equilibration of chemical potential of C at each step

SYS: @@ in temperature, thus allowing each already solidified

SYS: @@ part of the system to change its C concentration.

SYS:

SYS: @@ Note that there is a calculation type that calculates
SYS: @@ "real" back diffusion. See Console Mode example tce54.

SYS: @@ This model requires a kinetic (mobility) database

SYS: @@ in addition to the thermodynamic one.

SYS:

SYS: go scheil

SCHHEIL: save-file-name tce48a

SCHHEIL: start

THERMODYNAMIC DATABASE module

Database folder: C:\jenkins\workspace\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

Database /TCFE11/: FEDEMO

Current database: Iron Demo Database v4.0

VA /- DEFINED

Major element or alloy: fe

Composition input in mass (weight) percent? /Y/: Y

1st alloying element: c 1

2nd alloying element: cr 10

Next alloying element:

Temperature (C) /2000/: 2000

VA /- DEFINED

REINITIATING GES

FE DEFINED

C DEFINED

CR DEFINED

This database has following phases for the defined system

| | | |
|------------------|----------|----------------|
| GAS:G | LIQUID:L | BCC_A2 |
| LAIVES_PHASE_C14 | CBCC_A12 | CEMENTITE |
| CHI_A12 | CUB_A13 | DIAMOND_FCC_A4 |
| FCC_A1 | GRAPHITE | HCP_A3 |
| KSI_CARBIDE | M23C6 | M3C2 |
| M5C2 | M7C3 | SIGMA |

Reject phase(s) /NONE/: NONE

Restore phase(s) : /NONE/: NONE

The following phases are retained in this system:

| | | |
|------------------|----------|----------------|
| GAS:G | LIQUID:L | BCC_A2 |
| LAIVES_PHASE_C14 | CBCC_A12 | CEMENTITE |
| CHI_A12 | CUB_A13 | DIAMOND_FCC_A4 |
| FCC_A1 | GRAPHITE | HCP_A3 |
| KSI_CARBIDE | M23C6 | M3C2 |
| M5C2 | M7C3 | SIGMA |

OK? /Y/: Y

16:51:24,792 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

ELEMENTS

SPECIES

PHASES

Creating a new composition set FCC_A1#2

PARAMETERS ...

FUNCTIONS

List of references for assessed data

'A.T. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121 -127; Molar volumes'
'M. Ghasemi, Thermo-Calc Software AB, Sweden, 2019; Viscosity of metallic liquid'
'M Ghasemi, Thermo-Calc Software AB: assessing the surface tension of metallic liquid'
'M. Ghasemi, Thermo-Calc Software AB, Sweden, 2020; Unifying liquid volume'

database
 'Y. Tang, in TCCU2, Thermo-Calc Software AB, Stockholm, Sweden'
 'M. J. Assael, J. Phys. Chem. Ref. Data 35 (2006) 285; Fe, Al'
 'A.V. Khvan, B. Hallstedt, K. Chang, CALPHAD, 39, 54-61(2012); C -Cr-Nb'
 'A.V. Khvan, B. Hallstedt, C. Broeckmann, CALPHAD, 46, 24 -33(2014); Cr-Fe
 -C'
 'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-Fe'
 'B.J. Lee, CALPHAD, 17 (1993) 251-268; revision of Fe-Cr and Fe -Ni liquid'
 'J-O. Andersson, CALPHAD, 11 (1987) 271-276; TRITA 0314; C-CR'
 'X.G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
 'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
 'X.G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
 volumes'
 'J-O. Andersson, Metall. Trans. A, 19A (1988) 627-636 TRITA 0207 (1986); C
 -CR-FE'
 'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270
 (1986); CR-FE'
 'N. Saunders, COST 507 Report (1998); Cr-Ti'
 'B.J. Lee, unpublished work at KTH (1999); update of steel database'
 'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equilib., 19
 (1998) 441-448; Fe-Ti'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2019; Cr-Fe-Nb'
 'B.J. Lee, Metall. Trans. A, 24A (1993) 1017-1025; Fe-Cr-Mn-C'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, Volume data updated for
 TCFE9 database (TCFE v9.0, Jan, 2017).'
 'W. Huang, Metall. Trans. A, 21A (1990) 2115-2123; TRITA-MAC 411 (Rev
 1989); C-FE-MN'
 'B.J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
 'P. Villars, L.D. Calvert. Pearson's handbook of crystallographic data for
 intermetallic phases, Metals park, Ohio 1985: American society for
 metals'
 'B. Hallstedt, D. Djurovic, J. von Appen, R. Dronskowski, A. Dick, F.
 Koermann, T. Hickel, J. Neugebauer, CALPHAD, 34, 129 -33(2010); Fe-C'
 'P. Gustafson, TRITA-MAC 354 (1987); C-Cr-Fe-Mo-W'
 'J-O. Andersson, Metall. Trans. A, 19A (1988) 1385-1394; TRITA 0322 (1986);
 CR-FE-MO'
 'J. Bratberg, Z. Metallkd., 96 (2005) 335-344; Fe-Cr-Mo-C'
 'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2016; FCC Fe-Cr-C and C-Cr-Ni'
 'C. Qui, ISIJ International, 32 (1992), 1117-1127; Trita-MAC 482 (1992)
 Revision; C-Cr-Fe-Mo'
 'J-O. Andersson, CALPHAD, 12 (1988) 9-23; TRITA 0321 (1986); C -FE-MO'
 'P. Gustafson, Metall. Trans. A, 19A (1988) 2547-2554; TRITA-MAC 348,
 (1987); C-CR-FE-W'
 'H. Gohring, O. Fabrichnaya, A. Leineweber, E.J. Mittemeijer, Metall.
 Mater. Trans. A, 47A, 6173-86(2016); FE-N, and Fe-C-N'
 'K. Frisk, Metall. Trans. A, 21A (1990) 2477-2488; TRITA 0409 (1989); CR
 -FE-N'
 'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, Calphad 35.4
 (2011) 479-491; Fe-Mn-C'
 'B. Sundman et al., Report EUR 20315, Contract No 7210-PR/050, 2002; New
 Sigma model'
 -OK-

Should any phase have a miscibility gap check? /N/: N

LIQUID PHASE NAME: LIQUID

Fast diffusing components: /NONE/: C

This command is a combination of CHANGE_STATUS and SET_CONDITION
 to calculate directly when a phase may form by releasing one condition.
 You must release one of these conditions
 T=2273.15, W(C)=1E-2, W(CR)=0.1, P=100000, N=1 DEGREES OF FREEDOM 0
 PHASE CHANGE AT 1715.05468788

FCC_A1#2 forms

Testing POLY result by global minimization procedure
 Calculated 20164 grid points in 0 s
 CALCULATING USING NORMAL EQUILIBRIUM CONDITIONS
 ...OK

Phase Region from 1715.14 for:
 LIQUID
 Terminating at 1715.24
 Calculated 4 equilibria

Phase Region from 1715.14 for:
 LIQUID
 Global check of adding phase at 1.71505E+03
 Calculated 3 equilibria

Phase Region from 1715.05 for:
 LIQUID
 FCC_A1#2
 Global test at 1.70714E+03 OK
 Global test at 1.69714E+03 OK
 Global test at 1.68714E+03 OK
 Global test at 1.67714E+03 OK
 Global test at 1.66714E+03 OK
 Global test at 1.65714E+03 OK
 Global test at 1.64714E+03 OK
 Global test at 1.63714E+03 OK
 Global test at 1.62714E+03 OK
 Global test at 1.61714E+03 OK
 Global test at 1.60714E+03 OK
 Global check of removing phase at 1.59813E+03
 Calculated 120 equilibria

Phase Region from 1598.13 for:
 FCC_A1#2
 Calculated 4 equilibria
 *** Buffer saved on file: c:\jenkins\workspace\generate_console_examples\examples\tcex48\tcex48a.POLY3
 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes
 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

An EXP file c:\jenkins\WORKSP~1\GENERA~1\examples\tcex48\tcex48a_EQ.EXP
 has been created to store the equilibrium solidification results.

CALCULATING SCHEIL SOLIDIFICATION
 T(C) fraction solid
 1441.995 0.000000
 PHASE REGION:LIQUID + FCC_A1#1
 T(C) fraction solid
 1441.899 0.1329022E-03
 1440.899 0.2342642E-01
 1439.899 0.4585953E-01

| | |
|----------|---------------|
| 1438.899 | 0.6763138E-01 |
| 1437.899 | 0.8876763E-01 |
| 1436.899 | 0.1092937 |
| 1435.899 | 0.1292335 |
| 1434.899 | 0.1486098 |
| 1433.899 | 0.1674443 |
| 1432.899 | 0.1857574 |
| 1431.899 | 0.2035686 |
| 1430.899 | 0.2208963 |
| 1429.899 | 0.2377580 |
| 1428.899 | 0.2541705 |
| 1427.899 | 0.2701497 |
| 1426.899 | 0.2857107 |
| 1425.899 | 0.3008678 |
| 1424.899 | 0.3156350 |
| 1423.899 | 0.3300252 |
| 1422.899 | 0.3440509 |
| 1421.899 | 0.3577242 |
| 1420.899 | 0.3710564 |
| 1419.899 | 0.3840585 |
| 1418.899 | 0.3967408 |
| 1417.899 | 0.4091133 |
| 1416.899 | 0.4211856 |
| 1415.899 | 0.4329668 |
| 1414.899 | 0.4444657 |
| 1413.899 | 0.4556908 |
| 1412.899 | 0.4666499 |
| 1411.899 | 0.4773509 |
| 1410.899 | 0.4878012 |
| 1409.899 | 0.4980079 |
| 1408.899 | 0.5079779 |
| 1407.899 | 0.5177177 |
| 1406.899 | 0.5272337 |
| 1405.899 | 0.5365319 |
| 1404.899 | 0.5456182 |
| 1403.899 | 0.5544983 |
| 1402.899 | 0.5631775 |
| 1401.899 | 0.5716612 |
| 1400.899 | 0.5799544 |
| 1399.899 | 0.5880619 |
| 1398.899 | 0.5959884 |
| 1397.899 | 0.6037386 |
| 1396.899 | 0.6113168 |
| 1395.899 | 0.6187271 |
| 1394.899 | 0.6259739 |
| 1393.899 | 0.6330609 |
| 1392.899 | 0.6399920 |
| 1391.899 | 0.6467711 |
| 1390.899 | 0.6534016 |
| 1389.899 | 0.6598870 |
| 1388.899 | 0.6662309 |
| 1387.899 | 0.6724363 |
| 1386.899 | 0.6785066 |
| 1385.899 | 0.6844448 |
| 1384.899 | 0.6902539 |
| 1383.899 | 0.6959369 |
| 1382.899 | 0.7014966 |
| 1381.899 | 0.7069357 |
| 1380.899 | 0.7122570 |
| 1379.899 | 0.7174630 |
| 1378.899 | 0.7225564 |
| 1377.899 | 0.7275396 |
| 1376.899 | 0.7324150 |
| 1375.899 | 0.7371850 |
| 1374.899 | 0.7418519 |
| 1373.899 | 0.7464180 |
| 1372.899 | 0.7508854 |
| 1371.899 | 0.7552562 |
| 1370.899 | 0.7595327 |
| 1369.899 | 0.7637168 |
| 1368.899 | 0.7678105 |
| 1367.899 | 0.7718157 |
| 1366.899 | 0.7757345 |
| 1365.899 | 0.7795686 |
| 1364.899 | 0.7833198 |
| 1363.899 | 0.7869901 |
| 1362.899 | 0.7905810 |
| 1361.899 | 0.7940944 |
| 1360.899 | 0.7975319 |
| 1359.899 | 0.8008952 |
| 1358.899 | 0.8041858 |
| 1357.899 | 0.8074053 |
| 1356.899 | 0.8105553 |
| 1355.899 | 0.8136373 |
| 1354.899 | 0.8166528 |
| 1353.899 | 0.8196031 |
| 1352.899 | 0.8224898 |
| 1351.899 | 0.8253143 |
| 1350.899 | 0.8280778 |
| 1349.899 | 0.8307818 |
| 1348.899 | 0.8334275 |
| 1347.899 | 0.8360162 |
| 1346.899 | 0.8385492 |
| 1345.899 | 0.8410277 |
| 1344.899 | 0.8434529 |
| 1343.899 | 0.8458260 |
| 1342.899 | 0.8481482 |
| 1341.899 | 0.8504206 |
| 1340.899 | 0.8526443 |
| 1339.899 | 0.8548203 |
| 1338.899 | 0.8569498 |
| 1337.899 | 0.8590339 |
| 1336.899 | 0.8610734 |
| 1335.899 | 0.8630695 |
| 1334.899 | 0.8650231 |
| 1333.899 | 0.8669352 |
| 1332.899 | 0.8688067 |
| 1331.899 | 0.8706385 |
| 1330.899 | 0.8724315 |
| 1329.899 | 0.8741866 |
| 1328.899 | 0.8759047 |
| 1327.899 | 0.8775867 |
| 1326.899 | 0.8792332 |
| 1325.899 | 0.8808453 |
| 1324.899 | 0.8824235 |
| 1323.899 | 0.8839688 |

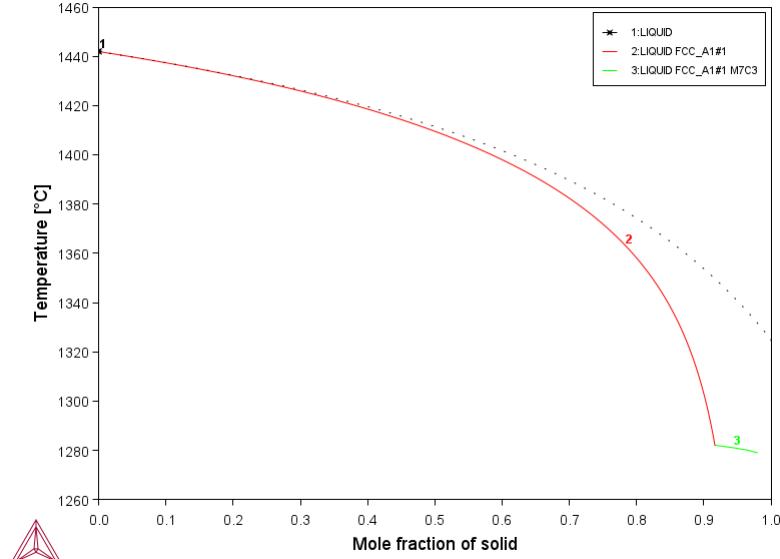
1322.899 0.8854819
 1321.899 0.8869634
 1320.899 0.8884142
 1319.899 0.8898350
 1318.899 0.8912264
 1317.899 0.8925891
 1316.899 0.8939237
 1315.899 0.8952310
 1314.899 0.8965116
 1313.899 0.8977660
 1312.899 0.8989948
 1311.899 0.9001988
 1310.899 0.9013784
 1309.899 0.9025342
 1308.899 0.9036667
 1307.899 0.9047766
 1306.899 0.9058642
 1305.899 0.9069302
 1304.899 0.9079750
 1303.899 0.9089992
 1302.899 0.9100032
 1301.899 0.9109874
 1300.899 0.9119524
 1299.899 0.9128985
 1298.899 0.9138263
 1297.899 0.9147361
 1296.899 0.9156283
 1295.899 0.9165035
 1294.899 0.9173618
 1293.899 0.9182039
 1292.899 0.9190299
 1291.899 0.9198404
 1290.899 0.9206356
 1289.899 0.9214159
 1288.899 0.9221816
 1287.899 0.9229331
 1286.899 0.9236708
 1285.899 0.9243949
 1284.899 0.9251057
 1283.899 0.9258036
 1282.899 0.9264888
 1282.038 0.9271048

PHASE REGION:LIQUID + FCC_A1#1 + M7C3

| T (C) | fraction solid |
|----------|----------------|
| 1282.007 | 0.9294370 |
| 1281.007 | 0.9559107 |
| 1280.007 | 0.9776564 |
| 1279.007 | 0.9907091 |

Calculating properties ...

Liquidus temperature: 1715.055 K

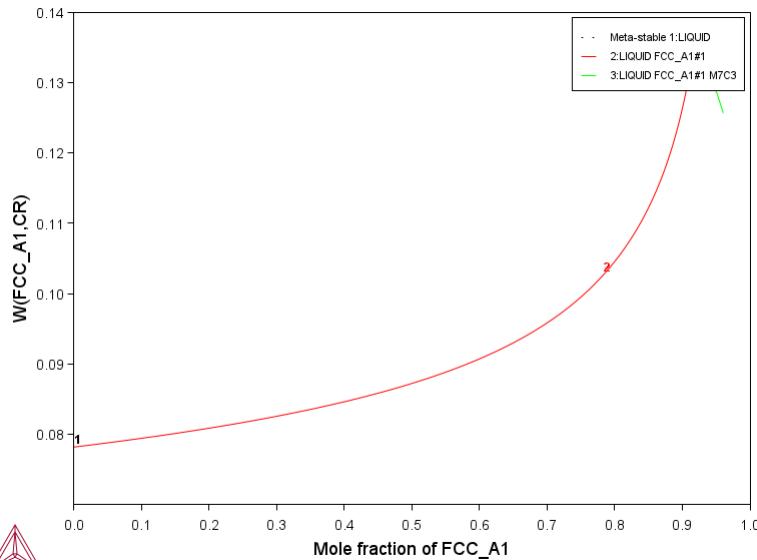


The following axis variables are available

T - Temperature in Celsius
 NL/BL/VL - Mole/mass/volume fraction of liquid
 NS/BS/VS - Mole/mass/volume fraction of all solid phases
 NS(ph)/BS(ph) - Mole/mass fraction of a solid phase
 VS(ph) - Volume fraction of a solid phase
 W(ph,el) - Weight fraction of an element in a phase
 X(ph,el) - Mole fraction of an element in a phase
 Y(ph,el) - Site fraction of an element in a phase
 NN(ph,el) - Distribution of an element in a phase
 NH/BH - Heat release and Latent heat per mole/gram
 CP/BCP - Apparent heat capacity per mole/gram
 NV/NV(ph) - Molar volume of the system or a phase
 DS/DS(ph) - Average density of the system or a phase
 BT - Apparent volumetric TEC of the system
 DVIS(ph) - Dynamic viscosity of a phase
 KVIS(ph) - Kinematic viscosity of phase
 SURF(ph) - Surface tension of a liquid phase
 ELRS/ELRS(ph) - Electrical resistivity of the system or a phase
 ELCD/ELCD(ph) - Electrical conductivity of the system or a phase
 THCD/THCD(ph) - Thermal conductivity of the system or a phase
 THRS/THRS(ph) - Thermal resistivity of the system or a phase
 THDF/THDF(ph) - Thermal diffusivity of the system or a phase
 DGV - Driving force for evaporation
 DHV - Evaporation enthalpy
 MMG - Molar mass of gas
 XAVG(el) - Mole fraction of an element in solid phases
 WAVG(el) - Mass fraction of an element in solid phases

"el" and "ph" are name of element and phase, respectively
"*" can be used as a wild character for "el" and "ph"

```
POST:Hit RETURN to continue
POST: make tce48a.exp y
POST:
POST: set-dia-ax x ns(fcc_a1)
POST: set-dia-ax y w(fcc_a1,cr)
POST: sel-plot new
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot.....
```



```
POST:Hit RETURN to continue
POST:
POST:
POST: make tce48b.exp y
POST:
POST: back
SCHEIL:
SCHEIL: @@ Ignore back diffusion of C in solids and do Scheil
SCHEIL: @@ with the same alloy by choosing option 3 from the
SCHEIL: @@ Scheil simulation option list.
SCHEIL: @@ Also plot solidification and microsegregation
SCHEIL: @@ diagrams and save to files
SCHEIL:
SCHEIL: save-file-name tce48b
SCHEIL: start
Database /TCFE11/: FEDEMO
Major element or alloy: fe
Composition input in mass (weight) percent? /Y/: Y
1st alloying element: c 1
2nd alloying element: cr 10
Next alloying element:
Temperature (C) /2000/: 1700
VA           /- DEFINED
REINITIATING GES .....
FE  DEFINED
C   DEFINED
CR  DEFINED
```

This database has following phases for the defined system

| | | |
|-----------------|----------|----------------|
| GAS:G | LIQUID:L | BCC_A2 |
| LAVES_PHASE_C14 | CBCC_A12 | CEMENTITE |
| CHI_A12 | CUB_A13 | DIAMOND_FCC_A4 |
| FCC_A1 | GRAPHITE | HCP_A3 |
| KSI_CARBIDE | M23C6 | M3C2 |
| M5C2 | M7C3 | SIGMA |

Reject phase(s) /NONE/: NONE
Restore phase(s): /NONE/: NONE

The following phases are retained in this system:

| | | |
|-----------------|----------|----------------|
| GAS:G | LIQUID:L | BCC_A2 |
| LAVES_PHASE_C14 | CBCC_A12 | CEMENTITE |
| CHI_A12 | CUB_A13 | DIAMOND_FCC_A4 |
| FCC_A1 | GRAPHITE | HCP_A3 |
| KSI_CARBIDE | M23C6 | M3C2 |
| M5C2 | M7C3 | SIGMA |

```
OK? /Y/: Y
ELEMENTS .....
SPECIES .....
PHASES .....
Creating a new composition set FCC_A1#2
PARAMETERS ...
FUNCTIONS ...
```

List of references for assessed data

'A.T. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
 'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121 -127; Molar volumes'
 'M. Ghasemi, Thermo-Calc Software AB, Sweden, 2019; Viscosity of metallic liquid'
 'M Ghasemi, Thermo-Calc Software AB: assessing the surface tension of metallic liquid'
 'M. Ghasemi, Thermo-Calc Software AB, Sweden, 2020; Unifying liquid volume database,
 'Y. Tang, in TCCU2, Thermo-Calc Software AB, Stockholm, Sweden'
 'M. J. Assael, J. Phys. Chem. Ref. Data 35 (2006) 285; Fe, Al'
 'A.V. Khvan, B. Hallstedt, K. Chang, CALPHAD, 39, 54-61(2012); C -Cr-Nb'
 'A.V. Khvan, B. Hallstedt, C. Broeckmann, CALPHAD, 46, 24 -33(2014); Cr-Fe -C'
 'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
 'B.J. Lee, CALPHAD, 17 (1993) 251-268; revision of Fe-Cr and Fe -Ni liquid'
 'J-O. Andersson, CALPHAD, 11 (1987) 271-276; TRITA 0314; C-CR'
 'X.G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
 'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
 'X.G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar volumes'
 'J-O. Andersson, Metall. Trans. A, 19A (1988) 627-636 TRITA 0207 (1986); C -CR-FE'
 'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270 (1986); CR-FE'
 'N. Saunders, COST 507 Report (1998); Cr-Ti'
 'B.J. Lee, unpublished work at KTH (1999); update of steel database'
 'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equilib., 19 (1998) 441-448; Fe-Ti'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2019; Cr-Fe-Nb'
 'B.J. Lee, Metall. Trans. A, 24A (1993) 1017-1025; Fe-Cr-Mn-C'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, Volume data updated for TCDF9 database (TCFE v9.0, Jan, 2017).'
 'W. Huang, Metall. Trans. A, 21A (1990) 2115-2123; TRITA-MAC 411 (Rev 1989); C-FE-MN'
 'B.J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
 'P. Villars, L.D. Calvert. Pearson's handbook of crystallographic data for intermetallic phases, Metals park, Ohio 1985: American society for metals'
 'B. Hallstedt, D. Djurovic, J. von Appen, R. Dronskowsk, A. Dick, F. Koermann, T. Hickel, J. Neugebauer, CALPHAD, 34, 129 -33(2010); Fe-C'
 'P. Gustafson, TRITA-MAC 354 (1987); C-Cr-Fe-Mo-W'
 'J-O. Andersson, Metall. Trans. A, 19A (1988) 1385-1394; TRITA 0322 (1986); CR-FE-MO'
 'J. Bratberg, Z. Metallkd., 96 (2005) 335-344; Fe-Cr-Mo-C'
 'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
 'R. Naraghi, Thermo-Calc Software AB, Sweden, 2016; FCC Fe-Cr-C and C-Cr-Ni'
 'C. Qui, ISIJ International, 32 (1992), 1117-1127; Trita-MAC 482 (1992) Revision; C-Cr-Fe-Mo'
 'J-O. Andersson, CALPHAD, 12 (1988) 9-23; TRITA 0321 (1986); C -FE-MO'
 'P. Gustafson, Metall. Trans. A, 19A (1988) 2547-2554; TRITA-MAC 348, (1987); C-CR-FE-W'
 'H. Gohring, O. Fabrichnaya, A. Leineweber, E.J. Mittemeijer, Metall. Mater. Trans. A, 47A, 6173-86(2016); FE-N, and Fe-C-N'
 'K. Frisk, Metall. Trans. A, 21A (1990) 2477-2488; TRITA 0409 (1989); CR -FE-N'
 'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowsk, Calphad 35.4 (2011) 479-491; Fe-Mn-C'
 'B. Sundman et al., Report EUR 20315, Contract No 7210-PR/050, 2002; New Sigma model'

-OK-

Should any phase have a miscibility gap check? /N/: N

LIQUID PHASE NAME: LIQUID

Fast diffusing components: /NONE/: NONE

This command is a combination of CHANGE_STATUS and SET_CONDITION to calculate directly when a phase may form by releasing one condition. You must release one of these conditions

T=1973.15, W(C)=1E-2, W(CR)=0.1, P=100000, N=1 DEGREES OF FREEDOM 0

PHASE CHANGE AT 1715.05468788

FCC_A1#1 forms

Testing POLY result by global minimization procedure
Calculated 20164 grid points in 0 s

CALCULATING USING NORMAL EQUILIBRIUM CONDITIONS

...OK

Phase Region from 1715.14 for:
LIQUID

Terminating at 1715.24

Calculated 4 equilibria

Phase Region from 1715.14 for:

LIQUID

Global check of adding phase at 1.71505E+03

Calculated 3 equilibria

Phase Region from 1715.05 for:

LIQUID

FCC_A1#1

Global test at 1.70714E+03 OK

Global test at 1.69714E+03 OK

Global test at 1.68714E+03 OK

Global test at 1.67714E+03 OK

Global test at 1.66714E+03 OK

Global test at 1.65714E+03 OK

Global test at 1.64714E+03 OK

Global test at 1.63714E+03 OK

Global test at 1.62714E+03 OK

Global test at 1.61714E+03 OK

Global test at 1.60714E+03 OK

Global check of removing phase at 1.59813E+03

Calculated 120 equilibria

Phase Region from 1598.13 for:

FCC_A1#1

Calculated 4 equilibria

*** Buffer saved on file: c:\jenkins\workspace\generate_console_examples\examples\tcex48\tcex48b.POLY3
POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

An EXP file c:\jenkins\WORKSP~1\GENERA~1\examples\tcex48\tcex48b_EQ.EXP has been created to store the equilibrium solidification results.

CALCULATING SCHEIL SOLIDIFICATION

T(C) fraction solid

1441.995 0.000000

PHASE REGION:LIQUID + FCC_A1#1

| T (C) | fraction solid |
|----------|----------------|
| 1441.899 | 0.1329022E-03 |
| 1440.899 | 0.2342642E-01 |
| 1439.899 | 0.4585862E-01 |
| 1438.899 | 0.6747197E-01 |
| 1437.899 | 0.8830633E-01 |
| 1436.899 | 0.1083992 |
| 1435.899 | 0.1277857 |
| 1434.899 | 0.1464991 |
| 1433.899 | 0.1645706 |
| 1432.899 | 0.1820295 |
| 1431.899 | 0.1989037 |
| 1430.899 | 0.2152193 |
| 1429.899 | 0.2310011 |
| 1428.899 | 0.2462723 |
| 1427.899 | 0.2610552 |
| 1426.899 | 0.2753706 |
| 1425.899 | 0.2892383 |
| 1424.899 | 0.3026771 |
| 1423.899 | 0.3157047 |
| 1422.899 | 0.3283380 |
| 1421.899 | 0.3405930 |
| 1420.899 | 0.3524849 |
| 1419.899 | 0.3640280 |
| 1418.899 | 0.3752362 |
| 1417.899 | 0.3861225 |
| 1416.899 | 0.3966992 |
| 1415.899 | 0.4069781 |
| 1414.899 | 0.4169706 |
| 1413.899 | 0.4266874 |
| 1412.899 | 0.4361386 |
| 1411.899 | 0.4453340 |
| 1410.899 | 0.4542829 |
| 1409.899 | 0.4629942 |
| 1408.899 | 0.4714763 |
| 1407.899 | 0.4797374 |
| 1406.899 | 0.4877852 |
| 1405.899 | 0.4956271 |
| 1404.899 | 0.5032702 |
| 1403.899 | 0.5107212 |
| 1402.899 | 0.5179866 |
| 1401.899 | 0.5250727 |
| 1400.899 | 0.5319853 |
| 1399.899 | 0.5387303 |
| 1398.899 | 0.5453131 |
| 1397.899 | 0.5517388 |
| 1396.899 | 0.5580126 |
| 1395.899 | 0.5641393 |
| 1394.899 | 0.5701234 |
| 1393.899 | 0.5759695 |
| 1392.899 | 0.5816819 |
| 1391.899 | 0.5872646 |
| 1390.899 | 0.5927217 |
| 1389.899 | 0.5980568 |
| 1388.899 | 0.6032737 |
| 1387.899 | 0.6083758 |
| 1386.899 | 0.6133667 |
| 1385.899 | 0.6182494 |
| 1384.899 | 0.6230272 |
| 1383.899 | 0.6277031 |
| 1382.899 | 0.6322800 |
| 1381.899 | 0.6367608 |
| 1380.899 | 0.6411480 |
| 1379.899 | 0.6454444 |
| 1378.899 | 0.6496525 |
| 1377.899 | 0.6537746 |
| 1376.899 | 0.6578132 |
| 1375.899 | 0.6617705 |
| 1374.899 | 0.6656487 |
| 1373.899 | 0.6694499 |
| 1372.899 | 0.6731762 |
| 1371.899 | 0.6768295 |
| 1370.899 | 0.6804118 |
| 1369.899 | 0.6839248 |
| 1368.899 | 0.6873704 |
| 1367.899 | 0.6907503 |
| 1366.899 | 0.6940662 |
| 1365.899 | 0.6973196 |
| 1364.899 | 0.7005122 |
| 1363.899 | 0.7036455 |
| 1362.899 | 0.7067209 |
| 1361.899 | 0.7097399 |
| 1360.899 | 0.7127038 |
| 1359.899 | 0.7156140 |
| 1358.899 | 0.7184717 |
| 1357.899 | 0.7212783 |
| 1356.899 | 0.7240349 |
| 1355.899 | 0.7267427 |
| 1354.899 | 0.7294029 |
| 1353.899 | 0.7320165 |
| 1352.899 | 0.7345847 |
| 1351.899 | 0.7371085 |
| 1350.899 | 0.7395889 |
| 1349.899 | 0.7420270 |
| 1348.899 | 0.7444235 |
| 1347.899 | 0.7467796 |
| 1346.899 | 0.7490960 |
| 1345.899 | 0.7513737 |
| 1344.899 | 0.7536136 |
| 1343.899 | 0.7558163 |
| 1342.899 | 0.7579829 |
| 1341.899 | 0.7601140 |
| 1340.899 | 0.7622104 |
| 1339.899 | 0.7642728 |
| 1338.899 | 0.7663021 |
| 1337.899 | 0.7682988 |
| 1336.899 | 0.7702636 |
| 1335.899 | 0.7721973 |
| 1334.899 | 0.7741005 |
| 1333.899 | 0.7759738 |
| 1332.899 | 0.7778178 |
| 1331.899 | 0.7796331 |
| 1330.899 | 0.7814204 |
| 1329.899 | 0.7831801 |
| 1328.899 | 0.7849129 |
| 1327.899 | 0.7866192 |

| | |
|---------------------------------------|----------------|
| 1326.899 | 0.7882996 |
| 1325.899 | 0.7899547 |
| 1324.899 | 0.7915848 |
| 1323.899 | 0.7931906 |
| 1322.899 | 0.7947724 |
| 1321.899 | 0.7963308 |
| 1320.899 | 0.7978662 |
| 1319.899 | 0.7993790 |
| 1318.899 | 0.8008697 |
| 1317.899 | 0.8023387 |
| 1316.899 | 0.8037865 |
| 1315.899 | 0.8052133 |
| 1314.899 | 0.8066196 |
| 1313.899 | 0.8080059 |
| 1312.899 | 0.8093723 |
| 1311.899 | 0.8107195 |
| 1310.899 | 0.8120476 |
| 1309.899 | 0.8133570 |
| 1308.899 | 0.8146482 |
| 1307.899 | 0.8159213 |
| 1306.899 | 0.8171768 |
| 1305.899 | 0.8184150 |
| 1304.899 | 0.8196361 |
| 1303.899 | 0.8208405 |
| 1302.899 | 0.8220285 |
| 1301.899 | 0.8232004 |
| 1300.899 | 0.8243564 |
| 1299.899 | 0.8254969 |
| 1298.899 | 0.8266221 |
| 1297.899 | 0.8277323 |
| 1296.899 | 0.8288277 |
| 1295.899 | 0.8299086 |
| 1294.899 | 0.8309753 |
| 1293.899 | 0.8320279 |
| 1292.899 | 0.8330668 |
| 1291.899 | 0.8340922 |
| 1290.899 | 0.8351043 |
| 1289.899 | 0.8361033 |
| 1288.899 | 0.8370895 |
| 1287.899 | 0.8380631 |
| 1286.899 | 0.8390242 |
| 1285.899 | 0.8399732 |
| 1284.899 | 0.8409101 |
| 1283.899 | 0.8418353 |
| 1282.899 | 0.8427488 |
| 1281.899 | 0.8436510 |
| 1280.899 | 0.8445419 |
| 1279.899 | 0.8454218 |
| 1278.899 | 0.8462908 |
| 1277.899 | 0.8471492 |
| 1276.899 | 0.8479970 |
| 1275.899 | 0.8488346 |
| 1274.899 | 0.8496620 |
| 1273.899 | 0.8504794 |
| 1272.899 | 0.8512869 |
| 1271.899 | 0.8520848 |
| 1270.899 | 0.8528732 |
| 1269.899 | 0.8536522 |
| 1268.899 | 0.8544220 |
| 1267.899 | 0.8551827 |
| 1267.548 | 0.8554471 |
| PHASE REGION:LIQUID + FCC_A1#1 + M7C3 | |
| T (C) | fraction solid |
| 1267.517 | 0.8556564 |
| 1266.517 | 0.8680204 |
| 1265.517 | 0.8787644 |
| 1264.517 | 0.8881677 |
| 1263.517 | 0.8964509 |
| 1262.517 | 0.9037902 |
| 1261.517 | 0.9103282 |
| 1260.517 | 0.9161808 |
| 1259.517 | 0.9214436 |
| 1258.517 | 0.9261957 |
| 1257.517 | 0.9305032 |
| 1256.517 | 0.9344216 |
| 1255.517 | 0.9379979 |
| 1254.517 | 0.9412721 |
| 1253.517 | 0.9442785 |
| 1252.517 | 0.9470463 |
| 1251.517 | 0.9496011 |
| 1250.517 | 0.9519649 |
| 1249.517 | 0.9541568 |
| 1248.517 | 0.9561939 |
| 1247.517 | 0.9580907 |
| 1246.517 | 0.9598604 |
| 1245.517 | 0.9615144 |
| 1244.517 | 0.9630630 |
| 1243.517 | 0.9645153 |
| 1242.517 | 0.9658794 |
| 1241.517 | 0.9671625 |
| 1240.517 | 0.9683712 |
| 1239.517 | 0.9695113 |
| 1238.517 | 0.9705881 |
| 1237.517 | 0.9716065 |
| 1236.517 | 0.9725706 |
| 1235.517 | 0.9734845 |
| 1234.517 | 0.9743516 |
| 1233.517 | 0.9751754 |
| 1232.517 | 0.9759587 |
| 1231.517 | 0.9767042 |
| 1230.517 | 0.9774144 |
| 1229.517 | 0.9780917 |
| 1228.517 | 0.9787380 |
| 1227.517 | 0.9793554 |
| 1226.517 | 0.9799457 |
| 1225.517 | 0.9805103 |
| 1224.517 | 0.9810510 |
| 1223.517 | 0.9815690 |
| 1222.517 | 0.9820657 |
| 1221.517 | 0.9825423 |
| 1220.517 | 0.9829999 |
| 1219.517 | 0.9834395 |
| 1218.517 | 0.9838622 |
| 1217.517 | 0.9842688 |
| 1216.517 | 0.9846601 |
| 1215.517 | 0.9850370 |

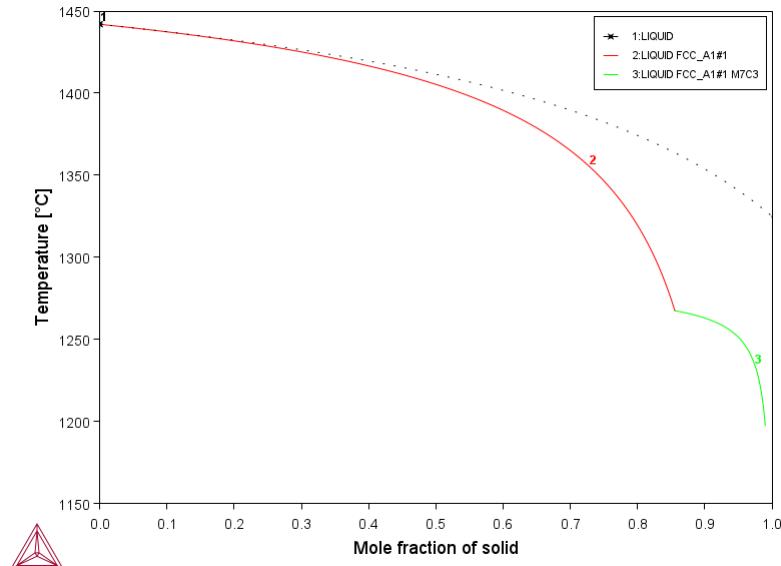
```

1214.517 0.9854002
1213.517 0.9857504
1212.517 0.9860882
1211.517 0.9864142
1210.517 0.9867291
1209.517 0.9870333
1208.517 0.9873273
1207.517 0.9876116
1206.517 0.9878867
1205.517 0.9881530
1204.517 0.9884108
1203.517 0.9886606
1202.517 0.9889027
1201.517 0.9891375
1200.517 0.9893652
1199.517 0.9895861
1198.517 0.9898005
1197.517 0.9900088

```

Calculating properties ...

Liquidus temperature: 1715.055 K



The following axis variables are available

```

T - Temperature in Celsius
NL/BL/VL - Mole/mass/volume fraction of liquid
NS/BS/VS - Mole/mass/volume fraction of all solid phases
NS(ph)/BS(ph) - Mole/mass fraction of a solid phase
VS(ph) - Volume fraction of a solid phase
W(ph,el) - Weight fraction of an element in a phase
X(ph,el) - Mole fraction of an element in a phase
Y(ph,el) - Site fraction of an element in a phase
NN(ph,el) - Distribution of an element in a phase
NH/BH - Heat release and Latent heat per mole/gram
CP/BCP - Apparent heat capacity per mole/gram
NV/NV(ph) - Molar volume of the system or a phase
DS/DS(ph) - Average density of the system or a phase
BT - Apparent volumetric TEC of the system
DVIS(ph) - Dynamic viscosity of a phase
KVIS(ph) - Kinematic viscosity of a phase
SURF(ph) - Surface tension of a liquid phase
ELRS/ELRS(ph) - Electrical resistivity of the system or a phase
ELCD/ELCD(ph) - Electrical conductivity of the system or a phase
THCD/THCD(ph) - Thermal conductivity of the system or a phase
THRS/THRS(ph) - Thermal resistivity of the system or a phase
THDF/THDF(ph) - Thermal diffusivity of the system or a phase
DGV - Driving force for evaporation
DHV - Evaporation enthalpy
MMG - Molar mass of gas
XAVG(el) - Mole fraction of an element in solid phases
WAVG(el) - Mass fraction of an element in solid phases

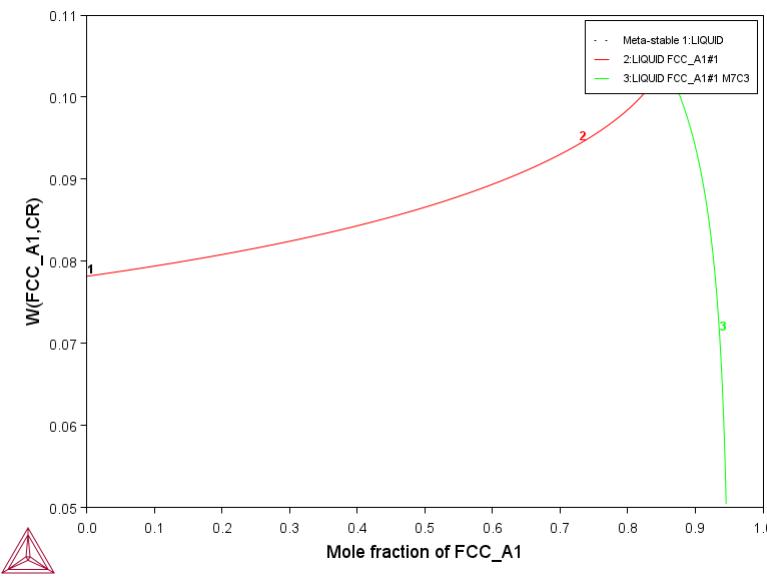
```

"el" and "ph" are name of element and phase, respectively
"**" can be used as a wild character for "el" and "ph"

```

POST:Hit RETURN to continue
POST: make tcecx48c.exp y
POST: set-dia=ax x ns(fcc_a1)
POST: set-dia=ax y w(fcc_a1,cr)
POST: sel-plot new
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot,,,,,

```



POST: make tcex48d.exp y

POST: back

SCHIEL:Hit RETURN to continue

SCHIEL: @@ Calculate simple equilibrium solidification of the SCHIEL: @@ same alloy and compare the results with those of

SCHIEL: @@ Scheil and ScheiC

SCHIEL: go p-3

POLY: read tcex48b

POLY: list-condition

T=1470.666563, P=100000, N(C)=1.712684283E-3, N(CR)=8.722254571E-4,
N(FE)=7.614560229E-3

DEGREES OF FREEDOM 0

POLY: list-equilibrium

OUTPUT TO SCREEN OR FILE /SCREEN/:

Options /VWCS/: VWCS

Output from POLY-3, equilibrium = 1, label A0 , database: FEDEMO

Conditions:

T=1470.666563, P=100000, N(C)=1.712684283E-3, N(CR)=8.722254571E-4,
N(FE)=7.614560229E-3

DEGREES OF FREEDOM 0

Temperature 1470.67 K (1197.52 C), Pressure 1.000000E+05
Number of moles of components 1.01995E-02, Mass in grams 4.91174E-01
Total Gibbs energy -7.59431E+02, Enthalpy 5.56424E+02, Volume 7.04651E-08

| Component | Moles | W-Fraction | Activity | Potential | Ref.stat |
|-----------|------------|------------|------------|-------------|----------|
| C | 1.7127E-03 | 4.1881E-02 | 5.7244E-02 | -3.4977E+04 | SER |
| CR | 8.7223E-04 | 9.2334E-02 | 2.0297E-04 | -1.0397E+05 | SER |
| FE | 7.6146E-03 | 8.6578E-01 | 1.4460E-03 | -7.9958E+04 | SER |

| LIQUID | Status | ENTERED | Driving force | 0.0000E+00 |
|--------|-------------|---|-----------------|------------|
| Moles | 9.9912E-03 | Mass 4.8105E-01, Volume fraction 9.8002E-01 | Mass fractions: | |
| FE | 8.66596E-01 | CR 9.14436E-02 | C 4.19606E-02 | |

| FCC_A1#1 | Status | ENTERED | Driving force | 0.0000E+00 |
|----------|-------------|---|-----------------|------------|
| Moles | 1.3784E-04 | Mass 7.1889E-03, Volume fraction 1.4059E-02 | Mass fractions: | |
| FE | 9.31133E-01 | CR 5.04939E-02 | C 1.83727E-02 | |

| M7C3 | Status | ENTERED | Driving force | 0.0000E+00 |
|-------|-------------|---|-----------------|------------|
| Moles | 7.0414E-05 | Mass 2.9323E-03, Volume fraction 5.9217E-03 | Mass fractions: | |
| FE | 5.72418E-01 | CR 3.41056E-01 | C 8.65257E-02 | |

POLY:Hit RETURN to continue

POLY:

POLY: reinit

POLY: set-condition t=1717.15 w(cr)=0.1 w(c)=0.01 p=1e5 n=1

POLY: c-e

Using global minimization procedure

Calculated 21475 grid points in 0 s
Found the set of lowest grid points in 0 s

Calculated POLY solution 0 s, total time 0 s

POLY: set-ax-var 1 t 500 1717.15 10

POLY: advanced

Which option? /STEP_AND_MAP/: break-condition

Break condition: np(liquid)=0

POLY: save tcex48c y

POLY: step normal

No initial equilibrium, trying to add one 0
Step will start from axis value 1717.15

Phase Region from 1717.15 for:
LIQUID

Calculated 4 equilibria

Phase Region from 1715.05 for:
LIQUID

FCC_A1#2

Calculated 14 equilibria

Phase Region from 1598.13 for:
FCC_A1#2

*** Buffer saved on file: c:\jenkins\workspace\generate_console_examples\examples\tcex48\tcex48c.POLY3

POLY: post

POST: @@ Define a function to get the amount of solids

POST: ent fun fs=1-np(liquid);

POST: @@ Plot a solidification diagram

POST: set-dia-ax x fs

POST: set-dia-ax y t-c

POST: append-exp y tcex48a tcex48c 0; 1; 0; 1;

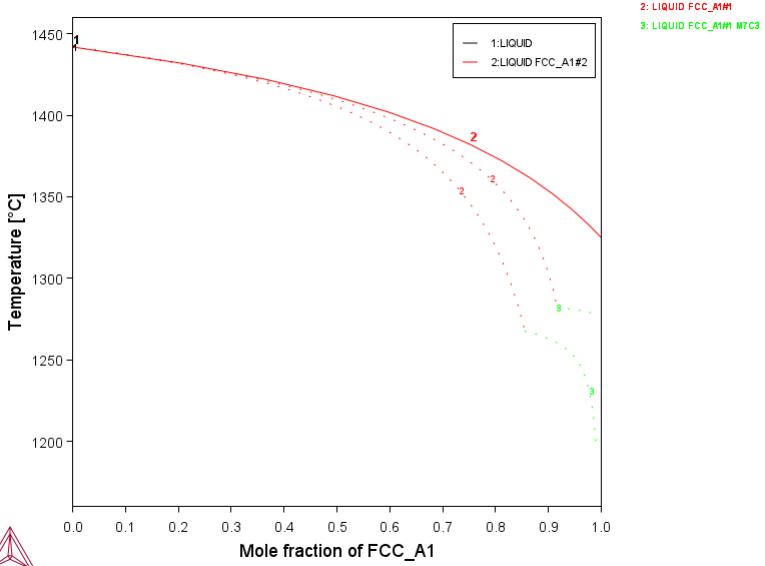
POST: set-ax-text x n

AXIS TEXT : Mole fraction of FCC_A1

```

POST: set-scaling-status y n 1160 1460
POST: set-title example 48e
POST: sel-plot new
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot

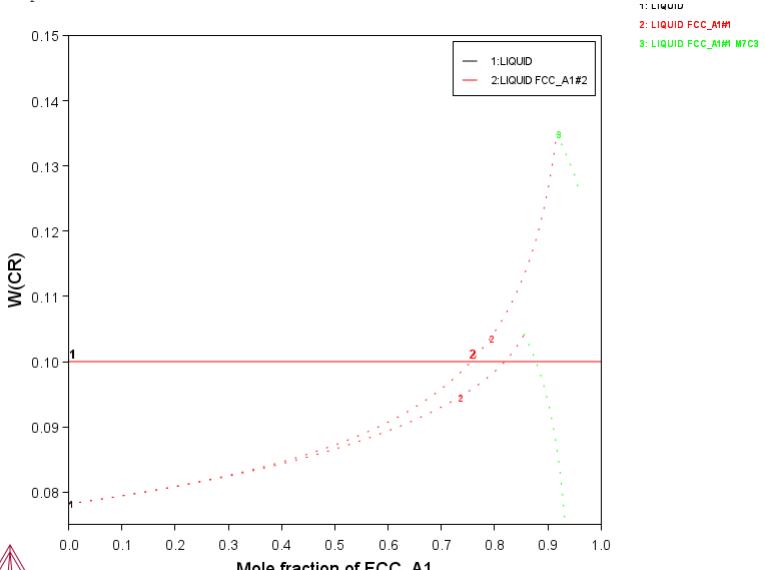
```



```

POST:
POST:Hit RETURN to continue
POST:
POST: @@ Plot microsegregation, which represents the composition
POST: @@ profile of the solid. For equilibrium solidification
POST: @@ there is no solute segregation and the composition of
POST: @@ solidified solid is uniform.
POST:
POST: set-dia-ax x fs
POST: set-dia-ax y w(cr)
POST: append-exp y tcex48b tcex48d 0; 1; 0; 1;
POST: set-ax-text x n
AXIS TEXT : Mole fraction of FCC_A1
POST: set-scaling y n 0.075 0.15
POST: set-title example 48f
POST: sel-plot new
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot

```



```

POST:
POST: set-inter
POST:

```

tce49

SYS:About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

```
SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce49\tce49.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Quasichemical model using the GES module
SYS:
SYS: @@ This example shows how to enter parameters
SYS: @@ for a FACT quasichemical liquid model and
SYS: @@ how to calculate the sulfur activity using
SYS: @@ the Gibbs energy system (GES) module commands.
SYS:
SYS: @@ This example uses some GES commands that are not yet
SYS: @@ supported by GES6. Therefore, we enforce the use of GES5.
SYS:
SYS: set-ges-version 5
SYS:
SYS: set-log ex49,,
SYS:
SYS: go gibbs
... the command in full is GOTO_MODULE
GIBBS ENERGY SYSTEM
GES5: ent-el /- VA CU S
... the command in full is ENTER_ELEMENT
THERMODYNAMIC DATABASE module
Database folder: C:\jenkins\workspace\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA           /- DEFINED
DICTRA_FCC_A1 REJECTED
GES5: am_el_d /- ELECTRON_GAS      0.0000E+00  0.0000E+00  0.0000E+00 1
... the command in full is AMEND_ELEMENT_DATA
GES5: am_el_d VA VACUUM          0.0000E+00  0.0000E+00  0.0000E+00 1
... the command in full is AMEND_ELEMENT_DATA
GES5: am_el_d CU FCC_A1        6.3546E+01  5.0041E+03  3.3150E+01 1
... the command in full is AMEND_ELEMENT_DATA
GES5: am_el_d S FC_ORTHORHOMBIC 3.2066E+01  0.0000E+00  0.0000E+00 1
... the command in full is AMEND_ELEMENT_DATA
GES5:
GES5:
GES5: @@ The quasichemical model requires species entered with the
GES5: @@ stoichiometry. The factor 2/ZZ is needed
GES5: @@ for the pure elements and 1/ZZ for the compounds.
GES5: @@ For Cu ZZ=0.9294 and 2/ZZ_Cu=2.15193
GES5: @@ For S ZZ=1.8366 and 2/ZZ_S=1.08897
GES5: @@ For CuS the stoichiometries are thus 1/ZZ_Cu=1.07596 and
GES5: @@ 1/ZZ_S=0.54448
GES5:
GES5: enter-specie CUQ           CU2.15193
... the command in full is ENTER_SPECIES
GES5: enter-specie CUQS          CU1.07596S0.54448
... the command in full is ENTER_SPECIES
GES5: enter-specie S2            S2
... the command in full is ENTER_SPECIES
GES5: enter-specie SQ            S1.08897
... the command in full is ENTER_SPECIES
GES5:
GES5:
GES5: @@ The Gibbs energy difference between FCC-Cu
GES5: @@ and quasichemical liquid-Cu
GES5:
GES5: ent-sym fun GQCU  2.98150E+02 +16547-7.6815*T;   6.00000E+03 N
... the command in full is ENTER_SYMBOL
GES5:
GES5:
GES5: @@ The Gibbs energy difference between GAS-S and
GES5: @@ quasichemical liquid-S
GES5:
GES5: ent-sym fun GQS   2.98150E+02 -65357+165.396*T-13.513*T*LN(T);
... the command in full is ENTER_SYMBOL
HIGH TEMPERATURE LIMIT /6000/: 6.00000E+03 N
GES5:
GES5:
GES5: @@ Gibbs energies for the pure elements and gases refered to SER
GES5: ent-sym fun GHSERCU 2.98150E+02 -7770.458+130.485403*T
... the command in full is ENTER_SYMBOL
& -24.112392*T*LN(T)-.00265684*T**2+1.29223E
& -07*T**3+52478*(-1); 1.35802E+03 Y
FUNCTION: -13542.33+183.804197*T-31.38*T*LN(T)+3.64643E+29*T**(-9);
HIGH TEMPERATURE LIMIT /6000/: 3.20000E+03 N
GES5: ent-sym fun GS2GAS  2.98150E+02 +117374.548+2.98629558*T
... the command in full is ENTER_SYMBOL
& -34.09678*T*LN(T)-.002325464*T**2+1.85480167E-07*T**3
& +128593.6*T**(-1); 1.00000E+03 Y
FUNCTION: +117352.438+2.50383258*T-34.04744*T*LN(T)-.0021150245*T**2
& +9.16602333E-08*T**3+175718.45*T**(-1); 3.40000E+03 Y
FUNCTION: +124361.091+14.5182895*T-36.1923*T*LN(T)-5.930925E-04*T**2
& -7.54259333E-09*T**3-7484105*T**(-1); 6.00000E+03 N
GES5: ent-sym fun GS1LIQ  2.98150E+02 -4001.549+77.889686*T
... the command in full is ENTER_SYMBOL
& -15.504*T*LN(T)-.018629*T**2-2.4942E-07*T**3
& -113945*T**(-1); 3.88360E+02 Y
FUNCTION: -5285183.35+118449.585*T-19762.4*T*LN(T)+32.79275*T**2
& -.0102214167*T**3+2.646735E+08*T**(-1); 4.28150E+02 Y
FUNCTION: -8174995.23+319914.078*T-57607.3*T*LN(T)+135.3045*T**2
& -.0529973333*T**3; 4.32250E+02 Y
```

```

FUNCTION: -219408.801+7758.83993*T-1371.85*T*LN(T)+2.845035*T**2
& -.00101380333*T**3; 4.53150E+02 Y
FUNCTION: +92539.872-1336.36627*T+202.958*T*LN(T)-.2531915*T**2
& +5.18835E-05*T**3-8202200*T**(-1); 7.17000E+02 Y
FUNCTION: -6889.972+176.35482*T-32*T*LN(T); 1.30000E+03 N
GES5: ent-sym fun GCULIQ 2.98150E+02 +12964.84-9.510243*T
... the command in full is ENTER_SYMBOL
& -5.83932E-21*T**7*GHSERCU; 1.35802E+03 Y
FUNCTION: +13495.4-9.920463*T-3.64643E+29*T**(-9)+GHSERCU ;
HIGH TEMPERATURE LIMIT /6000/: 3.20000E+03 N
GES5:
GES5:
GES5:
GES5: ent-phase GAS G, 1 S2 ; N N
... the command in full is ENTER_PHASE
GES5:
GES5:
GES5: ent-param G(GAS,S2;0) 2.98150E+02 +GS2GAS +RTLNP ;
... the command in full is ENTER_PARAMETER
G(GAS,S2;0)- 2 G(FC_ORTHORHOMBIC,S;0)
HIGH TEMPERATURE LIMIT /6000/: 6.00000E+03 N
GES5:
GES5:
GES5:
GES5: ent-phase FCC_A1 , 1 CU ; N N
... the command in full is ENTER_PHASE
GES5: amend_phase FCC_A1 magnetic -3.0 2.80000E-01
... the command in full is AMEND_PHASE_DESCRIPTION
GES5:
GES5:
GES5: ent-param G(FCC_A1,CU;0) 2.98150E+02 +GHSERCU; 3.20000E+03 N
... the command in full is ENTER_PARAMETER
G(FCC_A1,CU;0)-G(FCC_A1,CU;0)
GES5:
GES5:
GES5:
GES5: ent-phase QUASI L, 1 CUQ,CUQS,SQ ; N N
... the command in full is ENTER_PHASE
GES5:
GES5:
GES5: @@ The stoichiometry parameter for pure Cu is 2/ZZ,
GES5: @@ the stoichiometry ratio
GES5:
GES5: ent-param VK(QUASI,CUQ;0) 2.98150E+02 .9294; 6.00000E+03 N
... the command in full is ENTER_PARAMETER
VK(QUASI,CUQ;0)
GES5:
GES5: @@ The energy parameter for pure Cu (factor is 2/VK)
GES5:
GES5: ent-param G(QUASI,CUQ;0) 2.98150E+02 +2.15193*GCULIQ
... the command in full is ENTER_PARAMETER
G(QUASI,CUQ;0)-2.15193 G(FCC_A1,CU;0)
& +2.15193*GQCU ; 6.00000E+03 N
GES5:
GES5: @@ The Gibbs energy parameter for the molecule CUQS
GES5: @@ (factors 1/ZZ_cu and 1/ZZ_sq)
GES5:
GES5: ent-param G(QUASI,CUQS;0) 2.98150E+02 +1.07596*GCULIQ
... the command in full is ENTER_PARAMETER
G(QUASI,CUQS;0)-1.07596 G(FCC_A1,CU;0)-0.54448 G(FC_ORTHORHOMBIC,S;0)
& +1.075963*GQCU+.54448*GSSLIQ ; 6.00000E+03 N
GES5:
GES5:
GES5: @@ The stoichiometry parameter for pure S is 2/ZZ
GES5:
GES5: ent-param VK(QUASI,SQ;0) 2.98150E+02 1.8366; 6.00000E+03 N
... the command in full is ENTER_PARAMETER
VK(QUASI,SQ;0)
GES5:
GES5: @@ The energy parameter for pure S (factor is 2/VK)
GES5:
GES5: ent-param G(QUASI,SQ;0) 2.98150E+02 +1.08897*GSSLIQ ;
... the command in full is ENTER_PARAMETER
G(QUASI,SQ;0)-1.08897 G(FC_ORTHORHOMBIC,S;0)
HIGH TEMPERATURE LIMIT /6000/: 6.00000E+03 N
GES5:
GES5: @@ The mixing terms
GES5:
GES5: ent-param G(QUASI,CUQ,CUQS;0) 2.98150E+02 -82768; 6.00000E+03 N
... the command in full is ENTER_PARAMETER
G(QUASI,CUQ,CUQS;0)
GES5: ent-param G(QUASI,CUQ,CUQS;1) 2.98150E+02 -32070; 6.00000E+03 N
... the command in full is ENTER_PARAMETER
G(QUASI,CUQ,CUQS;1)
GES5: ent-param G(QUASI,CUQ,CUQS;2) 2.98150E+02 68734; 6.00000E+03 N
... the command in full is ENTER_PARAMETER
G(QUASI,CUQ,CUQS;2)
GES5: ent-param G(QUASI,CUQ,CUQS;3) 2.98150E+02 -84194+50*T;
... the command in full is ENTER_PARAMETER
G(QUASI,CUQ,CUQS;3)
HIGH TEMPERATURE LIMIT /6000/: 6.00000E+03 N
GES5: ent-param G(QUASI,CUQ,CUQS;4) 2.98150E+02 -43638; 6.00000E+03 N
... the command in full is ENTER_PARAMETER
G(QUASI,CUQ,CUQS;4)
GES5: ent-param G(QUASI,CUQ,CUQS;5) 2.98150E+02 +20*T; 6.00000E+03 N
... the command in full is ENTER_PARAMETER
G(QUASI,CUQ,CUQS;5)
GES5:
GES5:
GES5: @@ This command makes the entropy calculation according
GES5: @@ to FACT quasichemical model
GES5:
GES5: amend-phase-description QUASI quasi-fact00
GES5:
GES5: @@ Binary excess Legendre with 1 as independent
GES5: @@ Note that the order of the species are important.
GES5:
GES5: amend-phase-description QUASI excess
MODEL NAME /REDLICH-KISTER_MUGGANU/: mixed
First (the independent) constituent: CUQ
Second (the dependent) constituent: CUQS

```

Excess model type: /LEGENDRE/: Legendre

Any other non-Redlich-Kister binary excess parameters?

First (the independent) constituent: NONE

GES5:

GES5:

GES5:

GES5: list-data

OUTPUT TO SCREEN OR FILE /SCREEN/:

OPTIONS?:

1OUTPUT FROM GIBBS ENERGY SYSTEM ON PC/WINDOWS NT DATE 2023- 4-27
 FROM DATABASE: User data 2023.04.27

ALL DATA IN SI UNITS
 FUNCTIONS VALID FOR 298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED

| ELEMENT | STABLE ELEMENT | REFERENCE | MASS | H298-H0 | S298 |
|---------|----------------|-----------------|------------|------------|------------|
| -1 | /- | ELECTRON_GAS | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 0 | VA | VACUUM | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 1 | CU | FCC_A1 | 6.3546E+01 | 5.0041E+03 | 3.3150E+01 |
| 2 | S | FC_ORTHORHOMBIC | 3.2066E+01 | 0.0000E+00 | 0.0000E+00 |

| SPECIES | STOICHIOMETRY |
|---------|-------------------|
| 1 CU | CU |
| 2 CUQ | CU2.15193 |
| 3 CUQS | CU1.07596S0.54448 |
| 4 S | S |
| 5 S2 | S2 |
| 6 SQ | S1.08897 |
| 7 VA | VA |

GAS
 CONSTITUENTS: S2

$G(\text{GAS}, \text{S2}; 0) - 2 G(\text{FC}_\text{ORTHORHOMBIC}, \text{S}; 0) = +\text{GS2GAS} + \text{RTLNP}$

QUASI
 \$ QUASICHEMICAL-FACT00 ENTROPY CONTRIBUTION
 CONSTITUENTS: CUQ, CUQS, SQ

$VK(\text{QUASI}, \text{CUQ}; 0) = +.9294$
 $G(\text{QUASI}, \text{CUQ}; 0) - 2.15193 G(\text{FCC}_\text{A1}, \text{CU}; 0) = +2.15193 * \text{GCULIQ} + 2.15193 * \text{GQCU}$
 $G(\text{QUASI}, \text{CUQS}; 0) - 0.107596 G(\text{FCC}_\text{A1}, \text{CU}; 0) - 0.54448 G(\text{FC}_\text{ORTHORHOMBIC}, \text{S}; 0) = +1.07596 * \text{GCULIQ} + 1.07596 * \text{GQCU} + 5.4448 * \text{GSSLIQ}$
 $VK(\text{QUASI}, \text{SQ}; 0) = +1.8366$
 $G(\text{QUASI}, \text{SQ}; 0) - 1.08897 G(\text{FC}_\text{ORTHORHOMBIC}, \text{S}; 0) = +1.08897 * \text{GSSLIQ}$

\$ Binary excess model Legendre with CUQ as independent

$L(\text{QUASI}, \text{CUQ}, \text{CUQS}; 0) = -82768$
 $L(\text{QUASI}, \text{CUQ}, \text{CUQS}; 1) = -32070$
 $L(\text{QUASI}, \text{CUQ}, \text{CUQS}; 2) = +68734$
 $L(\text{QUASI}, \text{CUQ}, \text{CUQS}; 3) = -84194 + 50 * T$
 $L(\text{QUASI}, \text{CUQ}, \text{CUQS}; 4) = -43638$
 $L(\text{QUASI}, \text{CUQ}, \text{CUQS}; 5) = +20 * T$

FCC_A1
 ADDITIONAL CONTRIBUTION FROM MAGNETIC ORDERING
 Magnetic function below Curie Temperature
 $+1.860338755 * \text{TAO}^{**(-1)} - 1.17449124 * \text{TAO}^{**-3} - 0.00775516624 * \text{TAO}^{**9}$
 $-0.0017449124 * \text{TAO}^{**15}$
 Magnetic function above Curie Temperature
 $-0.0426902268 * \text{TAO}^{**(-5)} - 0.0013552453 * \text{TAO}^{**(-15)}$
 $-2.84601512E-04 * \text{TAO}^{**(-25)}$

CONSTITUENTS: CU

$G(\text{FCC}_\text{A1}, \text{CU}; 0) - G(\text{FCC}_\text{A1}, \text{CU}; 0) = 298.15 < T < 3200.00: +\text{GHSERCU}$

| SYMBOL | STATUS | VALUE/FUNCTION |
|-------------|---|---|
| FUNCTION R | 298.15 | 8.31451000000000 ; 6000 N REFO ! |
| 2 RTLNP | 20000000 | $+R^*T^*\ln(1E-05^*P)$ |
| 103 GQCU | 20000000 | $+16547-7.6815^*T$ |
| 104 GQS | 20000000 | $-65357+165.396^*T-13.513^*T^*\ln(T)$ |
| 105 GHSERCU | 20000000 | |
| | 298.15 < T < 1358.02: | $-7770.458+130.485403^*T-24.112392^*T^*\ln(T)$ |
| | $-.00265684^*T^{**2}+1.29223E-07^*T^{**3}+52478^*T^{**(-1)}$ | |
| | 1358.02 < T < 3200.00: | $-13542.33+183.804197^*T-31.38^*T^*\ln(T)$ |
| | $+3.64643E+29^*T^{**(-9)}$ | |
| 106 GS2GAS | 20000000 | $298.15 < T < 1000.00: +117374.548+2.98629558^*T-34.09678^*T^*\ln(T)$ |
| | $-.002325464^*T^{**2}+1.85480167E-07^*T^{**3}+128593.6^*T^{**(-1)}$ | |
| | 1000.00 < T < 3400.00: | $+117352.438+2.50383258^*T-34.04744^*T^*\ln(T)$ |
| | $-.0021150245^*T^{**2}+9.16602333E-08^*T^{**3}+175718.45^*T^{**(-1)}$ | |
| | 3400.00 < T < 6000.00: | $+124361.091+14.5182895^*T-36.1923^*T^*\ln(T)$ |
| | $-5.930925E-04^*T^{**2}-7.54259333E-09^*T^{**3}-7484105^*T^{**(-1)}$ | |
| 107 GSSLIQ | 20000000 | $298.15 < T < 388.36: -4001.549+77.889686^*T-15.504^*T^*\ln(T)-.018629^*T^{**2}$ |
| | $-0.4942E-07^*T^{**3}-113945^*T^{**(-1)}$ | |
| | 388.36 < T < 428.15: | $-5285183.35+118449.585^*T-19762.4^*T^*\ln(T)$ |
| | $+32.79275^*T^{**2}-0.0102214167^*T^{**3}+2.646735E+08^*T^{**(-1)}$ | |
| | 428.15 < T < 432.25: | $-8174995.23+319914.078^*T-57607.3^*T^*\ln(T)$ |
| | $+135.3045^*T^{**2}-0.0529973333^*T^{**3}$ | |
| | 432.25 < T < 453.15: | $-219408.801+7758.83993^*T-1371.85^*T^*\ln(T)$ |
| | $+2.845035^*T^{**2}-0.00101380333^*T^{**3}$ | |
| | 453.15 < T < 717.00: | $+92539.872-1336.36627^*T+202.958^*T^*\ln(T)$ |
| | $-.2531915^*T^{**2}+5.18835E-05^*T^{**3}-8202200^*T^{**(-1)}$ | |
| | 717.00 < T < 1300.00: | $-6889.972+176.35482^*T-32^*T^*\ln(T)$ |
| 108 GCULIQ | 20000000 | $298.15 < T < 1358.02: +12964.84-9.510243^*T-5.83932E-21^*T^{**7}+\text{GHSERCU}$ |
| | 1358.02 < T < 3200.00: | $+13495.4-9.920463^*T-3.64643E+29^*T^{**(-9)}+\text{GHSERCU}$ |

GES5:
GES5: Hit RETURN to continue
GES5: go p-3
 ... the command in full is GOTO_MODULE

POLY version 3.32
POLY:

```

POLY:
POLY:
POLY: l-st ph
    ... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES
PHASE           STATUS      DRIVING FORCE     MOLES
FCC_A1          ENTERED    0.000000E+00  0.000000E+00
QUASI          ENTERED    0.000000E+00  0.000000E+00
GAS             ENTERED    0.000000E+00  0.000000E+00
POLY: c-st p *=sus
    ... the command in full is CHANGE_STATUS
POLY: c-st p q gas
    ... the command in full is CHANGE_STATUS
Status: /ENTERED/: ENTERED
Start value, number of mole formula units /0/: 0
POLY:
POLY:
POLY: s-c t=1473 p=1e5 n=1 x(s)=.33
    ... the command in full is SET_CONDITION
POLY: c-e
    ... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated      1966 grid points in      0 s
Found the set of lowest grid points in      0 s
Calculated POLY solution      0 s, total time      0 s
POLY: l-e
    ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
Output from POLY-3, equilibrium =      1, label A0 , database: User dat

Conditions:
T=1473, P=100000, N=1, X(S)=0.33
DEGREES OF FREEDOM 0

Temperature   1473.00 K ( 1199.85 C), Pressure 1.000000E+05
Number of moles of components 1.000000E+00, Mass in grams 5.31576E+01
Total Gibbs energy -1.24169E+05, Enthalpy 1.52783E+04, Volume 0.000000E+00

Component      Moles      W-Fraction Activity Potential Ref.stat
CU            6.7000E-01  8.0094E-01 8.2231E-04 -8.6997E+04 SER
S             3.3000E-01  1.9906E-01 8.3318E-08 -1.9964E+05 SER

QUASI          Status ENTERED      Driving force 0.0000E+00
Moles 1.0000E+00, Mass 5.3158E+01, Volume fraction 0.0000E+00 Mass fractions:
CU 8.00936E-01 S 1.99064E-01
POLY:Hit RETURN to continue
POLY: s-r-s s gas
    ... the command in full is SET_REFERENCE_STATE
Temperature /*/: *
Pressure /1E5/: 1E5
POLY: sh acr(s)
    ... the command in full is SHOW_VALUE
ACR(S)=2.1652884E-3
POLY:Hit RETURN to continue
POLY: s-a-v 1 x(s)
    ... the command in full is SET_AXIS_VARIABLE
Min value /0/: .3
Max value /1/: .4
Increment /.0025/: .0025
POLY: save tcex49 y
    ... the command in full is SAVE_WORKSPACES
POLY: step normal
    ... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 0.330000
...OK

Phase Region from 0.330000 for:
    QUASI
Global test at 3.50000E-01 .... OK
Global check of adding phase at 3.61133E-01
Calculated 15 equilibria

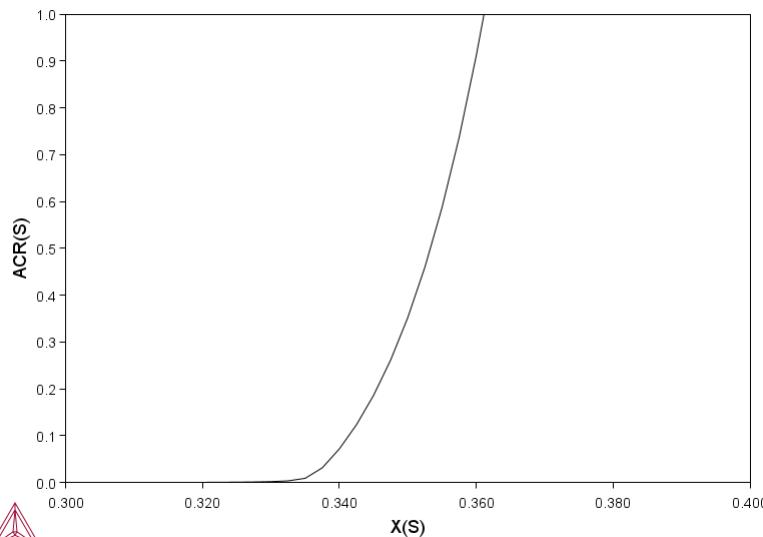
Phase Region from 0.361133 for:
    GAS
    QUASI
Global test at 3.80000E-01 .... OK
Terminating at 0.400000
Calculated 19 equilibria

Phase Region from 0.330000 for:
    QUASI
Global test at 3.10000E-01 .. Creating a new composition set QUASI#2
Backtracking to find phase change for QUASI#2
Global test at 3.27500E-01 .... OK
Global test at 3.22500E-01 .... OK
Global test at 3.17500E-01 .... OK
Global test at 3.12500E-01 .... OK
Global check of adding phase at 3.11581E-01
Calculated 11 equilibria

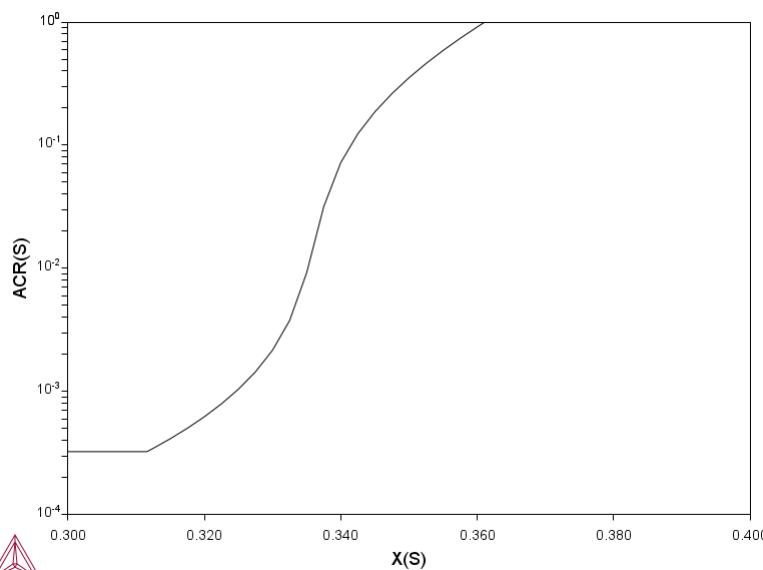
Phase Region from 0.311581 for:
    QUASI#1
    QUASI#2
Terminating at 0.300000
Calculated 8 equilibria
*** Buffer saved on file: c:\jenkins\workspace\generate_console_examples\examples\tcex49\tcex49.POLY3
POLY: po
    ... the command in full is POST
POLY-3 POSTPROCESSOR VERSION 3.2
POST: s-d-a x x(s)
    ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y acr(s)
    ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 49a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
    ... the command in full is MAKE_EXPERIMENTAL_DATAFILE
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
    ... the command in full is PLOT_DIAGRAM

```

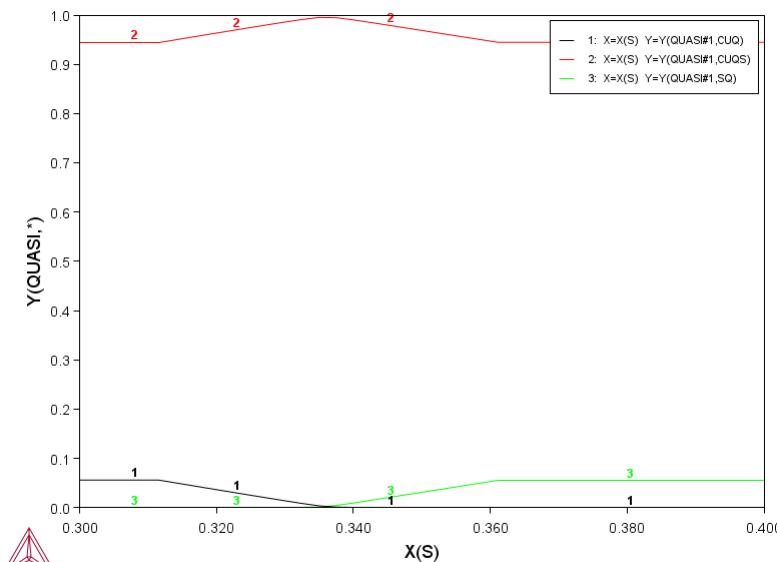
example 49a



```
POST:  
POST:Hit RETURN to continue  
POST: s-a-ty y log  
... the command in full is SET_AXIS_TYPE  
POST: set-title example 49b  
POST: sel-plot new  
... the command in full is SELECT_PLOT  
POST:  
POST:  
POST: SET_EXP_FILE_FORMAT 5  
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y  
... the command in full is MAKE_EXPERIMENTAL_DATAFILE  
POST: SET_EXP_FILE_FORMAT 10  
POST:  
POST: plot  
... the command in full is PLOT_DIAGRAM
```



```
POST:  
POST:Hit RETURN to continue  
POST: s-d-a y y(quasi,*)  
... the command in full is SET_DIAGRAM_AXIS  
COLUMN NUMBER /*:  
POST:  
POST: s-a-ty y lin  
... the command in full is SET_AXIS_TYPE  
POST: s-lab d  
... the command in full is SET_LABEL_CURVE_OPTION  
POST: set-title example 49c  
POST: sel-plot new  
... the command in full is SELECT_PLOT  
POST:  
POST:  
POST: SET_EXP_FILE_FORMAT 5  
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y  
... the command in full is MAKE_EXPERIMENTAL_DATAFILE  
POST: SET_EXP_FILE_FORMAT 10  
POST:  
POST: plot  
... the command in full is PLOT_DIAGRAM
```



```

POST:
POST:
POST:@?
POST: back
POLY: read tcex49
... the command in full is READ_WORKSPACES
POLY:
POLY:
POLY: s-c t=1573
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 1966 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 0.330000
...OK

Phase Region from 0.330000 for:
QUASI
Global test at 3.50000E-01 .... OK
Global check of adding phase at 3.56605E-01
Calculated 13 equilibria

Phase Region from 0.356605 for:
GAS
QUASI
Global test at 3.75000E-01 .... OK
Global test at 4.00000E-01 .... OK
Terminating at 0.400000
Calculated 21 equilibria

Phase Region from 0.330000 for:
QUASI
Global test at 3.10000E-01 .... OK
Terminating at 0.300000
Calculated 15 equilibria
*** Buffer saved on file: c:\jenkins\workspace\generate_console_examples\examples\tcex49\tcex49.POLY3
POLY:
POLY: read tcex49
... the command in full is READ_WORKSPACES
POLY:
POLY:
POLY: s-c t=1673
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 1966 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 0.330000
...OK

Phase Region from 0.330000 for:
QUASI
Global test at 3.50000E-01 .... OK
Global check of adding phase at 3.52789E-01
Calculated 12 equilibria

Phase Region from 0.352789 for:
GAS
QUASI
Global test at 3.72500E-01 .... OK
Global test at 3.97500E-01 .... OK
Terminating at 0.400000
Calculated 22 equilibria

Phase Region from 0.330000 for:
QUASI
Global test at 3.10000E-01 .... OK
Terminating at 0.300000
Calculated 15 equilibria
*** Buffer saved on file: c:\jenkins\workspace\generate_console_examples\examples\tcex49\tcex49.POLY3
POLY:

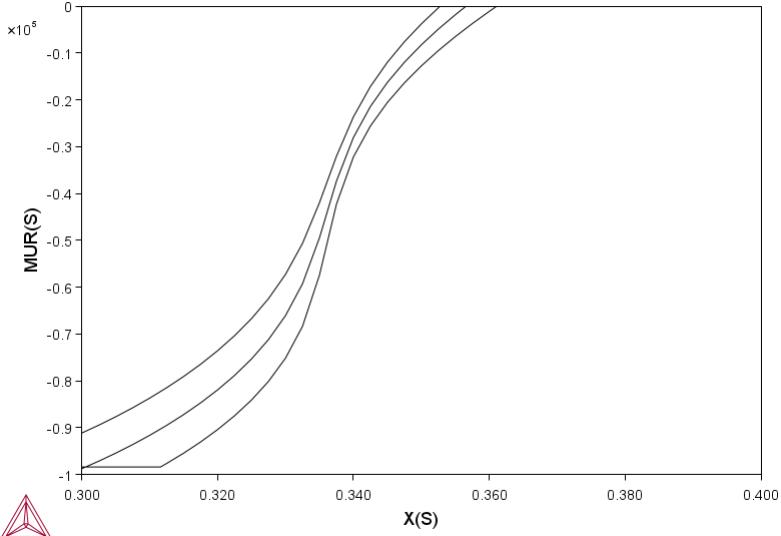
```

```

POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2
POST: s-d-a y mur(s)
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a x x(s)
... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 49d
POST: sel.plot new
... the command in full is SELECT_PLOT
*** ERROR 1037 IN GETINT: NO DIGIT
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
Creating a new composition set QUASI#2
The composition set QUASI#2 created from the store file
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 49d



```

POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:

```

tce51

SYS:About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce51\tce51.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Calculation of molar volume,
SYS: @@ thermal expansivity, and density.
SYS:
SYS: @@ This example uses the POLY3 module to calculate
SYS: @@ the molar volume, thermal expansivity, and density
SYS: @@ of the FCC_A1, BCC_A2 LIQUID, and liquid phases of C-Fe.
SYS:
SYS: set-log ex51,,
SYS:
SYS: go data
... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module
Database folder: C:\jenkins\workspace\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE11: sw FEDEMO
... the command in full is SWITCH_DATABASE
Current database: Iron Demo Database v4.0

VA /- DEFINED
TDB_FEDEMO:
TDB_FEDEMO: @@ Volume of a unary system
TDB_FEDEMO: d-sys fe
... the command in full is DEFINE_SYSTEM
FE DEFINED
TDB_FEDEMO: rej-ph * all
... the command in full is REJECT
LIQUID:L LAVES_PHASE_C14
 BCC_A2
CBCC_A12 CUB_A13
HCP_A3 REJECTED
TDB_FEDEMO: rest-ph fcc_a1,bcc_a2,liquid
... the command in full is RESTORE
FCC_A1 LIQUID:L
 BCC_A2
RESTORED
TDB_FEDEMO: get
... the command in full is GET_DATA
16:55:10,233 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES
ELEMENTS
SPECIES
PHASES
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS

List of references for assessed data

'A.T. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
'Y. Tang, in TCCU2, Thermo-Calc Software AB, Stockholm, Sweden'
'M. J. Assael, J. Phys. Chem. Ref. Data 35 (2006) 285; Fe, Al'
'M Ghasemi, Thermo-Calc Software AB: assessing the surface tension of
metallic liquid'
'X.G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
volumes'
-OK-
TDB_FEDEMO:
TDB_FEDEMO: go poly
... the command in full is GOTO_MODULE

POLY version 3.32
POLY: s-c t=400, n=1, p=1e5
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 3 grid points in 1 s
POLY: s-a-v 1 t 298 2000,,
... the command in full is SET_AXIS_VARIABLE
POLY:

POLY: save tce51 y
... the command in full is SAVE_WORKSPACES
POLY: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 400.000
...OK

Phase Region from 400.000 for:
 BCC_A2
Global test at 4.80000E+02 OK
Global test at 5.80000E+02 OK
Global test at 6.80000E+02 OK
Global test at 7.80000E+02 OK
Global test at 8.80000E+02 OK
Global test at 9.80000E+02 OK
Global test at 1.08000E+03 OK
Global test at 1.18000E+03 OK
Global check of adding phase at 1.18481E+03
Calculated 81 equilibria

```

Phase Region from    1184.81      for:
  BCC_A2
  FCC_A1
Calculated      2 equilibria

Phase Region from    1184.81      for:
  FCC_A1
Global test at 1.26000E+03 .... OK
Global test at 1.36000E+03 .... OK
Global test at 1.46000E+03 .... OK
Global test at 1.56000E+03 .... OK
Global test at 1.66000E+03 .... OK
Global check of adding phase at 1.666747E+03
Calculated      51 equilibria

Phase Region from    1667.47      for:
  BCC_A2
  FCC_A1
Calculated      2 equilibria

Phase Region from    1667.47      for:
  BCC_A2
Global test at 1.74000E+03 .... OK
Global check of adding phase at 1.81095E+03
Calculated      18 equilibria

Phase Region from    1810.95      for:
  LIQUID
  BCC_A2
Calculated      2 equilibria

Phase Region from    1810.95      for:
  LIQUID
Global test at 1.89000E+03 .... OK
Global test at 1.99000E+03 .... OK
Terminating at    2000.00
Calculated      22 equilibria

Phase Region from    400.000     for:
  BCC_A2
Global test at 3.20000E+02 .... OK
Terminating at    298.000
Calculated      14 equilibria
*** Buffer saved on file: c:\jenkins\workspace\generate_console_examples\examples\tcex51\tcex51.POLY3

```

POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

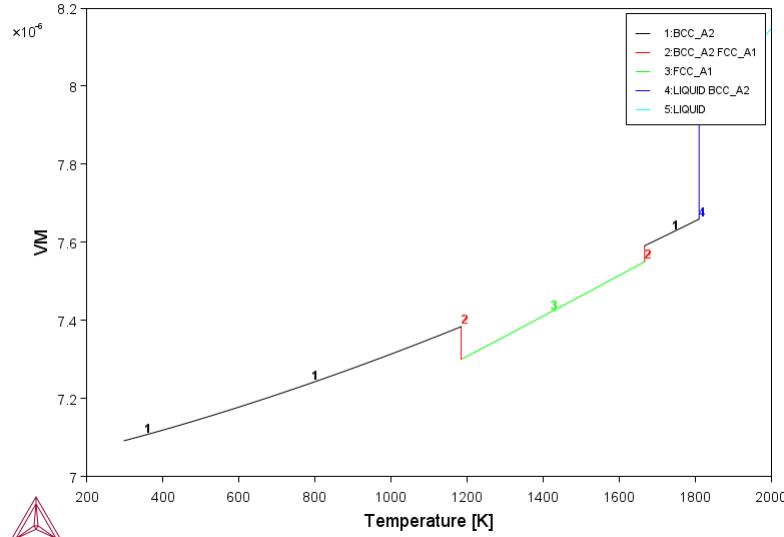
Setting automatic diagram axes

```

POST: s-d-a x t-k
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y vm
... the command in full is SET_DIAGRAM_AXIS
POST:
POST: set-title example 51a
POST: s-l e
... the command in full is SET_LABEL_CURVE_OPTION
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 51a



```

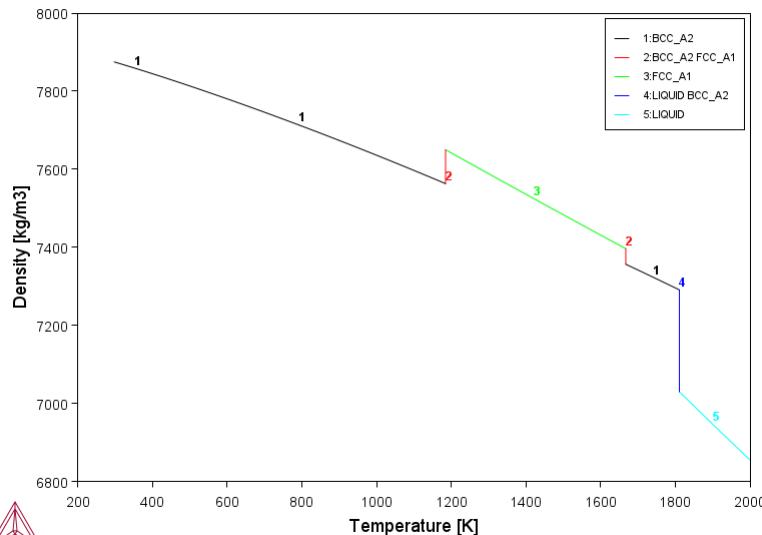
POST:
POST: Hit RETURN to continue
POST: @@ Define and plot density
POST: ent fun density=b*1e-3/vm;
... the command in full is ENTER_SYMBOL
POST: s-d-a y density
... the command in full is SET_DIAGRAM_AXIS
POST: set-axis-text y n
... the command in full is SET_AXIS_TEXT_STATUS
AXIS TEXT : Density [kg/m3]
POST: set-title example 51b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI

```

```

POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
example 51b

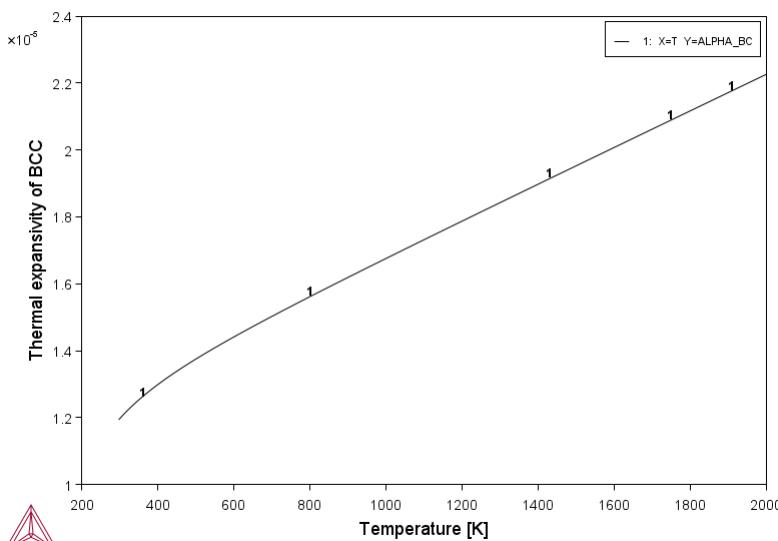
```



```

POST:
POST:Hit RETURN to continue
POST: @@ Define and plot coefficient of linear
POST: @@ thermal expansion
POST: ent fun alpha_bcc_a2=vm(bcc_a2).t/vm(bcc_a2)/3;
... the command in full is ENTER_SYMBOL
POST: s-d-a y alpha_bcc_a2
... the command in full is SET_DIAGRAM_AXIS
POST: s-l d
... the command in full is SET_LABEL_CURVE_OPTION
POST: set-axis-text y n
... the command in full is SET_AXIS_TEXT_STATUS
AXIS TEXT : Thermal expansivity of BCC
POST: set-title example 51c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFILE
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
example 51c

```



```

POST:
POST:Hit RETURN to continue
POST: back
POST: @@ Volume of Fe-C binary system
POST: go da
... the command in full is GOTO_MODULE
TDB_FEDEMO: rej sys
... the command in full is REJECT
VA                               /- DEFINED
REINITIATING GES .....
TDB_FEDEMO: de-sys fe c
... the command in full is DEFINE_SYSTEM
FE                               C DEFINED
TDB_FEDEMO: rej-ph * all
... the command in full is REJECT
GAS:G          LIQUID:L          BCC_A2
LAVES_PHASE_C14    CBCC_A12      CEMENTITE
CUB_A13         DIAMOND_FCC_A4   FCC_A1
GRAPHITE        HCP_A3          KSI_CARBIDE
M23C6           M5C2           M7C3
REJECTED

```

```

TDB_FEDEMO: res-ph fcc_a1,bcc_a2,cementite,liquid
... the command in full is RESTORE
  FCC_A1          BCC_A2          CEMENTITE
LIQUID:L RESTORED
TDB_FEDEMO: get
... the command in full is GET_DATA
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS .....
FUNCTIONS .....

List of references for assessed data

'A.T. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121 -127; Molar
  volumes'
'M. Ghasemi, Thermo-Calc Software AB, Sweden, 2019; Viscosity of metallic
  liquid'
'M Ghasemi, Thermo-Calc Software AB: assessing the surface tension of
  metallic liquid'
'Y. Tang, in TCCU2, Thermo-Calc Software AB, Stockholm, Sweden'
'M. J. Assael, J. Phys. Chem. Ref. Data 35 (2006) 285; Fe, Al'
'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
'M. Ghasemi, Thermo-Calc Software AB, Sweden, 2020; Unifying liquid volume
  database'
'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
'X.G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
'X.G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
  volumes'
'B. Hallstedt, D. Djurovic, J. von Appen, R. Dronskowski, A. Dick, F.
  Koermann, T. Hickel, J. Neugebauer, CALPHAD, 34, 129 -33(2010); Fe-C'
-OK-
TDB_FEDEMO:
TDB_FEDEMO: go poly
... the command in full is GOTO_MODULE

POLY version 3.32
POLY: s-c t=400, n=1, p=1e5
... the command in full is SET_CONDITION
POLY: s-c w(c)=.6e-2
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated       628 grid points in      0 s
Found the set of lowest grid points in      0 s
Calculated POLY solution      0 s, total time      0 s
POLY: s-a-v 1 t 298 2000,
... the command in full is SET_AXIS_VARIABLE
POLY:
POLY: save tce51 y
... the command in full is SAVE_WORKSPACES

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

POLY: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default -
Step will start from axis value    400.000
...OK

Phase Region from    400.000      for:
  BCC_A2
  CEMENTITE
Global test at  4.80000E+02 .... OK
Global test at  5.80000E+02 .... OK
Global test at  6.80000E+02 .... OK
Global test at  7.80000E+02 .... OK
Global test at  8.80000E+02 .... OK
Global test at  9.80000E+02 .... OK
Global check of adding phase at  9.99685E+02
Calculated      62 equilibria

Phase Region from    999.685      for:
  BCC_A2
  CEMENTITE
  FCC_A1
Calculated      2 equilibria

Phase Region from    999.685      for:
  BCC_A2
  FCC_A1
Global check of removing phase at  1.02363E+03
Calculated      6 equilibria

Phase Region from   1023.63      for:
  FCC_A1
Global test at  1.10000E+03 .... OK
Global test at  1.20000E+03 .... OK
Global test at  1.30000E+03 .... OK
Global test at  1.40000E+03 .... OK
Global test at  1.50000E+03 .... OK
Global test at  1.60000E+03 .... OK
Global check of adding phase at  1.69090E+03
Calculated      70 equilibria

Phase Region from   1690.90      for:
  LIQUID
  FCC_A1
Global check of removing phase at  1.76294E+03
Calculated      10 equilibria

Phase Region from   1762.94      for:
  LIQUID
Global test at  1.84000E+03 .... OK
Global test at  1.94000E+03 .... OK
Terminating at   2000.00
Calculated      27 equilibria

```

```

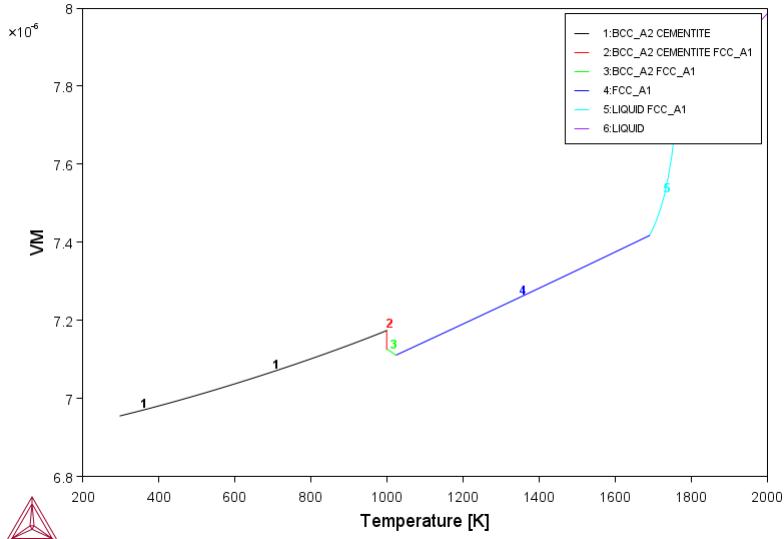
Phase Region from    400.000      for:
    BCC_A2
    CEMENTITE
Global test at  3.20000E+02 .... OK
Terminating at   298.000
Calculated   14 equilibria
*** Buffer saved on file: c:\jenkins\workspace\generate_console_examples\examples\tcex51\tcex51.POLY3
POST: post
  POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: s-d-a x t-k
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y vm
... the command in full is SET_DIAGRAM_AXIS
POST:
POST: set-title example 51d
POST: s-l e
... the command in full is SET_LABEL_CURVE_OPTION
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 51d



```

POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:

```

tce52

SYS:About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

```
SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce52\tce52.TCM.test"
SYS: set-echo
SYS:
SYS:
SYS: @@ Changing the excess models for interaction
SYS: @@ parameters in a solution phase
SYS:
SYS:
SYS: @@ This example shows how to change the excess models for binary
SYS: @@ and ternary interactions in a solution phase, either through
SYS: @@ direct interactive amendments of phase descriptions within
SYS: @@ the GES module, or enforced by specific type-definitions
SYS: @@ given in a database file retrieved by the TDB module.
SYS: @@
SYS: @@ For Binary Excess Model: from the default R-K model to
SYS: @@ Mixed-Excess-Model (the phase has to be a substitutional phase)
SYS: @@
SYS: @@ For Ternary Extrapolation Model: from the default R-K-M model to
SYS: @@ Toop_Kohler model
SYS: @@
SYS: set-log TCEX52.LOG
Heading: Example showing how to enter a TOOP binary extrapolation model
SYS:
SYS:
SYS: @@ This example uses features not supported by GES6.
SYS: @@ Therefore, we enforce the use of GES5.
SYS: set-ges-version 5
SYS:
SYS: go gibbs
... the command in full is GOTO_MODULE
GIBBS ENERGY SYSTEM
GES5: reinitiate ,,
Default element reference state symbol index /1/:
GES5: ent-el /- VA A B C
... the command in full is ENTER_ELEMENT
THERMODYNAMIC DATABASE module
Database folder: C:\jenkins\workspace\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA          /- DEFINED
DICTRA_FCC_A1 REJECTED

GES5: am_el_d /- ELECTRON_GAS      0.0000E+00  0.0000E+00  0.0000E+00 1
... the command in full is AMEND_ELEMENT_DATA
GES5: am_el_d VA VACUUM           0.0000E+00  0.0000E+00  0.0000E+00 1
... the command in full is AMEND_ELEMENT_DATA
GES5: am_el_d A UNKNOWN          1.0000E+01  0.0000E+00  0.0000E+00 2
... the command in full is AMEND_ELEMENT_DATA
GES5: am_el_d B BETA_RHOMBO_B    1.0811E+01  1.2220E+00  5.9000E+00 2
... the command in full is AMEND_ELEMENT_DATA
GES5: am_el_d C GRAPHITE         1.2011E+01  1.0540E+00  5.7400E+00 2
... the command in full is AMEND_ELEMENT_DATA
GES5:
GES5: ent-phase LIQUID L, 1 A,B,C ; N N
... the command in full is ENTER_PHASE
GES5:
GES5: ent-param G(LIQUID,A;0) 298.15 0; 6000 N!
... the command in full is ENTER_PARAMETER
G(LIQUID,A;0)-H298(UNKNOWN,A;0)
GES5: ent-param G(LIQUID,B;0) 298.15 0; 6000 N!
... the command in full is ENTER_PARAMETER
G(LIQUID,B;0)-H298(BETA_RHOMBO_B,B;0)
GES5: ent-param G(LIQUID,C;0) 298.15 0; 6000 N!
... the command in full is ENTER_PARAMETER
G(LIQUID,C;0)-H298(GRAPHITE,C;0)
GES5:
GES5: ent-param L(LIQUID,A,B;0) 298.15 10000; 6000 N
... the command in full is ENTER_PARAMETER
L(LIQUID,A,B;0)
GES5: ent-param L(LIQUID,A,B;1) 298.15 -10000; 6000 N
... the command in full is ENTER_PARAMETER
L(LIQUID,A,B;1)
GES5:
GES5: list-data ,,
```

1OUTPUT FROM GIBBS ENERGY SYSTEM ON PC/WINDOWS NT DATE 2023- 4-27
FROM DATABASE: User data 2023.04.27

ALL DATA IN SI UNITS
FUNCTIONS VALID FOR 298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED

| ELEMENT | STABLE ELEMENT REFERENCE | MASS | H298-H0 | S298 |
|---------|--------------------------|------------|------------|------------|
| -1 | /- ELECTRON_GAS | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 0 | VA VACUUM | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 1 | A UNKNOWN | 1.0000E+01 | 0.0000E+00 | 0.0000E+00 |
| 2 | B BETA_RHOMBO_B | 1.0811E+01 | 1.2220E+00 | 5.9000E+00 |
| 3 | C GRAPHITE | 1.2011E+01 | 1.0540E+00 | 5.7400E+00 |

| SPECIES | STOICHIOMETRY |
|---------|---------------|
| 1 A | A |
| 2 B | B |
| 3 C | C |
| 4 VA | VA |

```

LIQUID
EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
CONSTITUENTS: A,B,C

G(LIQUID,A;0)-H298(UNKNOWN,A;0) = 0.0
G(LIQUID,B;0)-H298(BETA_RHOMBO_B,B;0) = 0.0
G(LIQUID,C;0)-H298(GRAPHITE,C;0) = 0.0
L(LIQUID,A,B;0) = +10000
L(LIQUID,A,B;1) = -10000

SYMBOL      STATUS   VALUE/FUNCTION
FUNCTION R      298.15    8.314510000000000 ; 6000 N REFO !
2 RTLNP      20000000 +R*T*LN(1E-05*P)

```

GES5:Hit RETURN to continue

```

GES5: @ =====
GES5: @ Step 1: Amending the binary excess model:
GES5: @ =====
GES5: @ The default binary excess model is the Redlich-Kister Model
GES5: @ for all the three associated binary interaction pairs
GES5: @ (A-B, A-C and B-C) in the substitutional LIQUID solution
GES5: @ phase (without sublattice) that consists of three elements
GES5: @ (A, B and C).
GES5:
GES5: @ Before changing this default binary excess model for the
GES5: @ ternary LIQUID solution phase, one must have already entered
GES5: @ the G parameters (for standard Gibbs energies of all pure
GES5: @ end-members) and L parameters (for binary R-K excess
GES5: @ interaction energies), as shown here.
GES5:
GES5: @ In this particular example, we want to change from the
GES5: @ default R-K binary excess model to the Mixed-Excess-Model
GES5: @ (with three different binary excess models, namely Legendre,
GES5: @ Polynom and Redlich-Kister models, applied to the A-B,
GES5: @ A-C and B-C binaries, respectively), as demonstrated below:
GES5:
GES5: @ For the A-B interaction, the Legendre binary excess model
GES5: @ should be used (rather than the default Redlich-Kister
GES5: @ Model), with the first species (i.e. A) as the independent constituent,
GES5: @ and the second species (i.e. B) as the dependent constituent,
GES5: @ while the L parameters for the A-B interaction shall remain
GES5: @ the same as those handled by the R-K model.
GES5: amend-phase-description liquid

```

AMEND WHAT /COMPOSITION_SETS/: ?

```

You can amend
EXCESS_MODEL
MAGNETIC_ORDERING
DEBYE_HUCKEL
STATUS_BITS
NEW_CONSTITUENT
RENAME_PHASE
COMPOSITION_SETS
GLASS_TRANSITION
DISORDERED_PART
MAJOR_CONSTITUENT
ZRO2_TRANSITION
REMOVE_ADDITIONS
QUASICHEM_IONIC
QUASICHEM_FACT00
QUASICHEM_IRSID
TERNARY_EXTRAPOLAT
HKF_ELECTROSTATIC
DEFAULT_STABLE
SITE RATIOS
FRACTION LIMITS
NEVER_DISORDER_PAR

```

AMEND WHAT /COMPOSITION_SETS/: excess

MODEL NAME /REDLICH-KISTER_MUGGIANU/: ?

REDLICH-KISTER_MUGGIANU

REDLICH-KISTER_KOHLER

FLORY-HUGGINS POLYMER MODEL

MIXED-EXCESS-MODELS (R-K default)

HKF

PITZER

CENTRAL_ATOM_MODEL

MODEL NAME /REDLICH-KISTER_MUGGIANU/: mixed

First (the independent) constituent: ?

FILE SYSTEM ERROR IN FILHLP

ERROR 1717 READING HELP FILE

First (the independent) constituent: A

Second (the dependent) constituent: B

Excess model type: /LEGENDRE/: ?

Legal choices are: LEGENDRE, POLYNOM or REDLICH-KISTER

Excess model type: /LEGENDRE/: legendre

Any other non-Redlich-Kister binary excess parameters?

First (the independent) constituent: NONE

GES5:

GES5: list-data ,,

1OUTPUT FROM GIBBS ENERGY SYSTEM ON PC/WINDOWS NT DATE 2023- 4-27
FROM DATABASE: User data 2023.04.27

ALL DATA IN SI UNITS
FUNCTIONS VALID FOR 298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED

| ELEMENT | STABLE ELEMENT | REFERENCE | MASS | H298-H0 | S298 |
|---------|----------------|---------------|------------|------------|------------|
| -1 | /- | ELECTRON_GAS | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 0 | VA | VACUUM | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 1 | A | UNKNOWN | 1.0000E+01 | 0.0000E+00 | 0.0000E+00 |
| 2 | B | BETA_RHOMBO_B | 1.0811E+01 | 1.2220E+00 | 5.9000E+00 |
| 3 | C | GRAPHITE | 1.2011E+01 | 1.0540E+00 | 5.7400E+00 |

| SPECIES | STOICHIOMETRY |
|---------|---------------|
| 1 A | A |
| 2 B | B |
| 3 C | C |

4 VA

VA

```
LIQUID
EXCESS MODEL IS MIXED-EXCESS-MODELS (R-K default)
CONSTITUENTS: A,B,C

G(LIQUID,A;0)-H298(UNKNOWN,A;0) = 0.0
G(LIQUID,B;0)-H298(BETA_RHOMBO_B,B;0) = 0.0
G(LIQUID,C;0)-H298(GRAPHITE,C;0) = 0.0
$ Binary excess model Legendre with A as independent
L(LIQUID,A,B;0) = +10000
L(LIQUID,A,B;1) = -10000

SYMBOL      STATUS   VALUE/FUNCTION
FUNCTION R      298.15     8.314510000000000 ; 6000 N REFO !
2 RTLNP    20000000 +R*T*LN(1E-05*P)
```

GES5:Hit RETURN to continue

```
GES5:
GES5: @@ For the A-C interaction, the Polynom binary excess model
GES5: @@ should be used (rather than the default Redlich-Kister
GES5: @@ Model), with the second species (i.e. C) as the
GES5: @@ independent constituent and the first species (i.e. A)
GES5: @@ as the dependent constituent, while the L parameters for
GES5: @@ the A-C interaction shall remain the same as those
GES5: @@ handled by the R-K model.
GES5:
GES5: ent-param G(LIQUID,A,C;0) 298.15 10000; 6000 N
... the command in full is ENTER_PARAMETER
G(LIQUID,A,C;0)
GES5: ent-param G(LIQUID,A,C;1) 298.15 5000; 6000 N
... the command in full is ENTER_PARAMETER
G(LIQUID,A,C;1)
GES5:
GES5: amend-phase-des LIQUID excess mixed C A polynom
... the command in full is AMEND_PHASE_DESCRIPTION
```

Any other non-Redlich-Kister binary excess parameters?

First (the independent) constituent:

GES5: list-data ,,

1OUTPUT FROM GIBBS ENERGY SYSTEM ON PC/WINDOWS NT DATE 2023- 4-27
FROM DATABASE: User data 2023.04.27

ALL DATA IN SI UNITS
FUNCTIONS VALID FOR 298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED

| ELEMENT | STABLE ELEMENT | REFERENCE | MASS | H298-HO | S298 |
|---------|----------------|-----------|------------|------------|------------|
| -1 /- | ELECTRON_GAS | | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 0 VA | VACUUM | | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 1 A | UNKNOWN | | 1.0000E+01 | 0.0000E+00 | 0.0000E+00 |
| 2 B | BETA_RHOMBO_B | | 1.0811E+01 | 1.2220E+00 | 5.9000E+00 |
| 3 C | GRAPHITE | | 1.2011E+01 | 1.0540E+00 | 5.7400E+00 |

| SPECIES | STOICHIOMETRY |
|---------|---------------|
| 1 A | A |
| 2 B | B |
| 3 C | C |
| 4 VA | VA |

```
LIQUID
EXCESS MODEL IS MIXED-EXCESS-MODELS (R-K default)
CONSTITUENTS: A,B,C
```

```
G(LIQUID,A;0)-H298(UNKNOWN,A;0) = 0.0
G(LIQUID,B;0)-H298(BETA_RHOMBO_B,B;0) = 0.0
G(LIQUID,C;0)-H298(GRAPHITE,C;0) = 0.0
$ Binary excess model Legendre with A as independent
L(LIQUID,A,B;0) = +10000
L(LIQUID,A,B;1) = -10000
$ Binary excess model Polynom with C as independent
L(LIQUID,A,C;0) = +10000
L(LIQUID,A,C;1) = +5000

SYMBOL      STATUS   VALUE/FUNCTION
FUNCTION R      298.15     8.314510000000000 ; 6000 N REFO !
2 RTLNP    20000000 +R*T*LN(1E-05*P)
```

GES5:Hit RETURN to continue

```
GES5:
GES5: @@ For the B-C interaction, the default Redlich-Kister binary
GES5: @@ excess model shall still be used; so we do not need to
GES5: @@ amend anything regarding that.
GES5:
GES5: ent-param G(LIQUID,B,C;0) 298.15 10000; 6000 N
... the command in full is ENTER_PARAMETER
G(LIQUID,B,C;0)
GES5: ent-param G(LIQUID,B,C;1) 298.15 -2000; 6000 N
... the command in full is ENTER_PARAMETER
G(LIQUID,B,C;1)
GES5:
GES5: list-data ,,
```

1OUTPUT FROM GIBBS ENERGY SYSTEM ON PC/WINDOWS NT DATE 2023- 4-27
FROM DATABASE: User data 2023.04.27

ALL DATA IN SI UNITS
FUNCTIONS VALID FOR 298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED

| ELEMENT | STABLE ELEMENT | REFERENCE | MASS | H298-HO | S298 |
|---------|----------------|-----------|------------|------------|------------|
| -1 /- | ELECTRON_GAS | | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 0 VA | VACUUM | | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 1 A | UNKNOWN | | 1.0000E+01 | 0.0000E+00 | 0.0000E+00 |
| 2 B | BETA_RHOMBO_B | | 1.0811E+01 | 1.2220E+00 | 5.9000E+00 |
| 3 C | GRAPHITE | | 1.2011E+01 | 1.0540E+00 | 5.7400E+00 |

```

SPECIES                      STOICHIOMETRY
 1 A                         A
 2 B                         B
 3 C                         C
 4 VA                        VA

LIQUID
EXCESS MODEL IS MIXED-EXCESS-MODELS (R-K default)
CONSTITUENTS: A,B,C

G(LIQUID,A;0)-H298(UNKNOWN,A;0) = 0.0
G(LIQUID,B;0)-H298(BETA_RHOMBO_B,B;0) = 0.0
G(LIQUID,C;0)-H298(GRAPHITE,C;0) = 0.0
$ Binary excess model Legendre with A as independent
L(LIQUID,A,B;0) = +10000
L(LIQUID,A,B;1) = -10000
$ Binary excess model Polynom with C as independent
L(LIQUID,A,C;0) = +10000
L(LIQUID,A,C;1) = +5000
L(LIQUID,B,C;0) = +10000
L(LIQUID,B,C;1) = -2000

SYMBOL      STATUS   VALUE/FUNCTION
FUNCTION R    298.15   8.314510000000000 ; 6000 N REFO !
2 RTLNP     20000000 +R*T*LN(1E-05*p)

```

```

GES5:Hit RETURN to continue
GES5:
GES5: @@ =====
GES5: @@ Step 2: Amending the ternary extrapolation model:
GES5: @@ =====
GES5: @@ The default ternary excess model is the
GES5: @@ Redlich-Kister_Muggianu Model (i.e., the MUGGIANU_RESTOR
GES5: @@ method for ternary extrapolation based on binary parameters)
GES5: @@ for the associated ternary interaction terms; when no
GES5: @@ ternary L parameter is entered for that, such a default
GES5: @@ Redlich-Kister_Muggianu Model is thus to be used for
GES5: @@ extrapolation from binary excess energies to ternary
GES5: @@ interactions in the substitutional LIQUID solution phase
GES5: @@ (without sublattice) that consists of three elements
GES5: @@ (A, B and C).
GES5:
GES5: @@ However, in this particular example as follows.
GES5: @@ We shall change from this default R-K-M ternary excess
GES5: @@ model to the TOOP-KOHLER method for the ternary extrapolation
GES5: @@ method, with the species C as the Toop constituent, while
GES5: @@ the species A and B as the Kohler constituents (entering A
GES5: @@ and B, or B and A, as the basis constituent and first
GES5: @@ interacting constituent). This implicitly enforces that,
GES5: @@ during the ternary extrapolation, only the A-B binary
GES5: @@ interaction parameters are utilized in accordance with the
GES5: @@ Kohler ternary extrapolation formula for A-B-C ternary
GES5: @@ interaction, while any other binary interaction parameters
GES5: @@ involving the Toop species C (i.e., of A-C and B-C binaries)
GES5: @@ are used in line with the Toop-Kohler ternary extrapolation
GES5: @@ formula (for the A-C-B and B-C-A ternary interactions). This
GES5: @@ makes the extrapolated ternary excess interaction terms
GES5: @@ different from those handled either by the default
GES5: @@ MUGGIANU_RESTOR method or by the alternative KOHLER-ALL
GES5: @@ method.
GES5:
GES5: @@ Note that only when all the relevant binary excess energies
GES5: @@ in a ternary system are treated by the default Redlich-Kister
GES5: @@ Model (i.e., the Mixed-Excess-Model should have not been
GES5: @@ used), the MUGGIANU_RESTOR method for ternary extrapolations
GES5: @@ is equivalent to the Redlich-Kister_Muggianu Model, or the
GES5: @@ KOHLER-ALL method to the Redlich-Kister_Kohler Model.
GES5:
GES5: amend_phase-des LIQUID
... the command in full is AMEND_PHASE_DESCRIPTION
AMEND WHAT /COMPOSITION_SETS/: ?

```

You can amend

EXCESS_MODEL
MAGNETIC_ORDERING
DEBYE_HUCKEL
STATUS_BITS
NEW_CONSTITUENT
RENAME_PHASE
COMPOSITION_SETS
GLASS_TRANSITION
DISORDERED_PART
MAJOR_CONSTITUENT
ZRO2_TRANSITION
REMOVE_ADDITIONS
QUASICHEM_IONIC
QUASICHEM_FACT00
QUASICHEM_IRSID
TERNARY_EXTRAPOLAT
HKF_ELECTROSTATIC
DEFAULT_STABLE
SITE RATIOS
FRACTION_LIMITS
NEVER_DISORDER_PAR

AMEND WHAT /COMPOSITION_SETS/: TERN-EXT
Extrapolation method: /TOOP-KOHLER/: ?
Default method is Muggianu, you can use

TOOP-KOHLER
KOHLER-ALL
MUGGIANU_RESTOR

Extrapolation method: /TOOP-KOHLER/: TOOP-KOHLER
Constituent in sublattice 1: A
First interaction constituent: B
Toop constituent: C
GES5:
GES5: list-data ,,

ALL DATA IN SI UNITS
FUNCTIONS VALID FOR 298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED

| ELEMENT | STABLE ELEMENT REFERENCE | MASS | H298-H0 | S298 |
|---------|--------------------------|------------|------------|------------|
| -1 /- | ELECTRON_GAS | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 0 VA | VACUUM | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 1 A | UNKNOWN | 1.0000E+01 | 0.0000E+00 | 0.0000E+00 |
| 2 B | BETA_RHOMBO_B | 1.0811E+01 | 1.2220E+00 | 5.9000E+00 |
| 3 C | GRAPHITE | 1.2011E+01 | 1.0540E+00 | 5.7400E+00 |

| SPECIES | STOICHIOMETRY |
|---------|---------------|
| 1 A | A |
| 2 B | B |
| 3 C | C |
| 4 VA | VA |

LIQUID
EXCESS MODEL IS MIXED-EXCESS-MODELS (R-K default)
CONSTITUENTS: A,B,C

G(LIQUID,A;0)-H298(UNKNOWN,A;0) = 0.0
G(LIQUID,B;0)-H298(BETA_RHOMBO_B,B;0) = 0.0
G(LIQUID,C;0)-H298(GRAPHITE,C;0) = 0.0
\$ Binary excess model Legendre with A as independent
\$ Ternary extrapolation for LIQUID using KOHLER A B C
L(LIQUID,A,B;0) = +10000
L(LIQUID,A,B;1) = -10000
\$ Binary excess model Polynom with C as independent
\$ Ternary extrapolation for LIQUID using TOOP-KOHLER A C B
L(LIQUID,A,C;0) = +10000
L(LIQUID,A,C;1) = +5000
\$ Ternary extrapolation for LIQUID using TOOP-KOHLER B C A
L(LIQUID,B,C;0) = +10000
L(LIQUID,B,C;1) = -2000

| SYMBOL | STATUS | VALUE/FUNCTION |
|------------|----------|-----------------------------------|
| FUNCTION R | 298.15 | 8.314510000000000 ; 6000 N REFO ! |
| 2 RTLNP | 20000000 | +R*T*LN(1E-05*P) |

GES5:Hit RETURN to continue

GES5: @@ ======
GES5: @@ Step 3: Performing an equilibrium calculation using the
GES5: @@ entered and amended descriptions.
GES5: @@ ======
GES5:
GES5: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY: s-c t=1500 p=1e5 n=1 x(b)=.2 x(c)=.3
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 1965 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY: l-e , X
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: User dat

Conditions:
T=1500, P=100000, N=1, X(B)=0.2, X(C)=0.3
DEGREES OF FREEDOM 0

Temperature 1500.00 K (1226.85 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 1.07655E+01
Total Gibbs energy -1.08432E+04, Enthalpy 1.99843E+03, Volume 0.00000E+00

| Component | Moles | M-Fraction | Activity | Potential | Ref.stat |
|-----------|------------|------------|------------|-------------|----------|
| A | 5.0000E-01 | 5.0000E-01 | 4.7833E-01 | -9.1973E+03 | SER |
| B | 2.0000E-01 | 2.0000E-01 | 1.9875E-01 | -2.0151E+04 | SER |
| C | 3.0000E-01 | 3.0000E-01 | 5.5332E-01 | -7.3811E+03 | SER |

LIQUID Status ENTERED Driving force 0.0000E+00
Moles 1.0000E+00, Mass 1.0765E+01, Volume fraction 0.0000E+00 Mole fractions:
A 5.0000E-01 C 3.0000E-01 B 2.0000E-01

POLY: sh qf(*)
... the command in full is SHOW_VALUE
QF(LIQUID)=0.52168269
POLY: sh gm(*) dgm(*)
... the command in full is SHOW_VALUE
GM(LIQUID)=-10843.162
DGM(LIQUID)=0
POLY:

POLY: save TCEX52a.POLY3 y
... the command in full is SAVE_WORKSPACES
POLY:Hit RETURN to continue
POLY: @@ ======
POLY: @@ Step 4: Reading the same data from a small database and
POLY: @@ Performing the same equilibrium calculation.
POLY: @@ ======
POLY:
POLY: go data
... the command in full is GOTO_MODULE

TDB_TCFE11: rej sys
... the command in full is REJECT
VA /- DEFINED
DICTRA_FCC_A1 REJECTED
REINITIATING GES
TDB_TCFE11:
TDB_TCFE11: sw user TCEX52-TOOP.TDB
... the command in full is SWITCH_DATABASE
Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

VA /- DEFINED
TDB_USER: d-sys /all
... the command in full is DEFINE_SYSTEM

```

A          B          C
DEFINED
TDB_USER: l-sys const
... the command in full is LIST_SYSTEM
LIQUID:L      :A B C:
TDB_USER: get
... the command in full is GET_DATA
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS .....

List of references for assessed data

'Reference 2'
'Reference 1'
AFTER ...
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
-OK-
TDB_USER:
TDB_USER: Hit RETURN to continue
TDB_USER: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY:
POLY: s-c t=1500 p=1e5 n=1 x(b)=.2 x(c)=.3
... the command in full is SET_CONDITION
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated      1965 grid points in      0 s
Found the set of lowest grid points in      0 s
Calculated POLY solution      0 s, total time      0 s
POLY: l-e , X
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium =      1, label A0 , database: USER

Conditions:
T=1500, P=100000, N=1, X(B)=0.2, X(C)=0.3
DEGREES OF FREEDOM 0

Temperature 1500.00 K ( 1226.85 C), Pressure 1.000000E+05
Number of moles of components 1.000000E+00, Mass in grams 1.07655E+01
Total Gibbs energy -1.08432E+04, Enthalpy 1.99843E+03, Volume 0.000000E+00

Component      Moles      M-Fraction Activity Potential Ref.stat
A      5.0000E-01  5.0000E-01 4.7833E-01 -9.1973E+03 SER
B      2.0000E-01  2.0000E-01 1.9875E-01 -2.0151E+04 SER
C      3.0000E-01  3.0000E-01 5.5332E-01 -7.3811E+03 SER

LIQUID      Status ENTERED      Driving force 0.0000E+00
Moles 1.0000E+00, Mass 1.0765E+01, Volume fraction 0.0000E+00 Mole fractions:
A  5.0000E-01  C 3.0000E-01  B 2.0000E-01
POLY: sh qf(*)
... the command in full is SHOW_VALUE
QF(LIQUID)=0.52168269
POLY: sh gm(*) dgm(*)
... the command in full is SHOW_VALUE
GM(LIQUID)=-10843.162
DGM(LIQUID)=0
POLY:
POLY: save TCEX52b.POLY3 y
... the command in full is SAVE_WORKSPACES
POLY:
POLY:
POLY: @@ As you have noticed, the calculated equilibrium (using the
POLY: @@ small database) is exactly the same as the first
POLY: @@ calculation (with data amended in the GES module
POLY: @@ step-by-step, for the binary/ternary excess models).
POLY:
POLY:
POLY: set-inter
... the command in full is SET_INTERACTIVE
POLY:

```

tce53**SYS:About**

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

```
SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce53\tce53.TCM.test"
SYS: go sys
SYS: set-echo
SYS:
SYS: set-log TCEX53.LOG
Heading: Pourbaix Diagram Calculations through the TDB-GES-POLY-POST routine
SYS:
SYS: @@ Some Pourbaix diagrams
SYS:
SYS:
SYS: @@ =====
SYS: @@ Copyright: Thermo-Calc Software AB, Stockholm, Sweden
SYS: @@ Developer: Dr. Pingfang Shi, Thermo-Calc Software AB
SYS: @@ Date: 2014-05-26 (revision)
SYS: @@ Text updated July 2017 (AJW)
SYS:
SYS: @@ =====
SYS: @@ Example description:
SYS: @@ =====
SYS: @@ TCEX53 uses the PAQ2 database to calculate some Pourbaix
SYS: @@ diagrams. The DATABASE_RETRIEVAL (TDB),
SYS: @@ GIBBS_ENERGY_SYSTEM (GES), POLY3, and POSTA modules are
SYS: @@ used for the Fe-X-H2O-NaCl heterogeneous interaction
SYS: @@ system, where X = Cr-Ni-Co.
SYS:
SYS: @@ Note: The initial bulk composition of Fe-based alloy in
SYS: @@ this calculation is only preliminarily assigned, in which
SYS: @@ the BCC_A2 and/or FCC_A1 solution phase(s) are considered
SYS: @@ as of primarily interest. For practical calculations,
SYS: @@ you need more precise inputs for the initial bulk
SYS: @@ compositions of alloys.
SYS:
SYS: @@ =====
SYS: @@ Notes about the example and the PAQ2 database:
SYS: @@ =====
SYS: @@ The so-called Pourbaix diagram is actually a phase diagram
SYS: @@ with independently-varied electropotential (Eh) and
SYS: @@ acidity (pH), for an heterogeneous interaction system at a
SYS: @@ certain bulk composition (that is by default always set as
SYS: @@ 1 kg of water solving a specified amount of metals and
SYS: @@ other solutes), under defined temperature and pressure
SYS: @@ conditions.
SYS:
SYS: @@ The PAQ2 database is specially designed for Pourbaix
SYS: @@ diagram calculations (i.e., Eh-pH plots). It contains an
SYS: @@ AQUEOUS solution phase and REF_ELECTRODE phase (as a
SYS: @@ reference for electron in aqueous electrolyte systems),
SYS: @@ as well as some data for various solid phases (solution
SYS: @@ or stoichiometric) and a gaseous mixture phase.
SYS:
SYS: @@ For more Pourbaix diagram exercises, see TCEX40 and the
SYS: @@ extended examples TCEX40A to TCEX40E.
SYS:
SYS: @@ =====
SYS: @@ Step 1: Single-Point Calculations for H2O-NaCl system
SYS: @@ =====
SYS: @@ To demonstrate how to define the molality of NaCl
SYS: @@ in an aqueous-bearing heterogeneous interaction system
SYS:
SYS: @@ Retrieve data from the PAQ2 database:
SYS: go data
... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module
Database folder: C:\jenkins\workspace\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA           /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE11: rej sys
... the command in full is REJECT
VA           /- DEFINED
DICTRA_FCC_A1 REJECTED
REINITIATING GES ....
TDB_TCFE11: @@ Switch to the PAQ2 database
TDB_TCFE11: sw PAQ2
... the command in full is SWITCH_DATABASE
Current database: Public Aqueous Solution (SIT) v2.5

H          O          ZE
VA DEFINED
LIQUID:L REJECTED
GRAPHITE      DIAMOND_A4      FC_ORTHORHOMBIC
MONOCLINIC   REJECTED
CBCC_A12      CUB_A13      CHI_A12
FE4N         FECN_CHI REJECTED
CEMENTITE     M23C6       M7C3
M5C2          M3C2        KSI_CARBIDE
PI REJECTED
FE3C          NI3C        CR3C2
CR7C3         CR23C6 REJECTED
COCO3         FECO3       NAHCO3
NA2CO3_S1    NA2CO3_S2    NICO3
CRC606 REJECTED
CO3N          CRN         CR2N
FE2N          NI3N REJECTED
```

| | | |
|----------|-----------|-----------|
| NANO2_S1 | NANO2_S2 | NANO3 |
| REJECTED | | |
| COCL2 | CRCL2 | CRCL3 |
| FECL2 | FECL3 | NICL2 |
| REJECTED | | |
| FECLO | NACLO4_S1 | NACLO4_S2 |
| REJECTED | | |

TDB_PAQ2: data

... the command in full is DATABASE_INFORMATION
 Current database: Public Aqueous Solution (SIT) v2.5

PAQ2

Thermo-Calc PUBLIC AQUEOUS DATABASE FOR POURBAIX MODULE
 (based on and replacing AQ in TCC/TCW & PAQ in TCC-Demo/TCW-Demo)

 (Version 2.5, Feb. 2021)

Copyright © 1997-2008: Thermo-Calc Software AB, Sweden

This public aqueous solution database contains aqueous solution species, and gaseous mixture species and solid/liquid (pure and solution) phases in an 11-element system (Fe-Co-Cr-Na-Ni-C-H-O-N-S-Cl). As a demo version of the complete TCAQ2 Aqueous Solution Database, it is specially designed for uses with the apecial POURBAIX module which allows easy and automatic calculations of the sp-called Pourbaix diagrams (i.e., Eh-pH plots) and many types of property diagrams. It can also be used in normal TCC/TCW calculations for aqueous involved heterogeneous interaction systems. The TCAQ2 Aqueous Solution Database covers 83 elements (compatible with the SGTE PURE/SSUB/SSOL and other databases), and can be used together with the SIT (Specific Interaction Theory) Model for complex aqueous solution that has already implemented in Thermo-Calc.

PAQ has been developed since 1996, and gradually modified and expanded later on. PAQ2.4 combines 4 files from its previous version PAQ2 [i.e., PAQ2setup.TDB for defining elements, species and phases; PAQ2param.TDB for assigning various functions and parameters for standard properties of various phases; PAQ2inter.TDB for assigning binary or higher-order interaction parameters for non-ideal properties of aqueous solution phase; and PAQ2funct.TDB for entering extra functions referred in PAQ2param.TDB].

The AQUEOUS solution phase can be treated by the SIT Model, using the TCAQ2 (or PAQ2) database that can be applied to low PTX conditions (up to 100 bar, 350 C and 3 molality). However, if investigated heterogeneous interaction processes occur at high PTX (up to 5 kbar, 1000 C and 10 molality), the other aqueous solution database, called AQS2, which implies the complete Revised HKF (Helgeson-Kirkham-Flowers) Model, is required.

Data for pure elements are taken from the SGTE unary database (PURE) with explicit magnetic and pressure dependencies. The reference state is 298.15 K and 1 bar. All data follow the new temperature scale ITPS 90. For calculations of the so-called Pourbaix-diagrams (pH-Eh) and related property diagrams within either the POURBAIX-module or through normal TDB-GES-POLY-POST routines, following types of phases must be defined in the heterogeneous interaction systems:

AQUEOUS: from PAQ2 (or PAQS2) or TCAQ2 (or AQS2);
 REF_ELECTRODE: from PAQ2 (or PAQS2) or TCAQ2 (or AQS2);
 GAS: from PAQ2 (or PAQS2) or SSUB4 (or TCMP2);

Various Solids: from PAQ2 (or PAQS2) or SSOL4 (or TCFE6, TCMP2, etc.). There are many solid phases (stoichiometric or solution) and a metallic liquid mixture phase which are included in the public PAQ2 and PAQS2 databases. By default, however, many such phases have been rejected automatically. Of course, if one wishes to consider any of such phases (such as Cementite or M23C6) into a defined interaction system, they can be appropriately restored in the POURBAIX or TDB modules.

Either TCAQ2 or AQS2 databases can be used by the advanced, easy-to-use POURBAIX Module via its multiple-database option, or be utilized along with ordinary Thermo-Calc routines. For a gaseous mixture phase, one could append from the SSUB (SGTE PURE SUBSTANCES DATABASE, which treats the gas phase as an ideal mixture at all temperatures, pressures and compositions), or from some non-ideal gaseous/fluid mixture models implemented in the Thermo-Calc GES system (such as the SUPERFLUID model, i.e., the non-ideal EOS and non-ideal mixing for the C-H-O-S-N-Ar fluids; Shi and Saxena, 1992). For other condensed materials except for aqueous solution species, one could append data (of stoichiometric and solution solid phases) from any compatible Thermo-Calc database(s) [e.g., PURE, SSUB, SSOL, TCFE, TCNI, TCNF, CCCI, TTNI, TTTI, TTAl, TTMs, TTZr, NSLD, SEMC, TCMP, TCES, SALT, ION, SLAG, NOX, NUOX, SNUX, NUMT, GCE, and other substances/solutions databases], depending upon application systems and investigated aqueous-bearing heterogeneous interaction processes.

In a normal POLY calculation (single points, stepping, and/or mapping), one should always remember as the first step to appropriately redefine the components as follows:

DEF-COMP H2O H+1 Ze Fe Ni NaCl Cl-1 S <& other components>;

Then, one can appropriately define the equilibrium conditions, e.g., SET-COND P=1e5 T=300 B=1000 N(H+1)=0 N(Ze)=0 N(Fe)=1e-6 N(NaCl)=3...;

and set the necessary reference states for some components, e.g.,

SET-REFERENCE-STATE H2O AQUEOUS * 1E5 ;

SET-REFERENCE-STATE ZE REF_ELEC * 1E5 ;

SET-REFERENCE-STATE NaCl HALITE * 1E5 ;

SET-REFERENCE-STATE Fe BCC * 1E5 ;

The pH and Eh are thus defined by entering the following functions:

ENT-SYM FUNC pH=-log10(ACR(H+1)) ;

ENT-SYM FUNC Eh=MUR(ZE)/RNF ;

However, if the reference state for H+1 component has been defined by

SET-REFERENCE-STATE H+1 AQUEOUS * 1E5 ;

then the pH quantity should be alternatively entered as:

ENT-SYM FUNC pH=-log10(ACR(H+1,AQUEOUS)) ;

For defining activity and activity coefficients of the solvent, use:

ENT-SYM FUNC ACRH2O=ACR(H2O,AQUEOUS) ;

ENT-SYM FUNC RCH2O=ACR(H2O,AQUEOUS) ;

while for defining activity, activity coefficients and molality of a specific solute species "i", use:

ENT-SYM FUNC Aii=ACR(i,AQUEOUS)*AH2O ;

ENT-SYM FUNC RCI=ACR(i,AQUEOUS)*YH2O/Y(AQUEOUS,i) ;

ENT-SYM FUNC Mli=Y(AQUEOUS,i)*AH2O/YH2O ;

where RNF=96485.309, AH2O=55.508435 and YH2O=Y(AQUEOUS,H2O) as

predefined functions, and i=Fe+2 (for instance) as species name.

Important Note: The REF_ELECTRODE phase is the reference electrode which should always be included in a defined system involving aqueous solution for the purpose of calculating electron potential [MUR(ZE)], while this phase should always be SUSPENDED in all the POLY calculations.

For further information, please contact Dr. Pingfang Shi at TCSAB.

Release History: Version 1.0 initial release (as AQ), 1997
 Version 1.1 with minor improvements (as AQ), 1998
 Version 1.2 with minor improvements (as AQ), 2000
 Version 2.0 with major improvements (as PAQ2.0), 2002
 Version 2.1 with minor improvements (as PAQ2.1), 2003
 Version 2.2 with minor improvements (as PAQ2.2), 2006
 Version 2.3 with minor improvements (as PAQ2.3), 2007

Version 2.4 with major improvements (as PAQ2.4), 2008
 Edited by: Dr. Pingfang Shi (Thermo-Calc Software, 1997-2008).

```

=====
TDB_PAQ2: d-sys H O Na Cl
... the command in full is DEFINE_SYSTEM
NA          CL DEFINED
TDB_PAQ2: l-sys const
... the command in full is LIST_SYSTEM
AQUEOUS:A :H2O H2 H+1 OH-1 H2O2 HO2-1 O2 O3 CL2 CL-1 CLO2 CLO-1 CLO2-1
CLO3-1 CLO4-1 HCLO HCLO2 NA+1:
> Aqueous Solution: using the SIT Model (from TCAQ2 database)
REF ELECTRODE :ZE:
> Reference Electrode for ZE potentail; always SUSPENDED in POLY.
GAS:G      :CL CL2 CL1H1 CL1O1 CL1O2 CL1H1O1 CL2O1 CL1NA1 CL2NA2 CL3NA3 H
H1NA1 H1NA1O1 H1O1 H1O2 H2 H2NA2O2 H2O1 H2O2 NA NA1O1 NA2 NA2O1 NA2O2 O O2
O3:
> Gaseous Mixture, using the ideal gas model
FCC_A1     :NA O:VA:
> This is also the MX (X=C,N) solution phase.
BCC_A2     :NA O:VA:
> This is also the MX3 (X=C,N) solution phase.
HCP_A3     :NA:VA:
> This is also the M2X (X=C,N) solution phase.
HALITE     :NAICL1:
NAO2       :NA1O2:
NA2O_S1    :NA2O1:
NA2O_S2    :NA2O1:
NA2O_S3    :NA2O1:
NA2O2_S1   :NA2O2:
NA2O2_S2   :NA2O2:
NAOH_S1    :H1NA1O1:
NAOH_S2    :H1NA1O1:
TDB_PAQ2: get
... the command in full is GET_DATA
16:57:48,973 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS .....
FUNCTIONS .....

List of references for assessed data

'TCS public data set for gaseous mixture in the Fe-Co-Cr-Na-Ni-C-H-O-N-S
-Cl system.'
'TCS public data set for liquid mixture and alloy solutions in the Fe-Co
-Cr-Na-Ni-C-H-O-N-S-Cl system.'
'TCS public data set for stoichiometric solids and liquids in the Fe-Co-Cr
-Na-Ni-C-H-O-N-S-Cl system.'
'TCS Aqueous Solution Database, TCAQ2, v2.0 (2002/2003). Extracted data
only for Fe-Co-Cr-Na-Ni-C-H-O-N-S-Cl bearing aqueous solution species
from TCAQ2 which covers totally 83 elements and contains many more
aqueous solution species.'

-OK-
16:57:49,163 [Thread-0] WARN MacroProcessingContext: The handling of the excess model command is not yet supported in GES6.
16:57:49,163 [Thread-0] WARN MacroProcessingContext: The handling of the add contribution command is not yet supported in GES6.
16:57:49,164 [Thread-0] WARN MacroProcessingContext: The handling of the fraction limits command is not yet supported in GES6.
TDB_PAQ2: Hit RETURN to continue
TDB_PAQ2:
TDB_PAQ2: @@ Define the system-components and the reference states:
TDB_PAQ2: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY: d-com H2O H+1 ZE Na Cl
... the command in full is DEFINE_COMPONENTS
POLY: s-r-s H2O AQUEOUS * 1e5
... the command in full is SET_REFERENCE_STATE
POLY: s-r-s ZE REF_ELE * 1e5
... the command in full is SET_REFERENCE_STATE
POLY: l-st c
... the command in full is LIST_STATUS
*** STATUS FOR ALL COMPONENTS
COMPONENT      STATUS    REF. STATE      T (K)      P (Pa)
VA             ENTERED   SER
H2O            ENTERED   AQUEOUS      *
H+1            ENTERED   SER
ZE             ENTERED   REF_ELECTRODE  *
NA             ENTERED   SER
CL             ENTERED   SER
POLY:
POLY: @@ Define the equilibrium conditions
POLY: @@ -----
POLY: @@ Define P-T and bulk composition in the interaction system
POLY: @@ for the calculations of initial equilibria:
POLY:
POLY: s-c P=1e5 T=298.15 b(H2O)=1000
... the command in full is SET_CONDITION
POLY: s-in-am b(Na1Cl1)=5
... the command in full is SET_INPUT_AMOUNTS
POLY: s-c n(H+1)=0 n(ZE)=0
... the command in full is SET_CONDITION
Convergence in the equilibrium calculation can be hard to reach with zero amount conditions; It is recommended to suspend a component instead
Convergence in the equilibrium calculation can be hard to reach with zero amount conditions; It is recommended to suspend a component instead
POLY: l-c
... the command in full is LIST_CONDITIONS
P=100000, T=298.15, B(H2O)=1000, B(NA)=1.966861769, B(CL)=3.033138231,
N(H+1)=0, N(ZE)=0
DEGREES OF FREEDOM 0
POLY:
POLY: @@ Calculate an equilibrium with only AQUEOUS:
POLY: c-st p *=sus
... the command in full is CHANGE_STATUS
POLY: c-st p AQUEOUS=ent 55.8
... the command in full is CHANGE_STATUS

```

```

POLY: l-st p
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES
PHASE           STATUS      DRIVING FORCE    MOLES
AQUEOUS         ENTERED     0.000000E+00   1.785600E+03
SUSPENDED PHASES:
REF_ELECTRODE NAOH_S2 NAOH_S1 NAO2 NA2O_S3 NA2O_S2 NA2O_S1 NA2O2_S2 NA2O2_S1
HCP_A3 HALITE FCC_A1 BCC_A2 GAS
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated          1212 grid points in          0 s
Found the set of lowest grid points in          0 s
Creating a new composition set AQUEOUS#2
Calculated POLY solution          0 s, total time          0 s
POLY: l-e ,x
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium =      1, label A0 , database: PAQ2

Conditions:
P=100000, T=298.15, B(H2O)=1000, B(NA)=1.966861769, B(CL)=3.033138231,
N(H+1)=0, N(ZE)=0
DEGREES OF FREEDOM 0

Temperature 298.15 K ( 25.00 C), Pressure 1.000000E+05
Number of moles of components 5.56795E+01, Mass in grams 1.005000E+03
Total Gibbs energy -1.70630E+07, Enthalpy -1.59010E+07, Volume 0.000000E+00

Component       Moles      M-Fraction Activity Potential Ref.stat
H2O            5.5508E+01  9.9693E-01  9.9654E-01 -8.5871E+00 AQUEOUS#
H+1           -9.7239E-08 -1.7464E-09  1.0405E-07 -3.9858E+04 SER
ZE             8.6043E-08  1.5453E-09  3.4476E+12  7.1565E+04 REF_ELEC
NA             8.5554E-02  1.5365E-03  4.5046E-63 -3.5588E+05 SER
CL             8.5554E-02  1.5365E-03  4.1623E-18 -9.9210E+04 SER

AQUEOUS#1      Status ENTERED      Driving force 0.0000E+00
Moles 5.5680E+01, Mass 1.0050E+03, Volume fraction 0.0000E+00 Mole fractions:
H2O  9.96927E-01  NA  1.53654E-03  H+1 -1.74641E-09
CL  1.53654E-03  ZE  1.54532E-09
Constitution: SiteFraction Molality Activity log10Act
H2O  9.96927E-01  5.55084E+01  9.96605E-01 -0.0015
CL-1 1.53654E-03  8.55538E-02  6.73425E-02 -1.1717
NA+1 1.53654E-03  8.55538E-02  6.73424E-02 -1.1717
H+1  2.37132E-09  1.32034E-07  1.04050E-07 -6.9828
OH-1  2.19965E-09  1.22476E-07  9.63757E-08 -7.0160
O2   4.70270E-10  2.61844E-08  2.61828E-08 -7.5820
O3   1.00000E-12  0.00000E+00  2.70935E-38 -37.5671
HClO  1.00000E-12  0.00000E+00  3.25360E-20 -19.4876
H2O2  1.00000E-12  0.00000E+00  3.68420E-21 -20.4337
HClO2 1.00000E-12  0.00000E+00  1.28717E-37 -36.8904
H2   1.00000E-12  0.00000E+00  5.39110E-43 -42.2683
HO2-1 1.00000E-12  0.00000E+00  7.49315E-26 -25.1253
ClO4-1 1.00000E-12  0.00000E+00  8.09139E-33 -32.0920
ClO3-1 1.00000E-12  0.00000E+00  1.41605E-30 -29.8489
ClO2-1 1.00000E-12  0.00000E+00  1.29472E-32 -31.8878
ClO2  1.00000E-12  0.00000E+00  4.84011E-38 -37.3151
ClO-1  1.00000E-12  0.00000E+00  6.77886E-21 -20.1688
Cl2   1.00000E-12  0.00000E+00  4.80004E-25 -24.3188
Solution Properties: pH = 6.9828 Eh = 0.7417 V I = 0.0856
pe = 12.5375 Ah = 71.5647 kJ m* = 0.1711
Aw = 0.9966 Os = 1.1033 pKw = 13.9973
At1= 1.0000E-12 At2= 1.2248E-07 (equiv_mol/kg_H2O)

POLY: l-st p
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES
PHASE           STATUS      DRIVING FORCE    MOLES
AQUEOUS#2        ENTERED     0.000000E+00   0.000000E+00
AQUEOUS#1        ENTERED     0.000000E+00   5.567954E+01
SUSPENDED PHASES:
REF_ELECTRODE NAOH_S2 NAOH_S1 NAO2 NA2O_S3 NA2O_S2 NA2O_S1 NA2O2_S2 NA2O2_S1
HCP_A3 HALITE FCC_A1 BCC_A2 GAS
POLY: sh b n n(*)
... the command in full is SHOW_VALUE
B=1005.
N=55.679543
N(H2O)=55.508435, N(H+1)=-9.7239338E-8, N(ZE)=8.6042553E-8,
N(NA)=8.5553782E-2, N(CL)=8.5553803E-2
POLY:Hit RETURN to continue
POLY:
POLY: @@ Calculate an equilibrium with all phases (except for REF_ELE)
POLY:
POLY: c-st p *=ent 0
... the command in full is CHANGE_STATUS
POLY: c-st p AQUEOUS=ent 55.8
... the command in full is CHANGE_STATUS
POLY:
POLY: @@ Always set the REF_ELECTRODE phase as SUSPENDED:
POLY:
POLY: c-st p REF_ELE=sus
... the command in full is CHANGE_STATUS
POLY: l-st p
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES
PHASE           STATUS      DRIVING FORCE    MOLES
NAOH_S2          ENTERED     0.000000E+00   0.000000E+00
NAOH_S1          ENTERED     0.000000E+00   0.000000E+00
NAO2             ENTERED     0.000000E+00   0.000000E+00
NA2O_S3          ENTERED     0.000000E+00   0.000000E+00
NA2O_S2          ENTERED     0.000000E+00   0.000000E+00
NA2O_S1          ENTERED     0.000000E+00   0.000000E+00
NA2O2_S2         ENTERED     0.000000E+00   0.000000E+00
NA2O2_S1         ENTERED     0.000000E+00   0.000000E+00
HCP_A3           ENTERED     0.000000E+00   0.000000E+00
HALITE           ENTERED     0.000000E+00   0.000000E+00
FCC_A1           ENTERED     0.000000E+00   0.000000E+00
BCC_A2           ENTERED     0.000000E+00   0.000000E+00
AQUEOUS#2        ENTERED     0.000000E+00   0.000000E+00
AQUEOUS#1        ENTERED     0.000000E+00   5.580000E+01
GAS              ENTERED     0.000000E+00   0.000000E+00
SUSPENDED PHASES:
REF_ELECTRODE
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated          806 grid points in          2 s

```

```

Found the set of lowest grid points in          0 s
Calculated POLY solution      1 s, total time    3 s
POLY: l-e ,x
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium =      1, label A0 , database: PAQ2

Conditions:
P=100000, T=298.15, B(H2O)=1000, B(NA)=1.966861769, B(CL)=3.033138231,
N(H+1)=0, N(ZE)=0
DEGREES OF FREEDOM 0

Temperature   298.15 K (   25.00 C), Pressure 1.000000E+05
Number of moles of components 5.56795E+01, Mass in grams 1.00500E+03
Total Gibbs energy -1.70630E+07, Enthalpy -1.59010E+07, Volume 0.00000E+00

Component      Moles      M-Fraction  Activity  Potential  Ref.stat
H2O           5.5508E+01  9.9693E-01  9.9654E-01 -8.5871E+00 AQUEOUS#
H+1           -9.7239E-08 -1.7464E-09  1.0405E-07 -3.9858E+04 SER
ZE            8.6043E-08  1.5453E-09  3.4476E+12  7.1565E+04 REF_ELEC
NA            8.5554E-02   1.5365E-03  4.5046E-63 -3.5588E+05 SER
CL            8.5554E-02   1.5365E-03  4.1623E-18 -9.9210E+04 SER

AQUEOUS#1      Status ENTERED   Driving force 0.0000E+00
Moles 5.5680E+01, Mass 1.0050E+03, Volume fraction 0.0000E+00 Mole fractions:
H2O  9.96927E-01 NA  1.53654E-03 H+1 -1.74641E-09
CL  1.53654E-03 ZE  1.54532E-09
Constitution: SiteFraction Molality Activity log10Act
H2O       9.96927E-01  5.55084E+01  9.96605E-01 -0.0015
CL-1      1.53654E-03  8.55538E-02  6.73425E-02 -1.1717
NA+1      1.53654E-03  8.55538E-02  6.73424E-02 -1.1717
H+1       2.37132E-09  1.32034E-07  1.04050E-07 -6.9828
OH-1      2.19965E-09  1.22476E-07  9.63757E-08 -7.0160
O2        4.70270E-10  2.61844E-08  2.61828E-08 -7.5820
O3        1.00000E-12  0.00000E+00  2.70935E-38 -37.5671
HClO      1.00000E-12  0.00000E+00  3.25360E-20 -19.4876
H2O2      1.00000E-12  0.00000E+00  3.68420E-21 -20.4337
HClO2     1.00000E-12  0.00000E+00  1.28717E-37 -36.8904
H2        1.00000E-12  0.00000E+00  5.39110E-43 -42.2683
HO2-1     1.00000E-12  0.00000E+00  7.49315E-26 -25.1253
ClO4-1     1.00000E-12  0.00000E+00  8.09139E-33 -32.0920
ClO3-1     1.00000E-12  0.00000E+00  1.41605E-30 -29.8489
ClO2-1     1.00000E-12  0.00000E+00  1.29472E-32 -31.8878
ClO2      1.00000E-12  0.00000E+00  4.84011E-38 -37.3151
ClO-1      1.00000E-12  0.00000E+00  6.77886E-21 -20.1688
Cl2        1.00000E-12  0.00000E+00  4.80004E-25 -24.3188
Solution Properties: pH = 6.9828 Eh = 0.7417 V I = 0.0856
pe = 12.5375 Ah = 71.5647 kJ m* = 0.1711
Aw = 0.9966 Os = 1.1033 pKw = 13.9973
At1= 1.0000E-12 At2= 1.2248E-07 (equiv_mol/kg_H2O)

POLY: l-st p
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES
PHASE      STATUS      DRIVING FORCE      MOLES
AQUEOUS#2  ENTERED   0.000000E+00  0.000000E+00
AQUEOUS#1  ENTERED   0.000000E+00  5.567954E+01
GAS        ENTERED   -3.453482E+00  0.000000E+00
HALITE     ENTERED   -4.519288E+00  0.000000E+00
NAOH_S1    ENTERED   -1.737487E+01  0.000000E+00
BCC_A2     ENTERED   -1.752962E+01  0.000000E+00
FCC_A1     ENTERED   -1.752962E+01  0.000000E+00
NAOH_S2    ENTERED   -1.793977E+01  0.000000E+00
NAO2       ENTERED   -1.999496E+01  0.000000E+00
NA2O_S1    ENTERED   -2.605088E+01  0.000000E+00
NA2O_S2    ENTERED   -2.640940E+01  0.000000E+00
NA2O_S1    ENTERED   -4.241247E+01  0.000000E+00
ENTERED PHASES WITH DRIVING FORCE LESS THAN -4.257992E+01
NA2O_S2 NA2O_S3 HCP_A3
SUSPENDED PHASES:
REF_ELECTRODE
POLY: sh b n n(*)*
... the command in full is SHOW_VALUE
B=1005.
N=55.679543
N(H2O)=55.508435, N(H+1)=-9.7239338E-8, N(ZE)=8.6042552E-8,
N(NA)=8.5553782E-2, N(CL)=8.5553803E-2
POLY:
POLY: @@ As shown here, 0.5wt% of NaCl (in 1 kg of H2O) is
POLY: @@ equivalent to 0.085554 molality of NaCl.
POLY:
POLY: @@ Save the workspace for the H2O-NaCl system:
POLY: save TCEX53_a.POLY3_y
... the command in full is SAVE_WORKSPACES
POLY: Hit RETURN to continue
POLY:
POLY: @@ =====
POLY: @@ Step 2: Single-Point Calculations for Fe-X (X = Cr-Ni-Co)
POLY: @@ =====
POLY: @@ To demonstrate how to define the initial amount of alloy
POLY: @@ in an aqueous-bearing heterogeneous interaction system:
POLY: @@ -----
POLY: @@ Note: We are only interested in the BCC_A2 and FCC_A1
POLY: @@ phases in the Fe-based alloy, in the current testing
POLY: @@ calculation. If necessary, you can consider other
POLY: @@ phases (which exist in the applied steel material).
POLY:
POLY: go data
... the command in full is GOTO_MODULE
TDE_PAQ2: rej sys
... the command in full is REJECT
H          O          ZE
VA DEFINED
LIQUID:L REJECTED
GRAPHITE      DIAMOND_A4      FC_ORTHORHOMBIC
MONOCLINIC REJECTED
CBCC_A12      CUB_A13      CHI_A12
FE4N          FECN_CHI REJECTED
CEMENTITE     M23C6       M7C3
M5C2          M3C2       KSI_CARBIDE
PI REJECTED
FE3C          NI3C       CR3C2
CR7C3         CR23C6 REJECTED
COCO3          FECO3      NAHCO3
NA2CO3_S1    NA2CO3_S2      NICO3
CRC606 REJECTED
CO3N          CRN        CR2N

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```

FE2N          NI3N REJECTED
NANO2_S1      NANO2_S2          NANO3
    REJECTED
COCCL2        CRCL2           CRCL3
FECCL2        FECL3           NICL2
    REJECTED
FECLO         NACLO4_S1       NACLO4_S2
    REJECTED
REINITIATING GES .....
TDB_PAQ2: sw PAQ2
... the command in full is SWITCH_DATABASE
TDB_PAQ2: rej ele H O ZE
... the command in full is REJECT
H             O                   ZE
    REJECTED
TDB_PAQ2: d-sys Fe Cr Ni Co
... the command in full is DEFINE_SYSTEM
FE            CR                 NI
CO DEFINED
TDB_PAQ2: l-sys const
... the command in full is LIST_SYSTEM
GAS:G         :CO CR CR2 FE NI:
> Gaseous Mixture, using the ideal gas model
FCC_A1        :CO CR FE NI:VA:
> This is also the MX (X=C,N) solution phase.
BCC_A2        :CO CR FE NI:VA:
> This is also the MX3 (X=C,N) solution phase.
HCP_A3        :CO CR FE NI:VA:
> This is also the M2X (X=C,N) solution phase.
SIGMA         :CO FE NI:CR:CO CR FE NI:
TDB_PAQ2: rej-ph *
... the command in full is REJECT
GAS:G         FCC_A1           BCC_A2
HCP_A3        SIGMA REJECTED
TDB_PAQ2: rest-ph FCC_A1 BCC_A2
... the command in full is RESTORE
FCC_A1        BCC_A2 RESTORED
TDB_PAQ2: get
... the command in full is GET_DATA
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS .....
FUNCTIONS .....

List of references for assessed data

'TCS public data set for liquid mixture and alloy solutions in the Fe-Co
-Cr-Na-Ni-C-H-O-N-S-Cl system.'
-OK-
TDB_PAQ2: Hit RETURN to continue
TDB_PAQ2:
TDB_PAQ2: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY:
POLY: @@ You can turn on the Global Minimization:
POLY: Adv-Opt EQ_CALC Y Y !
... the command in full is ADVANCED_OPTIONS
Settings for the minimization of an equilibria:
POLY: Adv-Opt GLOBAL Y 20000 !
... the command in full is ADVANCED_OPTIONS
Settings for global minimization:
POLY:
POLY: s-c P=1e5 T=298.15
... the command in full is SET_CONDITION
POLY:
POLY: @@ The following conditions [system-size B and initial bulk
POLY: @@ composition w(i) of Fe-alloy] corresponds to the total
POLY: @@ initial amount of Fe-based alloy in the interaction,
POLY: @@ i.e., 1 gram of steel (Fe-10Cr-5Ni-1Co wt%).
POLY:
POLY: s-c B=1 w(Cr)=.10 w(Ni)=.05 w(Co)=.01
... the command in full is SET_CONDITION
POLY:
POLY: l-c
... the command in full is LIST CONDITIONS
P=100000, T=298.15, B=1, W(CR)=0.1, W(NI)=5E-2, W(CO)=1E-2
DEGREES OF FREEDOM 0
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated      39232 grid points in          1 s
Found the set of lowest grid points in      0 s
Creating a new composition set BCC_A2#2
Calculated POLY solution      1 s, total time      2 s
Creating a new composition set BCC_A2#3
POLY: l-e ,x
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium =      1, label A0 , database: PAQ2

Conditions:
P=100000, T=298.15, B=1, W(CR)=0.1, W(NI)=5E-2, W(CO)=1E-2
DEGREES OF FREEDOM 0

Temperature 298.15 K ( 25.00 C), Pressure 1.000000E+05
Number of moles of components 1.79859E-02, Mass in grams 1.000000E+00
Total Gibbs energy -1.58616E+02, Enthalpy -1.09889E+01, Volume 1.20553E-07

Component      Moles      M-Fraction Activity Potential Ref.stat
CO            1.6968E-04  9.4342E-03 4.4157E-08 -4.1983E+04 SER
CR            1.9232E-03  1.0693E-01 5.8926E-02 -7.0192E+03 SER
FE            1.5041E-02  8.3627E-01 3.7073E-02 -8.1679E+03 SER
NI            8.5193E-04  4.7367E-02 7.7089E-04 -1.7769E+04 SER

BCC_A2#3      Status ENTERED     Driving force 0.0000E+00
Moles 1.4641E-02, Mass 8.1821E-01, Volume fraction 8.5170E-01 Mole fractions:
FE 9.87131E-01 CO 1.15888E-02 NI 8.17873E-04 CR 4.61992E-04

BCC_A2#1      Status ENTERED     Driving force 0.0000E+00

```

Moles 1.9166E-03, Mass 9.9654E-02, Volume fraction 1.1495E-01 Mole fractions:
CR 9.99946E-01 FE 5.39522E-05 CO 9.25541E-12 NI 8.81026E-12

FCC_A1 Status ENTERED Driving force 0.0000E+00
Moles 1.4280E-03, Mass 8.2138E-02, Volume fraction 3.3346E-02 Mole fractions:
NI 5.88202E-01 FE 4.11792E-01 CO 5.30943E-06 CR 6.98908E-09

POLY: l-st cp
... the command in full is LIST_STATUS
*** STATUS FOR ALL COMPONENTS
COMPONENT STATUS REF. STATE T(K) P(Pa)
VA ENTERED SER
CO ENTERED SER
CR ENTERED SER
FE ENTERED SER
NI ENTERED SER
*** STATUS FOR ALL PHASES
PHASE STATUS DRIVING FORCE MOLES
FCC_A1 ENTERED 0.000000E+00 1.428010E-03
BCC_A2#3 ENTERED 0.000000E+00 1.464136E-02
BCC_A2#2 ENTERED 0.000000E+00 0.000000E+00
BCC_A2#1 ENTERED 0.000000E+00 1.916564E-03

POLY: sh b n n(*)
... the command in full is SHOW_VALUE
B=1.
N=1.7985937E-2
N(CO)=1.6968364E-4, N(CR)=1.9232249E-3, N(FE)=1.5041094E-2, N(NI)=8.5193389E-4
POLY: Hit RETURN to continue
POLY:
POLY: s-c T=1073.15
... the command in full is SET_CONDITION
POLY: l-c
... the command in full is LIST_CONDITIONS
P=100000, T=1073.15, B=1, W(CR)=0.1, W(NI)=5E-2, W(CO)=1E-2
DEGREES OF FREEDOM 0
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 39232 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY: l-e ,x
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: PAQ2
Conditions:
P=100000, T=1073.15, B=1, W(CR)=0.1, W(NI)=5E-2, W(CO)=1E-2
DEGREES OF FREEDOM 0
Temperature 1073.15 K (800.00 C), Pressure 1.000000E+05
Number of moles of components 1.79859E-02, Mass in grams 1.00000E+00
Total Gibbs energy -9.18150E+02, Enthalpy 5.59649E+02, Volume 1.23044E-07
Component Moles M-Fraction Activity Potential Ref.stat
CO 1.6968E-04 9.4342E-03 1.8364E-05 -9.7303E+04 SER
CR 1.9232E-03 1.0693E-01 3.0133E-03 -5.1794E+04 SER
FE 1.5041E-02 8.3627E-01 4.2352E-03 -4.8757E+04 SER
NI 8.5193E-04 4.7367E-02 1.1925E-04 -8.0610E+04 SER
FCC_A1 Status ENTERED Driving force 0.0000E+00
Moles 1.7986E-02, Mass 1.0000E+00, Volume fraction 1.0000E+00 Mole fractions:
FE 8.36270E-01 CR 1.06929E-01 NI 4.73667E-02 CO 9.43424E-03
POLY: l-st cp
... the command in full is LIST_STATUS
*** STATUS FOR ALL COMPONENTS
COMPONENT STATUS REF. STATE T(K) P(Pa)
VA ENTERED SER
CO ENTERED SER
CR ENTERED SER
FE ENTERED SER
NI ENTERED SER
*** STATUS FOR ALL PHASES
PHASE STATUS DRIVING FORCE MOLES
FCC_A1 ENTERED 0.000000E+00 1.798594E-02
BCC_A2#1 ENTERED -1.564120E-02 0.000000E+00
BCC_A2#3 ENTERED -1.564120E-02 0.000000E+00
BCC_A2#2 ENTERED -1.564120E-02 0.000000E+00

POLY: sh b n n(*)
... the command in full is SHOW_VALUE
B=1.
N=1.7985937E-2
N(CO)=1.6968364E-4, N(CR)=1.9232249E-3, N(FE)=1.5041094E-2, N(NI)=8.5193389E-4
POLY: @@
POLY: @@ As shown here, 1 gram of steel (Fe-10Cr-5Ni-1Co wt%)
POLY: @@ is equivalent to:
POLY: @@ n(Fe) = 1.5041094E-2
POLY: @@ n(Cr) = 1.9232249E-3
POLY: @@ n(Ni) = 8.5193389E-4
POLY: @@ n(Co) = 1.6968422E-4
POLY:
POLY: @@ Save the workspace for the Fe-Cr-Ni-Co system:
POLY: save TCEX53_b.POLY3_y
... the command in full is SAVE_WORKSPACES
POLY: Hit RETURN to continue
POLY:
POLY: @@ ======
POLY: @@ Step 3: Single-Point Calculations for Fe-Cr-Ni-Co + H2O-NaCl
POLY: @@ ======
POLY: @@ Bulk composition in the heterogeneous interaction system:
POLY: @@ b(H2O) = 1000
POLY: @@ n(NaCl) = 0.085554
POLY: @@ n(Fe) = 1.5041094E-2
POLY: @@ n(Cr) = 1.9232249E-3
POLY: @@ n(Ni) = 8.5193389E-4
POLY: @@ n(Co) = 1.6968422E-4
POLY:
POLY: @@ Retrieve data from the PAQ2 database:
POLY: go data
... the command in full is GOTO_MODULE
TDB_PAQ2: rej sys
... the command in full is REJECT
H O ZE
VA DEFINED
LIQUID:L REJECTED
GRAPHITE DIAMOND_A4 FC_ORTHORHOMBIC

FUNCTIONS

List of references for assessed data

'TCS public data set for gaseous mixture in the Fe-Co-Cr-Na-Ni-C-H-O-N-S
-Cl system.'
'TCS public data set for liquid mixture and alloy solutions in the Fe-Co
-Cr-Na-Ni-C-H-O-N-S-Cl system.'
'TCS public data set for stoichiometric solids and liquids in the Fe-Co-Cr
-Na-Ni-C-H-O-N-S-Cl system.'
'TCS Aqueous Solution Database, TCAQ2, v2.0 (2002/2003). Extracted data
only for Fe-Co-Cr-Na-Ni-C-H-O-N-S-Cl bearing aqueous solution species
from TCAQ2 which covers totally 83 elements and contains many more
aqueous solution species.'

-OK-

16:57:54,161 [Thread-0] WARN MacroProcessingContext: The handling of the excess model command is not yet supported in GES6.
16:57:54,161 [Thread-0] WARN MacroProcessingContext: The handling of the add contribution command is not yet supported in GES6.
16:57:54,162 [Thread-0] WARN MacroProcessingContext: The handling of the fraction limits command is not yet supported in GES6.

TDB_PAQ2:Hit RETURN to continue

TDB_PAQ2: @@ Define system-components and the reference states:
TDB_PAQ2: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32

POLY: d-com H2O H+1 ZE Na Cl Fe Cr Ni Co
... the command in full is DEFINE_COMPONENTS

POLY: s-r-s H2O AQUEOUS * 1e5
... the command in full is SET_REFERENCE_STATE

POLY: s-r-s ZE REF_ELE * 1e5
... the command in full is SET_REFERENCE_STATE

POLY: l-st c
... the command in full is LIST_STATUS

*** STATUS FOR ALL COMPONENTS

| COMPONENT | STATUS | REF. STATE | T (K) | P (Pa) |
|-----------|---------|---------------|-------|--------|
| VA | ENTERED | SER | | |
| H2O | ENTERED | AQUEOUS | * | 100000 |
| H+1 | ENTERED | SER | | |
| ZE | ENTERED | REF_ELECTRODE | * | 100000 |
| NA | ENTERED | SER | | |
| CL | ENTERED | SER | | |
| FE | ENTERED | SER | | |
| CR | ENTERED | SER | | |
| NI | ENTERED | SER | | |
| CO | ENTERED | SER | | |

POLY:

POLY: @@ Define some symbols (constants/variables/functions/tables):
POLY: @@ You can define some important ones e.g., RNF; pH, Eh
POLY: @@ ======
POLY: @@ Important: With the default reference state (SER) used for
POLY: @@ system-component H+1, the pH condition in aqueous solution
POLY: @@ should be defined as:
POLY: @@ pH = -log10(act(H+1,aqs)) (traditional)
POLY: @@ = -log10[acr(H+1,AQUEOUS)*55.508435] (Thermo-Calc)
POLY: @@ = -ln[acr(H+1,AQUEOUS)*55.508435]*2.302585093
POLY: @@ where
POLY: act(H+1,aqs) is molality_based activity of
POLY: H+1 species (as of the traditional concept);
POLY: acr(H+1,AQ)*AH2O is site-fraction_based activity of
POLY: H+1 species (calculated in Thermo-Calc).
POLY: @@
POLY: Such a definition not only gives correct pH values for all
POLY: thermodynamic models (SIT and HKF) but also does not affect
POLY: the calculation of ACR(H+1) [LNACR(H+1)] quantity that is
POLY: normally used as MAPPING/STEPPING variables in all modules
POLY: (POURBAIX & TDB/GESS5/POLY3/POST).
POLY: ======
POLY: @@ You can also choose to define many other symbols (for
POLY: @@ plotting) on the same scope of the POURBAIX module.
POLY:
POLY: @@ A list of valid symbols for the Fe-Cr-Ni-Co-H2O-NaCl
POLY: @@ heterogeneous interaction system on the scope same as the
POLY: @@ automatically defined symbols in the POURBAIX module can be
POLY: @@ found at the end of this MACRO file (but only as a reference).
POLY: @@ -----
POLY: @@ It is important to note that:
POLY: @@ * AH2O is always a constant, and YH2O is the site fraction
POLY: @@ of the solvent H2O, i.e.,
POLY: @@ AH2O = 55.508435
POLY: @@ YH2O = Y(AQ,H2O)
POLY:
POLY: @@ * The AYT and ART quantities are on the Site-Fraction basis:
POLY: @@ AYT for AC(i,AQ)
POLY: @@ ART for ACR(i,AQ)
POLY:
POLY: @@ * The AIT (AIi), RCT (RCi) and MLT (MLi) quantities are
POLY: @@ on the Molality basis:
POLY: @@ AIT for ACR(i,AQ)*AH2O
POLY: @@ as activity based on molality
POLY: @@ RCT for ACR(i,AQ)*YH2O/Y(AQ,i)
POLY: @@ as activity coefficient based on molality
POLY: @@ MLT for Y(AQ,i)*AH2O/YH2O
POLY: @@ as molality
POLY: @@ -----
POLY: @@ AIi = RCi * MLi
POLY: @@ = ACR(i,AQ)*YH2O/Y(AQ,i) * Y(AQ,i)*AH2O/YH2O
POLY: @@ = ACR(i,AQ)*AH2O
POLY:
POLY: @@ * It is always ACR(sp,AQ) = AC(sp,AQ)
POLY:
POLY: @@ * It is always the AIi=AIT(H+1) [=ACR(H+1,AQ)*AH2O]
POLY: @@ quantity, rather than ART(H+1) [=ACR(H+1,AQ)] quantity,
POLY: @@ that is the equivalent property for the acidity
POLY: @@ condition pH.
POLY: @@ -----
POLY: ent-sym const AH2O=55.508435
... the command in full is ENTER_SYMBOL
POLY: ent-sym const RNF =96485.309
... the command in full is ENTER_SYMBOL
POLY: ent-sym funct Eh = mur(ZE)/RNF;

```

... the command in full is ENTER_SYMBOL
POLY: ent-sym funct pH = -log10(acr(H+1,AQUEOUS)*AH2O);
... the command in full is ENTER_SYMBOL
POLY: l-sym
... the command in full is LIST_SYMBOLS
DEFINED CONSTANTS
AH2O=55.508435, RNF=96485.309
DEFINED FUNCTIONS AND VARIABLES%
EH=MUR(ZE)/RNF
PH=- LOG10(ACR(H+1,AQUEOUS)*AH2O )
POLY:
POLY: @@ Define the equilibrium conditions:
POLY: @@
POLY: @@ Define P-T and bulk composition in the interaction system
POLY: @@ for calculating starting point [at e.g pH=7 & Eh=0 (V)]:
POLY:
POLY: @@ P-T conditions:
POLY: s-c P=1e5 T=298.15
... the command in full is SET_CONDITION
POLY: @@
POLY: @@ Alternatively, it can be manually input as below:
POLY: @@ s-c P=
POLY: @@ @@Pressure_in_Pascal:

POLY: @@ s-c T=
POLY: @@ @@Temperature_In_Kelvin:
POLY:

POLY: @@ For Aqueous-involving interaction systems, it is always
POLY: @@ recommended to define 1 kg of H2O, so that it is
POLY: @@ convenient to consider molality quantities and other
POLY: @@ properties in aqueous solution.
POLY:
POLY: s-c b(H2O)=1000
... the command in full is SET_CONDITION
POLY:
POLY: @@ The following is equivalent to 0.085554 mole of NaCl
POLY: @@ in 1 kg of H2O:
POLY: s-c n(Na)=0.085554 n(Cl)=0.085554
... the command in full is SET_CONDITION
POLY:
POLY: @@ For calculating Pourbaix diagrams or other diagrams in
POLY: @@ aqueous-involving interaction system, it is important
POLY: @@ to consider the so-called "effective interaction rate".
POLY:
POLY: @@ The following is equivalent to 1 gram of specified
POLY: @@ steel (Fe-10Cr-5Ni-1Co wt%) in an effective interaction
POLY: @@ with 1 kg of H2O (dissolving 0.085554 mole of NaCl):
POLY:
POLY: s-c n(Fe)=1.5041094E-2 n(Cr)=1.9232249E-3
... the command in full is SET_CONDITION
POLY: s-c n(Ni)=8.5193389E-4 n(Co)=1.6968422E-4
... the command in full is SET_CONDITION
POLY:
POLY: @@ Let's calculate initial equilibrium at pH=7 & Eh=0 (V):
POLY: s-c lnacr(H+1)=-16.11809565 mur(ZE)=0
... the command in full is SET_CONDITION
POLY:
POLY: l-c
... the command in full is LIST_CONDITIONS
P=100000, T=298.15, B(H2O)=1000, N(NA)=8.5554E-2, N(CL)=8.5554E-2,
N(FE)=1.5041094E-2, N(CR)=1.9232249E-3, N(NI)=8.5193389E-4,
N(CO)=1.6968422E-4, LNACR(H+1)=-16.11809565, MUR(ZE)=0
DEGREES OF FREEDOM 0
POLY:
POLY: @@
POLY: @@ Turn off GLOBAL completely for aqueous calculations
POLY: @@
POLY: @@ Adv-Opt GLOBAL
POLY: @@ Use global minimization as much as possible /N/: N
POLY: @@ Use global minimization for test only? /N/: N
POLY: @@
POLY: @@
POLY: Adv-Opt GLOBAL N N !
... the command in full is ADVANCED_OPTIONS
Settings for global minimization:
POLY: @@
POLY: @@
POLY: @@ Adv-Opt EQ_CALC
POLY: @@ Force positive definite phase Hessian /Y/: N
POLY: @@ Control stepsize during minimization /Y/: Y
POLY: @@
POLY: Adv-Opt EQ_CALC N Y !
... the command in full is ADVANCED_OPTIONS
Settings for the minimization of an equilibria:
POLY:
POLY: @@
POLY: @@ Set numerical limits:
POLY: @@
POLY: @@ Notes:
POLY: @@ For equilibrium calculations (single-point, stepping or
POLY: @@ mapping) of complex aqueous-bearing heterogeneous
POLY: @@ interaction systems, it is recommended to modify the
POLY: @@ numerical limits.
POLY:
POLY: @@ The next command (changing the numerical limits from the
POLY: @@ default values "500 1E-6 1E-12 N" to "20000 1E-6 1E-20 Y")
POLY: @@ makes the following changes:
POLY: @@ 1) Changes "Maximum number of iterations" from the
POLY: @@ default 500 to 20000, which enforces 40 times more
POLY: @@ iterations for each of the calculations in order
POLY: @@ to obtain stable equilibria;
POLY: @@ 2) The "Required accuracy" remains the default value 1E-6.
POLY: @@ It can be changed to 1E-4, that allows less accurate
POLY: @@ calculations but makes it easier/faster to converge;
POLY: @@ 3) Changes "Smallest fraction" from the default site
POLY: @@ fraction of 1E-12 to 1E-20, which is more suitable
POLY: @@ for aqueous solution phases; and
POLY: @@ 4) The "Approximate driving force for metastable phases"
POLY: @@ is changed from the default of "N" to "Y" (meaning
POLY: @@ it should always approximately calculate driving

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POLY: @@ forces for metastable phases).
POLY:
POLY: @@ These changes in the numerical limits are essential and
POLY: @@ useful for making sure of finding a converged solution of
POLY: @@ stable equilibria, especially when the heterogeneous
POLY: @@ interaction system becomes more complicated.
POLY: @@
POLY: s-n-l 20000 1e-6 1e-20 Y
... the command in full is SET_NUMERICAL_LIMITS
LIMITATIONS of the present version of Thermo-Calc
Max number of elements : 80
Max number of species : 5000
Max number of sublattices in a phase : 10
Max number of constituents in a phase: : 200
Max number of constituents in an ideal phase :5000
POLY:
POLY:
POLY: @@ Calculate an equilibrium with only AQUEOUS:
POLY: c-st p *sus
... the command in full is CHANGE_STATUS
POLY: c-st p AQUEOUS=ent 55.8
... the command in full is CHANGE_STATUS
POLY: l-st p
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES
PHASE STATUS DRIVING FORCE MOLES
AQUEOUS ENTERED 0.000000E+00 6.138000E+03
SUSPENDED PHASES:
WUSTITE REF,ELECTRODE NIO_S2 NIO_S1 NIOOH NIO2H2 NIIF2O4 NICR2O4 NAOH_S2
NAOH_S1 NAO2 NA2O_S3 NA2O_S2 NA2O_S1 NA2O2_S2 NA2O2_S1 NA2FEO2 NA2CRO4_S2
NA2CRO4_S1 NA2CR2O4 MAGNETITE HEMATITE HALITE FEOOH FEO3H3 FEO2H2 FECR2O4
FE2O3_GAMMA FE2O2O2H2 FCC_A1 CRO3 CRO2 CR8O21 CR5O12 CR2O3 COO_S COO2H2
COFE2O4 COCR2O4 CO3O4 BCC_A2 GAS
POLY: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Global equilibrium calculation turned off, you can turn it on with
ADVANCED_OPTIONS GLOBAL_MINIMIZATION Y,,,
109 IT$ , CPU TIME USED 0 SECONDS
POLY: l-e ,x
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: PAQ2

Conditions:
P=100000, T=298.15, B(H2O)=1000, N(NA)=8.5554E-2, N(CL)=8.5554E-2,
N(FE)=1.5041094E-2, N(CR)=1.9232249E-3, N(NI)=8.5193389E-4,
N(CO)=1.6968422E-4, LNACR(H+1)=-16.11809565, MUR(ZE)=0
DEGREES OF FREEDOM 0

Temperature 298.15 K ( 25.00 C), Pressure 1.000000E+05
Number of moles of components 5.57254E+01, Mass in grams 1.00599E+03
Total Gibbs energy -1.70641E+07, Enthalpy -1.59024E+07, Volume -4.21624E-08

Component Moles M-Fraction Activity Potential Ref.stat
H2O 5.5508E+01 9.9611E-01 9.9606E-01 -9.7846E+00 AQUEOUS
H+1 -1.0027E-02 -1.7993E-04 1.0000E-07 -3.9956E+04 SER
ZE 3.7895E-02 6.8003E-04 1.0000E+00 0.0000E+00 REF_ELEC
NA 8.5554E-02 1.5353E-03 1.5211E-50 -2.8436E+05 SER
CL 8.5554E-02 1.5353E-03 1.1822E-30 -1.7083E+05 SER
FE 1.5041E-02 2.6991E-04 1.2285E-18 -1.0223E+05 SER
CR 1.9232E-03 3.4513E-05 1.6596E-45 -2.5561E+05 SER
NI 8.5193E-04 1.5288E-05 6.0058E-14 -7.5468E+04 SER
CO 1.6968E-04 3.0450E-06 3.2708E-16 -8.8391E+04 SER

AQUEOUS Status ENTERED Driving force 0.0000E+00
Moles 5.5725E+01, Mass 1.0060E+03, Volume fraction 1.0000E+00 Mole fractions:
H2O 9.96107E-01 ZE 6.80033E-04 NI 1.52881E-05
CL 1.53528E-03 FE 2.69915E-04 CO 3.04501E-06
NA 1.53528E-03 CR 3.45125E-05 H+1 -1.79930E-04
Constitution: SiteFraction Molality Activity log10Act
H2O 9.96604E-01 5.55084E+01 9.96157E-01 -0.0017
NA+1 1.53628E-03 8.55668E+02 6.59591E-02 -1.1807
CL-1 1.53628E-03 8.55668E+02 6.59412E-02 -1.1808
FE+2 1.56791E-04 8.73285E-03 3.08751E-03 -2.5104
FEOH+1 1.13299E-04 6.31049E-03 4.86919E-03 -2.3125
CRO+1 3.00740E-05 1.67505E-03 1.29247E-03 -2.8886
NI+2 1.52852E-05 8.51348E-04 3.02381E-04 -3.5194
CROH+2 3.38456E-06 1.88512E-04 6.68399E-05 -4.1750
CO+2 3.04698E-06 1.69710E-04 6.02711E-05 -4.2199
HCR02 1.05903E-06 5.89856E-05 5.89799E-05 -4.2293
NIOH+1 1.28111E-08 7.13548E-07 5.50574E-07 -6.2592
CR+3 1.12056E-08 6.24122E-07 6.07385E-08 -7.2165
CRO-1 6.16631E-09 3.43448E-07 2.65005E-07 -6.5767
OH-1 2.33522E-09 1.30066E-07 1.00231E-07 -6.9990
H+1 2.32641E-09 1.29576E-07 1.00000E-07 -7.0000
FEOH+2 1.10316E-12 6.14435E-11 2.17858E-11 -10.6618
CR+2 1.47493E-16 8.21498E-15 2.91275E-15 -14.5357
FE+3 6.69156E-17 3.72704E-15 3.61605E-16 -15.4418
FECL+2 3.43228E-17 1.91170E-15 6.77823E-16 -15.1689
H2 1.06276E-19 5.91933E-18 5.91876E-18 -17.2278
FE2O2H2+4 2.32944E-20 1.29744E-18 2.05117E-20 -19.6880
O2 1.00000E-20 0.00000E+00 2.17014E-58 -57.6635
FEO3H3-1 1.00000E-20 0.00000E+00 4.15261E-44 -43.3817
H2O2 1.00000E-20 0.00000E+00 3.35251E-46 -45.4746
CRO-4 1.00000E-20 0.00000E+00 1.67197E-26 -25.7768
HClO 1.00000E-20 0.00000E+00 2.78756E-45 -44.5548
HClO2 1.00000E-20 0.00000E+00 1.00400E-87 -86.9983
CR2O7-2 1.00000E-20 0.00000E+00 9.28118E-52 -51.0324
HCrO4-1 1.00000E-20 0.00000E+00 5.05292E-27 -26.2965
HO2-1 1.00000E-20 0.00000E+00 7.09471E-51 -50.1491
CO1H2O2 1.00000E-20 0.00000E+00 5.9656E-101 -100.2243
CO+3 1.00000E-20 0.00000E+00 7.96270E-38 -37.0989
O3 1.00000E-20 0.00000E+00 2.0444E-113 -112.6894
ClO4-1 1.00000E-20 0.00000E+00 5.44300E-133 -132.2642
ClO3-1 1.00000E-20 0.00000E+00 1.0463E-105 -104.9803
ClO2-1 1.00000E-20 0.00000E+00 1.05079E-82 -81.9785
ClO2 1.00000E-20 0.00000E+00 1.1394E-100 -99.9433
ClO-1 1.00000E-20 0.00000E+00 6.04311E-46 -45.2187
Cl2 1.00000E-20 0.00000E+00 3.87204E-50 -49.4121
Solution Properties: pH = 7.0000 Eh = 0.0000 V I = 0.1094
pe = 0.0000 Ah = 0.0000 kJ m* = 0.1891
Aw = 0.9962 Os = 1.1300 pKw = 13.9973
At1= 1.00000E-20 At2= 1.3007E-07 (equiv_mol/kg_H2O)
POLY: l-st p
... the command in full is LIST_STATUS

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*** STATUS FOR ALL PHASES
PHASE           STATUS      DRIVING FORCE    MOLES
AQUEOUS        ENTERED     0.000000E+00   5.572540E+01
SUSPENDED PHASES:
WUSTITE REF_ELECTRODE NIO_S2 NIO_S1 NIOOH NIO2H2 NIFE2O4 NICR2O4 NAOH_S2
NAOH_S1 NAO2_NAO2_S3 NA2O_S2 NA2O_S1 NA2O2_S2 NA2O2_S1 NA2FE02 NA2CRO4_S2
NA2CRO4_S1 NA2CR2O4 MAGNETITE HEMATITE HALITE FEOOH FEO3H3 FE02H2 FECR2O4
FE2O3_GAMMA FE2O2O2H2 FCC_A1 CRO3 CRO2 CR8021 CR5012 CR2O3 COO_S COO2H2
COFE2O4 COCR2O4 CO3O4 BCC_A2 GAS
POLY: sh b n n(*)  

... the command in full is SHOW_VALUE
B=1005.9899
N=55.725397
N(H2O)=55.508435, N(H+1)=-1.0026646E-2, N(ZE)=3.7895099E-2, N(NA)=8.5554E-2,
N(CL)=8.5554E-2, N(FE)=1.5041094E-2, N(CR)=1.9232249E-3,
N(NI)=8.5193389E-4, N(CO)=1.6968422E-4
POLY:Hit RETURN to continue
POLY:  

POLY: @@ Calculate an equilibrium with all phases (except for REF_ELE):
POLY:  

POLY: c-st p *=ent 0  

... the command in full is CHANGE_STATUS
POLY: c-st p AQUEOUS=ent 55.8
... the command in full is CHANGE_STATUS
POLY: @@ Always set the REF_ELECTRODE phase as SUSPENDED:
POLY: c-st p REF_ELE=sus
... the command in full is CHANGE_STATUS
POLY: l-st p  

... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES
PHASE           STATUS      DRIVING FORCE    MOLES
WUSTITE        ENTERED     0.000000E+00   0.000000E+00
NIO_S2          ENTERED     0.000000E+00   0.000000E+00
NIO_S1          ENTERED     0.000000E+00   0.000000E+00
NIOOH           ENTERED     0.000000E+00   0.000000E+00
NIO2H2          ENTERED     0.000000E+00   0.000000E+00
NIFE2O4         ENTERED     0.000000E+00   0.000000E+00
NICR2O4         ENTERED     0.000000E+00   0.000000E+00
NAOH_S2         ENTERED     0.000000E+00   0.000000E+00
NAOH_S1         ENTERED     0.000000E+00   0.000000E+00
NAO2             ENTERED     0.000000E+00   0.000000E+00
NA2O_S3          ENTERED     0.000000E+00   0.000000E+00
NA2O_S2          ENTERED     0.000000E+00   0.000000E+00
NA2O_S1          ENTERED     0.000000E+00   0.000000E+00
NA2O2_S2         ENTERED     0.000000E+00   0.000000E+00
NA2O2_S1         ENTERED     0.000000E+00   0.000000E+00
NA2FE02          ENTERED     0.000000E+00   0.000000E+00
NA2CRO4_S2       ENTERED     0.000000E+00   0.000000E+00
NA2CRO4_S1       ENTERED     0.000000E+00   0.000000E+00
NA2CR2O4         ENTERED     0.000000E+00   0.000000E+00
MAGNETITE        ENTERED     0.000000E+00   0.000000E+00
HEMATITE         ENTERED     0.000000E+00   0.000000E+00
HALITE            ENTERED     0.000000E+00   0.000000E+00
FEOOH             ENTERED     0.000000E+00   0.000000E+00
FEO3H3            ENTERED     0.000000E+00   0.000000E+00
FE02H2            ENTERED     0.000000E+00   0.000000E+00
FECR2O4           ENTERED     0.000000E+00   0.000000E+00
FE2O3_GAMMA       ENTERED     0.000000E+00   0.000000E+00
FE2O2O2H2         ENTERED     0.000000E+00   0.000000E+00
FCC_A1            ENTERED     0.000000E+00   0.000000E+00
CRO3              ENTERED     0.000000E+00   0.000000E+00
CRO2              ENTERED     0.000000E+00   0.000000E+00
CR8021            ENTERED     0.000000E+00   0.000000E+00
CR5012            ENTERED     0.000000E+00   0.000000E+00
CR2O3              ENTERED     0.000000E+00   0.000000E+00
COO_S              ENTERED     0.000000E+00   0.000000E+00
COO2H2            ENTERED     0.000000E+00   0.000000E+00
COFE2O4           ENTERED     0.000000E+00   0.000000E+00
COCR2O4           ENTERED     0.000000E+00   0.000000E+00
CO3O4              ENTERED     0.000000E+00   0.000000E+00
BCC_A2              ENTERED     0.000000E+00   0.000000E+00
AQUEOUS            ENTERED     0.000000E+00   5.583623E+01
GAS                ENTERED     0.000000E+00   0.000000E+00
SUSPENDED PHASES:
REF_ELECTRODE
POLY: c-e  

... the command in full is COMPUTE_EQUILIBRIUM
 78 ITS, CPU TIME USED 1 SECONDS
POLY: l-e ,x  

... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: PAQ2

Conditions:
P=100000, T=298.15, B(H2O)=1000, N(NA)=8.5554E-2, N(CL)=8.5554E-2,
N(FE)=1.5041094E-2, N(CR)=1.9232249E-3, N(NI)=8.5193389E-4,
N(CO)=1.6968422E-4, LNACR(H+1)=-16.11809565, MUR(ZE)=0
DEGREES OF FREEDOM 0

Temperature 298.15 K ( 25.00 C), Pressure 1.000000E+05
Number of moles of components 5.56976E+01, Mass in grams 1.00595E+03
Total Gibbs energy -1.70627E+07, Enthalpy -1.59010E+07, Volume -3.10120E-16

Component      Moles      M-Fraction Activity Potential Ref.stat
H2O            5.5508E+01  9.9660E-01  9.9654E-01 -8.5924E+00 AQUEOUS
H+1            -5.2910E-02 -9.4995E-04  1.0000E-07 -3.9956E+04 SER
ZE             5.2936E-02  9.5042E-04  1.0000E+00 -4.4035E-12 REF_ELEC
NA             8.5554E-02  1.5360E-03  1.5537E-50 -2.8431E+05 SER
CL             8.5554E-02  1.5360E-03  1.2078E-30 -1.7077E+05 SER
FE             1.5041E-02  2.7005E-04  5.2232E-26 -1.4431E+05 SER
CR             1.9232E-03  3.4530E-05  1.2572E-53 -3.0196E+05 SER
NI             8.5193E-04  1.5296E-05  1.0073E-15 -8.5603E+04 SER
CO             1.6968E-04  3.0465E-06  1.5331E-20 -1.1310E+05 SER

AQUEOUS          Status ENTERED      Driving force 0.0000E+00
Moles 5.5653E+01, Mass 1.0045E+03, Volume fraction 1.0000E+00 Mole fractions:
H2O  9.96925E-01 ZE  4.72606E-07 FE  1.08577E-11
CL  1.53727E-03 NI  2.36161E-07 CR  2.55062E-13
NA  1.53727E-03 CO  1.31447E-10 H+1 -2.25543E-10
Constitution: SiteFraction Molality Activity log10Act
H2O  9.96925E-01  5.55084E+01  9.96603E-01  -0.0015
CL-1 1.53727E-03  8.55948E-02  6.73703E-02  -1.1715
NA+1 1.53727E-03  8.55948E-02  6.73703E-02  -1.1715
NI+2 2.35950E-07  1.31376E-05  5.07139E-06  -5.2949
OH-1 2.28889E-09  1.27444E-07  1.00279E-07  -6.9988
H+1 2.27916E-09  1.26903E-07  1.00000E-07  -7.0000
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NIOH+1      2.10599E-10   1.17261E-08   9.23842E-09   -8.0344
CO+2        1.31447E-10   7.31890E-09   2.82496E-09   -8.5490
FE+2        6.13590E-12    3.41645E-10   1.31278E-10   -9.8818
FEOH+1      4.72178E-12    2.62907E-10   2.07132E-10   -9.6838
CRO+1       2.23303E-13    1.24334E-11   9.79571E-12   -11.0090
CROH+2     2.36100E-14    1.31459E-12   5.06585E-13   -12.2953
HCRO2       8.03267E-15    4.47256E-13   4.47228E-13   -12.3495
CR+3        7.04094E-17    3.92037E-15   4.60120E-16   -15.3371
CRO2-1     4.58077E-17    2.55056E-15   2.00946E-15   -14.6969
H2          1.06307E-19    5.91913E-18   5.91876E-18   -17.2278
FEOH+2      4.31923E-20    2.40493E-18   9.26752E-19   -18.0330
O3          1.00000E-20    0.00000E+00   2.0474E-113   -112.6888
FEO3H3-1   1.00000E-20    0.00000E+00   1.76819E-51   -50.7525
FECI+2      1.00000E-20    0.00000E+00   2.94449E-23   -22.5310
FE2O2H2+4  1.00000E-20    0.00000E+00   3.71178E-35   -34.4304
FE+3        1.00000E-20    0.00000E+00   1.53750E-23   -22.8132
H2O2        1.00000E-20    0.00000E+00   3.35574E-46   -45.4742
HCLO        1.00000E-20    0.00000E+00   2.84935E-45   -44.5453
CRO4-2      1.00000E-20    0.00000E+00   1.26903E-34   -33.8965
HCLO2       1.00000E-20    0.00000E+00   1.02675E-87   -86.9885
HCRO4-1    1.00000E-20    0.00000E+00   3.83517E-35   -34.4162
CR207-2    1.00000E-20    0.00000E+00   5.34416E-68   -67.2721
HO2-1       1.00000E-20    0.00000E+00   7.10153E-51   -50.1486
CR+2        1.00000E-20    0.00000E+00   2.20654E-23   -22.6563
CO1H2O2    1.00000E-20    0.00000E+00   2.7988E-105   -104.5530
CO+3        1.00000E-20    0.00000E+00   3.73219E-42   -41.4280
O2          1.00000E-20    0.00000E+00   2.17223E-58   -57.6631
CL04-1      1.00000E-20    0.00000E+00   5.57317E-133  -132.2540
CL03-1      1.00000E-20    0.00000E+00   1.0705E-105   -104.9704
CL02-1      1.00000E-20    0.00000E+00   1.07460E-82   -81.9688
CL02        1.00000E-20    0.00000E+00   1.1652E-100   -99.9336
CL0-1       1.00000E-20    0.00000E+00   6.17706E-46   -45.2092
CL2         1.00000E-20    0.00000E+00   4.04170E-50   -49.3934
Solution Properties: pH = 7.0000 Eh = -0.0000 V I = 0.0856
                     pe = -0.0000 Ah = -0.0000 kJ m* = 0.1712
                     Aw = 0.9966 Os = 1.1033 pKw = 13.9973
                     At1= 1.00000E-20 At2= 1.2744E-07 (equiv_mol/kg_H2O)

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HEMATITE      Status ENTERED   Driving force 0.0000E+00
Moles 3.3409E-02, Mass 1.0670E+00, Volume fraction 0.0000E+00 Mole fractions:
ZE 1.20000E+00 NI 0.00000E+00 NA 0.00000E+00
H2O 6.00000E-01 CR 0.00000E+00 CO 0.00000E+00
FE 4.00000E-01 CL 0.00000E+00 H+1 -1.20000E+00

```

```

NIFE204      Status ENTERED   Driving force 0.0000E+00
Moles 5.8715E-03, Mass 1.9660E-01, Volume fraction 0.0000E+00 Mole fractions:
ZE 1.14286E+00 NI 1.42857E-01 NA 0.00000E+00
H2O 5.71429E-01 CR 0.00000E+00 CO 0.00000E+00
FE 2.85714E-01 CL 0.00000E+00 H+1 -1.14286E+00

```

```

CR203      Status ENTERED   Driving force 0.0000E+00
Moles 3.9597E-03, Mass 1.2037E-01, Volume fraction 0.0000E+00 Mole fractions:
ZE 1.20000E+00 NI 0.00000E+00 NA 0.00000E+00
H2O 6.00000E-01 FE 0.00000E+00 CO 0.00000E+00
CR 4.00000E-01 CL 0.00000E+00 H+1 -1.20000E+00

```

```

COCR204      Status ENTERED   Driving force 0.0000E+00
Moles 1.1877E-03, Mass 3.8504E-02, Volume fraction 0.0000E+00 Mole fractions:
ZE 1.14286E+00 CO 1.42857E-01 NA 0.00000E+00
H2O 5.71429E-01 NI 0.00000E+00 FE 0.00000E+00
CR 2.85714E-01 CL 0.00000E+00 H+1 -1.14286E+00

```

POLY: 1-st p
... the command in full is LIST_STATUS

*** STATUS FOR ALL PHASES

| PHASE | STATUS | DRIVING FORCE | MOLES |
|-------------|---------|---------------|--------------|
| NIFE204 | ENTERED | 0.000000E+00 | 5.871536E-03 |
| HEMATITE | ENTERED | 0.000000E+00 | 3.340878E-02 |
| CR203 | ENTERED | 0.000000E+00 | 3.959678E-03 |
| COCR204 | ENTERED | 0.000000E+00 | 1.187738E-03 |
| AQUEOUS | ENTERED | 0.000000E+00 | 5.565313E+01 |
| FECR204 | ENTERED | -1.007600E-01 | 0.000000E+00 |
| FE2O2O2H2 | ENTERED | -1.872978E-01 | 0.000000E+00 |
| FEOH | ENTERED | -2.260402E-01 | 0.000000E+00 |
| COFE204 | ENTERED | -8.149192E-01 | 0.000000E+00 |
| FEO3H3 | ENTERED | -1.157510E+00 | 0.000000E+00 |
| NICR204 | ENTERED | -1.415362E+00 | 0.000000E+00 |
| FE2O3_GAMMA | ENTERED | -1.461433E+00 | 0.000000E+00 |
| MAGNETITE | ENTERED | -1.556302E+00 | 0.000000E+00 |
| NIO2H2 | ENTERED | -3.146330E+00 | 0.000000E+00 |
| NIO_S1 | ENTERED | -4.159999E+00 | 0.000000E+00 |

ENTERED PHASES WITH DRIVING FORCE LESS THAN -4.169527E+00

NIO_S2 HALITE COO2H2 FEO2H2 NA2CR2O4 NA2FE02 CO3O4 WUSTITE COO_S CRO2
NA2CRO4_S1 NA2CRO4_S2 NIOOH CR5O12 NAOH_S1 NAOH_S2 CR8O21 CRO3 GAS NA2O2_S1
NA2O2_S2 NA2O_S1 NA2O_S2 NA2O_S3 NAO2 FCC_A1 BCC_A2

SUSPENDED PHASES:

REF ELECTRODE

POLY: sh b n n(*)
... the command in full is SHOW_VALUE

B=1005.9467

N=55.697555

N(H2O)=55.508435, N(H+1)=-5.2909903E-2, N(ZE)=5.2936192E-2, N(NA)=8.5554E-2,
N(CL)=8.5554E-2, N(FE)=1.5041094E-2, N(CR)=1.9232249E-3,
N(NI)=8.5193389E-4, N(CO)=1.6968422E-4

POLY:

POLY: @@ Save the workspace for the single-point equilibrium

POLY: @@ of the Fe-Cr-Ni-Co + H2O-NaCl system:

POLY:

POLY: save TCEX53_c.POLY3 y

... the command in full is SAVE_WORKSPACES

POLY:Hit RETURN to continue

POLY:

POLY: @@ =====

POLY: @@ Step 4: Pourbaix Diagram Mapping for Fe-Cr-Ni-Co + H2O-NaCl

POLY: @@ =====

POLY:

POLY: @@ Define the mapping variables for Pourbaix diagram:

POLY: @@ pH from 0 to 14

POLY: @@ Eh from -1.2 to 1.5 (V)

POLY: s-a-v 1 lnacr(H+1) -32.22994 0 0.5

... the command in full is SET_AXIS_VARIABLE

POLY: s-a-v 2 mur(Ze) -150000 200000 5000

... the command in full is SET_AXIS_VARIABLE

POLY: l-a-v

... the command in full is LIST_AXIS_VARIABLE

Axis No 1: LNACR(H+1) Min: -32.22994 Max: 0 Inc: 0.5

Axis No 2: MUR(ZE) Min: -150000 Max: 200000 Inc: 5000

POLY:

POLY: @@ Add the starting points as initial equilibria:
 POLY: @@ These may be enforced in 2 or 4 directions with
 POLY: @@ the option >
 POLY:
 POLY: add 1>
 ... the command in full is ADD_INITIAL_EQUILIBRIUM
 POLY: add -1>
 ... the command in full is ADD_INITIAL_EQUILIBRIUM
 POLY: add 2>
 ... the command in full is ADD_INITIAL_EQUILIBRIUM
 POLY: add -2>
 ... the command in full is ADD_INITIAL_EQUILIBRIUM
 POLY: @@ You can have more starting points at other pH-Eh
 POLY: @@ conditions [corresponding to varied lnacr(H+1)
 POLY: @@ and mur(Ze) values], and add them as initial equilibria.
 POLY: @@ s-c lnacr(H+1)=-23.0
 POLY: @@ s-c mur(ZE)=-2000
 POLY: @@ l-c
 POLY: @@ c-e
 POLY: @@ l-e ,x
 POLY:
 POLY: li-in-eq
 ... the command in full is LIST_INITIAL_EQUILIBRIA

No 1 +1> P=100000, T=298.15, B(H₂O)=1000., N(NA)=8.5554E-2, N(CL)=8.5554E-2,
 N(FE)=1.5041094E-2, N(CR)=1.9232249E-3, N(NI)=8.5193389E-4,
 N(CO)=1.6968422E-4, LNACR(H+1)=-16.118096, MUR(ZE)=-4.4035374E-12

No 2 -1> P=100000, T=298.15, B(H₂O)=1000., N(NA)=8.5554E-2, N(CL)=8.5554E-2,
 N(FE)=1.5041094E-2, N(CR)=1.9232249E-3, N(NI)=8.5193389E-4,
 N(CO)=1.6968422E-4, LNACR(H+1)=-16.118096, MUR(ZE)=-4.4035374E-12

No 3 +2> P=100000, T=298.15, B(H₂O)=1000., N(NA)=8.5554E-2, N(CL)=8.5554E-2,
 N(FE)=1.5041094E-2, N(CR)=1.9232249E-3, N(NI)=8.5193389E-4,
 N(CO)=1.6968422E-4, LNACR(H+1)=-16.118096, MUR(ZE)=-4.4035374E-12

No 4 -2> P=100000, T=298.15, B(H₂O)=1000, N(NA)=8.5554E-2, N(CL)=8.5554E-2,
 N(FE)=1.5041094E-2, N(CR)=1.9232249E-3, N(NI)=8.5193389E-4,
 N(CO)=1.6968422E-4, LNACR(H+1)=-16.118096, MUR(ZE)=-4.4035374E-12

POLY:
 POLY: @@ Save the workspace for the Pourbaix diagram settings
 POLY: @@ of the Fe-Cr-Ni-Co + H₂O-NaCl system:
 POLY: save TCEX53.d.POLY3 y
 ... the command in full is SAVE_WORKSPACES
POLY:Hit RETURN to continue
POLY:
 POLY: @@ Perform the mapping calculation:
 POLY: @@ -----
 POLY: @@ Due to the complexity of the aqueous solution model (SIT),
 POLY: @@ a complete mapping calculation of the Pourbaix diagram
 POLY: @@ may take a long time. Be patient...
 POLY: @@ -----
 POLY: MAP
 Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Tie-lines not in the plane of calculation
 Generating start point 1
 Generating start point 2
 Generating start point 3
 Generating start point 4
 Generating start point 5
 Generating start point 6
 Generating start point 7
 Generating start point 8
 Generating start point 9
 Generating start point 10
 Working hard
 Generating start point 11
 Generating start point 12

Phase region boundary 1 at: -1.541E+01 -4.404E-12
 AQUEOUS
 COCR2O4
 CR2O3
 ** FECR2O4
 HEMATITE
 NIFE2O4
 Calculated.. 35 equilibria
 Terminating at axis limit.

Phase region boundary 2 at: -3.223E+01 -4.165E+04
 AQUEOUS
 COCR2O4
 CR2O3
 ** FECR2O4
 HEMATITE
 NIFE2O4
 Calculated. 38 equilibria

Phase region boundary 3 at: -1.404E+01 3.415E+03
 AQUEOUS
 COCR2O4
 CR2O3
 ** FECR2O4
 HEMATITE
 ** NIFE2O4
 Calculated. 7 equilibria

Phase region boundary 4 at: -1.404E+01 3.415E+03
 AQUEOUS
 COCR2O4
 CR2O3
 ** FECR2O4
 HEMATITE
 Calculated. 7 equilibria

Phase region boundary 5 at: -1.110E+01 1.070E+04
 AQUEOUS
 ** COCR2O4
 CR2O3
 ** FECR2O4
 HEMATITE

```

Phase region boundary  6 at: -1.110E+01  1.070E+04
    AQUEOUS
    CR2O3
    ** FECR2O4
    HEMATITE
Calculated.          8 equilibria

Phase region boundary  7 at: -7.729E+00  1.905E+04
    AQUEOUS
    CR2O3
    ** FECR2O4
    ** HEMATITE

Phase region boundary  8 at: -7.729E+00  1.905E+04
    AQUEOUS
    CR2O3
    ** FECR2O4
Calculated.          9 equilibria

Phase region boundary  9 at: -7.729E+00 -1.955E+04
    ** GAS
    AQUEOUS
    CR2O3
    ** FECR2O4

Phase region boundary 10 at: -7.729E+00 -1.955E+04
    GAS
    AQUEOUS
    CR2O3
    ** FECR2O4
Calculated.          3 equilibria

Phase region boundary 11 at: -7.169E+00 -1.817E+04
    GAS
    AQUEOUS
    ** CR2O3
    ** FECR2O4

Phase region boundary 12 at: -7.169E+00 -1.817E+04
    GAS
    AQUEOUS
    ** FECR2O4
Calculated.          44 equilibria

Phase region boundary 13 at: -7.169E+00 -1.817E+04
    GAS
    AQUEOUS
    ** CR2O3
Calculated.          2 equilibria

Phase region boundary 14 at: -7.259E+00 -1.839E+04
    ** GAS
    AQUEOUS
    ** CR2O3

Phase region boundary 15 at: -7.259E+00 -1.839E+04
    AQUEOUS
    ** CR2O3
Calculated.          10 equilibria

Phase region boundary 16 at: -7.259E+00  2.259E+04
    AQUEOUS
    ** CR2O3
    ** HEMATITE

Phase region boundary 17 at: -7.259E+00  2.259E+04
    AQUEOUS
    ** CR2O3
    HEMATITE
Calculated.          32 equilibria

Phase region boundary 18 at: -1.110E+01  7.654E+04
    AQUEOUS
    ** COCR2O4
    ** CR2O3
    HEMATITE

Phase region boundary 19 at: -1.110E+01  7.654E+04
    AQUEOUS
    COCR2O4
    ** CR2O3
    HEMATITE
Calculated.          7 equilibria

Phase region boundary 20 at: -1.404E+01  6.628E+04
    AQUEOUS
    COCR2O4
    ** CR2O3
    HEMATITE
    ** NIFE2O4

Phase region boundary 21 at: -1.404E+01  6.628E+04
    AQUEOUS
    COCR2O4
    ** CR2O3
    HEMATITE
    NIFE2O4
Calculated..         38 equilibria
Terminating at axis limit.

Phase region boundary 22 at: -1.404E+01  6.628E+04
    AQUEOUS
    COCR2O4
    HEMATITE
    ** NIFE2O4
Calculated.          1 equilibria

Phase region boundary 23 at: -1.404E+01  6.733E+04
    AQUEOUS
    ** CO3O4
    COCR2O4
    HEMATITE
    ** NIFE2O4

Phase region boundary 24 at: -1.404E+01  6.733E+04
    AQUEOUS

```

```

CO3O4
COCR2O4
HEMATITE
** NIFE2O4
Calculated.          2 equilibria

Phase region boundary 25 at: -1.404E+01 6.745E+04
    AQUEOUS
    CO3O4
    ** COCR2O4
    HEMATITE
    ** NIFE2O4

Phase region boundary 26 at: -1.404E+01 6.745E+04
    AQUEOUS
    CO3O4
    HEMATITE
    ** NIFE2O4
Calculated.          5 equilibria

Phase region boundary 27 at: -1.404E+01 8.332E+04
    ** GAS
    AQUEOUS
    CO3O4
    HEMATITE
    ** NIFE2O4

Phase region boundary 28 at: -1.404E+01 8.332E+04
    GAS
    AQUEOUS
    CO3O4
    HEMATITE
    ** NIFE2O4
Calculated.          11 equilibria

Phase region boundary 29 at: -1.257E+01 8.794E+04
    GAS
    AQUEOUS
    CO3O4
    ** HALITE
    HEMATITE
    ** NIFE2O4

Phase region boundary 30 at: -1.257E+01 8.794E+04
    GAS
    AQUEOUS
    CO3O4
    HALITE
    HEMATITE
    ** NIFE2O4
Calculated.          33 equilibria

Phase region boundary 31 at: -1.257E+01 8.794E+04
    GAS
    AQUEOUS
    CO3O4
    ** HALITE
    HEMATITE
Calculated.          9 equilibria

Phase region boundary 32 at: -8.749E+00 9.740E+04
    GAS
    AQUEOUS
    ** CO3O4
    ** HALITE
    HEMATITE

Phase region boundary 33 at: -8.749E+00 9.740E+04
    GAS
    AQUEOUS
    ** HALITE
    HEMATITE
Calculated.          18 equilibria

Phase region boundary 34 at: -1.463E+00 1.159E+05
    GAS
    AQUEOUS
    ** HALITE
    ** HEMATITE

Phase region boundary 35 at: -1.463E+00 1.159E+05
    GAS
    AQUEOUS
    ** HALITE
Calculated.          47 equilibria

Phase region boundary 36 at: -1.463E+00 1.159E+05
    GAS
    AQUEOUS
    ** HEMATITE
Calculated.          5 equilibria

Phase region boundary 37 at: -1.463E+00 1.159E+05
    GAS
    AQUEOUS
    HALITE
    ** HEMATITE
Calculated.          27 equilibria

Phase region boundary 38 at: -8.749E+00 9.740E+04
    GAS
    AQUEOUS
    ** CO3O4
    HEMATITE
Calculated.          8 equilibria

Phase region boundary 39 at: -1.021E+01 9.281E+04
    ** GAS
    AQUEOUS
    ** CO3O4
    HEMATITE

Phase region boundary 40 at: -1.021E+01 9.281E+04
    AQUEOUS
    ** CO3O4
    HEMATITE

```

Calculated. 5 equilibria
 Phase region boundary 41 at: -1.211E+01 7.398E+04
 AQUEOUS
 ** CO3O4
 ** COCR2O4
 HEMATITE
 Phase region boundary 42 at: -1.211E+01 7.398E+04
 AQUEOUS
 ** CO3O4
 COCR2O4
 HEMATITE
 Calculated. 5 equilibria
 Terminating at known equilibrium
 Phase region boundary 43 at: -1.211E+01 7.398E+04
 AQUEOUS
 CO3O4
 ** COCR2O4
 HEMATITE
 Calculated. 4 equilibria
 Terminating at known equilibrium
 Phase region boundary 44 at: -1.211E+01 7.398E+04
 AQUEOUS
 CO3O4
 ** COCR2O4
 HEMATITE
 Calculated. 5 equilibria
 Terminating at known equilibrium
 Phase region boundary 45 at: -1.021E+01 9.281E+04
 ** GAS
 AQUEOUS
 HEMATITE
 Calculated. 20 equilibria
 Phase region boundary 46 at: -1.208E+00 1.151E+05
 ** GAS
 AQUEOUS
 ** HEMATITE
 Calculated.. 4 equilibria
 Terminating at axis limit.
 Phase region boundary 48 at: -1.208E+00 1.151E+05
 AQUEOUS
 ** HEMATITE
 Calculated. 28 equilibria
 Terminating at known equilibrium
 Phase region boundary 49 at: -1.208E+00 1.151E+05
 GAS
 AQUEOUS
 ** HEMATITE
 Calculated 14 equilibria
 Phase region boundary 50 at: -1.021E+01 9.281E+04
 ** GAS
 AQUEOUS
 CO3O4
 HEMATITE
 Calculated. 9 equilibria
 Terminating at known equilibrium
 Phase region boundary 51 at: -8.749E+00 9.740E+04
 GAS
 AQUEOUS
 ** CO3O4
 HALITE
 HEMATITE
 Calculated 39 equilibria
 Phase region boundary 52 at: -1.257E+01 8.794E+04
 GAS
 AQUEOUS
 CO3O4
 ** HALITE
 HEMATITE
 NIFE2O4
 Calculated.. 41 equilibria
 Terminating at axis limit.
 Phase region boundary 53 at: -1.404E+01 8.332E+04
 ** GAS
 AQUEOUS
 CO3O4
 HEMATITE
 NIFE2O4
 Calculated.. 38 equilibria
 Terminating at axis limit.
 Phase region boundary 54 at: -1.404E+01 6.745E+04
 AQUEOUS
 CO3O4
 ** COCR2O4
 HEMATITE
 NIFE2O4
 Calculated. 27 equilibria
 Phase region boundary 55 at: -2.249E+01 3.456E+04
 AQUEOUS
 CO3O4
 ** COCR2O4
 ** COFE2O4
 HEMATITE
 NIFE2O4
 Phase region boundary 56 at: -2.249E+01 3.456E+04
 AQUEOUS
 CO3O4
 ** COCR2O4
 COFE2O4

```

HEMATITE
NIFE2O4
#####
Phase region boundary 57 at: -2.249E+01 3.456E+04
    AQUEOUS
    CO3O4
    ** COFE2O4
    HEMATITE
    NIFE2O4
Calculated..          21 equilibria
Terminating at axis limit.

Phase region boundary 58 at: -2.249E+01 3.456E+04
    AQUEOUS
    CO3O4
    COCR2O4
    ** COFE2O4
    HEMATITE
    NIFE2O4
Calculated.          2 equilibria

Phase region boundary 59 at: -2.239E+01 3.480E+04
    AQUEOUS
    ** CO3O4
    COCR2O4
    ** COFE2O4
    HEMATITE
    NIFE2O4
Calculated..          21 equilibria
Terminating at axis limit.

Phase region boundary 60 at: -2.239E+01 3.480E+04
    AQUEOUS
    COCR2O4
    ** COFE2O4
    HEMATITE
    NIFE2O4
Calculated..          21 equilibria
Terminating at known equilibrium

Phase region boundary 61 at: -2.239E+01 3.480E+04
    AQUEOUS
    ** CO3O4
    COCR2O4
    HEMATITE
    NIFE2O4
Calculated.          18 equilibria
Terminating at known equilibrium

Phase region boundary 62 at: -2.239E+01 3.480E+04
    AQUEOUS
    ** CO3O4
    COCR2O4
    COFE2O4
    HEMATITE
    NIFE2O4
Calculated.          2 equilibria
Terminating at known equilibrium

Phase region boundary 63 at: -1.404E+01 6.628E+04
    AQUEOUS
    COCR2O4
    CR2O3
    HEMATITE
    ** NIFE2O4
Calculated.          14 equilibria
Terminating at known equilibrium

Phase region boundary 64 at: -1.110E+01 7.654E+04
    AQUEOUS
    ** COCR2O4
    CR2O3
    HEMATITE
Calculated.          15 equilibria
Terminating at known equilibrium

Phase region boundary 65 at: -7.259E+00 2.259E+04
    AQUEOUS
    CR2O3
    ** HEMATITE
Calculated.          2 equilibria
Terminating at known equilibrium

Phase region boundary 66 at: -7.259E+00 -1.839E+04
    ** GAS
    AQUEOUS
Calculated..          16 equilibria
Terminating at axis limit.

Phase region boundary 67 at: -7.259E+00 -1.839E+04
    ** GAS
    AQUEOUS
    CR2O3
Calculated.          2 equilibria
Terminating at known equilibrium

Phase region boundary 68 at: -7.169E+00 -1.817E+04
    GAS
    AQUEOUS
    ** CR2O3
    FECR2O4
Calculated.          3 equilibria

Phase region boundary 69 at: -7.752E+00 -1.961E+04
    ** GAS
    AQUEOUS
    ** CR2O3
    FECR2O4
Calculated.          9 equilibria

Phase region boundary 70 at: -7.752E+00 -1.961E+04
    AQUEOUS
    ** CR2O3
    FECR2O4
Calculated.          9 equilibria

Phase region boundary 71 at: -7.752E+00 1.899E+04
    AQUEOUS

```

```

** CR2O3
  FECR2O4
  ** HEMATITE

Phase region boundary 72 at: -7.752E+00 1.899E+04
  AQUEOUS
  ** CR2O3
  FECR2O4
  HEMATITE
Calculated.          8 equilibria
Terminating at known equilibrium

Phase region boundary 73 at: -7.752E+00 1.899E+04
  AQUEOUS
  FECR2O4
  ** HEMATITE
Calculated.          16 equilibria

Phase region boundary 74 at: -1.286E+01 -1.893E+04
  AQUEOUS
  FECR2O4
  ** HEMATITE
  MAGNETITE
Calculated.          4 equilibria

Phase region boundary 75 at: -1.286E+01 -1.893E+04
  AQUEOUS
  COFE2O4
  FECR2O4
  ** HEMATITE
  MAGNETITE
Calculated.          2 equilibria

Phase region boundary 76 at: -1.395E+01 -2.164E+04
  AQUEOUS
  COFE2O4
  FECR2O4
  ** HEMATITE
  MAGNETITE
Calculated.          2 equilibria

Phase region boundary 77 at: -1.395E+01 -2.164E+04
  AQUEOUS
  COFE2O4
  FECR2O4
  ** HEMATITE
  MAGNETITE
  NIFE2O4
Calculated.          2 equilibria

Phase region boundary 78 at: -1.404E+01 -2.186E+04
  AQUEOUS
  COFE2O4
  FECR2O4
  ** HEMATITE
  MAGNETITE
  NIFE2O4
Calculated..         38 equilibria
Terminating at axis limit.

Phase region boundary 80 at: -1.404E+01 -2.186E+04
  AQUEOUS
  COFE2O4
  FECR2O4
  MAGNETITE
  ** NIFE2O4
Calculated.          5 equilibria

Phase region boundary 81 at: -1.555E+01 -3.682E+04
  AQUEOUS
  ** BCC_A2
  COFE2O4
  FECR2O4
  MAGNETITE
  ** NIFE2O4
Calculated..         35 equilibria
Terminating at axis limit.

Phase region boundary 82 at: -1.555E+01 -3.682E+04
  AQUEOUS
  BCC_A2
  COFE2O4
  FECR2O4
  MAGNETITE
  ** NIFE2O4
Calculated..         35 equilibria
Terminating at axis limit.

Phase region boundary 83 at: -1.555E+01 -3.682E+04
  AQUEOUS
  ** BCC_A2
  COFE2O4
  FECR2O4
  MAGNETITE
Calculated.          2 equilibria

Phase region boundary 84 at: -1.548E+01 -3.681E+04
  AQUEOUS
  ** BCC_A2
  ** COFE2O4
  FECR2O4
  MAGNETITE
Calculated.          4 equilibria

Phase region boundary 85 at: -1.548E+01 -3.681E+04
  AQUEOUS
  ** BCC_A2
  FECR2O4
  MAGNETITE
Calculated.          4 equilibria

Phase region boundary 86 at: -1.473E+01 -3.690E+04
  ** GAS
  AQUEOUS
  ** BCC_A2

```

```

FECR2O4
MAGNETITE

Phase region boundary 87 at: -1.473E+01 -3.690E+04
  GAS
  AQUEOUS
** BCC_A2
FECR2O4
MAGNETITE
Calculated.          5 equilibria

Phase region boundary 88 at: -1.390E+01 -3.486E+04
  GAS
  AQUEOUS
** BCC_A2
FECR2O4
** MAGNETITE

Phase region boundary 89 at: -1.390E+01 -3.486E+04
  GAS
  AQUEOUS
** BCC_A2
FECR2O4
Calculated.          8 equilibria

Phase region boundary 90 at: -1.280E+01 -3.214E+04
  GAS
  AQUEOUS
** BCC_A2
FECR2O4
** HALITE

Phase region boundary 91 at: -1.280E+01 -3.214E+04
  GAS
  AQUEOUS
** BCC_A2
FECR2O4
HALITE
Calculated          201 equilibria

Phase region boundary 92 at: -1.280E+01 -3.214E+04
  GAS
  AQUEOUS
FECR2O4
** HALITE
Calculated.          14 equilibria

Phase region boundary 93 at: -7.005E+00 -1.778E+04
  GAS
  AQUEOUS
** FECR2O4
** HALITE

Phase region boundary 94 at: -7.005E+00 -1.778E+04
  GAS
  AQUEOUS
** HALITE
Calculated..          16 equilibria
Terminating at axis limit.

Phase region boundary 95 at: -7.005E+00 -1.778E+04
  GAS
  AQUEOUS
** FECR2O4
  HALITE
Calculated          62 equilibria

Phase region boundary 96 at: -7.005E+00 -1.778E+04
  GAS
  AQUEOUS
** FECR2O4
  HALITE
Calculated.          6 equilibria

Phase region boundary 97 at: -1.280E+01 -3.214E+04
  GAS
  AQUEOUS
  BCC_A2
FECR2O4
** HALITE
Calculated.          6 equilibria

Phase region boundary 98 at: -1.381E+01 -3.464E+04
  GAS
  AQUEOUS
  BCC_A2
FECR2O4
** HALITE
** MAGNETITE
Calculated..          38 equilibria
Terminating at axis limit.

Phase region boundary 100 at: -1.381E+01 -3.464E+04
  GAS
  AQUEOUS
  BCC_A2
FECR2O4
** MAGNETITE
Calculated          61 equilibria
+
++
```

```

Phase region boundary 102 at: -1.390E+01 -3.486E+04
  GAS
  AQUEOUS
  FECR2O4
  ** MAGNETITE
Calculated.          3 equilibria

Phase region boundary 103 at: -1.472E+01 -3.688E+04
  ** GAS
  AQUEOUS
  FECR2O4
  ** MAGNETITE
Calculated.          5 equilibria
Terminating at known equilibrium

Phase region boundary 104 at: -1.472E+01 -3.688E+04
  AQUEOUS
  FECR2O4
  ** MAGNETITE
Calculated.          15 equilibria
Terminating at known equilibrium

Phase region boundary 105 at: -1.472E+01 -3.688E+04
  ** GAS
  AQUEOUS
  FECR2O4
  MAGNETITE
Calculated.          2 equilibria
Terminating at known equilibrium

Phase region boundary 107 at: -1.390E+01 -3.486E+04
  GAS
  AQUEOUS
  BCC_A2
  FECR2O4
  ** MAGNETITE
Calculated.          46 equilibria

Phase region boundary 108 at: -1.473E+01 -3.690E+04
  ** GAS
  AQUEOUS
  BCC_A2
  FECR2O4
  MAGNETITE
Calculated..         38 equilibria
Terminating at axis limit.

Phase region boundary 109 at: -1.548E+01 -3.681E+04
  AQUEOUS
  ** COFE2O4
  FECR2O4
  MAGNETITE
Calculated.          5 equilibria
Terminating at known equilibrium

Phase region boundary 110 at: -1.548E+01 -3.681E+04
  AQUEOUS
  BCC_A2
  COFE2O4
  FECR2O4
  MAGNETITE
Calculated..         37 equilibria
Terminating at axis limit.

Phase region boundary 111 at: -1.555E+01 -3.682E+04
  AQUEOUS
  ** BCC_A2
  COFE2O4
  FECR2O4
  MAGNETITE
  NIFE2O4
Calculated..         35 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 112 at: -1.404E+01 -2.186E+04
  AQUEOUS
  COFE2O4
  FECR2O4
  HEMATITE
  MAGNETITE
  ** NIFE2O4
Calculated.          1 equilibria

Phase region boundary 113 at: -1.404E+01 -2.186E+04
  AQUEOUS
  COFE2O4
  FECR2O4
  HEMATITE
  ** MAGNETITE
  ** NIFE2O4
Calculated.          4 equilibria

Phase region boundary 114 at: -1.404E+01 -2.186E+04
  AQUEOUS
  COFE2O4
  FECR2O4
  HEMATITE
  ** NIFE2O4
Calculated.          4 equilibria

Phase region boundary 115 at: -1.404E+01 -1.073E+04
  AQUEOUS
  ** COCR2O4
  COFE2O4
  FECR2O4
  HEMATITE
  ** NIFE2O4
Calculated.          4 equilibria

Phase region boundary 116 at: -1.404E+01 -1.073E+04
  AQUEOUS
  COCR2O4

```

```

COFE2O4
FECR2O4
HEMATITE
** NIFE2O4
Calculated.          1 equilibria
Terminating at known equilibrium

Phase region boundary 117 at: -1.404E+01 -1.073E+04
    AQUEOUS
    ** COCR2O4
    COFE2O4
    FECR2O4
    HEMATITE
Calculated.          2 equilibria

Phase region boundary 118 at: -1.395E+01 -1.051E+04
    AQUEOUS
    ** COCR2O4
    ** COFE2O4
    FECR2O4
    HEMATITE
Calculated.          7 equilibria
Terminating at known equilibrium

Phase region boundary 119 at: -1.395E+01 -1.051E+04
    AQUEOUS
    ** COCR2O4
    FECR2O4
    HEMATITE
Calculated.          3 equilibria
Terminating at known equilibrium

Phase region boundary 120 at: -1.395E+01 -1.051E+04
    AQUEOUS
    ** COFE2O4
    FECR2O4
    HEMATITE
Calculated.          3 equilibria

Phase region boundary 121 at: -1.395E+01 -2.164E+04
    AQUEOUS
    ** COFE2O4
    FECR2O4
    HEMATITE
    ** MAGNETITE
Calculated.          1 equilibria
Terminating at known equilibrium

Phase region boundary 122 at: -1.395E+01 -2.164E+04
    AQUEOUS
    ** COFE2O4
    FECR2O4
    HEMATITE
    MAGNETITE
Calculated.          4 equilibria
Terminating at known equilibrium

Phase region boundary 123 at: -1.395E+01 -2.164E+04
    AQUEOUS
    FECR2O4
    HEMATITE
    ** MAGNETITE
Calculated.          2 equilibria
Terminating at known equilibrium

Phase region boundary 124 at: -1.395E+01 -2.164E+04
    AQUEOUS
    COFE2O4
    FECR2O4
    HEMATITE
    ** MAGNETITE
Calculated.          2 equilibria
Terminating at known equilibrium

Phase region boundary 125 at: -1.395E+01 -1.051E+04
    AQUEOUS
    COCR2O4
    ** COFE2O4
    FECR2O4
    HEMATITE
    NIFE2O4
Calculated.          2 equilibria
Terminating at known equilibrium

Phase region boundary 126 at: -1.404E+01 -1.073E+04
    AQUEOUS
    ** COCR2O4
    COFE2O4
    FECR2O4
    HEMATITE
    NIFE2O4
Calculated..         38 equilibria
Terminating at axis limit.

Phase region boundary 127 at: -1.404E+01 -2.186E+04
    AQUEOUS
    COFE2O4
    FECR2O4
    HEMATITE
    ** MAGNETITE
    NIFE2O4
Calculated..         38 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 128 at: -7.752E+00  1.899E+04
    AQUEOUS
    CR2O3
    FECR2O4
    ** HEMATITE
Calculated.          2 equilibria
Terminating at known equilibrium

Phase region boundary 129 at: -7.752E+00 -1.961E+04
    ** GAS
    AQUEOUS
    CR2O3
    FECR2O4
Calculated.          2 equilibria
Terminating at known equilibrium

```

```

Phase region boundary 130 at: -1.110E+01 1.070E+04
    AQUEOUS
    ** COCR2O4
    CR2O3
    FECR2O4
    HEMATITE
Calculated.          1 equilibria
Terminating at known equilibrium

Phase region boundary 131 at: -1.404E+01 3.415E+03
    AQUEOUS
    COCR2O4
    CR2O3
    FECR2O4
    HEMATITE
    ** NIFE2O4
Calculated.          1 equilibria
Terminating at known equilibrium

Phase region boundary 132 at: -1.541E+01 -4.404E-12
    AQUEOUS
    COCR2O4
    CR2O3
    ** FECR2O4
    HEMATITE
    NIFE2O4
Calculated.          4 equilibria
Terminating at known equilibrium

Phase region boundary 133 at: -3.020E+01 -4.404E-12
    AQUEOUS
    COCR2O4
    ** CR2O3
    HEMATITE
    NIFE2O4
Calculated..         9 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 134 at: -3.020E+01 -4.404E-12
    AQUEOUS
    COCR2O4
    ** CR2O3
    HEMATITE
    NIFE2O4
Calculated.          54 equilibria
Terminating at known equilibrium

Phase region boundary 135 at: -1.610E+01 5.964E+04
    AQUEOUS
    ** CO3O4
    COCR2O4
    HEMATITE
    NIFE2O4
Calculated.          21 equilibria
Terminating at known equilibrium

Phase region boundary 136 at: -1.610E+01 5.964E+04
    AQUEOUS
    ** CO3O4
    COCR2O4
    HEMATITE
    NIFE2O4
Calculated.          7 equilibria
Terminating at known equilibrium

Phase region boundary 137 at: -1.612E+01 5.959E+04
    AQUEOUS
    ** CO3O4
    COCR2O4
    HEMATITE
    NIFE2O4
Calculated.          14 equilibria
Terminating at known equilibrium

Phase region boundary 138 at: -1.612E+01 5.959E+04
    AQUEOUS
    ** CO3O4
    COCR2O4
    HEMATITE
    NIFE2O4
Calculated.          6 equilibria
Terminating at known equilibrium

Phase region boundary 139 at: -1.612E+01 5.825E+04
    AQUEOUS
    COCR2O4
    ** CR2O3
    HEMATITE
    NIFE2O4
Calculated..         34 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 140 at: -1.612E+01 5.825E+04
    AQUEOUS
    COCR2O4
    ** CR2O3
    HEMATITE
    NIFE2O4
Calculated.          6 equilibria
Terminating at known equilibrium

Phase region boundary 141 at: -1.612E+01 -1.748E+03
    AQUEOUS
    COCR2O4
    CR2O3
    ** FECR2O4
    HEMATITE
    NIFE2O4
Calculated..         34 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 142 at: -1.612E+01 -1.748E+03
    AQUEOUS

```

```

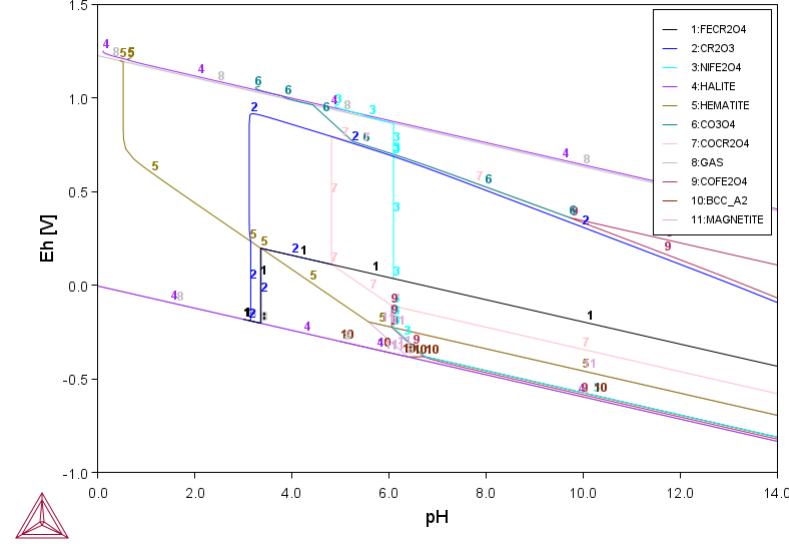
COCR2O4
CR2O3
** FECR2O4
HEMATITE
NIFE2O4
Calculated.          6 equilibria
Terminating at known equilibrium
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\generate_console_examples\examples\tcex53\TCEX53_d.POLY3
CPU time for mapping      745 seconds
POLY:
POLY: @@ Plot the calculated Pourbaix diagram (and others):
POLY: @@ -----
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: l-sym
... the command in full is LIST_SYMBOLS
DEFINED CONSTANTS
AH2O=55.508435, RNF=96485.309, ZERO=0
DEFINED FUNCTIONS AND VARIABLES%
EH=MUR(ZE)/RNF
PH=- LOG10(ACR(H+1,AQUEOUS)*AH2O )
TEMP_C=T-273.15
POST:Hit RETURN to continuePOST:
POST:
s-d-a x pH
... the command in full is SET_DIAGRAM_AXIS
POST: s-a-text x n pH
... the command in full is SET_AXIS_TEXT_STATUS
POST:
POST: s-d-a y Eh
... the command in full is SET_DIAGRAM_AXIS
POST: s-a-text y n Eh [V]
... the command in full is SET_AXIS_TEXT_STATUS
POST:
POST: s-t-m-s y
... the command in full is SET_TRUE_MANUAL_SCALING
COMMAND NOT SUPPORTED IN THIS PLOT DRIVER
POST: s-l-c e
... the command in full is SET_LABEL_CURVE_OPTION
POST:
POST: s-s-s x n 0 14
... the command in full is SET_SCALING_STATUS
POST: s-s-s y n -1.0 1.5
... the command in full is SET_SCALING_STATUS
POST: s-title Thermo-Calc Example 53-a
... the command in full is SET_TITLE
POST: pl...
... the command in full is PLOT DIAGRAM

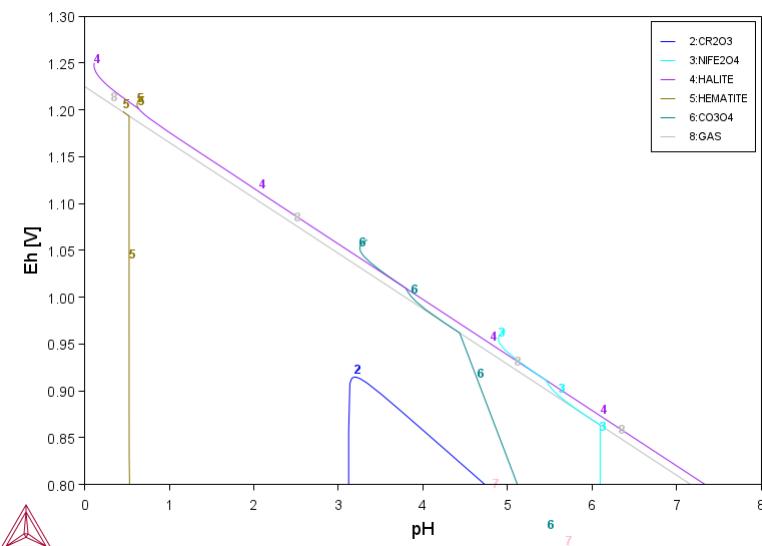
```

Thermo-Calc Example 53-a



POST: make TCEX53.EXP y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST:Hit RETURN to continue
POST:
POST:
POST: sel-pl new
... the command in full is SELECT_PLOT
POST:
POST: s-s-s x n 0 8
... the command in full is SET_SCALING_STATUS
POST: s-s-s y n .8 1.3
... the command in full is SET_SCALING_STATUS
POST: s-title Thermo-Calc Example 53-b
... the command in full is SET_TITLE
POST:
POST: pl...
... the command in full is PLOT_DIAGRAM

Thermo-Calc Example 53-b



POST: Hit RETURN to continue

POST:

POST: sel-pl new

... the command in full is SELECT_PLOT

POST:

POST: s-s-s y n - .4 .4

... the command in full is SET_SCALING_STATUS

POST: s-title Thermo-Calc Example 53-c

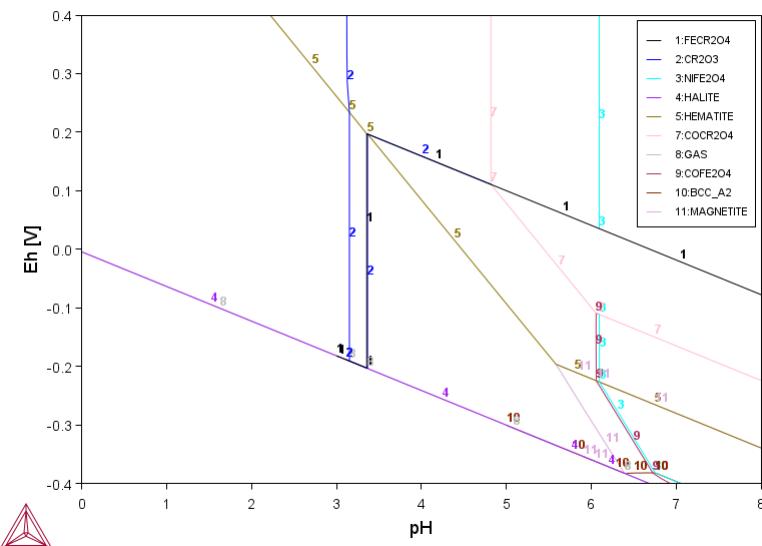
... the command in full is SET_TITLE

POST:

POST: pl,,,

... the command in full is PLOT_DIAGRAM

Thermo-Calc Example 53-c



POST: Hit RETURN to continue

POST:

POST:

POST: @@ -----
POST: @@ From the same mapping calculations, you can plot more
POST: @@ diagrams, using different X-Y axis variables (for such
POST: @@ purposes, it is convenient to use pre-defined symbols as
POST: @@ listed at the end of this macro file).

POST: @@ -----

POST:

POST: SET-INTERACTIVE

... the command in full is SET_INTERACTIVE_MODE

POST:

tce54**SYS:About**

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce54\tce54.TCM.test"

SYS: SET_ECHO

SYS:

SYS: @@ Simulating the solidification of a Al-2.1Cu-1Si alloy

SYS: @@ with a Scheil calculation including back diffusion

SYS:

SYS: @@ This is an example of a solidification simulation

SYS: @@ of a Al-2.1Cu-1Si alloy. The back diffusion option

SYS: @@ in the Scheil module is used, i.e. there is back

SYS: @@ diffusion in the primary phase, which is FCC_A1.

SYS:

SYS: GO SCHEIL

SCHEIL: USE-BACK-DIFFUSION YES

SCHEIL: START-WIZARD

 THERMODYNAMIC DATABASE module

 Database folder: C:\jenkins\workspace\generate_console_examples\databases\data

 Current database: Steels/Fe-Alloys v11.0

 VA /- DEFINED

 DICTRA_FCC A1 REJECTED

Database /TCFE11/: ALDEMO

 Current database: Aluminum Demo Database v4.1

 VA /- DEFINED

Major element or alloy: AL

Composition input in mass (weight) percent? /Y/: N

 Composition will be taken to be in mole percent

1st alloying element: CU

Mole percent /1/: 2.1

2nd alloying element: SI

Mole percent /1/: 1.0

Next alloying element:

Temperature (C) /2000/: 1000

 VA /- DEFINED

 REINITIATING GES

 AL DEFINED

 CU DEFINED

 SI DEFINED

This database has following phases for the defined system

| | | |
|-----------------|---------------|----------------|
| LIQUID:L | AL2CU_C16 | ALCU_DEL |
| ALCU_EPS | ALCU_ETA | ALCU_ZETA |
| ALZR2_B82 | BCC_A2 | BCC_B2 |
| C14_LAVES | C15_LAVES | C36_LAVES |
| CU15Si4_EPSILON | CU33Si7_DELTA | CU56Si11_GAMMA |
| CUSI_ETA | DIAMOND_A4 | FCC_A1 |
| GAMMA_D83 | GAMMA_H | HCP_A3 |

Reject phase(s) /NONE/: NONE

Restore phase(s): /NONE/: NONE

.....
The following phases are retained in this system:

| | | |
|-----------------|---------------|----------------|
| LIQUID:L | AL2CU_C16 | ALCU_DEL |
| ALCU_EPS | ALCU_ETA | ALCU_ZETA |
| ALZR2_B82 | BCC_A2 | BCC_B2 |
| C14_LAVES | C15_LAVES | C36_LAVES |
| CU15Si4_EPSILON | CU33Si7_DELTA | CU56Si11_GAMMA |
| CUSI_ETA | DIAMOND_A4 | FCC_A1 |
| GAMMA_D83 | GAMMA_H | HCP_A3 |

.....
OK? /Y/: Y

17:09:21,021 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

FUNCTIONS

List of references for assessed data

'A. Dinsdale, Calphad,15 317-425 (1991)'
'Volume data from TCFE4, 2006'
'H-L Chen, in TCAL7.0, Evaluation and modeling of electrical resistivity thermal conductivity'
'M J Assael, High Temp High Press 41 (2012); Sb, Pb, Bi, Ni, Ag'
'M Ghasemi, Thermo-Calc Software AB (2020)'
'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89; Molar volumes'
'M J Assael, J Phys Chem Ref Data 39 (2010) 033105; Cu, Sn'
'M J Assael, J Phys Chem Ref Data 41 (2012) 033101; Cd, Co, Ga, In, Hg, Si, Ti, Zn'
'I. Ansara (Editor), COST 507, (1998)'
'M Ghasemi, Thermo-Calc Software AB (2019)'
'C.-Y. He,Calphad, 33,200-210 (2009),Al-Cu-Si'
'J. Groebner,Calphad,20(2)247-254(1996),Al-C-Si'
'X.Y. Yan,J. Alloy and Compd. 308, 221-229 (2000),CU-Si'
'L. Kjellqvist, Thermo-Calc Software AB, Stockholm, 2010; Unassessed parameter, linear combination of unary volume data'
'H-L Chen, in TCAL3.0, Assessment, extrapolation and assumption'
'Hai-Lin Chen, electrical resistivity thermal conductivity (2020)'

'L. Kjellqvist, Thermo-Calc Software AB, Sweden 2012; Molar volumes'
'H-L Chen, Evaluation of molar volume'
'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
'N. Dupin, Calphad, 25(2)279-298(2001), Al-Cr-Ni'
'Nathalie Dupin, in TCNI6.0, Refinement of Al-Ni'
'Volume data, N. Dupin 2008'
'H-L Chen, in TCAL2.0, Assessment, extrapolation and assumption'
'J.R.Zhao, Y.Du, to be submitted, 2010, Sn-Sr, Cu-Mg-Si'
'W.H. Sun, unpublished (2010), Cu-Si-Zn, Cu-Ni-Zn'
'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
'H-L Chen, in TCAL1.2, assessment of Al-Cu-Mg-Si'

-OK-

Should any phase have a miscibility gap check? /N/: N

Mobility Database /MALDEMO/: MALDEMO

Current database: Al-Alloys Mobility demo database v2.0.1

VA /- DEFINED
AL DEFINED
CU DEFINED
SI DEFINED

This database has following phases for the defined system

LIQUID:L FCC_A1
Reject phase(s) /NONE/: NONE
Restore phase(s): /NONE/: NONE

The following phases are retained in this system:

LIQUID:L FCC_A1

OK? /Y/: Y
ELEMENTS
SPECIES
PHASES
PARAMETERS ...
FUNCTIONS

List of references for assessed data

'This parameter has not been assessed'
'Lijun Zhang, Yong Du et al., "Atomic mobilities and diffusivities in the fcc, L12 and B2 phases of the Ni-Al system", 2010'
'G. Ghosh, Acta Mater., 2001, 49, 2609-2624'
'D.D. Liu, L.J. Zhang et al. "The assessment of atomic mobilities of Al and Cu in fcc Al-Cu alloys", CALPHAD, 2009, 33, 761-768'
'D.D. Liu, L.J. Zhang et al., "The assessment of atomic mobilities of Al, Cu and Si in fcc Al-Cu-Si system", 2010'
'L. Zhang et al., Acta Mater., 58(2010)3664.'
'Y. Du et al., Mat. Sci. Eng. A363(2003)140.'

INFO: Forcing option USE_POLY3 for complex phase ALZR2_B82

INFO: Forcing option USE_POLY3 for complex phase BCC_A2

-OK-

Should any phase have a miscibility gap check? /N/: N

LIQUID PHASE NAME: LIQUID

Fast diffusing components: /NONE/: NONE

Temperature time dependence /LINEAR/: LINEAR

Cooling rate (K/s) /1/: 0.1

Expression for secondary dendrite arm spacing /CONSTANT/: POWER LAW

Power law in the form c*(cooling rate)^~-n

Exponent n /.33/: 0.33

Scaling factor c /5E-05/: 5.0E-5

Secondary dendrite arm spacing 0.1069E-03 m

Primary phase /AUTOMATIC/: AUTOMATIC

This command is a combination of CHANGE_STATUS and SET_CONDITION to calculate directly when a phase may form by releasing one condition. You must release one of these conditions.

T=1273.15, X(CU)=2.1E-2, X(SI)=1E-2, P=100000, N=1 DEGREES OF FREEDOM 0

PHASE CHANGE AT 914.742752934

FCC_A1#1 forms

Testing POLY result by global minimization procedure

Calculated 17676 grid points in 0 s

CALCULATING USING NORMAL EQUILIBRIUM CONDITIONS

...OK

Phase Region from 914.833 for:

LIQUID

Terminating at 914.933

Calculated 4 equilibria

Phase Region from 914.833 for:

LIQUID

Global check of adding phase at 9.14743E+02

Calculated 3 equilibria

Phase Region from 914.743 for:

LIQUID

FCC_A1

Global test at 9.06833E+02 OK

Global test at 8.96833E+02 OK

Global test at 8.86833E+02 OK

Global test at 8.76833E+02 OK

Global test at 8.66833E+02 OK

Global test at 8.56833E+02 OK

Global test at 8.46833E+02 OK

Global test at 8.36833E+02 OK

Global test at 8.26833E+02 OK

Global test at 8.16833E+02 OK

Global test at 8.06833E+02 OK

Global test at 7.96833E+02 OK

Global check of removing phase at 7.94498E+02

Backtracking to find phase change for DIAMOND_A4#1

Global test at 7.95833E+02 OK

Global check of adding phase at 7.95274E+02

Calculated 123 equilibria

Phase Region from 795.274 for:

LIQUID

DIAMOND_A4

FCC_A1

```

Global check of removing phase at 7.94976E+02
Calculated      3 equilibria

Phase Region from    794.976      for:
  DIAMOND_A4
  FCC_A1
Calculated      4 equilibria
*** Buffer saved on file: C:\Users\azureuser\AppData\Local\Temp\SCHEIL_2572.POLY3
POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes
POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

An EXP file C:\Users\AZUREU~1\AppData\Local\Temp\SCHEIL_EQ_2572.EXP
has been created to store the equilibrium solidification results.
CALCULATING SCHEIL SOLIDIFICATION
FCC_A1#1 set as the primary phase
  T(C)      fraction solid
  641.6828      0.000000
PHASE REGION:LIQUID + FCC_A1
  T(C)      fraction solid
  641.5871      0.3328777E-03
  640.5871      0.5644985E-01
  639.5871      0.1069005
  638.5871      0.1524234
  637.5871      0.1936937
  636.5871      0.2312698
  635.5871      0.2656170
  634.5871      0.2971265
  633.5871      0.3261293
  632.5871      0.3529072
  631.5871      0.3777019
  630.5871      0.4007215
  629.5871      0.4221464
  628.5871      0.4421334
  627.5871      0.4608199
  626.5871      0.4783264
  625.5871      0.4947590
  624.5871      0.5102119
  623.5871      0.5247683
  622.5871      0.5385028
  621.5871      0.5514818
  620.5871      0.5637648
  619.5871      0.5754054
  618.5871      0.5864519
  617.5871      0.5969479
  616.5871      0.6069329
  615.5871      0.6164428
  614.5871      0.6255102
  613.5871      0.6341648
  612.5871      0.6424338
  611.5871      0.6503422
  610.5871      0.6579126
  609.5871      0.6651662
  608.5871      0.6721220
  607.5871      0.6787981
  606.5871      0.6852106
  605.5871      0.6913748
  604.5871      0.6973048
  603.5871      0.7030135
  602.5871      0.7085130
  601.5871      0.7138145
  600.5871      0.7189286
  599.5871      0.7238649
  598.5871      0.7286325
  597.5871      0.7332399
  596.5871      0.7376950
  595.5871      0.7420052
  594.5871      0.7461775
  593.5871      0.7502185
  592.5871      0.7541341
  591.5871      0.7579302
  590.5871      0.7616122
  589.5871      0.7651851
  588.5871      0.7686538
  587.5871      0.7720227
  586.5871      0.7752961
  585.5871      0.7784781
  584.5871      0.7815724
  583.5871      0.7845827
  582.5871      0.7875122
  581.5871      0.7903644
  580.5871      0.7931421
  579.5871      0.7958484
  578.5871      0.7984858
  577.5871      0.8010572
  576.5871      0.8035649
  575.5871      0.8060112
  574.5871      0.8083985
  573.5871      0.8107288
  572.5871      0.8130043
  571.5871      0.8152267
  570.5871      0.8173981
  569.5871      0.8195201
  568.5871      0.8215943
  567.5871      0.8236226
  566.5871      0.8256062
  565.5871      0.8275468
  564.5871      0.8294457
  563.5871      0.8313043
  562.5871      0.8331238
  561.5871      0.8349055
  560.5871      0.8366505
  559.5871      0.8383601
  558.5871      0.8400352
  557.5871      0.8416770
  556.5871      0.8432863
  555.5871      0.8448642
  554.5871      0.8464117
  553.5871      0.8479295
  552.5871      0.8494185
  551.5871      0.8508797
  550.5871      0.8523136

```

549.5871 0.8537212
 548.5871 0.8551031
 547.5871 0.8564601
 546.5871 0.8577928
 545.5871 0.8591019
 544.5871 0.8603880
 543.5871 0.8616518
 542.5871 0.8628937
 541.5871 0.8641145
 540.5871 0.8653146
 539.5871 0.8664947
 538.5871 0.8676551
 537.5871 0.8687964
 536.5871 0.8699191
 535.5871 0.8710236
 534.5871 0.8721105
 533.5871 0.8731801
 532.5871 0.8742329
 531.5871 0.8752693
 530.5871 0.8762896
 529.5871 0.8772944
 528.5871 0.8782839
 527.5871 0.8792586
 526.5871 0.8802187

PHASE REGION:LIQUID + AL2CU_C16 + FCC_A1

| | |
|----------|----------------|
| T (C) | fraction solid |
| 525.9815 | 0.8807600 |
| 524.9815 | 0.8868168 |
| 523.9815 | 0.8922526 |
| 522.9815 | 0.8972197 |
| 521.9815 | 0.9017762 |
| 520.9815 | 0.9059714 |
| 519.9815 | 0.9098471 |
| 518.9815 | 0.9134392 |
| 517.9815 | 0.9167784 |
| 516.9815 | 0.9198913 |

Not true equilibrium, recalculating with global minimization

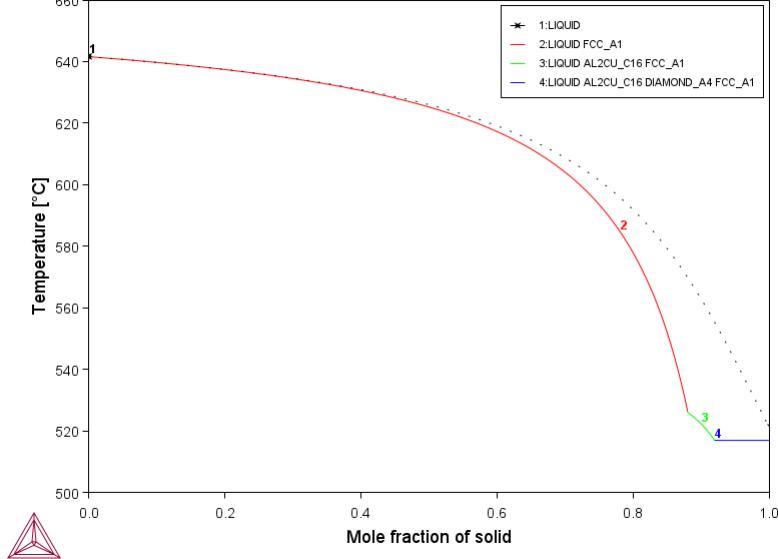
PHASE REGION:AL2CU_C16 + DIAMOND_A4 + FCC_A1

| | |
|----------|----------------|
| T (C) | fraction solid |
| 516.9496 | 1.000000 |

Calculating properties ...

Liquidus temperature: 914.743 K

Solidus temperature: 790.100 K



The following axis variables are available

T - Temperature in Celsius
 NL/BL/VL - Mole/mass/volume fraction of liquid
 NS/BS/VS - Mole/mass/volume fraction of all solid phases
 NS(ph)/BS(ph) - Mole/mass fraction of a solid phase
 VS(ph) - Volume fraction of a solid phase
 W(ph,el) - Weight fraction of an element in a phase
 X(ph,el) - Mole fraction of an element in a phase
 Y(ph,el) - Site fraction of an element in a phase
 NN(ph,el) - Distribution of an element in a phase
 NH/BH - Heat release and Latent heat per mole/gram
 CP/BCP - Apparent heat capacity per mole/gram
 NV/NV(ph) - Molar volume of the system or a phase
 DS/DS(ph) - Average density of the system or a phase
 BT - Apparent volumetric TEC of the system
 DVIS(ph) - Dynamic viscosity of a phase
 KVIS(ph) - Kinematic viscosity of a phase
 SURF(ph) - Surface tension of a liquid phase
 ELRS/ELRS(ph) - Electrical resistivity of the system or a phase
 ELCD/ELCD(ph) - Electrical conductivity of the system or a phase
 THCD/THCD(ph) - Thermal conductivity of the system or a phase
 THRS/THRS(ph) - Thermal resistivity of the system or a phase
 THDF/THDF(ph) - Thermal diffusivity of the system or a phase
 DGV - Driving force for evaporation
 DHV - Evaporation enthalpy
 MMG - Molar mass of gas
 XAVG(el) - Mole fraction of an element in solid phases
 WAVG(el) - Mass fraction of an element in solid phases

"el" and "ph" are name of element and phase, respectively
 "*" can be used as a wild character for "el" and "ph"

.....
POST:
POST: BACK
SCHEIL: SET-INTER
--OK--
SCHEIL:

tce55**SYS:About**

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

```
SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce55\tce55.TCM.test"
SYS:
SYS: @@ Plotting viscosity of Cr-Ni at 1873 K
SYS:
SYS: @@ Plotting viscosity of Cr-Ni at 1873 K
SYS: @@ The example includes an experimental
SYS: @@ data (*.exp) file called Cr-Ni_1873K.exp.
SYS:
SYS:
SYS: set-echo
SYS:
SYS: go da
THERMODYNAMIC DATABASE module
Database folder: C:\jenkins\workspace\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA           /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE11: sw FEDEMO
Current database: Iron Demo Database v4.0

VA           /- DEFINED
TDB_FEDEMO: def-system ni cr
NI          CR DEFINED
TDB_FEDEMO: reject-phase *
LIQUID:L      BCC_A2          LAVES_PHASE_C14
CBCC_A12     CHI_A12         CUB_A13
FCC_A1       HCP_A3          SIGMA
REJECTED

TDB_FEDEMO: restore-phase liquid
LIQUID:L RESTORED
TDB_FEDEMO: get
17:11:06,940 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ...

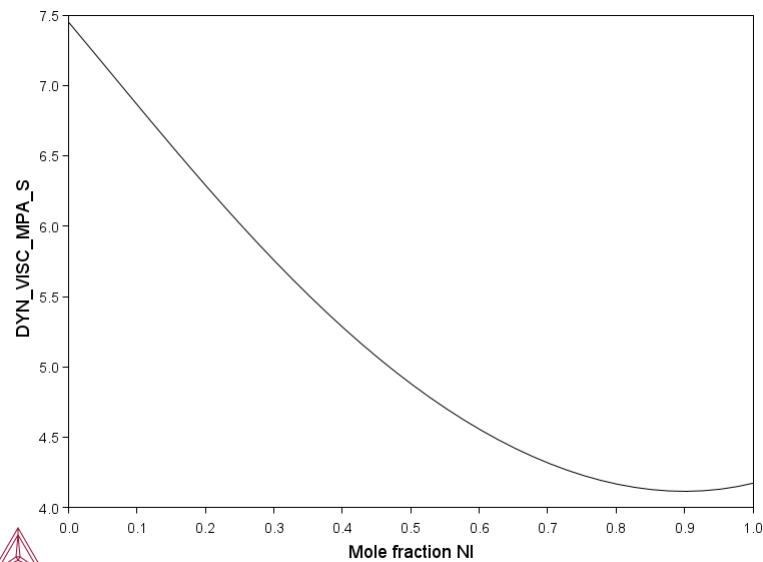
List of references for assessed data

'A.T. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
'M. Ghasemi, Thermo-Calc Software AB, Sweden, 2020; Unifying liquid volume
database'
'M. Ghasemi, Thermo-Calc Software AB, Sweden, 2019; Viscosity of metallic
liquid'
'M Ghasemi, Thermo-Calc Software AB: assessing the surface tension of
metallic liquid'
'Y. Tang, in TCCU2, Thermo-Calc Software AB, Stockholm, Sweden'
'M. J. Assael, High Temp. High Press., 41 (2012); Sb, Pb, Bi, Ni, Ag'
'B.J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
-OK-
TDB_FEDEMO:
TDB_FEDEMO: go poly

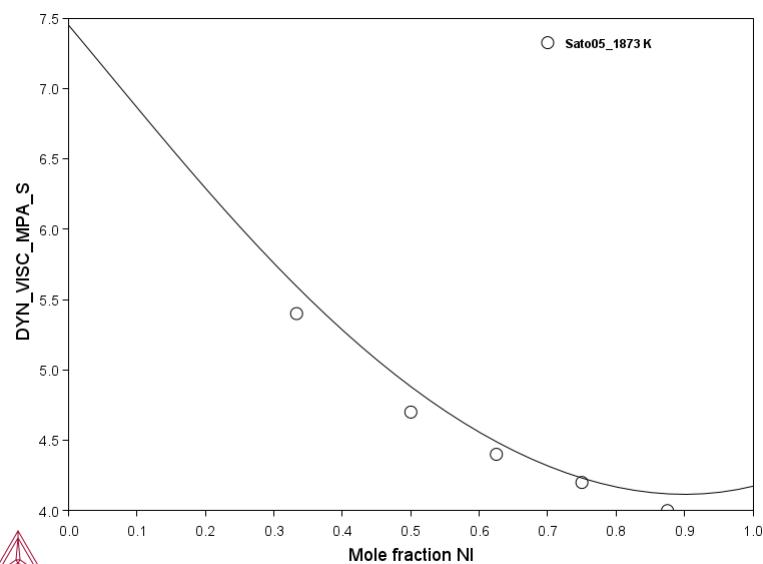
POLY version 3.32
POLY: s-c t=1873 n=1 p=1e5 x(ni)=.2
POLY: c-e
Using global minimization procedure
Calculated      209 grid points in      1 s
Found the set of lowest grid points in      0 s
Calculated POLY solution      1 s, total time      2 s
POLY: s-a-v 1 x(ni) 0 1 ,
POLY: step sep

Phase Region from 0.502463      for:
LIQUID

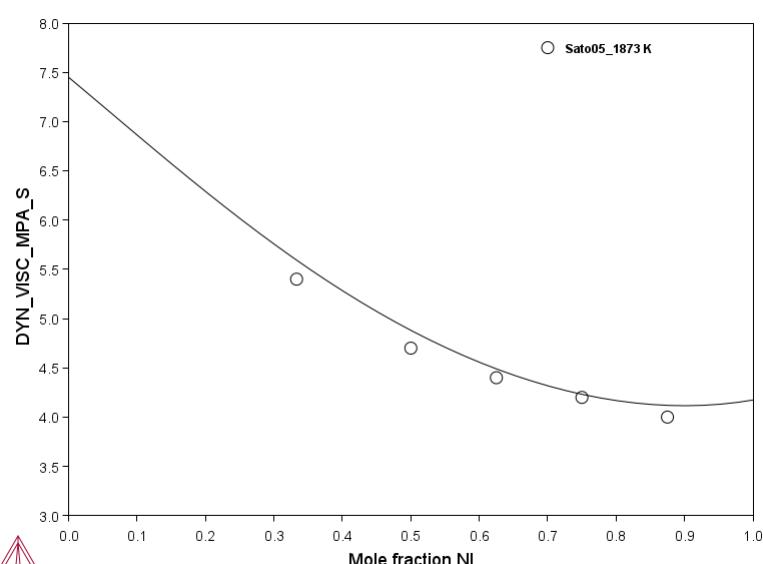
Phase Region from 0.502463      for:
LIQUID
*** Buffer saved on file *** C:\Users\azureuser\AppData\Local\Temp\RESULT_002.POLY3
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2
POST: ent-sym fun Dyn_visc_mPa_s=DVIS(liquid)*1000;
POST: s-d-a y Dyn_visc_mPa_s
POST: s-d-a x m-f ni
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
```



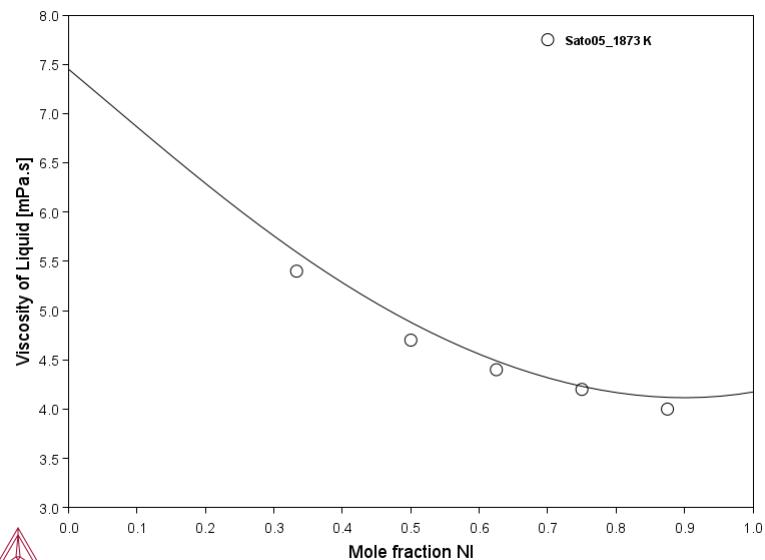
POST:
POST: ap-ex y Cr-Ni_1873K.exp 1:1
POST: pl



POST: s-s-s y n 3 8
POST: pl



POST:
POST:
POST: set-axis-text y N Viscosity of Liquid [mPa.s]
POST: pl



POST:
POST: set-inter
POST:

tce56**SYS:About**

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce56\tce56.TCM.test"
SYS: @@ Plotting Surface Tension of Cu-Zr at 1373 K
SYS:
SYS: @@ Plotting Surface Tension of Cu-Zr at 1373 K. The
SYS: @@ example includes an experimental data (*.exp) file
SYS: @@ called Cr-Zr_ALDEMO.exp.
SYS:
SYS: set-echo
SYS:
SYS: go data
THERMODYNAMIC DATABASE module
Database folder: C:\jenkins\workspace\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE11: sw aldemo
Current database: Aluminum Demo Database v4.1

VA /- DEFINED
TDB_ALDEMO:
TDB_ALDEMO: de-system cu zr
CU ZR DEFINED
TDB_ALDEMO: rej-phase *
LIQUID:L AL2CU_C16 ALCU_EPS
ALCU_ETA ALZR2_B82 BCC_A2
BCC_B2 C14_LAVES C15_LAVES
C36_LAVES FCC_A1 HCP_A3
REJECTED
TDB_ALDEMO: res-phase liquid
LIQUID:L RESTORED
TDB_ALDEMO: get
17:13:34,345 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES
ELEMENTS
SPECIES
PHASES
PARAMETERS ...
FUNCTIONS ...

List of references for assessed data

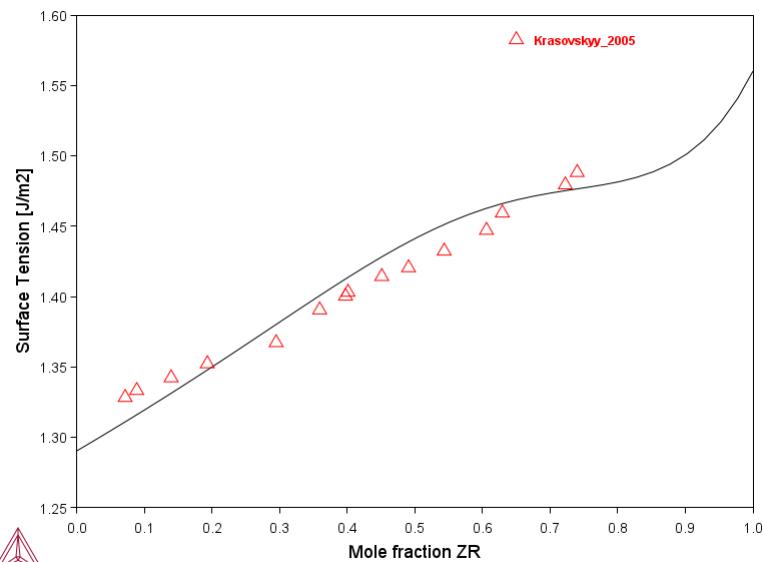
'A. Dinsdale, Calphad,15 317-425 (1991)'
'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
 Molar volumes'
'H-L Chen, in TCAL7.0, Evaluation and modeling of electrical resistivity
 thermal conductivity'
'M J Assael, J Phys Chem Ref Data 39 (2010) 033105; Cu, Sn'
'M Ghasemi, Thermo-Calc Software AB (2020)'
'A. Dinsdale, pure elements, volume, private communication, 2004'
'T Ishikawa, Meas Sci Technol 23 (2012) 025305; Ti, Ni, Zr, Nb, Ru, Rh, Hf,
 Ir, Pt, Tb'
'I. Ansara (Editor), COST 507, (1998)'
'M Ghasemi, Thermo-Calc Software AB (2019)'
-OK-
TDB_ALDEMO:
TDB_ALDEMO: go poly

POLY version 3.32
POLY: s-c t=1373 n=1 p=1e5 x(zr)=.2
POLY: c-e
Using global minimization procedure
Calculated 209 grid points in 2 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 2 s
POLY:

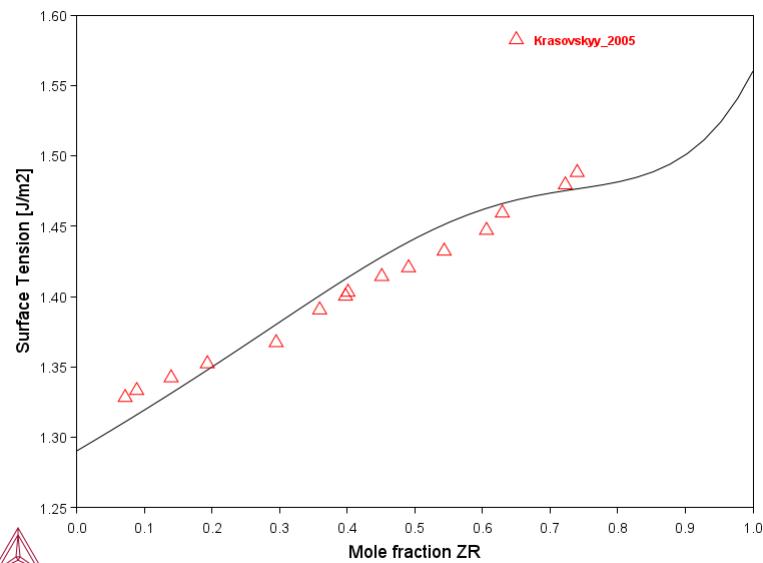
POLY: set-axis-var 1 x(zr) 0 1 ,,
POLY: step sep

Phase Region from 0.502463 for:
 LIQUID

Phase Region from 0.502463 for:
 LIQUID
*** Buffer saved on file *** C:\Users\azureuser\AppData\Local\Temp\RESULT_002.POLY3
POLY:
POLY: post
 POLY-3 POSTPROCESSOR VERSION 3.2
POST: set-diagram-axis y surf(liq)
POST: set-diagram-axis x m-f zr
POST:
POST: ap-exp y Cu-Zr_ALDEMO.exp 1:
POST:
POST:
POST: set-axis
 Ambiguous command use HELP
POST: set-axis-te
Axes (X, Y OR Z) : y
AUTOMATIC AXIS TEXT (Y OR N) /N/: N
AXIS TEXT : Surface Tension [J/m2]
POST: pl



```
POST:  
POST:  
POST: SET_EXP_FILE_FORMAT 5  
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y  
POST: SET_EXP_FILE_FORMAT 10  
POST:  
POST: plot
```



```
POST:  
POST: set-inter  
POST:
```

tce57

SYS:About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

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Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce57\tce57.TCM.test"

SYS: set-echo

SYS:

SYS: @@ Calculating a Scheil with Solute Trapping Solidification in a Al-Si-Cu system

SYS:

SYS: set-log ex57,,,

SYS:

SYS: go scheil

... the command in full is GOTO_MODULE

SCHEIL:

SCHEIL: SOLUTE_TRAPPING Y

SCHEIL:

SCHEIL: start

... the command in full is START_WIZARD

THERMODYNAMIC DATABASE module

Database folder: C:\jenkins\workspace\generate_console_examples\databases\data

Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED

DICTRA_FCC_A1 REJECTED

Database /TCFE11/: ALDEMO

Current database: Aluminum Demo Database v4.1

VA /- DEFINED

Major element or alloy: al

Composition input in mass (weight) percent? /Y/: Y

1st alloying element: si

Mass (weight) percent /1/: 7.5

2nd alloying element: cu

Mass (weight) percent /1/: 0.2

Next alloying element:

Temperature (C) /2000/: 2500

VA /- DEFINED

REINITIATING GES

... the command in full is DEFINE_ELEMENTS

AL DEFINED

... the command in full is DEFINE_ELEMENTS

SI DEFINED

... the command in full is DEFINE_ELEMENTS

CU DEFINED

This database has following phases for the defined system

| | | |
|------------------|---------------|----------------|
| LIQUID:L | AL2CU_C16 | ALCU_DEL |
| ALCU_EPS | ALCU_ETA | ALCU_ZETA |
| ALZR2_B82 | BCC_A2 | BCC_B2 |
| C14_LAVES | C15_LAVES | C36_LAVES |
| CU15Si14_EPSILON | CU33Si7_DELTA | CU56Si11_GAMMA |
| CUSI_ETA | DIAMOND_A4 | FCC_A1 |
| GAMMA_D83 | GAMMA_H | HCP_A3 |

Reject phase(s) /NONE/: NONE

Restore phase(s) : /NONE/: NONE

.....

The following phases are retained in this system:

| | | |
|------------------|---------------|----------------|
| LIQUID:L | AL2CU_C16 | ALCU_DEL |
| ALCU_EPS | ALCU_ETA | ALCU_ZETA |
| ALZR2_B82 | BCC_A2 | BCC_B2 |
| C14_LAVES | C15_LAVES | C36_LAVES |
| CU15Si14_EPSILON | CU33Si7_DELTA | CU56Si11_GAMMA |
| CUSI_ETA | DIAMOND_A4 | FCC_A1 |
| GAMMA_D83 | GAMMA_H | HCP_A3 |

.....

OK? /Y/: Y

17:15:17,185 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***

ELEMENTS

SPECIES

PHASES

... the command in full is AMEND_PHASE_DESCRIPTION

PARAMETERS

FUNCTIONS

List of references for assessed data

'A. Dinsdale, Calphad,15 317-425 (1991)'
'Volume data from TCFE4, 2006'
'H-L Chen, in TCAL7.0, Evaluation and modeling of electrical resistivity thermal conductivity'
'M J Assael, High Temp High Press 41 (2012); Sb, Pb, Bi, Ni, Ag'
'M Ghasemi, Thermo-Calc Software AB (2020)'
'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89; Molar volumes'
'M J Assael, J Phys Chem Ref Data 39 (2010) 033105; Cu, Sn'
'M J Assael, J Phys Chem Ref Data 41 (2012) 033101; Cd, Co, Ga, In, Hg, Si, Tl, Zn'
'I. Ansara (Editor), COST 507, (1998)'
'M Ghasemi, Thermo-Calc Software AB (2019)'
'C.-Y. He,Calphad, 33,200-210 (2009),Al-Cu-Si'
'J. Groebner,Calphad,20(2)247-254(1996),Al-C-Si'

```

'X.Y. Yan,J. Alloy and Compd. 308, 221-229 (2000),CU-Si'
'L. Kjellqvist, Thermo-Calc Software AB, Stockholm, 2010; Unassessed
    parameter, linear combination of unary volume data'
'H-L Chen, in TCAL3.0, Assessment, extrapolation and assumption'
'Hai-Lin Chen, electrical resistivity
    thermal conductivity (2020)'
'L. Kjellqvist, Thermo-Calc Software AB, Sweden 2012; Molar volumes'
'H-L Chen, Evaluation of molar volume'
'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
'N. Dupin, Calphad, 25(2)279-298(2001),Al-Cr-Ni'
'Nathalie Dupin, in TCNI6.0, Refinement of Al-Ni'
'Volume data, N. Dupin 2008'
'H-L Chen, in TCAL2.0, Assessment, extrapolation and assumption'
'J.R.Zhao, Y.Du, to be submitted, 2010,Sn-Sr,Cu-Mg-Si'
'W.H. Sun, unpublished (2010),Cu-Si-Zn,Cu-Ni-Zn'
'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
'H-L Chen, in TCAL1.2, assessment of Al-Cu-Mg-Si'
-OK-
Should any phase have a miscibility gap check? /N/: N
LIQUID PHASE NAME: LIQUID
Expression for solidification speed /SCANNING_SPEED_AND_ANGLE/: SCANNING_SPEED_AND_ANGLE
Solidification speed (m/s) is calculated as V = (scanning speed) * cos(alpha)
Scanning speed (m/s) /1/: 1
Alpha (degrees) /45/: 45
Solidification speed 0.7071 m/s
Primary phase /AUTOMATIC/: AUTOMATIC
... the command in full is COMPUTE_TRANSITION
This command is a combination of CHANGE_STATUS and SET_CONDITION
to calculate directly when a phase may form by releasing one condition.
You must release one of these conditions
T=2773.15, W(SI)=7.5E-2, W(CU)=2E-3, P=100000, N=1      DEGREES OF FREEDOM 0
PHASE CHANGE AT 885.72250905
FCC_A1#1 forms
Testing POLY result by global minimization procedure
Calculated 17676 grid points in           0 s
CALCULATING USING NORMAL EQUILIBRIUM CONDITIONS
... the command in full is ADD_INITIAL_EQUILIBRIUM
... the command in full is ENTER_SYMBOL
... the command in full is ADVANCED_OPTIONS
... the command in full is STEP_WITH_OPTIONS
....OK

Phase Region from 885.813 for:
    LIQUID
Terminating at 885.913
Calculated 4 equilibria

Phase Region from 885.813 for:
    LIQUID
Global check of adding phase at 8.85723E+02
Calculated 3 equilibria

Phase Region from 885.723 for:
    LIQUID
    FCC_A1
Global test at 8.77813E+02 .... OK
Global test at 8.67813E+02 .... OK
Global test at 8.57813E+02 .... OK
Global check of adding phase at 8.49559E+02
Calculated 39 equilibria

Phase Region from 849.559 for:
    LIQUID
    DIAMOND_A4
    FCC_A1
Global check of removing phase at 8.46181E+02
Calculated 6 equilibria

Phase Region from 846.181 for:
    DIAMOND_A4
    FCC_A1
Calculated 4 equilibria
*** Buffer saved on file: C:\Users\azureuser\AppData\Local\Temp\SCHEIL_864.POLY3
POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes
POSTPROCESSOR VERSION 3.2
Setting automatic diagram axes

... the command in full is ENTER_SYMBOL
... the command in full is MAKE_EXPERIMENTAL_DATAFI
An EXP file C:\Users\AZUREU~1\AppData\Local\Temp\SCHEIL_EQ_864.EXP
has been created to store the equilibrium solidification results.
... the command in full is READ_WORKSPACES
CALCULATING SCHEIL SOLIDIFICATION
FCC_A1#1 set as the primary phase
    T(C)      fraction solid
    612.6625  0.000000
    611.6625  0.000000
    610.6625  0.000000
    610.2481  0.000000
PHASE REGION:LIQUID + FCC_A1
    T(C)      fraction solid
    610.2163  0.3148145E-03
    609.2163  0.2406990E-01
    608.2163  0.4679047E-01
    607.2163  0.6854047E-01
    606.2163  0.8937880E-01
    605.2163  0.1093598
    604.2163  0.1285336
    603.2163  0.1469466
    602.2163  0.1646419
    601.2163  0.1816592
    600.2163  0.1980355
    599.2163  0.2138054
    598.2163  0.2290009
    597.2163  0.2436518
    596.2163  0.2577860
    595.2163  0.2714295
    594.2163  0.2846067
    593.2163  0.2973404
    592.2163  0.3096520
    591.2163  0.3215615
    590.2163  0.3330877

```

```

589.2163 0.3442483
588.2163 0.3550599
587.2163 0.3655382
586.2163 0.3756979
585.2163 0.3855530
584.2163 0.3951166
583.2163 0.4044010
582.2163 0.4134180
581.2163 0.4221787
580.2163 0.4306935
579.2163 0.4389724
578.2163 0.4470249
577.2163 0.4548598
576.4194 0.4609507

```

PHASE REGION:LIQUID + DIAMOND_A4 + FCC_A1

T (C) fraction solid

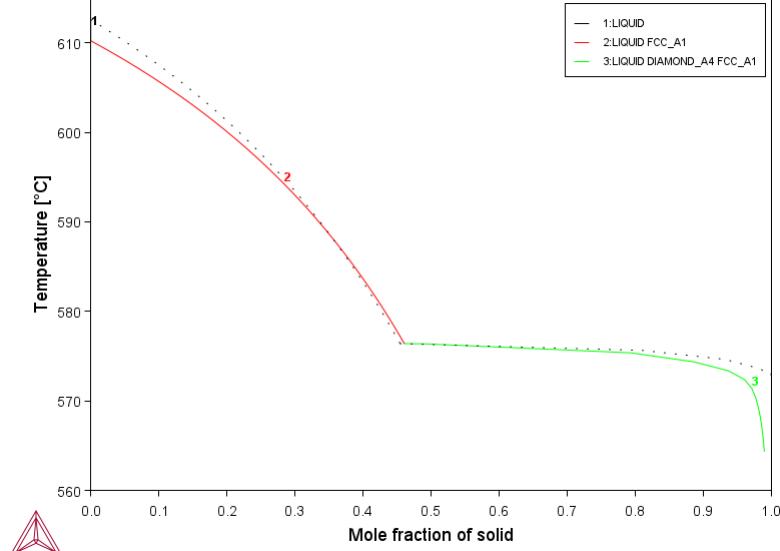
| T (C) | fraction solid |
|----------|----------------|
| 576.3875 | 0.4921089 |
| 575.3875 | 0.7935046 |
| 574.3875 | 0.8862770 |
| 573.3875 | 0.9372088 |
| 572.3875 | 0.9613926 |
| 571.3875 | 0.9719953 |
| 570.3875 | 0.9774242 |
| 569.3875 | 0.9811188 |
| 568.3875 | 0.9839099 |
| 567.3875 | 0.9860544 |
| 566.3875 | 0.9877322 |
| 565.3875 | 0.9890754 |
| 564.3875 | 0.9901738 |

Calculating properties ...

Liquidus temperature: 883.398 K

... the command in full is SET_LABEL_CURVE_OPTION

... the command in full is APPEND EXPERIMENTAL_DATA



The following axis variables are available

T - Temperature in Celsius
 NL/BL/VL - Mole/mass/volume fraction of liquid
 NS/BS/VS - Mole/mass/volume fraction of all solid phases
 NS(ph)/BS(ph) - Mole/mass fraction of a solid phase
 VS(ph) - Volume fraction of a solid phase
 W(ph,el) - Weight fraction of an element in a phase
 X(ph,el) - Mole fraction of an element in a phase
 Y(ph,el) - Site fraction of an element in a phase
 NN(ph,el) - Distribution of an element in a phase
 NH/BH - Heat release and Latent heat per mole/gram
 CP/BCP - Apparent heat capacity per mole/gram
 NV/NV(ph) - Molar volume of the system or a phase
 DS/DS(ph) - Average density of the system or a phase
 BT - Apparent volumetric TEC of the system
 DVIS(ph) - Dynamic viscosity of a phase
 KVVIS(ph) - Kinematic viscosity of a phase
 SURF(ph) - Surface tension of a liquid phase
 ELRS/ELRS(ph) - Electrical resistivity of the system or a phase
 ELCD/ELCD(ph) - Electrical conductivity of the system or a phase
 THCD/THCD(ph) - Thermal conductivity of the system or a phase
 THRS/THRS(ph) - Thermal resistivity of the system or a phase
 THDF/THDF(ph) - Thermal diffusivity of the system or a phase
 DGV - Driving force for evaporation
 DHV - Evaporation enthalpy
 MMG - Molar mass of gas
 XAVG(el) - Mole fraction of an element in solid phases
 WAVG(el) - Mass fraction of an element in solid phases

"el" and "ph" are name of element and phase, respectively

"*" can be used as a wild character for "el" and "ph"

POST:

POST:

POST: set-inter

... the command in full is SET_INTERACTIVE_MODE

POST:

tce58

SYS:About

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Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce58\tce58.TCM.test"
SYS: @@ Calculate volumetric thermal expansion coefficients
SYS: @@ of the L12-type Al3Sc.
SYS:
SYS: GO DA
THERMODYNAMIC DATABASE module
Database folder: C:\jenkins\workspace\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE11: SW Aldemo
Current database: Aluminum Demo Database v4.1

VA /- DEFINED
TDB_ALDEMO: DEF-ELE AL SC SC DEFINED
TDB_ALDEMO: GET
17:17:05,910 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES
ELEMENTS
SPECIES
PHASES
PARAMETERS ...
FUNCTIONS

List of references for assessed data

'A. Dinsdale, Calphad,15 317-425 (1991)'
'Volume data from TCFE4, 2006'
'H-L Chen, in TCAL7.0, Evaluation and modeling of electrical resistivity
 thermal conductivity'
'M J Assael, High Temp High Press 41 (2012); Sb, Pb, Bi, Ni, Ag'
'M Ghasemi, Thermo-Calc Software AB (2020)'
'L. Kjellqvist, Thermo-Calc Software AB, Sweden 2012; Molar volumes'
'M Ghasemi, Thermo-Calc Software AB (2019)'
'H. Bo, JALCOM 490 (2010) 318-325 Al-Sc, Al-Cu-SC'
'I. Ansara (Editor), COST 507, (1998)'
'L. Kjellqvist, Thermo-Calc Software AB, Stockholm, 2010; Unassessed
 parameter, linear combination of unary volume data'
'Hai-Lin Chen, electrical resistivity
 thermal conductivity (2020)'
'H-L Chen, in TCAL5.0, Modeling of the Al-Sc-Zr ternary system'
'H-L Chen, Evaluation of molar volume'
'N. Dupin, Calphad, 25(2)279-298(2001),Al-Cr-Ni'
'Nathalie Dupin, in TCNI6.0, Refinement of Al-Ni'
'W.H Sun,S.H. Liu,added to make this phase less stable, 2010'
'Volume data, N. Dupin 2008'
'H-L Chen, in TCAL3.0, Assessment, extrapolation and assumption'
'Z.P. Cao, modified by HL Chen, in the TCAL project. Ni-Sc'
'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
 Molar volumes'
-OK-
TDB_ALDEMO:
TDB_ALDEMO: go p-3

POLY version 3.32
POLY:

POLY: c-s ph *=sus
POLY: c-s ph al3sc,liquid,fcc_a1=ent 1
POLY:
POLY: s-c n=1 p=1e5
POLY:
POLY: s-c x(sc)=0.25 t=273
POLY:
POLY: ent func avAl3Sc=vm(al3sc).t/vm(al3sc);
POLY:
POLY: c-e
Using global minimization procedure
Calculated 419 grid points in 1 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 1 s, total time 2 s
POLY:
POLY: s-a-v 1 t 100 2000.,
POLY:
POLY: step
Option? /NORMAL/:
No initial equilibrium, using default
Step will start from axis value 273.000
...OK

Phase Region from 273.000 for:
 AL3SC
 FCC_A1
Global test at 3.53000E+02 OK
Global test at 4.53000E+02 OK
Global check of adding phase at 5.52137E+02
Calculated 30 equilibria

Phase Region from 552.137 for:
 LIQUID
 AL3SC
 FCC_A1
Calculated 2 equilibria

```

Phase Region from      552.137      for:
    LIQUID
    AL3SC
Global test at  6.23000E+02 .... OK
Global test at  7.23000E+02 .... OK
Global test at  8.23000E+02 .... OK
Global test at  9.23000E+02 .... OK
Global test at  1.02300E+03 .... OK
Global test at  1.12300E+03 .... OK
Global test at  1.22300E+03 .... OK
Global test at  1.32300E+03 .... OK
Global test at  1.42300E+03 .... OK
Global test at  1.52300E+03 .... OK
QBSMER trying to find equilibrium at  1.5970000E+03
QBSMER forced phase set change at   1597.000000000000
Calculated   109 equilibria

```

```

Phase Region from     1597.00      for:
    LIQUID
Global test at  1.66900E+03 .... OK
Global test at  1.76900E+03 .... OK
Global test at  1.86900E+03 .... OK
Global test at  1.96900E+03 .... OK
Terminating at   2000.00
Calculated    45 equilibria

```

```

Phase Region from     273.000      for:
    AL3SC
    FCC_A1
Global test at  1.93000E+02 .... OK
Global test at  1.00000E+02 .... OK
Terminating at   100.000
Calculated    21 equilibria
*** Buffer saved on file: C:\Users\azureuser\AppData\Local\Temp\RESULT_002.POLY3

```

```

POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

```

```

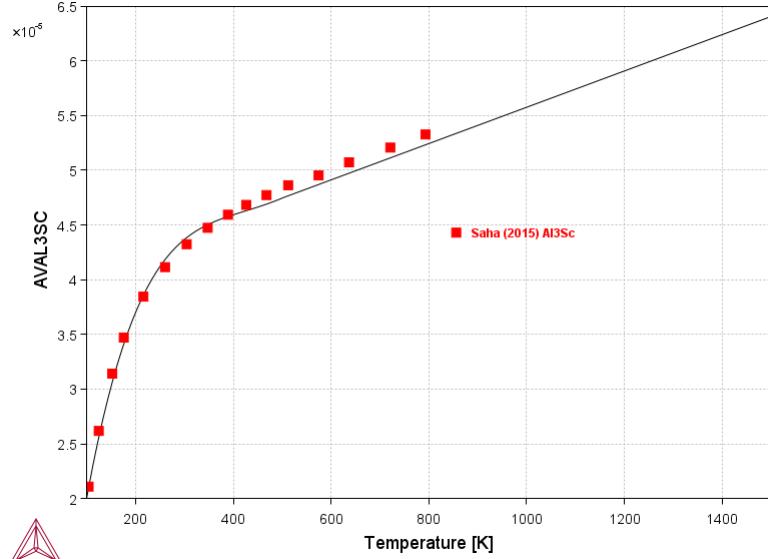
Setting automatic diagram axes

```

```

POST:
POST:@?plot_expansion_coefficient
POST: a-e y Al3X.exp
PROLOGUE NUMBER: /0/: 1
DATASET NUMBER(s): /-1/: 1
POST:
POST: set-ras Y,,
POST: s-d-a x t-k
POST: s-s-s x n 100 1500
POST: s-d-a y avAl3Sc
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot,,,

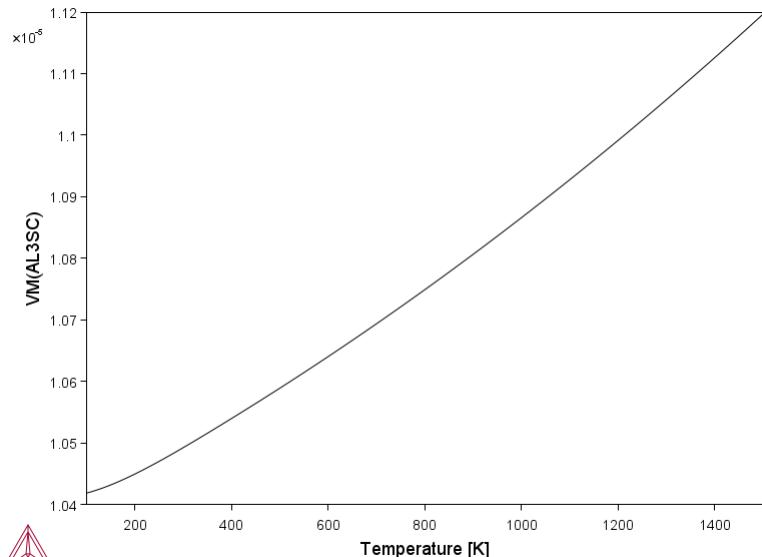
```



```

POST:
POST:@?plot_molar_volume
POST: select,,,
POST: s-d-a y vm(al3sc)
POST: a_e n,,,
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot,,,

```



POST:
POST: set-inter
POST:

tce59

SYS:About

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Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce59\tce59.TCM.test"
SYS: @@ Calculate volumetric thermal expansion coefficients
SYS: @@ of the L12-type Al3Zr.
SYS:
SYS: GO DA
THERMODYNAMIC DATABASE module
Database folder: C:\jenkins\workspace\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE11: SW Aldemo
Current database: Aluminum Demo Database v4.1

VA /- DEFINED
TDB_ALDEMO: DEF-ELE AL Zr
AL ZR DEFINED
TDB_ALDEMO: GET
17:18:27,007 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES
ELEMENTS
SPECIES
PHASES
PARAMETERS ...
FUNCTIONS

List of references for assessed data

'A. Dinsdale, Calphad,15 317-425 (1991)'
'Volume data from TCFE4, 2006'
'H-L Chen, in TCAL7.0, Evaluation and modeling of electrical resistivity
 thermal conductivity'
'M J Assael, High Temp High Press 41 (2012); Sb, Pb, Bi, Ni, Ag'
'M Ghasemi, Thermo-Calc Software AB (2020)'
'A. Dinsdale, pure elements, volume, private communication, 2004'
'T Ishikawa, Meas Sci Technol 23 (2012) 025305; Ti, Ni, Zr, Nb, Ru, Rh, Hf,
 Ir, Pt, Tb'
'I. Ansara (Editor), COST 507, (1998)'
'M Ghasemi, Thermo-Calc Software AB (2019)'
'L. Kjellqvist, Thermo-Calc Software AB, Stockholm, 2010; Unassessed
 parameter, linear combination of unary volume data'
'H-L Chen, in TCAL2.0, Assessment, extrapolation and assumption'
'H-L Chen, in TCAL5.0, Modeling of the Al-Sc-Zr ternary system'
'Hai-Lin Chen, electrical resistivity
 thermal conductivity (2020)'
'L. Kjellqvist, Thermo-Calc Software AB, Sweden 2012; Molar volumes'
'H-L Chen, Evaluation of molar volume'
'H-L Chen, in TCAL3.1, Assessment, extrapolation and assumption'
'N. Dupin, Calphad, 25(2)279-298(2001),Al-Cr-Ni'
'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
 Molar volumes'
'Nathalie Dupin, in TCNI6.0, Refinement of Al-Ni'
'Volume data, N. Dupin 2008'
'Unary parameter for Laves phases'
'N. Dupin, Unpublished work on molar volumes.'
'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
-OK-
TDB_ALDEMO:
TDB_ALDEMO: go p-3

POLY version 3.32
POLY:

POLY: c-s ph *=sus
POLY: c-s ph al3sc,liquid,fcc_a1=ent 1
POLY:
POLY: s-c n=1 p=1e5
POLY:
POLY: s-c x(Zr)=0.25 t=273
POLY:
POLY: ent func avAl3Zr=vm(al3sc).t/vm(al3sc);
POLY:
POLY: c-e
Using global minimization procedure
Calculated 419 grid points in 1 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 1 s
POLY:
POLY: s-a-v 1 t 100 2000,,
POLY:
POLY: step
Option? /NORMAL/:
No initial equilibrium, using default
Step will start from axis value 273.000
...OK

Phase Region from 273.000 for:
 AL3SC
 FCC_A1
Global Test at 3.53000E+02 OK
Global test at 4.53000E+02 OK
Global test at 5.53000E+02 OK
Global test at 6.53000E+02 OK
Global test at 7.53000E+02 OK
Global test at 8.53000E+02 OK
Global test at 9.53000E+02 OK
Global test at 1.05300E+03 OK

```

Global check of adding phase at 1.09736E+03
Calculated 85 equilibria

Phase Region from 1097.36 for:
  LIQUID
  AL3SC
  FCC_A1
Calculated 2 equilibria

Phase Region from 1097.36 for:
  LIQUID
  AL3SC
Global test at 1.17300E+03 .... OK
Global test at 1.27300E+03 .... OK
Global test at 1.37300E+03 .... OK
Global test at 1.47300E+03 .... OK
Global test at 1.57300E+03 .... OK
Global test at 1.67300E+03 .... OK
Global test at 1.77300E+03 .... OK
QBSMER trying to find equilibrium at 1.7990000E+03
QBSMER forced phase set change at 1799.000000000000
Calculated 75 equilibria

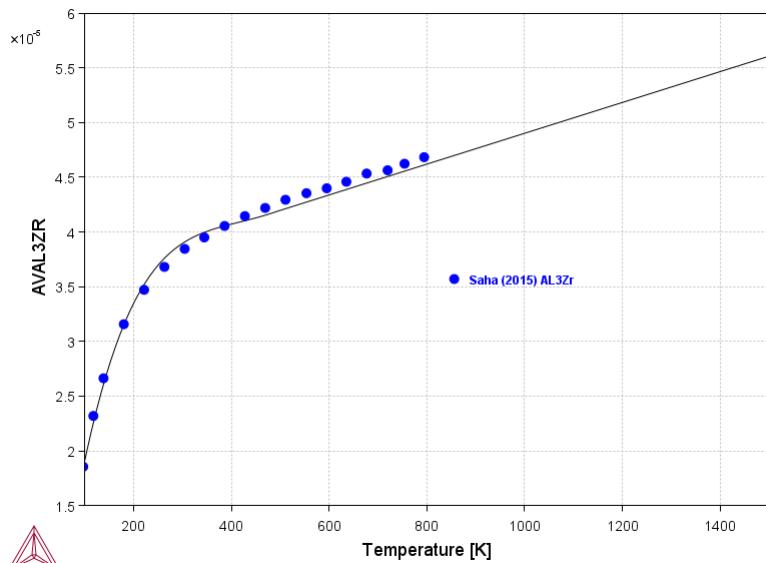
Phase Region from 1799.00 for:
  LIQUID
Global test at 1.87100E+03 .... OK
Global test at 1.97100E+03 .... OK
Terminating at 2000.00
Calculated 24 equilibria

Phase Region from 273.000 for:
  AL3SC
  FCC_A1
Global test at 1.93000E+02 .... OK
Global test at 1.00000E+02 .... OK
Terminating at 100.000
Calculated 21 equilibria
*** Buffer saved on file: C:\Users\azureuser\AppData\Local\Temp\RESULT_002.POLY3
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST:
POST:@?plot_expansion_coefficient
POST: a-e y Al3X.exp
PROLOGUE NUMBER: /0/: 1
DATASET NUMBER(s): /-1/: 2
POST:
POST: set-ras Y,,
POST: s-d-a x t-k
POST: s-s-s x n 100 1500
POST: s-d-a y avAl3Zr
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot,,,

```

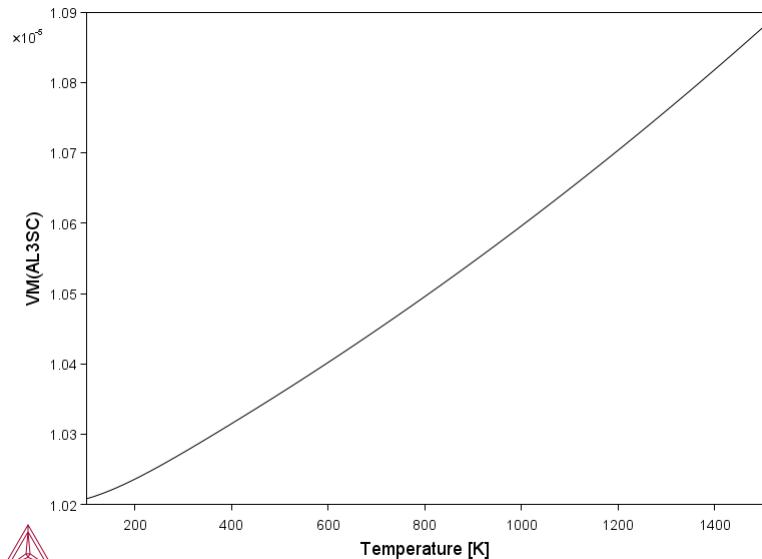




```

POST:
POST:@?plot_molar_volume
POST: select,,,
POST: s-d-a y vm(al3sc)
POST: a_e n,,,
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot,,,

```



POST:
POST:
POST: set-inter
POST:

tce60

SYS:About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

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Stockholm, Sweden

Software (build 27991) running on WinNT 64-bit wordlength
Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
License library version: 9.7.0.0036
Linked: Thu Apr 27 13:25:22 2023

```
SYS:SYS:MACRO "c:\jenkins\workspace\generate_console_examples\examples\tce60\tce60.TCM.test"
SYS: @@ Calculate the electrical resistivity (ELRS) and
SYS: @@ thermal conductivity (THCD) from FCC_A1 to liquid.
SYS:
SYS:
SYS: @@ This example makes a step calculation of pure Cu
SYS: @@ over a wide temperature range, covering both the
SYS: @@ FCC_A1 state and the liquid state. It plots thermal @@ conductivity of the system (pure Cu, for both
SYS: @@ FCC_A1 and liquid) and that of a single phase
SYS: @@ (taking FCC_A1 as an example), respectively.
SYS: @@ Also plots electrical resistivity of the system
SYS: @@ and that of FCC_A1.
SYS:
SYS: go da
THERMODYNAMIC DATABASE module
Database folder: C:\jenkins\workspace\generate_console_examples\databases\data
Current database: Steels/Fe-Alloys v11.0

VA           /*- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE11: sw aldemo
Current database: Aluminum Demo Database v4.1

VA           /*- DEFINED
TDB_ALDEMO: def-ele Cu
CU DEFINED
TDB_ALDEMO: get
17:19:47,752 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS .....
FUNCTIONS .....

List of references for assessed data

'A. Dinsdale, Calphad,15 317-425 (1991)'
'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
    Molar volumes'
'H.-L Chen, in TCAL7.0, Evaluation and modeling of electrical resistivity
    thermal conductivity'
'M J Assael, J Phys Chem Ref Data 39 (2010) 033105; Cu, Sn'
'M Ghasemi, Thermo-Calc Software AB (2020)'
'I. Ansara (Editor), COST 507, (1998)'
'L. Kjellqvist, Thermo-Calc Software AB, Sweden 2012; Molar volumes'
'L. Kjellqvist, Thermo-Calc Software AB, Stockholm, 2010; Unassessed
    parameter, linear combination of unary volume data'
'Hai-Lin Chen, electrical resistivity
    thermal conductivity (2020)'
'H-L Chen, Evaluation of molar volume'
'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
'N. Dupin, Calphad, 25(2)279-298(2001),Al-Cr-Ni'
-OK-
TDB_ALDEMO:
TDB_ALDEMO: go p-3

POLY version 3.32
POLY: s-c n=1 p=1e5 t=300
POLY:

POLY: c-s ph *
Status: /ENTERED/: sus
POLY: c-s ph fcc_a1 liquid
Status: /ENTERED/: ENTERED
Start value, number of mole formula units /0/: 1
POLY:
POLY: c-e
Using global minimization procedure
Calculated          2 grid points in      1 s
POLY:
POLY: s-a-v 1 t 200 6000
Increment /145/: 67.5
POLY:
POLY: step
Option? /NORMAL/: NORMAL
No initial equilibrium, using default
Step will start from axis value   300.000
...OK

Phase Region from  300.000     for:
    FCC_A1
Global test at  3.80000E+02 .... OK
Global test at  4.80000E+02 .... OK
Global test at  5.80000E+02 .... OK
Global test at  6.80000E+02 .... OK
Global test at  7.80000E+02 .... OK
Global test at  8.80000E+02 .... OK
Global test at  9.80000E+02 .... OK
Global test at  1.08000E+03 .... OK
Global test at  1.18000E+03 .... OK
Global test at  1.28000E+03 .... OK
Global check of adding phase at  1.35777E+03
Calculated  108 equilibria

Phase Region from  1357.77     for:
    LIQUID
```

```

FCC_A1
Calculated      2 equilibria
Phase Region from    1357.77      for:
LIQUID
Global test at  1.43000E+03 .... OK
Global test at  1.53000E+03 .... OK
Global test at  1.63000E+03 .... OK
Global test at  1.73000E+03 .... OK
Global test at  1.83000E+03 .... OK
Global test at  1.93000E+03 .... OK
Global test at  2.03000E+03 .... OK
Global test at  2.13000E+03 .... OK
Global test at  2.23000E+03 .... OK
Global test at  2.33000E+03 .... OK
Global test at  2.43000E+03 .... OK
Global test at  2.53000E+03 .... OK
Global test at  2.63000E+03 .... OK
Global test at  2.73000E+03 .... OK
Global test at  2.83000E+03 .... OK
Global test at  2.93000E+03 .... OK
Global test at  3.03000E+03 .... OK
Global test at  3.13000E+03 .... OK
Global test at  3.23000E+03 .... OK
Global test at  3.33000E+03 .... OK
Global test at  3.43000E+03 .... OK
Global test at  3.53000E+03 .... OK
Global test at  3.63000E+03 .... OK
Global test at  3.73000E+03 .... OK
Global test at  3.83000E+03 .... OK
Global test at  3.93000E+03 .... OK
Global test at  4.03000E+03 .... OK
Global test at  4.13000E+03 .... OK
Global test at  4.23000E+03 .... OK
Global test at  4.33000E+03 .... OK
Global test at  4.43000E+03 .... OK
Global test at  4.53000E+03 .... OK
Global test at  4.63000E+03 .... OK
Global test at  4.73000E+03 .... OK
Global test at  4.83000E+03 .... OK
Global test at  4.93000E+03 .... OK
Global test at  5.03000E+03 .... OK
Global test at  5.13000E+03 .... OK
Global test at  5.23000E+03 .... OK
Global test at  5.33000E+03 .... OK
Global test at  5.43000E+03 .... OK
Global test at  5.53000E+03 .... OK
Global test at  5.63000E+03 .... OK
Global test at  5.73000E+03 .... OK
Global test at  5.83000E+03 .... OK
Global test at  5.93000E+03 .... OK
Terminating at   6000.00
Calculated    468 equilibria

```

```

Phase Region from    300.000      for:
FCC_A1
Global test at  2.20000E+02 .... OK
Terminating at   200.000
Calculated    13 equilibria
*** Buffer saved on file: C:\Users\azureuser\AppData\Local\Temp\RESULT_002.POLY3

```

```

POLY:
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2

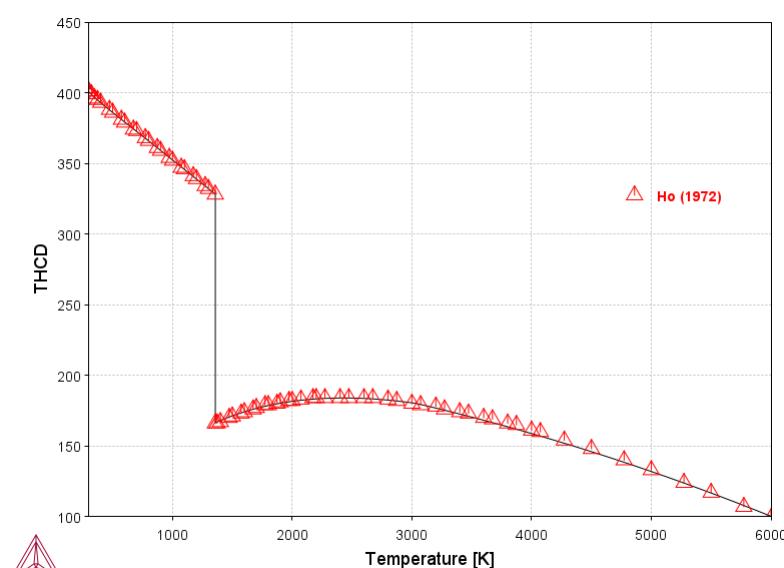
```

```
Setting automatic diagram axes
```

```

POST:
POST:@?plot_thcd_of_system
POST: s-d-a x t-k
POST: s-d-a y thcd
POST: s-s-s x n 200 6000
POST: a-e y 1972Ho_cu_thcd
PROLOGUE NUMBER: /0/: 1
DATASET NUMBER(s): /-1/: 1 2 3
POST: set-ray y
POST: set-tic 4
POST: pl,,

```



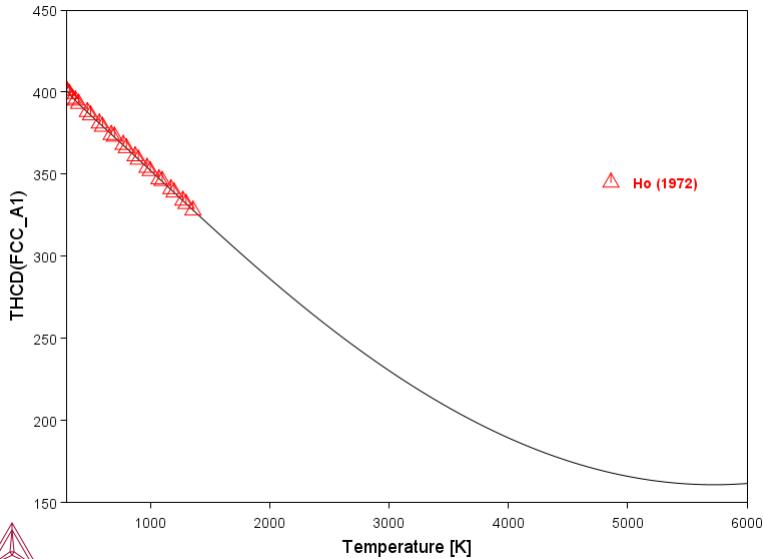
```

POST:
POST:@?plot_thcd_of_fcc_a1_only
POST: select,,,
POST: s-d-a y thcd(fcc_a1)
POST: s-s-s x n 200 6000

```

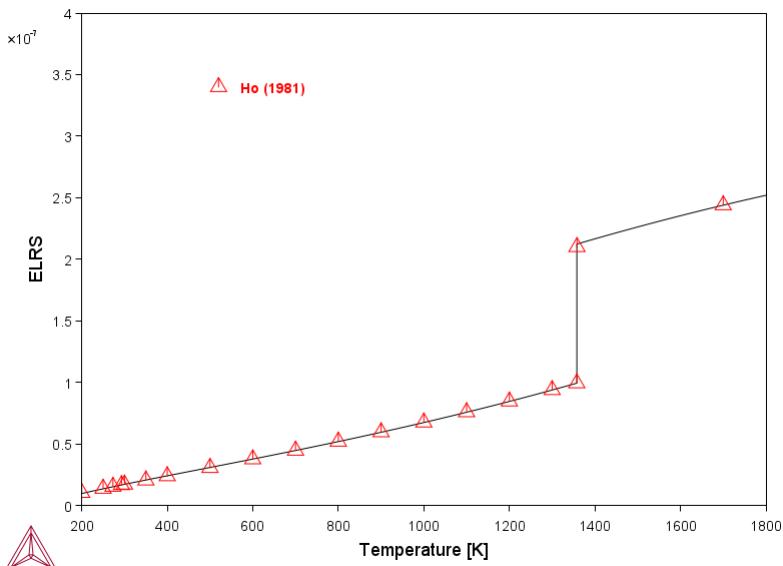
```

POST: a-e y 1972Ho_cu_thcd
PROLOGUE NUMBER: /1/: 1
DATASET NUMBER(s): /-1/: 1 2
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot,,,
```



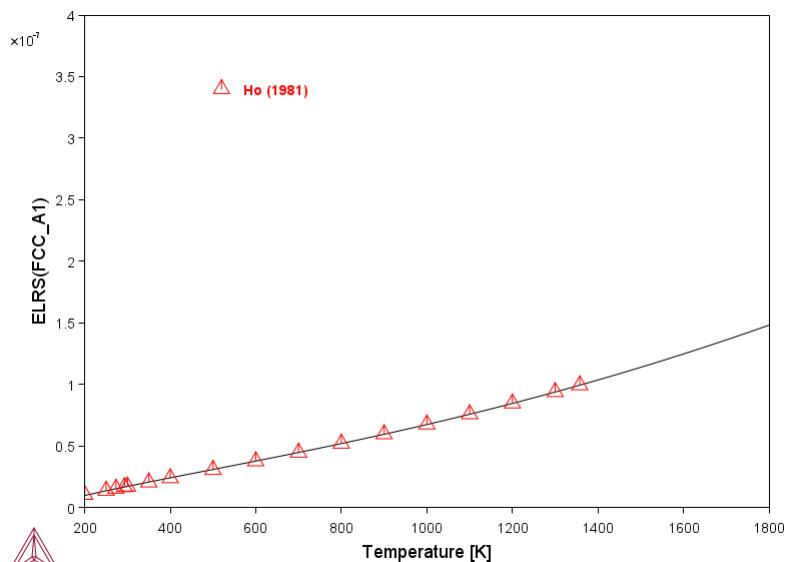
```

POST:
POST:@?plot_elrs_of_system
POST: select,,,
POST: s-d-a y elrs
POST: s-s-s y n 0 4e-7
POST: a-e y 1981Ho_cu_elrs
PROLOGUE NUMBER: /1/: 1
DATASET NUMBER(s): /-1/: 1 2 3
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot,,
```



```

POST:
POST:@?plot_elrs_of_fcc_a1_only
POST: select,,,
POST: s-d-a y elrs(fcc_a1)
POST: s-s-s y n 0 4e-7
POST: a-e y 1981Ho_cu_elrs
PROLOGUE NUMBER: /1/: 1
DATASET NUMBER(s): /-1/: 1 2
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_console_examples\unite\distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot,,
```



POST:
POST: set-inter
POST:

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