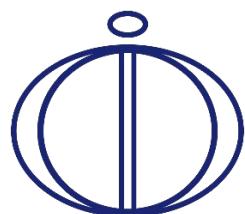


# **Diffusion Module (DICTRA) Example Macros**

**Thermo-Calc Version 2023b**



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## [exa1](#)

One-phase problem. Homogenization of a binary Fe-Ni alloy. In this example it is assumed there is initially a linear Ni-concentration profile.

## [exa2a](#)

One-phase problem. Homogenization of a binary Fe-Ni alloy. A Ni rich and a Ni lean alloy are put together and initially there is a step profile.

## [exa2b](#)

One-phase problem. Homogenization of a binary Fe-Ni alloy. This example is identical to a2a but instead it uses implicit time integration instead of the trapezoidal method for solving the PDEs.

## [exa3](#)

One-phase problem. Uphill diffusion in an Fe-Si-C alloy. This is an example to simulate uphill diffusion in a ternary single phase austenite matrix due to the classical Darken experiment published by L.S. Darken: Trans. Aime, v.180 (1949), pp. 430-438.

## [exa4](#)

One-phase problem. Carburization of binary Fe-C alloy: Comparison to an analytical erf solution. This is a simple binary simulation with a single phase region. The numerical simulation is compared with an analytical erf solution. For this reason a special database erf.tdb is created where the diffusion coefficient is set to a concentration independent value.

## [exa5](#)

One-phase problem. Carburization of a binary Fe-0.15 wt% C alloy. A mixture of 40% N<sub>2</sub> and 60% cracked methanol is used as carrier gas. The carburizing "carbon potential" in the gas is 0.85 wt%. A surface reaction controls the flux of C at the surface.

## [exa6](#)

One-phase problem. Diffusion through a tube wall. A simple example about diffusion through a tube wall. The tube material is an Fe-0.6Mn-0.7Si-0.05C alloy. On the inside wall a carbon activity of 0.9 is maintained whereas on the outside the C-activity is very low. This example demonstrates the use of the command SET-FIRST-INTERFACE as well as the MIXED boundary conditions.

## [exa7](#)

One phase example. Homogenization heat treatment. The initial segregation profile is created from a Scheil calculation (see macro create\_initial\_profile.TCM). The command INPUT\_SCHEIL\_PROFILE in the DICTRA MONITOR performs most of the set up. Only time and temperature must be entered after the INPUT\_SCHEIL\_PROFILE command is executed.

## [exb1a](#)

Moving boundary problem. Austenite to ferrite transformation in a binary Fe-C alloy. This example calculates a ferrite(BCC)/austenite(FCC) transformation in a binary Fe-C alloy. The initial state is an austenite of 2mm thickness. The composition of the austenite is Fe-0.15wt%C.

## [exb1b](#)

Moving boundary problem. Austenite to ferrite transformation in a binary Fe-C alloy. This is the same example as in exb1a but now the problem is with ferrite as an inactive phase adjacent to the initial austenite.

## [exb1c](#)

Moving boundary problem. Austenite to ferrite transformation in a binary Fe-C alloy. This is the same example as in exb1a and exb1b but now the simulation starts at a higher temperature and assumes a gradual cooling down to 1050 K.

## [exb2](#)

Moving boundary problem. Cementite dissolution in an Fe-Cr-C alloy. This example calculates the dissolution of a spherical cementite particle in an austenite matrix. This case is from Z.-K. Liu, L. Håglund, B. Jähnsson and J. Ågren: Metall. Trans.A, v.22A (1991), pp. 1745-1752.

## [exb3](#)

Moving boundary example. Dissolution of 23-carbide in an austenitic matrix. This example calculates the dissolution of an M23C6 particle in an austenite matrix. A film of ferrite is allowed to nucleate around the carbide during the precipitation.

## [exb4a](#)

Moving boundary problem. Solidification path of an Fe-18%Cr-8%Ni alloy: Eutectic reaction. This example demonstrates the solidification path of an Fe-18%Cr-8%Ni alloy. A eutectic reaction is assumed, LIQUID -> BCC + FCC. Hence the BCC and FCC regions should be on separate sides of the liquid region. Comparison is made with both a Scheil-Gulliver simulation and equilibrium solidification conditions, both done in Thermo-Calc.

## [exb4b](#)

Moving boundary problem. Solidification path of an Fe-18%Cr-8%Ni alloy: Peritectic reaction. This example is the same as exb4a but now a peritectic reaction is assumed: LIQUID + BCC -> FCC. Hence the FCC region should appear in between the LIQUID and the BCC. Comparison is made with both a Scheil-Gulliver simulation and equilibrium solidification conditions, both done in Thermo-Calc.

## [exb4c](#)

Moving boundary problem. Solidification path of an Fe-18%Cr-8%Ni alloy. This example is the same as exb4b but now the diffusivity data is amended for the LIQUID and a high value for the diffusivity is used to simulate a case where it is assumed that the composition in the LIQUID is always homogeneous. This example is less realistic than exb4b. Comparison is made with both a Scheil-Gulliver simulation and equilibrium solidification conditions, both done in Thermo-Calc.

## [exb4d](#)

Moving boundary problem. Solidification path of an Fe-18%Cr-8%Ni alloy. This example is the same as exb4b but instead of controlling the temperature the amount of heat extracted is given. Comparison is made with both a Scheil-Gulliver simulation and equilibrium solidification conditions, both done in Thermo-Calc.

## [exb5](#)

Moving boundary problem. Ternary diffusion couple of Fe-Ni-Cr alloys. This example demonstrates the evaluation of a ternary Fe-Cr-Ni diffusion couple. A thin slice of alpha phase (38%Cr, 0%Ni) is clamped between two thicker slices of gamma phase (27%Cr, 20%Ni). The assembly is subsequently heat treated at 1373 K. This example corresponds to diffusion couple A in M. Kajihara, C.-B. Lim and M. Kikuchi: ISIJ International 33 (1993), pp. 498-507. See also M. Kajihara and M. Kikuchi: Acta Metall.Mater. 41 (1993), pp.2045-2059.

## [exb6](#)

Moving boundary problem. Microsegregation of phosphorus. This example illustrates the effect of microsegregation of phosphorus during peritectic solidification in steel.

## [exb7](#)

This example modifies the database interactively, which is not yet supported by GES6. Therefore, we enforce the use of GES5.

## [exc1](#)

Cell calculation. Carbon cannon in ferrite/austenite: Fe-C system, 2-cell calculation This example simulates what happens to a ferrite plate that has inherited the carbon content of its parent austenite. The ferrite plate formed is embedded in an austenite matrix. This setup corresponds to a proposed mechanism for formation of Widmannst tten ferrite or for the ferrite phase of the bainite structure. It is assumed that the phase boundary between ferrite and austenite is immobile, this is achieved in the simulation by putting the ferrite and the austenite in two different cells. See also M. Hillert, L. H glund and J.  gren: Acta Metall. Mater. 41 (1993), pp.1951-1957.

## [exc2](#)

Cell calculation. Cementite dissolution in an Fe-Cr-C alloy: Three particle sizes and three different cells This example calculates the dissolution of cementite particles in an austenite matrix. This example is the same as exc1 but instead there are three particle sizes. A total of six particles are considered using three different cells. This is to represent some size distribution among the cementite particles. See also Z.-K. Liu, L. H glund, B. J nsson and J.  gren: Metall.Trans.A, v. 22A (1991), pp. 1745-1752.

## [exd1a](#)

Diffusion in dispersed systems. Carburization of Ni-25%Cr alloy: Dispersed system model This example is about carburization of a Ni-25Cr alloy. In this case the M3C2 and M7C3 carbides are entered as spheroid phases in a FCC matrix. This simulation can be run with either the DISPERSED SYSTEM MODEL or the HOMOGENIZATION MODEL. In this example the DISPERSED SYSTEM MODEL is used, which requires that the default HOMOGENIZATION MODEL is disabled. With the DISPERSED SYSTEM MODEL the command ENTER\_LABYRINTH\_FUNCTION is used to take into account the impeding effect of dispersed phases on long-range diffusion. For the HOMOGENIZATION MODEL the command ENTER\_HOMOGENIZATION\_FUNCTION should be used. This case is from A. Engstr m, L. H glund and J.  gren: Metall.Trans.A v. 25A (1994), pp. 1127-1134.

## [exd1b](#)

Diffusion in dispersed systems. Carburization of Ni-25%Cr alloy: Homogenization model This example is about carburization of a Ni-25Cr alloy. In this case the M3C2 and M7C3 carbides are entered as spheroid phases in a FCC matrix. This case is from A. Engstr m, L. H glund and J.  gren: Metall.Trans. A, v.25A (1994), pp. 1127-1134. This simulation can be run with the DISPERSED SYSTEM MODEL or HOMOGENIZATION MODEL. The default HOMOGENIZATION MODEL is used and then ENTER\_HOMOGENIZATION\_FUNCTION should be used instead of ENTER\_LABYRINTH\_FUNCTION.

## [exd2a](#)

Diffusion in dispersed systems. Diffusion couple of Fe-Cr-Ni alloys: Dispersed system model This example calculates the interdiffusion in a diffusion couple between a two-phase (FCC+BCC) and a single-phase (FCC) Fe-Ni-Cr alloy. This case is from A. Engstr m: Scand. J. Met., v. 24, 1995, pp.12-20. This simulation can be run with either the DISPERSED SYSTEM MODEL or the HOMOGENIZATION MODEL. In this example the DISPERSED SYSTEM MODEL is used, which requires that the default HOMOGENIZATION MODEL is disabled. With the DISPERSED SYSTEM MODEL the command ENTER\_LABYRINTH\_FUNCTION is used to take into account the impeding effect of dispersed phases on long-range diffusion. For the HOMOGENIZATION MODEL the command ENTER\_HOMOGENIZATION\_FUNCTION should be used.

## [exd2b](#)

Diffusion in dispersed systems. Diffusion couple of Fe-Cr-Ni alloys: Homogenization model This example calculates the interdiffusion in a diffusion couple between a two-phase (FCC+BCC) and a single-phase (FCC) Fe-Ni-Cr alloy. This case is from A. Engstr m: Scand. J. Met., v. 24, 1995, pp.12-20. This simulation can be run with either the DISPERSED SYSTEM MODEL or the HOMOGENIZATION MODEL. Here the default HOMOGENIZATION MODEL is used and then ENTER\_HOMOGENIZATION\_FUNCTION should be used instead of ENTER\_LABYRINTH\_FUNCTION.

## [exd3](#)

Diffusion in dispersed systems. Diffusion couple of Fe-Cr-Ni alloys: Homogenization model This example uses the homogenization model. It is taken from H. Larsson and A. Engstr m, Acta. Mater. v.54 (2006), pp. 2431-2439. Experimental data from A. Engstr m, Scand J Metall, v.243 (1995), p.12. The homogenization model can be used for multiphase simulations like the dispersed system model, but unlike the dispersed system model there is no need to have a single continuous matrix phase and, furthermore, there is no need to limit the size of time-steps. The set-up is performed in the same manner as for the dispersed system model, which means that a certain phase is entered as the matrix phase and the other phases are entered as spheroidal, but the choice of matrix phase will not affect the simulation.

## [exe1](#)

Cooperative growth. Growth of pearlite in an Fe-Mn-C alloy An example of pearlite growth in an Fe-0.50wt%C-0.91wt%Mn steel.

## [exf1](#)

Coarsening problem. Coarsening of M6C precipitate in an Fe-Mo-C alloy This example calculates the Ostwald-ripening of a spherical M6C carbide in an austenite matrix.

## [exg1](#)

Kinetic data example. Checking mobilities and diffusivities in an Fe-Ni alloy This is an example file to check the mobilities and diffusivities in an Fe-Ni alloy.

## [exg2](#)

Kinetic data example. Optimization of mobilities in Ni-Al fcc alloys A file for reading thermodynamic data and setting up the kinetic parameters that are needed for an optimization of the FCC phase in the binary Ni-Al system. See also A. Engstr m and J.  gren: ("Assessment of Diffusional Mobilities in Face-Centered Cubic Ni-Cr-Al Alloys" in Z. Metallkunde, Feb. 1996).

## [exh1](#)

Deviation from local equilibrium. Ferrite/austenite diffusion couple with interface mobility This example calculates the growth of ferrite into austenite with a limited interface mobility. this is done by adding a Gibbs-energy contribution to the ferrite using the SET-SURFACE-ENERGY command.

## [exh2](#)

Deviation from local equilibrium. Ferrite/austenite para-equilibrium in an Fe-Ni-C alloy This example calculates the growth of ferrite into austenite in an Fe-2.02%Ni-0.0885%C alloy using the para-equilibrium model. The results are compared with experimental information from Hutchinson, C. R., A. Fuchsmann, and Yves Brechet. "The diffusional formation of ferrite from austenite in Fe-C-Ni alloys." Metall. Mat. Trans. A 35.4 (2004): 1211-1221.

## [exh3](#)

Deviation from local equilibrium. Diffusion induced by a temperature gradient (thermomigration) This calculation shows how a temperature gradient induces diffusion.

## [exi1](#)

Diffusion in complex phases. Diffusion in a system with B2 ordering This example shows diffusion in a system with B2 ordering. The datafile AlFeNi-data.TDB contains both a thermodynamic and kinetic description for the ordered and disordered BCC.

## [exi2](#)

Diffusion in complex phases. Diffusion of carbon in cementite This example demonstrates the use of the model for calculation of diffusion through a stoichiometric phase. The flux of a component in the stoichiometric phase is assumed to be proportional to the difference in chemical potential at each side of the stoichiometric phase multiplied with the mobility for the component in the phase. The mobility is assessed from experimental information and is basically the tracer diffusivity for the component.

## [exi3a](#)

Diffusion in complex phases. Diffusion in iron oxide (FeO) This example shows the oxidation of an iron sample and the consequent growth of an oxide layer.

## [exi3b](#)



## One-Phase Problems



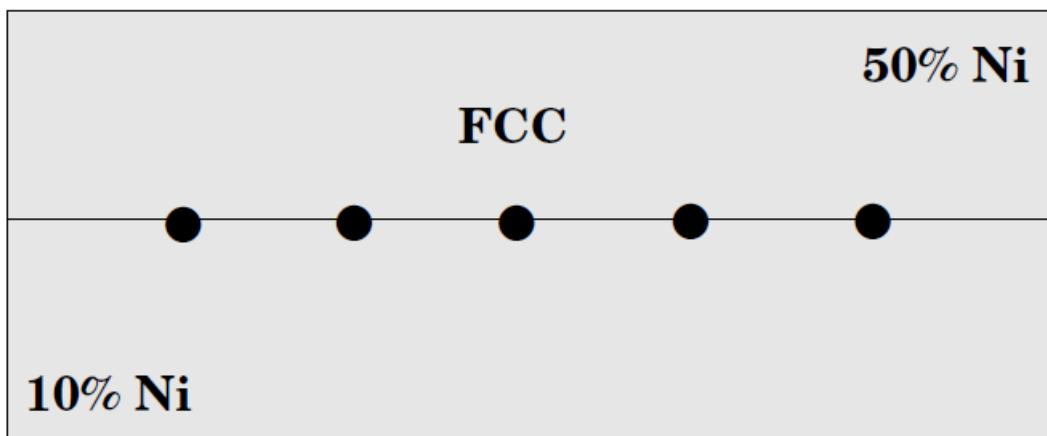


## Example exa1

### Homogenization of a binary Fe-Ni alloy: Linear Concentration Profile

Simple homogenization of a binary Fe-Ni alloy. It is assumed there is initially a linear Ni-concentration profile.

$$T = 1400 \text{ K}$$



$$1E-4$$

Diffusion in complex phases. Diffusion in iron oxide (FeO) with a grain boundary contribution This example shows the oxidation of an iron sample and consequent growth of an oxide layer using the grain boundary diffusion contribution model.

## Results

### exa1-setup

#### 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\_dictra\_console\_examples\examples\exa1\setup.DCM.test"

SYS: @@  
SYS: @@ One-phase problem.  
SYS: @@ Homogenization of a binary Fe-Ni alloy.  
SYS: @@ In this example it is assumed there is initially a linear  
SYS: @@ Ni-concentration profile.  
SYS: -----

NO SUCH COMMAND, USE HELP

SYS:  
SYS: @@  
SYS: @@ START BY GOING TO THE DATABASE MODULE  
SYS: @@

SYS: goto\_module  
MODULE NAME: data  
THERMODYNAMIC DATABASE module  
Database folder:  
C:\jenkins\workspace\generate\_dictra\_console\_examples\databases\data  
Current database: Steels/Fe-Alloys v12.0

VA /- DEFINED

DICTRA\_FCC\_A1 REJECTED

TDB\_TCFE12: @@

TDB\_TCFE12: @@ USE THERMODYNAMIC DATABASE TO RETRIEVE DATA

TDB\_TCFE12: @@

TDB\_TCFE12: switch\_database  
Use one of these databases

TCFE12 = Steels/Fe-Alloys v12.0  
TCFE9 = Steels/Fe-Alloys v9.3  
SSUB6 = SGTE Substances v6.0  
FEDEMO = Iron Demo Database v4.0  
MOB2 = Alloys Mobility v2.7  
MOBFE2 = Steels/Fe-Alloys Mobility v2.0  
MOBFE4 = Steels/Fe-Alloys Mobility v4.0  
MOBFE7 = Steels/Fe-Alloys Mobility v7.1  
MFEDEMO = Fe-Alloys Mobility demo database v2.0  
USER = User defined Database

DATABASE NAME /TCFE12/: fedemo

Current database: Iron Demo Database v4.0

VA /- DEFINED

TDB\_FEDEMO: @@

TDB\_FEDEMO: @@ DEFINE THE SYSTEM TO WORK WITH

TDB\_FEDEMO: @@

TDB\_FEDEMO: define\_system

ELEMENTS: fe ni

FE NI DEFINED

TDB\_FEDEMO: @@

TDB\_FEDEMO: @@

TDB\_FEDEMO: @@ EXCLUDE THE THERMODYNAMIC DATA FOR THE PHASES THAT ARE NOT NEEDED

TDB\_FEDEMO: @@

TDB\_FEDEMO: reject

ELEMENTS, SPECIES, PHASES, CONSTITUENT OR SYSTEM: /PHASES/: phase

PHASES: \*

LIQUID:L BCC\_A2 LAVES\_PHASE\_C14  
CBCC\_A12 CUB\_A1 FCC\_A1

HCP\_A3 REJECTED

TDB\_FEDEMO: @@

TDB\_FEDEMO: @@ RESTORE THE THERMODYNAMIC DATA FOR THE FCC PHASE

TDB\_FEDEMO: @@

TDB\_FEDEMO: restore

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

PHASES: fcc

FCC\_A1 RESTORED

TDB\_FEDEMO: @@

TDB\_FEDEMO: @@ RETRIEVE DATA FROM THE DATABASE FILE

TDB\_FEDEMO: @@

TDB\_FEDEMO: get\_data

14:59:13,665 [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'  
'X.G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar  
volumes'

```

'A.T. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); FE-NI'
'X.G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
-OK-
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ MOBILITY/DIFFUSIVITY DATA ARE STORED IN A SEPARATE DATABASE FILE.
TDB_FEDEMO: @@ SWITCH TO THE MOBILITY DATABASE TO RETRIEVE DATA
TDB_FEDEMO: @@
TDB_FEDEMO: append_database
Use one of these databases

TCFE12 = Steels/Fe-Alloys v12.0
TCFE9 = Steels/Fe-Alloys v9.3
SSUB6 = SGTE Substances v6.0
FEDEMO = Iron Demo Database v4.0
MOB2 = Alloys Mobility v2.7
MOBFE2 = Steels/Fe-Alloys Mobility v2.0
MOBFE4 = Steels/Fe-Alloys Mobility v4.0
MOBFE7 = Steels/Fe-Alloys Mobility v7.1
MFEDEMO = Fe-Alloys Mobility demo database v2.0
USER = User defined Database

DATABASE NAME /FEDEMO:/: mfedemo
Current database: Fe-Alloys Mobility demo database v2.0

VA DEFINED
APP: define_system
ELEMENTS: fe ni
    FE           NI   DEFINED
APP: reject
ELEMENTS, SPECIES, PHASES, CONSTITUENT OR SYSTEM: /PHASES/: phase
PHASES: *
    BCC_A2          FCC_A1  REJECTED
APP:
APP: restore
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /ELEMENTS/: phase
PHASES: fcc
    FCC_A1 RESTORED
APP:
APP: get_data
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

List of references for assessed data

'This parameter has not been assessed'
'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
-Ni'
'Xia, C. H. et al. JAC, 2021, 853, 157165.'
'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Ni self-diffusion'
-OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP
APP: @@
APP: goto_module
MODULE NAME: dictra_monitor
NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set_condition
GLOBAL OR BOUNDARY CONDITION /GLOBAL/: global
VARIABLE : T
LOW TIME LIMIT /0/: 0
T(TIME,X)= 1400;
HIGH TIME LIMIT /*/: *
ANY MORE RANGES /N/: N
DIC>
DIC> @@
DIC> @@ START BY ENTERING A REGION
DIC> @@
DIC> enter_region
REGION NAME : austenite
DIC>
DIC> @@
DIC> @@ ENTER A GRID INTO THE REGION
DIC> @@
DIC> @@ FOR SIMPLICITY, AN EQUIDISTANT GRID IS USED
DIC> @@
DIC> enter_grid_coordinates
REGION NAME : /AUSTENITE/: austenite
WIDTH OF REGION /1/: 1e-4
TYPE /LINEAR/: AUTO
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE active PHASE INTO THE REGION
DIC> @@
DIC> enter_phase_in_region
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /AUSTENITE/: austenite
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC> @@
DIC> @@ ENTER AN INITIAL Ni COMPOSITION INTO THE PHASE. A LINEAR
DIC> @@ VARIATION IN THE REGION IS ASSUMED.
DIC> @@
DIC> enter_compositions
REGION NAME : /AUSTENITE/: austenite
PHASE NAME: /FCC_A1/: fcc#1
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: weight_percent
PROFILE FOR /NI/: ni
TYPE /LINEAR/: linear
VALUE OF FIRST POINT : 10
VALUE OF LAST POINT : /10/: 50

```

```
DIC>
DIC> @@
DIC> @@ THE BOUNDARY CONDITION IS A CLOSED SYSTEM AS WE DO NOT SPECIFY
DIC> @@ ANYTHING ELSE
DIC> @@
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set_simulation_time
END TIME FOR INTEGRATION /.1/: 1E6
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /100000/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO FILE AND EXIT
DIC> @@
DIC> save_workspaces exa1 Y
DIC>
DIC> set_interactive
--OK---
DIC>
```

**exal-run**

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exal\run.DCM.test"
DIC>
DIC>
DIC> @@ exal_run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING EXAMPLE a1
DIC> @@
DIC> goto module
MODULE NAME: dictra_monitor
TIME STEP AT TIME 0.00000E+00
DIC>
DIC> read_workspaces exal
OK
DIC>
DIC> @@
DIC> @@ Start the simulation
DIC> @@
DIC> simulate_reaction
Region: AUSTENITE
linear grid 75
DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
U-FRACTION IN SYSTEM: FE = .709680136600384 NI = .290319863399616
TOTAL SIZE OF SYSTEM: 1E-04 [m]
U-FRACTION IN SYSTEM: FE = .709680136600384 NI = .290319863399616
TOTAL SIZE OF SYSTEM: 1E-04 [m]
TIME = 0.1000000E-06 DT = 0.1000000E-06 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680136600384 NI = .290319863399616
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.1001000E-03 DT = 0.1000000E-03 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680136600384 NI = .290319863399616
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.40010010 DT = 0.40000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680136600384 NI = .290319863399616
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 183.71515 DT = 183.31505 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680136600384 NI = .290319863399616
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 550.34526 DT = 366.63011 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680136600384 NI = .290319863399616
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 1 seconds
TIME = 1283.6055 DT = 733.26022 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680136600384 NI = .290319863399616
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 2750.1259 DT = 1466.5204 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680136600384 NI = .290319863399616
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 5683.1668 DT = 2933.0409 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680136600385 NI = .290319863399616
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 11549.249 DT = 5866.0817 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680136600384 NI = .290319863399616
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 23281.412 DT = 11732.163 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680136600384 NI = .290319863399616
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 46745.739 DT = 23464.327 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680136600384 NI = .290319863399616
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 93674.393 DT = 46928.654 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680136600385 NI = .290319863399616
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 187531.70 DT = 93857.308 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680136600384 NI = .290319863399615
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 287531.70 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680136600382 NI = .290319863399618
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 387531.70 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680136600383 NI = .290319863399617
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 487531.70 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680136600383 NI = .290319863399617
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 587531.70 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680136600382 NI = .290319863399618
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 687531.70 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680136600382 NI = .290319863399618
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 787531.70 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680136600382 NI = .290319863399618
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 887531.70 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680136600382 NI = .290319863399618
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 987531.70 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680136600383 NI = .290319863399617
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
```

```
TIME = 1000000.0 DT = 12468.299 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680136600383 NI = .290319863399617
TOTAL SIZE OF SYSTEM: 1E-04 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 0.0000000
DELETING TIME-RECORD FOR TIME 0.10000000E-06
DELETING TIME-RECORD FOR TIME 0.10010000E-03
DELETING TIME-RECORD FOR TIME 0.40010010
DELETING TIME-RECORD FOR TIME 183.71515
DELETING TIME-RECORD FOR TIME 550.34526
DELETING TIME-RECORD FOR TIME 1283.6055
DELETING TIME-RECORD FOR TIME 2750.1259
DELETING TIME-RECORD FOR TIME 5683.1668
DELETING TIME-RECORD FOR TIME 11549.249
DELETING TIME-RECORD FOR TIME 23281.412
DELETING TIME-RECORD FOR TIME 46745.739
DELETING TIME-RECORD FOR TIME 93674.393
DELETING TIME-RECORD FOR TIME 187531.70
DELETING TIME-RECORD FOR TIME 287531.70
DELETING TIME-RECORD FOR TIME 387531.70
DELETING TIME-RECORD FOR TIME 487531.70
DELETING TIME-RECORD FOR TIME 587531.70
DELETING TIME-RECORD FOR TIME 687531.70
DELETING TIME-RECORD FOR TIME 787531.70
DELETING TIME-RECORD FOR TIME 887531.70

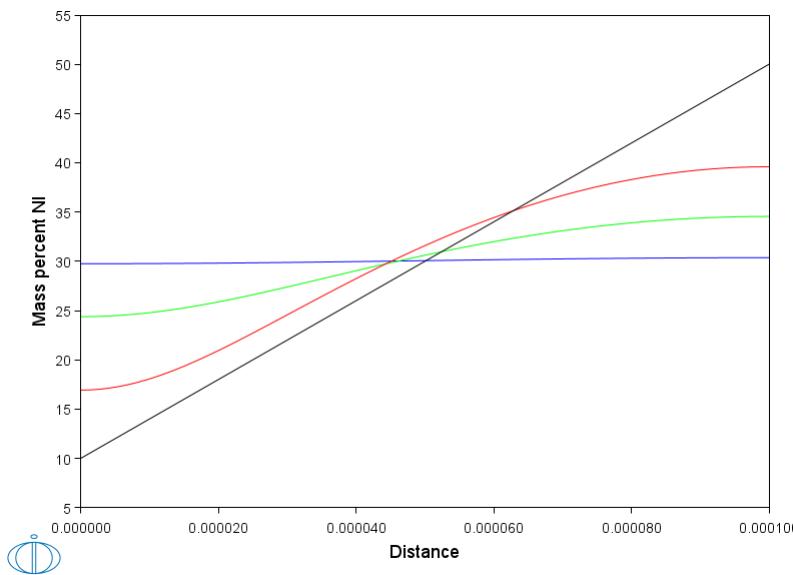
KEEPING TIME-RECORD FOR TIME 987531.70
AND FOR TIME 1000000.0
WORKSPACE RECLAIMED
```

```
TIMESTEP AT 1000000.00 SELECTED

DIC>
DIC> @@
DIC> @@ THE SIMULATION IS FINISHED
DIC> @@
DIC>
DIC> set_interactive
--OK---
DIC>
```

**exal-plot**

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exal\plot.DCM.test"
DIC>
DIC>
DIC> @@ exal_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE a1
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> goto_module
MODULE NAME: dictra_monitor
TIME STEP AT TIME 1.00000E+06
DIC> read_workspaces exal
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post_processor
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1:
POST-1: @@
POST-1: @@ PLOT SOME CONCENTRATION PROFILES
POST-1: @@
POST-1: set_diagram_axis
AXIS (X, Y OR Z) : x
VARIABLE : distance
INFO: Distance is set as independent variable
DISTANCE : /GLOBAL/: global
POST-1:
POST-1: set_diagram_axis
AXIS (X, Y OR Z) : y
VARIABLE : weight-percent
FOR COMPONENT : ni
POST-1:
POST-1: set_plot_condition
CONDITION /TIME/: time
VALUE(S) /LAST/: 0 1e5 3e5 1e6
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot_diagram
```



```
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: set_interactive
--OK---
POST-1:
```

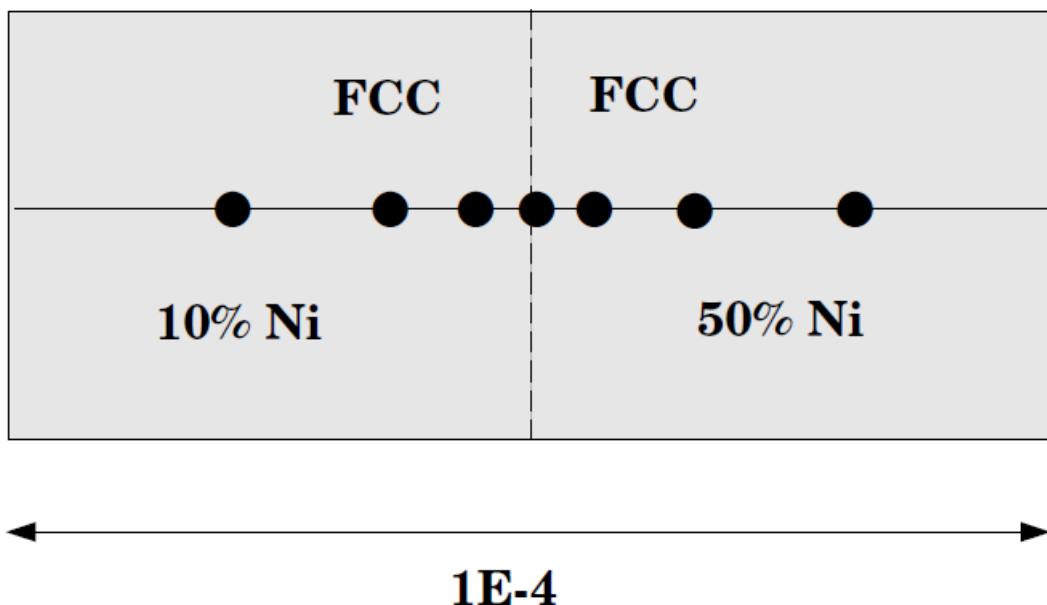


## Example exa2a

### Homogenization of a binary Fe-Ni alloy: Step-profile

Simple homogenization of a binary Fe-Ni alloy. A Ni rich and a Ni lean alloy are put together and initially there is a step profile.

$$T = 1400 \text{ K}$$



**exa2a-setup****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_dictra_console_examples\examples\exa2a\setup.DCM.test"
SYS: @@
SYS: @@ One-phase problem.
SYS: @@ Homogenization of a binary Fe-Ni alloy.
SYS: @@ A Ni rich and a Ni lean alloy are put together and initially
SYS: @@ there is a step profile.
SYS: -----
NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exa2a_setup.DCM
SYS:
SYS: @@
SYS: @@ IN exa1 ALL THE COMMANDS WERE WRITTEN IN FULL BUT NOW ABBREVIATED
SYS: @@ COMMANDS ARE USED
SYS: @@
SYS:
SYS: @@
SYS: @@ FIRST DEFINE A LOG-FILE FOR THIS EXAMPLE
SYS: @@
SYS: set_log_file setup
Heading:
SYS: @@
SYS: @@ NOW GO TO THE DATABASE MODULE
SYS: @@
SYS: go da
... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\generate_dictra_console_examples\databases\data
Current database: Steels/Fe-Alloys v12.0

VA           /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE12: @@
TDB_TCFE12: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA
TDB_TCFE12: @@
TDB_TCFE12: sw FEDEMO
... the command in full is SWITCH_DATABASE
Current database: Iron Demo Database v4.0

VA           /- DEFINED
TDB_FEDEMO: @@
TDB_FEDEMO: @@ DEFINE THE SYSTEM TO WORK WITH
TDB_FEDEMO: @@
TDB_FEDEMO: def-system fe ni
... the command in full is DEFINE_SYSTEM
FE          NI DEFINED
TDB_FEDEMO: @@
TDB_FEDEMO: @@ EXCLUDE THE THERMODYNAMIC DATA FOR THE PHASES THAT ARE NOT NEEDED
TDB_FEDEMO: @@
TDB_FEDEMO: rej ph * all
... the command in full is REJECT
LIQUID:L      BCC_A2          LAVES_PHASE_C14
CBCC_A12     CUB_A13        FCC_A1
HCP_A3       REJECTED
TDB_FEDEMO: res ph fcc
... the command in full is RESTORE
FCC_A1       RESTORED
TDB_FEDEMO: @@
TDB_FEDEMO: @@ RETRIEVE DATA FROM THE DATABASE FILE
TDB_FEDEMO: @@
TDB_FEDEMO: get
... the command in full is GET_DATA
15:02:27,976 [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.T. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
'X.G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
    volumes'
'A.T. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); FE-NI'
'X.G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
-OK-
TDB_FEDEMO: @@
TDB_FEDEMO: @@ MOBILITY/DIFFUSIVITY DATA ARE STORED IN A SEPARATE DATABASE FILE.
TDB_FEDEMO: @@ SWITCH TO THE MOBILITY DATABASE TO RETRIEVE DATA
TDB_FEDEMO: @@
TDB_FEDEMO: app
... the command in full is APPEND_DATABASE
Use one of these databases

TCFE12 = Steels/Fe-Alloys v12.0
TCFE9  = Steels/Fe-Alloys v9.3
SSUB6  = SGTE Substances v6.0
```





```
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 1E6
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /100000/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO FILE AND EXIT
DIC> @@
DIC> save exa2a Y
... the command in full is SAVE_WORKSPACES
DIC>
DIC> set-inter
... the command in full is SET_INTERACTIVE
--OK--
DIC>
```

**exa2a-run**

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exa2a\run.DCM.test"
... the command in full is MACRO_FILE_OPEN
DIC>
DIC>
DIC> @@ exa2a_run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING EXAMPLE a2a
DIC> @@
DIC>
DIC> @@
DIC> @@ LET US DEFINE A LOG-FILE FOR THIS EXAMPLE
DIC> @@
DIC> @@set-log-file run
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA MONITOR AN READ SETUP FROM FILE
DIC> @@
DIC> go d-m
... the command in full is GOTO_MODULE
TIME STEP AT TIME 0.00000E+00
DIC>
DIC> read exa2a
... the command in full is READ_WORKSPACES
... the command in full is DEFINE_COMPONENTS
... the command in full is SELECT_EQUILIBRIUM
OK
DIC>
DIC> @@
DIC> @@ START THE SIMULATION
DIC> @@
DIC> simulate
... the command in full is SIMULATEREACTION
DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
... the command in full is SET_NUMERICAL_LIMITS
U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
2 GRIDPOINT(S) ADDED TO CELL #1 REGION: AUSTENITE
TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.10010000E-03 DT = 0.10000000E-03 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.40010010 DT = 0.40000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 8.1787785 DT = 7.7786784 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 23.736135 DT = 15.557357 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 54.850849 DT = 31.114714 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 117.08028 DT = 62.229428 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 241.53913 DT = 124.45886 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 490.45684 DT = 248.91771 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 1 seconds
TIME = 988.29226 DT = 497.83542 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 1983.9631 DT = 995.67084 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 3975.3048 DT = 1991.3417 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 7957.9881 DT = 3982.6834 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 15923.355 DT = 7965.3667 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 31854.088 DT = 15930.733 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 63715.555 DT = 31861.467 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406171 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 127438.49 DT = 63722.934 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406174 NI = .291111754593826
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 227438.49 DT = 100000.00 SUM OF SQUARES = 0.0000000
```

```

U-FRACTION IN SYSTEM: FE = .708888245406174 NI = .291111754593826
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 327438.49 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406173 NI = .291111754593827
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 427438.49 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406172 NI = .291111754593828
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 627438.49 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406173 NI = .291111754593827
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 827438.49 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406172 NI = .291111754593828
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 927438.49 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406172 NI = .291111754593828
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 1000000.0 DT = 72561.511 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406172 NI = .291111754593828
TOTAL SIZE OF SYSTEM: 1E-04 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 0.0000000
DELETING TIME-RECORD FOR TIME 0.10000000E-06
DELETING TIME-RECORD FOR TIME 0.10010000E-03
DELETING TIME-RECORD FOR TIME 0.40010010
DELETING TIME-RECORD FOR TIME 8.1787785
DELETING TIME-RECORD FOR TIME 23.736135
DELETING TIME-RECORD FOR TIME 54.850849
DELETING TIME-RECORD FOR TIME 117.08028
DELETING TIME-RECORD FOR TIME 241.53913
DELETING TIME-RECORD FOR TIME 490.45684
DELETING TIME-RECORD FOR TIME 988.29226
DELETING TIME-RECORD FOR TIME 1983.9631
DELETING TIME-RECORD FOR TIME 3975.3048
DELETING TIME-RECORD FOR TIME 7957.9881
DELETING TIME-RECORD FOR TIME 15923.355
DELETING TIME-RECORD FOR TIME 31854.088
DELETING TIME-RECORD FOR TIME 63715.555
DELETING TIME-RECORD FOR TIME 127438.49
DELETING TIME-RECORD FOR TIME 227438.49
DELETING TIME-RECORD FOR TIME 327438.49
DELETING TIME-RECORD FOR TIME 427438.49
DELETING TIME-RECORD FOR TIME 527438.49
DELETING TIME-RECORD FOR TIME 627438.49
DELETING TIME-RECORD FOR TIME 727438.49
DELETING TIME-RECORD FOR TIME 827438.49

KEEPING TIME-RECORD FOR TIME 927438.49
AND FOR TIME 1000000.0
WORKSPACE RECLAIMED

```

```

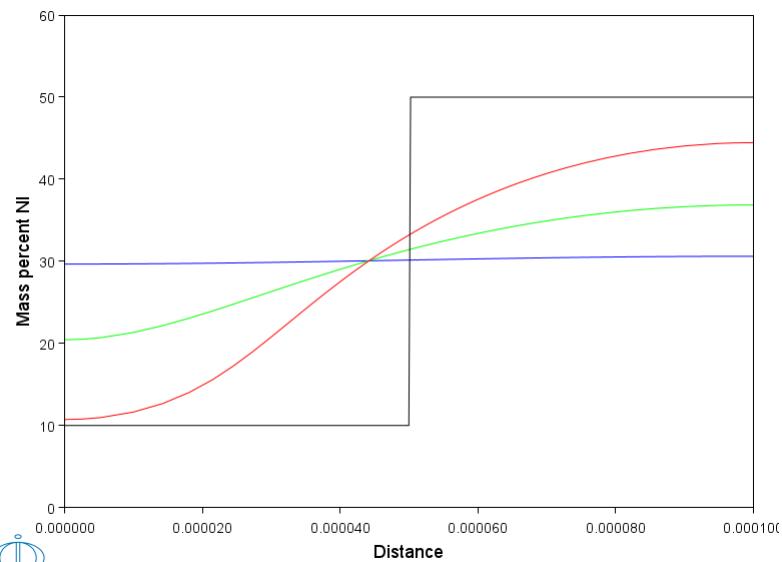
TIMESTEP AT 1000000.00 SELECTED

DIC>
DIC> @@
DIC> @@ THE SIMULATION IS FINISHED
DIC> @@
DIC>
DIC> set-inter
... the command in full is SET_INTERACTIVE
--OK--
DIC>

```

**exa2a-plot**

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exa2a\plot.DCM.test"
... the command in full is MACRO_FILE_OPEN
DIC>
DIC>
DIC> @@ exa2a_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE a2a
DIC> @@
DIC>
DIC> @@
DIC> @@ LET US DEFINE A LOG-FILE FOR THIS EXAMPLE
DIC> @@
DIC> set-log-file plot
AMBIGUOUS COMMAND, USE HELP
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
... the command in full is GOTO_MODULE
TIME STEP AT TIME 1.00000E+06
DIC>
DIC> read exa2a
... the command in full is READ_WORKSPACES
... the command in full is DEFINE_COMPONENTS
... the command in full is SELECT_EQUILIBRIUM
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
... the command in full is POST_PROCESSOR
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1:
POST-1: @@
POST-1: @@ PLOT SOME NI-CONCENTRATION PROFILES
POST-1: @@
POST-1: s-d-a
... the command in full is SET_DIAGRAM_AXIS
AXIS (X, Y OR Z) : x
VARIABLE : dist
INFO: Distance is set as independent variable
... the command in full is SET_INDEPENDENT_VARIABLE
DISTANCE : /GLOBAL/: glo
POST-1:
POST-1: s-d-a
... the command in full is SET_DIAGRAM_AXIS
AXIS (X, Y OR Z) : y
VARIABLE : weight-percent
FOR COMPONENT : ni
POST-1:
POST-1: s-p-c
... the command in full is SET_PLOT_CONDITION
CONDITION /TIME/: time
VALUE(S) /LAST/: 0 1e5 3e5 1e6
POST-1:
POST-1: @@
POST-1: @@ SET SCALING ON Y-AXIS BEFORE PLOTTING
POST-1: @@
POST-1: s-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 : 60
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFILE
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
... the command in full is PLOT_DIAGRAM
```



```
POST-1:  
POST-1:  
POST-1:  
POST-1:@?<Hit_return_to_continue>  
POST-1:  
POST-1: set-inter  
... the command in full is SET_INTERACTIVE_MODE  
--OK--  
POST-1:
```

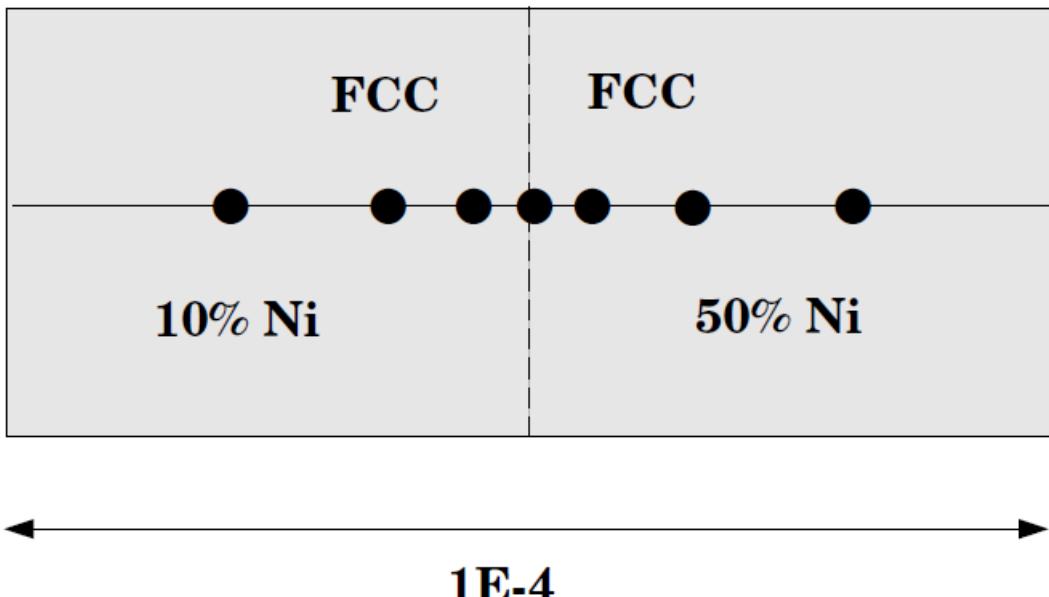


## Example exa2b

### Homogenization of a binary Fe-Ni alloy

Simple homogenization of a binary Fe-Ni alloy. We have put together a Ni rich and a Ni lean alloy. This example is identical to exa2a. However, in this example implicit time integration is used instead of the trapezoidal method for solving the PDEs.

**T = 1400 K**



**exa2b-setup****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_dictra_console_examples\examples\exa2b\setup.DCM.test"
SYS: @@
SYS: @@ One-phase problem.
SYS: @@ Homogenization of a binary Fe-Ni alloy.
SYS: @@ This example is identical to a2a but instead it uses implicit time
SYS: @@ integration instead of the trapezoidal method for solving the PDEs.
SYS: -----
NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exa2b_setup.DCM
SYS:
SYS: @@
SYS: @@ FIRST DEFINE A LOG-FILE FOR THIS EXAMPLE
SYS: @@
SYS: set_log_file setup
Heading:
SYS: @@
SYS: @@ THEN GO TO THE DATABASE MODULE
SYS: @@
SYS: go da
... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\generate_dictra_console_examples\databases\data
Current database: Steels/Fe-Alloys v12.0

VA           /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE12:
TDB_TCFE12: @@
TDB_TCFE12: @@ USE THE TCFE DATABASE FOR THERMODYNAMIC DATA
TDB_TCFE12: @@
TDB_TCFE12: sw fedemo
... the command in full is SWITCH_DATABASE
Current database: Iron Demo Database v4.0

VA           /- DEFINED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ DEFINE THE SYSTEM TO WORK WITH
TDB_FEDEMO: @@
TDB_FEDEMO: def-system fe ni
... the command in full is DEFINE_SYSTEM
FE           NI DEFINED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ EXCLUDE THE THERMODYNAMIC DATA FOR THE PHASES THAT ARE NOT NEEDED
TDB_FEDEMO: @@
TDB_FEDEMO: rej ph * all
... the command in full is REJECT
LIQUID:L      BCC_A2          LAVES_PHASE_C14
CBCC_A12      CUB_A13        FCC_A1
HCP_A3        REJECTED
TDB_FEDEMO: res ph fcc
... the command in full is RESTORE
FCC_A1        RESTORED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ RETRIEVE DATA FROM THE DATABASE FILE
TDB_FEDEMO: @@
TDB_FEDEMO: get
... the command in full is GET_DATA
15:05:41,817 [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.T. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
'X.G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
    volumes'
'A.T. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); FE-NI'
'X.G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
-OK
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ MOBILITY/DIFFUSIVITY DATA ARE STORED IN A SEPARATE DATABASE FILE.
TDB_FEDEMO: @@ SWITCH TO THE MOBILITY DATABASE TO RETRIEVE DATA.
TDB_FEDEMO: @@
TDB_FEDEMO: app
... the command in full is APPEND_DATABASE
Use one of these databases

TCFE12 = Steels/Fe-Alloys v12.0
TCFE9 = Steels/Fe-Alloys v9.3
SSUB6 = SGTE Substances v6.0
FEDEMO = Iron Demo Database v4.0
MOB2 = Alloys Mobility v2.7
MOBFE2 = Steels/Fe-Alloys Mobility v2.0
MOBFE4 = Steels/Fe-Alloys Mobility v4.0
MOBFE7 = Steels/Fe-Alloys Mobility v7.1
```





```
DIC> s-s-c
... the command in full is SET_SIMULATION_CONDITION
NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /AUTO/:
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPLICITY WHEN INTEGRATING PDES (AUTO, 0 -> 0.5 -> 1): /AUTO/: 1.0
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/: @@ SET THE SIMULATION TIME
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 1E6
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /100000/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO FILE AND EXIT
DIC> @@
DIC> save exa2b Y
... the command in full is SAVE_WORKSPACES
DIC>
DIC> set-inter
... the command in full is SET_INTERACTIVE
--OK---
DIC>
```

**exa2b-run**

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exa2b\run.DCM.test"
... the command in full is MACRO_FILE_OPEN
DIC>
DIC>
DIC> @@ exa2b_run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING EXAMPLE a2b
DIC> @@
DIC> @@
DIC> @@
DIC> @@ LET US DEFINE A LOG-FILE FOR THIS EXAMPLE
DIC> @@
DIC> set-log-file run
AMBIGUOUS COMMAND, USE HELP
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA MONITOR AND READ SETUP FROM FILE
DIC> @@
DIC> go d-m
... the command in full is GOTO_MODULE
TIME STEP AT TIME 0.00000E+00
DIC> read exa2b
... the command in full is READ_WORKSPACES
... the command in full is DEFINE_COMPONENTS
... the command in full is SELECT_EQUILIBRIUM
OK
DIC>
DIC> @@
DIC> @@ Start the simulation
DIC> @@
DIC> simulate
... the command in full is SIMULATE_REACTION
... the command in full is SET_NUMERICAL_LIMITS
U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
2 GRIDPOINT(S) ADDED TO CELL #1 REGION: AUSTENITE
TIME = 0.1000000E-06 DT = 0.1000000E-06 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.1001000E-03 DT = 0.1000000E-03 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.40010010 DT = 0.40000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 8.1713545 DT = 7.7712544 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 23.713863 DT = 15.542509 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 54.798881 DT = 31.085018 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 116.96892 DT = 62.170036 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 241.30899 DT = 124.34007 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 489.98913 DT = 248.68014 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 987.34941 DT = 497.36028 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 1982.0700 DT = 994.72057 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 3971.5111 DT = 1989.4411 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 7950.3934 DT = 3978.8823 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 15908.158 DT = 7957.7646 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .291111754593831
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 31823.687 DT = 15915.529 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .291111754593831
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 63654.745 DT = 31831.058 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406168 NI = .291111754593832
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 127316.86 DT = 63662.116 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406166 NI = .291111754593834
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 227316.86 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .70888824540616 NI = .29111175459384
```

```

TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep          0 seconds
TIME = 327316.86 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406157 NI = .291111754593843
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep          0 seconds
TIME = 427316.86 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406158 NI = .291111754593842
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep          0 seconds
TIME = 527316.86 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406155 NI = .291111754593846
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep          0 seconds
TIME = 627316.86 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406157 NI = .291111754593842
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep          0 seconds
TIME = 727316.86 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406153 NI = .291111754593847
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep          0 seconds
TIME = 827316.86 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406154 NI = .291111754593846
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep          0 seconds
TIME = 927316.86 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406153 NI = .291111754593847
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep          0 seconds
TIME = 1000000.0 DT = 72683.138 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406156 NI = .291111754593844
TOTAL SIZE OF SYSTEM: 1E-04 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 0.0000000
DELETING TIME-RECORD FOR TIME 0.10000000E-06
DELETING TIME-RECORD FOR TIME 0.10010000E-03
DELETING TIME-RECORD FOR TIME 0.40010010
DELETING TIME-RECORD FOR TIME 8.1713545
DELETING TIME-RECORD FOR TIME 23.713863
DELETING TIME-RECORD FOR TIME 54.798881
DELETING TIME-RECORD FOR TIME 116.96892
DELETING TIME-RECORD FOR TIME 241.30899
DELETING TIME-RECORD FOR TIME 489.98913
DELETING TIME-RECORD FOR TIME 987.34941
DELETING TIME-RECORD FOR TIME 1982.0700
DELETING TIME-RECORD FOR TIME 3971.5111
DELETING TIME-RECORD FOR TIME 7950.3934
DELETING TIME-RECORD FOR TIME 15908.158
DELETING TIME-RECORD FOR TIME 31823.687
DELETING TIME-RECORD FOR TIME 63654.745
DELETING TIME-RECORD FOR TIME 127316.86
DELETING TIME-RECORD FOR TIME 227316.86
DELETING TIME-RECORD FOR TIME 327316.86
DELETING TIME-RECORD FOR TIME 427316.86
DELETING TIME-RECORD FOR TIME 527316.86
DELETING TIME-RECORD FOR TIME 627316.86
DELETING TIME-RECORD FOR TIME 727316.86
DELETING TIME-RECORD FOR TIME 827316.86

KEEPING TIME-RECORD FOR TIME 927316.86
AND FOR TIME 1000000.0
WORKSPACE RECLAIMED

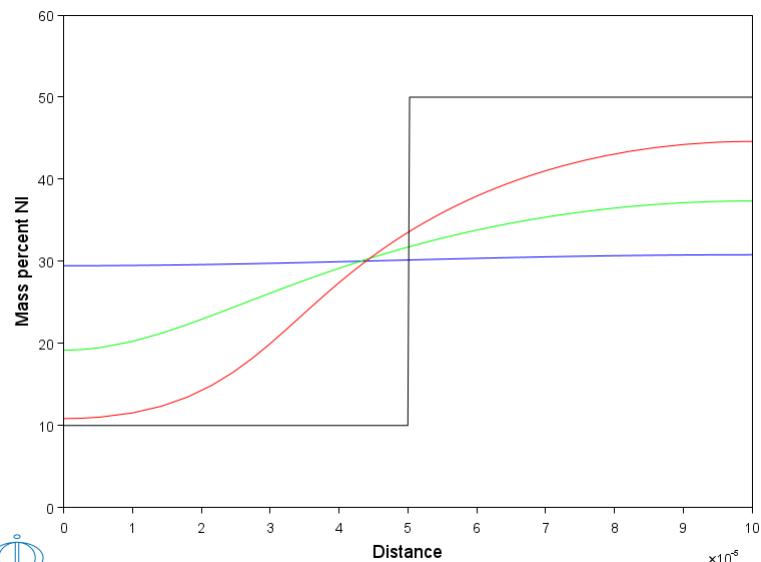
TIMESTEP AT 1000000.00 SELECTED
```

```

DIC>
DIC> @@
DIC> @@ THE SIMULATION IS FINISHED
DIC> @@
DIC>
DIC> set-inter
... the command in full is SET_INTERACTIVE
--OK--
DIC>
```

**exa2b-plot**

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exa2b\plot.DCM.test"
... the command in full is MACRO_FILE_OPEN
DIC>
DIC>
DIC> @@ exa2b_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE a2b
DIC> @@
DIC> @@
DIC> @@ LET US DEFINE A LOG-FILE FOR THIS EXAMPLE
DIC> @@
DIC> set-log-file plot
AMBIGUOUS COMMAND, USE HELP
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
... the command in full is GOTO_MODULE
TIME STEP AT TIME 1.00000E+06
DIC> read exa2b
... the command in full is READ_WORKSPACES
... the command in full is DEFINE_COMPONENTS
... the command in full is SELECT_EQUILIBRIUM
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
... the command in full is POST_PROCESSOR
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1:
POST-1: @@
POST-1: @@ PLOT SOME CONCENTRATION PROFILES
POST-1: @@
POST-1: s-d-a
... the command in full is SET_DIAGRAM_AXIS
AXIS (X, Y OR Z) : x
VARIABLE : dist
INFO: Distance is set as independent variable
... the command in full is SET_INDEPENDENT_VARIABLE
DISTANCE : /GLOBAL/: glo
POST-1:
POST-1: s-d-a
... the command in full is SET_DIAGRAM_AXIS
AXIS (X, Y OR Z) : y
VARIABLE : w-p
FOR COMPONENT : ni
POST-1:
POST-1: s-p-c
... the command in full is SET_PLOT_CONDITION
CONDITION /TIME/: time
VALUE(S) /LAST/: 0 1e5 3e5 1e6
POST-1:
POST-1: @@
POST-1: @@ SET SCALING ON Y-AXIS BEFORE PLOTTING
POST-1: @@
POST-1: s-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 : 60
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFILE
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
... the command in full is PLOT_DIAGRAM
```



POST-1:  
POST-1:  
POST-1:  
POST-1:@?<Hit\_return\_to\_continue>  
POST-1:  
POST-1: set-inter  
... the command in full is SET\_INTERACTIVE\_MODE  
--OK--  
POST-1:



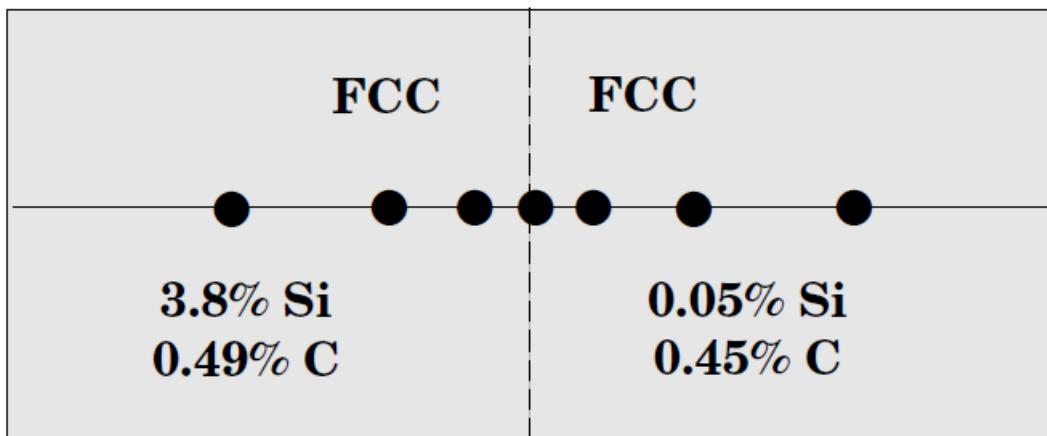
## Example exa3

### Uphill diffusion in an Fe-Si-C alloy

Simulation of uphill diffusion in a ternary single phase austenite matrix due to the classical darken experiment published by L.S. Darken (Trans. Aime, v.180 (1949), pp. 430-438).

In this example, two pieces of austenite (3.80 wt%Si, 0.49 wt%C) and (0.05 wt%Si, 0.45 wt%C) are put together and are subsequently annealed at 1050 C for 13 days. As both pieces are austenite they must be entered into the same region. This is done by giving the compositions of Si and C in each gridpoint individually. These data are then stored on file.

$$T = 1323 \text{ K}$$



**exa3-setup****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_dictra_console_examples\examples\exa3\setup.DCM.test"
SYS: @@
SYS: @@ One-phase problem.
SYS: @@ Uphill diffusion in an Fe-Si-C alloy
SYS: @@ This is an example to simulate uphill diffusion in a ternary single
SYS: @@ phase austenite matrix due to the classical Darken experiment published
SYS: @@ by L.S. Darken: Trans. Aime, v.180 (1949), pp. 430-438.
SYS: @@
SYS: @@ In this example two pieces of austenite (3.80 wt%Si, 0.49 wt%C) and
SYS: @@ (0.05 wt%Si, 0.45 wt%C) are put together and are subsequently annealed
SYS: @@ at 1050C for 13 days. As both pieces are austenite they must be entered
SYS: @@ into the same region. This is done by individually giving the compositions
SYS: @@ of Si and C in each grid point. These data are then stored to file.
SYS: -----
NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ darken_setup.DCM
SYS:
SYS: @@
SYS: @@ Note that LOG-FILES used previously in examples a2a and a2b are
SYS: @@ no longer used.
SYS: @@
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASE
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\generate_dictra_console_examples\databases\data
Current database: Steels/Fe-Alloys v12.0

VA          /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE12:
TDB_TCFE12: @@
TDB_TCFE12: @@ USE A TCFE DATABASE FOR THE THERMODYNAMIC DATA
TDB_TCFE12: @@
TDB_TCFE12: sw tcfe9
Current database: Steels/Fe-Alloys v9.3

VA          /- DEFINED
L12_FCC      B2_BCC           DICTRA_FCC_A1
REJECTED
TDB_TCFE9: def-sys fe si c
FE           SI               C
DEFINED
TDB_TCFE9: rej ph * all
GAS:G          LIQUID:L        BCC_A2
FCC_A1         HCP_A3         CBCC_A12
CUB_A13        DIAMOND_FCC_A4 GRAPHITE
CEMENTITE      M23C6          M7C3
M5C2          KSI_CARBIDE    FE4N_LP1
FECN_CHI        LAVES_PHASE_C14 M3SI
CR3SI          FE2SI          FESI2_H
FESI2_L         MSI            M5SI3
AL4C3          FE8SI2C      SIC
AL5FE4        MP_B31         M2P_C22
M203C:I REJECTED
TDB_TCFE9: res ph fcc
FCC_A1 RESTORED
TDB_TCFE9: get
15:08:55,694 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS .....
FUNCTIONS .....

List of references for assessed data

'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
'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. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
'J. Lacaze and B. Sundman, Metall. Mater. Trans. A, 22A (1991) 2211-2223;
  Fe-Si and Fe-Si-C'
'J. Miettinen and B. Hallstedt, CALPHAD, 22 (1998) 231-256; Fe-Si and Fe
  -Si-C'
-OK-
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE MOBILITY DATA
TDB_TCFE9: @@
TDB_TCFE9: app mobfe4
Current database: Steels/Fe-Alloys Mobility v4.0

VA  DEFINED
B2_BCC REJECTED
APP: def-sys fe si c
FE           SI               C
DEFINED
```

```

APP: rej ph * all
      CEMENTITE          FCC_A1
      FE4N_LP1           HCP_A3        LIQUID:L
      REJECTED

APP: res ph fcc
      FCC_A1 RESTORED
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS .....

List of references for assessed data

'This parameter has not been assessed'
'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'
'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
-Ni'
'D. Bergner et al., Defect and Diffusion Forum 66-69(1989)409. Impurity
diffusion of Si in fcc Fe.'

-OK-
APP:
APP: @@ ENTER THE DICTRA MONITOR
APP: @@ go d-m
NO TIME STEP DEFINED
DIC>
DIC> @@ ENTER GLOBAL CONDITION T
DIC> @@ set-cond glob T 0 1323; * N
DIC>
DIC> @@ ENTER THE REGION austenite
DIC> @@ enter-region
REGION NAME : austenite
DIC>
DIC> @@ ENTER THE GRID
DIC> @@ NOTE THAT GRID POINT DISTANCES ARE SMALLEST AROUND THE MIDDLE
DIC> @@ enter-grid
REGION NAME : /AUSTENITE/: austenite
WIDTH OF REGION /1/: 50E-3
TYPE /LINEAR/: AUTO
DIC>
DIC> @@ ENTER THE PHASE INTO A REGION (BOTH PIECES ARE AUSTENITIC)
DIC> @@ enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /AUSTENITE/: austenite
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC> @@ ENTER COMPOSITIONS INTO THE PHASE
DIC> @@ enter-composition
REGION NAME : /AUSTENITE/: austenite
PHASE NAME: /FCC_A1/: fcc#1
DEPENDENT COMPONENT ? /SI/: FE
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: C func 0.49-0.04*hs(x-25e-3);
PROFILE FOR /SI/: Si func 3.80-3.75*hs(x-25e-3);
DIC>
DIC> @@ SET THE SIMULATION TIME AND OTHER SIMULATION PARAMETERS
DIC> @@ set-simulation-time
END TIME FOR INTEGRATION /.1/: 1e10
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /1E+09/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC> save exa3 Y
DIC>
DIC> set-inter
--OK---
DIC>
```

**exa3-run**

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exa3\run.DCM.test"
DIC>
DIC>
DIC> @@ darken_run.DCM
DIC>
DIC>
DIC> @@ ENTER THE DICTRA MONITOR
DIC> @@
DIC> go d-m
TIME STEP AT TIME 0.00000E+00
DIC>
DIC> @@
DIC> @@ READ SETUP FROM FILE AND START SIMULATION
DIC> @@
DIC> read exa3
OK
DIC>
DIC> sim
Region: AUSTENITE
double geometric
coarse at outer boundaries dense at 0.25047E-01
lower part 0.80000      22
upper part 1.2500       22
DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
U-FRACTION IN SYSTEM: C = .0215351122808224 FE = .96291921367461
SI = .0370807863253901
TOTAL SIZE OF SYSTEM: .05 [m]
U-FRACTION IN SYSTEM: C = .0215351122808224 FE = .96291921367461
SI = .0370807863253901
TOTAL SIZE OF SYSTEM: .05 [m]
TIME = 0.1000000E-06 DT = 0.1000000E-06 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351122808224 FE = .96291921367461
SI = .0370807863253901
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep          0 seconds
TIME = 0.1001000E-03 DT = 0.1000000E-03 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351122808224 FE = .96291921367461
SI = .0370807863253901
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep          0 seconds
TIME = 0.40010010 DT = 0.40000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351122808224 FE = .96291921367461
SI = .0370807863253901
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep          0 seconds
TIME = 21.165600 DT = 20.765500 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351122808224 FE = .96291921367461
SI = .0370807863253901
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep          0 seconds
TIME = 62.696601 DT = 41.531000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351122808224 FE = .96291921367461
SI = .0370807863253901
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep          0 seconds
TIME = 145.75860 DT = 83.062001 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351122808224 FE = .96291921367461
SI = .0370807863253901
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep          0 seconds
TIME = 311.88260 DT = 166.12400 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351122808223 FE = .96291921367461
SI = .0370807863253901
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep          0 seconds
TIME = 644.13060 DT = 332.24800 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351122808223 FE = .96291921367461
SI = .0370807863253901
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep          0 seconds
TIME = 1308.6266 DT = 664.49600 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351122808225 FE = .96291921367461
SI = .0370807863253901
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep          0 seconds
TIME = 2637.6186 DT = 1328.9920 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .021535112280823 FE = .96291921367461
SI = .0370807863253901
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep          0 seconds
TIME = 5295.6026 DT = 2657.9840 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351122808237 FE = .96291921367461
SI = .0370807863253901
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep          1 seconds
TIME = 10611.571 DT = 5315.9680 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351122808241 FE = .96291921367461
SI = .0370807863253901
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep          0 seconds
TIME = 21243.507 DT = 10631.936 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351122808231 FE = .96291921367461
SI = .0370807863253901
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep          0 seconds
TIME = 42507.379 DT = 21263.872 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .02153511228082 FE = .96291921367461
SI = .0370807863253901
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep          0 seconds
TIME = 85035.123 DT = 42527.744 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351122808147 FE = .96291921367461
SI = .0370807863253901
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep          0 seconds
TIME = 170090.61 DT = 85055.489 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351122808122 FE = .96291921367461
SI = .0370807863253901
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep          0 seconds
```

```

TIME = 340201.59 DT = 170110.98 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351122808355 FE = .96291921367461
SI = .03708078632539
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep 0 seconds
TIME = 680423.54 DT = 340221.95 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351122809501 FE = .96291921367461
SI = .03708078632539
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep 0 seconds
TIME = 1360867.5 DT = 680443.91 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351122812752 FE = .96291921367461
SI = .03708078632539
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep 0 seconds
TIME = 2721755.3 DT = 1360887.8 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351122812751 FE = .96291921367461
SI = .03708078632539
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep 0 seconds
TIME = 5443530.9 DT = 2721775.6 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351122811051 FE = .96291921367461
SI = .03708078632539
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep 0 seconds
TIME = 10887082. DT = 5443551.3 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351122807858 FE = .96291921367461
SI = .03708078632539
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep 1 seconds
TIME = 21774185. DT = 10887103. SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351122805261 FE = .96291921367461
SI = .03708078632539
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep 0 seconds
TIME = 43548390. DT = 21774205. SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351122804139 FE = .96291921367461
SI = .03708078632539
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep 0 seconds
TIME = 87096800. DT = 43548410. SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351122803542 FE = .96291921367461
SI = .03708078632539
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep 0 seconds
TIME = 0.17419362E+09 DT = 87096820. SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .021535112280344 FE = .96291921367461
SI = .03708078632539
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep 0 seconds
TIME = 0.34838726E+09 DT = 0.17419364E+09 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351122804181 FE = .96291921367461
SI = .0370807863253899
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep 0 seconds
TIME = 0.69677454E+09 DT = 0.34838728E+09 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351122804583 FE = .96291921367461
SI = .03708078632539
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep 0 seconds
TIME = 0.13935491E+10 DT = 0.69677456E+09 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351122806053 FE = .96291921367461
SI = .03708078632539
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep 0 seconds
TIME = 0.23935491E+10 DT = 0.10000000E+10 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351122806321 FE = .96291921367461
SI = .03708078632539
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep 0 seconds
TIME = 0.33935491E+10 DT = 0.10000000E+10 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351122806242 FE = .96291921367461
SI = .03708078632539
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep 0 seconds
TIME = 0.43935491E+10 DT = 0.10000000E+10 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351122808473 FE = .96291921367461
SI = .03708078632539
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep 0 seconds
TIME = 0.53935491E+10 DT = 0.10000000E+10 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351122816121 FE = .96291921367461
SI = .03708078632539
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep 0 seconds
TIME = 0.63935491E+10 DT = 0.10000000E+10 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351122822195 FE = .96291921367461
SI = .03708078632539
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep 1 seconds
TIME = 0.73935491E+10 DT = 0.10000000E+10 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351122824683 FE = .96291921367461
SI = .03708078632539
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep 0 seconds
TIME = 0.83935491E+10 DT = 0.10000000E+10 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351122826702 FE = .96291921367461
SI = .03708078632539
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep 0 seconds
TIME = 0.93935491E+10 DT = 0.10000000E+10 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351122828045 FE = .96291921367461
SI = .03708078632539
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep 0 seconds
TIME = 0.10000000E+11 DT = 0.60645090E+09 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351122828368 FE = .96291921367461
SI = .03708078632539
TOTAL SIZE OF SYSTEM: .05 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 0.0000000
DELETING TIME-RECORD FOR TIME 0.10000000E-06
DELETING TIME-RECORD FOR TIME 0.10010000E-03
DELETING TIME-RECORD FOR TIME 0.40010010

```

DELETING TIME-RECORD FOR TIME 21.165600  
DELETING TIME-RECORD FOR TIME 62.696601  
DELETING TIME-RECORD FOR TIME 145.75860  
DELETING TIME-RECORD FOR TIME 311.88260  
DELETING TIME-RECORD FOR TIME 644.13060  
DELETING TIME-RECORD FOR TIME 1308.6266  
DELETING TIME-RECORD FOR TIME 2637.6186  
DELETING TIME-RECORD FOR TIME 5295.6026  
DELETING TIME-RECORD FOR TIME 10611.571  
DELETING TIME-RECORD FOR TIME 21243.507  
DELETING TIME-RECORD FOR TIME 42507.379  
DELETING TIME-RECORD FOR TIME 85035.123  
DELETING TIME-RECORD FOR TIME 170090.61  
DELETING TIME-RECORD FOR TIME 340201.59  
DELETING TIME-RECORD FOR TIME 680423.54  
DELETING TIME-RECORD FOR TIME 1360867.5  
DELETING TIME-RECORD FOR TIME 2721755.3  
DELETING TIME-RECORD FOR TIME 5443530.9  
DELETING TIME-RECORD FOR TIME 10887082.  
DELETING TIME-RECORD FOR TIME 21774185.  
DELETING TIME-RECORD FOR TIME 43548390.  
DELETING TIME-RECORD FOR TIME 87096800.  
DELETING TIME-RECORD FOR TIME 0.17419362E+09  
DELETING TIME-RECORD FOR TIME 0.34838726E+09  
DELETING TIME-RECORD FOR TIME 0.69677454E+09  
DELETING TIME-RECORD FOR TIME 0.13935491E+10  
DELETING TIME-RECORD FOR TIME 0.23935491E+10  
DELETING TIME-RECORD FOR TIME 0.33935491E+10  
DELETING TIME-RECORD FOR TIME 0.43935491E+10  
DELETING TIME-RECORD FOR TIME 0.53935491E+10  
DELETING TIME-RECORD FOR TIME 0.63935491E+10  
DELETING TIME-RECORD FOR TIME 0.73935491E+10  
DELETING TIME-RECORD FOR TIME 0.83935491E+10

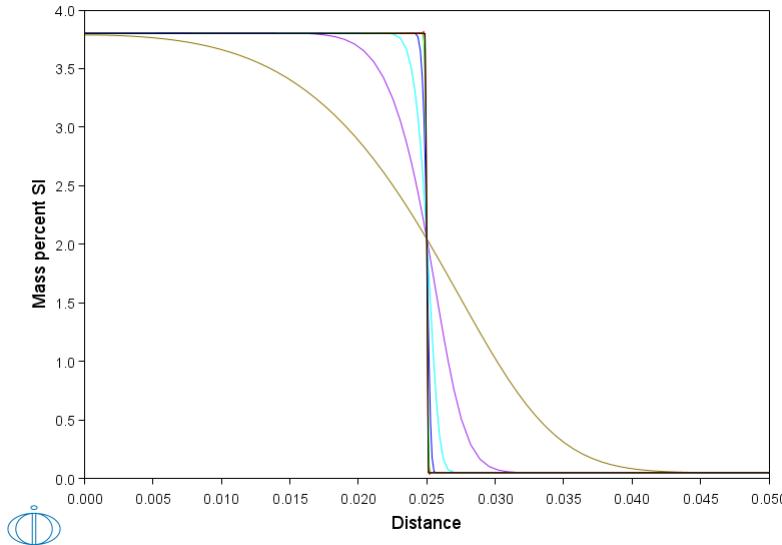
KEEPING TIME-RECORD FOR TIME 0.93935491E+10  
AND FOR TIME 0.10000000E+11  
WORKSPACE RECLAIMED

TIMESTEP AT 0.100000000E+11 SELECTED

DIC>  
DIC> set-inter  
--OK---  
DIC>

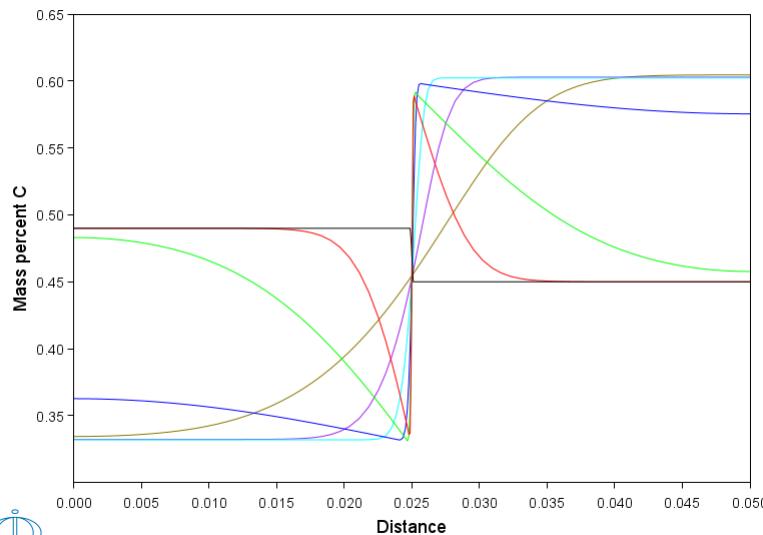
**exa3-plot**

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exa3\plot.DCM.test"
DIC>
DIC>
DIC> @@ darken_plot.DCM
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA MODULE AND SPECIFY THE STORE-RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 1.00000E+10
DIC> read exa3
OK
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA POST PROCESSOR
DIC> @@
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1: @@
POST-1: @@ PLOT THE CONCENTRATION PROFILE FOR Si AT TIMES 0, 1E5, 1123200, 1E7,
POST-1: @@ 1E8, 1E9 AND 1E10 S
POST-1: @@
POST-1: @@ SET DISTANCE IN SYSTEM AS X-AXIS, WEIGHT-% SI ON Y-AXIS AND SPECIFY
POST-1: @@ FOR WHICH SIMULATION TIMES TO PLOT THE PROFILES.
POST-1: @@
POST-1: set-diagram-axis x distance global
INFO: Distance is set as independent variable
POST-1: set-diagram-axis y weight-percent si
POST-1: set-plot-condition time 0 1E5 1123200 1e7 1E8 1E9 1E10
POST-1:
POST-1: @@
POST-1: @@ PLOT THE DIAGRAM
POST-1: @@
POST-1: set-title
TITLE : Figure a3.1
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

**Figure a3.1**

```
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1: @@
POST-1: @@ PLOT THE CONCENTRATION PROFILES FOR C
POST-1: @@
POST-1: @@ WE ONLY NEED TO CHANGE THE Y-AXIS
POST-1: @@
POST-1: set-diagram-axis y w-p c
POST-1: set-title Figure a3.2
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

**Figure a3.2**

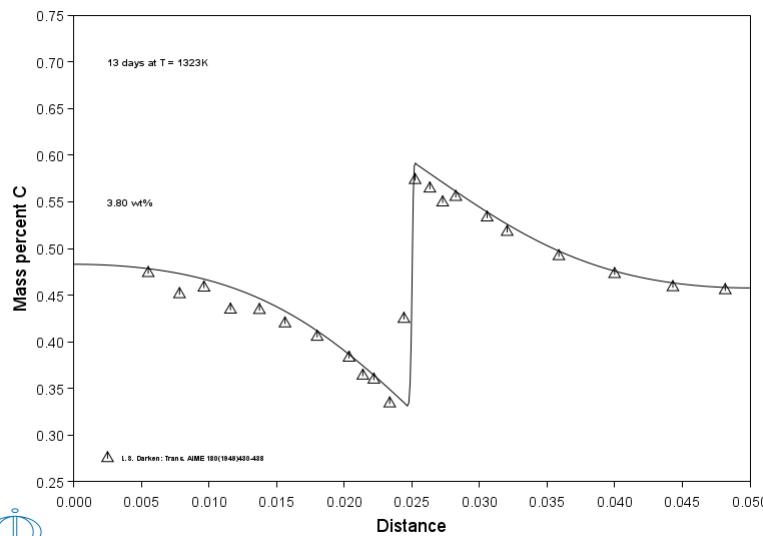


```

POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1: @@
POST-1: @@ COMPARE WITH DARKEN'S EXPERIMENTS
POST-1: @@
POST-1: append_experimental_data yes exa3.exp 0; 1
POST-1:
POST-1: set-plot-condition time 1123200
POST-1:
POST-1: s-s-s
AXIS (X, Y OR Z) : y
AUTOMATIC SCALING (Y OR N) /N/: n
MIN VALUE : 0.25
MAX VALUE : 0.75
POST-1:
POST-1: set-title Figure a3.3
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

```

**Figure a3.3**



```

POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1: set-inter
--OK--
POST-1:

```

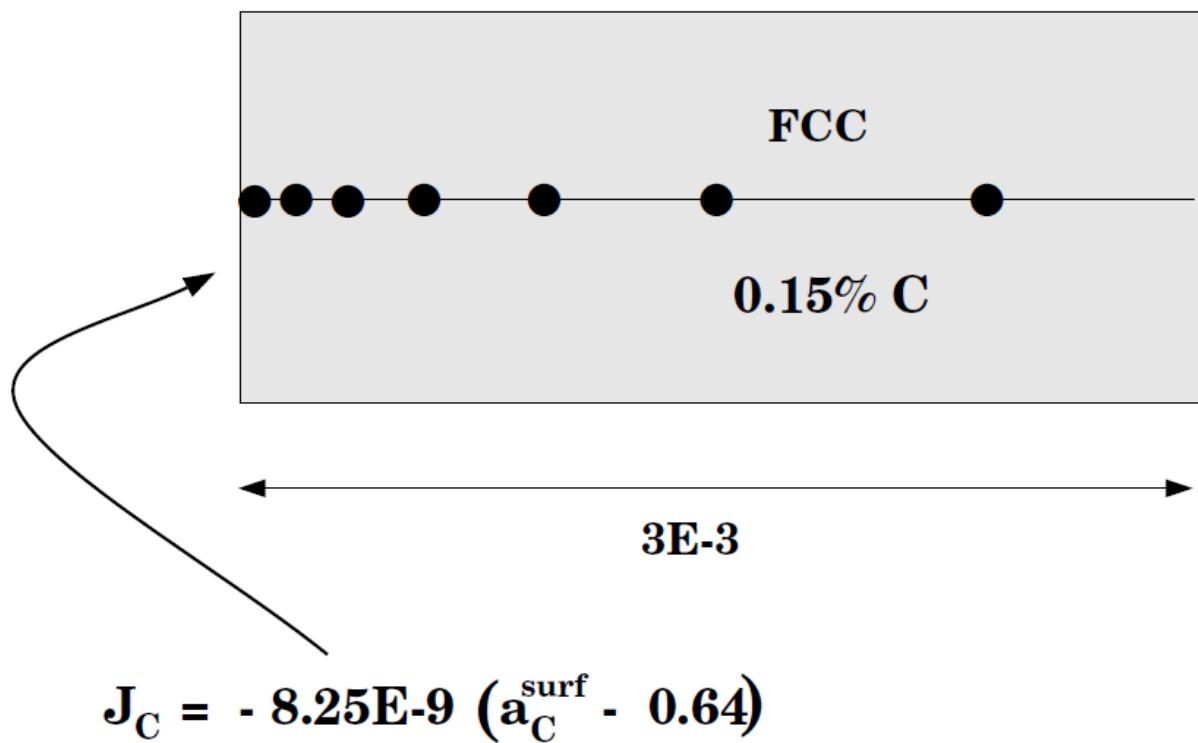


## Example exa5

### Carburization of a binary Fe-0.15 wt% C alloy: A surface reaction controls the flux of C at the surface

A mixture of 40% N<sub>2</sub> and 60% cracked methanol is used as carrier gas. The carburizing "carbon potential" in the gas is 0.85 wt%.

$$T = 1173 \text{ K}$$



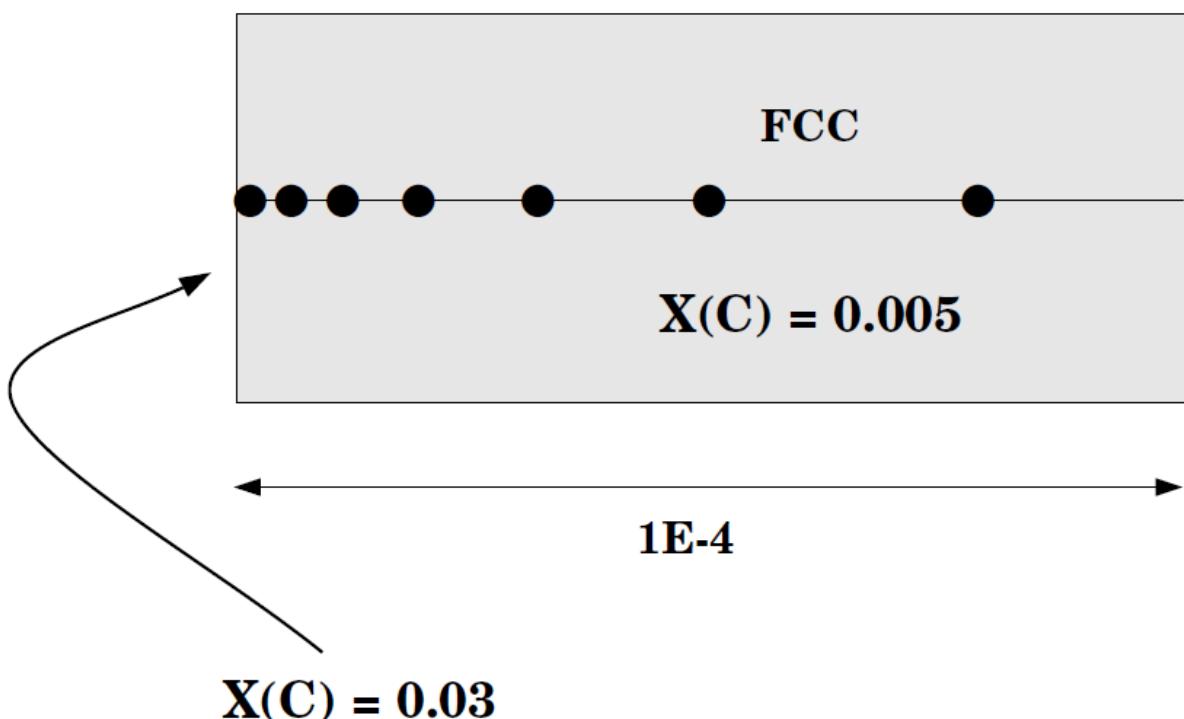


## Example exa4

### Carburization of a binary Fe-C alloy: Comparison to analytical erf solution

This is a simple binary simulation with one single phase region. It compares a numerical simulation with an analytical erf-solution. For this reason a special database is created (*erf.tdb*) where the diffusion coefficient is set to a concentration independent value.

**T = 1200 K**



**exa4-setup****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\_dictra\_console\_examples\examples\exa4\setup.DCM.test"**  
**SYS: @@**  
**SYS: @@ One-phase problem.**  
**SYS: @@ Carburization of binary Fe-C alloy: Comparison to an analytical erf solution**  
**SYS: @@ This is a simple binary simulation with a single phase region.**  
**SYS: @@ The numerical simulation is compared with an analytical erf solution.**  
**SYS: @@ For this reason a special database erf.tdb is created where the**  
**SYS: @@ diffusion coefficient is set to a concentration independent value.**  
**SYS: -----**  
NO SUCH COMMAND, USE HELP  
**SYS:**  
**SYS: @@ exa4\_setup.DCM**  
**SYS:**  
**SYS:**  
**SYS: @@**  
**SYS: @@ READ THE DATA FROM THE DATABASES**  
**SYS: @@**  
**SYS: go da**  
THERMODYNAMIC DATABASE module  
Database folder:  
C:\jenkins\workspace\generate\_dictra\_console\_examples\databases\data  
Current database: Steels/fe-Alloys v12.0  
  
VA                   /- DEFINED  
DICTRA\_FCC\_A1 REJECTED  
**TDB\_TCFE12: sw FEDEMO**  
Current database: Iron Demo Database v4.0  
  
VA                   /- DEFINED  
**TDB\_FEDEMO: def-system fe,c**  
FE                   C DEFINED  
**TDB\_FEDEMO: rej-ph \***  
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: rest-ph fcc**  
FCC\_A1 RESTORED  
**TDB\_FEDEMO: get**  
15:12:16,029 [Thread-0] INFO JavaWrapper: \*\*\* Invoking Gibbs Energy System v6 \*\*\*  
REINITIATING GES ....  
ELEMENTS ....  
SPECIES ....  
PHASES .....  
PARAMETERS ....  
FUNCTIONS ....  
  
List of references for assessed data  
  
'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'  
'X.G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'  
'A.T. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'  
'X.G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar  
volumes'  
-OK-  
**TDB\_FEDEMO:**  
**TDB\_FEDEMO: append user exa4.TDB**  
Current database: User defined Database  
This database does not support the DATABASE\_INFORMATION command  
  
VA DEFINED  
15:12:16,200 [Thread-0] INFO TDBFileParser: USER\_1740327838\_14, number of lines read: 29  
15:12:16,251 [Thread-0] INFO DatabaseUtils: Parsing of USER\_1740327838\_14 completed in 72 ms  
**TDB\_APP: def-system fe,c**  
FE                   C DEFINED  
**TDB\_APP: rej-ph \***  
FCC\_A1 REJECTED  
**TDB\_APP: rest-ph fcc**  
FCC\_A1 RESTORED  
**TDB\_APP: get**  
ELEMENTS ....  
SPECIES ....  
PHASES .....  
PARAMETERS ....  
FUNCTIONS ....  
-OK-  
**TDB\_APP:**  
**TDB\_APP: @@**  
**TDB\_APP: @@ GO TO THE DICTRA MODULE AND SET UP THE SYSTEM**  
**TDB\_APP: @@**  
**TDB\_APP: go d-m**  
NO TIME STEP DEFINED  
**DIC>**  
**DIC> @@**  
**DIC> @@ ENTER GLOBAL CONDITION T**  
**DIC> @@**  
**DIC> set-cond glob T 0 1200; \* N**  
**DIC>**  
**DIC> @@**  
**DIC> @@ ENTER THE REGION steel**  
**DIC> @@**  
**DIC> enter-region**  
**REGION NAME : steel**  
**DIC>**

```

DIC> @@
DIC> @@ ENTER THE GRID
DIC> @@ CARBON ENTERS THE SYSTEM FROM THE LOWER BOUNDARY AND CONSEQUENTLY
DIC> @@ MORE POINTS ARE REQUIRED AT THAT BOUNDARY. THIS IS WHY A GEOMETRIC
DIC> @@ GRID IS USED.
DIC> @@
DIC> enter-grid
REGION NAME : /STEEL/: steel
WIDTH OF REGION /1/: 1E-4
TYPE /LINEAR/: AUTO
DIC>
DIC> @@
DIC> @@ ENTER THE PHASE INTO THE REGION
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /STEEL/: steel
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITION IN THE FCC PHASE
DIC> @@
DIC> enter-composition
REGION NAME : /STEEL/: steel
PHASE NAME: /FCC_A1/: fcc#1
COMPOSITION TYPE /MOLE_FRACTION/: mole-fraction
PROFILE FOR /C/: c
TYPE /LINEAR/: linear
VALUE OF FIRST POINT : 0.005
VALUE OF LAST POINT : /5E-3/: 0.005
15:12:16,806 [Thread-0] INFO Database: Preparing system for use: USER_1740327838_14
15:12:17,719 [Thread-0] INFO Phase: Preparing phase for use: FCC_A1
DIC>
DIC> @@
DIC> @@ SET A FIXED COMPOSITION AS THE BOUNDARY VALUE
DIC> @@
DIC> set-condition
GLOBAL OR BOUNDARY CONDITION /GLOBAL/: boundary
BOUNDARY /LOWER/: lower
CONDITION TYPE /CLOSED_SYSTEM/: state-variable-value
State variable expression #1 : /N=1/: n=1
State variable expression #2 : x(c)=0.03
DIC>
DIC> @@
DIC> @@ SET A SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 100
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /10/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC>
DIC> save exa4 Y
DIC>
DIC> set-inter
--OK---
DIC>

```

**exa4-run**

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exa4\run.DCM.test"
DIC>
DIC>
DIC> @@ exa4_run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING EXAMPLE a4
DIC> @@
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 0.00000E+00
DIC> read exa4
OK
DIC>
DIC> @@
DIC> @@ START THE SIMULATION
DIC> @@
DIC> sim
Region: STEEL
single geometric dense at 0.0000
1.1388 96
DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
U-FRACTION IN SYSTEM: C = .0050251256281407 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
U-FRACTION IN SYSTEM: C = .0050251256281407 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
TIME = 0.1000000E-06 DT = 0.1000000E-06 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00502599895421297 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.26001020E-05 DT = 0.25001020E-05 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00502674234772398 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.76003060E-05 DT = 0.50002040E-05 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00502762855271361 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.17600714E-04 DT = 0.10000408E-04 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00502880490898696 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.37601530E-04 DT = 0.20000816E-04 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00503042289514107 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.77603162E-04 DT = 0.40001632E-04 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00503268130112881 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.15760643E-03 DT = 0.80003264E-04 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00503585491527872 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.31761295E-03 DT = 0.16000653E-03 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00504032903043467 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.63762601E-03 DT = 0.32001306E-03 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00504664654067874 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.12776521E-02 DT = 0.64002611E-03 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00505557392100181 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.25577043E-02 DT = 0.12800522E-02 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00506819425567398 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.51178088E-02 DT = 0.25601044E-02 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00508603865206295 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.10238018E-01 DT = 0.51202089E-02 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00511127199989312 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.20478435E-01 DT = 0.10240418E-01 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0051469556180961 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 1 seconds
TIME = 0.40959271E-01 DT = 0.20480836E-01 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00519741865567008 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.81920942E-01 DT = 0.40961671E-01 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0052687830573381 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.16384428 DT = 0.81923342E-01 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00536970755217346 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.32769097 DT = 0.16384468 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00551243555924854 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.65538434 DT = 0.32769337 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00571428313781583 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 1.3107711 DT = 0.65538674 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00599973850521004 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 2.6215446 DT = 1.3107735 SUM OF SQUARES = 0.0000000
```

```

U-FRACTION IN SYSTEM: C = .00640343298842195 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 5.2430915 DT = 2.6215470 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00697433052866847 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 10.486185 DT = 5.2430939 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00778159421638383 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 20.486185 DT = 10.000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00887736257293564 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 30.486185 DT = 10.000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00972196664325369 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 40.486185 DT = 10.000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .010436351986536 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 50.486185 DT = 10.000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0110669328932657 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 60.486185 DT = 10.000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0116377078880251 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 70.486185 DT = 10.000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0121630223717782 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 90.486185 DT = 10.000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0131119785059757 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 100.00000 DT = 9.5138146 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .013526298212787 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 0.0000000
DELETING TIME-RECORD FOR TIME 0.10000000E-06
DELETING TIME-RECORD FOR TIME 0.26001020E-05
DELETING TIME-RECORD FOR TIME 0.76003060E-05
DELETING TIME-RECORD FOR TIME 0.17600714E-04
DELETING TIME-RECORD FOR TIME 0.37601530E-04
DELETING TIME-RECORD FOR TIME 0.77603162E-04
DELETING TIME-RECORD FOR TIME 0.15760643E-03
DELETING TIME-RECORD FOR TIME 0.31761295E-03
DELETING TIME-RECORD FOR TIME 0.63762601E-03
DELETING TIME-RECORD FOR TIME 0.12776521E-02
DELETING TIME-RECORD FOR TIME 0.25577043E-02
DELETING TIME-RECORD FOR TIME 0.51178088E-02
DELETING TIME-RECORD FOR TIME 0.10238018E-01
DELETING TIME-RECORD FOR TIME 0.20478435E-01
DELETING TIME-RECORD FOR TIME 0.40959271E-01
DELETING TIME-RECORD FOR TIME 0.81920942E-01
DELETING TIME-RECORD FOR TIME 0.16384428
DELETING TIME-RECORD FOR TIME 0.32769097
DELETING TIME-RECORD FOR TIME 0.65538434
DELETING TIME-RECORD FOR TIME 1.3107711
DELETING TIME-RECORD FOR TIME 2.6215446
DELETING TIME-RECORD FOR TIME 5.2430915
DELETING TIME-RECORD FOR TIME 10.486185
DELETING TIME-RECORD FOR TIME 20.486185
DELETING TIME-RECORD FOR TIME 30.486185
DELETING TIME-RECORD FOR TIME 40.486185
DELETING TIME-RECORD FOR TIME 50.486185
DELETING TIME-RECORD FOR TIME 60.486185
DELETING TIME-RECORD FOR TIME 70.486185
DELETING TIME-RECORD FOR TIME 80.486185

KEEPING TIME-RECORD FOR TIME 90.486185
AND FOR TIME 100.00000
WORKSPACE RECLAIMED

```

```

TIMESTEP AT 100.000000 SELECTED

DIC>
DIC> @@
DIC> @@ THE SIMULATION IS FINISHED
DIC> @@
DIC>
DIC> set-inter
--OK--
DIC>

```

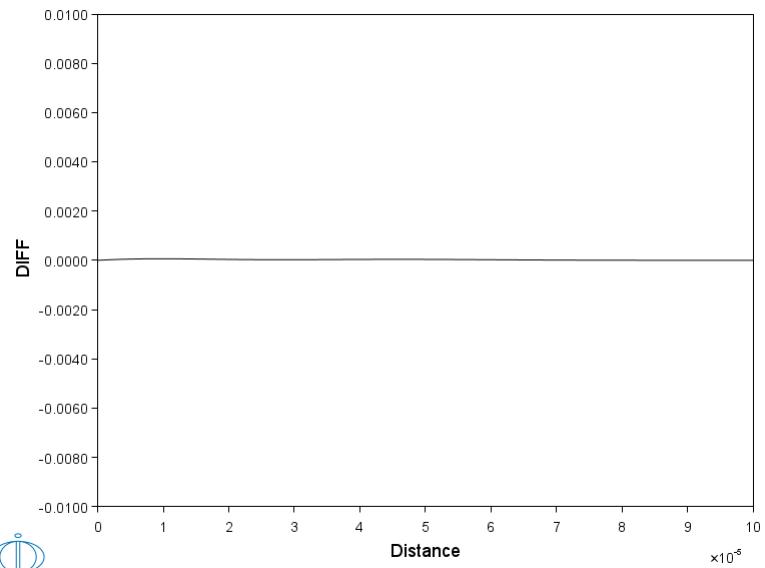
**exa4-plot**

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exa4\plot.DCM.test"
DIC>
DIC>
DIC> @@ exa4_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE exa4
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 1.00000E+02
DIC> read exa4
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1: @@
POST-1: @@ PLOT A COMPOSITION PROFILE
POST-1: @@
POST-1: s-d-a x distance global
INFO: Distance is set as independent variable
POST-1: s-d-a y x(c)
POST-1: s-p-c time 25
POST-1: @@
POST-1: @@
POST-1: @@ ENTER THE ANALYTICAL SOLUTION, CALLED ERFSOL
POST-1: @@
POST-1: enter-symbol
Function or table /FUNCTION/: function
NAME: erfsol
FUNCTION: 0.03-0.025*erf(gd/sqrt(4*dc(fcc,c,c,fe)*25));
POST-1:
POST-1: @@
POST-1: @@ COMPARE THE ANALYTICAL AND NUMERICAL SOLUTIONS
POST-1: @@
POST-1: enter-symbol
Function or table /FUNCTION/: table
NAME: aaa
Variable(s) x(c) erfsol
POST-1:
POST-1: s-d-a y aaa
COLUMN NUMBER /*/: 1 2
POST-1:
POST-1: set-axis-text
AXIS (X, Y OR Z) : y
AUTOMATIC AXIS TEXT (Y OR N) /N/: n
AXIS TEXT : Mole fraction C
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```



```
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: @@
POST-1: @@ PLOT THE DIFFERENCE
POST-1: @@
POST-1: enter func diff=x(c)-erfsol;
POST-1: s-d-a y diff
POST-1: s-s-s y n -1e-2 1e-2
POST-1:
```

```
POST-1:  
POST-1: SET_EXP_FILE_FORMAT 5  
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples/unite/distribution\macroResult.exp Y  
POST-1: SET_EXP_FILE_FORMAT 10  
POST-1:  
POST-1: plot
```



```
POST-1:  
POST-1:  
POST-1:  
POST-1:@?<Hit_return_to_continue>  
POST-1:  
POST-1: set-interactive  
--OK--  
POST-1:
```

**exa5-setup****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\_dictra\_console\_examples\examples\exa5\setup.DCM.test"**

**SYS:** i>\_@  
NO SUCH COMMAND, USE HELP  
**SYS:** @@ One-phase problem.  
**SYS:** @@ Carburization of a binary Fe-0.15 wt% C alloy.  
**SYS:** @@ A mixture of 40% N2 and 60% cracked methanol is used as carrier gas.  
**SYS:** @@ The carburizing "carbon potential" in the gas is 0.85 wt%.  
**SYS:** @@ A surface reaction controls the flux of C at the surface.  
**SYS:** -----

NO SUCH COMMAND, USE HELP  
**SYS:**  
**SYS:** @@ exa5\_setup.DCM  
**SYS:**  
**SYS:** @@  
**SYS:** @@ GO TO THE DATABASES AND READ THE THERMODYNAMIC AND KINETIC DATA  
**SYS:** @@  
**SYS:** go da  
THERMODYNAMIC DATABASE module  
Database folder:  
C:\jenkins\workspace\generate\_dictra\_console\_examples\databases\data  
Current database: Steels/Fe-Alloys v12.0

VA                           /- DEFINED  
DICTRA\_FCC\_A1 REJECTED  
**TDB\_TCFE12:** sw FEDEMO  
Current database: Iron Demo Database v4.0  
  
VA                           /- DEFINED  
**TDB\_FEDEMO:** def-sys fe,c  
FE                           C DEFINED  
**TDB\_FEDEMO:** rej-ph \*  
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                     MSC2                           M7C3  
REJECTED  
**TDB\_FEDEMO:** rest-ph fcc graphite  
FCC\_A1                    GRAPHITE RESTORED  
**TDB\_FEDEMO:** get  
15:15:31,545 [Thread-0] INFO JavaWrapper: \*\*\* Invoking Gibbs Energy System v6 \*\*\*  
REINITIATING GES ....  
ELEMENTS ....  
SPECIES ....  
PHASES ....  
PARAMETERS ...  
FUNCTIONS ....

List of references for assessed data

'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'  
'X.G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'  
'A.T. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'  
'X.G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar  
volumes'  
'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121 -127; Molar  
volumes'

-OK-

**TDB\_FEDEMO:@**

**TDB\_FEDEMO:** append

Use one of these databases

TCFE12 = Steels/Fe-Alloys v12.0  
TCFE9 = Steels/Fe-Alloys v9.3  
SSUB6 = SGTE Substances v6.0  
FEDEMO = Iron Demo Database v4.0  
MOB2 = Alloys Mobility v2.7  
MOBFE2 = Steels/Fe-Alloys Mobility v2.0  
MOBFE4 = Steels/Fe-Alloys Mobility v4.0  
MOBFE7 = Steels/Fe-Alloys Mobility v7.1  
MFEDEMO = Fe-Alloys Mobility demo database v2.0  
USER = User defined Database

**DATABASE NAME /FEDEMO:/:** mfedemo

Current database: Fe-Alloys Mobility demo database v2.0

VA DEFINED  
**APP:** def-sys fe,c  
FE                           C DEFINED  
**APP:** rej-ph \*  
BCC\_A2                    FCC\_A1                      CEMENTITE  
REJECTED  
**APP:** rest-ph fcc  
FCC\_A1 RESTORED  
**APP:** get  
ELEMENTS ....  
SPECIES ....  
PHASES ....  
PARAMETERS ...  
FUNCTIONS ....

List of references for assessed data

'This parameter has not been assessed'  
'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'  
'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe  
-Ni'

```

-OK-
APP: @?
APP: @@ GO TO THE DICTRA MONITOR TO SET UP THE INITIAL STATE OF THE SPECIMEN
APP: @@
APP: go d-m
NO TIME STEP DEFINED
*** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
DIC>
DIC> set-cond glob T 0 1173; * N
DIC>
DIC> @@
DIC> @@ SELECT A REFERENCE STATE FOR THE C ACTIVITY
DIC> @@
DIC> set-ref-state
Component: c
Reference state: graph
Temperature /*/: *
Pressure /100000/: 1e5
DIC>
DIC> @@
DIC> @@ ENTER A REGION, GRID, PHASE AND COMPOSITION
DIC> @@
DIC> enter-region
REGION NAME : steel
DIC>
DIC> enter-grid
REGION NAME : /STEEL/: steel
WIDTH OF REGION /1/: 3E-3
TYPE /LINEAR/: AUTO
DIC>
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /STEEL/: steel
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC> enter-composition
REGION NAME : /STEEL/: steel
PHASE NAME: /FCC_A1/: fcc#1
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: c
TYPE /LINEAR/: lin
VALUE OF FIRST POINT : 0.15
VALUE OF LAST POINT : /0.15/: 0.15
DIC>
DIC> @@
DIC> @@ NOW SET THE BOUNDARY CONDITIONS. WE ARE ONLY INTERESTED IN THE
DIC> @@ SURFACE REGION, FOR EXAMPLE IT IS SUFFICIENT TO SET CONDITIONS AT THE
DIC> @@ LOWER BOUNDARY.
DIC> @@
DIC>
DIC> @@
DIC> @@ Specify the activity flux function which controls the uptake of C.
DIC> @@
DIC> @@ The functions f and g and the parameter N has to be specified.
DIC> @@ k k
DIC> @@
DIC> @@ N
DIC> @@ J V = f (variables)*(ACTIVITY -g (variables)) (1)
DIC> @@ k m k k
DIC> @@
DIC> @@ f and g in equation 1 is the mass-transfer coefficient and
DIC> @@ k k
DIC> @@ the activity of k in the gas, respectively. ACTIVITY in eq. 1 means
DIC> @@ the actual activity of species k at the surface.
DIC> @@
DIC>
DIC> @@
DIC> @@ The main carburizing reaction for our atmosphere is:
DIC> @@
DIC> @@ CO + H -> C + H O (I)
DIC> @@ 2 <- - 2
DIC> @@
DIC> @@ Following Sproge and Å...gren (J. Heat Treating, v6, no 1, 1988 pp. 9-19)
DIC> @@ we calculate the mass-transfer coefficient for carbon, f in
DIC> @@ eq. 1 above by means of eq. 3, 4 and 12 in Sproge and Å...gren's paper.
DIC> @@
DIC> @@
DIC> @@ A * K * P * sqrt( P )
DIC> @@ I CO H
DIC> @@
DIC> @@ f = ----- / gamma (2)
DIC> @@ a + B * K * P * sqrt( P )
DIC> @@ C I CO H
DIC> @@
DIC> @@ K is the equilibrium constant for reaction (I)
DIC> @@ I
DIC> @@
DIC> @@ A and B are constants defined in Sproge and Å...gren's paper. gamma
DIC> @@ is the activity coefficient for carbon in the steel.
DIC> @@
DIC> @@ Assume a constant value for P * sqrt( P ) = 0.14
DIC> @@ CO H
DIC> @@
DIC> @@ The carbon activity in the gas is controlled by the partial
DIC> @@ pressure of water as can be understood from reaction (I).
DIC> @@
DIC> @@ Assume that the carbon activity, a of the gas is 0.64
DIC> @@ C
DIC> @@ which corresponds to a carburizing "carbon potential" of 0.85 wt%.
DIC> @@
DIC> @@ In this way we may calculate f to 8.25E-9 mol/s.
DIC> @@
DIC>
DIC> set-cond
GLOBAL OR BOUNDARY CONDITION /GLOBAL/: bound
BOUNDARY /LOWER/: lower
CONDITION TYPE /CLOSED_SYSTEM/: activity_flux_function

```

ENTER THE EXPRESSION AS:

```
N
J V = f (variables)*(ACTIVITY -g (variables))
k m k k
FLUX OF FCC_A1,C
LOW TIME LIMIT /0/: 0
f(T,P,TIME)= -8.25E-9;
HIGH TIME LIMIT /*/: *
ANY MORE RANGES /N/: N
N /1/: 1
LOW TIME LIMIT /0/: 0
g(T,P,TIME)= 0.64;
HIGH TIME LIMIT /*/: *
ANY MORE RANGES /N/: N
DIC>
DIC> @@
DIC> @@ SPECIFY A SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 18000
AUTOMATIC Timestep CONTROL /YES/:
MAX Timestep DURING INTEGRATION /1800/:
INITIAL Timestep : /1E-07/:
SMALLEST ACCEPTABLE Timestep : /1E-07/:
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO FILE
DIC> @@
DIC> Save exa5 Y
DIC>
DIC> set-inter
--OK--
```

**exa5-run**

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exa5\run.DCM.test"
DIC>
DIC>
DIC> @@ exa5_run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING EXAMPLE a5
DIC> @@
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 0.00000E+00
*** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
DIC> read exa5
OK
DIC>
DIC> @@
DIC> @@ Start the simulation
DIC> @@
DIC> sim
Region: STEEL
single geometric dense at 0.0000
1.2176 101
DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
U-FRACTION IN SYSTEM: C = .00698495916383109 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
U-FRACTION IN SYSTEM: C = .00698495916383109 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
TIME = 0.1000000E-06 DT = 0.1000000E-06 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698495916398349 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 0.24659766E-05 DT = 0.23659766E-05 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698495916758908 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 1 seconds
TIME = 0.71979297E-05 DT = 0.47319532E-05 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698495917479988 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 0.16661836E-04 DT = 0.94639063E-05 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698495918922068 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 0.35589649E-04 DT = 0.18927813E-04 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698495921806013 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 0.73445274E-04 DT = 0.37855625E-04 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698495927573319 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 0.14915652E-03 DT = 0.75711250E-04 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698495939106305 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 1 seconds
TIME = 0.30057903E-03 DT = 0.15142250E-03 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0069849596216772 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 0.60342403E-03 DT = 0.30284500E-03 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0069849600827771 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 0.24204940E-02 DT = 0.12113800E-02 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698496284726693 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 0.48432541E-02 DT = 0.24227600E-02 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698496652968263 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 0.96887741E-02 DT = 0.48455200E-02 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698497388635673 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 0.19379814E-01 DT = 0.96910401E-02 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0069849885766828 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 1 seconds
TIME = 0.38761894E-01 DT = 0.19382080E-01 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698501789240893 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 0.77526054E-01 DT = 0.38764160E-01 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698507634097207 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 0.15505437 DT = 0.77528320E-01 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698519272377668 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 0.31011102 DT = 0.15505664 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698542404641377 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 0.62022430 DT = 0.31011328 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698588265674895 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 1.2404509 DT = 0.62022656 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698678864751835 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 1 seconds
```

```

TIME = 2.4809040 DT = 1.2404531 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698856957978377 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 4.9618102 DT = 2.4809063 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0069920463860113 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 9.9236228 DT = 4.9618125 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0069987699663246 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 19.847248 DT = 9.9236250 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00701160601590709 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 39.694498 DT = 19.847250 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00703569376361481 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 79.388998 DT = 39.694500 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00707989462116312 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 1 seconds
TIME = 158.77800 DT = 79.389000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00715874757109899 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 317.55600 DT = 158.77800 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0072947413875038 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 635.11200 DT = 317.55600 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00752054375503549 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 1270.2240 DT = 635.11200 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00788106518443744 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 2540.4480 DT = 1270.2240 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00843611780537169 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 1 seconds
TIME = 4340.4480 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00904710226999854 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 6140.4480 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00955134567260692 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 7940.4480 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00999113675765003 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 9740.4480 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0103863764716782 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 1 seconds
TIME = 11540.448 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0107484090267306 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 13340.448 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0110844421240379 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 15140.448 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0113993948509716 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 16940.448 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0116968050295535 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 1 seconds
TIME = 18000.000 DT = 1059.5520 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0118647499013306 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 0.0000000
DELETING TIME-RECORD FOR TIME 0.10000000E-06
DELETING TIME-RECORD FOR TIME 0.24659766E-05
DELETING TIME-RECORD FOR TIME 0.71979297E-05
DELETING TIME-RECORD FOR TIME 0.16661836E-04
DELETING TIME-RECORD FOR TIME 0.35589649E-04
DELETING TIME-RECORD FOR TIME 0.73445274E-04
DELETING TIME-RECORD FOR TIME 0.14915652E-03
DELETING TIME-RECORD FOR TIME 0.30057903E-03
DELETING TIME-RECORD FOR TIME 0.60342403E-03
DELETING TIME-RECORD FOR TIME 0.12091140E-02
DELETING TIME-RECORD FOR TIME 0.24204940E-02
DELETING TIME-RECORD FOR TIME 0.48432541E-02
DELETING TIME-RECORD FOR TIME 0.96887741E-02
DELETING TIME-RECORD FOR TIME 0.19379814E-01
DELETING TIME-RECORD FOR TIME 0.38761894E-01
DELETING TIME-RECORD FOR TIME 0.77526054E-01
DELETING TIME-RECORD FOR TIME 0.15505437
DELETING TIME-RECORD FOR TIME 0.31011102
DELETING TIME-RECORD FOR TIME 0.62022430
DELETING TIME-RECORD FOR TIME 1.2404509
DELETING TIME-RECORD FOR TIME 2.4809040
DELETING TIME-RECORD FOR TIME 4.9618102
DELETING TIME-RECORD FOR TIME 9.9236228
DELETING TIME-RECORD FOR TIME 19.847248
DELETING TIME-RECORD FOR TIME 39.694498
DELETING TIME-RECORD FOR TIME 79.388998
DELETING TIME-RECORD FOR TIME 158.77800
DELETING TIME-RECORD FOR TIME 317.55600
DELETING TIME-RECORD FOR TIME 635.11200
DELETING TIME-RECORD FOR TIME 1270.2240
DELETING TIME-RECORD FOR TIME 2540.4480
DELETING TIME-RECORD FOR TIME 4340.4480
DELETING TIME-RECORD FOR TIME 6140.4480

```

DELETING TIME-RECORD FOR TIME 7940.4480  
DELETING TIME-RECORD FOR TIME 9740.4480  
DELETING TIME-RECORD FOR TIME 11540.448  
DELETING TIME-RECORD FOR TIME 13340.448  
DELETING TIME-RECORD FOR TIME 15140.448

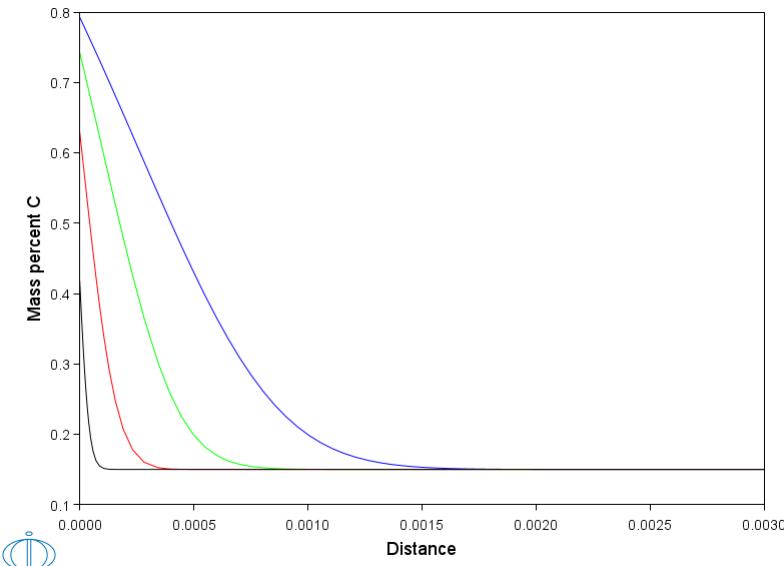
KEEPING TIME-RECORD FOR TIME 16940.448  
AND FOR TIME 18000.000  
WORKSPACE RECLAIMED

TIMESTEP AT 18000.0000 SELECTED

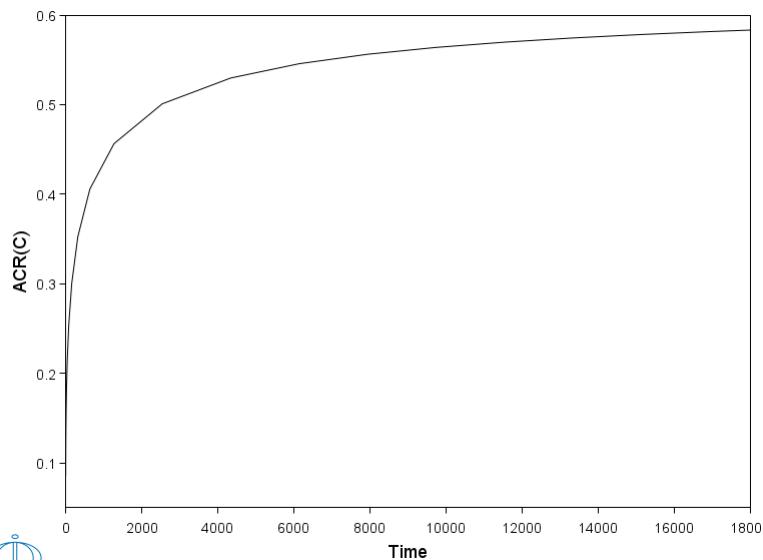
DIC>  
DIC> set-inter  
--OK--  
DIC>

## exa5-plot

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exa5\plot.DCM.test"
DIC>
DIC>
DIC> @@ exa5_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE a5
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 1.80000E+04
*** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
DIC> read exa5
OK
DIC>
DIC> @@
DIC> @@ ENTER THE POST PROCESSOR
DIC> @@
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1: @@
POST-1: @@ PLOT SOME DIFFERENT CONCENTRATION PROFILES
POST-1: @@
POST-1: s-d-a x dist glo
INFO: Distance is set as independent variable
POST-1: s-d-a y w-p c
POST-1: s-p-c time 100 1000 5000 18000
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```



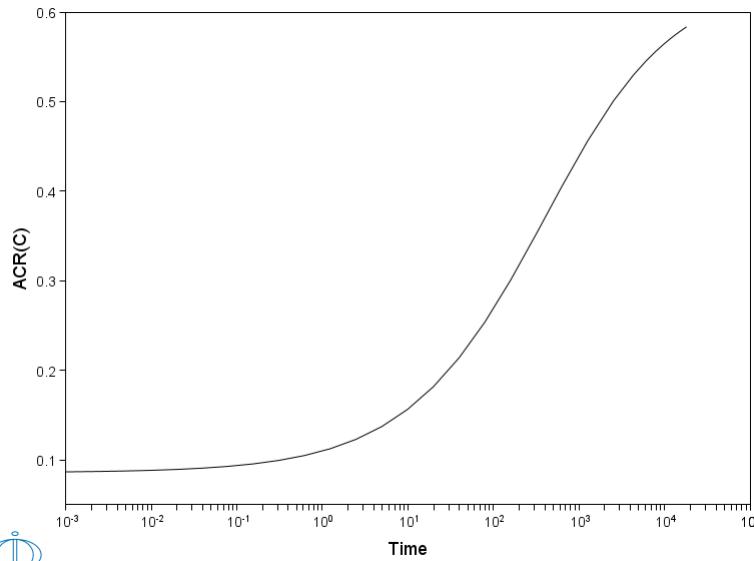
```
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: @@
POST-1: @@ PLOT THE VARIATION OF THE C ACTIVITY AT THE SURFACE
POST-1: @@
POST-1: s-d-a y acr(c)
POST-1:
POST-1: s-d-a x time
INFO: Time is set as independent variable
POST-1:
POST-1: s-p-c
CONDITION /TIME/: interface
INTERFACE : first
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```



```

POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: @@
POST-1: @@ USE A LOGARITHMIC SCALE ON THE X-AXIS
POST-1: @@
POST-1: set-axis-type
AXIS (X, Y OR Z) : x
AXIS TYPE /LINEAR/: logarithmic
POST-1:
POST-1: s-s-s x n 0.001 2e4
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

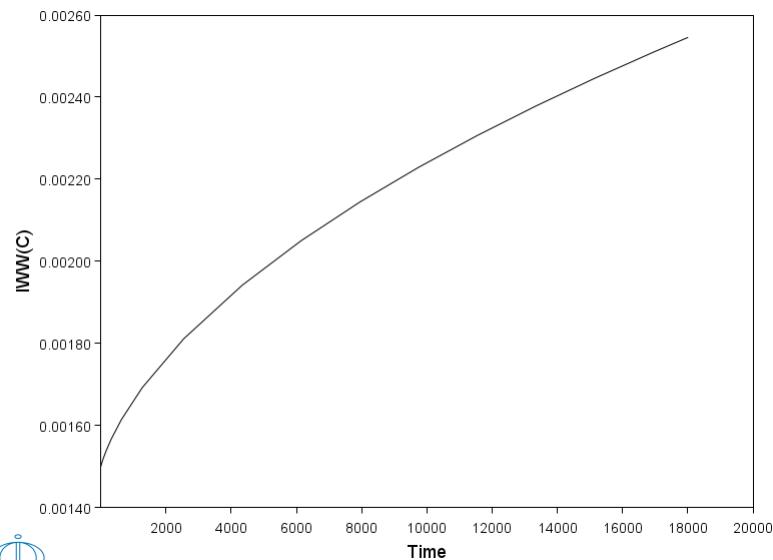
```



```

POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: @@
POST-1: @@ PLOT THE AVERAGE WEIGHT FRACTION OF C IN THE SPECIMEN
POST-1: @@
POST-1: s-d-a y iww(c)
POST-1:
POST-1: set-ax-ty
AXIS (X, Y OR Z) : x
AXIS TYPE /LINEAR/: linear
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
    OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

```



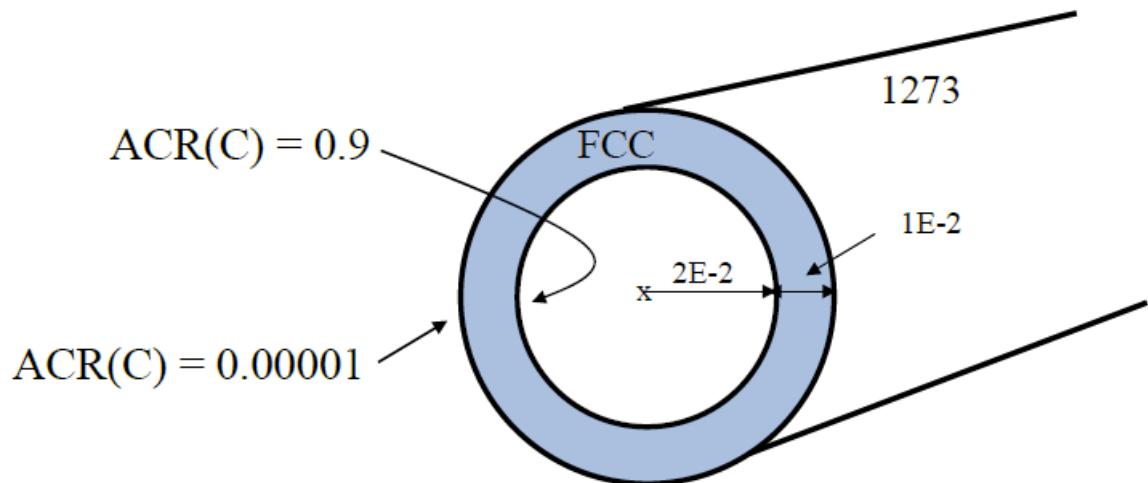
```
POST-1:  
POST-1:  
POST-1:  
POST-1:@?<Hit_return_to_continue>  
POST-1:  
POST-1:  
POST-1:  
POST-1: set-inter  
--OK---  
POST-1:
```



## Example exa6

### Diffusion through a tube wall: Boundary conditions result in a gradient in C-activity

A simple example of diffusion through a tube wall. The tube-material is an Fe-0.6%Mn-0.7%Si-0.05%C alloy. On the inside wall a carbon activity of 0.9 is maintained whereas on the outside the C-activity is very low. This example demonstrates the use of the command SET-FIRST-INTERFACE as well as the use of MIXED boundary conditions.



**exa6-setup****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_dictra_console_examples\examples\exa6\setup.DCM.test"
SYS: @@
SYS: @@ One-phase problem.
SYS: @@ Diffusion through a tube wall.
SYS: @@ A simple example about diffusion through a tube wall.
SYS: @@ The tube material is an Fe-0.6%Mn-0.7%Si-0.05%C alloy. On
SYS: @@ the inside wall a carbon activity of 0.9 is maintained whereas on
SYS: @@ the outside the C-activity is very low. This example demonstrates
SYS: @@ the use of the command SET-FIRST-INTERFACE as well as the MIXED
SYS: @@ boundary conditions.
SYS: -----
NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ setup.DCM
SYS:
SYS:
SYS: @@
SYS: @@ GO TO THE DATABASE MODULE
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\generate_dictra_console_examples\databases\data
Current database: Steels/Fe-Alloys v12.0

VA          /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE12: @@
TDB_TCFE12: @@ USE THE TCFE DATABASE FOR THERMODYNAMIC DATA
TDE_TCFE12: @@
TDB_TCFE12: sw tcfef9
Current database: Steels/Fe-Alloys v9.3

VA          /- DEFINED
L12_FCC      B2_BCC           DICTRA_FCC_A1
REJECTED
TDE_TCFE9: def-sys fe si mn c
FE           SI               MN
C  DEFINED
TDE_TCFE9: rej ph * all
GAS:G          LIQUID:L        BCC_A2
FCC_A1         HCP_A3          CBCC_A12
CUB_A13        DIAMOND_FCC_A4 GRAPHITE
CEMENTITE      M23C6           M7C3
M5C2          KSI_CARBIDE    FE4N_LP1
FECN_CHI        LAVES_PHASE_C14 M3SI-
MN9Si2         MN11Si19       MN6SI
G_PHASE         CR3SI          FE2SI
FESI2_H         FESI2_L        MSI
M5Si3          AL4C3          FE8Si2C
SIC            MN5SiC         CUZN_EPSILON
AL5Fe4         MP_B31         M2P_C22
FLUORITE_C1:I   ZRO2_TETR:I  M2O3C:I
M2O3H:I        REJECTED
TDB_TCFE9: res ph fcc,grap
FCC_A1         GRAPHITE RESTORED
TDE_TCFE9: get
15:18:54,094 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS .....

List of references for assessed data

'A. 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, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
  volumes'
'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
'P. Gustafsson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, CALPHAD, 34, 279
  -85(2010); Mn-C'
'J. Lacaze and B. Sundman, Metall. Mater. Trans. A, 22A (1991) 2211-2223;
  Fe-Si and Fe-Si-C'
'W. Huang, CALPHAD, 13 (1989) 243-252; TRITA-MAC 388 (rev 1989); FE-MN'
'W. Zheng, J. Alloys Compd., 632 (2015) 661-675'
'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, CALPHAD,
  submitted, 2011; Fe-Mn-C'
'J. Miettinen and B. Hallstedt, CALPHAD, 22 (1998) 231-256; Fe-Si and Fe
  -Si-C'
'A. Forsberg and J. Agren, J. Phase Equilib., 14 (1993) 354-363; Fe-Mn-Si'
-OK-
TDE_TCFE9:
TDB_TCFE9: @@
TDE_TCFE9: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE KINETIC DATA
TDB_TCFE9: @@
TDB_TCFE9: app
Use one of these databases
TCFE12 = Steels/Fe-Alloys v12.0
```

```

TCFE9      = Steels/Fe-Alloys v9.3
SSUB6      = SGT Substances v6.0
FEDEMO     = Iron Demo Database v4.0
MOB2       = Alloys Mobility v2.7
MOBFE2     = Steels/Fe-Alloys Mobility v2.0
MOBFE4     = Steels/Fe-Alloys Mobility v4.0
MOBFE7     = Steels/Fe-Alloys Mobility v7.1
MFDEMO     = Fe-Alloys Mobility demo database v2.0
USER       = User defined Database

DATABASE NAME /TCFE9/: mobfe4
Current database: Steels/Fe-Alloys Mobility v4.0

VA DEFINED
B2_BCC REJECTED
APP: def-sys fe si mn c
    FE                      SI                  MN
    C DEFINED
APP: rej ph * all
    BCC_A2                 CEMENTITE          FCC_A1
    FE4N_LP1                HCP_A3             LIQUID:L
    REJECTED
APP: res ph fcc
    FCC_A1 RESTORED
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS .....
FUNCTIONS .....

List of references for assessed data

'This parameter has not been assessed'
'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'
'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
-Ni'
'Y. Liu, L. Zhang, et al. CALPHAD 33(2009)614-23; Fe-Mn-C (fcc)'
'M. Yin, et al. (2010) unpublished work.'
'W. Zheng, et al., J. Alloys and Compounds, 632 (2015) 661-675; Fe-Mn-Si
(fcc)'
'D. Bergner et al., Defect and Diffusion Forum 66-69(1989)409. Impurity
diffusion of Si in fcc Fe.'

-OK-
APP:
APP: @@ 
APP: @@ ENTER THE DICTRA MONITOR WHERE THE PROBLEM IS SET UP
APP: @@
APP: go d-m
NO TIME STEP DEFINED
*** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
DIC>
DIC> @@
DIC> @@ ENTER GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 1273; * N
DIC>
DIC> @@
DIC> @@ SET THE REFERENCE STATE FOR CARBON
DIC> @@
DIC> set-ref C grap * 101325
DIC>
DIC> @@
DIC> @@ ENTER A REGION
DIC> @@
DIC> enter-region aus
DIC>
DIC> @@
DIC> @@ ENTER A DOUBLE GEOMETRIC GRID INTO THE REGION
DIC> @@
DIC> enter-grid
REGION NAME : /AUS/: aus
WIDTH OF REGION /1/: 1e-2
TYPE /LINEAR/: AUTO
DIC>
DIC> @@
DIC> @@ SET THE GEOMETRY (1 = CYLINDER)
DIC> @@
DIC> enter-geo
GEOMETRICAL EXPONENT /0/: 1
DIC>
DIC> @@
DIC> @@ SET THE FIRST INTERFACE => TUBE
DIC> @@
DIC> set-first-interface
COORDINATE FOR FIRST INTERFACE /0/: 2e-2
DIC>
DIC> @@
DIC> @@ ENTER AN active PHASE IN THE REGION
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /AUS/: aus
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc_a1#1
DIC>
DIC> @@
DIC> @@ ENTER INITIAL COMPOSITIONS INTO THE PHASE
DIC> @@
DIC> enter-composition
REGION NAME : /AUS/: aus
PHASE NAME: /FCC_A1/: fcc#1
DEPENDENT COMPONENT ? /SI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: si lin 0.7 0.7
PROFILE FOR /MN/: mn lin 0.6 0.6
PROFILE FOR /SI/: c lin 5e-2 5e-2
DIC>
DIC> @@
DIC> @@ SET THE BOUNDARY CONDITIONS ON BOTH THE LOWER AND UPPER PART OF THE REGION
DIC> @@
DIC> @@ USE MIXED CONDITIONS: AN ACTIVITY CONDITION FOR C AND CLOSED

```

```
DIC> @@ SYSTEMS FOR MN AND SI.
DIC> @@
DIC> set-cond
GLOBAL OR BOUNDARY CONDITION /GLOBAL/: boundary
BOUNDARY /LOWER/: lower
CONDITION TYPE /CLOSED_SYSTEM/: mixed
Dependent substitutional element:FE
Dependent interstitial element:VA
TYPE OF CONDITION FOR COMPONENT C /ZERO_FLUX/: activity
LOW TIME LIMIT /0/: 0
ACR(C) (TIME)= 0.9;
HIGH TIME LIMIT /*/: *
ANY MORE RANGES /N/: N
TYPE OF CONDITION FOR COMPONENT MN /ZERO_FLUX/: zero_flux
TYPE OF CONDITION FOR COMPONENT SI /ZERO_FLUX/: zero_flux
DIC>
DIC> set-cond
GLOBAL OR BOUNDARY CONDITION /GLOBAL/: boundary
BOUNDARY /UPPER/: upper
CONDITION TYPE /CLOSED_SYSTEM/: mixed
Dependent substitutional element:FE
Dependent interstitial element:VA
TYPE OF CONDITION FOR COMPONENT C /ZERO_FLUX/: activity
LOW TIME LIMIT /0/: 0
ACR(C) (TIME)= 1e-5;
HIGH TIME LIMIT /*/: *
ANY MORE RANGES /N/: N
TYPE OF CONDITION FOR COMPONENT MN /ZERO_FLUX/: zero_flux
TYPE OF CONDITION FOR COMPONENT SI /ZERO_FLUX/: zero_flux
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 1e9
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /100000000/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC> @@
DIC> @@ SAVE TO FILE
DIC> @@
DIC> save exa6 y
DIC>
DIC> set-inter
--OK---
DIC>
```

**exa6-run**

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exa6\run.DCM.test"
DIC>
DIC>
DIC> @@ run.DCM
DIC>
DIC> @@
DIC> FILE FOR RUNNING exa6
DIC> @@
DIC>
DIC> @@
DIC> ENTER THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 0.00000E+00
*** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
DIC> read exa6
OK
DIC>
DIC> @@
DIC> Start the simulation
DIC> @@
DIC> simulate
Region: AUS
double geometric
dense at outer boundaries, coarse at 0.50000E-02
lower part 1.2500 22
upper part 0.80000 22
DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
U-FRACTION IN SYSTEM: C = .00115488575879621 FE = .490055682684517
MN = .00302988813183616 SI = .00691442924890042
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
U-FRACTION IN SYSTEM: C = .00115488575879621 FE = .490055682684517
MN = .00302988813183616 SI = .00691442924890042
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00116822817821891 FE = .490055682684517
MN = .00302988813183616 SI = .00691442924890042
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 1 seconds
TIME = 0.10010000E-03 DT = 0.10000000E-03 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00116829188694328 FE = .490055682684517
MN = .00302988813183616 SI = .00691442924890042
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds
TIME = 3.0557610 DT = 3.0556609 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00118959189435653 FE = .490055682684521
MN = .00302988813183664 SI = .00691442924889593
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds
TIME = 9.1670828 DT = 6.1113218 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00121111672154579 FE = .490055682684524
MN = .00302988813183702 SI = .00691442924889251
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds
TIME = 21.389726 DT = 12.222644 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00123890626455181 FE = .490055682684528
MN = .00302988813183746 SI = .00691442924888853
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 1 seconds
TIME = 45.835013 DT = 24.445287 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00127670303015352 FE = .490055682684532
MN = .00302988813183797 SI = .00691442924888392
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds
TIME = 94.725588 DT = 48.890574 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00132921753226138 FE = .490055682684536
MN = .00302988813183855 SI = .00691442924887889
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds
TIME = 192.50674 DT = 97.781148 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00140291029963708 FE = .49005568268454
MN = .00302988813183909 SI = .00691442924887446
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds
TIME = 388.06903 DT = 195.56230 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00150683893865951 FE = .490055682684541
MN = .00302988813183934 SI = .00691442924887331
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds
TIME = 779.19363 DT = 391.12459 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00165382101622263 FE = .490055682684533
MN = .00302988813183861 SI = .00691442924888217
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 1 seconds
TIME = 1561.4428 DT = 782.24919 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00186208912002594 FE = .49005568268452
MN = .00302988813183733 SI = .00691442924889648
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds
TIME = 3125.9412 DT = 1564.4984 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00215763950853838 FE = .490055682684545
MN = .00302988813184034 SI = .00691442924886802
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds
TIME = 6254.9379 DT = 3128.9967 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00257762247234064 FE = .490055682684614
MN = .00302988813184873 SI = .0069144292487913
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds
TIME = 12512.931 DT = 6257.9935 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00317612553687887 FE = .490055682684701
MN = .00302988813186053 SI = .00691442924869196
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 1 seconds
TIME = 25028.918 DT = 12515.987 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00403212708748458 FE = .490055682684788
MN = .00302988813187388 SI = .00691442924859185
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds
TIME = 50060.892 DT = 25031.974 SUM OF SQUARES = 0.0000000
```

```

U-FRACTION IN SYSTEM: C = .00526185946385771 FE = .490055682684867
MN = .00302988813188714 SI = .00691442924849985
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds
TIME = 100124.84 DT = 50063.948 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00703878462392718 FE = .490055682684956
MN = .00302988813189985 SI = .00691442924839735
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 1 seconds
TIME = 200252.74 DT = 100127.90 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00961468135205802 FE = .490055682685084
MN = .0030298881319146 SI = .00691442924825484
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds

output ignored...

... output resumed

CPU time used in timestep 0 seconds
TIME = 1602043.3 DT = 801023.17 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .016516584267494 FE = .490055682687091
MN = .00302988813214933 SI = .00691442924601361
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 1 seconds
TIME = 307117.5 DT = 1469074.2 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0165253458723486 FE = .490055682689399
MN = .00302988813240263 SI = .00691442924345169
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds
TIME = 5521426.5 DT = 2450309.1 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0165254570895423 FE = .490055682693946
MN = .00302988813287881 SI = .00691442923842824
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds
TIME = 9715746.1 DT = 4194319.5 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0165253215591159 FE = .490055682703382
MN = .00302988813383215 SI = .00691442922803932
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds
TIME = 17813876. DT = 8098130.0 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0165250052909415 FE = .490055682726195
MN = .00302988813607049 SI = .00691442920298777
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds
TIME = 34010136. DT = 16196260. SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0165246276464079 FE = .490055682784398
MN = .00302988814169422 SI = .00691442913916063
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds
TIME = 66402656. DT = 32392520. SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0165243580713321 FE = .490055682920989
MN = .00302988815540702 SI = .00691442898885753
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 1 seconds
TIME = 0.13118770E+09 DT = 64785040. SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0165244582014692 FE = .490055683192306
MN = .00302988818558275 SI = .00691442868736454
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds
TIME = 0.23061023E+09 DT = 99422537. SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0165263917143567 FE = .490055683555767
MN = .00302988823056496 SI = .00691442827892098
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds
TIME = 0.33012543E+09 DT = 99515198. SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0165303267851657 FE = .49005568386721
MN = .00302988827178368 SI = .0069144279262599
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 1 seconds
TIME = 0.42970616E+09 DT = 99580728. SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0165336326908904 FE = .490055684142115
MN = .00302988830951066 SI = .00691442761362775
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds
TIME = 0.52934108E+09 DT = 99634921. SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0165366300962672 FE = .490055684390274
MN = .0030298883443561 SI = .00691442733062356
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds
TIME = 0.62902222E+09 DT = 99681143. SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0165394384249253 FE = .490055684617852
MN = .00302988837682077 SI = .00691442707058051
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 1 seconds
TIME = 0.72874408E+09 DT = 99721854. SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0165421143527838 FE = .490055684829008
MN = .00302988840729343 SI = .00691442682895181
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds
TIME = 0.82850228E+09 DT = 99758206. SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0165446894756979 FE = .490055685026688
MN = .00302988843607474 SI = .00691442660249091
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds
TIME = 0.92829328E+09 DT = 99791002. SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0165471833610488 FE = .490055685213062
MN = .00302988846340021 SI = .0069144263887909
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 1 seconds
TIME = 0.98979354E+09 DT = 61500257. SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0165498694311615 FE = .490055685322987
MN = .00302988847959189 SI = .006914426267452
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds
TIME = 0.10000000E+10 DT = 10206459. SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0165516055116168 FE = .490055685340902
MN = .00302988848223566 SI = .00691442624211591
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 0.0000000

```

```
DELETING TIME-RECORD FOR TIME 0.1000000E-06
DELETING TIME-RECORD FOR TIME 0.1001000E-03
DELETING TIME-RECORD FOR TIME 3.0557610
DELETING TIME-RECORD FOR TIME 9.1670828
DELETING TIME-RECORD FOR TIME 21.389726
DELETING TIME-RECORD FOR TIME 45.835013
DELETING TIME-RECORD FOR TIME 94.725588
DELETING TIME-RECORD FOR TIME 192.50674
DELETING TIME-RECORD FOR TIME 388.06903
DELETING TIME-RECORD FOR TIME 779.19363
DELETING TIME-RECORD FOR TIME 1561.4428
DELETING TIME-RECORD FOR TIME 3125.9412
DELETING TIME-RECORD FOR TIME 6254.9379
DELETING TIME-RECORD FOR TIME 12512.931
DELETING TIME-RECORD FOR TIME 25028.918
DELETING TIME-RECORD FOR TIME 50060.892
DELETING TIME-RECORD FOR TIME 100124.84
DELETING TIME-RECORD FOR TIME 200252.74
DELETING TIME-RECORD FOR TIME 400508.53
DELETING TIME-RECORD FOR TIME 801020.11
DELETING TIME-RECORD FOR TIME 1602043.3
DELETING TIME-RECORD FOR TIME 3071117.5
DELETING TIME-RECORD FOR TIME 5521426.5
DELETING TIME-RECORD FOR TIME 9715746.1
DELETING TIME-RECORD FOR TIME 17813876.
DELETING TIME-RECORD FOR TIME 34010136.
DELETING TIME-RECORD FOR TIME 66402656.
DELETING TIME-RECORD FOR TIME 0.13118770E+09
DELETING TIME-RECORD FOR TIME 0.23061023E+09
DELETING TIME-RECORD FOR TIME 0.33012543E+09
DELETING TIME-RECORD FOR TIME 0.42970616E+09
DELETING TIME-RECORD FOR TIME 0.52934108E+09
DELETING TIME-RECORD FOR TIME 0.62902222E+09
DELETING TIME-RECORD FOR TIME 0.72874408E+09
DELETING TIME-RECORD FOR TIME 0.82850228E+09
DELETING TIME-RECORD FOR TIME 0.92829328E+09
```

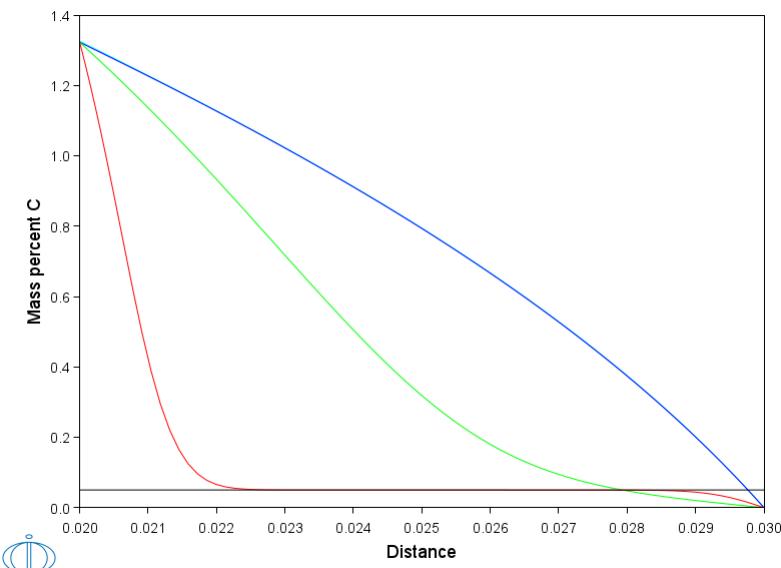
```
KEEPING TIME-RECORD FOR TIME 0.98979354E+09
AND FOR TIME 0.10000000E+10
WORKSPACE RECLAIMED
```

```
TIMESTEP AT 0.10000000E+10 SELECTED
```

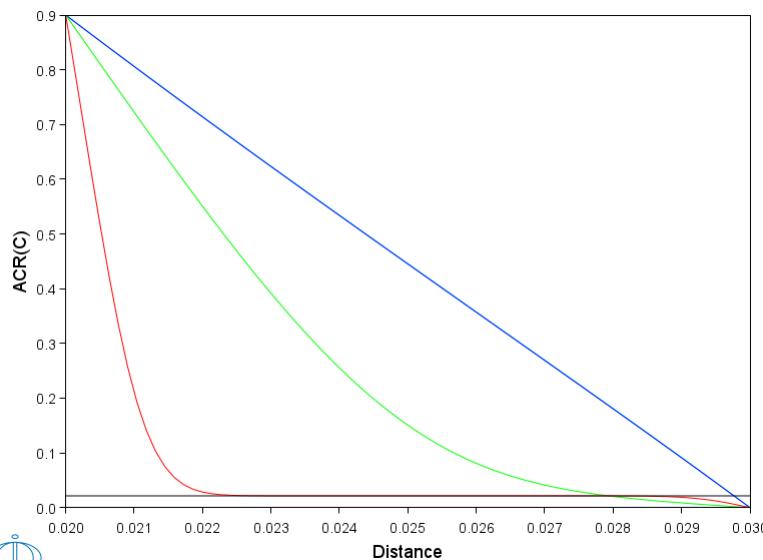
```
DIC>
DIC> @@
DIC> @@ THE SIMULATION IS FINISHED
DIC> @@
DIC>
DIC> set-inter
--OK---
DIC>
```

## exa6-plot

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exa6\plot.DCM.test"
DIC>
DIC>
DIC> @@ exa6_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE exa6
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 1.00000E+09
*** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
DIC> read exa6
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1:
POST-1: @@
POST-1: @@ PLOT THE CONCENTRATION OF C AT DIFFERENT TIMES
POST-1: @@
POST-1: s-d-a x distance global
INFO: Distance is set as independent variable
POST-1: s-d-a y w-p c
POST-1: s-p-c time 0,1e4,2e5,1e7,1e9
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```



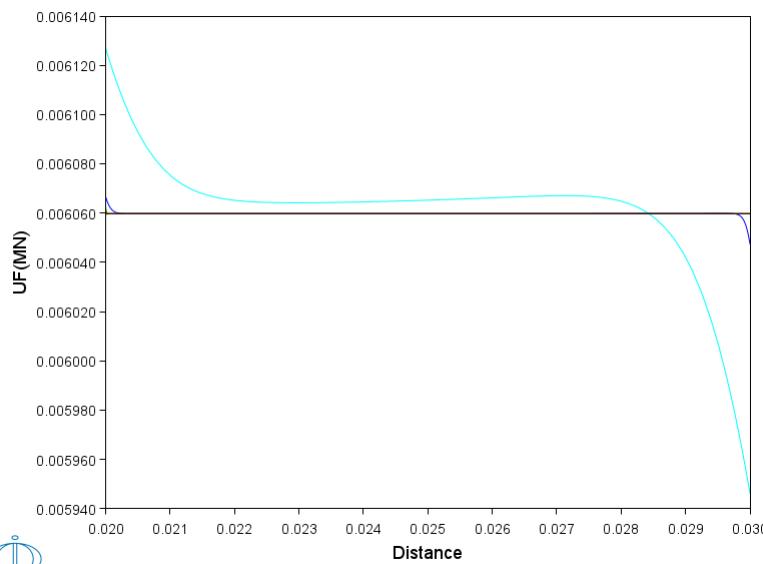
```
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ PLOT THE ACTIVITY OF C
POST-1: @@
POST-1:
POST-1: s-d-a y acr(c)
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```



```

 $\odot$ 
POST-1:
POST-1:
POST-1:
POST-1: Hit RETURN to continue
POST-1:
POST-1: @@ 
POST-1: @@ LET US LOOK AT THE MN AND SI PROFILES
POST-1: @@
POST-1: @@ WE PLOT THE U-FRACTION OF MN AND SI WHICH WILL BE INDEPENDENT
POST-1: @@ OF THE C-CONCENTRATION.
POST-1: @@
POST-1: s-d-a y u-f mn
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

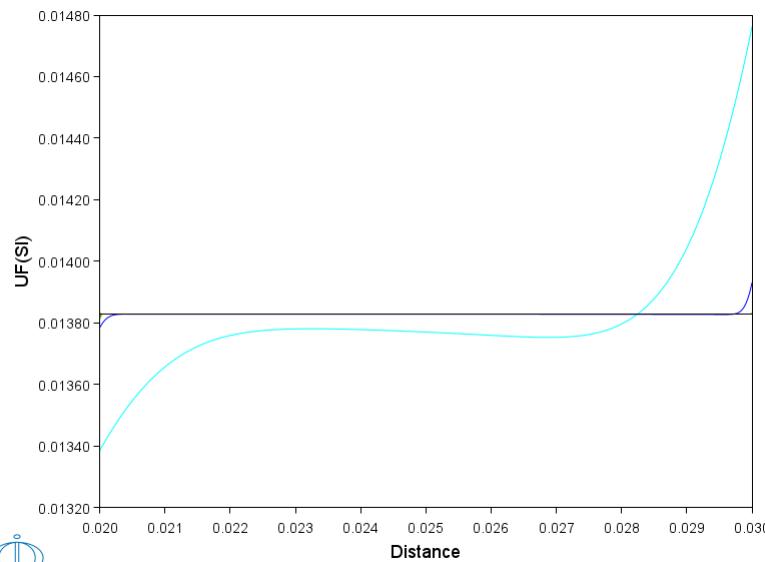
```



```

 $\odot$ 
POST-1:
POST-1:
POST-1:
POST-1:
POST-1: Hit RETURN to continue
POST-1:
POST-1: s-d-a y u-f si
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

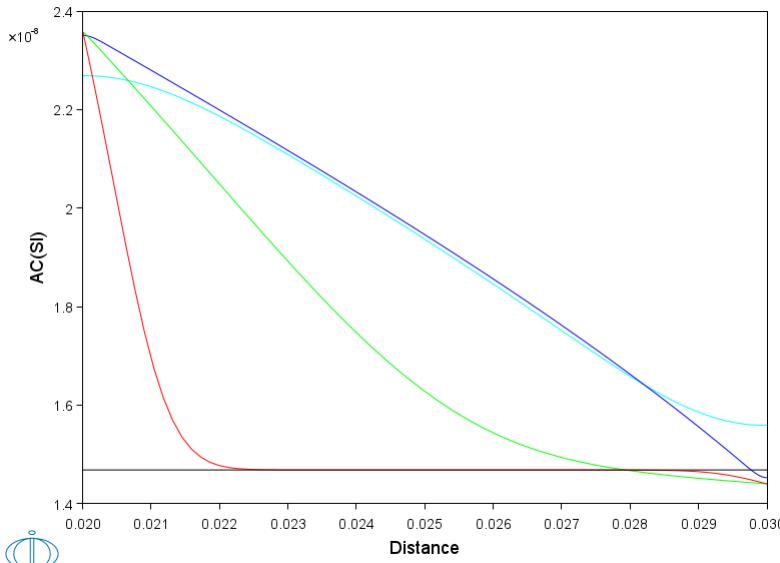
```



```

 $\odot$ 
POST-1:
POST-1:
POST-1:
POST-1:
POST-1: Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ FINALLY, LOOK AT THE ACTIVITY PROFILES OF SI
POST-1: @@
POST-1: s-d-a y ac(si)
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

```



```

 $\odot$ 
POST-1:
POST-1:
POST-1:
POST-1:
POST-1: Hit RETURN to continue
POST-1:
POST-1: set-inter
--OK--
POST-1:

```

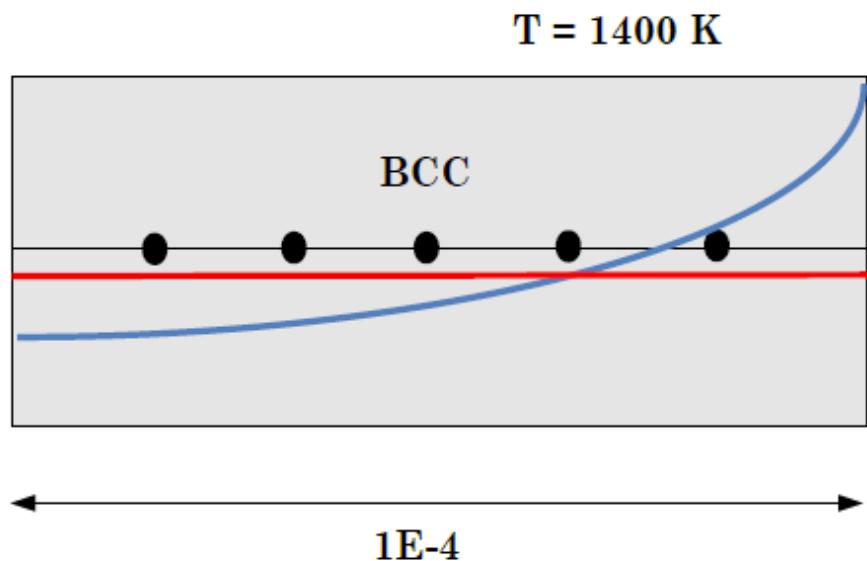


## Example exa7

### Homogenization heat-treatment

(Initial profile imported from Scheil simulation)

The initial segregation profile is created from a Scheil calculation (see macro `create_initial_profile.TCM`). The command `INPUT_SCHEIL_PROFILE` in the DICTRA monitor performs most of the setup. Only time and temperature must be entered after the `INPUT_SCHEIL_PROFILE` command is executed.



**exa7-setup****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\_dictra\_console\_examples\examples\exa7\setup.DCM.test"**

**SYS:** @@ One phase example.

**SYS:** @@ Homogenization heat treatment

**SYS:** @@ The initial segregation profile is created from a Scheil

**SYS:** @@ calculation (see macro create\_initial\_profile.TCM). The command

**SYS:** @@ INPUT\_SCHEIL\_PROFILE in the DICTRA MONITOR performs most of the

**SYS:** @@ set up. Only time and temperature must be entered after the

**SYS:** @@ INPUT\_SCHEIL\_PROFILE command is executed.

**SYS:** -----

NO SUCH COMMAND, USE HELP

**SYS:**

**SYS:** @@ In this example only a single phase, ferrite, is entered in the simulation

**SYS:** go da

  THERMODYNAMIC DATABASE module

  Database folder:

  C:\jenkins\workspace\generate\_dictra\_console\_examples\databases\data

  Current database: Steels/Fe-Alloys v12.0

  VA                           /- DEFINED

  DICTRA\_FCC\_A1 REJECTED

**TDB\_FEDEMO:** sw FEDEMO

  Current database: Iron Demo Database v4.0

  VA                           /- DEFINED

**TDB\_FEDEMO:** def-sys fe cr ni mn

  FE                           CR                           NI

  MN DEFINED

**TDB\_FEDEMO:** rej ph \*

  LIQUID:L                   BCC\_A2                   LAVES\_PHASE\_C14

  CBCC\_A12                  CHI\_A12                  CUB\_A13

  DIAMOND\_FCC\_A4           FCC\_A1                   HCP\_A3

  SIGMA REJECTED

**TDB\_FEDEMO:** rest ph bcc

  BCC\_A2 RESTORED

**TDB\_FEDEMO:** get

15:22:44,304 [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'

'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'

'B.J. Lee, Metall. Trans. A, 24A (1993) 1919-1933; Cr-Mn, Fe-Cr -Mn'

'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'

'A.T. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); CR -NI'

'W. Huang, CALPHAD, 13 (1989) 243-252; TRITA-MAC 388 (rev 1989); FE-MN'

'L.J. Zhang, Int.J. Mater. Res.,100(2) 160-175 (2009),Fe-Mn-Ni'

'A.T. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); FE-NI'

'Shuhong Liu, unpublished work (2010),Mn-Ni,Al-Mn-Ni,Mn-Ni-Zn, Al-Cu-Fe-Mg

-Mn-Si'

-OK-

**TDB\_FEDEMO:**

**TDB\_FEDEMO:** app MFEDEMO

  Current database: Fe-Alloys Mobility demo database v2.0

  VA DEFINED

**APP:** def-sys fe cr ni mn

  FE                           CR                           NI

  MN DEFINED

**APP:** rej ph \*

  BCC\_A2                  FCC\_A1 REJECTED

**APP:** rest ph bcc

  BCC\_A2 RESTORED

**APP:** get

  ELEMENTS .....

  SPECIES .....

  PHASES .....

  PARAMETERS ....

  FUNCTIONS ....

List of references for assessed data

'This parameter has not been assessed'

'B. Jonsson: ISIJ International, 35(1995)1415-1421; Cr, Fe and Ni diffusion bcc Cr-Fe-Ni'

'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion in bcc Fe'

'M. Xing, Thermo-Calc Software AB, Sweden, 2023.'

'S. Deng, et al., CALPHAD, 56 (2017) 230-240.'

'Assessed from data presented in Landolt-Bornstein, Vol. 26, ed. H. Mehrer, Springer (1990); Impurity diff of Mn in bcc Fe.'

'W. Zheng, et al., Metall Mater Trans, 48 (2017) 536-550; Fe-Mn-Mo (fcc and bcc)'

-OK-

**APP:**

**APP:** go dict-mon

  NO TIME STEP DEFINED

```
DIC>
DIC>
DIC> @@ THE INPUT_SCHEIL_PROFILE COMMAND PERFORMS MOST OF THE SET UP
DIC> input_scheil_profile
INFO: SCHEIL_REGION CREATED
FILE NAME /XP.TXT/: segregation_profile.TXT
ENTER WIDTH OF REGION /1/: 100e-6
INFO: LINEAR GRID IN SCHEIL_REGION ENTERED WITH 100 GRID POINTS
ENTER MAIN SOLID SOLUTION PHASE
PHASE NAME: bcc#1
INFO: CHANGING DEPENDENT COMPONENT FROM NI TO FE
INFO: COMPOSITION PROFILE ENTERED IN REGION
SHOULD MORE PHASES BE ENTERED IN THE REGION /NO/: n
INFO: TO COMPLETE SETUP, ENTER TEMPERATURE AND
SIMULATION TIME
DIC>
DIC>
DIC> @@ ENTER THE HEAT TREATMENT TEMPERATURE
DIC> s-cond
GLOBAL OR BOUNDARY CONDITION /GLOBAL/: glob
VARIABLE : t
LOW TIME LIMIT /0/: 0 1473; * n
DIC>
DIC>
DIC> @@ ENTER A SIMULATION TIME
DIC> se-si-ti
END TIME FOR INTEGRATION /1/: 3600
AUTOMATIC TIMESTEP CONTROL /YES/: y
MAX TIMESTEP DURING INTEGRATION /360/: 360
INITIAL TIMESTEP : /1E-07/: 1e-7
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/: 1e-9
DIC>
DIC>
DIC> save exa7 y
DIC>
DIC> set-inter
--OK--
DIC>
```

**exa7-run**

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exa7\run.DCM.test"
DIC> go dict-mon
TIME STEP AT TIME 0.00000E+00
DIC>
DIC> read exa7
OK
DIC>
DIC> sim
DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
U-FRACTION IN SYSTEM: CR = .180420497424242 FE = .796498787878788
MN = .0099901687828288 NI = .0130905459141414
TOTAL SIZE OF SYSTEM: 1E-04 [m]
U-FRACTION IN SYSTEM: CR = .180420497424242 FE = .796498787878788
MN = .0099901687828288 NI = .0130905459141414
TOTAL SIZE OF SYSTEM: 1E-04 [m]
TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .180420497424242 FE = .796498787878788
MN = .0099901687828288 NI = .0130905459141414
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 1 seconds
TIME = 0.10010000E-03 DT = 0.10000000E-03 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .180420497424242 FE = .796498787878788
MN = .0099901687828288 NI = .0130905459141414
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.43088419 DT = 0.43078409 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .180420497424242 FE = .796498787878788
MN = .0099901687828289 NI = .0130905459141414
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 1 seconds
TIME = 1.2924524 DT = 0.86156818 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .180420497424243 FE = .796498787878788
MN = .0099901687828290 NI = .0130905459141414
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 3.0155887 DT = 1.7231364 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .180420497424243 FE = .796498787878787
MN = .0099901687828290 NI = .0130905459141415
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 6.4618615 DT = 3.4462727 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .180420497424241 FE = .796498787878781
MN = .00999016878283681 NI = .0130905459141414
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 13.354407 DT = 6.8925455 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .180420497424229 FE = .79649878787749
MN = .00999016878287913 NI = .0130905459141424
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 27.139498 DT = 13.785091 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .180420497424222 FE = .796498787878759
MN = .0099901687828793 NI = .0130905459141401
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 1 seconds
TIME = 54.709680 DT = 27.570182 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .180420497424197 FE = .79649878787879
MN = .00999016878287965 NI = .0130905459141337
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 109.85004 DT = 55.140364 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .180420497424141 FE = .796498787878856
MN = .00999016878288083 NI = .0130905459141224
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 220.13077 DT = 110.28073 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .180420497424055 FE = .796498787878951
MN = .00999016878288577 NI = .0130905459141089
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 440.69223 DT = 220.56145 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .180420497423961 FE = .79649878787904
MN = .00999016878289932 NI = .0130905459140991
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 800.69223 DT = 360.00000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .180420497423904 FE = .796498787879084
MN = .00999016878291493 NI = .0130905459140971
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 1 seconds
TIME = 1160.6922 DT = 360.00000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .180420497423885 FE = .796498787879096
MN = .00999016878292099 NI = .0130905459140983
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 1520.6922 DT = 360.00000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .180420497423872 FE = .796498787879108
MN = .00999016878292251 NI = .0130905459140985
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 1880.6922 DT = 360.00000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .18042049742386 FE = .796498787879119
MN = .00999016878292204 NI = .0130905459140978
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 2240.6922 DT = 360.00000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .180420497424024 FE = .79649878787892
MN = .00999016878295024 NI = .0130905459141057
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 2600.6922 DT = 360.00000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .18042049742418 FE = .79649878787873
MN = .00999016878297173 NI = .0130905459141176
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 2960.6922 DT = 360.00000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .180420497424307 FE = .796498787878573
MN = .00999016878299033 NI = .0130905459141292
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
```

```
TIME = 3320.6922 DT = 360.00000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .180420497424408 FE = .796498787878447
MN = .00999016878300546 NI = .0130905459141394
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 3600.0000 DT = 279.30777 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .180420497424462 FE = .796498787878379
MN = .00999016878301344 NI = .0130905459141448
TOTAL SIZE OF SYSTEM: 1E-04 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 0.0000000
DELETING TIME-RECORD FOR TIME 0.10000000E-06
DELETING TIME-RECORD FOR TIME 0.10010000E-03
DELETING TIME-RECORD FOR TIME 0.43088419
DELETING TIME-RECORD FOR TIME 1.2924524
DELETING TIME-RECORD FOR TIME 3.0155887
DELETING TIME-RECORD FOR TIME 6.4618615
DELETING TIME-RECORD FOR TIME 13.354407
DELETING TIME-RECORD FOR TIME 27.139498
DELETING TIME-RECORD FOR TIME 54.709680
DELETING TIME-RECORD FOR TIME 109.85004
DELETING TIME-RECORD FOR TIME 220.13077
DELETING TIME-RECORD FOR TIME 440.69223
DELETING TIME-RECORD FOR TIME 800.69223
DELETING TIME-RECORD FOR TIME 1160.6922
DELETING TIME-RECORD FOR TIME 1520.6922
DELETING TIME-RECORD FOR TIME 1880.6922
DELETING TIME-RECORD FOR TIME 2240.6922
DELETING TIME-RECORD FOR TIME 2600.6922
DELETING TIME-RECORD FOR TIME 2960.6922

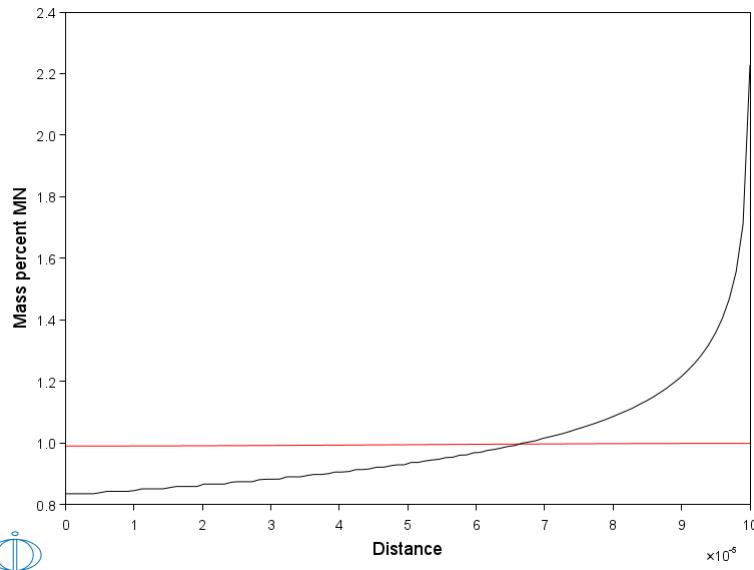
KEEPING TIME-RECORD FOR TIME 3320.6922
AND FOR TIME 3600.0000
WORKSPACE RECLAIMED
```

```
TIMESTEP AT 3600.00000 SELECTED
```

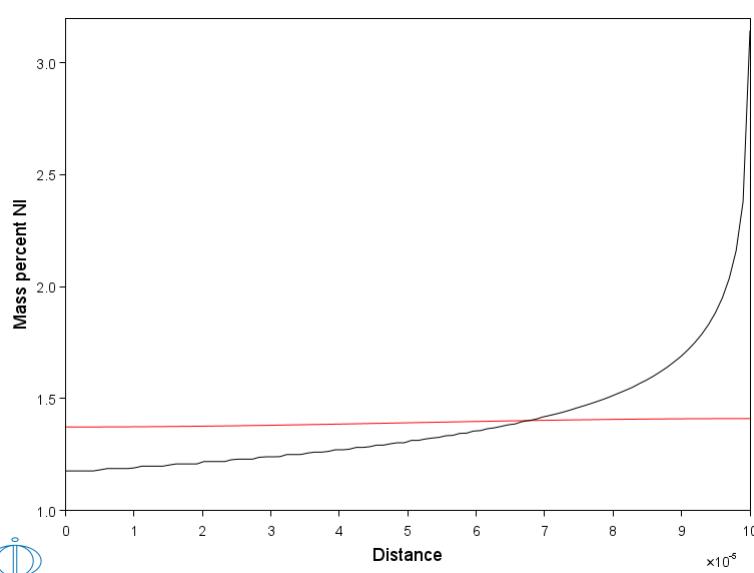
```
DIC>
DIC> set-inter
--OK---
DIC>
```

**exa7-plot**

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exa7\plot.DCM.test"
DIC> go dict-mon
TIME STEP AT TIME 3.60000E+03
DIC>
DIC> read exa7
OK
DIC>
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1: s-p-c time 0,3600
POST-1: s-d-a x d g
INFO: Distance is set as independent variable
POST-1: s-d-a y w-p mn
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```



```
POST-1:
POST-1: @@ Hit enter for the next plot
POST-1:@?
POST-1:
POST-1: s-d-a y w-p ni
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```



```
POST-1:
POST-1: set-inter
--OK---
POST-1:
```



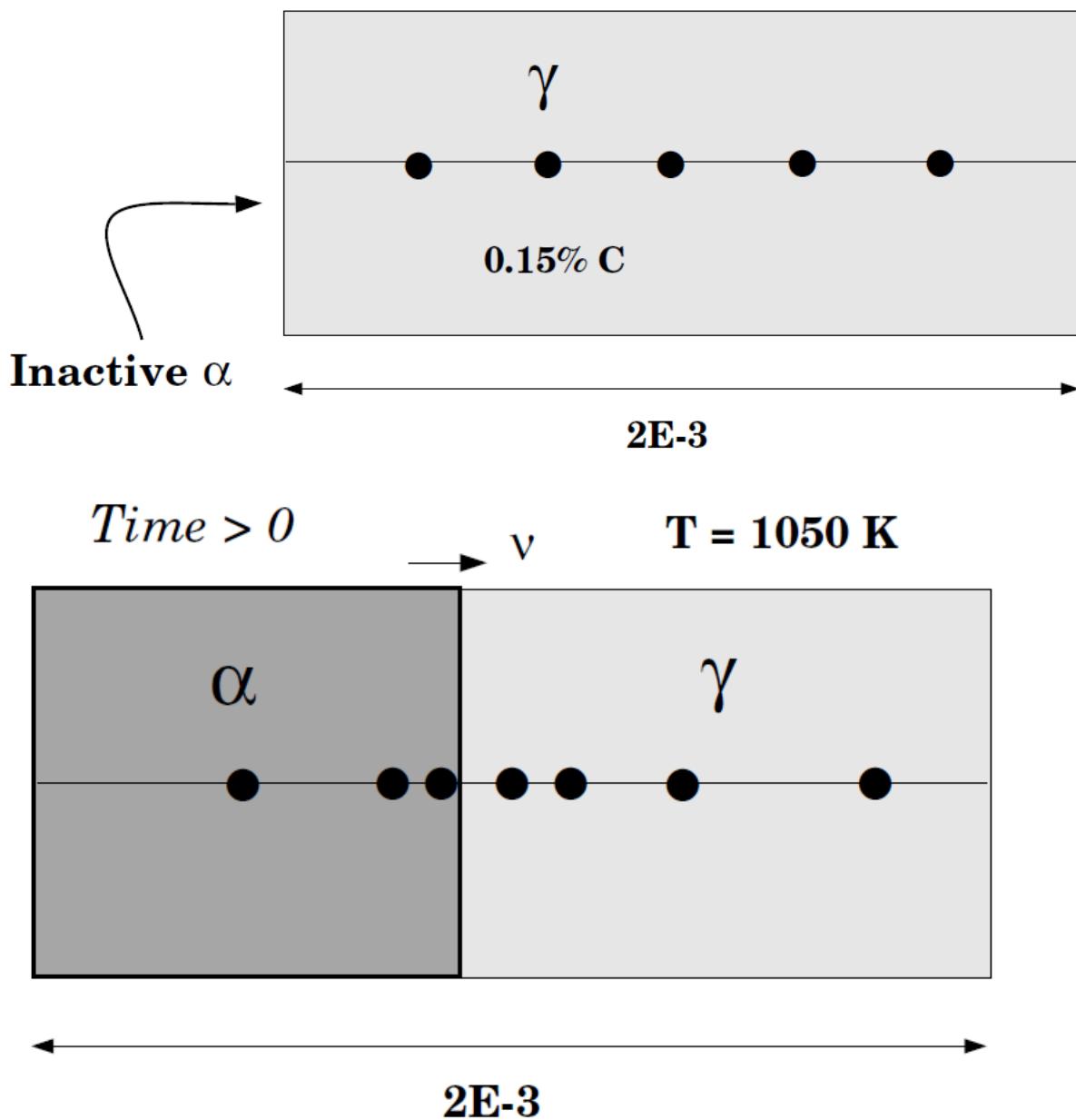
## Example exb1b

## **$\gamma$ to $\alpha$ transformation in a binary Fe-C alloy: Inactive $\alpha$**

This is the same example as in exb1a but now the problem is with ferrite as an inactive phase adjacent to the initial austenite.

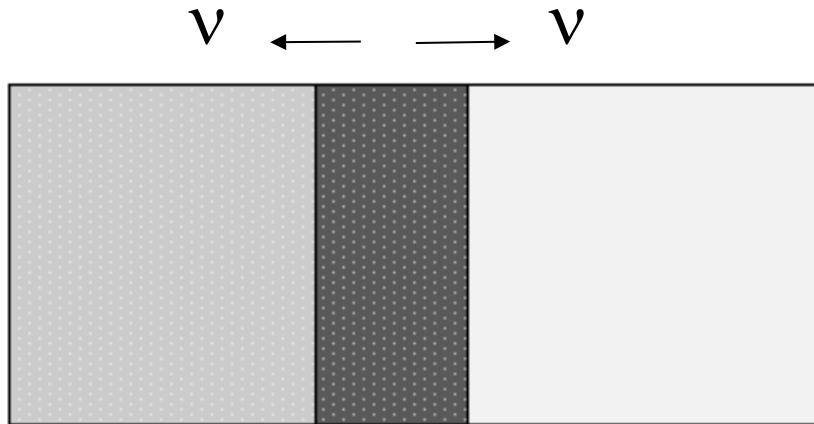
*Time = 0*

**T = 1050 K**





## Moving Boundary Problems



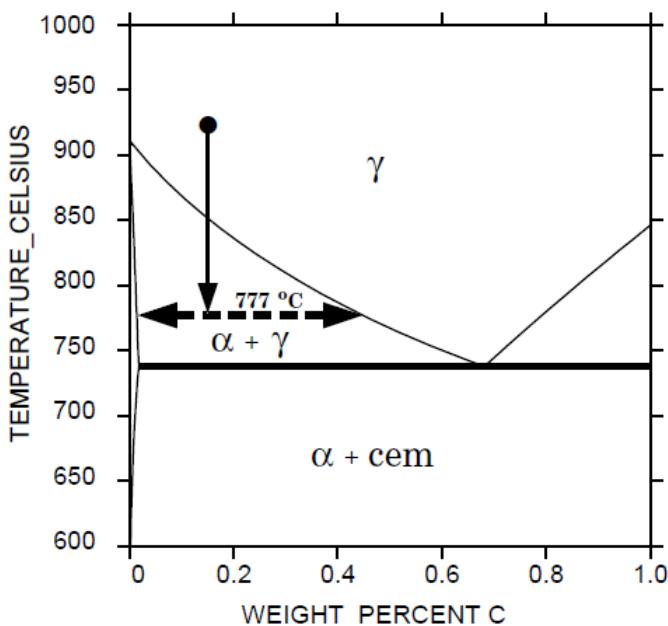


## Example exb1a

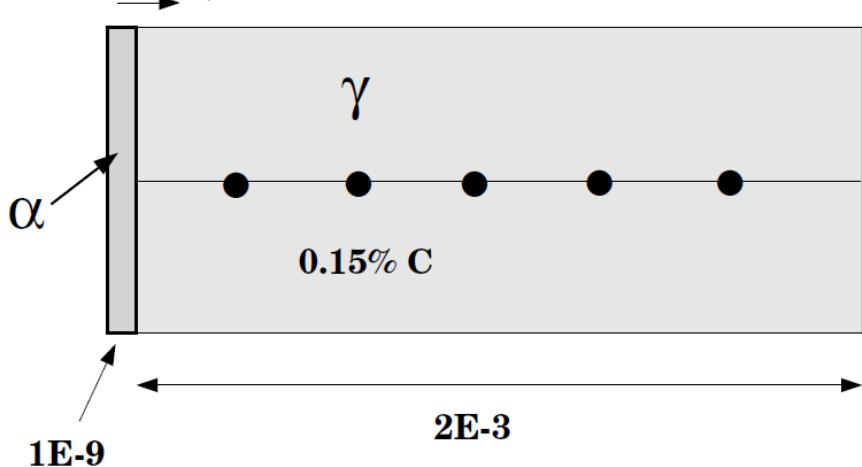
### $\gamma$ to $\alpha$ transformation in a binary Fe-C alloy

This example calculates a ferrite (BCC)/austenite (FCC) transformation in a binary Fe-C alloy. The initial state is an austenite of 2 mm thickness. The composition of the austenite is Fe-0.15wt%C. After austenitization the specimen has been quenched down to 1050K. The system is assumed closed, no boundary conditions are set (a closed system is the default). Ferrite is expected to grow into the austenite. For this reason you start with a thin region with ferrite adjacent to the austenite.

Fe - C Phase diagram



$T = 1050$  K



**exbla-setup****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_dictra_console_examples\examples\exbla\setup.DCM.test"
SYS: @@
SYS: @@ Moving boundary problem.
SYS: @@ Austenite to ferrite transformation in a binary Fe-C alloy
SYS: @@ This example calculates a ferrite(BCC)/austenite(FCC)transformation
SYS: @@ in a binary Fe-C alloy. The initial state is an austenite of 2mm
SYS: @@ thickness. The composition of the austenite is Fe-0.15wt%C.
SYS: @@
SYS: @@ After austenitization the specimen is quenched down to 1050K.
SYS: @@ The system is assumed closed, so no boundary conditions are set
SYS: @@ (a closed system is the default). Ferrite is expected to grow
SYS: @@ into the austenite, which is why we start with a thin
SYS: @@ region with ferrite adjacent to the austenite.
SYS: -----
NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exbla_setup.DCM
SYS:
SYS:
SYS: @@
SYS: @@ START BY GOING TO THE DATABASE MODULE
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\generate_dictra_console_examples\databases\data
Current database: Steels/Fe-Alloys v12.0

VA          /- DEFINED
DICTRA_FCC_A1  REJECTED
TDB_TCFE12: @@
TDB_TCFE12: @@
TDB_TCFE12: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE THE DATA
TDB_TCFE12: @@
TDB_TCFE12: sw FEDEMO
Current database: Iron Demo Database v4.0

VA          /- DEFINED
TDB_FEDEMO: @@
TDB_FEDEMO: @@ DEFINE THE SYSTEM TO WORK WITH
TDB_FEDEMO: @@
TDB_FEDEMO: def-sys fe c
FE          C DEFINED
TDB_FEDEMO: @@
TDB_FEDEMO: @@
TDB_FEDEMO: @@ EXCLUDE THE THERMODYNAMIC DATA FOR THE PHASES THAT ARE NOT NEEDED
TDB_FEDEMO: @@
TDB_FEDEMO: rej ph * all
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 bcc
FCC_A1          BCC_A2  RESTORED
TDB_FEDEMO: @@
TDB_FEDEMO: @@ RETRIEVE DATA FROM THE DATABASE FILE
TDB_FEDEMO: @@
TDB_FEDEMO: get
15:26:00,768 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS .....

List of references for assessed data

'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'
'X.G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
'A.T. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
'X.G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
volumes'

-OK-
TDB_FEDEMO: @@
TDB_FEDEMO: @@ MOBILITY/DIFFUSIVITY DATA ARE STORED IN A SEPARATE DATABASE FILE.
TDB_FEDEMO: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE DATA
TDB_FEDEMO: @@
TDB_FEDEMO: append
Use one of these databases

TCFE12 = Steels/Fe-Alloys v12.0
TCFE9 = Steels/Fe-Alloys v9.3
SSUB6 = SGTE Substances v6.0
FEDEMO = Iron Demo Database v4.0
MOB2 = Alloys Mobility v2.7
MOBFE2 = Steels/Fe-Alloys Mobility v2.0
MOBFE4 = Steels/Fe-Alloys Mobility v4.0
MOBFE7 = Steels/Fe-Alloys Mobility v7.1
MFEDEMO = Fe-Alloys Mobility demo database v2.0
```

```

USER      = User defined Database

DATABASE NAME /FEDEMO/: MFDEMO
Current database: Fe-Alloys Mobility demo database v2.0

VA  DEFINED
APP: def-sys fe c
    C  DEFINED
APP: rej ph * all
BCC_A2          FCC_A1           CEMENTITE
REJECTED
APP: res ph fcc bcc
FCC_A1          BCC_A2  RESTORED
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS .....

List of references for assessed data

'This parameter has not been assessed'
'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'
'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
-Ni'
'B. Jonsson: Z. Metallkunde 85(1994)498-501; C and N diffusion in bcc Cr
-Fe-Ni'
'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
in bcc Fe'

-OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP
APP: @@
APP: go d-m
NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER GLOBAL CONDITION T
DIC> @@
DIC> set-condition global T 0 1050; * N
DIC>
DIC> @@
DIC> @@ START BY ENTERING THE REGIONS ferrite AND austenite WHERE WE
DIC> @@ PUT THE BCC AND FCC PHASE, RESPECTIVELY. THE FERRITE REGION IS
DIC> @@ ASSUMED INITIALLY TO BE VERY THIN, 1E-9 METERS.
DIC> @@
DIC> enter-region
REGION NAME : ferrite
DIC>
DIC> enter-region
REGION NAME : austenite
ATTACH TO REGION NAMED /FERRITE/:
ATTACHED TO THE RIGHT OF FERRITE /YES/:
DIC>
DIC> @@
DIC> @@ ENTER GRIDS INTO THE REGIONS
DIC> @@
DIC> enter-grid
REGION NAME : /FERRITE/: ferrite
WIDTH OF REGION /1/: 1e-9
TYPE /LINEAR/: linear
NUMBER OF POINTS /50/: 10
DIC>
DIC> enter-grid austenite
WIDTH OF REGION /1/: 20e-4
TYPE /LINEAR/: geo
NUMBER OF POINTS /50/: 100
VALUE OF R IN THE GEOMETRICAL SERIE : 1.05
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ ENTER active PHASES INTO THE REGIONS
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /FERRITE/: ferrite
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: bcc
DIC>
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /AUSTENITE/: austenite
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ ENTER AN INITIAL COMPOSITION INTO BCC
DIC> @@
DIC> enter-composition
REGION NAME : /FERRITE/: ferrite
PHASE NAME: /BCC_A2/: bcc
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: C
TYPE /LINEAR/: linear
VALUE OF FIRST POINT : 0.01
VALUE OF LAST POINT : /1E-2/: 0.01
DIC>
DIC> @@
DIC> @@ ENTER AN INITIAL COMPOSITION INTO FCC
DIC> @@
DIC> enter-composition
REGION NAME : /AUSTENITE/: austenite
PHASE NAME: /FCC_A1/: fcc#1
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: C
TYPE /LINEAR/: linear

```

```
VALUE OF FIRST POINT : 0.15
VALUE OF LAST POINT : /0.15/: 0.15
DIC>
DIC>
DIC> @@
DIC> @@ THE BOUNDARY CONDITION IS A CLOSED SYSTEM AS WE DO NOT SPECIFY
DIC> @@ ANYTHING ELSE
DIC> @@
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 1e9
AUTOMATIC TIMESTEP CONTROL /YES/: YES
MAX TIMESTEP DURING INTEGRATION /100000000/: 1e8
INITIAL TIMESTEP : /1E-07/: 1E-7
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/: 1E-7
DIC>
DIC>
DIC> @@
DIC> @@ IMPLICIT (1) TIME INTEGRATION IS USED INSTEAD OF THE MORE ACCURATE
DIC> @@ (BUT LESS STABLE) TRAPEZOIDAL METHOD WHICH IS THE DEFAULT.
DIC> @@
DIC> s-s-c
NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /AUTO/:
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPURITY WHEN INTEGRATING PDES (AUTO, 0 -> 0.5 -> 1) : /AUTO/: 1.0
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:
ALWAYS CALCULATE STIFFNESS MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/:
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exbla Y
DIC>
DIC> set-inter
--OK--
DIC>
```

**exbla-run**

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exbla\run.DCM.test"
DIC>
DIC>
DIC> @@ exbla_run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING EXAMPLE b1a
DIC> @@
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 0.00000E+00
DIC> read exbla
OK
DIC>
DIC> @@
DIC> @@ START THE SIMULATION
DIC> @@
DIC> simulate
Trying old scheme          3
U-FRACTION IN SYSTEM: C = .00698495590385911  FE = 1
TOTAL SIZE OF SYSTEM: .002000001 [m]
U-FRACTION IN SYSTEM: C = .00698495590385911  FE = 1
TOTAL SIZE OF SYSTEM: .002000001 [m]
4 GRIDPOINT(S) ADDED TO CELL #1 REGION: FERRITE
1 GRIDPOINT(S) ADDED TO CELL #1 REGION: AUSTENITE
0.115717401092456          0.115717856446352          111.048198612396          0.112984276756263          0.104050478927888          9.078830400089431
002    7.040904692738453E-002          3.472489874813312E-002          1.786881065983819E-003          9.193856999783227E-
006    1.857932499491210E-009          6.954562748969641E-020          TIME = 0.10000000E-06 DT = 0.10000000E-
06 SUM OF SQUARES = 0.69545627E-19
CELL # 1 VELOCITY AT INTERFACE # 2 IS 9.7160434 AND 9.7160434
POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.97260434E-06
U-FRACTION IN SYSTEM: C = .0069849386866348 FE = 1
TOTAL SIZE OF SYSTEM: .002000001 [m]
11 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: FERRITE
11 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: AUSTENITE

CPU time used in timestep          0 seconds
3.924867797203495E-003          3.925632782419901E-003          2.584529936625708E-005          1.486336645533285E-005          1.819317601377473E-
006    2.382918753471705E-009          8.205875381529106E-010          1.188244672679580E-010          1.387526115512604E-
021    TIME = 0.30000000E-06 DT = 0.20000000E-06 SUM OF SQUARES = 0.13875261E-20
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.39725772E-05 AND 0.39725772E-05
POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.97260514E-06
U-FRACTION IN SYSTEM: C = .00698493868664155 FE = 1
TOTAL SIZE OF SYSTEM: .002000001 [m]
CPU time used in timestep          0 seconds
3.646820050949611E-009          3.608769024242698E-009          9.804145357096042E-014          2.593396189298117E-019          TIME = 0.70000000E-
06 DT = 0.40000000E-06 SUM OF SQUARES = 0.25933962E-18
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.39679420E-05 AND 0.39679420E-05
POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.97260672E-06
U-FRACTION IN SYSTEM: C = .00698493868663973 FE = 1
TOTAL SIZE OF SYSTEM: .002000001 [m]
CPU time used in timestep          0 seconds
4.098598145867339E-009          4.058536706115315E-009          2.032937233572303E-015          1.674083532969155E-019          TIME = 0.15000000E-
05 DT = 0.80000000E-06 SUM OF SQUARES = 0.16740835E-18
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.39678989E-05 AND 0.39678989E-05
POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.97260990E-06
U-FRACTION IN SYSTEM: C = .0069849386866361 FE = 1
TOTAL SIZE OF SYSTEM: .002000001 [m]
1 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: FERRITE

CPU time used in timestep          0 seconds
4.09386269160249E-009          4.053797957014362E-009          1.173125463773368E-017          TIME = 0.31000000E-05 DT = 0.16000000E-
05 SUM OF SQUARES = 0.11731255E-16
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.39678132E-05 AND 0.39678132E-05
POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.97261625E-06
U-FRACTION IN SYSTEM: C = .00698493868662881 FE = 1
TOTAL SIZE OF SYSTEM: .002000001 [m]
1 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: FERRITE

CPU time used in timestep          0 seconds
4.084126643589076E-009          4.044153223609211E-009          5.413131685350729E-015          1.876149027657953E-023          TIME = 0.63000000E-
05 DT = 0.32000000E-05 SUM OF SQUARES = 0.18761490E-22
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.39676284E-05 AND 0.39676284E-05
POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.97262894E-06
U-FRACTION IN SYSTEM: C = .00698493868661433 FE = 1
TOTAL SIZE OF SYSTEM: .002000001 [m]
1 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: FERRITE

CPU time used in timestep          0 seconds
4.066800294220374E-009          4.026871951297030E-009          TIME = 0.10000000E-05 DT = 0.10000000E-05
output ignored...

... output resumed

1 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: AUSTENITE

CPU time used in timestep          0 seconds
1.903878495914222E-004          1.904040719369463E-004          1.509925713236157E-
018    TIME = 0.61258999E+09 DT = 0.10000000E+09 SUM OF SQUARES = 0.15099257E-17
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.38832374E-16 AND 0.38832374E-16
POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.13795631E-02
U-FRACTION IN SYSTEM: C = .00698478094673415 FE = 1
TOTAL SIZE OF SYSTEM: .002000001 [m]
2 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: FERRITE

CPU time used in timestep          0 seconds
7.135878186050930E-005          7.137189516735779E-005          1.224404141804395E-
025    TIME = 0.71258999E+09 DT = 0.10000000E+09 SUM OF SQUARES = 0.12244041E-24
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.33638036E-17 AND -0.33638036E-17
POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.13795628E-02
U-FRACTION IN SYSTEM: C = .0069847843769304 FE = 1
TOTAL SIZE OF SYSTEM: .002000001 [m]
1 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: AUSTENITE
```

CPU time used in timestep 0 seconds  
 2.276970266630391E-004 2.276970266630391E-004 2.819025009160587E-018  
 TIME = 0.81258999E+09 DT = 0.10000000E+09 SUM OF SQUARES = 0.28190250E-17  
 CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.70690954E-16 AND 0.70690954E-16  
 POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.13795699E-02  
 U-FRACTION IN SYSTEM: C = .00698471229072272 FE = 1  
 TOTAL SIZE OF SYSTEM: .002000001 [m]  
 3 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: FERRITE

CPU time used in timestep 0 seconds  
 5.175372179088760E-006 5.176015048274887E-006 4.805688098157295E-019  
 TIME = 0.91258999E+09 DT = 0.10000000E+09 SUM OF SQUARES = 0.48056881E-18  
 CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.42268448E-16 AND -0.42268448E-16  
 POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.13795656E-02  
 U-FRACTION IN SYSTEM: C = .00698475539343863 FE = 1  
 TOTAL SIZE OF SYSTEM: .002000001 [m]  
 1 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: AUSTENITE

CPU time used in timestep 0 seconds  
 1.971234376368413E-004 1.971471608276373E-004 3.234169931384480E-019  
 TIME = 0.10000000E+10 DT = 87410009. SUM OF SQUARES = 0.32341699E-18  
 CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.27418465E-16 AND 0.27418465E-16  
 POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.13795680E-02  
 U-FRACTION IN SYSTEM: C = .00698473095392153 FE = 1  
 TOTAL SIZE OF SYSTEM: .002000001 [m]  
 MUST SAVE WORKSPACE ON FILE  
 WORKSPACE SAVED ON FILE  
 RECLAIMING WORKSPACE  
 DELETING TIME-RECORD FOR TIME 0.0000000  
 DELETING TIME-RECORD FOR TIME 0.10000000E-06  
 DELETING TIME-RECORD FOR TIME 0.30000000E-06  
 DELETING TIME-RECORD FOR TIME 0.70000000E-06  
 DELETING TIME-RECORD FOR TIME 0.15000000E-05  
 DELETING TIME-RECORD FOR TIME 0.31000000E-05  
 DELETING TIME-RECORD FOR TIME 0.63000000E-05  
 DELETING TIME-RECORD FOR TIME 0.12700000E-04  
 DELETING TIME-RECORD FOR TIME 0.25500000E-04  
 DELETING TIME-RECORD FOR TIME 0.51100000E-04  
 DELETING TIME-RECORD FOR TIME 0.10230000E-03  
 DELETING TIME-RECORD FOR TIME 0.20470000E-03  
 DELETING TIME-RECORD FOR TIME 0.40950000E-03  
 DELETING TIME-RECORD FOR TIME 0.81910000E-03  
 DELETING TIME-RECORD FOR TIME 0.16383000E-02  
 DELETING TIME-RECORD FOR TIME 0.32767000E-02  
 DELETING TIME-RECORD FOR TIME 0.65535000E-02  
 DELETING TIME-RECORD FOR TIME 0.13107100E-01  
 DELETING TIME-RECORD FOR TIME 0.26214300E-01  
 DELETING TIME-RECORD FOR TIME 0.52428700E-01  
 DELETING TIME-RECORD FOR TIME 0.10485750  
 DELETING TIME-RECORD FOR TIME 0.20971510  
 DELETING TIME-RECORD FOR TIME 0.41943030  
 DELETING TIME-RECORD FOR TIME 0.83886070  
 DELETING TIME-RECORD FOR TIME 1.6777215  
 DELETING TIME-RECORD FOR TIME 3.3554431  
 DELETING TIME-RECORD FOR TIME 6.7108863  
 DELETING TIME-RECORD FOR TIME 13.421773  
 DELETING TIME-RECORD FOR TIME 26.843545  
 DELETING TIME-RECORD FOR TIME 53.687091  
 DELETING TIME-RECORD FOR TIME 107.37418  
 DELETING TIME-RECORD FOR TIME 214.74836  
 DELETING TIME-RECORD FOR TIME 429.49673  
 DELETING TIME-RECORD FOR TIME 858.99346  
 DELETING TIME-RECORD FOR TIME 1717.9869  
 DELETING TIME-RECORD FOR TIME 3435.9738  
 DELETING TIME-RECORD FOR TIME 6871.9477  
 DELETING TIME-RECORD FOR TIME 13743.895  
 DELETING TIME-RECORD FOR TIME 27487.791  
 DELETING TIME-RECORD FOR TIME 54975.581  
 DELETING TIME-RECORD FOR TIME 109951.16  
 DELETING TIME-RECORD FOR TIME 219902.33  
 DELETING TIME-RECORD FOR TIME 439804.65  
 DELETING TIME-RECORD FOR TIME 879609.30  
 DELETING TIME-RECORD FOR TIME 1759218.6  
 DELETING TIME-RECORD FOR TIME 3518437.2  
 DELETING TIME-RECORD FOR TIME 7036874.4  
 DELETING TIME-RECORD FOR TIME 14073749.  
 DELETING TIME-RECORD FOR TIME 28147498.  
 DELETING TIME-RECORD FOR TIME 56294995.  
 DELETING TIME-RECORD FOR TIME 0.11258999E+09  
 DELETING TIME-RECORD FOR TIME 0.21258999E+09  
 DELETING TIME-RECORD FOR TIME 0.31258999E+09  
 DELETING TIME-RECORD FOR TIME 0.41258999E+09  
 DELETING TIME-RECORD FOR TIME 0.51258999E+09  
 DELETING TIME-RECORD FOR TIME 0.61258999E+09  
 DELETING TIME-RECORD FOR TIME 0.71258999E+09  
 DELETING TIME-RECORD FOR TIME 0.81258999E+09

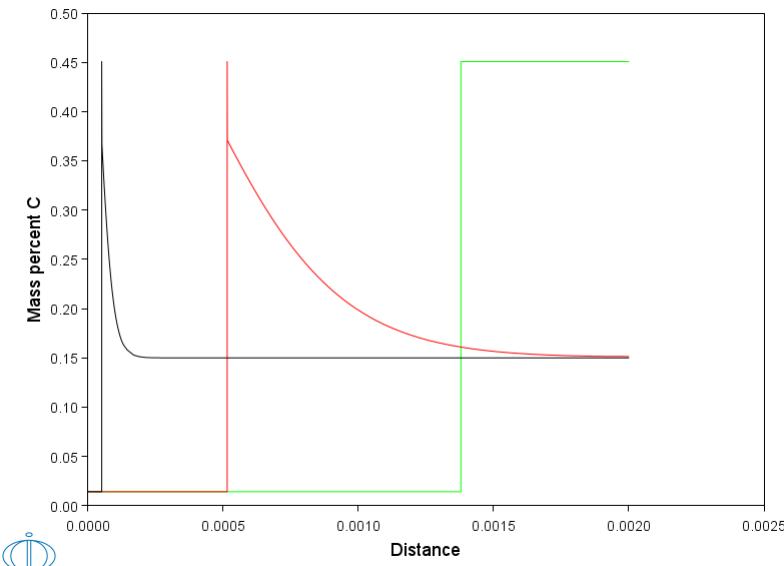
KEEPING TIME-RECORD FOR TIME 0.91258999E+09  
 AND FOR TIME 0.10000000E+10  
 WORKSPACE RECLAIMED

TIMESTEP AT 0.10000000E+10 SELECTED

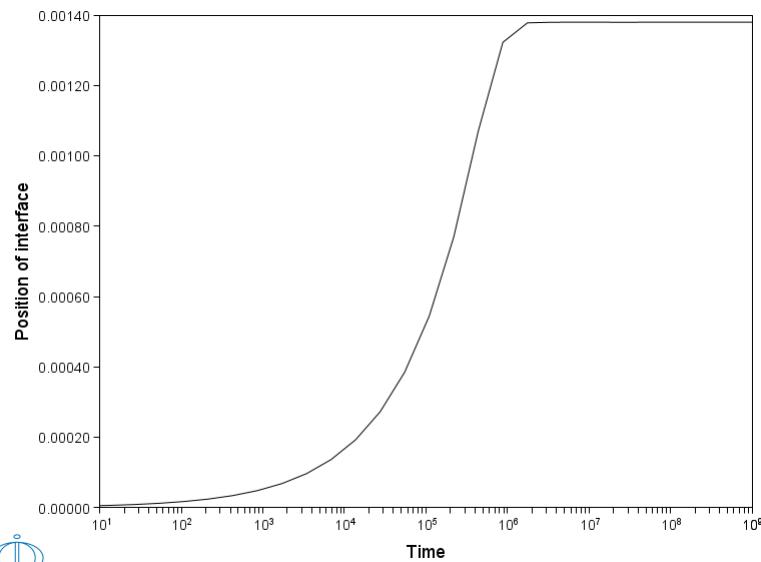
**DIC>**  
**DIC>**  
**DIC>**  
**DIC> @@**  
**DIC> @@ THE SIMULATION IS FINISHED**  
**DIC> @@**  
**DIC>**  
**DIC> set-inter**  
**--OK--**  
**DIC>**

## exbla-plot

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exbla\plot.DCM.test"
DIC>
DIC>
DIC> @@ exbla_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE bia
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 1.00000E+09
DIC> read exbla
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1:
POST-1: @@
POST-1: @@ PLOT THE CARBON CONCENTRATIONS AT DIFFERENT TIMES
POST-1: @@
POST-1: s-d-a x distance global
INFO: Distance is set as independent variable
POST-1: s-d-a y w-p c
POST-1: s-p-c time le3,1e5,1e9
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```



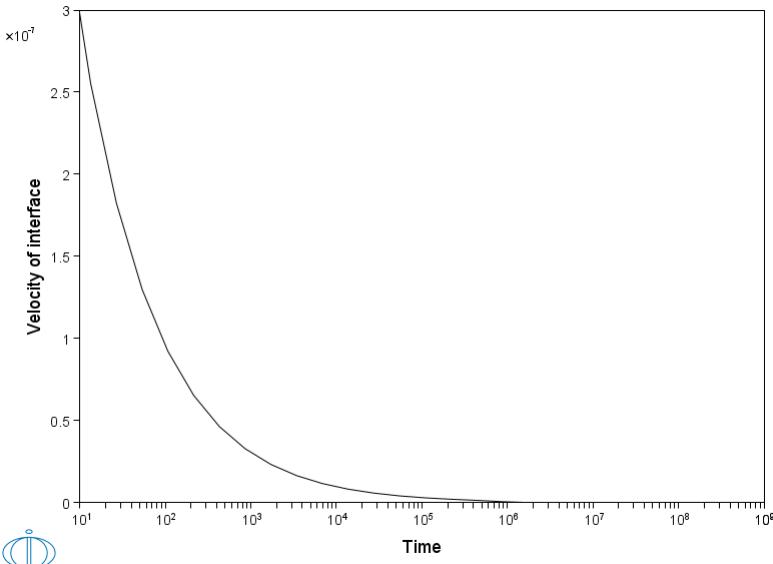
```
POST-1:
POST-1:
POST-1:@?
POST-1:
POST-1: sel-plot new
POST-1:
POST-1:
POST-1: @@
POST-1: @@ PLOT THE POSITION OF THE BCC/FCC INTERPHASE
POST-1: @@
POST-1: s-d-a x time
INFO: Time is set as independent variable
POST-1: s-d-a y
VARIABLE : pos
INTERFACE : aus
UPPER OR LOWER INTERFACE OF REGION AUSTENITE#1 /LOWER/: lower
POST-1:
POST-1: set_axis_type
AXIS (X, Y OR Z) : x
AXIS TYPE /LINEAR/: log
POST-1:
POST-1: s-s-s
AXIS (X, Y OR Z) : x
AUTOMATIC SCALING (Y OR N) /N/: n
MIN VALUE : 10
MAX VALUE : 1e9
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
    OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```



```

POST-1:
POST-1:@?
POST-1:
POST-1: sel-plot new
POST-1:
POST-1:
POST-1: @@ PLOT THE VELOCITY OF THE BCC/FCC INTERPHASE
POST-1: @@
POST-1: s-d-a
AXIS (X, Y OR Z) : y
VARIABLE : velocity
INTERFACE : aus
UPPER OR LOWER INTERFACE OF REGION AUSTENITE#1 /LOWER/: lower
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
      OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

```



```

POST-1:
POST-1:
POST-1:
POST-1:
POST-1: set-inter
--OK--
POST-1:

```

**exblb-setup****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\_dictra\_console\_examples\examples\exblb\setup.DCM.test"**

**SYS: @@**  
**SYS: @@ Moving boundary problem.**  
**SYS: @@ Austenite to ferrite transformation in a binary Fe-C alloy**  
**SYS: @@ This is the same example as in exbla but now the problem is with**  
**SYS: @@ ferrite as an inactive phase adjacent to the initial austenite.**  
**SYS: -----**  
NO SUCH COMMAND, USE HELP  
**SYS:**  
**SYS: @@ exblb\_setup.DCM**  
**SYS:**  
**SYS: @@**  
**SYS: @@ START BY GOING TO THE DATABASE MODULE**  
**SYS: @@**  
**SYS: go da**  
THERMODYNAMIC DATABASE module  
Database folder:  
C:\jenkins\workspace\generate\_dictra\_console\_examples\databases\data  
Current database: Steels/Fe-Alloys v12.0  
  
VA /- DEFINED  
DICTRA\_FCC\_A1 REJECTED  
**TDB\_TCFE12:**  
**TDB\_TCFE12: @@**  
**TDB\_TCFE12: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA**  
**TDB\_TCFE12: @@**  
**TDB\_TCFE12: sw FEDEMO**  
Current database: Iron Demo Database v4.0  
  
VA /- DEFINED  
**TDB\_FEDEMO:**  
**TDB\_FEDEMO: @@**  
**TDB\_FEDEMO: @@ DEFINE THE SYSTEM TO WORK WITH**  
**TDB\_FEDEMO: @@**  
**TDB\_FEDEMO: def-sys fe c**  
FE C DEFINED  
**TDB\_FEDEMO:**  
**TDB\_FEDEMO: @@**  
**TDB\_FEDEMO: @@ EXCLUDE THE THERMODYNAMIC DATA FOR THE PHASES THAT ARE NOT NEEDED**  
**TDB\_FEDEMO: @@**  
**TDB\_FEDEMO: rej ph \* all**  
GAS:G LIQUID:L  
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 bcc**  
FCC\_A1 BCC\_A2 RESTORED  
**TDB\_FEDEMO:**  
**TDB\_FEDEMO: @@**  
**TDB\_FEDEMO: @@ RETRIEVE DATA FROM THE DATABASE FILE**  
**TDB\_FEDEMO: @@**  
**TDB\_FEDEMO: get**  
15:29:17,518 [Thread-0] INFO JavaWrapper: \*\*\* Invoking Gibbs Energy System v6 \*\*\*  
REINITIATING GES ....  
ELEMENTS .....  
SPECIES .....  
PHASES .....  
PARAMETERS ...  
FUNCTIONS ....  
  
List of references for assessed data  
  
'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'  
'X.G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'  
'A.T. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'  
'X.G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar  
volumes'  
-OK-  
**TDB\_FEDEMO:**  
**TDB\_FEDEMO: @@**  
**TDB\_FEDEMO: @@ MOBILITY/DIFFUSIVITY DATA ARE STORED IN A SEPARATE DATABASE FILE.**  
**TDB\_FEDEMO: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE THE DATA.**  
**TDB\_FEDEMO: @@**  
**TDB\_FEDEMO: app**  
Use one of these databases  
  
TCFE12 = Steels/Fe-Alloys v12.0  
TCFE9 = Steels/Fe-Alloys v9.3  
SSUB6 = SGTE Substances v6.0  
FEDEMO = Iron Demo Database v4.0  
MOB2 = Alloys Mobility v2.7  
MOBFE2 = Steels/Fe-Alloys Mobility v2.0  
MOBFE4 = Steels/Fe-Alloys Mobility v4.0  
MOBFE7 = Steels/Fe-Alloys Mobility v7.1  
MFEDEMO = Fe-Alloys Mobility demo database v2.0  
USER = User defined Database  
  
**DATABASE NAME /FEDEMO/: MFEDEMO**  
Current database: Fe-Alloys Mobility demo database v2.0  
  
VA DEFINED  
**APP: def-sys fe c**  
FE C DEFINED

```

APP: rej ph * all
BCC A2           FCC_A1
REJECTED
APP: res ph fcc bcc
FCC_A1          BCC_A2 RESTORED
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS .....

List of references for assessed data

'This parameter has not been assessed'
'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'
'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
-Ni'
'B. Jonsson: Z. Metallkunde 85(1994)498-501; C and N diffusion in bcc Cr
-Fe-Ni'
'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
in bcc Fe'

-OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP
APP: @@
APP: go d-m
NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 1050; * N
DIC>
DIC> @@
DIC> @@ START BY ENTERING THE REGION austenite WHERE WE PUT THE fcc PHASE
DIC> @@
DIC> enter-region
REGION NAME : austenite
DIC>
DIC> @@
DIC> @@ ENTER THE GRID INTO THE REGION
DIC> @@
DIC> enter-grid
REGION NAME : /AUSTENITE/: austenite
WIDTH OF REGION /1/: 20e-4
TYPE /LINEAR/: GEO
NUMBER OF POINTS /50/: 100
VALUE OF R IN THE GEOMETRICAL SERIE : 1.05
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE active PHASES INTO THE REGIONS
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /AUSTENITE/: austenite
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC> @@
DIC> @@ ENTER THE inactive PHASES INTO THE REGIONS
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inactive
ATTACH TO REGION NAMED /AUSTENITE/: austenite
ATTACHED TO THE RIGHT OF AUSTENITE /YES/: no
PHASE NAME: /NONE/: bcc
REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-5
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITION FOR FCC
DIC> @@
DIC> enter-composition
REGION NAME : /AUSTENITE/: austenite
PHASE NAME: /FCC_A1/: fcc#1
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: C
TYPE /LINEAR/: lin
VALUE OF FIRST POINT : 0.15
VALUE OF LAST POINT : /0.15/: 0.15
DIC>
DIC> @@
DIC> @@ THE BOUNDARY CONDITION IS A CLOSED SYSTEM AS WE DO NOT SPECIFY
DIC> @@ ANYTHING ELSE
DIC> @@
DIC>
DIC> list-prof,,,
INTERFACE AT GLOBAL CORRDINATE X = 0.00000E+00
REGION AUSTENITE
COORDINATE      NP(FCC_A1)      X(FCC_A1,C)      X(FCC_A1,FE)
0               1              .00693651     .993063
8.04898E-07    1              .00693651     .993063
1.65004E-06    1              .00693651     .993063
2.53744E-06    1              .00693651     .993063
3.46921E-06    1              .00693651     .993063
4.44757E-06    1              .00693651     .993063
5.47485E-06    1              .00693651     .993063
6.55349E-06    1              .00693651     .993063
7.68606E-06    1              .00693651     .993063
8.87526E-06    1              .00693651     .993063
1.01239E-05    1              .00693651     .993063
1.1435E-05     1              .00693651     .993063
1.28117E-05    1              .00693651     .993063
1.42572E-05    1              .00693651     .993063
1.57749E-05    1              .00693651     .993063
1.73685E-05    1              .00693651     .993063
1.90419E-05    1              .00693651     .993063
2.07989E-05    1              .00693651     .993063
2.26437E-05    1              .00693651     .993063

```

```

2.45808E-05 1 .00693651 .993063
2.66147E-05 1 .00693651 .993063
2.87504E-05 1 .00693651 .993063
3.09928E-05 1 .00693651 .993063
3.33473E-05 1 .00693651 .993063
3.58196E-05 1 .00693651 .993063
3.84155E-05 1 .00693651 .993063
4.11411E-05 1 .00693651 .993063
4.40031E-05 1 .00693651 .993063
4.70081E-05 1 .00693651 .993063
5.01634E-05 1 .00693651 .993063
5.34765E-05 1 .00693651 .993063
5.69552E-05 1 .00693651 .993063
6.06079E-05 1 .00693651 .993063
6.44432E-05 1 .00693651 .993063
6.84703E-05 1 .00693651 .993063
7.26987E-05 1 .00693651 .993063
7.71385E-05 1 .00693651 .993063
8.18003E-05 1 .00693651 .993063
8.66952E-05 1 .00693651 .993063
9.18349E-05 1 .00693651 .993063
9.72315E-05 1 .00693651 .993063
1.02898E-04 1 .00693651 .993063
1.08848E-04 1 .00693651 .993063
1.15095E-04 1 .00693651 .993063
1.21655E-04 1 .00693651 .993063
1.28542E-04 1 .00693651 .993063
1.35774E-04 1 .00693651 .993063
1.43368E-04 1 .00693651 .993063
1.51341E-04 1 .00693651 .993063
1.59713E-04 1 .00693651 .993063
1.68504E-04 1 .00693651 .993063
1.77734E-04 1 .00693651 .993063
1.87426E-04 1 .00693651 .993063
1.97602E-04 1 .00693651 .993063
2.08287E-04 1 .00693651 .993063
2.19506E-04 1 .00693651 .993063
2.31286E-04 1 .00693651 .993063
2.43655E-04 1 .00693651 .993063
2.56643E-04 1 .00693651 .993063
2.7028E-04 1 .00693651 .993063
2.84599E-04 1 .00693651 .993063
2.99634E-04 1 .00693651 .993063
3.1542E-04 1 .00693651 .993063
3.31996E-04 1 .00693651 .993063
3.49401E-04 1 .00693651 .993063
3.67676E-04 1 .00693651 .993063
3.86865E-04 1 .00693651 .993063
4.07013E-04 1 .00693651 .993063
4.28168E-04 1 .00693651 .993063
4.50382E-04 1 .00693651 .993063
4.73706E-04 1 .00693651 .993063
4.98196E-04 1 .00693651 .993063
5.2391E-04 1 .00693651 .993063
5.50911E-04 1 .00693651 .993063
5.79261E-04 1 .00693651 .993063
6.09029E-04 1 .00693651 .993063
6.40286E-04 1 .00693651 .993063
6.73105E-04 1 .00693651 .993063
7.07565E-04 1 .00693651 .993063
7.43748E-04 1 .00693651 .993063
7.8174E-04 1 .00693651 .993063
8.21632E-04 1 .00693651 .993063
8.63519E-04 1 .00693651 .993063
9.075E-04 1 .00693651 .993063
9.5368E-04 1 .00693651 .993063
.00100217 1 .00693651 .993063
.00105308 1 .00693651 .993063
.00110654 1 .00693651 .993063
.00116267 1 .00693651 .993063
.00122161 1 .00693651 .993063
.0012835 1 .00693651 .993063
.00134848 1 .00693651 .993063
.00141671 1 .00693651 .993063
.00148835 1 .00693651 .993063
.00156357 1 .00693651 .993063
.00164255 1 .00693651 .993063
.00172548 1 .00693651 .993063
.00181256 1 .00693651 .993063
.001904 1 .00693651 .993063
.002 1 .00693651 .993063
INTERFACE AT GLOBAL CORRDINATE X = 2.00000E-03
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /1/: 1e9
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /100000000/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ IMPLICIT (1) TIME INTEGRATION IS USED INSTEAD OF THE MORE ACCURATE
DIC> @@ (BUT LESS STABLE) TRAPETZOIDAL METHOD WHICH IS THE DEFAULT.
DIC> @@
DIC> s-s-c
NSO1A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /AUTO/:
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPLICITY WHEN INTEGRATING PDES (AUTO, 0 -> 0.5 -> 1): /AUTO/: 1.0
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/:
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT

```

```
DIC> @@  
DIC> save exblb Y  
DIC>  
DIC> set-inter  
--OK---  
DIC>
```

**exb1b-run**

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exb1b\run.DCM.test"
DIC>
DIC>
DIC> @@ exb1b_run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING EXAMPLE b1b
DIC> @@
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 0.00000E+00
DIC> read exb1b
OK
DIC>
DIC> @@
DIC> @@ START THE SIMULATION
DIC> @@
DIC> sim y
U-FRACTION IN SYSTEM: C = .00698495916383108 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
U-FRACTION IN SYSTEM: C = .00698495916383108 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
1 GRIDPOINT(S) ADDED TO CELL #1 REGION: AUSTENITE
INFO: PHASE BCC_A2 IS SCHEDULED TO APPEAR
1 GRIDPOINT(S) ADDED TO CELL #1 REGION: AUSTENITE
REGION STATUS CHANGE, ITERATING: TIME= 0.50000000E-07
1 GRIDPOINT(S) ADDED TO CELL #1 REGION: AUSTENITE
REGION STATUS CHANGE, ITERATING: TIME= 0.25000000E-07
TIME = 0.25000000E-07 DT = 0.25000000E-07
U-FRACTION IN SYSTEM: C = .00698495916383108 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE

KEEPING TIME-RECORD FOR TIME 0.000000
AND FOR TIME 0.25000000E-07
WORKSPACE RECLAIMED
Trying old scheme 3
START VALUE(S) FOR INTERFACE #2 R_BCC_A2/AUSTENITE, CELL #1
-----
11 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: AUSTENITE

Trying old scheme 3
U-FRACTION IN SYSTEM: C = .00698156310125388 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
U-FRACTION IN SYSTEM: C = .00698156310125388 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
1 GRIDPOINT(S) ADDED TO CELL #1 REGION: R_BCC_A2
0.117127671162475 0.117128128916111 114.061443788323 0.114375906531175 0.105392179246106 9.205187146557051
002 7.158223455443510E-002 3.55870384097867E-002 2.021962532141424E-003 1.121279031038779E-
005 1.860868180040830E-009 2.255960336898259E-017 TIME = 0.12500000E-06 DT = 0.10000000E-
06 SUM OF SQUARES = 0.22559603E-16
CELL # 1 VELOCITY AT INTERFACE # 2 IS 9.7403076 AND 9.7403076
POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS 0.19740308E-05
U-FRACTION IN SYSTEM: C = .00698153921639083 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 0 seconds
1.105926481475599E-004 1.10633597837903E-004 7.720383379543468E-006 2.580905732333360E-006 1.887737382731095E-
007 1.041889226901693E-012 7.56290643860871E-013 8.50532976325443E-014 1.067827284524753E-
012 1.656757278471121E-016 5.561058959448397E-013 1.510019030704305E-017 TIME = 0.15721135E-03 DT = 0.15708635E-
03 SUM OF SQUARES = 0.15100190E-16
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.13219662E-04 AND 0.13219662E-04
POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS 0.19761074E-05
U-FRACTION IN SYSTEM: C = .00698153616291106 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 0 seconds
25 GRIDPOINT(S) ADDED TO CELL #1 REGION: R_BCC_A2
1.39576485658342E-007 1.396548518201008E-007 3.547022050121580E-015 8.173273215014309E-023 TIME = 0.47138404E-
03 DT = 0.31417269E-03 SUM OF SQUARES = 0.81732732E-22
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.83404798E-05 AND 0.83404798E-05
POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS 0.19787277E-05
U-FRACTION IN SYSTEM: C = .00698153616144201 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 1 seconds
2 GRIDPOINT(S) ADDED TO CELL #1 REGION: R_BCC_A2
4.935457367475106E-009 4.842416578234144E-009 2.360375795843106E-019 TIME = 0.10997294E-02 DT = 0.62834538E-
03 SUM OF SQUARES = 0.23603758E-18
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.82599760E-05 AND 0.82599760E-05
POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS 0.19839179E-05
U-FRACTION IN SYSTEM: C = .0069815361599996 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 0 seconds
7.49972043768404E-009 7.615438607914891E-009 2.958840402399737E-018 TIME = 0.23564202E-02 DT = 0.12566908E-
02 SUM OF SQUARES = 0.29588404E-17
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.79894423E-05 AND 0.79894423E-05

output ignored...

... output resumed

POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS 0.13798800E-02
U-FRACTION IN SYSTEM: C = .00698154236718254 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
5 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: R_BCC_A2

CPU time used in timestep 0 seconds
1.038299116519649E-004 1.038420219855692E-004 5.444368651887415E-
017 TIME = 0.67271826E+09 DT = 0.10000000E+09 SUM OF SQUARES = 0.54443687E-16
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.20826096E-16 AND -0.20826096E-16
POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS 0.13798779E-02
U-FRACTION IN SYSTEM: C = .00698156360434208 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
1 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: AUSTENITE
```

CPU time used in timestep 1 seconds  
 1.929994543956659E-004 1.930110199665162E-004 1.558390641553055E-018  
 TIME = 0.77271826E+09 DT = 0.10000000E+09 SUM OF SQUARES = 0.15583906E-17  
 CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.47708044E-16 AND 0.47708044E-16  
 POSITION OF INTERFACE R\_BCC\_A2 / AUSTENITE IS 0.13798827E-02  
 U-FRACTION IN SYSTEM: C = .00698151495464328 FE = 1  
 TOTAL SIZE OF SYSTEM: .002 [m]  
 7 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: R\_BCC\_A2

CPU time used in timestep 0 seconds  
 5.005184255490110E-003 5.005319176317448E-003 1.019280681735454E-015 5.584854986157855E-029  
 TIME = 0.87271826E+09 DT = 0.10000000E+09 SUM OF SQUARES = 0.55848550E-28  
 CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.30013588E-15 AND -0.30013588E-15  
 POSITION OF INTERFACE R\_BCC\_A2 / AUSTENITE IS 0.13798527E-02  
 U-FRACTION IN SYSTEM: C = .00698182101457197 FE = 1  
 TOTAL SIZE OF SYSTEM: .002 [m]  
 1 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: AUSTENITE

CPU time used in timestep 0 seconds  
 6.555274976143166E-005 6.556246389530778E-005 1.016616411613121E-022  
 TIME = 0.97271826E+09 DT = 0.10000000E+09 SUM OF SQUARES = 0.10166164E-21  
 CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.10285440E-15 AND 0.10285440E-15  
 POSITION OF INTERFACE R\_BCC\_A2 / AUSTENITE IS 0.13798630E-02  
 U-FRACTION IN SYSTEM: C = .00698171613003814 FE = 1  
 TOTAL SIZE OF SYSTEM: .002 [m]  
 14 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: R\_BCC\_A2

CPU time used in timestep 0 seconds  
 6.079841876333348E-006 6.080855698457493E-006 2.647075620323817E-026  
 TIME = 0.10000000E+10 DT = 27281736. SUM OF SQUARES = 0.26470756E-25  
 CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.20103042E-16 AND -0.20103042E-16  
 POSITION OF INTERFACE R\_BCC\_A2 / AUSTENITE IS 0.13798624E-02  
 U-FRACTION IN SYSTEM: C = .00698172172274839 FE = 1  
 TOTAL SIZE OF SYSTEM: .002 [m]  
 MUST SAVE WORKSPACE ON FILE  
 WORKSPACE SAVED ON FILE  
 RECLAIMING WORKSPACE  
 DELETING TIME-RECORD FOR TIME 0.0000000  
 DELETING TIME-RECORD FOR TIME 0.25000000E-07  
 DELETING TIME-RECORD FOR TIME 0.12500000E-06  
 DELETING TIME-RECORD FOR TIME 0.15721135E-03  
 DELETING TIME-RECORD FOR TIME 0.47138404E-03  
 DELETING TIME-RECORD FOR TIME 0.10997294E-02  
 DELETING TIME-RECORD FOR TIME 0.23564202E-02  
 DELETING TIME-RECORD FOR TIME 0.48698017E-02  
 DELETING TIME-RECORD FOR TIME 0.98965648E-02  
 DELETING TIME-RECORD FOR TIME 0.19950091E-01  
 DELETING TIME-RECORD FOR TIME 0.40057143E-01  
 DELETING TIME-RECORD FOR TIME 0.80271248E-01  
 DELETING TIME-RECORD FOR TIME 0.16069946  
 DELETING TIME-RECORD FOR TIME 0.32155588  
 DELETING TIME-RECORD FOR TIME 0.64326871  
 DELETING TIME-RECORD FOR TIME 1.2866944  
 DELETING TIME-RECORD FOR TIME 2.5735457  
 DELETING TIME-RECORD FOR TIME 5.1472484  
 DELETING TIME-RECORD FOR TIME 10.294654  
 DELETING TIME-RECORD FOR TIME 20.589465  
 DELETING TIME-RECORD FOR TIME 41.179086  
 DELETING TIME-RECORD FOR TIME 82.358329  
 DELETING TIME-RECORD FOR TIME 164.71682  
 DELETING TIME-RECORD FOR TIME 329.43379  
 DELETING TIME-RECORD FOR TIME 658.86773  
 DELETING TIME-RECORD FOR TIME 1317.7356  
 DELETING TIME-RECORD FOR TIME 2635.4714  
 DELETING TIME-RECORD FOR TIME 5270.9430  
 DELETING TIME-RECORD FOR TIME 10541.886  
 DELETING TIME-RECORD FOR TIME 21083.772  
 DELETING TIME-RECORD FOR TIME 42167.545  
 DELETING TIME-RECORD FOR TIME 84335.090  
 DELETING TIME-RECORD FOR TIME 168670.18  
 DELETING TIME-RECORD FOR TIME 337340.36  
 DELETING TIME-RECORD FOR TIME 674680.72  
 DELETING TIME-RECORD FOR TIME 13493361.4  
 DELETING TIME-RECORD FOR TIME 2698722.9  
 DELETING TIME-RECORD FOR TIME 5397445.7  
 DELETING TIME-RECORD FOR TIME 10794891.  
 DELETING TIME-RECORD FOR TIME 21589783.  
 DELETING TIME-RECORD FOR TIME 43179566.  
 DELETING TIME-RECORD FOR TIME 86359132.  
 DELETING TIME-RECORD FOR TIME 0.17271826E+09  
 DELETING TIME-RECORD FOR TIME 0.27271826E+09  
 DELETING TIME-RECORD FOR TIME 0.37271826E+09  
 DELETING TIME-RECORD FOR TIME 0.47271826E+09  
 DELETING TIME-RECORD FOR TIME 0.57271826E+09  
 DELETING TIME-RECORD FOR TIME 0.67271826E+09  
 DELETING TIME-RECORD FOR TIME 0.77271826E+09  
 DELETING TIME-RECORD FOR TIME 0.87271826E+09

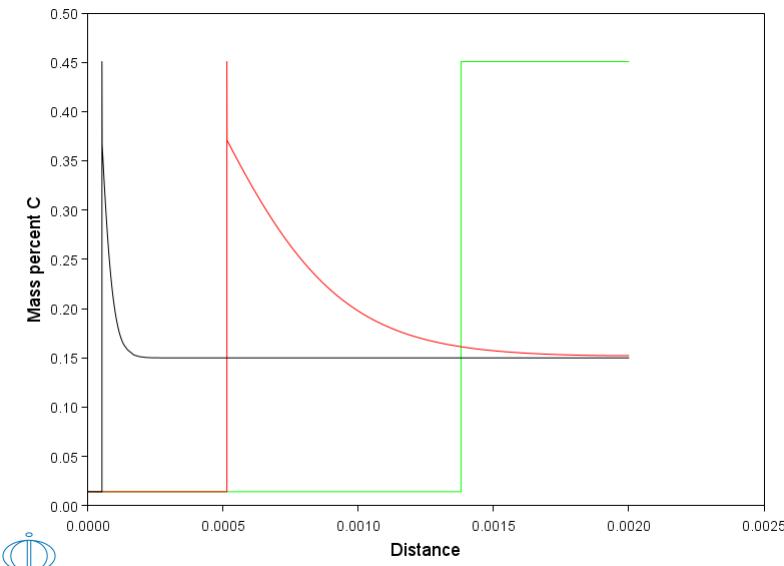
KEEPING TIME-RECORD FOR TIME 0.97271826E+09  
 AND FOR TIME 0.10000000E+10  
 WORKSPACE RECLAIMED

TIMESTEP AT 0.100000000E+10 SELECTED

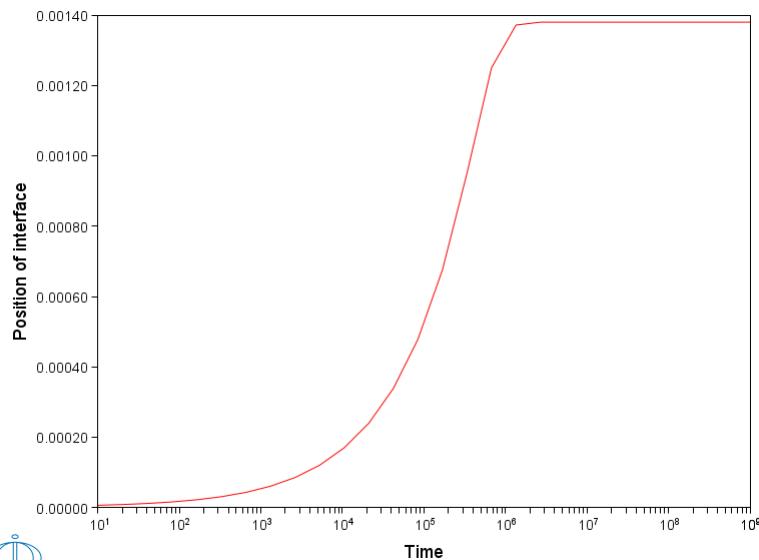
DIC>  
 DIC>  
 DIC>  
 DIC>  
 DIC>  
 DIC>  
 DIC> @@  
 DIC> @@ THE SIMULATION IS FINISHED  
 DIC> @@  
 DIC>  
 DIC> set-inter  
 --OK--  
 DIC>

## exb1b-plot

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exb1b\plot.DCM.test"
DIC>
DIC>
DIC> @@ exb1b_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE b1b
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 1.00000E+09
DIC> read exb1b
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1:
POST-1: @@
POST-1: @@ PLOT THE CARBON CONCENTRATIONS AT DIFFERENT TIMES
POST-1: @@
POST-1: s-d-a y w-p c
POST-1: s-d-a x dist glob
INFO: Distance is set as independent variable
POST-1: s-p-c time 1e3,1e5,1e9
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```



```
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: sel-plot new
POST-1:
POST-1: @@
POST-1: @@ PLOT THE POSITION OF THE BCC/FCC INTERPHASE
POST-1: @@
POST-1: s-d-a x time
INFO: Time is set as independent variable
POST-1: s-d-a y
VARIABLE : pos
INTERFACE : aus
UPPER OR LOWER INTERFACE OF REGION AUSTENITE#1 /LOWER/: lower
POST-1:
POST-1: set_axis_type
AXIS (X, Y OR Z) : x
AXIS TYPE /LINEAR/: log
POST-1:
POST-1: s-s-s
AXIS (X, Y OR Z) : x
AUTOMATIC SCALING (Y OR N) /N/: n
MIN VALUE : 10
MAX VALUE : 1e9
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
ORKING ...
OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

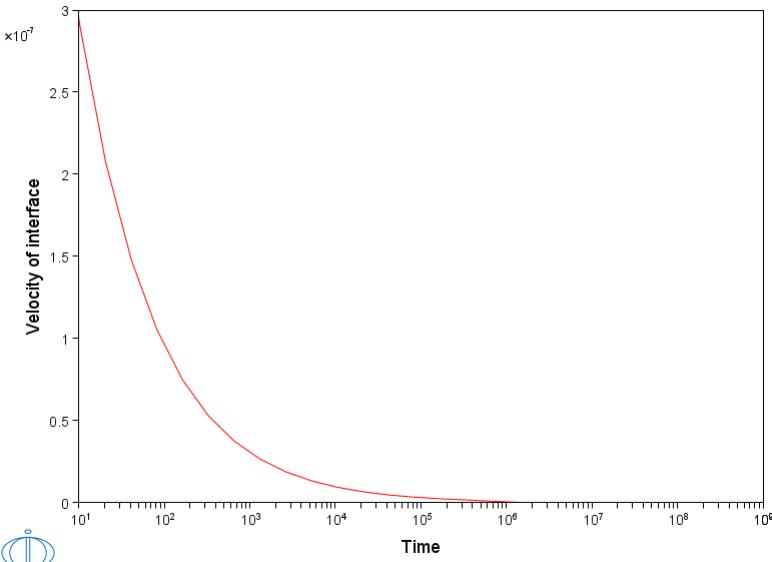


©

```

POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: sel-plot new
POST-1:
POST-1: @@ PLOT THE VELOCITY OF THE BCC/FCC INTERPHASE
POST-1: @@
POST-1: s-d-a
AXIS (X, Y OR Z) : y
VARIABLE : velocity
INTERFACE : aus
UPPER OR LOWER INTERFACE OF REGION AUSTENITE#1 /LOWER/: lower
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
ORKING ...
          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

```



©

```

POST-1:
POST-1:
POST-1:
POST-1:
POST-1: set-inter
--OK--
POST-1:

```



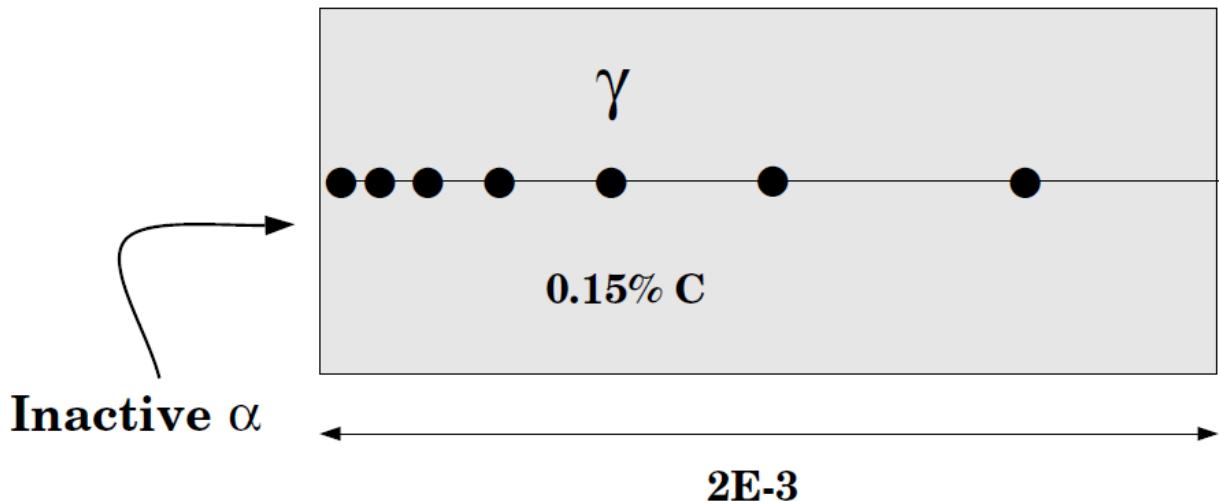
## Example exb1c

### $\gamma$ to $\alpha$ transformation in a binary Fe-C alloy: Gradual cool down to 1050 K

This is the same example as in exb1a and exb1b but now the simulation starts at a higher temperature and assumes a gradual cooling down to 1050 K. When 1050 K is reached, the temperature is kept constant and thus has an isothermal transformation. As in exb1b, ferrite is in an inactive phase adjacent to the initial austenite.

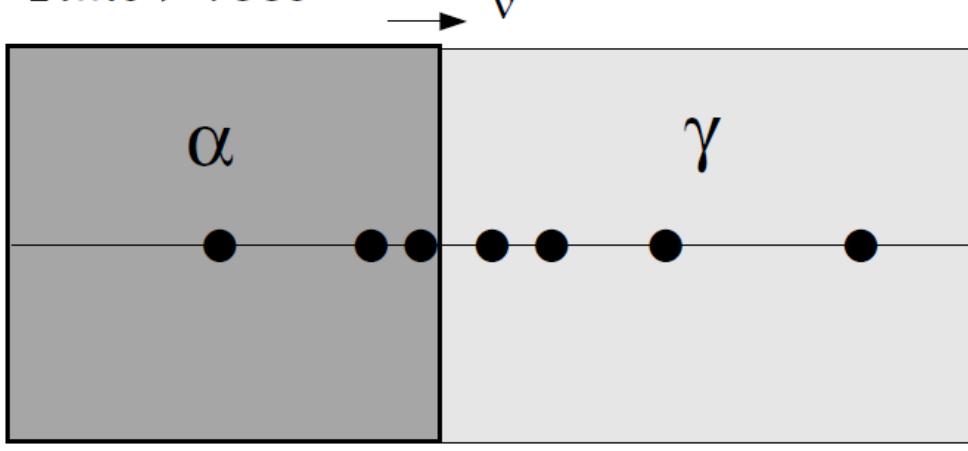
Time = 0

T = 1173 - Time \* 0.1667



Time > 738s

T = 1050 K



2E-3

**exblc-setup****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_dictra_console_examples\examples\exblc\setup.DCM.test"
SYS: @@
SYS: @@ Moving boundary problem.
SYS: @@ Austenite to ferrite transformation in a binary Fe-C alloy
SYS: @@ This is the same example as in exbla and exlbl but now the
SYS: @@ simulation starts at a higher temperature and assumes a gradual cooling
SYS: @@ down to 1050 K.
SYS: @@
SYS: @@ When 1050 K is reached, the temperature is kept constant and thus has an
SYS: @@ isothermal transformation. As in exlbl ferrite is an inactive
SYS: @@ phase adjacent to the initial austenite.
SYS: -----
NO SUCH COMMAND, USE HELP
SYS:
SYS: @@
SYS: @@ START BY GOING TO THE DATABASE MODULE
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\generate_dictra_console_examples\databases\data
Current database: Steels/Fe-Alloys v12.0

VA          /- DEFINED
DICTRA_FCC_A1  REJECTED
TDB_TCFE12:
TDB_TCFE12: @@
TDB_TCFE12: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA
TDB_TCFE12: @@
TDB_TCFE12: sw FEDEMO
Current database: Iron Demo Database v4.0

VA          /- DEFINED
TDB_FEDEMO: @@
TDB_FEDEMO: @@ DEFINE THE SYSTEM TO WORK WITH
TDB_FEDEMO: @@
TDB_FEDEMO: def-sys fe c
FE          C  DEFINED
TDB_FEDEMO: @@
TDB_FEDEMO: @@ EXCLUDE THE THERMODYNAMIC DATA FOR THE PHASES THAT ARE NOT NEEDED
TDB_FEDEMO: @@
TDB_FEDEMO: rej ph * all
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 bcc
FCC_A1          BCC_A2  RESTORED
TDB_FEDEMO: @@
TDB_FEDEMO: @@ RETRIEVE DATA FROM THE DATABASE FILE
TDB_FEDEMO: @@
TDB_FEDEMO: get
15:32:34,090 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS .....

List of references for assessed data

'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'
'X.G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
'A.T. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
'X.G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
    volumes'
-OK-
TDB_FEDEMO: @@
TDB_FEDEMO: @@ MOBILITY/DIFFUSIVITY DATA ARE STORED IN A SEPARATE DATABASE FILE.
TDB_FEDEMO: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE DATA
TDB_FEDEMO: @@
TDB_FEDEMO: app
Use one of these databases

TCFE12 = Steels/Fe-Alloys v12.0
TCFE9  = Steels/Fe-Alloys v9.3
SSUB6  = SGTE Substances v6.0
FEDEMO = Iron Demo Database v4.0
MOB2   = Alloys Mobility v2.7
MOBFE2 = Steels/Fe-Alloys Mobility v2.0
MOBFE4 = Steels/Fe-Alloys Mobility v4.0
MOBFE7 = Steels/Fe-Alloys Mobility v7.1
MFEDEMO = Fe-Alloys Mobility demo database v2.0
USER   = User defined Database

DATABASE NAME /FEDEMO/: MFEDEMO
```

Current database: Fe-Alloys Mobility demo database v2.0

```
VA DEFINED
APP: def-sys fe c
FE C DEFINED
APP: rej ph * all
BCC_A2 FCC_A1 CEMENTITE
REJECTED
APP: res ph fcc bcc
FCC_A1 BCC_A2 RESTORED
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS .....
FUNCTIONS .....

List of references for assessed data

'This parameter has not been assessed'
'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'
'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
-Ni'
'B. Jonsson: Z. Metallkunde 85(1994)498-501; C and N diffusion in bcc Cr
-Fe-Ni'
'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
in bcc Fe'

-OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP
APP: @@
APP: go d-m
NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER GLOBAL CONDITION T
DIC> @@
DIC> @@ ASSUME THAT THE COOLING RATE IS 10K/MINUTE DOWN TO 1050K
DIC> @@
DIC> set-cond
GLOBAL OR BOUNDARY CONDITION /GLOBAL/: glob
VARIABLE : T
LOW TIME LIMIT /0/: 0
T(TIME,X)= 1173-time*0.1667;
HIGH TIME LIMIT /*/: 738
ANY MORE RANGES /N/: y
T(TIME,X)= 1050;
HIGH TIME LIMIT /*/: *
ANY MORE RANGES /N/: N
DIC>
DIC> @@
DIC> @@ START BY ENTERING THE REGION austenite WHERE WE PUT THE fcc PHASE
DIC> @@
DIC> enter-region
REGION NAME : austenite
DIC>
DIC> @@
DIC> @@ ENTER THE GRID INTO THE REGION
DIC> @@
DIC> enter-grid
REGION NAME : /AUSTENITE/: austenite
WIDTH OF REGION /1/: 20e-4
TYPE /LINEAR/: AUTO
DIC>
DIC> @@
DIC> @@ ENTER THE active PHASES INTO THE REGIONS
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /AUSTENITE/: austenite
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC> @@
DIC> @@ ENTER THE inactive PHASES INTO THE REGIONS
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inact
ATTACH TO REGION NAMED /AUSTENITE/: austenite
ATTACHED TO THE RIGHT OF AUSTENITE /YES/: no
PHASE NAME: /NONE/: bcc
REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-5
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITION FOR FCC
DIC> @@
DIC> enter-composition
REGION NAME : /AUSTENITE/: austenite
PHASE NAME: /FCC_A1/: fcc#1
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: C
TYPE /LINEAR/: lin
VALUE OF FIRST POINT : 0.15
VALUE OF LAST POINT : /0.15/: 0.15
DIC>
DIC> @@
DIC> @@ THE BOUNDARY CONDITION IS A CLOSED SYSTEM AS WE DO NOT SPECIFY
DIC> @@ ANYTHING ELSE.
DIC> @@
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /1/: 738
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /73.8/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
```

```
DIC>
DIC>
DIC> @@ IMPLICIT (1) TIME INTEGRATION IS USED INSTEAD OF THE MORE ACCURATE
DIC> @@ (BUT LESS STABLE) TRAPEZOIDAL METHOD WHICH IS THE DEFAULT.
DIC> @@
DIC> s-s-c
NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA Timesteps IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /AUTO/:
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -> 1): /AUTO/: 1.0
MAX Timestep Change per timestep : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/:
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exb1c Y
DIC>
DIC> set-inter
--OK--
DIC>
```

**exb1c-run**

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exb1c\run.DCM.test"
DIC>
DIC>
DIC> @@ exb1c_run.DCM
DIC>
DIC> @@ FILE FOR RUNNING EXAMPLE exb1c
DIC> @@
DIC> go d-m
TIME STEP AT TIME 0.00000E+00
DIC> read exb1c
OK
DIC>
DIC> @@
DIC> @@ START THE SIMULATION
DIC> @@
DIC> sim
Region: AUSTENITE
single geometric dense at 0.0000
1.2084 101
U-FRACTION IN SYSTEM: C = .00698495916383108 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
U-FRACTION IN SYSTEM: C = .00698495916383108 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
TIME = 0.1000000E-06 DT = 0.1000000E-06 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698495916383108 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 0 seconds
TIME = 0.24660033E-05 DT = 0.23660033E-05 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698495916383108 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 0 seconds
TIME = 0.71980098E-05 DT = 0.47320065E-05 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698495916383108 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 0 seconds
TIME = 0.16662023E-04 DT = 0.94640131E-05 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698495916383108 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 0 seconds
TIME = 0.35590049E-04 DT = 0.18928026E-04 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698495916383108 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 0 seconds
TIME = 0.73446101E-04 DT = 0.37856052E-04 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698495916383108 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 0 seconds
TIME = 0.14915821E-03 DT = 0.75712105E-04 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698495916383108 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 0 seconds
TIME = 0.30058242E-03 DT = 0.15142421E-03 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698495916383108 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 0 seconds
TIME = 0.60343083E-03 DT = 0.30284842E-03 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698495916383108 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 0 seconds
TIME = 0.12091277E-02 DT = 0.60569684E-03 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698495916383108 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 1 seconds
TIME = 0.24205213E-02 DT = 0.12113937E-02 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698495916383108 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 0 seconds
TIME = 0.48433087E-02 DT = 0.24227873E-02 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698495916383108 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 0 seconds
TIME = 0.9688834E-02 DT = 0.48455747E-02 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698495916383108 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 0 seconds
TIME = 0.19380033E-01 DT = 0.96911494E-02 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698495916383108 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 0 seconds
TIME = 0.38762332E-01 DT = 0.19382299E-01 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698495916383108 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 0 seconds
TIME = 0.77526929E-01 DT = 0.38764598E-01 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698495916383109 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 0 seconds
TIME = 0.15505612 DT = 0.77529195E-01 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698495916383109 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 0 seconds
TIME = 0.31011451 DT = 0.15505839 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698495916383109 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 0 seconds
TIME = 0.62023129 DT = 0.31011678 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698495916383109 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 0 seconds
TIME = 1.2404649 DT = 0.62023356 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698495916383109 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 0 seconds
TIME = 2.4809320 DT = 1.2404671 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698495916383109 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 0 seconds
TIME = 4.9618662 DT = 2.4809342 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698495916383109 FE = 1
```

TOTAL SIZE OF SYSTEM: .002 [m]  
 CPU time used in timestep 0 seconds  
 TIME = 9.9237347 DT = 4.9618685 SUM OF SQUARES = 0.0000000  
 U-FRACTION IN SYSTEM: C = .0069849591638311 FE = 1  
 TOTAL SIZE OF SYSTEM: .002 [m]  
 CPU time used in timestep 0 seconds  
 TIME = 19.847472 DT = 9.9237370 SUM OF SQUARES = 0.0000000  
 U-FRACTION IN SYSTEM: C = .00698495916383107 FE = 1  
 TOTAL SIZE OF SYSTEM: .002 [m]  
 CPU time used in timestep 0 seconds  
 TIME = 39.694946 DT = 19.847474 SUM OF SQUARES = 0.0000000  
 U-FRACTION IN SYSTEM: C = .00698495916383105 FE = 1  
 TOTAL SIZE OF SYSTEM: .002 [m]  
 CPU time used in timestep 0 seconds  
 TIME = 76.594946 DT = 36.900000 SUM OF SQUARES = 0.0000000  
 U-FRACTION IN SYSTEM: C = .00698495916383098 FE = 1  
 TOTAL SIZE OF SYSTEM: .002 [m]  
 CPU time used in timestep 0 seconds

output ignored...

... output resumed

TIME = 0.44452637E+09 DT = 0.10000000E+09 SUM OF SQUARES = 0.43377185E-21  
 CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.50045449E-16 AND 0.50045449E-16  
 POSITION OF INTERFACE R\_BCC\_A2 / AUSTENITE IS 0.13793348E-02  
 U-FRACTION IN SYSTEM: C = .0069871020918711 FE = 1  
 TOTAL SIZE OF SYSTEM: .002 [m]  
 4 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: R\_BCC\_A2

CPU time used in timestep 0 seconds  
 1.355588490500316E-006 1.355821418555050E-006 3.813755816508475E-028  
 029 TIME = 0.54452637E+09 DT = 0.10000000E+09 SUM OF SQUARES = 0.38137558E-28  
 CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.80435336E-17 AND -0.80435336E-17  
 POSITION OF INTERFACE R\_BCC\_A2 / AUSTENITE IS 0.13793340E-02  
 U-FRACTION IN SYSTEM: C = .00698711029416879 FE = 1  
 TOTAL SIZE OF SYSTEM: .002 [m]  
 1 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: AUSTENITE

CPU time used in timestep 0 seconds  
 3.303539951570819E-004 3.303598391958185E-004 2.572637178395358E-017  
 017 TIME = 0.64452637E+09 DT = 0.10000000E+09 SUM OF SQUARES = 0.25726372E-16  
 CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.81236552E-16 AND 0.81236552E-16  
 POSITION OF INTERFACE R\_BCC\_A2 / AUSTENITE IS 0.13793421E-02  
 U-FRACTION IN SYSTEM: C = .00698702745417951 FE = 1  
 TOTAL SIZE OF SYSTEM: .002 [m]  
 6 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: R\_BCC\_A2

CPU time used in timestep 0 seconds  
 3.782772525035657E-006 3.782772525035657E-006 2.661361147697371E-019  
 019 TIME = 0.74452637E+09 DT = 0.10000000E+09 SUM OF SQUARES = 0.26613611E-18  
 CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.15744654E-16 AND -0.15744654E-16  
 POSITION OF INTERFACE R\_BCC\_A2 / AUSTENITE IS 0.13793406E-02  
 U-FRACTION IN SYSTEM: C = .00698704350959976 FE = 1  
 TOTAL SIZE OF SYSTEM: .002 [m]  
 1 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: AUSTENITE

CPU time used in timestep 0 seconds  
 7.0235575076397174E-007 7.018301498991900E-007 1.367197279746478E-027  
 027 TIME = 0.84452637E+09 DT = 0.10000000E+09 SUM OF SQUARES = 0.13671973E-26  
 CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.19538992E-16 AND -0.19538992E-16  
 POSITION OF INTERFACE R\_BCC\_A2 / AUSTENITE IS 0.13793386E-02  
 U-FRACTION IN SYSTEM: C = .00698706343424927 FE = 1  
 TOTAL SIZE OF SYSTEM: .002 [m]  
 1 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: AUSTENITE

CPU time used in timestep 0 seconds  
 2.017748798134671E-006 2.016639494127638E-006 2.662669048478394E-020  
 020 TIME = 0.94452637E+09 DT = 0.10000000E+09 SUM OF SQUARES = 0.26626690E-19  
 CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.26113115E-16 AND -0.26113115E-16  
 POSITION OF INTERFACE R\_BCC\_A2 / AUSTENITE IS 0.13793360E-02  
 U-FRACTION IN SYSTEM: C = .00698709006278274 FE = 1  
 TOTAL SIZE OF SYSTEM: .002 [m]  
 1 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: AUSTENITE

CPU time used in timestep 0 seconds  
 1.682906541555828E-005 1.682478352364456E-005 4.489539105948096E-020  
 020 TIME = 0.10000000E+10 DT = 55473634. SUM OF SQUARES = 0.44895391E-19  
 CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.45705454E-16 AND -0.45705454E-16  
 POSITION OF INTERFACE R\_BCC\_A2 / AUSTENITE IS 0.13793335E-02  
 U-FRACTION IN SYSTEM: C = .00698711591770347 FE = 1  
 TOTAL SIZE OF SYSTEM: .002 [m]  
 MUST SAVE WORKSPACE ON FILE  
 WORKSPACE SAVED ON FILE  
 RECLAIMING WORKSPACE  
 DELETING TIME-RECORD FOR TIME 738.00000  
 DELETING TIME-RECORD FOR TIME 755.22880  
 DELETING TIME-RECORD FOR TIME 789.68640  
 DELETING TIME-RECORD FOR TIME 858.60160  
 DELETING TIME-RECORD FOR TIME 996.43199  
 DELETING TIME-RECORD FOR TIME 1272.0928  
 DELETING TIME-RECORD FOR TIME 1823.4144  
 DELETING TIME-RECORD FOR TIME 2926.0575  
 DELETING TIME-RECORD FOR TIME 5131.3439  
 DELETING TIME-RECORD FOR TIME 9541.9165  
 DELETING TIME-RECORD FOR TIME 18363.062  
 DELETING TIME-RECORD FOR TIME 36005.353  
 DELETING TIME-RECORD FOR TIME 71289.934  
 DELETING TIME-RECORD FOR TIME 141859.10  
 DELETING TIME-RECORD FOR TIME 282997.42  
 DELETING TIME-RECORD FOR TIME 565274.07  
 DELETING TIME-RECORD FOR TIME 1129827.4  
 DELETING TIME-RECORD FOR TIME 2258934.0  
 DELETING TIME-RECORD FOR TIME 4517147.2  
 DELETING TIME-RECORD FOR TIME 9033573.6  
 DELETING TIME-RECORD FOR TIME 18066426.  
 DELETING TIME-RECORD FOR TIME 36132132.  
 DELETING TIME-RECORD FOR TIME 72263543.  
 DELETING TIME-RECORD FOR TIME 0.14452637E+09  
 DELETING TIME-RECORD FOR TIME 0.24452637E+09  
 DELETING TIME-RECORD FOR TIME 0.34452637E+09  
 DELETING TIME-RECORD FOR TIME 0.44452637E+09  
 DELETING TIME-RECORD FOR TIME 0.54452637E+09

DELETING TIME-RECORD FOR TIME 0.64452637E+09  
DELETING TIME-RECORD FOR TIME 0.74452637E+09  
DELETING TIME-RECORD FOR TIME 0.84452637E+09

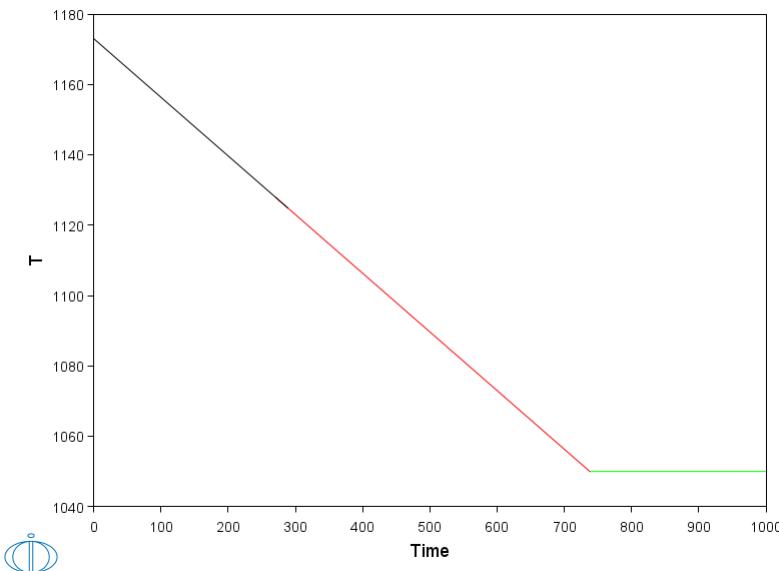
KEEPING TIME-RECORD FOR TIME 0.94452637E+09  
AND FOR TIME 0.10000000E+10  
WORKSPACE RECLAIMED

TIMESTEP AT 0.10000000E+10 SELECTED

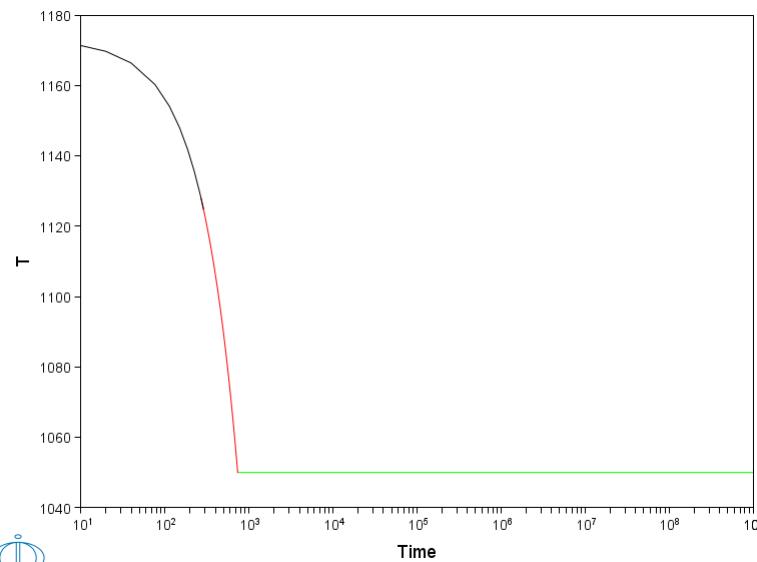
DIC>  
DIC>  
DIC>  
DIC>  
DIC>  
DIC>  
DIC>  
DIC> @@  
DIC> @@ THE SIMULATION IS FINISHED  
DIC> @@  
DIC>  
DIC> set-inter  
--OK---  
DIC>

**exb1c-plot**

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exb1c\plot.DCM.test"
DIC>
DIC>
DIC> @@ exb1c_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE b1c
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 1.00000E+09
DIC> read exb1c
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1: @@
POST-1: @@ PLOT TEMPERATURE VS. TIME
POST-1: @@
POST-1: s-d-a y t
POST-1: s-d-a x time
INFO: Time is set as independent variable
POST-1: s-p-c
CONDITION /TIME/: interface
INTERFACE : austenite
UPPER OR LOWER INTERFACE OF REGION AUSTENITE#1 /LOWER/: lower
POST-1: s-s-s x n 0 1000
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
ORKING ...
OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```



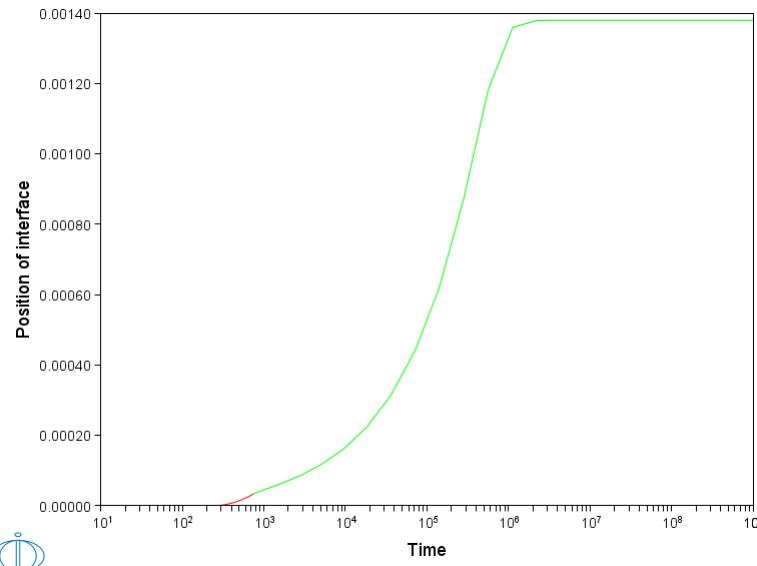
```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: @@
POST-1: @@ PLOT VS. LOG TIME
POST-1: @@
POST-1: set-axis-type x log
POST-1: s-s-s x n 10 1e9
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```



```

POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: @@
POST-1: @@ PLOT THE POSITION OF THE BCC/FCC INTERPHASE
POST-1: @@
POST-1: s-d-a
AXIS (X, Y OR Z) : y
VARIABLE : position
INTERFACE : austenite
UPPER OR LOWER INTERFACE OF REGION AUSTENITE#1 /LOWER/: lower
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
ORKING ... OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

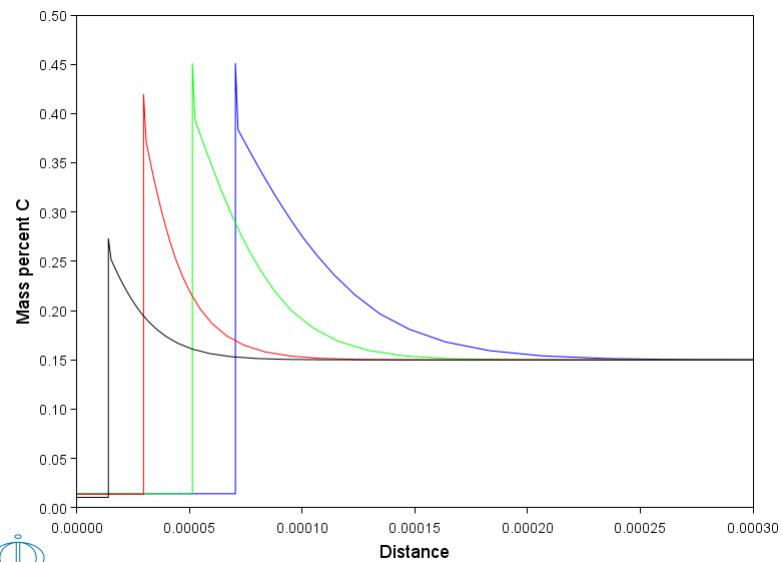
```



```

POST-1:
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: @@
POST-1: @@ PLOT THE CARBON CONCENTRATION VS. DISTANCE
POST-1: @@
POST-1: s-d-a y w-p c
POST-1: s-d-a x dis glob
INFO: Distance is set as independent variable
POST-1: s-p-c time 500,700,1200,2000
POST-1: set-axis-type x lin
POST-1: s-s-s x n 0 3e-4
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
ORKING ... OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

```



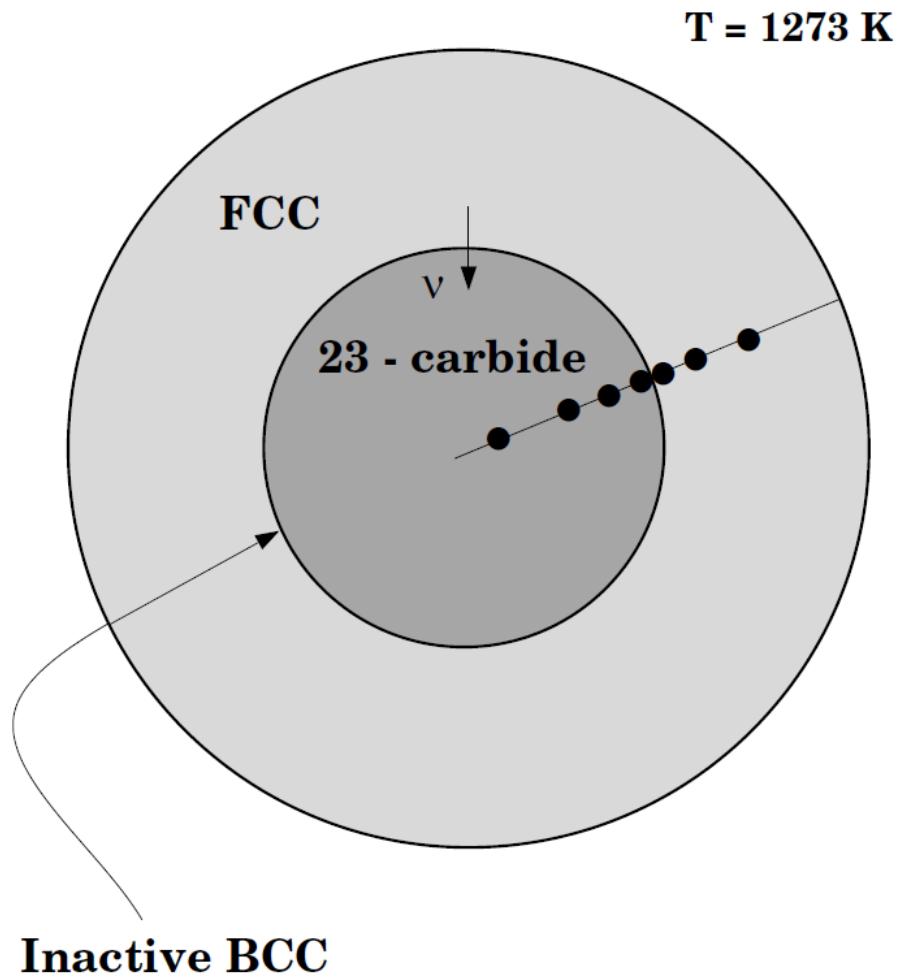
```
POST-1:  
POST-1:  
POST-1:  
POST-1:  
POST-1:@?<Hit_return_to_continue>  
POST-1: set-inter  
---OK---  
POST-1:
```



## Example exb3

### Dissolution of 23-carbide in an austenitic matrix

This example calculates the dissolution of an M<sub>23</sub>C<sub>6</sub> particle in an austenite matrix. A film of ferrite is allowed to nucleate around the carbide during the precipitation.

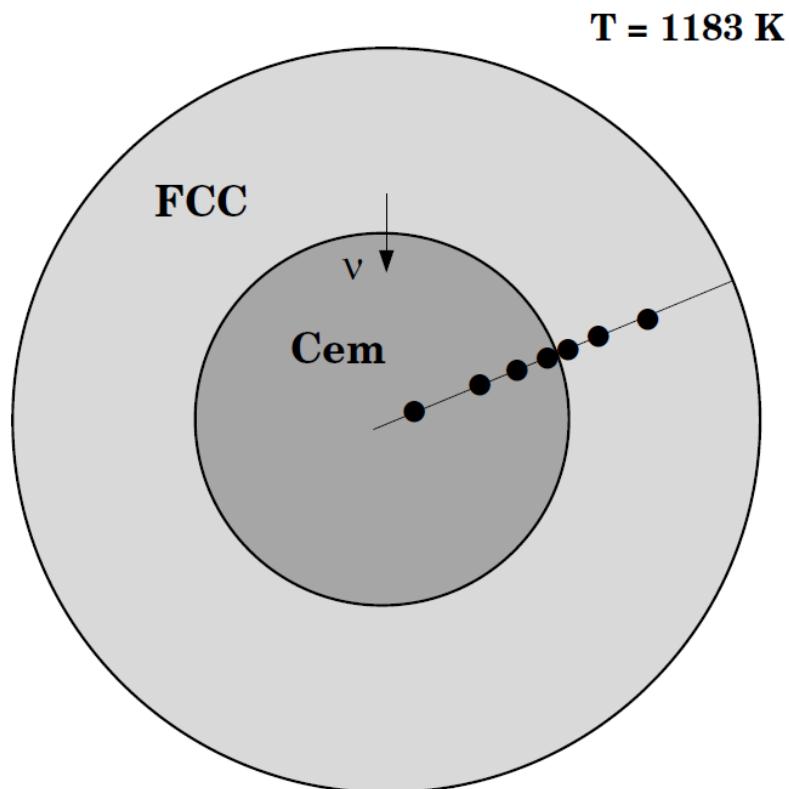




## Example exb2

### Cementite dissolution in an Fe-Cr-C alloy

This example calculates the dissolution of a spherical cementite particle in an austenite matrix. This case is from Z.-K. Liu, L. Höglund, B. Jönsson and J. Ågren (Metall. Trans.A, v.22A, 1991, pp. 1745-1752). In order to achieve the correct average composition in the calculation it is necessary to take into account the fact that the calculation is set up using the volume fraction of the phases. To calculate the initial state at the heat treatment temperature we need first to determine the state at the normalizing temperature. To calculate the volume fraction of the phases we need to enter a number of functions that calculate these quantities.



**exb2-setup****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_dictra_console_examples\examples\exb2\setup.DCM.test"
SYS: i>_@_
NO SUCH COMMAND, USE HELP
SYS: @@ Moving boundary problem.
SYS: @@ Cementite dissolution in an Fe-Cr-C alloy
SYS: @@ This example calculates the dissolution of a spherical cementite
SYS: @@ particle in an austenite matrix.
SYS: @@ This case is from Z.-K. Liu, L. Hågglund, B. Jähnsson and J. Ångren:
SYS: @@ Metall. Trans.A, v.22A (1991), pp. 1745-1752.
SYS: -----
NO SUCH COMMAND, USE HELP
SYS: @@
SYS: @@ In order to achieve the correct average composition in the calculation
SYS: @@ it is necessary to take into account that the calculation is set up
SYS: @@ using the volume fraction of the phases. To calculate the initial
SYS: @@ state at the heat treatment temperature we first need to determine
SYS: @@ the state at the normalizing temperature. To calculate the volume
SYS: @@ fraction of the phases we need to enter a number of functions
SYS: @@ that calculate these quantities. NOTE: The volume fractions are
SYS: @@ determined by assuming that only the substitutional components
SYS: @@ contribute to the volume of a system, whereas the interstitial
SYS: @@ components do not.
SYS: @@
SYS: @@ The total radius of the system can be calculated from the relation:
SYS: @@
SYS: @@ 
$$\frac{R}{V_{tot}} = \frac{V_{cem}}{V_{cem}}$$

SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASES
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\generate_dictra_console_examples\databases\data
Current database: Steels/Fe-Alloys v12.0

VA           /- DEFINED
TDB_FCC_A1  REJECTED
TDB_TCFE12: @@
TDB_TCFE12: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE THE DATA
TDB_TCFE12: @@
TDB_TCFE12: sw FEDEMO
Current database: Iron Demo Database v4.0

VA           /- DEFINED
TDB_FEDEMO: def-sys fe cr c
FE          CR
      C
      DEFINED
TDB_FEDEMO: rej ph * all
GAS:G        LIQUID:L
LAVES_PHASE_C14  CBCC_A12
CHI_A12      CUB_A13
FCC_A1       GRAPHITE
KSI_CARBIDE M23C6
M5C2         M7C3
      SIGMA
      REJECTED
TDB_FEDEMO: res ph fcc bcc cem
FCC_A1       BCC_A2
      CEMENTITE
      RESTORED
TDB_FEDEMO: get
15:35:53,793 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
Creating a new composition set FCC_A1#2
PARAMETERS ...
FUNCTIONS .....

List of references for assessed data
'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'
'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
'A.T. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
'X.G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
    volumes'
'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'
'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 1995: 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. 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'
-OK-
TDB_FEDEMO:
TDE_FEDEMO: @@
TDB_FEDEMO: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE THE MOBILITY DATA
TDE_FEDEMO: @@
TDE_FEDEMO: app mobfe4
Current database: Steels/Fe-Alloys Mobility v4.0

VA DEFINED
B2_BCC REJECTED
APP: def-sp fe cr c
FE CR
APP: rej ph * all
BCC_A2 CEMENTITE FCC_A1
FE4N_LP1 HCP_A3 LIQUID:L
REJECTED
APP: res ph fcc cementite
FCC_A1 CEMENTITE RESTORED
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS .....
FUNCTIONS .....

List of references for assessed data

'This parameter has not been assessed'
'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'
'B. Jonsson: Z. Metallkunde 85(1994)502-509; C diffusion in fcc Cr-Fe-Ni'
'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Fe diffusion fcc Cr-Fe'
'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
-Ni'
'This parameter has been estimated'
-OK-
APP:
APP: @@
APP: @@ ENTER THE POLY-3 MONITOR
APP: @@
APP: go p-3

POLY version 3.32
POLY:

POLY: @@
POLY: @@ SET THE CONDITIONS AT THE NORMALIZING TEMPERATURE
POLY: @@
POLY: set-cond T=1008,P=101325,N=1
POLY: set-cond X(CR)=0.0206,X(C)=0.0391
POLY:
POLY:
POLY: @@
POLY: @@ ENTER FUNCTIONS TO DETERMINE THE VOLUME-FRACTIONS
POLY: @@
POLY:
POLY: @@
POLY: @@ Radius of the cementite particle
POLY: ent-symb var rcem=0.5255e-6;
POLY:
POLY: @@ total number of moles of substitutional components
POLY: ent-symb func nstot=n(fe)+n(cr);
POLY:
POLY: @@ number of moles of substitutional components in cementite
POLY: ent-symb func nscem=n(cem,fe)+n(cem,cr);
POLY:
POLY: @@ volume fraction (U-fraction) of cementite
POLY: ent-symb func vfcm=nscem/nstot;
POLY:
POLY: @@ total radius of the system
POLY: ent-symb func rtot=rcem/vfcm** (1/3);
POLY:
POLY: @@ radius of the surrounding austenite matrix
POLY: ent-symb func rmat=rtot-rcem;
POLY:
POLY:
POLY: @@
POLY: @@ COMPUTE THE EQUILIBRIUM
POLY: @@
POLY: compute-eq
Using global minimization procedure
Calculated 4113 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:
POLY:
POLY: @@
POLY: @@ SHOW THE COMPUTED VALUES TO BE USED IN THE DICTRA CALCULATION
POLY: @@
POLY: show rmat
RMAT=5.3924863E-7
POLY: show w(cem,cr),w(bcc,cr),w(bcc,c)
W(CEMENTITE,CR)=0.12581645
W(BCC_A2,CR)=4.4332285E-3
W(BCC_A2,C)=1.510215E-4
POLY:
POLY: ent var wmatcr=w(bcc,cr);
POLY: ent var wmatc=w(bcc,c);
POLY: ent var wcemcr=w(cem,cr);
POLY:
POLY: @@
POLY: @@ ENTER THE DICTRA MONITOR
POLY: @@
POLY: go d-m
NO TIME STEP DEFINED
*** ENTERING BCC_A2 AS A DIFFUSION NONE PHASE
DIC>
```

```

DIC> @@
DIC> @@ ENTER GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob t 0 1183; * n
DIC>
DIC> @@
DIC> @@ ENTER THE REGIONS carb AND aus
DIC> @@
DIC> enter-region
REGION NAME : carb
DIC>
DIC> enter-region
REGION NAME : aus
ATTACH TO REGION NAMED /CARB/:
ATTACHED TO THE RIGHT OF CARB /YES/:
DIC> @@
DIC> @@ ENTER GEOMTRICAL GRIDS INTO THE REGIONS
DIC> @@
DIC>
DIC> @@
DIC> @@ THE INITIAL SIZE OF THE CEMENTITE PARTICLE IS ASSUMED TO BE KNOWN
DIC> @@ (IN THIS CASE THE VALUE IS TAKEN FROM LIU ET AL. WHO ESTIMATED THE
DIC> @@ AVERAGE INITIAL DIAMETER OF THE PARTICLES TO 1.051E-6 METERS).
DIC> @@
DIC> enter-grid
REGION NAME : /CARB/: carb
WIDTH OF REGION /1/: rcm
TYPE /LINEAR/: AUTO
DIC>
DIC> @@
DIC> @@ THE SIZE OF THE FCC REGION CAN BE CALCULATED FROM A MASS BALANCE
DIC> @@ AFTER ESTIMATING THE INITIAL COMPOSITIONS IN THE TWO PHASES
DIC> @@
DIC> enter-grid
REGION NAME : /AUS/: aus
WIDTH OF REGION /1/: rmat
TYPE /LINEAR/: AUTO
DIC>
DIC> @@
DIC> @@ ENTER PHASES INTO REGIONS
DIC> @@
DIC> enter-phase act carb matrix cementite
DIC> enter-phase act aus matrix fcc#1
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITIONS IN THE PHASES
DIC> @@
DIC> enter-composition
REGION NAME : /CARB/: carb
PHASE NAME: /CEMENTITE/: cementite
COMPOSITION TYPE /MOLE_FRACTION/: weig-fraction
PROFILE FOR /CR/: cr lin wcemcr wcemcr
DIC>
DIC> enter-composition
REGION NAME : /AUS/: aus
PHASE NAME: /FCC_A1#1/: fcc#1
DEPENDENT COMPONENT ? /FE/: fe
COMPOSITION TYPE /MOLE_FRACTION/: weig-fraction
PROFILE FOR /C/: CR lin wmatcr wmatcr
PROFILE FOR /CR/: C lin wmatc wmatc
DIC>
DIC> @@
DIC> @@ SET TO A SPHERICAL GEOMETRY
DIC> @@
DIC> enter-geo
GEOMETRICAL EXPONENT /0/: 2
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME AND OTHER SIMULATION PARAMETERS
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /1/: 10000
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /1000/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exb2 Y
DIC>
DIC> set-inter
--OK---
DIC>

```

**exb2-run**

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exb2\run.DCM.test"
DIC>
DIC>
DIC> @@ exb2_run.DCM
DIC>
DIC>
DIC> @@ READ THE SET UP FROM FILE AND START THE SIMULATION
DIC> @@
DIC>
DIC>
DIC> go d-m
TIME STEP AT TIME  0.00000E+00
*** ENTERING BCC_A2 AS A DIFFUSION NONE PHASE
DIC> read exb2
OK
DIC> sim
Region: CARB
single geometric dense at  0.52550E-06
0.85084   96
Region: AUS
single geometric dense at  0.0000
1.0072   63
DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
Trying old scheme          4
GENERATING STARTING VALUES FOR CELL # 1 INTERFACE # 2
DETERMINING INITIAL EQUILIBRIUM VALUES
CALCULATING STARTING VALUES:      9    EQUILIBRIUM CALCULATIONS           DONE       6 OUT OF      9
04
U-FRACTION IN SYSTEM: C = .0406910188418179 CR = .0214382349908298
FE = .978561765139677
TOTAL SIZE OF SYSTEM: 5.0562655986E-18 [m^3]
U-FRACTION IN SYSTEM: C = .0406910188418179 CR = .0214382349908298
FE = .978561765139677
TOTAL SIZE OF SYSTEM: 5.0562655986E-18 [m^3]
0.175650510569693   0.175691773365777   0.175650565704887   2.957532598305099E-003   7.754437973902466E-
005   5.789560110638669E-006   8.570927948261712E-007   3.747773449054368E-007   3.453239602567087E-
007   1.349945520965789E-007   1.350781378777377E-007   1.346761780040160E-007   1.361219741567956E-
007   1.343486158187189E-007   1.340757896497654E-007   1.335307279086690E-007   1.344901657987451E-
007   1.324431149502718E-007   1.302779707752355E-007   1.259882989092764E-007   1.269270676242141E-
007   1.175749112140888E-007   1.014430318623444E-007   7.21795337839238E-008   7.299680976072143E-
008   2.728135259936651E-008   7.241610557431686E-011   4.089073975800423E-014   7.514683315310822E-
019   TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.15641202E-18
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.39436721E-02 AND -0.39436721E-02
POSITION OF INTERFACE CARB / AUS IS 0.52510563E-06
U-FRACTION IN SYSTEM: C = .040729015482772 CR = .0214383281162587
FE = .978561672014248
TOTAL SIZE OF SYSTEM: 5.0562655986E-18 [m^3]
15 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: CARB

CPU time used in timestep          1 seconds
2.248325209321158E-005   2.248775172894889E-005   2.248323619911258E-005   1.887681971785783E-009   1.633889346556181E-
009   1.019554384038724E-009   6.882195845839138E-010   6.885275294802593E-010   2.216755169621960E-
010   6.151372771543853E-014   2.128400055077280E-017   TIME = 0.30000000E-06 DT = 0.20000000E-
06 SUM OF SQUARES = 0.18330541E-18
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.22443437E-04 AND -0.22443437E-04
POSITION OF INTERFACE CARB / AUS IS 0.52510114E-06
U-FRACTION IN SYSTEM: C = .04072976539935 CR = .0214383291134799
FE = .978561671017027
TOTAL SIZE OF SYSTEM: 5.0562655986E-18 [m^3]
CPU time used in timestep          0 seconds
6.026886171006244E-004   6.026583061736450E-004   6.026723276374160E-004   8.498836241942660E-005   3.515902363183597E-
005   2.728069475198861E-007   4.04929651693932E-010   6.350486825359254E-015   2.881549266615981E-
018   TIME = 0.70000000E-06 DT = 0.40000000E-06 SUM OF SQUARES = 0.13123592E-18
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.46375286E-05 AND -0.46375286E-05
POSITION OF INTERFACE CARB / AUS IS 0.52509929E-06
U-FRACTION IN SYSTEM: C = .0407315536943019 CR = .0214383294273154
FE = .978561670703191
TOTAL SIZE OF SYSTEM: 5.0562655986E-18 [m^3]
CPU time used in timestep          1 seconds
2.365053654994453E-004   2.365034011193425E-004   2.364987464518160E-004   7.190707106424921E-005   1.444190616366121E-
007   4.667910968230499E-011   2.104087464936592E-014   2.043433015732732E-017   TIME = 0.15000000E-05 DT = 0.80000000E-
06 SUM OF SQUARES = 0.59644760E-18
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.40628788E-05 AND -0.40628788E-05
POSITION OF INTERFACE CARB / AUS IS 0.52509604E-06
U-FRACTION IN SYSTEM: C = .0407314707249636 CR = .0214383297893152
FE = .978561670341192
TOTAL SIZE OF SYSTEM: 5.0562655986E-18 [m^3]

output ignored...

... output resumed

2.665669006532875E-009   5.237408957649139E-014   3.862303376798767E-
019   TIME = 8301.5667 DT = 1000.0000 SUM OF SQUARES = 0.22983948E-18
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.10714300E-10 AND -0.10714300E-10
POSITION OF INTERFACE CARB / AUS IS 0.24630882E-06
U-FRACTION IN SYSTEM: C = .040763456619809 CR = .0214383907682669
FE = .97856160936224
TOTAL SIZE OF SYSTEM: 5.0562655986E-18 [m^3]
CPU time used in timestep          1 seconds
8.021013850733219E-009   8.076199852417704E-009   8.037960234130764E-009   2.650858755431560E-009   9.260001949187760E-
010   5.030462419597751E-015   3.756929409274618E-
018   TIME = 9301.5667 DT = 1000.0000 SUM OF SQUARES = 0.37532071E-17
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.10120585E-10 AND -0.10120585E-10
POSITION OF INTERFACE CARB / AUS IS 0.23618823E-06
U-FRACTION IN SYSTEM: C = .0407634751645684 CR = .0214383896425145
FE = .978561610487993
TOTAL SIZE OF SYSTEM: 5.0562655986E-18 [m^3]
CPU time used in timestep          1 seconds
7.716032811257552E-007   7.711887701630558E-007   7.708715590379299E-007   6.765610938268225E-008   1.033751320413251E-
013   2.628446794668101E-017   TIME = 10000.0000 DT = 698.43330 SUM OF SQUARES = 0.24417362E-16
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.95749019E-11 AND -0.95749019E-11
POSITION OF INTERFACE CARB / AUS IS 0.22950080E-06
U-FRACTION IN SYSTEM: C = .0407634745654968 CR = .0214383889005123
FE = .978561611229995
TOTAL SIZE OF SYSTEM: 5.0562655986E-18 [m^3]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
```

RECLAIMING WORKSPACE

DELETING TIME-RECORD FOR TIME 0.0000000  
DELETING TIME-RECORD FOR TIME 0.10000000E-06  
DELETING TIME-RECORD FOR TIME 0.30000000E-06  
DELETING TIME-RECORD FOR TIME 0.70000000E-06  
DELETING TIME-RECORD FOR TIME 0.15000000E-05  
DELETING TIME-RECORD FOR TIME 0.31000000E-05  
DELETING TIME-RECORD FOR TIME 0.63000000E-05  
DELETING TIME-RECORD FOR TIME 0.12700000E-04  
DELETING TIME-RECORD FOR TIME 0.25500000E-04  
DELETING TIME-RECORD FOR TIME 0.51100000E-04  
DELETING TIME-RECORD FOR TIME 0.99418841E-04  
DELETING TIME-RECORD FOR TIME 0.17900385E-03  
DELETING TIME-RECORD FOR TIME 0.30071417E-03  
DELETING TIME-RECORD FOR TIME 0.47831765E-03  
DELETING TIME-RECORD FOR TIME 0.72934329E-03  
DELETING TIME-RECORD FOR TIME 0.10758312E-02  
DELETING TIME-RECORD FOR TIME 0.15428938E-02  
DELETING TIME-RECORD FOR TIME 0.21467122E-02  
DELETING TIME-RECORD FOR TIME 0.29017133E-02  
DELETING TIME-RECORD FOR TIME 0.38194432E-02  
DELETING TIME-RECORD FOR TIME 0.49085135E-02  
DELETING TIME-RECORD FOR TIME 0.61737016E-02  
DELETING TIME-RECORD FOR TIME 0.76140450E-02  
DELETING TIME-RECORD FOR TIME 0.92225149E-02  
DELETING TIME-RECORD FOR TIME 0.10986151E-01  
DELETING TIME-RECORD FOR TIME 0.12887549E-01  
DELETING TIME-RECORD FOR TIME 0.14913628E-01  
DELETING TIME-RECORD FOR TIME 0.17051229E-01  
DELETING TIME-RECORD FOR TIME 0.19290844E-01  
DELETING TIME-RECORD FOR TIME 0.21633465E-01  
DELETING TIME-RECORD FOR TIME 0.24076421E-01  
DELETING TIME-RECORD FOR TIME 0.26619478E-01  
DELETING TIME-RECORD FOR TIME 0.29264709E-01  
DELETING TIME-RECORD FOR TIME 0.32010278E-01  
DELETING TIME-RECORD FOR TIME 0.34862213E-01  
DELETING TIME-RECORD FOR TIME 0.37829432E-01  
DELETING TIME-RECORD FOR TIME 0.40921190E-01  
DELETING TIME-RECORD FOR TIME 0.44135912E-01  
DELETING TIME-RECORD FOR TIME 0.47480207E-01  
DELETING TIME-RECORD FOR TIME 0.50960807E-01  
DELETING TIME-RECORD FOR TIME 0.54592579E-01  
DELETING TIME-RECORD FOR TIME 0.58382957E-01  
DELETING TIME-RECORD FOR TIME 0.62356658E-01  
DELETING TIME-RECORD FOR TIME 0.66520761E-01  
DELETING TIME-RECORD FOR TIME 0.68801534E-01  
DELETING TIME-RECORD FOR TIME 0.71495808E-01  
DELETING TIME-RECORD FOR TIME 0.74611177E-01  
DELETING TIME-RECORD FOR TIME 0.78157596E-01  
DELETING TIME-RECORD FOR TIME 0.82113712E-01  
DELETING TIME-RECORD FOR TIME 0.86489284E-01  
DELETING TIME-RECORD FOR TIME 0.91274871E-01  
DELETING TIME-RECORD FOR TIME 0.96471058E-01  
DELETING TIME-RECORD FOR TIME 0.10205818  
DELETING TIME-RECORD FOR TIME 0.10804601  
DELETING TIME-RECORD FOR TIME 0.11444776  
DELETING TIME-RECORD FOR TIME 0.12132749  
DELETING TIME-RECORD FOR TIME 0.12873099  
DELETING TIME-RECORD FOR TIME 0.13674515  
DELETING TIME-RECORD FOR TIME 0.14543216  
DELETING TIME-RECORD FOR TIME 0.15494171  
DELETING TIME-RECORD FOR TIME 0.16560505  
DELETING TIME-RECORD FOR TIME 0.17785673  
DELETING TIME-RECORD FOR TIME 0.19238367  
DELETING TIME-RECORD FOR TIME 0.21033391  
DELETING TIME-RECORD FOR TIME 0.23438453  
DELETING TIME-RECORD FOR TIME 0.27062133  
DELETING TIME-RECORD FOR TIME 0.33531950  
DELETING TIME-RECORD FOR TIME 0.41255614  
DELETING TIME-RECORD FOR TIME 0.50834603  
DELETING TIME-RECORD FOR TIME 0.63458020  
DELETING TIME-RECORD FOR TIME 0.81556832  
DELETING TIME-RECORD FOR TIME 0.91469959  
DELETING TIME-RECORD FOR TIME 1.0981843  
DELETING TIME-RECORD FOR TIME 1.4390940  
DELETING TIME-RECORD FOR TIME 1.6570155  
DELETING TIME-RECORD FOR TIME 2.0571419  
DELETING TIME-RECORD FOR TIME 2.8315122  
DELETING TIME-RECORD FOR TIME 4.3109178  
DELETING TIME-RECORD FOR TIME 7.1209891  
DELETING TIME-RECORD FOR TIME 12.538354  
DELETING TIME-RECORD FOR TIME 23.255021  
DELETING TIME-RECORD FOR TIME 44.688355  
DELETING TIME-RECORD FOR TIME 87.555022  
DELETING TIME-RECORD FOR TIME 173.28836  
DELETING TIME-RECORD FOR TIME 344.75503  
DELETING TIME-RECORD FOR TIME 687.68836  
DELETING TIME-RECORD FOR TIME 1373.5550  
DELETING TIME-RECORD FOR TIME 2301.5667  
DELETING TIME-RECORD FOR TIME 3301.5667  
DELETING TIME-RECORD FOR TIME 4301.5667  
DELETING TIME-RECORD FOR TIME 5301.5667  
DELETING TIME-RECORD FOR TIME 6301.5667  
DELETING TIME-RECORD FOR TIME 7301.5667  
DELETING TIME-RECORD FOR TIME 8301.5667

KEEPING TIME-RECORD FOR TIME 9301.5667  
AND FOR TIME 10000.000  
WORKSPACE RECLAIMED

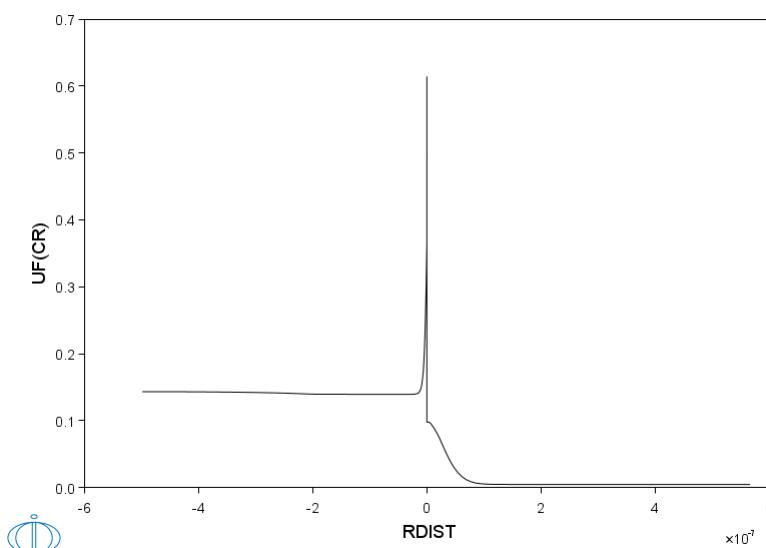
TIMESTEP AT 10000.0000 SELECTED

DIC>  
DIC> set-inter  
--OK--  
DIC>

**exb2-plot**

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exb2\plot.DCM.test"
DIC>
DIC>
DIC> @@ exb2_plot.DCM
DIC>
DIC> @@
DIC> FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE b2
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 1.00000E+04
*** ENTERING BCC_A2 AS A DIFFUSION NONE PHASE
DIC> read exb2
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1: @@
POST-1: @@ LET US PLOT CHROMIUM CONCENTRATION PROFILES
POST-1: @@ WE THEN SET THE DISTANCE AS X-AXIS (NOTE THAT DISTANCE IS AUTOMATICALLY
POST-1: @@ SET AS THE INDEPENDENT VARIABLE) AND U-FRACTION CARBON AS Y-AXIS
POST-1: @@ REMEMBER THAT THE PLOT CONDITION ALSO MUST BE SET.
POST-1: @@
POST-1: @@ NOTICE THAT ALL DISTANCES IN THE DATA FILE ARE GIVEN RELATIVE TO THE
POST-1: @@ CEM/FCC INTERFACE. FOR THIS REASON AN OFFSET MUST BE GIVEN TO THE
POST-1: @@ DATA ACCORDING TO THE ACTUAL PARTICLE RADIUS AT THE SPECIFIED TIME.
POST-1: @@
POST-1: enter-symb
Function or table /FUNCTION/: func
NAME: rdist
FUNCTION: gd-poi(carb,u);
POST-1:
POST-1: s-d-a x rdist
POST-1:
POST-1: s-i-v
VARIABLE /TIME/: dist
DISTANCE : /GLOBAL/: glo
POST-1:
POST-1: s-d-a y uf(cr)
POST-1:
POST-1: s-p-c time 10
POST-1:
POST-1: @@
POST-1: @@ SET THE TITLE ON THE PLOT
POST-1: @@
POST-1: set-title Figure b2.1
POST-1:
POST-1: @@
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

**Figure b2.1**



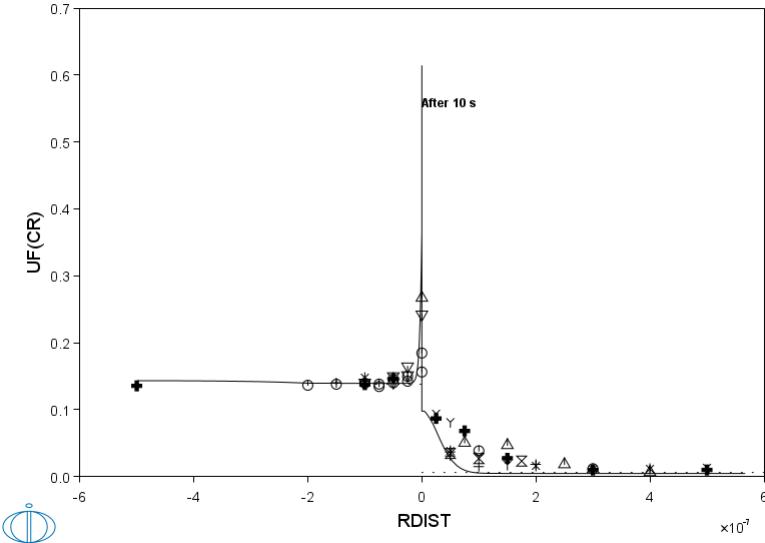
```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: @@
POST-1: @@ INCLUDE EXPERIMENTAL DATA POINTS ON THE PLOT FOR COMPARISION
POST-1: @@
POST-1: @@ FIRST LIST DATASETS
POST-1: @@
POST-1: app y exb2.exp
PROLOGUE NUMBER: /0/: 0
```

```

DATASET NUMBER(s): /-1/: -1
DATASET 1 CONCENTRATION PROFILE T=10S
DATASET 2 CONCENTRATION PROFILE T=100S
DATASET 3 CONCENTRATION PROFILE T=1000S
DATASET 4 CONCENTRATION PROFILE T=10000S
DATASET 5 VOLUME FRACTION CEMENTITE VS. TIME
DATASET 6 MEAN PARTICLE DIAMETER VS. TIME
POST-1:
POST-1: @@
POST-1: @@ SELECT THE PROPER DATASET
POST-1: @@
POST-1: app y exb2.exp
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 1
POST-1:
POST-1: set-title Figure b2.2
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

```

Figure b2.2

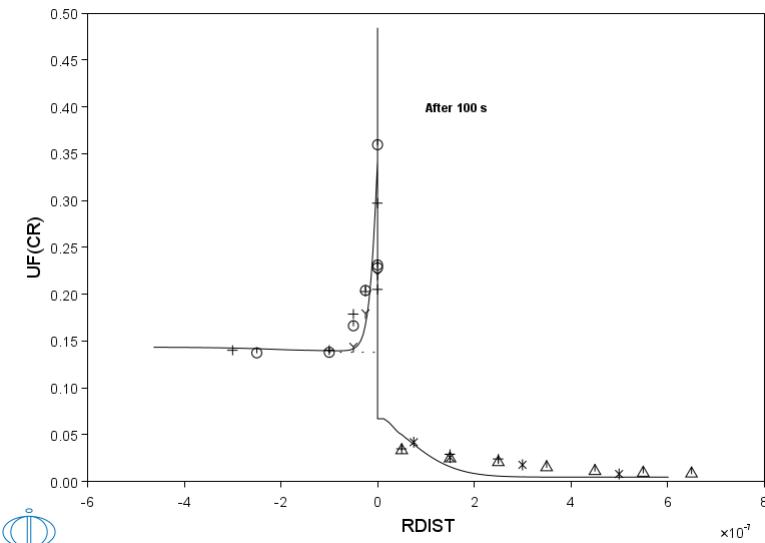


```

POST-1:
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: @@
POST-1: @@ PLOT ALSO FOR 100, 1000 AND 10000 seconds
POST-1: @@
POST-1:
POST-1: s-p-c time 100
POST-1:
POST-1: app y exb2.exp
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 2
POST-1:
POST-1: set-title Figure b2.3
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

```

Figure b2.3



```

POST-1:
POST-1:

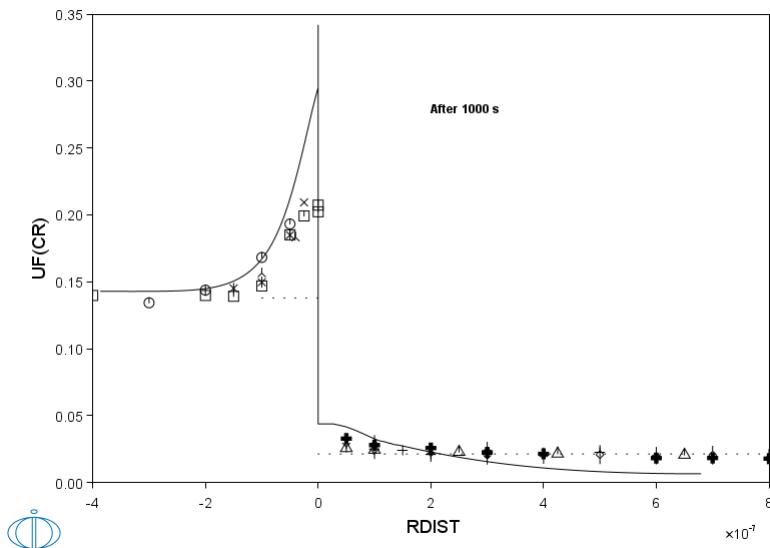
```

```

POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1:
POST-1: s-p-c time 1000
POST-1:
POST-1: app y exb2.exp
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 3
POST-1:
POST-1: set-title Figure b2.4
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

```

Figure b2.4

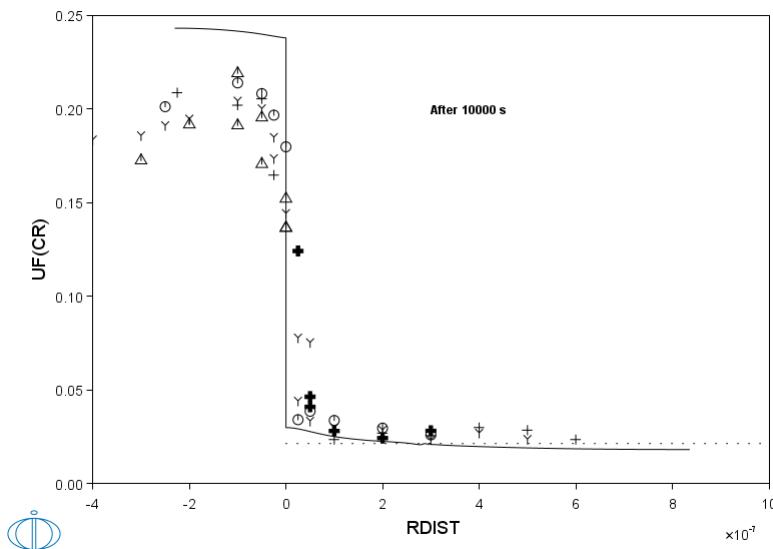


```

POST-1:
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1:
POST-1: s-p-c time 10000
POST-1:
POST-1: app y exb2.exp
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 4
POST-1:
POST-1: set-title Figure b2.5
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

```

Figure b2.5



```

POST-1:
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: @@
POST-1: @@ ALSO PLOT HOW THE VOLUME FRACTION OF CEMENTITE VARIES
POST-1: @@ WITH TIME
POST-1: @@

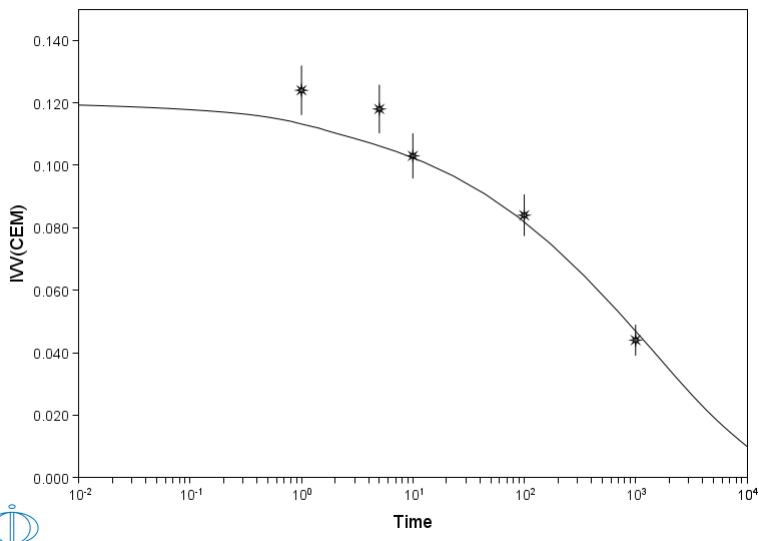
```

```

POST-1: s-d-a y ivv(cem)
POST-1: s-s-s y n 0 .15
POST-1:
POST-1: s-d-a x time
INFO: Time is set as independent variable
POST-1: set-axis-type x log
POST-1: s-s-s x n .01 10000
POST-1:
POST-1: s-p-c integral
POST-1:
POST-1: app y exb2.exp
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 5
POST-1:
POST-1: set-title Figure b2.6
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

```

Figure b2.6

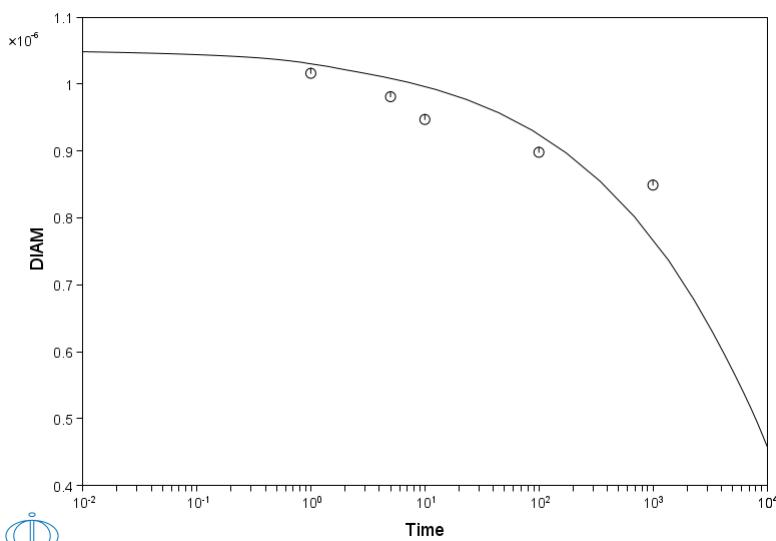


```

POST-1:
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: @@
POST-1: @@ ALSO PLOT HOW THE DIAMETER OF CEMENTITE VARIES WITH TIME
POST-1: @@
POST-1: enter func diam=2*poi(carb,u);
POST-1: s-d-a y diam
POST-1:
POST-1: s-p-c interface carb upper
POST-1:
POST-1: app y exb2.exp
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 6
POST-1:
POST-1: set-title Figure b2.7
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

```

Figure b2.7



```
POST-1:
```

```
POST-1:  
POST-1:  
POST-1:  
POST-1:@?<_hit_return_to_continue_>  
POST-1:  
POST-1: set-inter  
--OK---  
POST-1:
```



FUNCTIONS ....

List of references for assessed data

'This parameter has not been assessed'  
'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'  
'B. Jonsson: Z. Metallkunde 85(1994)502-509; C diffusion in fcc Cr-Fe-Ni'  
'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Fe diffusion fcc Cr-Fe'  
'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe  
-Ni'  
'B. Jonsson: Z. Metallkunde 85(1994)498-501; C and N diffusion in bcc Cr  
-Fe-Ni'  
'B. Jonsson: ISIJ International, 35(1995)1415-1421; Cr, Fe and Ni  
diffusion bcc Cr-Fe-Ni'  
'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion  
in bcc Fe'  
-OK-  
**APP:**  
**APP: @@**  
**APP: @@ ENTER THE DICTRA MONITOR**  
**APP: @@**  
**APP: go d-m**  
NO TIME STEP DEFINED  
\*\*\* ENTERING M23C6 AS A DIFFUSION NONE PHASE  
**DIC>**  
**DIC>**  
**DIC> @@ THE MOBILITY DATABASE LACKS KINETIC DATA FOR THE M23-CARBIDE**  
**DIC> @@ SO AN ESTIMATE FOR THE MOBILITIES IN THIS PHASE ARE ENTERED.**  
**DIC> ent-mob-est M23 c**  
**M[M23,C](T)= 0;**  
**DIC>**  
**DIC> ent-mob-est M23 cr**  
**M[M23,CR](T)= 3e-11\*exp(-278000/8.3145/T);**  
**DIC>**  
**DIC> ent-mob-est M23 fe**  
**M[M23,FE](T)= 1e-11\*exp(-275000/8.3145/T);**  
**DIC>**  
**DIC> @@**  
**DIC> @@ ENTER GLOBAL CONDITION T**  
**DIC> @@**  
**DIC> set-cond glob T 0 1273; \* N**  
**DIC>**  
**DIC> @@**  
**DIC> @@ ENTER THE REGIONS carbide AND matrix**  
**DIC> @@**  
**DIC> enter-region carbide**  
**DIC> enter-region matrix**  
**ATTACH TO REGION NAMED /CARBIDE/:**  
**ATTACHED TO THE RIGHT OF CARBIDE /YES/:**  
**DIC> @@**  
**DIC> @@ ASSUME SOME REASONABLE SIZE OF THE CARBIDE PARTICLE**  
**DIC> @@**  
**DIC> enter-grid carbide 5.0000000E-7 AUTO**  
**DIC> @@**  
**DIC> @@ THE SIZE OF THE FCC REGION WE CAN CALCULATE FROM A MASS BALANCE**  
**DIC> @@ AFTER ESTIMATING THE INITIAL COMPOSITIONS IN THE TWO PHASES.**  
**DIC> @@**  
**DIC> enter-grid matrix 5.55859755E-7 AUTO**  
**DIC> @@**  
**DIC> @@ ENTER PHASES INTO THE REGION MATRIX. BOUNDARY CONDITIONS ARE GIVEN**  
**DIC> @@ IF THE INACTIVE PHASE bcc IS NUCLEATED**  
**DIC> @@**  
**DIC> enter-phase**  
**ACTIVE OR INACTIVE PHASE /ACTIVE/: act**  
**REGION NAME : /CARBIDE/: matrix**  
**PHASE TYPE /MATRIX/: matrix**  
**PHASE NAME: /NONE/: fcc#1**  
**DIC>**  
**DIC> enter-phase**  
**ACTIVE OR INACTIVE PHASE /ACTIVE/: inact**  
**ATTACH TO REGION NAMED /MATRIX/: matrix**  
**ATTACHED TO THE RIGHT OF MATRIX /YES/: no**  
**PHASE NAME: /NONE/: bcc#1**  
**DEPENDENT COMPONENT ? /FE/: fe**  
**REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/**  
**CONDITION TYPE /CLOSED\_SYSTEM/: closed**  
**DIC>**  
**DIC> @@**  
**DIC> @@ ENTER THE PHASE INTO THE REGION carbide**  
**DIC> @@**  
**DIC> enter-phase**  
**ACTIVE OR INACTIVE PHASE /ACTIVE/: act**  
**REGION NAME : /CARBIDE/: carbide**  
**PHASE TYPE /MATRIX/: matrix**  
**PHASE NAME: /NONE/: m23c6**  
**DIC>**  
**DIC> @@**  
**DIC> @@ ENTER COMPOSITIONS INTO THE PHASES**  
**DIC> @@**  
**DIC> enter-composition**  
**REGION NAME : /CARBIDE/: carbide**  
**PHASE NAME: /M23C6/: m23c6**  
**DEPENDENT COMPONENT ? /FE/: fe**  
**COMPOSITION TYPE /MOLE\_FRACTION/: mole-fraction**  
**PROFILE FOR /CR/: cr lin 0.55079807 0.55079807**  
**DIC>**  
**DIC>**  
**DIC> enter-composition**  
**REGION NAME : /MATRIX/: matrix**  
**PHASE NAME: /FCC\_A1#1/: fcc#1**  
**DEPENDENT COMPONENT ? /FE/: fe**  
**COMPOSITION TYPE /MOLE\_FRACTION/: mole-fraction**  
**PROFILE FOR /C/: cr lin 8.5203899E-2 8.5203899E-2**  
**PROFILE FOR /CR/: c lin 1.8072433E-4 1.8072433E-4**  
**DIC>**  
**DIC> @@**  
**DIC> @@ SET TO A SPHERICAL GEOMETRY**  
**DIC> @@**  
**DIC> enter-geo**  
**GEOMETRICAL EXPONENT /0/: 2**  
**DIC>**

```
DIC> @@
DIC> @@ SET THE SIMULATION TIME AND OTHER SIMULATION PARAMETERS
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 8000
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /800/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exb3 Y
DIC>
DIC>
DIC>
DIC> set-inter
--OK---
DIC>
```

**exb3-run**

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exb3\run.DCM.test"
DIC>
DIC>
DIC> @@ exb3_run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING EXAMPLE b3
DIC> @@
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA MONITOR AND READ THE SET UP FROM FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 0.00000E+00
DIC> read exb3
OK
DIC>
DIC> @@
DIC> @@ WHEN THE FERRITE NUCLEATES WE USE DEFAULT VALUES
DIC> @@ AS STARTING VALUES FOR THE WIDTH OF THE NEW REGION
DIC> @@ AND THE VELOCITY OF THE INTERFACES
DIC> @@
DIC>
DIC> @@
DIC> @@ START THE SIMULATION
DIC> @@
DIC> sim yes
Region: CARBIDE
single geometric dense at 0.50000E-06
0.83296 92
Region: MATRIX
single geometric dense at 0.0000
1.0051 62
DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
Trying old scheme 4
GENERATING STARTING VALUES FOR CELL # 1 INTERFACE # 2
DETERMINING INITIAL EQUILIBRIUM VALUES
CALCULATING STARTING VALUES: 9 EQUILIBRIUM CALCULATIONS DONE 6 OUT OF 9
U-FRACTION IN SYSTEM: C = .0278637912207471 CR = .149918318671311
FE = .850081681459196
TOTAL SIZE OF SYSTEM: 4.93068569406E-18 [m^3]
U-FRACTION IN SYSTEM: C = .0278637912207471 CR = .149918318671311
FE = .850081681459196
TOTAL SIZE OF SYSTEM: 4.93068569406E-18 [m^3]
0.565663007975141 0.565797019192576 0.565663812089353 1.015925208843506E-002 3.012654895297374E-
004 4.77345260290525E-005 2.96573903808362E-006 7.21536208790236E-007 8.262638058237679E-
007 4.246506052258363E-008 4.119324775544587E-008 3.974271203490607E-008 4.355497133377958E-
008 3.870625294980521E-008 3.673410109462362E-008 3.294771045509524E-008 3.668595706368702E-
008 2.600355363977916E-008 1.460917538496769E-008 1.658190605030451E-009 4.335933840560691E-
012 1.279149121605197E-015 2.899183614917506E-017 TIME = 0.10000000E-06 DT = 0.10000000E-
06 SUM OF SQUARES = 0.83673774E-18
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.17310735E-02 AND -0.17310735E-02
POSITION OF INTERFACE CARBIDE / MATRIX IS 0.49982689E-06
U-FRACTION IN SYSTEM: C = .0278769048021911 CR = .149918499752463
FE = .850081500378044
TOTAL SIZE OF SYSTEM: 4.93068569406E-18 [m^3]
16 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: CARBIDE

CPU time used in timestep 5 seconds
1.096405342624917E-004 1.09662644588033E-004 1.096405350852260E-004 5.301312566822289E-008 2.238795316374124E-
008 6.726062370086679E-011 8.23261579318133E-014 3.182642174509809E-019 TIME = 0.30000000E-06 DT = 0.20000000E-
06 SUM OF SQUARES = 0.20442551E-18
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.29934902E-05 AND -0.29934902E-05
POSITION OF INTERFACE CARBIDE / MATRIX IS 0.49982629E-06
U-FRACTION IN SYSTEM: C = .0278774003819474 CR = .149918500361418
FE = .850081499769089
TOTAL SIZE OF SYSTEM: 4.93068569406E-18 [m^3]
1 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: MATRIX

CPU time used in timestep 0 seconds
1.2178349596313E-004 1.217822143854386E-004 1.217736602724578E-004 6.952195104151467E-007 2.897692712754018E-
009 5.944748189095357E-012 3.496865204311504E-016 2.035021782261392E-022 TIME = 0.70000000E-06 DT = 0.40000000E-
06 SUM OF SQUARES = 0.20257338E-21
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.28086480E-05 AND -0.28086480E-05
POSITION OF INTERFACE CARBIDE / MATRIX IS 0.49982517E-06
U-FRACTION IN SYSTEM: C = .027877419496498 CR = .149918501468152
FE = .850081498662355
TOTAL SIZE OF SYSTEM: 4.93068569406E-18 [m^3]

output ignored...

... output resumed

TIME = 5410.6612 DT = 800.00000 SUM OF SQUARES = 0.99762170E-17
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.73712262E-12 AND -0.73712262E-12
POSITION OF INTERFACE CARBIDE / MATRIX IS 0.39357102E-06
U-FRACTION IN SYSTEM: C = .0278015157550372 CR = .149767573703472
FE = .850232426427035
TOTAL SIZE OF SYSTEM: 4.93068569406E-18 [m^3]
1 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: MATRIX

CPU time used in timestep 0 seconds
7.015624378228012E-008 7.017688495326688E-008 7.008589902670440E-008 4.426507946389554E-008 3.471895036950963E-
008 1.769880807680145E-008 5.85576643512253E-010 7.017102799860972E-016 2.852547377460861E-
018 TIME = 6210.6612 DT = 800.00000 SUM OF SQUARES = 0.28524369E-17
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.30980547E-12 AND -0.30980547E-12
POSITION OF INTERFACE CARBIDE / MATRIX IS 0.39332317E-06
U-FRACTION IN SYSTEM: C = .0278015171702384 CR = .149767574150767
FE = .85023242597974
TOTAL SIZE OF SYSTEM: 4.93068569406E-18 [m^3]
1 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: MATRIX

CPU time used in timestep 1 seconds
2.35027544398883E-008 2.35077646243124E-008 2.346113833901093E-008 1.535816969162443E-008 1.387526823006116E-
008 1.184263808147993E-008 6.58366354524535E-009 6.584768513872619E-009 1.062628885898886E-
009 4.145145332811724E-015 5.48049284168976E-
```

```

019      TIME =    7010.6612    DT =     800.00000    SUM OF SQUARES =   0.54793392E-18
CELL # 1 VELOCITY AT INTERFACE # 2 IS   -0.67756298E-13 AND   -0.67756298E-13
POSITION OF INTERFACE CARBIDE / MATRIX IS   0.39326897E-06
U-FRACTION IN SYSTEM: C = .0278015204411016 CR = .149767574502582
FE = .850232425627925
TOTAL SIZE OF SYSTEM: 4.93068569406E-18 [m^3]
1 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: MATRIX

CPU time used in timestep          1 seconds
7.805179964189818E-009    7.805809523970721E-009    7.780599797891480E-009    5.027993348845369E-009    4.922913714587291E-
009     4.700587203673256E-009    4.285804770208922E-009    4.286385142459803E-009    3.500314303177902E-
009     2.177116540697416E-009    4.752268298982334E-010    5.000374667320044E-014    2.445698574235898E-
018     TIME =    7810.6612    DT =     800.00000    SUM OF SQUARES =   0.24448113E-17
CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.68735069E-13 AND   0.68735069E-13
POSITION OF INTERFACE CARBIDE / MATRIX IS   0.39332396E-06
U-FRACTION IN SYSTEM: C = .0278015157664164 CR = .149767574512603
FE = .850232425617904
TOTAL SIZE OF SYSTEM: 4.93068569406E-18 [m^3]
30 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: CARBIDE
1 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: MATRIX

CPU time used in timestep          1 seconds
5.324979273216256E-008    5.324852889533831E-008    5.352220575550326E-008    2.366787624559008E-008    2.344415446545753E-
008     2.293205072017713E-008    2.198804179203802E-008    2.199551475311726E-008    2.010431897491741E-
008     1.664222958296746E-008    1.065292826244636E-008    1.065353610665117E-008    2.838728589913421E-
009     3.450337562891720E-017    TIME =    8000.0000    DT =    189.33884    SUM OF SQUARES =   0.37473966E-17
CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.34820009E-12 AND   0.34820009E-12
POSITION OF INTERFACE CARBIDE / MATRIX IS   0.39338988E-06
U-FRACTION IN SYSTEM: C = .0278015148252938 CR = .149767574514193
FE = .850232425616315
TOTAL SIZE OF SYSTEM: 4.93068569406E-18 [m^3]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME    61.635951
DELETING TIME-RECORD FOR TIME    68.483888
DELETING TIME-RECORD FOR TIME    68.483898
DELETING TIME-RECORD FOR TIME    68.483918
DELETING TIME-RECORD FOR TIME    68.483958
DELETING TIME-RECORD FOR TIME    68.484038
DELETING TIME-RECORD FOR TIME    68.484198
DELETING TIME-RECORD FOR TIME    68.484518
DELETING TIME-RECORD FOR TIME    68.485158
DELETING TIME-RECORD FOR TIME    68.486438
DELETING TIME-RECORD FOR TIME    68.488998
DELETING TIME-RECORD FOR TIME    68.494118
DELETING TIME-RECORD FOR TIME    68.504358
DELETING TIME-RECORD FOR TIME    68.524838
DELETING TIME-RECORD FOR TIME    68.565798
DELETING TIME-RECORD FOR TIME    68.647718
DELETING TIME-RECORD FOR TIME    68.811558
DELETING TIME-RECORD FOR TIME    69.139238
DELETING TIME-RECORD FOR TIME    69.794598
DELETING TIME-RECORD FOR TIME    71.105318
DELETING TIME-RECORD FOR TIME    73.726758
DELETING TIME-RECORD FOR TIME    78.969638
DELETING TIME-RECORD FOR TIME    89.455398
DELETING TIME-RECORD FOR TIME    110.42692
DELETING TIME-RECORD FOR TIME    152.36996
DELETING TIME-RECORD FOR TIME    236.25604
DELETING TIME-RECORD FOR TIME    404.02820
DELETING TIME-RECORD FOR TIME    739.57252
DELETING TIME-RECORD FOR TIME    1410.6612
DELETING TIME-RECORD FOR TIME    2210.6612
DELETING TIME-RECORD FOR TIME    3010.6612
DELETING TIME-RECORD FOR TIME    3810.6612
DELETING TIME-RECORD FOR TIME    4610.6612
DELETING TIME-RECORD FOR TIME    5410.6612
DELETING TIME-RECORD FOR TIME    6210.6612
DELETING TIME-RECORD FOR TIME    7010.6612

KEEPING TIME-RECORD FOR TIME    7810.6612
AND FOR TIME    8000.0000
WORKSPACE RECLAIMED

Timestep at    8000.00000    Selected

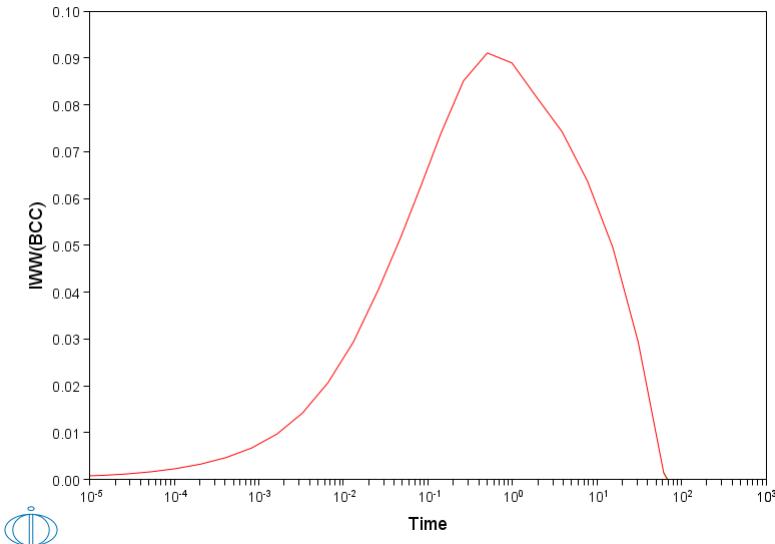
DIC>
DIC> set-inter
--OK--
DIC>

```

### exb3-plot

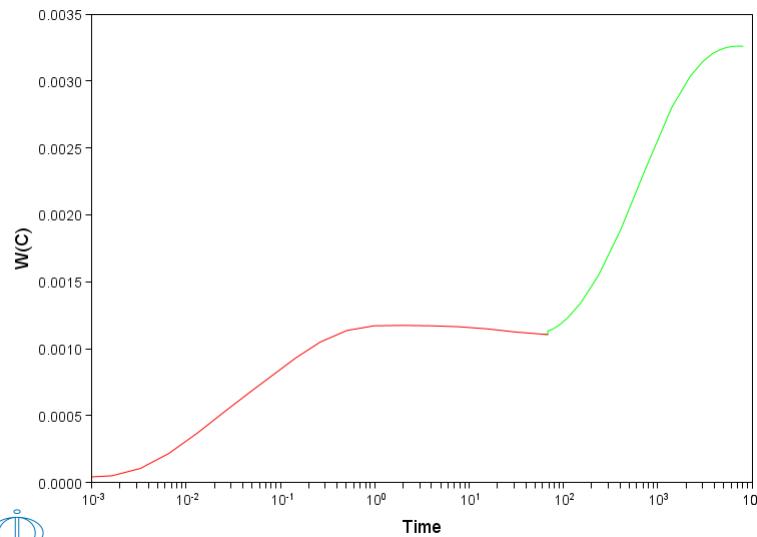
```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exb3\plot.DCM.test"
DIC>
DIC>
DIC> @@ exb3_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE b3
DIC> @@
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA MODULE AND SPECIFY THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 8.00000E+03
DIC> read exb3
OK
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA POST PROCESSOR
DIC> @@
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1: @@
POST-1: @@ LET US SEE HOW THE AMOUNT OF FERRITE VARIED DURING THE
POST-1: @@ SIMULATION
POST-1: @@
POST-1: s-d-a y iww(bcc)
POST-1: s-d-a x time
INFO: Time is set as independent variable
POST-1: s-ax-typ x log
POST-1: s-s-s x n 1E-5 1E3
POST-1: s-s-s y n 0 0.1
POST-1:
POST-1: set-tit Figure b3.1
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
ORKING ...
OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

Figure b3.1



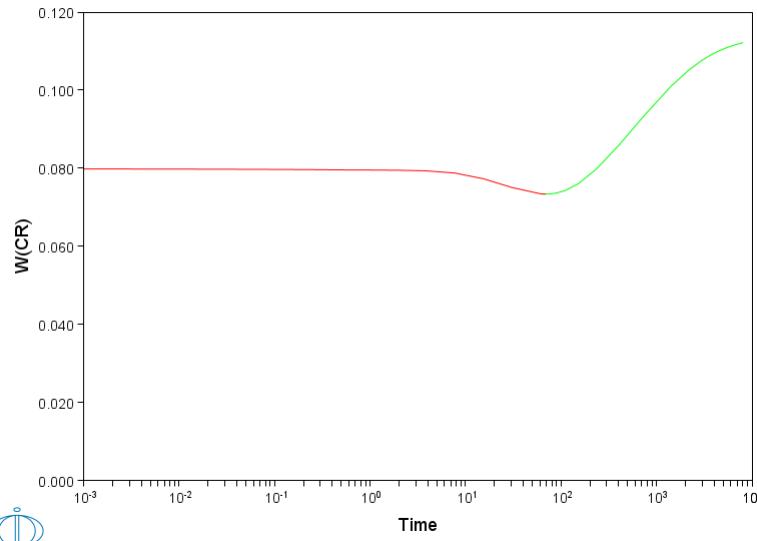
```
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: @@
POST-1: @@ NOW LOOK AT THE ALLOYING ELEMENTS AT THE UPPER BOUND OF THE SYSTEM
POST-1: @@
POST-1: s-d-a y w(c)
POST-1: s-s-s x n 1E-3 1E4
POST-1: s-p-c interface last
POST-1:
POST-1: set-tit Figure b3.2
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
ORKING ...
OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

**Figure b3.2**



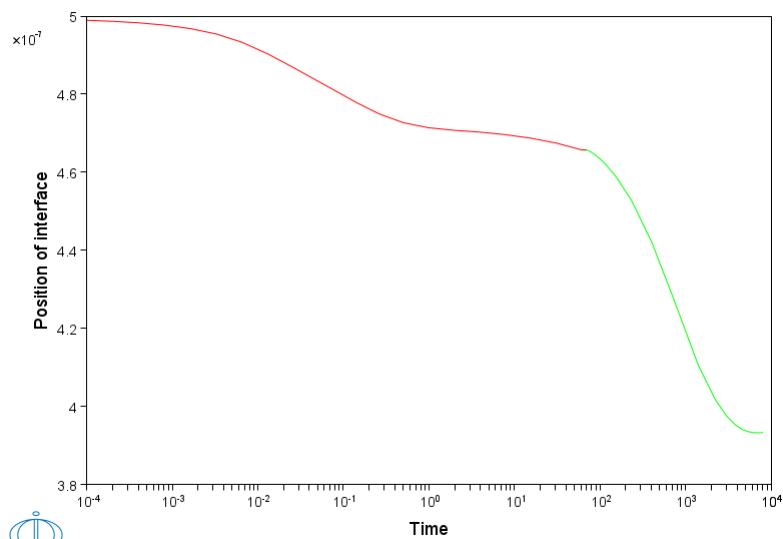
POST-1:  
POST-1:  
POST-1:@?<\_hit\_return\_to\_continue\_>  
POST-1:  
POST-1: s-d-a y w(cr)  
POST-1: s-s-s y n 0 0.12  
POST-1:  
POST-1: set-tit Figure b3.3  
POST-1:  
POST-1:  
POST-1: SET\_EXP\_FILE\_FORMAT 5  
POST-1: MAKE c:\jenkins\workspace\generate\_dictra\_console\_examples\unite\distribution\macroResult.exp Y  
ORKING ... OST-1: SET\_EXP\_FILE\_FORMAT 10  
POST-1:  
POST-1: plot

**Figure b3.3**



POST-1:  
POST-1:  
POST-1:@?<\_hit\_return\_to\_continue\_>  
POST-1:  
POST-1: @@  
POST-1: @@ AND FINALLY LOOK AT THE CHANGE OF RADIUS OF THE M23-CARBIDE  
POST-1: @@  
POST-1: s-d-a y position carbide upper  
POST-1: s-s-s x n 1E-4 1E4  
POST-1:  
POST-1: set-tit Figure b3.4  
POST-1:  
POST-1:  
POST-1: SET\_EXP\_FILE\_FORMAT 5  
POST-1: MAKE c:\jenkins\workspace\generate\_dictra\_console\_examples\unite\distribution\macroResult.exp Y  
ORKING ... OST-1: SET\_EXP\_FILE\_FORMAT 10  
POST-1:  
POST-1: plot

**Figure b3.4**



POST-1:  
POST-1:  
POST-1:@?<\_hit\_return\_to\_continue\_>  
POST-1:  
POST-1:  
POST-1: set-inter  
---OK---  
POST-1:



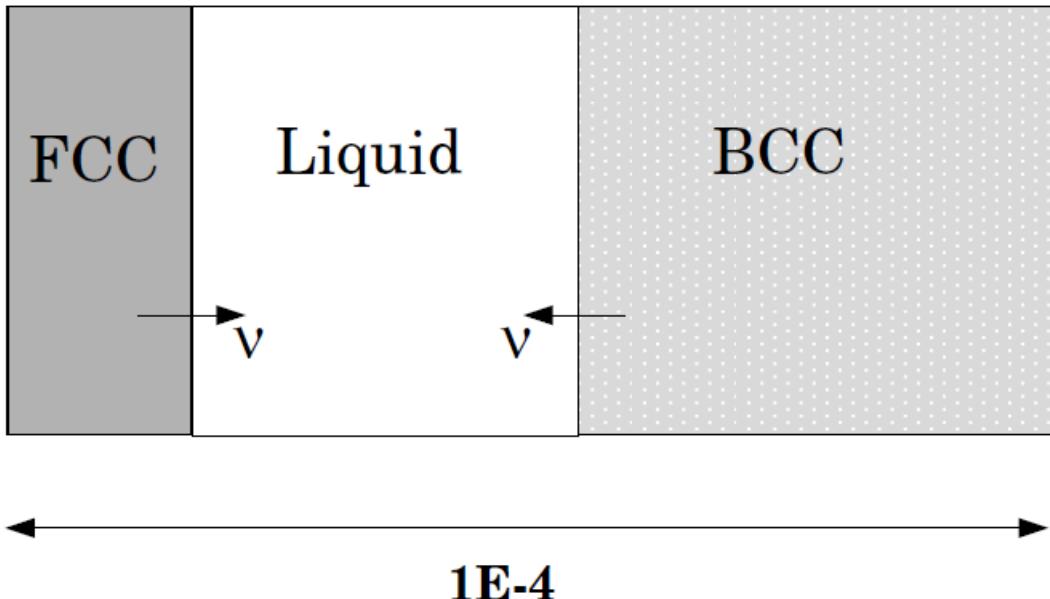
## Example exb4a

### Solidification path of a Fe-18%Cr-8%Ni alloy: Eutectic reaction

This example demonstrates the solidification path of an Fe-18%Cr-8%Ni alloy. A eutectic reaction is assumed, LIQUID  $\rightarrow$  BCC + FCC. Hence the BCC and FCC regions should be on separate sides of the liquid region. Comparison is made with both a Scheil-Gulliver simulation and equilibrium solidification conditions, both made with Thermo-Calc.

$$Time > 0$$

$$T = 1900 - 1 * \text{Time} \text{ K}$$



**exb4a-setup****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_dictra_console_examples\examples\exb4a\setup.DCM.test"
SYS: @@
SYS: @@ Moving boundary problem.
SYS: @@ Solidification path of an Fe-18%Cr-8%Ni alloy: Eutectic reaction
SYS: @@ This example demonstrates the solidification path of an Fe-18%Cr-8%Ni
SYS: @@ alloy. A eutectic reaction is assumed, LIQUID -> BCC + FCC. Hence the
SYS: @@ BCC and FCC regions should be on separate sides of the liquid region.
SYS: @@ Comparison is made with both a Scheil-Gulliver simulation and equilibrium
SYS: @@ solidification conditions, both done in Thermo-Calc.
SYS: -----
NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exb4a_setup.DCM
SYS:
SYS:
SYS: @@
SYS: @@ START BY GOING TO THE DATABASE MODULE
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\generate_dictra_console_examples\databases\data
Current database: Steels/Fe-Alloys v12.0

VA           /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE12:
TDB_TCFE12: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA
TDB_TCFE12: sw tcfef9
Current database: Steels/Fe-Alloys v9.3

VA           /- DEFINED
L12_FCC      B2_BCC          DICTRA_FCC_A1
REJECTED
TDB_TCFE9:
TDB_TCFE9: @@ DEFINE THE SYSTEM TO WORK WITH
TDB_TCFE9: def-sys fe ni cr
FE           NI             CR
DEFINED
TDB_TCFE9:
TDB_TCFE9: @@ EXCLUDE THE THERMODYNAMIC DATA FOR THE PHASES THAT ARE NOT NEEDED
TDB_TCFE9: rej ph /all
LIQUID:L     BCC_A2          FCC_A1
HCP_A3       CBCC_A12        CUB_A13
SIGMA        CHI_A12         LAVES_PHASE_C14
CR3SI        NBNI3          NI3TI
CRZN17       BETA1           GAMMA
AL5FE4       FLUORITE_C1:I  ZRO2_TETR:I
M203C:I     CEN12          CEN15
REJECTED
TDB_TCFE9: res ph fcc liq bcc
FCC A1       LIQUID:L        BCC_A2
RESTORED
TDB_TCFE9:
TDB_TCFE9: @@ RETRIEVE DATA FROM THE DATABASE FILE
TDB_TCFE9: get
15:48:43,359 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS .....
FUNCTIONS .....

List of references for assessed data

'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
'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'
'J. Brillo and I. Egry, Int. J. Thermophysics, 24, 1155-1170'
'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'
'B.-J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
'A. Dinsdale and T. Chart, MTDS NPL, Unpublished work (1986); CR-NI'
'A. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); FE-NI'
-OK-
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ MOBILITY/DIFFUSIVITY DATA ARE STORED IN A SEPARATE DATABASE FILE.
TDB_TCFE9: @@ SWITCH TO A MOBILITY DATABASE AND APPEND THE DATA
TDB_TCFE9: @@
TDB_TCFE9: app
Use one of these databases

TCFE12 = Steels/Fe-Alloys v12.0
TCFE9 = Steels/Fe-Alloys v9.3
SSUB6 = SGTE Substances v6.0
FEDEMO = Iron Demo Database v4.0
MOB2 = Alloys Mobility v2.7
MOBFE2 = Steels/Fe-Alloys Mobility v2.0
MOBFE4 = Steels/Fe-Alloys Mobility v4.0
MOBFE7 = Steels/Fe-Alloys Mobility v7.1
MFEDEMO = Fe-Alloys Mobility demo database v2.0
USER = User defined Database
```

```

DATABASE NAME /TCFE9/: mobfe4
Current database: Steels/Fe-Alloys Mobility v4.0

VA DEFINED
B2_BCC REJECTED
APP: def-sys fe ni cr
    FE           NI          CR
    DEFINED
APP: rej ph /all
    BCC_A2      FCC_A1      HCP_A3
    LIQUID:L   REJECTED
APP: res ph fcc liq bcc
    FCC_A1      LIQUID:L   BCC_A2
    RESTORED
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS .....

List of references for assessed data

'This parameter has not been assessed'
'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Fe diffusion fcc Cr-Fe'
'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Ni diffusion fcc Cr-Ni'
'B. Jonsson: Z. Metallkunde 86(1995)686-692; Cr, Fe and Ni diffusion fcc
    Cr-Fe-Ni'
'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
    -Ni'
'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Ni self-diffusion'
'B. Jonsson: ISIJ International, 35(1995)1415-1421; Cr, Fe and Ni
    diffusion bcc Cr-Fe-Ni'
'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
    in bcc Fe'
'No assessed or estimated parameters'
'Estimation by using the modified Sutherland equation from Chen et al.,
    Phil. Magazine 94 (2014) 1552.'
'L. Zhang et al., Acta Mater., 58(2010)3664.'

-OK-
APP: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP
APP: @@
APP: go d-m
NO TIME STEP DEFINED
DIC> @@
DIC> @@ ENTER GLOBAL CONDITION T
DIC> @@
DIC> @@ LOWER THE TEMPERATURE TO A RATE OF 1 K/s
DIC> @@
DIC> set-cond glob T 0 1900-1*TIME; * N
DIC>
DIC> @@
DIC> @@ ENTER A REGION CALLED smalta
DIC> @@
DIC> enter-region smalta
DIC>
DIC> @@
DIC> @@ ENTER A DOUBLE GEOMETRIC GRID INTO THE REGION
DIC> @@
DIC> enter-grid
REGION NAME : /SMALTA/: smalta
WIDTH OF REGION /1/: 1e-4
TYPE /LINEAR/: AUTO
DIC>
DIC>
DIC> @@
DIC> @@ ENTER active PHASES INTO THE REGION
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /SMALTA/: smalta
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: liq
DIC>
DIC> @@
DIC> @@ ENTER inactive PHASES INTO THE REGION: ONE PHASE ON EACH SIDE OF THE LIQUID
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inact
ATTACH TO REGION NAMED /SMALTA/: smalta
ATTACHED TO THE RIGHT OF SMALTA /YES/: no
PHASE NAME: /NONE/: fcc#1
DEPENDENT COMPONENT ? /NI/: fe
REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-5
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inact
ATTACH TO REGION NAMED /SMALTA/: smalta
ATTACHED TO THE RIGHT OF SMALTA /YES/: yes
PHASE NAME: /NONE/: bcc#1
DEPENDENT COMPONENT ? /NI/: fe
REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-5
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> @@
DIC> @@ ENTER A START COMPOSITION FOR THE LIQUID
DIC> @@
DIC> enter-composition
REGION NAME : /SMALTA/: smalta
PHASE NAME: /LIQUID/: liq
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /CR/: cr lin 18 18
PROFILE FOR /NI/: ni lin 8 8
DIC>
DIC> @@
DIC> @@ THE BOUNDARY CONDITION IS A CLOSED SYSTEM (THE DEFAULT) AS WE DO NOT SPECIFY

```

```
DIC> @@ ANYTHING ELSE.
DIC> @@
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 200
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /20/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC> @@
DIC> @@ CHECK THE INTERFACE POSITION. THIS IS TO MAKE SURE THAT THE
DIC> @@ LIQUID REGION DOES NOT SHRINK TOO MUCH DURING A TIMESTEP.
DIC> @@ IN ADDITION THE TIMESTEP IS CONTROLLED BY THE PHASE INTERFACE
DIC> @@ DISPLACEMENT DURING THE SIMULATION.
DIC> @@
DIC> s-s-c
NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /AUTO/: AUTO
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -> 1): /AUTO/:
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/:
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exb4a Y
DIC>
DIC> set-inter
--OK--
DIC>
```

**exb4a-run**

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exb4a\run.DCM.test"
DIC>
DIC>
DIC> @@ exb4a_run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING EXAMPLE b4a
DIC> @@
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA MONITOR AND READ THE SET UP FROM FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 0.00000E+00
DIC> read exb4a
OK
DIC>
DIC> @@
DIC> @@ START THE SIMULATION
DIC> @@
DIC> sim yes
Region: SMALTA
double geometric
dense at outer boundaries, coarse at 0.50000E-04
lower part 1.2275 22
upper part 0.81465 22
DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
INFO: TIMESTEP IS CONTROLLED BY INTERFACE POSITION
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882254
TOTAL SIZE OF SYSTEM: 1E-04 [m]
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882254
TOTAL SIZE OF SYSTEM: 1E-04 [m]
TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291
NI = .0754116207882254
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 1 seconds
TIME = 0.26028659E-05 DT = 0.25028659E-05 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291
NI = .0754116207882254
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 1 seconds
TIME = 0.76085978E-05 DT = 0.50057319E-05 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882254
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 1 seconds
TIME = 0.17620062E-04 DT = 0.10011464E-04 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882254
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.37642989E-04 DT = 0.20022928E-04 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291
NI = .0754116207882254
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.77688844E-04 DT = 0.40045855E-04 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291
NI = .0754116207882255
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.15778055E-03 DT = 0.80091710E-04 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291
NI = .0754116207882255
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.31796397E-03 DT = 0.16018342E-03 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882255
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.63833082E-03 DT = 0.32036684E-03 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291
NI = .0754116207882255
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.12790645E-02 DT = 0.64073368E-03 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882255
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.25605319E-02 DT = 0.12814674E-02 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291
NI = .0754116207882255
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 1 seconds
TIME = 0.51234666E-02 DT = 0.25629347E-02 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291
NI = .0754116207882255
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.10249336E-01 DT = 0.51258694E-02 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882255
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.20501075E-01 DT = 0.10251739E-01 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882255
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.41004553E-01 DT = 0.20503478E-01 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291
NI = .0754116207882255
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.82011508E-01 DT = 0.41006956E-01 SUM OF SQUARES = 0.0000000
```

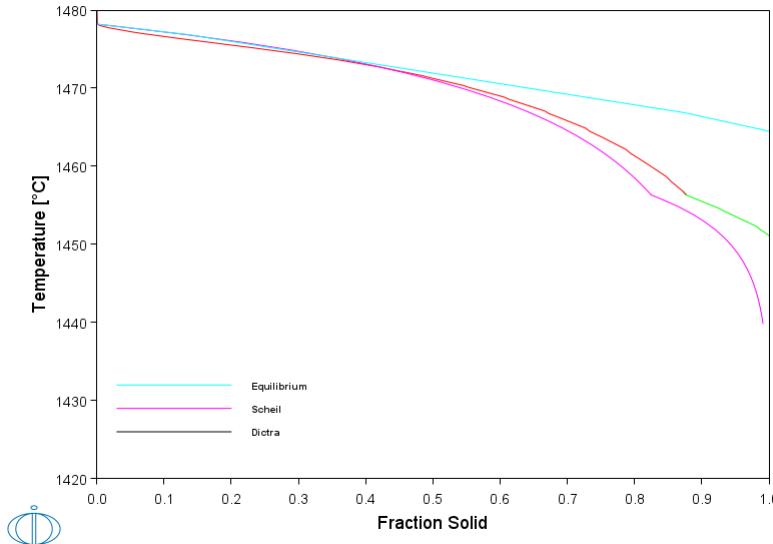


```
DIC> @@  
DIC>  
DIC> set-inter  
--OK---  
DIC>
```

**exb4a-plot**

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exb4a\plot.DCM.test"
DIC>
DIC>
DIC> @@ exb4a_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE b4a
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 2.00000E+02
DIC> read exb4a
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1: set-title Fe-18%Cr-8%Ni
POST-1:
POST-1: @@
POST-1: @@ PLOT THE FRACTION OF SOLID AND COMPARE WITH A SCHEIL-GULLIVER SIMULATION
POST-1: @@ AND EQUILIBRIUM SOLIDIFICATION (DATA ON FILE exb4.exp)
POST-1: @@
POST-1: enter function fs=1-ivv(liquid);
POST-1: s-d-a x fs
POST-1: s-s-s x n 0 1
POST-1: set-axis-text
AXIS (X, Y OR Z) : x
AUTOMATIC AXIS TEXT (Y OR N) /N/: n
AXIS TEXT : Fraction Solid
POST-1:
POST-1: s-d-a y t-c
POST-1: s-s-s y n 1420 1480
POST-1:
POST-1: s-p-c interface smalta lower
POST-1:
POST-1: app y exb4a.exp 0; 1
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
ORKING ...orking ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

Fe-18%Cr-8%Ni



```
POST-1:
POST-1:
POST-1: set-inter
--OK---
POST-1:
```



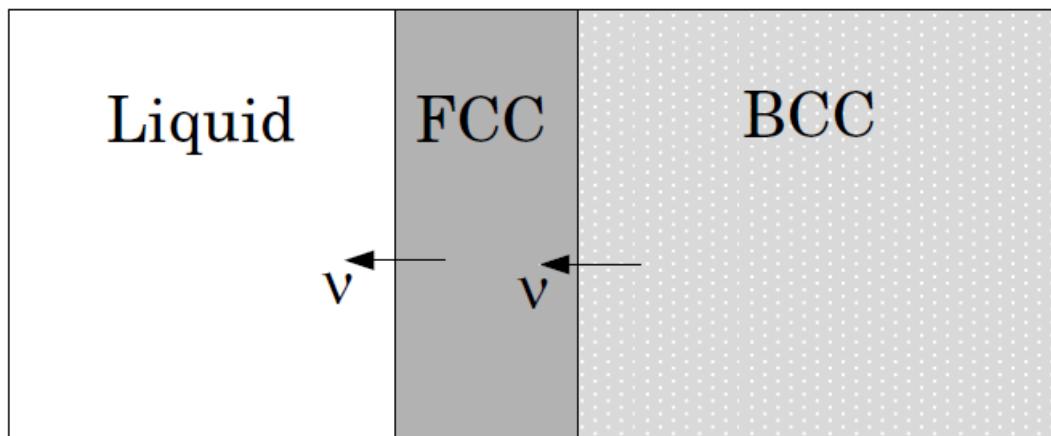
## Example exb4b

### Solidification path of an Fe-18%Cr-8%Ni alloy: Peritectic reaction

This example is the same as exb4a but now a peritectic reaction is assumed, LIQUID + BCC  $\rightarrow$  FCC. Hence the FCC region should appear in between the LIQUID and the BCC. Comparison is made with both a Scheil-Gulliver simulation and equilibrium solidification conditions, both made with Thermo-Calc.

*Time > 0*

$$T = 1900 - 1 * \text{Time} \text{ K}$$



← →  
**1E-4**

**exb4b-setup****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_dictra_console_examples\examples\exb4b\setup.DCM.test"
SYS: @@
SYS: @@ Moving boundary problem.
SYS: @@ Solidification path of an Fe-18%Cr-8%Ni alloy: Peritectic reaction
SYS: @@ This example is the same as exb4 but now a peritectic reaction is assumed:
SYS: @@ LIQUID + BCC -> FCC. Hence the FCC region should appear in between the LIQUID
SYS: @@ and the BCC. Comparison is made with both a Scheil-Gulliver simulation and
SYS: @@ equilibrium solidification conditions, both done in Thermo-Calc.
SYS: -----
NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exb4b_setup.DCM
SYS:
SYS:
SYS: @@
SYS: @@ START BY GOING TO THE DATABASE MODULE
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\generate_dictra_console_examples\databases\data
Current database: Steels/Fe-Alloys v12.0

VA           /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE12:
TDB_TCFE12: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA
TDB_TCFE12: sw fedemo
Current database: Iron Demo Database v4.0

VA           /- DEFINED
TDB_FEDEMO:
TDB_FEDEMO: @@ DEFINE THE SYSTEM TO WORK WITH
TDB_FEDEMO: def-sys fe ni cr
FE          NI          CR
DEFINED
TDB_FEDEMO:
TDB_FEDEMO: @@ EXCLUDE THE THERMODYNAMIC DATA FOR THE PHASES THAT ARE NOT NEEDED
TDB_FEDEMO: rej ph /all
LIQUID:L      BCC_A2      LAVES_PHASE_C14
CBCC_A12     CHI_A12     CUB_A13
FCC_A1       HCP_A3      SIGMA
REJECTED
TDB_FEDEMO: res ph fcc liq bcc
FCC_A1       LIQUID:L    BCC_A2
RESTORED
TDB_FEDEMO:
TDB_FEDEMO: @@ RETRIEVE DATA FROM THE DATABASE FILE
TDB_FEDEMO: get
15:55:04,124 [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'
-OK-
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ MOBILITY/DIFFUSIVITY DATA ARE STORED IN A SEPARATE DATABASE FILE.
TDB_FEDEMO: @@ SWITCH TO A MOBILITY DATABASE AND APPEND THE DATA.
TDB_FEDEMO: @@
TDB_FEDEMO: app
Use one of these databases
TCFE12 = Steels/Fe-Alloys v12.0
TCFE9 = Steels/Fe-Alloys v9.3
SSUB6 = SGTE Substances v6.0
FEDEMO = Iron Demo Database v4.0
MOB2 = Alloys Mobility v2.7
MOBFE2 = Steels/Fe-Alloys Mobility v2.0
MOBFE4 = Steels/Fe-Alloys Mobility v4.0
MOBFE7 = Steels/Fe-Alloys Mobility v7.1
MFEDEMO = Fe-Alloys Mobility demo database v2.0
USER = User defined Database
```

```

DATABASE NAME /FEDEMO/: mobfe4
Current database: Steels/Fe-Alloys Mobility v4.0

VA DEFINED
B2_BCC REJECTED
APP: def-sys fe ni cr
    FE           NI          CR
    DEFINED
APP: rej ph /all
    FCC_A2      FCC_A1      HCP_A3
    LIQUID:L REJECTED
APP: res ph fcc liq bcc
    FCC_A1      LIQUID:L   BCC_A2
    RESTORED
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS .....

List of references for assessed data

'This parameter has not been assessed'
'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Fe diffusion fcc Cr-Fe'
'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Ni diffusion fcc Cr-Ni'
'B. Jonsson: Z. Metallkunde 86(1995)686-692; Cr, Fe and Ni diffusion fcc
    Cr-Fe-Ni'
'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
    -Ni'
'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Ni self-diffusion'
'B. Jonsson: ISIJ International, 35(1995)1415-1421; Cr, Fe and Ni
    diffusion bcc Cr-Fe-Ni'
'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
    in bcc Fe'
'No assessed or estimated parameters'
'Estimation by using the modified Sutherland equation from Chen et al.,
    Phil. Magazine 94 (2014) 1552.'
'L. Zhang et al., Acta Mater., 58(2010)3664.'

-OK-
APP: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP
APP: @@
APP: go d-m
NO TIME STEP DEFINED
DIC> @@
DIC> @@ ENTER GLOBAL CONDITION T
DIC> @@
DIC> @@ LOWER THE TEMPERATURE TO A RATE OF 1 K/s
DIC> @@
DIC> set-cond glob T 0 1900-1*TIME; * N
DIC>
DIC> @@
DIC> @@ ENTER A REGION CALLED smalta
DIC> @@
DIC> enter-region smalta
DIC>
DIC> @@
DIC> @@ ENTER A GEOMETRIC GRID INTO THE REGION
DIC> @@
DIC> enter-grid
REGION NAME : /SMALTA/: smalta
WIDTH OF REGION /1/: 1e-4
TYPE /LINEAR/: AUTO
DIC>
DIC> @@
DIC> @@ ENTER active PHASES INTO THE REGION
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /SMALTA/: smalta
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: liq
DIC>
DIC> @@
DIC> @@ ENTER inactive PHASES INTO THE REGION, WITH BOTH PHASES ON THE SAME
DIC> @@ SIDE OF THE LIQUID REGION IN ORDER TO GET A PERITECTIC REACTION.
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inact
ATTACH TO REGION NAMED /SMALTA/: smalta
ATTACHED TO THE RIGHT OF SMALTA /YES/: yes
PHASE NAME: /NONE/: fcc#1
DEPENDENT COMPONENT ? /NI/: fe
REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-5
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inact
ATTACH TO REGION NAMED /SMALTA/: smalta
ATTACHED TO THE RIGHT OF SMALTA /YES/: yes
PHASE NAME: /NONE/: bcc#1
DEPENDENT COMPONENT ? /NI/: fe
REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-5
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> @@
DIC> @@ ENTER THE START COMPOSITION FOR THE LIQUID
DIC> @@
DIC> enter-composition
REGION NAME : /SMALTA/: smalta
PHASE NAME: /LIQUID/: liq
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /CR/: cr lin 18 18
PROFILE FOR /NI/: ni lin 8 8
DIC>
DIC> @@
DIC> @@ THE BOUNDARY CONDITION IS A CLOSED SYSTEM (DEFAULT) AS WE DO NOT SPECIFY

```

```
DIC> @@ ANYTHING ELSE.
DIC> @@
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 200
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /20/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC> @@
DIC> @@ CHECK THE INTERFACE POSITION. THIS IS TO MAKE SURE THAT THE LIQUID REGION
DIC> @@ DOES NOT SHRINK TOO MUCH DURING A TIMESTEP. IN ADDITION, THE TIMESTEP IS
DIC> @@ CONTROLLED BY THE PHASE INTERFACE DISPLACEMENT DURING THE SIMULATION.
DIC> @@
DIC> s-s-c
NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /AUTO/: yes
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -> 1): /AUTO/:
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/: @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exb4b Y
DIC>
DIC> set-inter
--OK---
DIC>
```

**exb4b-run**

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exb4b\run.DCM.test"
DIC>
DIC> @@ exb4b_run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING EXAMPLE b4b
DIC> @@
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA MONITOR AND READ THE SET UP FROM FILE
DIC> @@
DIC>
DIC> go d-m
TIME STEP AT TIME 0.00000E+00
DIC> read exb4b
OK
DIC>
DIC> @@
DIC> @@ START THE SIMULATION
DIC> @@
DIC> sim yes
Region: SMALTA
single geometric dense at 0.10000E-03
0.93810          83
DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882254
TOTAL SIZE OF SYSTEM: 1E-04 [m]
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882254
TOTAL SIZE OF SYSTEM: 1E-04 [m]
TIME = 0.1000000E-06 DT = 0.1000000E-06 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882254
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep           2 seconds
TIME = 0.27420944E-05 DT = 0.26420944E-05 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291
NI = .0754116207882254
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep           0 seconds
TIME = 0.80262833E-05 DT = 0.52841888E-05 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882254
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep           0 seconds
TIME = 0.18594661E-04 DT = 0.10568378E-04 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882254
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep           0 seconds
TIME = 0.39731416E-04 DT = 0.21136755E-04 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882254
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep           0 seconds
TIME = 0.82004927E-04 DT = 0.42273511E-04 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882254
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep           0 seconds
TIME = 0.16655195E-03 DT = 0.845457022E-04 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882254
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep           0 seconds
TIME = 0.33564599E-03 DT = 0.16909404E-03 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882254
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep           0 seconds
TIME = 0.67383408E-03 DT = 0.33818809E-03 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291
NI = .0754116207882254
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep           0 seconds
TIME = 0.13502102E-02 DT = 0.67637617E-03 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882254
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep           1 seconds
TIME = 0.27029626E-02 DT = 0.13527523E-02 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291
NI = .0754116207882254
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep           0 seconds
TIME = 0.54084673E-02 DT = 0.27055047E-02 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291
NI = .0754116207882254
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep           0 seconds
TIME = 0.10819477E-01 DT = 0.54110094E-02 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291
NI = .0754116207882255
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep           0 seconds
TIME = 0.21641495E-01 DT = 0.10822019E-01 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882253
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep           0 seconds
TIME = 0.43285533E-01 DT = 0.21644038E-01 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291
NI = .0754116207882252
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep           0 seconds
TIME = 0.86573608E-01 DT = 0.43288075E-01 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291
NI = .0754116207882254
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep           0 seconds
```

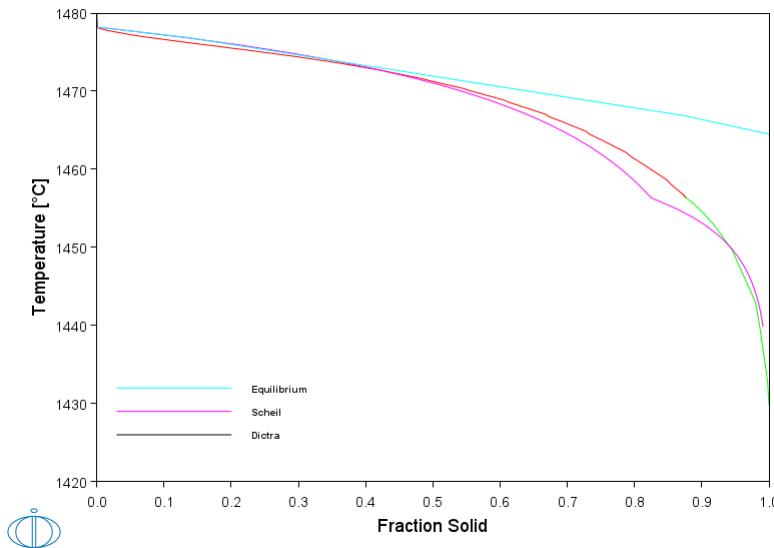




## exb4b-plot

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exb4b\plot.DCM.test"
DIC>
DIC>
DIC> @@ exb4b_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE b4b
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 2.00000E+02
DIC> read exb4b
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1: set-title Fe-18%Cr-8%Ni
POST-1:
POST-1: @@
POST-1: @@ PLOT THE FRACTION OF SOLID AND COMPARE WITH A SCHEIL-GULLIVER
POST-1: @@ SIMULATION AND EQUILIBRIUM SOLIDIFICATION (DATA ON FILE exb4.exp)
POST-1: @@
POST-1: enter func fs=1-ivv(liquid);
POST-1: s-d-a x fs
POST-1: s-s-s x n 0 1
POST-1: s-ax-te x n Fraction Solid
POST-1:
POST-1: s-d-a y t-c
POST-1: s-s-s y n 1420 1480
POST-1:
POST-1: s-p-c interf smalta lower
POST-1:
POST-1: app y exb4b.exp 0; 1
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
ORKING ...orking ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

Fe-18%Cr-8%Ni



```
POST-1:
POST-1:
POST-1:
POST-1: set-inter
--OK---
POST-1:
```



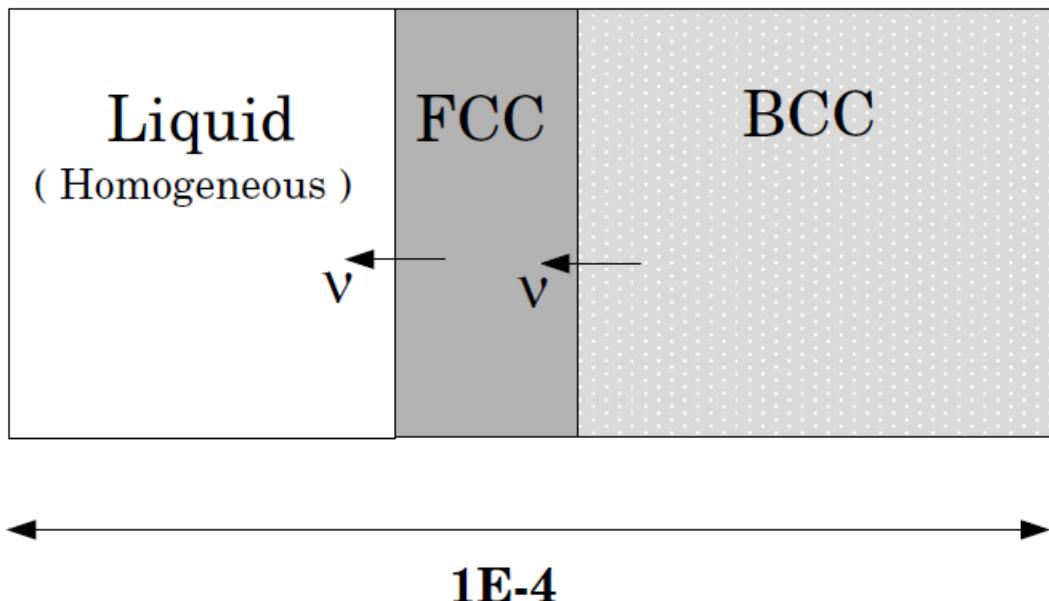
## Example exb4c

### Solidification path of an Fe-18%Cr-8%Ni alloy: Peritectic reaction, homogeneous liquid

This example is the same as exb4b but now the diffusivity data is amended for the LIQUID and a very high value for the diffusivity is used in order to simulate a case where we assume that the composition in the LIQUID is always homogeneous. This case should be considered less realistic than exb4b. Comparison is made with both a Scheil-Gulliver simulation and equilibrium solidification conditions, both made with Thermo-Calc.

*Time > 0*

$$T = 1900 - 1 * \text{Time} \text{ K}$$



**exb4c-setup****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_dictra_console_examples\examples\exb4c\setup.DCM.test"
SYS: @@
SYS: @@ Moving boundary problem.
SYS: @@ Solidification path of an Fe-18%Cr-8%Ni alloy
SYS: @@ This example is the same as exb4b but now the diffusivity data is amended
SYS: @@ for the LIQUID and a high value for the diffusivity is used to simulate a
SYS: @@ case where it is assumed that the composition in the LIQUID is always
SYS: @@ homogeneous. This example is less realistic than exb4b.
SYS: @@ Comparison is made with both a Scheil-Gulliver simulation and equilibrium
SYS: @@ solidification conditions, both done in Thermo-Calc.
SYS: -----
NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exb4c_setup.DCM
SYS:
SYS: @@
SYS: @@ START BY GOING TO THE DATABASE MODULE
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\generate_dictra_console_examples\databases\data
Current database: Steels/Fe-Alloys v12.0

VA           /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE12:
TDB_TCFE12: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA
TDB_TCFE12: sw tcfef9
Current database: Steels/Fe-Alloys v9.3

VA           /- DEFINED
L12_FCC      B2_BCC          DICTRA_FCC_A1
REJECTED
TDB_TCFE9:
TDB_TCFE9: @@ DEFINE THE SYSTEM TO WORK WITH
TDB_TCFE9: def-sys fe ni cr
FE           NI             CR
DEFINED
TDB_TCFE9:
TDB_TCFE9: @@ EXCLUDE THE THERMODYNAMIC DATA FOR THE PHASES THAT ARE NOT NEEDED
TDB_TCFE9: rej ph /all
LIQUID:L      BCC_A2          FCC_A1
HCP_A3        CBCC_A12         CUB_A13
SIGMA         CHI_A12         LAVES_PHASE_C14
CR3SI         NBNI3           NI3TI
CRZN17        BETA1           GAMMA
AL5FE4        FLUORITE_C1:I  ZRO2_TETR:I
M203C:I       CEN12           CEN15
REJECTED
TDB_TCFE9: res ph fcc liq bcc
FCC A1        LIQUID:L        BCC_A2
RESTORED
TDB_TCFE9:
TDB_TCFE9: @@ RETRIEVE DATA FROM THE DATABASE FILE
TDB_TCFE9: get
16:02:14,113 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS .....
FUNCTIONS .....

List of references for assessed data

'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
'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'
'J. Brillo and I. Egry, Int. J. Thermophysics, 24, 1155-1170'
'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'
'B.-J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
'A. Dinsdale and T. Chart, MTDS NPL, Unpublished work (1986); CR-NI'
'A. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); FE-NI'
-OK-
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ MOBILITY/DIFFUSIVITY DATA ARE STORED IN A SEPARATE DATABASE FILE.
TDB_TCFE9: @@ SWITCH TO A MOBILITY DATABASE AND APPEND THE DATA.
TDB_TCFE9: @@
TDB_TCFE9: app
Use one of these databases

TCFE12 = Steels/Fe-Alloys v12.0
TCFE9 = Steels/Fe-Alloys v9.3
SSUB6 = SGTE Substances v6.0
FEDEMO = Iron Demo Database v4.0
MOB2 = Alloys Mobility v2.7
MOBFE2 = Steels/Fe-Alloys Mobility v2.0
MOBFE4 = Steels/Fe-Alloys Mobility v4.0
MOBFE7 = Steels/Fe-Alloys Mobility v7.1
MFEDEMO = Fe-Alloys Mobility demo database v2.0
USER = User defined Database
```

```

DATABASE NAME /TCFE9/: mobfe4
Current database: Steels/Fe-Alloys Mobility v4.0

VA DEFINED
B2_BCC REJECTED
APP: def-sys fe ni cr
    FE           NI          CR
    DEFINED
APP: rej ph /all
    FCC_A2      FCC_A1      HCP_A3
    LIQUID:L   REJECTED
APP: res ph fcc liq bcc
    FCC_A1      LIQUID:L   BCC_A2
    RESTORED
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ...

List of references for assessed data

'This parameter has not been assessed'
'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Fe diffusion fcc Cr-Fe'
'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Ni diffusion fcc Cr-Ni'
'B. Jonsson: Z. Metallkunde 86(1995)686-692; Cr, Fe and Ni diffusion fcc
Cr-Fe-Ni'
'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
-Ni'
'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Ni self-diffusion'
'B. Jonsson: ISIJ International, 35(1995)1415-1421; Cr, Fe and Ni
diffusion bcc Cr-Fe-Ni'
'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
in bcc Fe'
'No assessed or estimated parameters'
'Estimation by using the modified Sutherland equation from Chen et al.,
Phil. Magazine 94 (2014) 1552.'
'L. Zhang et al., Acta Mater., 58(2010)3664.'

-OK-
APP: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP
APP: @@
APP: go d-m
NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ LIST THE MOBILITIES IN THE LIQUID
DIC> @@
DIC> list-mobility-data
Sorry, LIST-DATA disabled for this database
DIC>
DIC>
DIC> liquid
NO SUCH COMMAND, USE HELP
DIC>
DIC>
DIC> @@
DIC> @@ AMEND THE DIFFUSIVITY DATA IN THE LIQUID
DIC> @@
DIC> @@ CHANGE TO A DIFFUSIVITY THAT IS 1000 TIMES HIGHER THAN THE
DIC> @@ VALUE IN THE MOBILITY DATABASE. THIS SHOULD BE ENOUGH IN ORDER TO
DIC> @@ ASSUME THAT THE COMPOSITION IN THE LIQUID IS AT ALL TIMES HOMOGENEOUS.
DIC> @@
DIC> amend_mobility_data
PARAMETER:
*** ERROR, PLEASE RE-ENTER EACH PART SEPARATELY
IDENTIFIER: dq
PHASE NAME: liquid&cr
CONSTITUENT: cr
INTERACTING CONSTITUENT:
DQ(LIQUID&CR#1,CR;0) = Sorry, database encrypted
Do you want to change the number of ranges /NO/: yes
Reenter ranges
DQ(LIQUID&CR#1,CR;0) =
LOW TEMPERATURE LIMIT /298.15/: 298.15
FUNCTION: +R*T*LN(1E-06);
HIGH TEMPERATURE LIMIT /6000/: 6000
ANY MORE RANGES /N/: no

*** WARNING, NO MAGNETIC CONTRIBUTION DEFINED

DIC>
DIC> amend_mobility_data
PARAMETER: dq(liquid&cr,fe;0)
DQ(LIQUID&CR#1,FE;0) = Sorry, database encrypted
Do you want to change the number of ranges /NO/: y
Reenter ranges
DQ(LIQUID&CR#1,FE;0) =
LOW TEMPERATURE LIMIT /298.15/: 298.15 +R*T*LN(1E-06); 6000 n

*** WARNING, NO MAGNETIC CONTRIBUTION DEFINED

DIC>
DIC> am-mob dq(liquid&cr,ni;0)
DQ(LIQUID&CR#1,NI;0) = Sorry, database encrypted
Do you want to change the number of ranges /NO/: y
Reenter ranges
DQ(LIQUID&CR#1,NI;0) =
LOW TEMPERATURE LIMIT /298.15/: 298.15 +R*T*LN(1E-06); 6000 n

*** WARNING, NO MAGNETIC CONTRIBUTION DEFINED

DIC>
DIC> am-mob dq(liquid&ni,cr;0)
DQ(LIQUID&NI#1,CR;0) = Sorry, database encrypted
Do you want to change the number of ranges /NO/: y
Reenter ranges

```

```

DQ(LIQUID&NI#1,CR;0) =
LOW TEMPERATURE LIMIT /298.15/: 298.15 +R*T*LN(1E-06); 6000 n

*** WARNING, NO MAGNETIC CONTRIBUTION DEFINED

DIC>
DIC> am-mob dq(liquid&ni,fe;0)
DQ(LIQUID&NI#1,FE;0) = Sorry, database encrypted
Do you want to change the number of ranges /NO/: y
Reenter ranges
DQ(LIQUID&NI#1,FE;0) =
LOW TEMPERATURE LIMIT /298.15/: 298.15 +R*T*LN(1E-06); 6000 n

*** WARNING, NO MAGNETIC CONTRIBUTION DEFINED

DIC>
DIC> am-mob dq(liquid&ni,ni;0)
DQ(LIQUID&NI#1,NI;0) = Sorry, database encrypted
Do you want to change the number of ranges /NO/: y
Reenter ranges
DQ(LIQUID&NI#1,NI;0) =
LOW TEMPERATURE LIMIT /298.15/: 298.15 +R*T*LN(1E-06); 6000 n

*** WARNING, NO MAGNETIC CONTRIBUTION DEFINED

DIC>
DIC> am-mob dq(liquid&fe,cr;0)
DQ(LIQUID&FE#1,CR;0) = Sorry, database encrypted
Do you want to change the number of ranges /NO/: y
Reenter ranges
DQ(LIQUID&FE#1,CR;0) =
LOW TEMPERATURE LIMIT /298.15/: 298.15 +R*T*LN(1E-06); 6000 n

*** WARNING, NO MAGNETIC CONTRIBUTION DEFINED

DIC>
DIC> am-mob dq(liquid&fe,fe;0)
DQ(LIQUID&FE#1,FE;0) = Sorry, database encrypted
Do you want to change the number of ranges /NO/: y
Reenter ranges
DQ(LIQUID&FE#1,FE;0) =
LOW TEMPERATURE LIMIT /298.15/: 298.15 +R*T*LN(1E-06); 6000 n

*** WARNING, NO MAGNETIC CONTRIBUTION DEFINED

DIC>
DIC> am-mob dq(liquid&fe,ni;0)
DQ(LIQUID&FE#1,NI;0) = Sorry, database encrypted
Do you want to change the number of ranges /NO/: y
Reenter ranges
DQ(LIQUID&FE#1,NI;0) =
LOW TEMPERATURE LIMIT /298.15/: 298.15 +R*T*LN(1E-06); 6000 n

*** WARNING, NO MAGNETIC CONTRIBUTION DEFINED

DIC>
DIC> li-mob
AMBIGUOUS COMMAND, USE HELP
DIC>
DIC>
DIC> liquid
NO SUCH COMMAND, USE HELP
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> @@ LOWER THE TEMPERATURE TO A RATE OF 1 K/s
DIC> set-cond glob T 0 1900-1*TIME; * N
DIC>
DIC> @@
DIC> @@ ENTER A REGION CALLED smalta
DIC> @@
DIC> enter-region smalta
DIC>
DIC> @@
DIC> @@ ENTER A GEOMETRIC GRID INTO THE REGION
DIC> @@
DIC> enter-grid
REGION NAME : /SMALTA/: smalta
WIDTH OF REGION /1/: 1e-4
TYPE /LINEAR/: AUTO
DIC>
DIC> @@
DIC> @@ ENTER active PHASES INTO THE REGION
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /SMALTA/: smalta
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: liq
DIC>
DIC> @@
DIC> @@ ENTER inactive PHASES INTO THE REGION, BOTH PHASES ON THE SAME SIDE
DIC> @@ OF THE LIQUID REGION IN ORDER TO GET A PERITECTIC REACTION.
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inact
ATTACH TO REGION NAMED /SMALTA/: smalta
ATTACHED TO THE RIGHT OF SMALTA /YES/: yes
PHASE NAME: /NONE/: fcc#1
DEPENDENT COMPONENT ? /NI/: fe
REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-5
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> enter-phase

```

```
ACTIVE OR INACTIVE PHASE /ACTIVE/: inact
ATTACH TO REGION NAMED /SMALTA/: smalta
ATTACHED TO THE RIGHT OF SMALTA /YES/: yes
PHASE NAME: /NONE/: bcc#1
DEPENDENT COMPONENT ? /NI/: fe
REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-5
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> @@
DIC> @@ ENTER THE START COMPOSITION FOR THE LIQUID
DIC> @@
DIC> enter-composition
REGION NAME : /SMALTA/: smalta
PHASE NAME: /LIQUID/: liq
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /CR/: cr lin 18 18
PROFILE FOR /NI/: ni lin 8 8
16:02:17,652 [Thread-0] INFO Database: Preparing system for use: MOBFE4_MODIFIED_168261133643117
16:02:18,552 [Thread-0] INFO Phase: Preparing phase for use: LIQUID
DIC>
DIC> @@
DIC> @@ THE BOUNDARY CONDITION IS A CLOSED SYSTEM (DEFAULT) AS WE DO NOT SPECIFY
DIC> @@ ANYTHING ELSE
DIC> @@
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 200
AUTOMATIC TIMESTEP CONTROL /YES/: yes
MAX TIMESTEP DURING INTEGRATION /20/: 1
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ CHECK THE INTERFACE POSITION. THIS IS TO MAKE SURE THAT THE LIQUID
DIC> @@ REGION DOES NOT SHRINK TOO MUCH DURING A TIMESTEP. IN ADDITION THE TIMESTEP
DIC> @@ IS CONTROLLED BY THE PHASE INTERFACE DISPLACEMENT DURING THE SIMULATION.
DIC> @@
DIC> s-s-c
NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /AUTO/: yes
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPLICITY WHEN INTEGRATING PDES (AUTO, 0 -> 0.5 -> 1): /AUTO/:
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/: @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exb4c Y
DIC>
DIC> set-inter
--OK---
DIC>
```

**exb4c-run**

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exb4c\run.DCM.test"
DIC>
DIC> @@ exb4c_run.DCM
DIC>
DIC> @@
DIC> FILE FOR RUNNING EXAMPLE b4b
DIC> @@
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA MONITOR AND READ THE SET UP FROM FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 0.00000E+00
DIC> read exb4c
OK
DIC>
DIC> @@
DIC> @@ START THE SIMULATION
DIC> @@
DIC> sim yes
Region: SMALTA
single geometric dense at 0.10000E-03
0.99375 62
DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882254
TOTAL SIZE OF SYSTEM: 1E-04 [m]
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882254
TOTAL SIZE OF SYSTEM: 1E-04 [m]
16:03:14,773 [Thread-0] INFO Phase: Preparing phase for use: BCC_A2
16:03:15,447 [Thread-0] INFO Phase: Preparing phase for use: FCC_A1
TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882254
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 5 seconds
TIME = 0.10773101E-05 DT = 0.97731005E-06 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882254
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.30319302E-05 DT = 0.19546201E-05 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882254
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.69411704E-05 DT = 0.39092402E-05 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882254
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.14759651E-04 DT = 0.78184804E-05 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882254
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.30396612E-04 DT = 0.15636961E-04 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882254
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.61670533E-04 DT = 0.31273922E-04 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882254
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.12421838E-03 DT = 0.62547843E-04 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882255
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 1 seconds
TIME = 0.24931406E-03 DT = 0.12509569E-03 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882255
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.49950544E-03 DT = 0.25019137E-03 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882255
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.99988818E-03 DT = 0.50038275E-03 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882255
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.20006537E-02 DT = 0.10007655E-02 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992482 FE = .733068011219293
NI = .0754116207882257
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.40021847E-02 DT = 0.20015310E-02 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992482 FE = .733068011219293
NI = .0754116207882259
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.80052466E-02 DT = 0.40030620E-02 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992478 FE = .733068011219298
NI = .0754116207882241
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.16011371E-01 DT = 0.80061240E-02 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992479 FE = .733068011219296
NI = .0754116207882191
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.32023619E-01 DT = 0.16012248E-01 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992493 FE = .733068011219288
NI = .0754116207882191
```

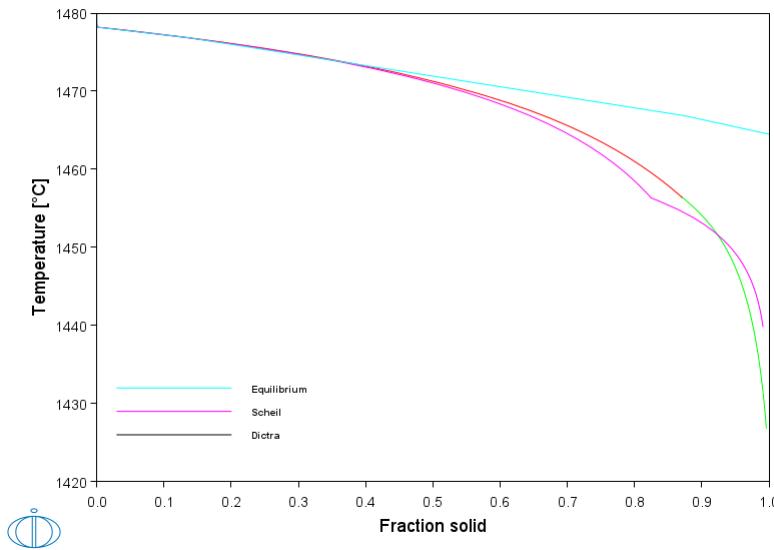


```
DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ THE SIMULATION IS FINISHED
DIC> @@
DIC>
DIC>
DIC> set-inter
--OK---
DIC>
```

## exb4c-plot

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exb4c\plot.DCM.test"
DIC>
DIC>
DIC> @@ exb4c_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE b4c
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 2.00000E+02
DIC> read exb4c
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1: set-title Fe-18%Cr-8%Ni
POST-1:
POST-1: @@
POST-1: @@ PLOT THE FRACTION OF SOLID AND COMPARE WITH A SCHEIL-GULLIVER
POST-1: @@ SIMULATION AND EQUILIBRIUM SOLIDIFICATION (DATA ON FILE exb4.exp).
POST-1: @@ IN THIS CASE WE CAN SEE THAT ALL THREE LINES INITIALLY FALL
POST-1: @@ ON THE SAME LINE.
POST-1: @@
POST-1: enter func fs=1-ivv(liquid);
POST-1: s-d-a x fs
POST-1: s-s-s x n 0 1
POST-1: s-ax-te x n Fraction solid
POST-1:
POST-1: s-d-a y t-c
POST-1: s-s-s y n 1420 1480
POST-1:
POST-1: s-p-c interf smalta lower
POST-1:
POST-1: app y exb4c.exp 0; 1
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
ORKING ...
OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

Fe-18%Cr-8%Ni



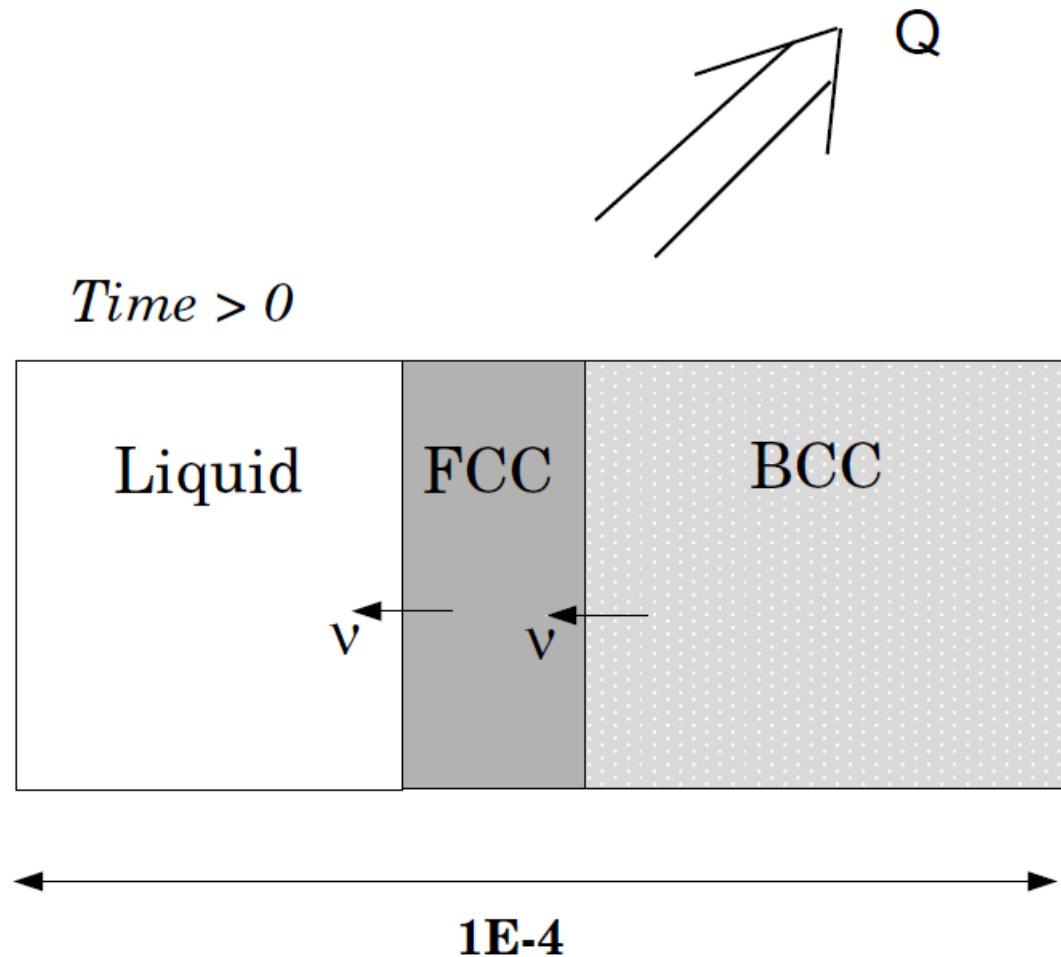
```
POST-1:
POST-1:
POST-1:
POST-1: set-inter
--OK---
POST-1:
```



## Example exb4d

### Solidification path of an Fe-18%Cr-8%Ni alloy: Peritectic reaction, heat-flux controls the temperature

This example is the same as exb4b but instead of controlling the temperature the amount heat extracted is given. Comparison is made with both a Scheil-Gulliver simulation and equilibrium solidification conditions, both made with Thermo-Calc.



**exb4d-setup****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\_dictra\_console\_examples\examples\exb4d\setup.DCM.test"**  
**SYS: @@**  
**SYS: @@ Moving boundary problem.**  
**SYS: @@ Solidification path of an Fe-18%Cr-8%Ni alloy**  
**SYS: @@ This example is the same as exb4b but instead of controlling the temperature**  
**SYS: @@ the amount of heat extracted is given. Comparison is made with both a**  
**SYS: @@ Scheil-Gulliver simulation and equilibrium solidification conditions,**  
**SYS: @@ both done in Thermo-Calc.**  
**SYS: -----**  
NO SUCH COMMAND, USE HELP  
**SYS:**  
**SYS: @@ exb4d\_setup.DCM**  
**SYS:**  
**SYS: @@**  
**SYS: @@ START BY GOING TO THE DATABASE MODULE**  
**SYS: @@**  
**SYS: go da**  
THERMODYNAMIC DATABASE module  
Database folder:  
C:\jenkins\workspace\generate\_dictra\_console\_examples\databases\data  
Current database: Steels/Fe-Alloys v12.0  
  
VA                           /- DEFINED  
DICTRA\_FCC\_A1 REJECTED  
**TDB\_TCFE12:**  
**TDB\_TCFE12: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA**  
**TDB\_TCFE12: sw fedemo**  
Current database: Iron Demo Database v4.0  
  
VA                           /- DEFINED  
**TDB\_FEDEMO:**  
**TDB\_FEDEMO: @@ DEFINE THE SYSTEM TO WORK WITH**  
**TDB\_FEDEMO: def-sys fe ni cr**  
FE                           NI                           CR  
DEFINED  
**TDB\_FEDEMO:**  
**TDB\_FEDEMO: @@ EXCLUDE THE THERMODYNAMIC DATA FOR THE PHASES THAT ARE NOT NEEDED**  
**TDB\_FEDEMO: rej ph /all**  
LIQUID:L                   BCC\_A2                   LAVES\_PHASE\_C14  
CBCC\_A12                   CHI\_A12                   CUB\_A13  
FCC\_A1                     HCP\_A3                   SIGMA  
REJECTED  
**TDB\_FEDEMO: res ph fcc liq bcc**  
FCC\_A1                     LIQUID:L                   BCC\_A2  
RESTORED  
**TDB\_FEDEMO:**  
**TDB\_FEDEMO: @@ RETRIEVE DATA FROM THE DATABASE FILE**  
**TDB\_FEDEMO: get**  
16:08:46,663 [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, SGT 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'  
-OK-  
**TDB\_FEDEMO:**  
**TDB\_FEDEMO: @@**  
**TDB\_FEDEMO: @@ MOBILITY/DIFFUSIVITY DATA ARE STORED IN A SEPARATE DATABASE FILE.**  
**TDB\_FEDEMO: @@ SWITCH TO THE MOBILITY DATABASE AND APPEND THE DATA**  
**TDB\_FEDEMO: @@**  
**TDB\_FEDEMO: app**  
Use one of these databases  
  
TCFE12 = Steels/Fe-Alloys v12.0  
TCFE9 = Steels/Fe-Alloys v9.3  
SSUB6 = SGT Data for Pure Elements, CALPHAD, 15 (1991) 317-425  
FEDEMO = Iron Demo Database v4.0  
MOB2 = Alloys Mobility v2.7  
MOBFE2 = Steels/Fe-Alloys Mobility v2.0  
MOBFE4 = Steels/Fe-Alloys Mobility v4.0  
MOBFE7 = Steels/Fe-Alloys Mobility v7.1  
MFDEMO = Fe-Alloys Mobility demo database v2.0  
USER = User defined Database

```

DATABASE NAME /FEDEMO/: mobfe2
Current database: Steels/Fe-Alloys Mobility v2.0
TCS Steel Mobility Database Version 2.0 from 2011-12-09.

VA DEFINED

*** WARNING: This database cannot be used with GES6, temporarily reverting to G
ESS5

APP: def-sys fe ni cr
    FE           NI          CR
    DEFINED
APP: rej ph /all
    BCC_A2      FCC_A1      HCP_A3
    LIQUID:L   REJECTED
APP: res ph fcc liq bcc
    FCC_A1      LIQUID:L   BCC_A2
    RESTORED
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS .....
FUNCTIONS .....

List of references for assessed data

'This parameter has not been assessed'
'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Fe diffusion fcc Cr-Fe'
'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Ni diffusion fcc Cr-Ni'
'B. Jonsson: Z. Metallkunde 86(1995)686-692; Cr, Fe and Ni diffusion fcc
    Cr-Fe-Ni'
'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
    -Ni'
'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Ni self-diffusion'
'B. Jonsson: ISIJ International, 35(1995)1415-1421; Cr, Fe and Ni
    diffusion bcc Cr-Fe-Ni'
'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
    in bcc Fe'

-OK-
APP:
APP: @@ 
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP
APP: @@ 
APP: go d-m
NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ EXTRACT HEAT 91.19 J/mole/s
DIC> @@
DIC> set-cond glob Q 0 91.19; * N
DIC>
DIC> @@
DIC> @@ ENTER AN INITIAL TEMPERATURE
DIC> @@
DIC> set-initial-temp 1900
DIC>
DIC> @@
DIC> @@ ENTER A REGION CALLED smalta
DIC> @@
DIC> enter-region smalta
DIC>
DIC> @@
DIC> @@ ENTER A GEOMETRIC GRID INTO THE REGION
DIC> @@
DIC> enter-grid
REGION NAME : /SMALTA/: smalta
WIDTH OF REGION /1/: 1e-4
TYPE /LINEAR/: AUTO
DIC>
DIC>
DIC> @@
DIC> @@ ENTER active PHASES INTO THE REGION
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /SMALTA/: smalta
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: liq
DIC>
DIC> @@
DIC> @@ ENTER inactive PHASES INTO THE REGION, BOTH PHASES ON THE
DIC> @@ SAME SIDE OF THE LIQUID REGION TO GET A PERITECTIC REACTION.
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inact
ATTACH TO REGION NAMED /SMALTA/: smalta
ATTACHED TO THE RIGHT OF SMALTA /YES/: yes
PHASE NAME: /NONE/: fcc#1
DEPENDENT COMPONENT ? /NI/: fe
REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-3
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inact
ATTACH TO REGION NAMED /SMALTA/: smalta
ATTACHED TO THE RIGHT OF SMALTA /YES/: yes
PHASE NAME: /NONE/: bcc#1
DEPENDENT COMPONENT ? /NI/: fe
REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-3
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> @@
DIC> @@ ENTER A START COMPOSITION FOR THE LIQUID
DIC> @@
DIC> enter-composition
REGION NAME : /SMALTA/: smalta
PHASE NAME: /LIQUID/: liq
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /CR/: cr lin 18 18
PROFILE FOR /NI/: ni lin 8 8

```

```
DIC>
DIC> @@
DIC> @@ THE BOUNDARY CONDITION IS A CLOSED SYSTEM (DEFAULT) AS WE DO NOT SPECIFY
DIC> @@ ANYTHING ELSE
DIC> @@
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /1/: 200
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /20/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ CHECK THE INTERFACE POSITION. THIS IS TO MAKE SURE THAT THE LIQUID REGION
DIC> @@ DOES NOT SHRINK TOO MUCH DURING A TIMESTEP. IN ADDITION THE TIMESTEP IS
DIC> @@ CONTROLLED BY THE PHASE INTERFACE DISPLACEMENT DURING THE SIMULATION.
DIC> @@
DIC> s-s-c
NSO1A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /AUTO/: yes
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/: no
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPLICITY WHEN INTEGRATING PDES (AUTO, 0 -> 0.5 -> 1) : /AUTO/:
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/: @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exb4d Y
DIC>
DIC> set-inter
--OK---
DIC>
```

**exb4d-run**

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exb4d\run.DCM.test"
DIC>
DIC> @@ exb4d_run.DCM
DIC>
DIC> @@
DIC> FILE FOR RUNNING EXAMPLE b4b
DIC> @@
DIC>
DIC> @@
DIC> ENTER THE DICTRA MONITOR AND READ THE SET UP FROM FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 0.00000E+00
DIC> read exb4d
OK
DIC>
DIC> @@
DIC> @@ START THE SIMULATION
DIC> @@
DIC> sim
Region: SMALTA
single geometric dense at 0.10000E-03
0.92197 87
DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
TEMPERATURE: 1900.0000 ENTHALPY: 73940.238
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882254
TOTAL SIZE OF SYSTEM: 1E-04 [m]
TEMPERATURE: 1900.0000 ENTHALPY: 73940.238
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882254
TOTAL SIZE OF SYSTEM: 1E-04 [m]
3.863918610051459E-003 3.86469145661233E-003 3.837208638551419E-012 3.816464753926110E-021 TIME = 0.10000000E-
06 DT = 0.10000000E-06 SUM OF SQUARES = 0.38164648E-20
TEMPERATURE: 1900.0000 ENTHALPY: 73940.238
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882254
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
3.863391026320342E-003 3.864163722589357E-003 3.853401261337085E-012 3.843259701995471E-021 TIME = 0.26002472E-
05 DT = 0.25002472E-05 SUM OF SQUARES = 0.38432597E-20
TEMPERATURE: 1900.0000 ENTHALPY: 73940.238
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882254
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
1.545296500120001E-004 1.545605588204789E-004 6.483839778845627E-015 6.483839778845627E-015 TIME = 1.752158783167687E-
012 3.485949864582234E-027 TIME = 0.76007416E-05 DT = 0.50004944E-05 SUM OF SQUARES = 0.34859499E-26
TEMPERATURE: 1900.0000 ENTHALPY: 73940.238
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882254
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
1.545143195209232E-004 1.54542268041278E-004 5.953822578370995E-015 5.953822578370995E-015 TIME = 1.743271464499436E-
012 1.549311070034878E-027 TIME = 0.17601730E-04 DT = 0.10000989E-04 SUM OF SQUARES = 0.15493111E-26
TEMPERATURE: 1900.0000 ENTHALPY: 73940.236
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882254
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
1.544836608300040E-004 1.545145650479135E-004 5.949046235387195E-015 5.949046235387195E-015 TIME = 1.743189863755022E-
012 1.54931108253759E-027 TIME = 0.37603708E-04 DT = 0.20001978E-04 SUM OF SQUARES = 0.15493111E-26
TEMPERATURE: 1899.9999 ENTHALPY: 73940.235
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882254
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
1.544223525710398E-004 1.544532506482932E-004 6.497872790021408E-015 6.497872790021408E-015 TIME = 1.752389233746494E-
012 2.478897895506436E-026 TIME = 0.77607664E-04 DT = 0.40003955E-04 SUM OF SQUARES = 0.24788979E-25
TEMPERATURE: 1899.9999 ENTHALPY: 73940.231
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882254
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
1.542997725366472E-004 1.543306583501994E-004 6.477658832716117E-015 6.477658832716117E-015 TIME = 1.752057874212783E-
012 1.549311337567070E-027 TIME = 0.15761557E-03 DT = 0.80007911E-04 SUM OF SQUARES = 0.15493113E-26
TEMPERATURE: 1899.9997 ENTHALPY: 73940.224
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882255
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
1.542066247921270E-005 2.353241149621661E-008 1.773340958976166E-013 3.806810471789864E-016 3.837214312499011E-
019 TIME = 197.37514 DT = 1.0007812 SUM OF SQUARES = 0.34004843E-18
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.72699313E-07 AND 0.72699313E-07
POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS 0.55751529E-05
TEMPERATURE: 1704.9920 ENTHALPY: 55979.121
U-FRACTION IN SYSTEM: CR = .191391778337222 FE = .733228660767811
NI = .0753795608949664
TOTAL SIZE OF SYSTEM: 1E-04 [m]
3 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: R_FCC_A1

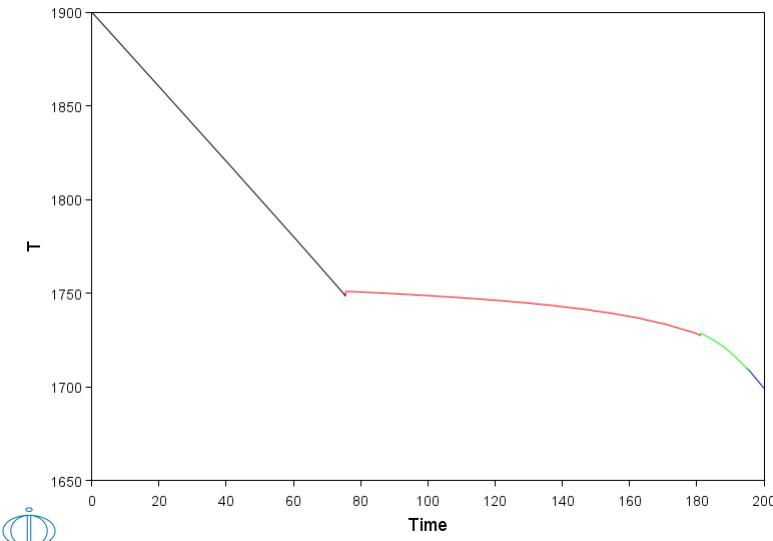
CPU time used in timestep 1 seconds
9.357586306924341E-002 9.357551717940230E-002 9.357594168160094E-002 9.357496299293516E-002 6.844730878844204E-
004 1.219390771921775E-006 1.03988492876086E-009 5.649386022982683E-014 4.716374080095207E-
016 8.04418304514580E-013 4.770065364100804E-016 2.476299699783943E-012 4.803192277670716E-
016 1.227566490259846E-013 4.849893846363009E-016 7.979623838142825E-013 4.849893846385736E-
016 2.476299699783943E-012 4.703634005094377E-016 1.282098294232727E-013 8.743551043691272E-
020 TIME = 199.37670 DT = 2.0015625 SUM OF SQUARES = 0.87428453E-19
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.92564682E-07 AND 0.92564682E-07
POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS 0.57604269E-05
TEMPERATURE: 1700.6542 ENTHALPY: 55796.599
U-FRACTION IN SYSTEM: CR = .19139177833486 FE = .733228660768288
NI = .0753795608968521
```



## exb4d-plot

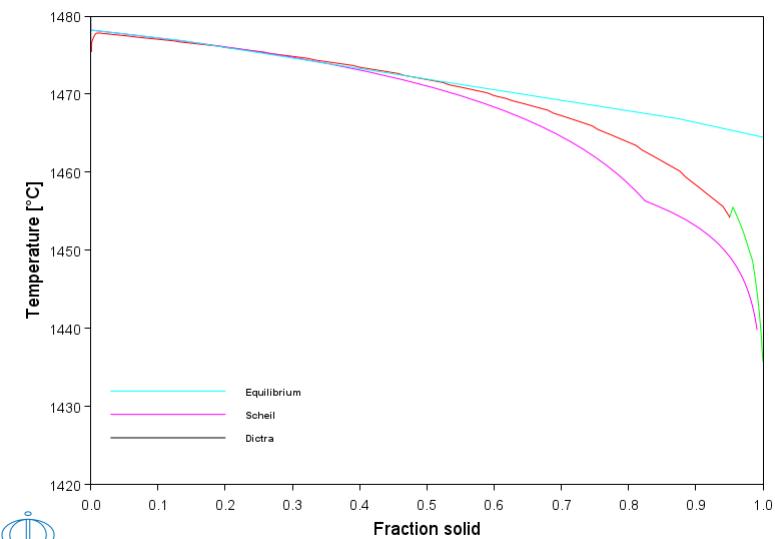
```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exb4d\plot.DCM.test"
DIC>
DIC>
DIC> @@ exb4d_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE b4b
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 2.00000E+02
DIC> read exb4d
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1: set-title Fe-18%Cr-8%Ni
POST-1:
POST-1: @@
POST-1: @@ PLOT THE FRACTION OF SOLID AND COMPARE WITH SCHEIL-GULLIVER
POST-1: @@ SIMULATION AND EQUILIBRIUM SOLIDIFICATION (DATA ON FILE exb4.exp)
POST-1: @@
POST-1: s-d-a x time
INFO: Time is set as independent variable
POST-1: s-d-a y T
POST-1: s-p-c inter first
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
ORKING ...orking ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

Fe-18%Cr-8%Ni



```
POST-1:
POST-1:Hit RETURN to continue
POST-1: enter func fs=1-ivv(liquid);
POST-1: s-d-a x fs
POST-1: s-s-s x n 0 1
POST-1: s-ax-te x n Fraction solid
POST-1:
POST-1: s-d-a y t-c
POST-1: s-s-s y n 1420 1480
POST-1:
POST-1: s-p-c interf smalta lower
POST-1:
POST-1: app y exb4d.exp 0; 1
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
ORKING ...orking ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

### Fe-18%Cr-8%Ni



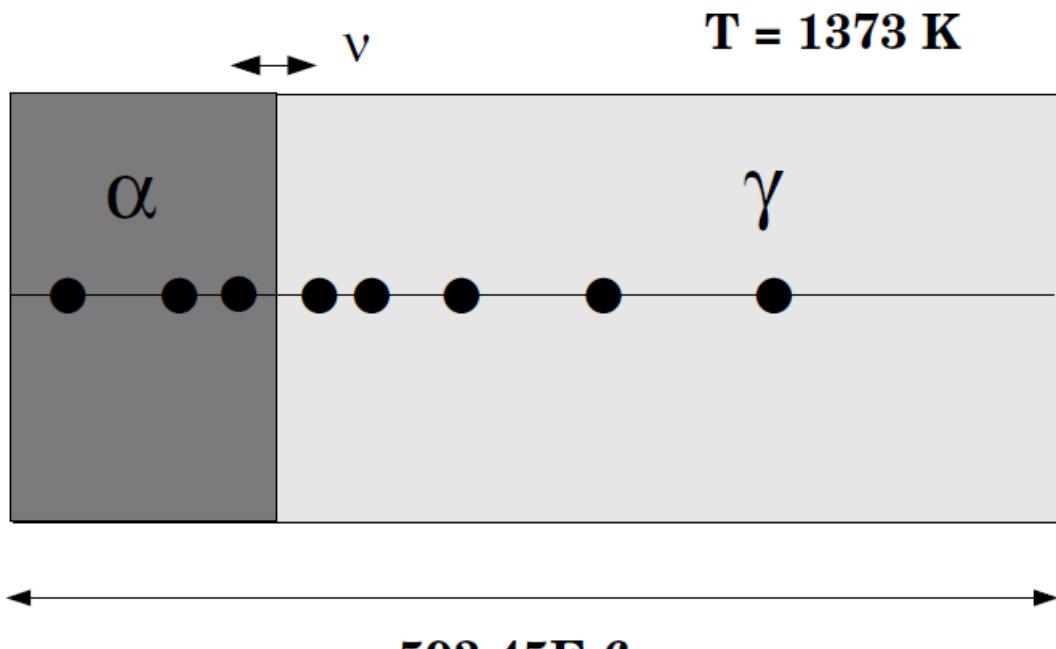
```
POST-1:  
POST-1:  
POST-1:  
POST-1: set-inter  
--OK---  
POST-1:
```



## Example exb5

### $\gamma/\alpha/\gamma$ diffusion couple of Fe-Ni-Cr alloys

This example demonstrates the evaluation of a ternary Fe-Cr-Ni diffusion couple. A thin slice of  $\alpha$  phase (38%Cr, 0%Ni) is clamped between two thicker slices of  $\gamma$  phase (27%Cr, 20%Ni). The assembly is subsequently heat treated at 1373K. This setup corresponds to diffusion couple A in M. Kajihara, C.-B. Lim and M. Kikuchi: ISIJ International 33 (1993), pp. 498-507. See also M. Kajihara and M. Kikuchi: Acta Metall.Mater. 41 (1993), pp.2045-2059.



**exb5-setup****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\_dictra\_console\_examples\examples\exb5\setup.DCM.test"**

**SYS: @@**  
**SYS: @@** Moving boundary problem.  
**SYS: @@** Ternary diffusion couple of Fe-Ni-Cr alloys  
**SYS: @@** This example demonstrates the evaluation of a ternary Fe-Cr-Ni diffusion  
**SYS: @@** couple. A thin slice of alpha phase (38%Cr, 0%Ni) is clamped between  
**SYS: @@** two thicker slices of gamma phase (27%Cr, 20%Ni). The assembly is  
**SYS: @@** subsequently heat treated at 1373 K. This example corresponds to diffusion  
**SYS: @@** couple A in M. Kajihara, C.-B. Lim and M. Kikuchi: ISIJ International  
**SYS: @@** 33 (1993), pp. 498-507. See also M. Kajihara and M. Kikuchi: Acta Metall.Mater.  
**SYS: @@** 41 (1993), pp.2045-2059.

**SYS: -----**

NO SUCH COMMAND, USE HELP

**SYS:**  
**SYS: @@**  
**SYS: @@** GO TO A DATABASE AND READ THE THERMODYNAMIC AND KINETIC DATA  
**SYS: @@**

**SYS: go da**

THERMODYNAMIC DATABASE module

Database folder:

C:\jenkins\workspace\generate\_dictra\_console\_examples\databases\data  
Current database: Steels/Fe-Alloys v12.0

VA /- DEFINED

DICTRA\_FCC\_A1 REJECTED

**TDB\_TCFE12: sw fedemo**

Current database: Iron Demo Database v4.0

VA /- DEFINED

**TDB\_FEDEMO: def-sys cr fe ni**  
CR FE NI

DEFINED

**TDB\_FEDEMO: rej-ph /all**  
LIQUID:L BCC\_A2 LAVES\_PHASE\_C14  
CBCC\_A12 CHI\_A12 CUB\_A13  
FCC\_A1 HCP\_A3 SIGMA

REJECTED

**TDB\_FEDEMO: res-ph bcc,fcc**  
BCC\_A2 FCC\_A1 RESTORED

**TDB\_FEDEMO: get**

16:14:49,958 [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'  
'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'  
'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'  
'A.T. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); CR -NI'  
'A.T. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); FE-NI'

-OK-

**TDB\_FEDEMO:**

**TDB\_FEDEMO: app**

Use one of these databases

TCFE12 = Steels/Fe-Alloys v12.0  
TCFE9 = Steels/Fe-Alloys v9.3  
SSUB6 = SGTE Substances v6.0  
FEDEMO = Iron Demo Database v4.0  
MOB2 = Alloys Mobility v2.7  
MOBFE2 = Steels/Fe-Alloys Mobility v2.0  
MOBFE4 = Steels/Fe-Alloys Mobility v4.0  
MOBFE7 = Steels/Fe-Alloys Mobility v7.1  
MFEDEMO = Fe-Alloys Mobility demo database v2.0  
USER = User defined Database

**DATABASE NAME /FEDEMO:/: mfedemo**

Current database: Fe-Alloys Mobility demo database v2.0

VA DEFINED

**APP: def-sys cr fe ni**

CR FE NI

DEFINED

**APP: rej-ph /all**  
BCC\_A2 FCC\_A1 REJECTED

**APP: res-ph bcc,fcc**  
BCC\_A2 FCC\_A1 RESTORED

**APP: get**

ELEMENTS .....

SPECIES .....

PHASES .....

PARAMETERS ...

FUNCTIONS ....

List of references for assessed data

```

'This parameter has not been assessed'
'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Fe diffusion fcc Cr-Fe'
'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Ni diffusion fcc Cr-Ni'
'B. Jonsson: Z. Metallkunde 86(1995)686-692; Cr, Fe and Ni diffusion fcc
'Cr-Fe-Ni'
'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
'-Ni'
'Xia, C. H. et al. JAC, 2021, 853, 157165.'
'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Ni self-diffusion'
'B. Jonsson: ISIJ International, 35(1995)1415-1421; Cr, Fe and Ni
'diffusion bcc Cr-Fe-Ni'
'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
'in bcc Fe'

--OK-
APP:
APP: @@ GO TO THE DICTRA MODULE TO SET UP THE SIMULATION
APP: @@ go d-m
NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ SET THE GLOBAL CONDITIONS
DIC> @@
DIC> set-cond glob T 0 1373; * N
DIC>
DIC> @@
DIC> @@ ENTER TWO REGIONS, ONE FOR EACH PHASE
DIC> @@
DIC> enter-region alpha
DIC> enter-region gamma
ATTACH TO REGION NAMED /ALPHA/:
ATTACHED TO THE RIGHT OF ALPHA /YES/:
DIC> @@
DIC> @@ ENTER THE GRID SIZE AND SPACINGS
DIC> @@
DIC> enter-grid alpha 93.45E-6 AUTO
DIC> enter-grid gamma 500.0E-6 AUTO
DIC>
DIC> @@
DIC> @@ SPECIFY WHICH PHASE GOES INTO WHICH REGION
DIC> @@
DIC> enter-phase act alpha matrix bcc
DIC> enter-phase act gamma matrix fcc
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITIONS IN THE PHASES
DIC> @@ IT IS IMPORTANT NOT TO PUT 0%NI IN PHASE BCC,
DIC> @@ ENTER SOME SMALL VALUE INSTEAD
DIC> @@
DIC> enter-composition
REGION NAME : /ALPHA/: alpha
PHASE NAME: /BCC_A2/: bcc
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-f
PROFILE FOR /CR/: cr lin .38 .38
PROFILE FOR /NI/: ni lin 1e-5 1e-5
DIC>
DIC> enter-composition
REGION NAME : /GAMMA/: gamma
PHASE NAME: /FCC_A1/: fcc
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-f
PROFILE FOR /CR/: cr lin .27 .27
PROFILE FOR /NI/: ni lin .28 .28
DIC>
DIC> @@
DIC> @@ SPECIFY THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 36E5
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /360000/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC> SAVE exb5 Y
DIC>
DIC> set-inter
--OK---
DIC>
```

**exb5-run**

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exb5\run.DCM.test"
DIC>
DIC>
DIC> @@ exb5_run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING EXAMPLE b5
DIC> @@
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA MONITOR AND READ THE SET UP FROM FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 0.00000E+00
DIC> read exb5
OK
DIC>
DIC> @@
DIC> @@ START THE SIMULATION
DIC> @@
DIC> simulate
Region: ALPHA
single geometric dense at 0.93450E-04
0.80000 36
Region: GAMMA
single geometric dense at 0.0000
1.2500 103
DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
Trying old scheme 4
GENERATING STARTING VALUES FOR CELL # 1 INTERFACE # 2
DETERMINING INITIAL EQUILIBRIUM VALUES
CALCULATING STARTING VALUES: 9 EQUILIBRIUM CALCULATIONS *** ERROR 1611 IN QTHISS: TOO MANY ITERATIONS
Give the command INFO TROUBLE for help
DONE 6 OUT OF 9 *** ERROR 1611 IN QTHISS: TOO MANY ITERATIONS
Give the command INFO TROUBLE for help
DONE 9 OUT OF 9 try 1 failed
try 2 failed
try 3 failed
DETERMINED ACTIVITIES ACR(NI) 2.00457405352E-04
UNABLE TO OBTAIN GOOD STARTING VALUE USING THE OLD SCHEME
USE NEW SCHEME /YES:
Trying new scheme
GENERATING STARTING VALUES FOR CELL # 1 INTERFACE # 2
DETERMINING INITIAL EQUILIBRIUM VALUES
CALCULATING STARTING VALUES: 18 EQUILIBRIUM CALCULATIONS DONE 1 OUT OF 18
04
U-FRACTION IN SYSTEM: CR = .305280432605602 FE = .471672082221692
NI = .223047485172706
TOTAL SIZE OF SYSTEM: 5.9345E-04 [m]
U-FRACTION IN SYSTEM: CR = .305280432605602 FE = .471672082221692
NI = .223047485172706
TOTAL SIZE OF SYSTEM: 5.9345E-04 [m]
3.503057562890267E-002 3.503838978370250E-002 3.503070722825020E-002 6.010860850726212E-004 4.996105706031839E-
004 3.843187703297066E-004 2.950242505081373E-004 2.951615357478117E-004 1.282240365502392E-
004 1.415607653199716E-007 1.955426406535891E-009 4.891072072428393E-011 2.356759560239555E-
015 9.643498967181070E-022 TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.73857918E-22
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.16001447 AND 0.16001447
POSITION OF INTERFACE ALPHA / GAMMA IS 0.93466001E-04
U-FRACTION IN SYSTEM: CR = .305280432536186 FE = .471672082122531
TOTAL SIZE OF SYSTEM: 5.9345E-04 [m]
26 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: GAMMA

CPU time used in timestep 0 seconds
9.795982644299397E-004 9.797941939216723E-004 9.795986845933737E-004 2.251217783118110E-012 1.908561997053581E-
012 1.862630659905408E-012 2.156599195709713E-012 7.359572650265387E-012 1.738570243408562E-
012 1.698130957899166E-012 1.706072891801743E-012 6.521088610529210E-012 1.693481728433165E-
012 1.692572480378887E-012 1.694702315318739E-012 6.464482669340281E-012 1.692327747944229E-
012 1.691636341818396E-012 1.690849106694576E-012 6.462570157934684E-012 1.690142864948186E-
012 1.689035147642133E-012 1.687602169176906E-012 6.46124286559346E-012 1.685135296062395E-
012 1.682410878389070E-012 1.676508508025022E-012

output ignored...

... output resumed

1.235822247056106E-008 4.714422625736839E-010 6.181920013957396E-014 2.498118349384551E-
019 TIME = 2324446.5 DT = 360000.00 SUM OF SQUARES = 0.17222933E-21
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.71764430E-11 AND -0.71764430E-11
POSITION OF INTERFACE ALPHA / GAMMA IS 0.93084783E-04
U-FRACTION IN SYSTEM: CR = .305280443031972 FE = .471672053155458
TOTAL SIZE OF SYSTEM: 5.9345E-04 [m]
NI = .22304750381257
8 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: GAMMA

CPU time used in timestep 1 seconds
1.232097985101387E-006 1.234292658654382E-006 1.228319008605722E-006 8.058105517324265E-009 1.530517558718996E-
009 5.437984387953843E-014 9.626773161308310E- 021 TIME = 2684446.5 DT = 360000.00 SUM OF SQUARES = 0.53699539E-22
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.62690554E-11 AND -0.62690554E-11
POSITION OF INTERFACE ALPHA / GAMMA IS 0.90827923E-04
U-FRACTION IN SYSTEM: CR = .305280443234724 FE = .471672053027
TOTAL SIZE OF SYSTEM: 5.9345E-04 [m]
NI = .223047503738276
8 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: GAMMA

CPU time used in timestep 1 seconds
4.709610878493658E-007 4.721549439646296E-007 4.686527475442992E-007 2.508781083457050E-009 3.420934356949292E-
010 2.221750348485615E-012 3.208924402956165E-
018 TIME = 3044446.5 DT = 360000.00 SUM OF SQUARES = 0.10753149E-21
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.57307740E-11 AND -0.57307740E-11
POSITION OF INTERFACE ALPHA / GAMMA IS 0.88764845E-04
U-FRACTION IN SYSTEM: CR = .305280443459185 FE = .471672052736094
NI = .223047503804721
TOTAL SIZE OF SYSTEM: 5.9345E-04 [m]
6 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: GAMMA

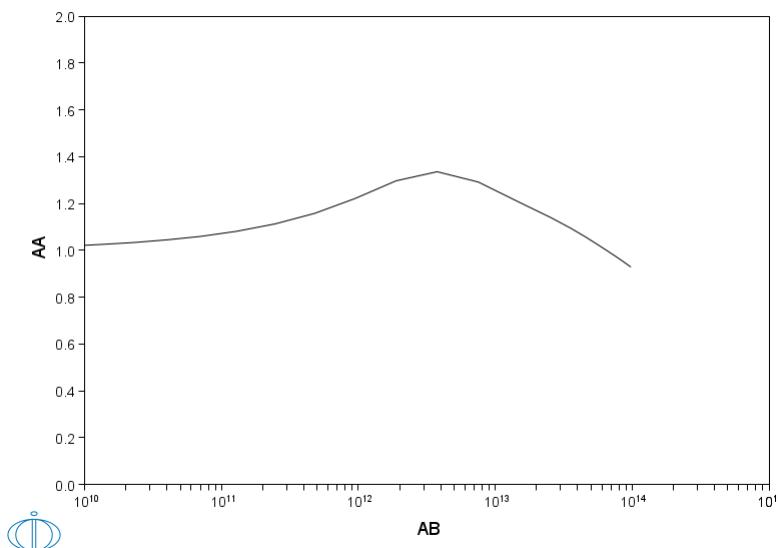
CPU time used in timestep 1 seconds
```

3.282917581441741E-007 3.292090288391608E-007 3.263904716258317E-007 2.179592456441579E-009 7.129622734406629E-000  
 010 1.08224330351970E-016 TIME = 3404446.5 DT = 360000.00 SUM OF SQUARES = 0.36917997E-17  
 CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.52536389E-11 AND -0.52536389E-11  
 POSITION OF INTERFACE ALPHA / GAMMA IS 0.86873535E-04  
 U-FRACTION IN SYSTEM: CR = .30528044370406 FE = .471672052293244  
 NI = .223047504002696  
 TOTAL SIZE OF SYSTEM: 5.9345E-04 [m]  
 5 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: GAMMA  
 CPU time used in timestep 0 seconds  
 2.072317568521768E-007 2.071961282481910E-007 2.075229854268564E-007 4.640298257299180E-009 7.016175495325838E-000  
 014 8.181461605380313E-021 TIME = 3600000.0 DT = 195553.51 SUM OF SQUARES = 0.52825946E-21  
 CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.47680762E-11 AND -0.47680762E-11  
 POSITION OF INTERFACE ALPHA / GAMMA IS 0.85941120E-04  
 U-FRACTION IN SYSTEM: CR = .305280443847066 FE = .47167205201273  
 NI = .223047504140204  
 TOTAL SIZE OF SYSTEM: 5.9345E-04 [m]  
 MUST SAVE WORKSPACE ON FILE  
 WORKSPACE SAVED ON FILE  
 RECLAIMING WORKSPACE  
 DELETING TIME-RECORD FOR TIME 0.000000  
 DELETING TIME-RECORD FOR TIME 0.1000000E-06  
 DELETING TIME-RECORD FOR TIME 0.87548762E-05  
 DELETING TIME-RECORD FOR TIME 0.26064629E-04  
 DELETING TIME-RECORD FOR TIME 0.60684133E-04  
 DELETING TIME-RECORD FOR TIME 0.12992314E-03  
 DELETING TIME-RECORD FOR TIME 0.26840116E-03  
 DELETING TIME-RECORD FOR TIME 0.54535720E-03  
 DELETING TIME-RECORD FOR TIME 0.10992693E-02  
 DELETING TIME-RECORD FOR TIME 0.22070934E-02  
 DELETING TIME-RECORD FOR TIME 0.44227417E-02  
 DELETING TIME-RECORD FOR TIME 0.88540383E-02  
 DELETING TIME-RECORD FOR TIME 0.17716632E-01  
 DELETING TIME-RECORD FOR TIME 0.35441818E-01  
 DELETING TIME-RECORD FOR TIME 0.70892191E-01  
 DELETING TIME-RECORD FOR TIME 0.10629850  
 DELETING TIME-RECORD FOR TIME 0.17711111  
 DELETING TIME-RECORD FOR TIME 0.21589677  
 DELETING TIME-RECORD FOR TIME 0.26420716  
 DELETING TIME-RECORD FOR TIME 0.36082792  
 DELETING TIME-RECORD FOR TIME 0.41374930  
 DELETING TIME-RECORD FOR TIME 0.51959205  
 DELETING TIME-RECORD FOR TIME 0.73127754  
 DELETING TIME-RECORD FOR TIME 1.0213988  
 DELETING TIME-RECORD FOR TIME 1.6016412  
 DELETING TIME-RECORD FOR TIME 2.7621260  
 DELETING TIME-RECORD FOR TIME 4.6143302  
 DELETING TIME-RECORD FOR TIME 8.3187385  
 DELETING TIME-RECORD FOR TIME 15.727555  
 DELETING TIME-RECORD FOR TIME 21.090183  
 DELETING TIME-RECORD FOR TIME 31.815440  
 DELETING TIME-RECORD FOR TIME 53.265954  
 DELETING TIME-RECORD FOR TIME 96.166981  
 DELETING TIME-RECORD FOR TIME 119.66484  
 DELETING TIME-RECORD FOR TIME 166.66056  
 DELETING TIME-RECORD FOR TIME 260.65200  
 DELETING TIME-RECORD FOR TIME 343.66057  
 DELETING TIME-RECORD FOR TIME 509.67770  
 DELETING TIME-RECORD FOR TIME 807.21566  
 DELETING TIME-RECORD FOR TIME 1402.2916  
 DELETING TIME-RECORD FOR TIME 2425.8615  
 DELETING TIME-RECORD FOR TIME 4473.0012  
 DELETING TIME-RECORD FOR TIME 8567.2807  
 DELETING TIME-RECORD FOR TIME 16755.840  
 DELETING TIME-RECORD FOR TIME 33132.957  
 DELETING TIME-RECORD FOR TIME 65887.193  
 DELETING TIME-RECORD FOR TIME 131395.66  
 DELETING TIME-RECORD FOR TIME 262412.61  
 DELETING TIME-RECORD FOR TIME 524446.49  
 DELETING TIME-RECORD FOR TIME 884446.49  
 DELETING TIME-RECORD FOR TIME 1244446.5  
 DELETING TIME-RECORD FOR TIME 1604446.5  
 DELETING TIME-RECORD FOR TIME 1964446.5  
 DELETING TIME-RECORD FOR TIME 2324446.5  
 DELETING TIME-RECORD FOR TIME 2684446.5  
 DELETING TIME-RECORD FOR TIME 3044446.5  
 KEEPING TIME-RECORD FOR TIME 3404446.5  
 AND FOR TIME 3600000.0  
 WORKSPACE RECLAIMED  
 TIMESTEP AT 3600000.00 SELECTED  
**DIC>** set-inter  
--OK--  
**DIC>**

**exb5-plot**

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exb5\plot.DCM.test"
DIC>
DIC>
DIC> @@ exb5_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE b5
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 3.60000E+06
DIC> read exb5
OK
DIC>
DIC> @@
DIC> @@ ENTER THE POST PROCESSOR, PLOT SOME QUANTITIES AND COMPARE WITH EXPERIMENTS
DIC> @@
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1: set-title Diffusion Couple A
POST-1:
POST-1: @@
POST-1: @@ WE ARE INTERESTED IN THE POSITION OF THE UPPER INTERFACE OF REGION ALPHA
POST-1: @@
POST-1: s-p-c interf alpha upper
POST-1:
POST-1: @@
POST-1: @@ 10 IS THE INITIAL THICKNESS USED FOR NORMALIZATION
POST-1: @@
POST-1: enter func l0=186.9e-6;
POST-1: enter func aa=2*poi(alpha,u)/l0;
POST-1: enter func ab=time/10**2;
POST-1: s-i-v time
POST-1:
POST-1: s-d-a x ab
POST-1: s-s-s x n 1e10 1e15
POST-1: s-ax-ty x log
POST-1:
POST-1: s-d-a y aa
POST-1: s-s-s y n 0 2
POST-1:
POST-1: app y exb5.exp
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 7
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

Diffusion Couple A

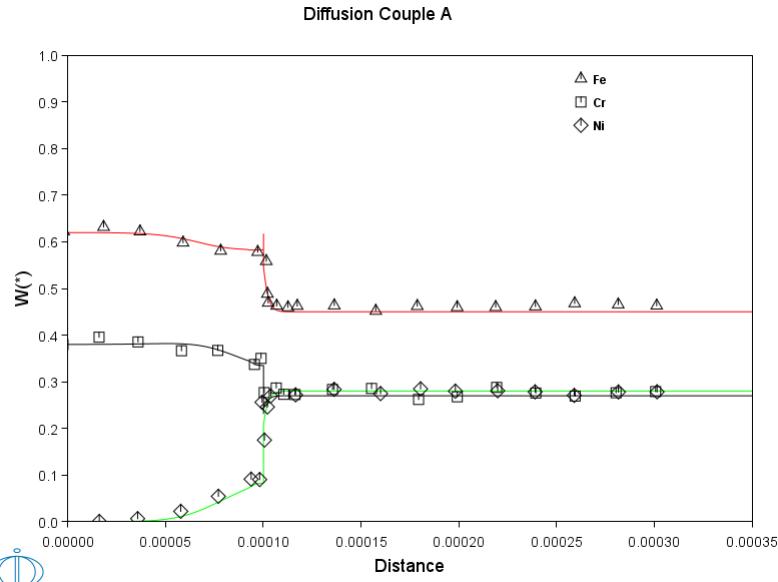


```
POST-1:
POST-1:
POST-1:
POST-1: Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ PLOT THE CONCENTRATION PROFILES FOR DIFFERENT ANNEALING TIMES
POST-1: @@
POST-1: s-d-a x dist glo
INFO: Distance is set as independent variable
POST-1: s-ax-ty x lin
POST-1: s-s-s x n 0 350e-6
POST-1:
POST-1: s-d-a y w(*)
POST-1: s-s-s y n 0 1
POST-1:
POST-1: s-p-c time 3600
POST-1:
```

```

POST-1: app y exb5.exp 0; 1
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

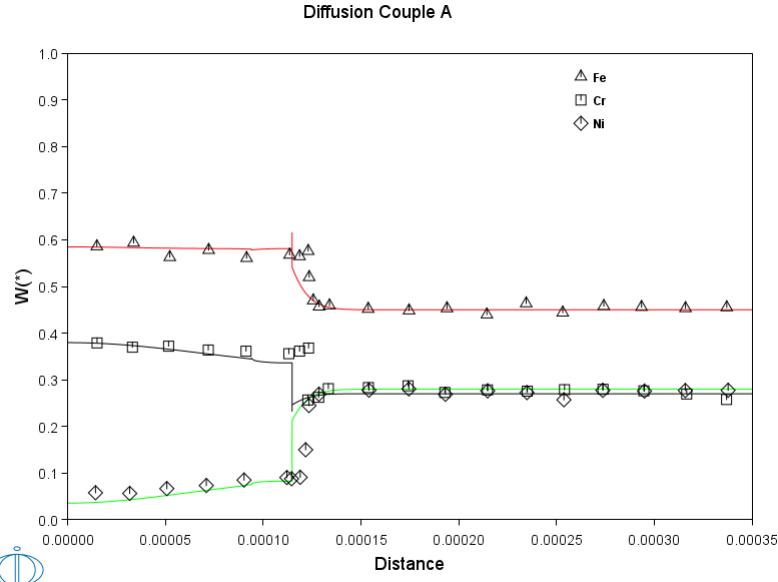
```



```

POST-1:
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: s-p-c time 36000
POST-1: app y exb5.exp 0; 2
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

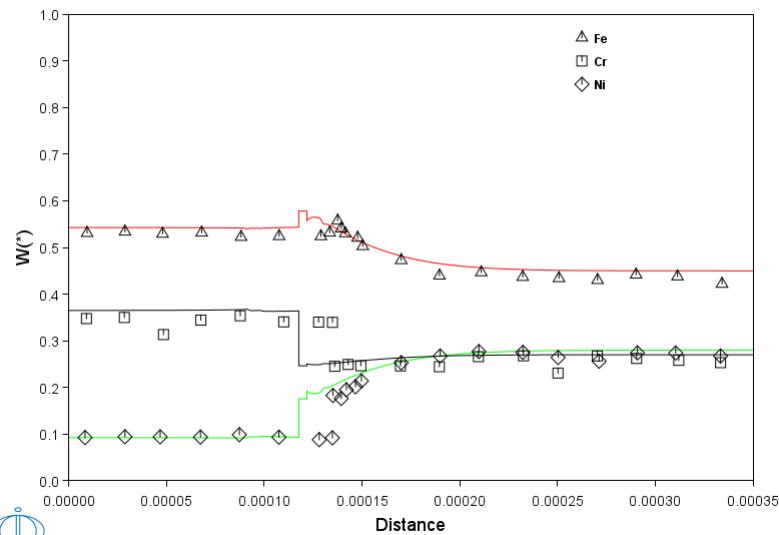
```



```

POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: s-p-c time 360000
POST-1: app y exb5.exp 0; 3
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

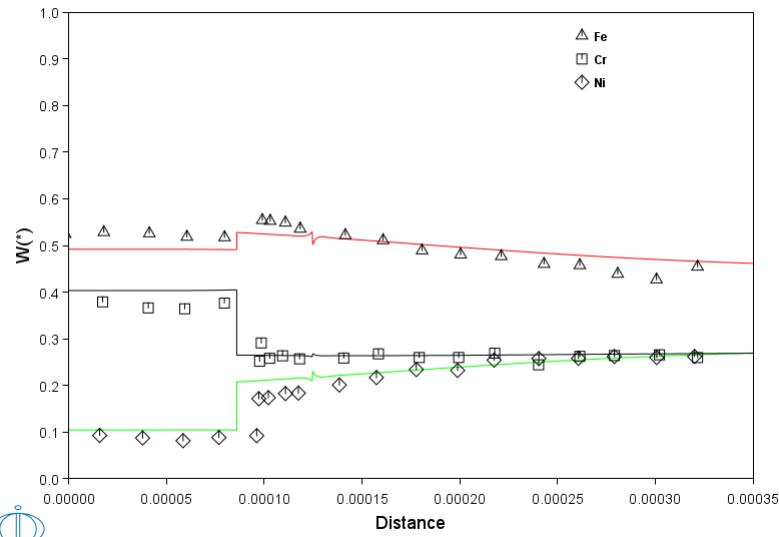
```

**Diffusion Couple A**

```

POST-1:
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: s-p-c time 3600000
POST-1: app y exb5.exp 0; 4
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

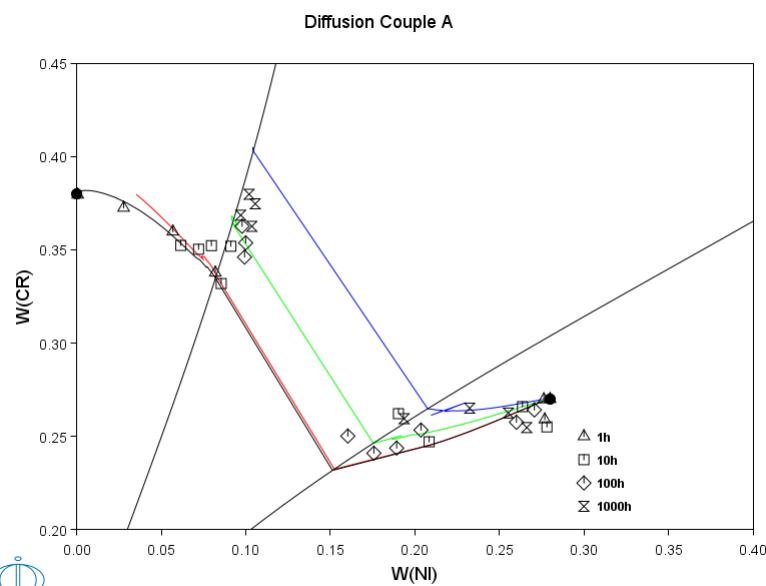
```

**Diffusion Couple A**

```

POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@ 
POST-1: @@ FINALLY PLOT DIFFUSION PATHS.
POST-1: @@
POST-1: s-d-a x w(ni)
POST-1: s-s-s x n .00 .40
POST-1:
POST-1: s-d-a y w(cr)
POST-1: s-s-s y n .20 .45
POST-1:
POST-1: s-i-v dist glob
POST-1:
POST-1: s-p-c time 3600,36000,360000,3600000
POST-1:
POST-1: app y exb5.exp 0; 5 6
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

```



```

POST-1:
POST-1:
POST-1:
POST-1: set-inter
--OK---
POST-1:

```



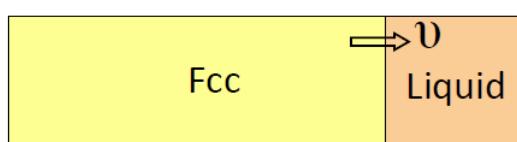
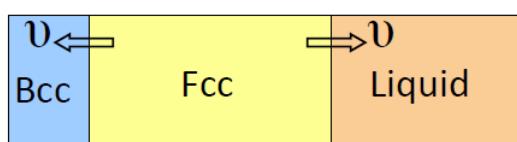
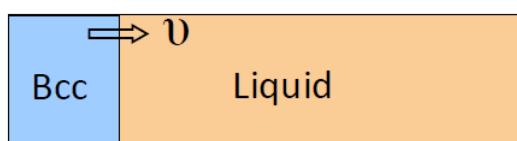
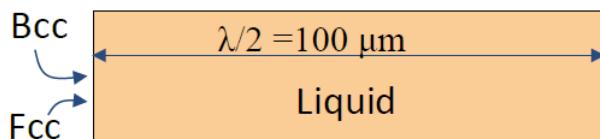
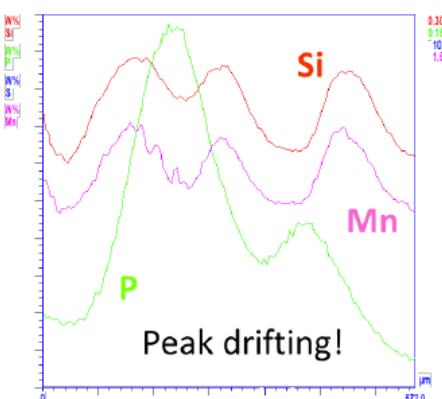
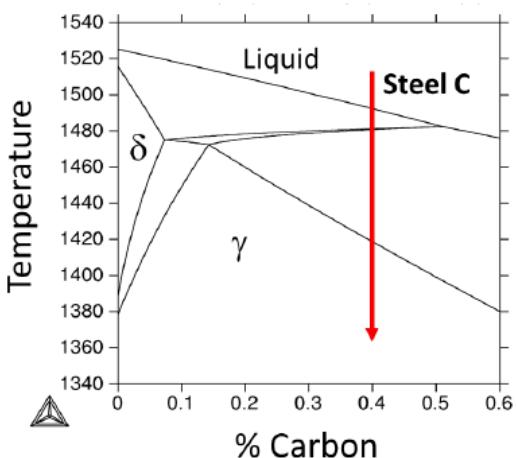
## Example exb6

### Micro-segregation of phosphorus

This example illustrates the effect of microsegregation of phosphorus during peritectic solidification in steel.

Steel C:

Fe - 0.8% Mn - 0.7% Si - 0.03% P - 0.4% C



**exb6-setup****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_dictra_console_examples\examples\exb6\setup.DCM.test"
SYS: @@
SYS: @@ Moving boundary problem.
SYS: @@ Microsegregation of phosphorus
SYS: @@ This example illustrates the effect of microsegregation
SYS: @@ of phosphorus during peritectic solidification in steel.
SYS: -----
NO SUCH COMMAND, USE HELP
SYS: @@
SYS: @@ START BY GOING TO THE DATABASE MODULE
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\generate_dictra_console_examples\databases\data
Current database: Steels/Fe-Alloys v12.0

VA           /*- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE12:
TDB_TCFE12: @@ USE A TCFE DATABASE FOR THERMODYNAMIC DATA
TDB_TCFE12: sw tcfef9
Current database: Steels/Fe-Alloys v9.3

VA           /*- DEFINED
L12_FCC      B2_BCC          DICTRA_FCC_A1
REJECTED
TDB_TCFE9:
TDB_TCFE9: @@ DEFINE THE SYSTEM TO WORK WITH
TDB_TCFE9: def-sys fe c si mn p
FE           C               SI
MN           P   DEFINED
TDB_TCFE9:
TDB_TCFE9: @@ EXCLUDE THE THERMODYNAMIC DATA FOR THE PHASES THAT ARE NOT NEEDED
TDB_TCFE9: rej ph /all
GAS:G         LIQUID:L        BCC_A2
FCC_A1        HCP_A3          CBCC_A12
CUB_A13       DIAMOND_FCC_A4  RED_P
WHITE_P        GRAPHITE        CEMENTITE
M23CG_        M7C3            M5C2
KSI_CARBIDE   FE4N_LP1        FECN_CHI
LAVES_PHASE_C14 MSS1_           MNSS1_2
MN118SI19    MN6SI           G_PHASE
CR3SI         FE2SI           FESI2_H
FESI2_L        MSI             M5Si3_
AL4C3         FE8Si2C         SIC
MN5SiC        CUZN_EPSILON    AL5FE4
MF_B31        CU3P_D021       M2P_C22
M3P_D0E       MN3P_D0E        FENBP
FESI4P4       SIP             SIP2
FLUORITE_C1:I ZRO2_TETR:I    M2O3C:I
M2O3H:I      REJECTED
TDB_TCFE9: res ph fcc liq bcc
FCC_A1        LIQUID:L        BCC_A2
RESTORED
TDB_TCFE9:
TDB_TCFE9: @@ RETRIEVE DATA FROM THE DATABASE FILE
TDB_TCFE9: get
16:18:55,717 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS .....

List of references for assessed data

'A. 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'
'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar volumes'
'L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2012; Molar volumes'
'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
'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, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowsk, CALPHAD, 34, 279 -85(2010); Mn-C'
'W. Huang, Metall. Trans. A, 21A (1990) 2115-2123; TRITA-MAC 411 (Rev 1989); C-FE-MN'
'J.-H. Shim, C.-S. Oh, and D.N. Lee, Z. Metallkd., 2000, 91, p 114-120; Fe -C-P'
'J. Grobner, H.L. Lukas and F. Aldinger, CALPHAD, 20 (1996) 247-254; Si-C and Al-Si-C'
'J. Lacaze and B. Sundman, Metall. Mater. Trans. A, 22A (1991) 2211-2223; Fe-Si and Fe-Si-C'
'W. Huang, CALPHAD, 13 (1989) 243-252; TRITA-MAC 388 (rev 1989); FE-MN'
'J.-H. Shim, C.-S. Oh and D.N. Lee, J. Korean Inst. Met. Mater., 34 (1996) 1385-1393; Fe-P'
'J. Miettinen, G. Vassilev, J. Phase Equilib. Diffus. 59 (2014) 601-607; Cr-Fe-P'
'J. Miettinen and B. Hallstedt, CALPHAD, 22 (1998) 231-256; Fe-Si and Fe -Si-C'
```

```

'J. Miettinen, G. Vassilev, J. Phase Equilib. Diffus, 35(5), 2014, 587-594;
 . Mn-P and Fe-Mn-P'
'W. Zheng, J. Alloys Compd., 632 (2015) 661-675'
'S.-M. Liang and R. Schmid-Fetzer, J. Phase Equilib., 2014, 35, 24-35'
'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, CALPHAD,
 submitted, 2011; Fe-Mn-C'
'R. Naraghi, Thermo-Calc Software AB, Sweden, 2014; Revision of the liquid
 C-Fe-Si description'
'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'
'J. Miettinen, G. Vassilev, J. Phase Equilib. Diffus, 37(5) 2016, 283-290;
 Fe-P-Si'

```

-OK-

**TDB\_TCFE9:**

**TDB\_TCFE9: @@**

**TDB\_TCFE9: @@ MOBILITY/DIFFUSIVITY DATA ARE STORED IN A SEPARATE DATABASE FILE.**

**TDB\_TCFE9: @@ SWITCH TO A MOBILITY DATABASE AND APPEND THE DATA.**

**TDB\_TCFE9: @@**

**TDB\_TCFE9: app**

Use one of these databases

```

TCFE12 = Steels/Fe-Alloys v12.0
TCFE9 = Steels/Fe-Alloys v9.3
SSUB6 = SGTE Substances v6.0
FEDEMO = Iron Demo Database v4.0
MOB2 = Alloys Mobility v2.7
MOBFE2 = Steels/Fe-Alloys Mobility v2.0
MOBFE4 = Steels/Fe-Alloys Mobility v4.0
MOBFE7 = Steels/Fe-Alloys Mobility v7.1
MFEDEMO = Fe-Alloys Mobility demo database v2.0
USER = User defined Database

```

**DATABASE NAME /TCFE9: mobfe4**

Current database: Steels/Fe-Alloys Mobility v4.0

VA DEFINED

B2\_BCC REJECTED

**APP: def-sys fe c si mn p**

FE	C	SI
MN	P DEFINED	

**APP: rej ph /all**

BCC_A2	CEMENTITE	FCC_A1
FE4N_LP1	HCP_A3	LIQUID:L

REJECTED

**APP: res ph fcc liq bcc**

FCC_A1	LIQUID:L	BCC_A2
--------	----------	--------

RESTORED

**APP: get**

ELEMENTS .....

SPECIES .....

PHASES .....

PARAMETERS ....

FUNCTIONS ....

List of references for assessed data

```

'This parameter has not been assessed'
'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'
'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
 -Ni'
'Y. Liu, L. Zhang, et al. CALPHAD 33(2009)614-23; Fe-Mn-C (fcc)'
'M. Yin, et al. (2010) unpublished work.'
'W. Zheng, et al., J. Alloys and Compounds, 632 (2015) 661-675; Fe-Mn-Si
 (fcc)'
'V. V. Mural and P. L. Gruzin, Phys. Met. Metallogr. (English Transl.) 17
 (5) (1964)154.; Impurity diff of P in fcc Fe.'
'D. Bergner et al., Defect and Diffusion Forum 66-69(1989)409. Impurity
 diffusion of Si in fcc Fe.'
'B. Jonsson: Z. Metallkunde 85(1994)498-501; C and N diffusion in bcc Cr
 -Fe-Ni'
'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
 in bcc Fe'
'S. Deng, et al., CALPHAD, 56 (2017) 230-240.'
'B. Jonsson: Unpublished research bcc Fe-Si 1994'
'Assessed from data presented in Landolt-Bornstein, Vol. 26, ed. H.
 Mehrer, springer (1990); Impurity diff of Mn in bcc Fe.'
'Assessed from data presented in Landolt-Bornstein, Vol. 26, ed. H.
 Mehrer, springer (1990); Impurity diff of P in bcc Fe.'
'No assessed or estimated parameters'
'Estimation by using the modified Sutherland equation from Chen et al.,
 Phil. Magazine 94 (2014) 1552.'
'L. Zhang et al., Acta Mater., 58(2010)3664.'
'S.Q. Wang et al., Int J Mater Res, 104 (2013) 721-735.'
'G. Barreau et al., C. R. Acad. Sci. (Paris) C 272(1971)618.; Impurity
 diffusion of Cr in fcc Cu.'
'Y. Tang et al., CALPHAD, 49(2015)58.'

```

-OK-

**APP:**

**APP: @@**

**APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP**

**APP: @@**

**APP: go d-m**

NO TIME STEP DEFINED

**DIC>**

**DIC> @@**

**DIC> @@ ENTER THE GLOBAL CONDITION T**

**DIC> @@**

**DIC> @@ LOWER THE TEMPERATURE TO A RATE OF 0.2 K/s**

**DIC> @@**

**DIC> set-cond glob T 0 1780-0.2\*TIME; \* N**

**DIC>**

**DIC> @@**

**DIC> @@ ENTER A REGION CALLED smalta**

**DIC> @@**

**DIC> enter-region smalta**

**DIC>**

**DIC> @@**

**DIC> @@ ENTER A DOUBLE GEOMETRIC GRID INTO THE REGION**

**DIC> @@**

**DIC> enter-grid**

**REGION NAME : /SMALTA/: smalta**

**WIDTH OF REGION /1/: 1e-4**

**TYPE /LINEAR/: AUTO**

**DIC>**

```

DIC> @@
DIC> @@ ENTER active PHASES INTO THE REGION
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /SMALTA/: smalta
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: liq
DIC>
DIC> @@
DIC> @@ ENTER inactive PHASES INTO THE REGION, BOTH PHASES ON THE SAME SIDE
DIC> @@ OF THE LIQUID REGION TO GET A PERITECTIC REACTION.
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inact
ATTACH TO REGION NAMED /SMALTA/: smalta
ATTACHED TO THE RIGHT OF SMALTA /YES/: no
PHASE NAME: /NONE/: fcc#1
DEPENDENT COMPONENT ? /SI/: fe
REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-5
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inact
ATTACH TO REGION NAMED /SMALTA/: smalta
ATTACHED TO THE RIGHT OF SMALTA /YES/: no
PHASE NAME: /NONE/: bcc#1
DEPENDENT COMPONENT ? /SI/: fe
REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-5
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> @@
DIC> @@ ENTER A START COMPOSITION FOR THE LIQUID
DIC> @@
DIC> enter-composition
REGION NAME : /SMALTA/: smalta
PHASE NAME: /LIQUID/: liq
DEPENDENT COMPONENT ? /SI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: c lin^0.4 0.4
PROFILE FOR /MN/: si lin 0.7 0.7
PROFILE FOR /P/: mn lin 0.8 0.8
PROFILE FOR /SI/: p lin 0.03 0.03
DIC>
DIC> @@
DIC> @@ THE BOUNDARY CONDITION IS A CLOSED SYSTEM (DEFAULT) AS WE DO NOT SPECIFY
DIC> @@ ANYTHING ELSE
DIC> @@
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /1/: 3000
AUTOMATIC TIMESTEP CONTROL /YES/: yes
MAX TIMESTEP DURING INTEGRATION /300/: 15
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC>
DIC>
DIC> @@ CHECK THE INTERFACE POSITION. THIS IS TO MAKE SURE THAT THE LIQUID REGION
DIC> @@ DOES NOT SHRINK TOO MUCH DURING A TIMESTEP. IN ADDITION THE TIMESTEP IS
DIC> @@ CONTROLLED BY THE PHASE INTERFACE DISPLACEMENT DURING THE SIMULATION.
DIC> @@
DIC> s-s-c
NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /AUTO/: yes
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPLICITY WHEN INTEGRATING PDES (AUTO, 0 -> 0.5 -> 1): /AUTO/:
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/:
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exb6 Y
DIC>
DIC> set-inter
--OK---
DIC>

```

**exb6-run**

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exb6\run.DCM.test"
DIC>
DIC>
DIC> @@ exb6_run.DCM
DIC>
DIC> @@
DIC> @@ READ THE SET UP FROM FILE AND START THE SIMULATION
DIC> @@
DIC>
DIC>
DIC> go d-m
TIME STEP AT TIME 0.00000E+00
DIC> read exb6
OK
DIC> sim
Region: SMALTA
single geometric dense at 0.0000
1.0649 83
DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
U-FRACTION IN SYSTEM: C = .0185375871047351 FE = .977481861209078
MN = .00810568126669964 P = 5.3913352823733E-04
SI = .0138733239959838
TOTAL SIZE OF SYSTEM: 1E-04 [m]
U-FRACTION IN SYSTEM: C = .0185375871047351 FE = .977481861209078
MN = .00810568126669964 P = 5.3913352823733E-04
SI = .0138733239959838
TOTAL SIZE OF SYSTEM: 1E-04 [m]
TIME = 0.1000000E-06 DT = 0.1000000E-06 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0185375871047351 FE = .977481861209078
MN = .00810568126669964 P = 5.3913352823733E-04
SI = .0138733239959838
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 3 seconds
TIME = 0.22705714E-05 DT = 0.21705714E-05 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0185375871047351 FE = .977481861209078
MN = .00810568126669964 P = 5.3913352823733E-04
SI = .0138733239959838
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.66117143E-05 DT = 0.43411429E-05 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0185375871047351 FE = .977481861209078
MN = .00810568126669964 P = 5.3913352823733E-04
SI = .0138733239959838
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.1529400E-04 DT = 0.86822858E-05 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0185375871047351 FE = .977481861209078
MN = .00810568126669964 P = 5.3913352823733E-04
SI = .0138733239959838
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 1 seconds
TIME = 0.32658572E-04 DT = 0.17364572E-04 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0185375871047351 FE = .977481861209078
MN = .00810568126669964 P = 5.3913352823733E-04
SI = .0138733239959838
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.67387715E-04 DT = 0.34729143E-04 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0185375871047351 FE = .977481861209078
MN = .00810568126669964 P = 5.3913352823733E-04
SI = .0138733239959838
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.13684600E-03 DT = 0.69458286E-04 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0185375871047351 FE = .977481861209078
MN = .00810568126669964 P = 5.3913352823733E-04
SI = .0138733239959838
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.27576257E-03 DT = 0.13891657E-03 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0185375871047351 FE = .977481861209078
MN = .00810568126669964 P = 5.3913352823733E-04
SI = .0138733239959838
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.55359572E-03 DT = 0.27783314E-03 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0185375871047351 FE = .977481861209078
MN = .00810568126669964 P = 5.3913352823733E-04
SI = .0138733239959838
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 1 seconds
TIME = 0.11092620E-02 DT = 0.55566629E-03 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .018537587104735 FE = .977481861209078
MN = .00810568126669964 P = 5.3913352823733E-04
SI = .0138733239959838
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.22205946E-02 DT = 0.11113326E-02 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .018537587104735 FE = .977481861209078
MN = .00810568126669965 P = 5.3913352823733E-04
SI = .0138733239959838
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.44432597E-02 DT = 0.22226652E-02 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0185375871047351 FE = .977481861209078
MN = .00810568126669965 P = 5.3913352823733E-04
SI = .0138733239959838
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.88885901E-02 DT = 0.44453303E-02 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0185375871047351 FE = .977481861209078
MN = .00810568126669964 P = 5.3913352823733E-04
SI = .0138733239959838
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.17779251E-01 DT = 0.88906606E-02 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0185375871047351 FE = .977481861209078
MN = .00810568126669963 P = 5.3913352823733E-04
SI = .0138733239959838
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
```

```

TIME = 0.35560572E-01 DT = 0.17781321E-01 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0185375871047351 FE = .977481861209078
MN = .00810568126669965 P = 5.39133528237329E-04
SI = .0138733239959838
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.71123215E-01 DT = 0.35562643E-01 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0185375871047355 FE = .977481861209078
MN = .00810568126669967 P = 5.39133528237328E-04
SI = .0138733239959839
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 1 seconds
TIME = 0.14224850 DT = 0.71125285E-01 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0185375871047348 FE = .977481861209078
MN = .0081056812666996 P = 5.39133528237325E-04
SI = .0138733239959839
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.28449907 DT = 0.14225057 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0185375871047348 FE = .977481861209078
MN = .00810568126669969 P = 5.39133528237324E-04

```

output ignored...

... output resumed

```

DELETING TIME-RECORD FOR TIME 920.10258
DELETING TIME-RECORD FOR TIME 935.10258
DELETING TIME-RECORD FOR TIME 950.10258
DELETING TIME-RECORD FOR TIME 965.10258
DELETING TIME-RECORD FOR TIME 980.10258
DELETING TIME-RECORD FOR TIME 995.10258
DELETING TIME-RECORD FOR TIME 1010.1026
DELETING TIME-RECORD FOR TIME 1025.1026
DELETING TIME-RECORD FOR TIME 1040.1026
DELETING TIME-RECORD FOR TIME 1055.1026
DELETING TIME-RECORD FOR TIME 1070.1026
DELETING TIME-RECORD FOR TIME 1085.1026
DELETING TIME-RECORD FOR TIME 1100.1026
DELETING TIME-RECORD FOR TIME 1115.1026
DELETING TIME-RECORD FOR TIME 1130.1026
DELETING TIME-RECORD FOR TIME 1145.1026
DELETING TIME-RECORD FOR TIME 1160.1026
DELETING TIME-RECORD FOR TIME 1175.1026
DELETING TIME-RECORD FOR TIME 1190.1026
DELETING TIME-RECORD FOR TIME 1205.1026
DELETING TIME-RECORD FOR TIME 1220.1026
DELETING TIME-RECORD FOR TIME 1235.1026
DELETING TIME-RECORD FOR TIME 1250.1026
DELETING TIME-RECORD FOR TIME 1265.1026
DELETING TIME-RECORD FOR TIME 1280.1026
DELETING TIME-RECORD FOR TIME 1295.1026
DELETING TIME-RECORD FOR TIME 1310.1026
DELETING TIME-RECORD FOR TIME 1325.1026
DELETING TIME-RECORD FOR TIME 1340.1026
DELETING TIME-RECORD FOR TIME 1355.1026
DELETING TIME-RECORD FOR TIME 1370.1026
DELETING TIME-RECORD FOR TIME 1385.1026
DELETING TIME-RECORD FOR TIME 1400.1026
DELETING TIME-RECORD FOR TIME 1415.1026
DELETING TIME-RECORD FOR TIME 1430.1026
DELETING TIME-RECORD FOR TIME 1445.1026
DELETING TIME-RECORD FOR TIME 1460.1026
DELETING TIME-RECORD FOR TIME 1475.1026
DELETING TIME-RECORD FOR TIME 1490.1026
DELETING TIME-RECORD FOR TIME 1505.1026
DELETING TIME-RECORD FOR TIME 1520.1026
DELETING TIME-RECORD FOR TIME 1535.1026
DELETING TIME-RECORD FOR TIME 1550.1026
DELETING TIME-RECORD FOR TIME 1565.1026
DELETING TIME-RECORD FOR TIME 1580.1026
DELETING TIME-RECORD FOR TIME 1595.1026
DELETING TIME-RECORD FOR TIME 1610.1026
DELETING TIME-RECORD FOR TIME 1625.1026
DELETING TIME-RECORD FOR TIME 1640.1026
DELETING TIME-RECORD FOR TIME 1655.1026
DELETING TIME-RECORD FOR TIME 1670.1026
DELETING TIME-RECORD FOR TIME 1685.1026
DELETING TIME-RECORD FOR TIME 1700.1026
DELETING TIME-RECORD FOR TIME 1715.1026
DELETING TIME-RECORD FOR TIME 1730.1026
DELETING TIME-RECORD FOR TIME 1745.1026
DELETING TIME-RECORD FOR TIME 1760.1026
DELETING TIME-RECORD FOR TIME 1775.1026
DELETING TIME-RECORD FOR TIME 1790.1026
DELETING TIME-RECORD FOR TIME 1805.1026
DELETING TIME-RECORD FOR TIME 1820.1026
DELETING TIME-RECORD FOR TIME 1835.1026
DELETING TIME-RECORD FOR TIME 1850.1026
DELETING TIME-RECORD FOR TIME 1865.1026
DELETING TIME-RECORD FOR TIME 1880.1026
DELETING TIME-RECORD FOR TIME 1895.1026
DELETING TIME-RECORD FOR TIME 1910.1026
DELETING TIME-RECORD FOR TIME 1925.1026
DELETING TIME-RECORD FOR TIME 1940.1026
DELETING TIME-RECORD FOR TIME 1955.1026
DELETING TIME-RECORD FOR TIME 1970.1026
DELETING TIME-RECORD FOR TIME 1985.1026
DELETING TIME-RECORD FOR TIME 2000.1026
DELETING TIME-RECORD FOR TIME 2015.1026
DELETING TIME-RECORD FOR TIME 2030.1026
DELETING TIME-RECORD FOR TIME 2045.1026
DELETING TIME-RECORD FOR TIME 2060.1026
DELETING TIME-RECORD FOR TIME 2075.1026
DELETING TIME-RECORD FOR TIME 2090.1026
DELETING TIME-RECORD FOR TIME 2105.1026
DELETING TIME-RECORD FOR TIME 2120.1026
DELETING TIME-RECORD FOR TIME 2135.1026
DELETING TIME-RECORD FOR TIME 2150.1026
DELETING TIME-RECORD FOR TIME 2165.1026
DELETING TIME-RECORD FOR TIME 2180.1026
DELETING TIME-RECORD FOR TIME 2195.1026
DELETING TIME-RECORD FOR TIME 2210.1026

```

DELETING TIME-RECORD FOR TIME 2225.1026  
DELETING TIME-RECORD FOR TIME 2240.1026  
DELETING TIME-RECORD FOR TIME 2255.1026  
DELETING TIME-RECORD FOR TIME 2270.1026  
DELETING TIME-RECORD FOR TIME 2285.1026  
DELETING TIME-RECORD FOR TIME 2300.1026  
DELETING TIME-RECORD FOR TIME 2315.1026  
DELETING TIME-RECORD FOR TIME 2330.1026  
DELETING TIME-RECORD FOR TIME 2345.1026  
DELETING TIME-RECORD FOR TIME 2360.1026  
DELETING TIME-RECORD FOR TIME 2375.1026  
DELETING TIME-RECORD FOR TIME 2390.1026  
DELETING TIME-RECORD FOR TIME 2405.1026  
DELETING TIME-RECORD FOR TIME 2420.1026  
DELETING TIME-RECORD FOR TIME 2435.1026  
DELETING TIME-RECORD FOR TIME 2450.1026  
DELETING TIME-RECORD FOR TIME 2465.1026  
DELETING TIME-RECORD FOR TIME 2480.1026  
DELETING TIME-RECORD FOR TIME 2495.1026  
DELETING TIME-RECORD FOR TIME 2510.1026  
DELETING TIME-RECORD FOR TIME 2525.1026  
DELETING TIME-RECORD FOR TIME 2540.1026  
DELETING TIME-RECORD FOR TIME 2555.1026  
DELETING TIME-RECORD FOR TIME 2570.1026  
DELETING TIME-RECORD FOR TIME 2585.1026  
DELETING TIME-RECORD FOR TIME 2600.1026  
DELETING TIME-RECORD FOR TIME 2615.1026  
DELETING TIME-RECORD FOR TIME 2630.1026  
DELETING TIME-RECORD FOR TIME 2645.1026  
DELETING TIME-RECORD FOR TIME 2660.1026  
DELETING TIME-RECORD FOR TIME 2675.1026  
DELETING TIME-RECORD FOR TIME 2690.1026  
DELETING TIME-RECORD FOR TIME 2705.1026  
DELETING TIME-RECORD FOR TIME 2720.1026  
DELETING TIME-RECORD FOR TIME 2735.1026  
DELETING TIME-RECORD FOR TIME 2750.1026  
DELETING TIME-RECORD FOR TIME 2765.1026  
DELETING TIME-RECORD FOR TIME 2780.1026  
DELETING TIME-RECORD FOR TIME 2795.1026  
DELETING TIME-RECORD FOR TIME 2810.1026  
DELETING TIME-RECORD FOR TIME 2825.1026  
DELETING TIME-RECORD FOR TIME 2840.1026  
DELETING TIME-RECORD FOR TIME 2855.1026  
DELETING TIME-RECORD FOR TIME 2870.1026  
DELETING TIME-RECORD FOR TIME 2885.1026  
DELETING TIME-RECORD FOR TIME 2900.1026  
DELETING TIME-RECORD FOR TIME 2915.1026  
DELETING TIME-RECORD FOR TIME 2930.1026  
DELETING TIME-RECORD FOR TIME 2945.1026  
DELETING TIME-RECORD FOR TIME 2960.1026  
DELETING TIME-RECORD FOR TIME 2975.1026

KEEPING TIME-RECORD FOR TIME 2990.1026  
AND FOR TIME 3000.0000  
WORKSPACE RECLAIMED

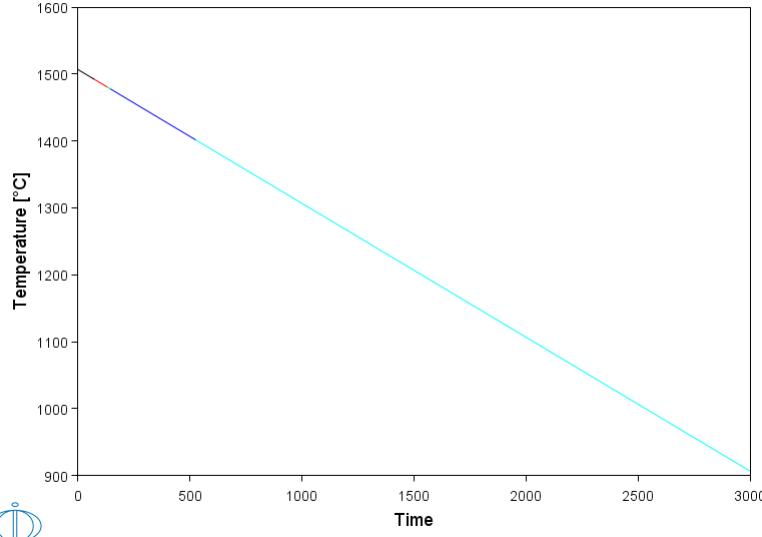
TIMESTEP AT 3000.00000 SELECTED

DIC>  
DIC> set-inter  
--OK---  
DIC>

**exb6-plot**

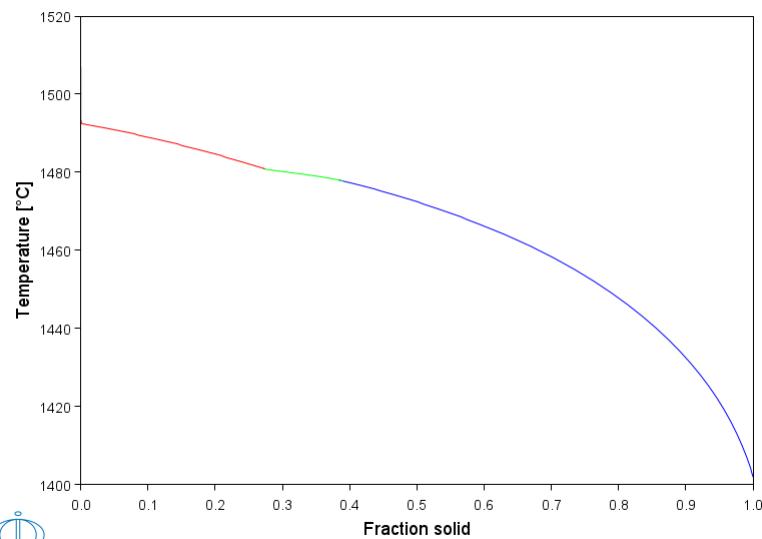
```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exb6\plot.DCM.test"
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 3.00000E+03
DIC> read exb6
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1: set-title Fe-0.4%C-0.7%Si-0.8%Mn-0.03%P
POST-1:
POST-1: s-d-a y t-c
POST-1: s-d-a x time
INFO: Time is set as independent variable
POST-1: s-p-c interf first
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples/unite/distribution\macroResult.exp Y
ORKING ...orking ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

Fe-0.4%C-0.7%Si-0.8%Mn-0.03%P



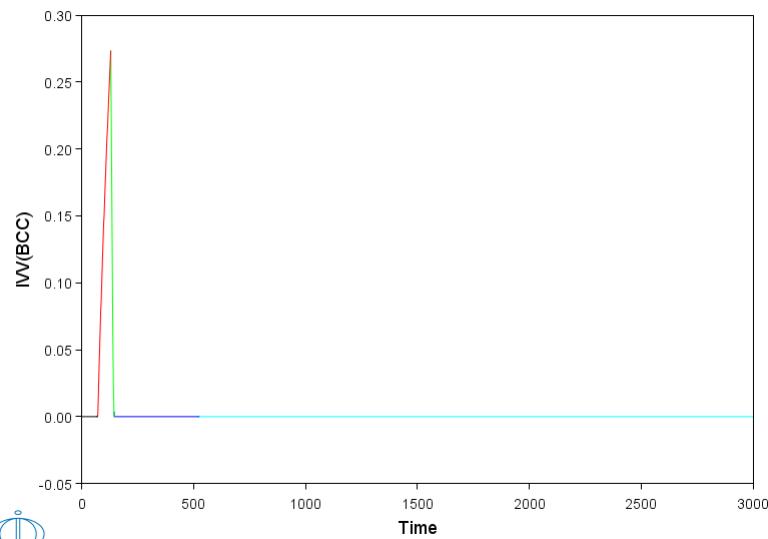
```
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ PLOT THE FRACTION OF SOLID
POST-1: @@
POST-1: enter func fs=1-ivv(liq);
POST-1: s-d-a x fs
POST-1: s-s-s x n 0 1
POST-1: s-ax-te x n Fraction solid
POST-1:
POST-1: s-d-a y t-c
POST-1:
POST-1:
POST-1: s-p-c interf smalta lower
POST-1:
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples/unite/distribution\macroResult.exp Y
ORKING ...orking ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

**Fe-0.4%C-0.7%Si-0.8%Mn-0.03%P**



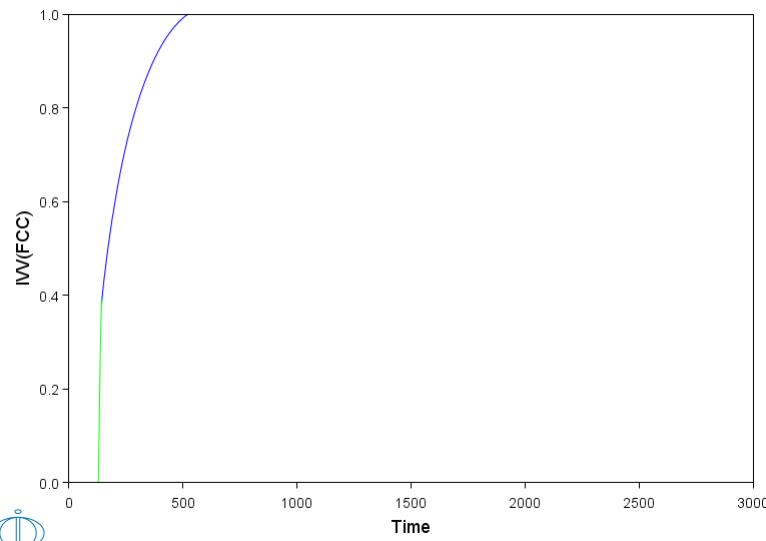
```
POST-1:  
POST-1:Hit RETURN to continue  
POST-1: s-d-a y ivv(bcc)  
POST-1: s-d-a x time  
INFO: Time is set as independent variable  
POST-1:  
POST-1:  
POST-1: SET_EXP_FILE_FORMAT 5  
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y  
ORKING ...orking ... OST-1: SET_EXP_FILE_FORMAT 10  
POST-1:  
POST-1: plot
```

**Fe-0.4%C-0.7%Si-0.8%Mn-0.03%P**



```
POST-1:  
POST-1:Hit RETURN to continue  
POST-1:  
POST-1: s-d-a y ivv(fcc)  
POST-1:  
POST-1: SET_EXP_FILE_FORMAT 5  
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y  
ORKING ...orking ... OST-1: SET_EXP_FILE_FORMAT 10  
POST-1:  
POST-1: plot
```

### Fe-0.4%C-0.7%Si-0.8%Mn-0.03%P

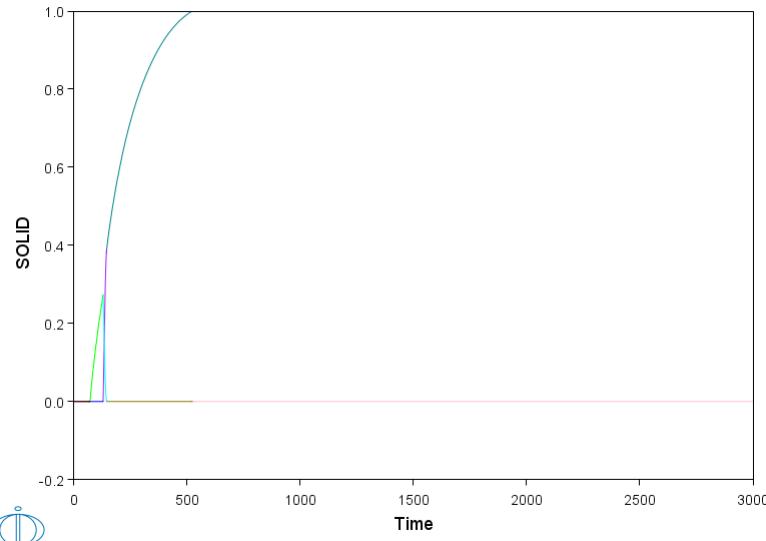


```

POST-1:
POST-1:Hit RETURN to continue
POST-1: ent table solid
Variable(s) ivv(bcc) ivv(fcc)
POST-1:
POST-1: s-d-a y solid
COLUMN NUMBER /*/:
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
ORKING ...orking ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

```

### Fe-0.4%C-0.7%Si-0.8%Mn-0.03%P

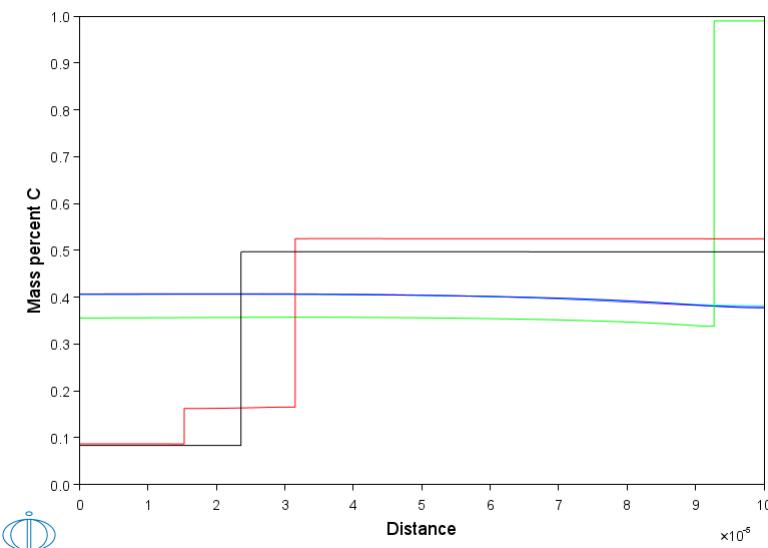


```

POST-1:
POST-1:Hit RETURN to continue
POST-1: s-d-a y w-p c
POST-1: s-d-a x dis gl
INFO: Distance is set as independent variable
POST-1: s-p-c time 120,135,400,700,1500,3000
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
ORKING ...orking ...OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

```

### Fe-0.4%C-0.7%Si-0.8%Mn-0.03%P

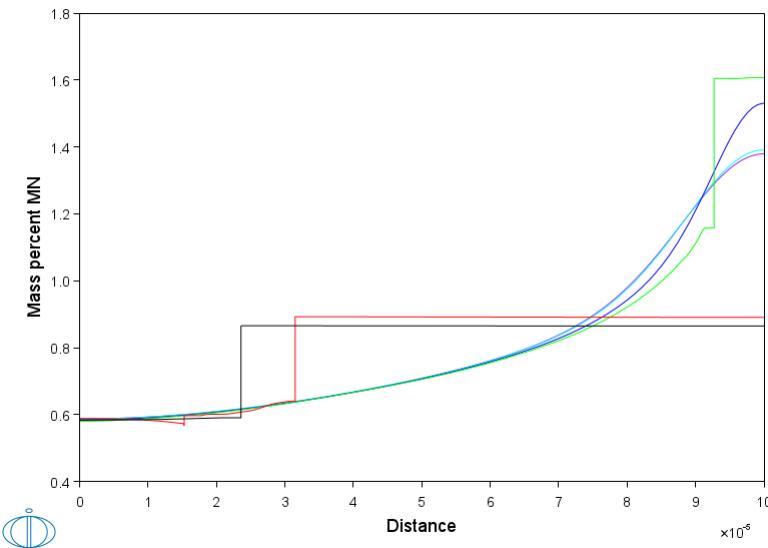


```

POST-1:
POST-1:Hit RETURN to continue
POST-1: s-d-a y w-p mn
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
ORKING ...orking ...OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

```

### Fe-0.4%C-0.7%Si-0.8%Mn-0.03%P

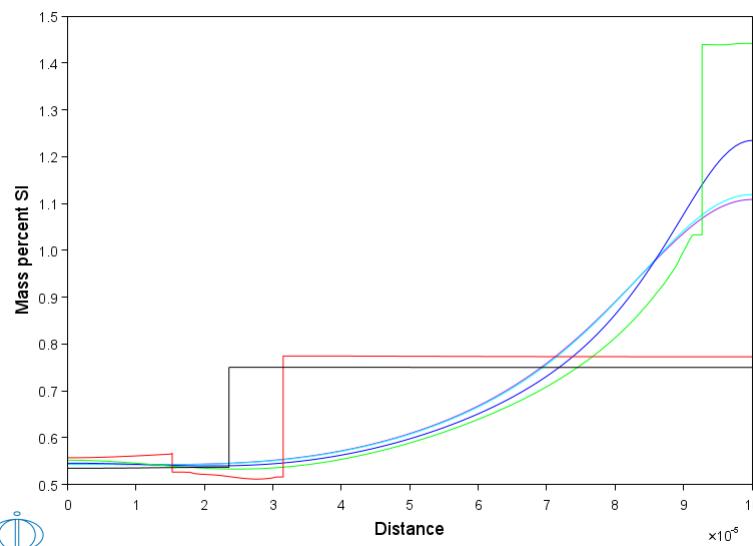


```

POST-1:
POST-1:Hit RETURN to continue
POST-1: s-d-a y w-p si
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
ORKING ...orking ...OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

```

### Fe-0.4%C-0.7%Si-0.8%Mn-0.03%P

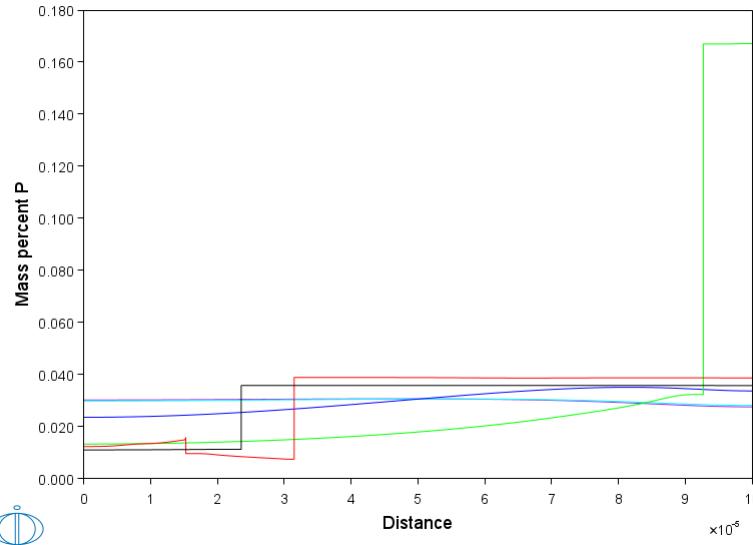


```

POST-1:
POST-1: Hit RETURN to continue
POST-1: s-d-a y w-p p
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
ORKING ...orking ...OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

```

### Fe-0.4%C-0.7%Si-0.8%Mn-0.03%P

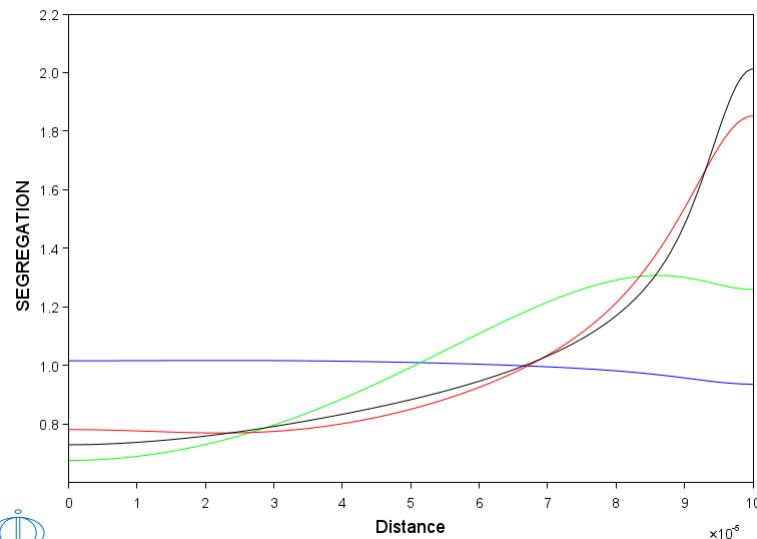


```

POST-1:
POST-1: Hit RETURN to continue
POST-1:
POST-1: ent function mnn
FUNCTION: w(mn)/0.008
&
POST-1: ent function sin
FUNCTION: w(si)/0.007
&
POST-1: ent function pn
FUNCTION: w(p)/0.0003
&
POST-1: ent function cn
FUNCTION: w(c)/0.004
&
POST-1: ent tabel segregation
Variable(s) mnn sin pn cn
POST-1:
POST-1:
POST-1: s-d-a y segregation
COLUMN NUMBER /*:
POST-1:
POST-1:
POST-1: s-p-c time 610
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

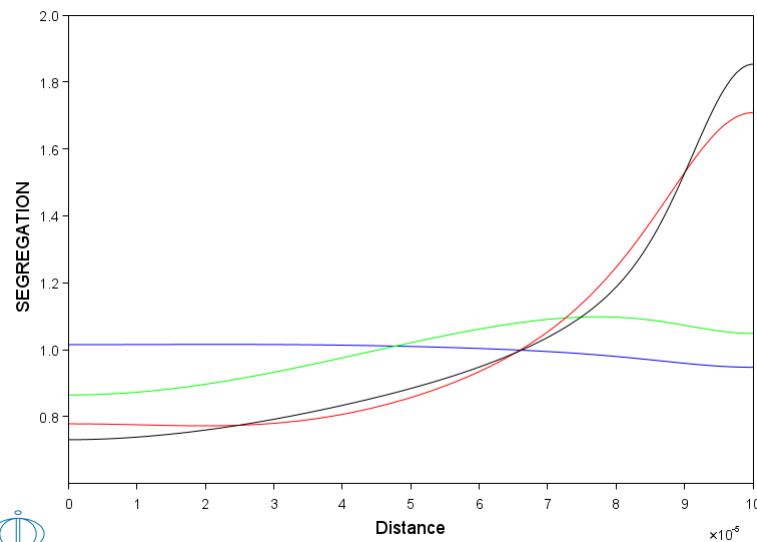
```

**Fe-0.4%C-0.7%Si-0.8%Mn-0.03%P**



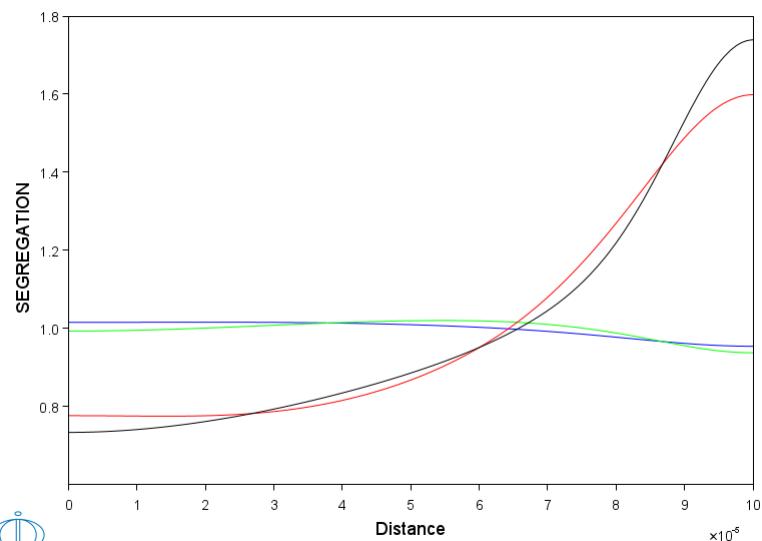
```
POST-1:  
POST-1:Hit RETURN to continue  
POST-1:  
POST-1: s-p-c time 800  
POST-1:  
POST-1: SET_EXP_FILE_FORMAT 5  
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y  
POST-1: SET_EXP_FILE_FORMAT 10  
POST-1:  
POST-1: plot
```

**Fe-0.4%C-0.7%Si-0.8%Mn-0.03%P**



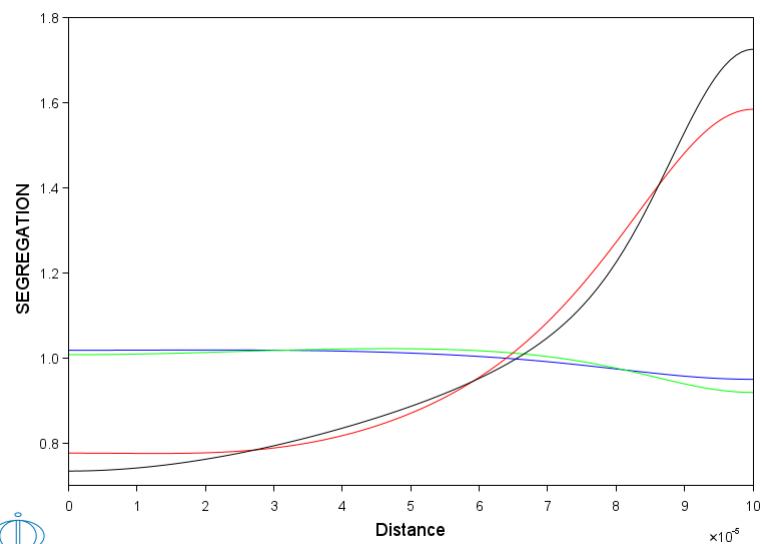
```
POST-1:  
POST-1:Hit RETURN to continue  
POST-1:  
POST-1: s-p-c time 1500  
POST-1:  
POST-1: SET_EXP_FILE_FORMAT 5  
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y  
POST-1: SET_EXP_FILE_FORMAT 10  
POST-1:  
POST-1: plot
```

**Fe-0.4%C-0.7%Si-0.8%Mn-0.03%P**



```
POST-1:  
POST-1:Hit RETURN to continue  
POST-1:  
POST-1: s-p-c time 3000  
POST-1:  
POST-1: SET_EXP_FILE_FORMAT 5  
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y  
POST-1: SET_EXP_FILE_FORMAT 10  
POST-1:  
POST-1: plot
```

**Fe-0.4%C-0.7%Si-0.8%Mn-0.03%P**



```
POST-1:  
POST-1:Hit RETURN to continue  
POST-1: set-inter  
--OK--  
POST-1:
```

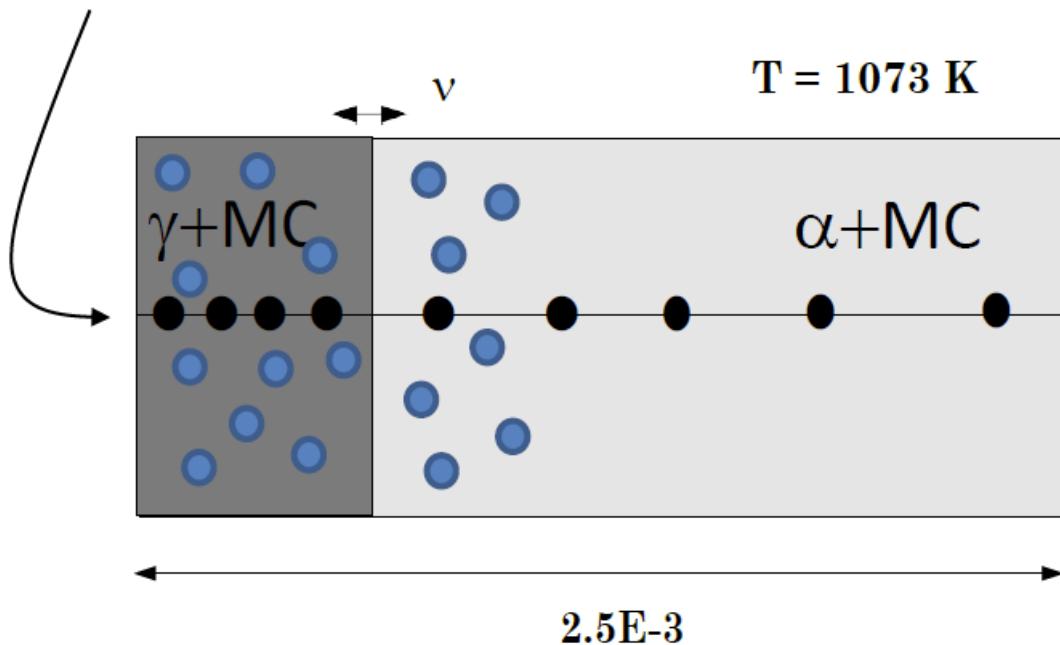


## Example exb7

### Moving boundary problem with multiple phases on each side of the boundary

This example shows how to enter dispersed phases on either side of a phase interface. The particular case shows how the kinetics of a ferrite to austenite transformation is affected by simultaneous precipitation of niobium carbide. The transformation is caused by carburization.

$$\text{ACR}(\text{C}) = 1$$



**exb7-setup****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_dictra_console_examples\examples\exb7\setup.DCM"
SYS: @@ This example modifies the database interactively, which is not
SYS: @@ yet supported by GES6. Therefore, we enforce the use of GES5.
SYS: set-ges-version 5
SYS:
SYS: @@
SYS: @@ Moving boundary problem.
SYS: @@ Moving boundary problem with multiple phases on each side
SYS: @@ This example shows how to enter dispersed phases on either side
SYS: @@ of a phase interface. The particular case shows how
SYS: @@ the kinetics of a ferrite to austenite transformation is
SYS: @@ affected by simultaneous precipitation of niobium carbide.
SYS: @@ The transformation is caused by carburization.
SYS: -----
NO SUCH COMMAND, USE HELP
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASE
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\generate_dictra_console_examples\databases\data
Current database: Steels/Fe-Alloys v12.0

VA           /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE12: @@
TDB_TCFE12: @@
TDB_TCFE12: @@ USE A TCFE DATABASE FOR THERMODYNAMIC DATA
TDB_TCFE12: @@
TDB_TCFE12: sw tcfef9
Current database: Steels/Fe-Alloys v9.3

VA           /- DEFINED
L12_FCC      B2_BCC          DICTRA_FCC_A1
REJECTED
TDB_TCFE9: @@
TDB_TCFE9: @@ DEFINE THE SYSTEM TO WORK WITH
TDB_TCFE9: @@
TDB_TCFE9: def-species fe c nb
FE           C               NB
DEFINED
TDB_TCFE9: @@
TDB_TCFE9: @@
TDB_TCFE9: @@ EXCLUDE THE THERMODYNAMIC DATA FOR THE PHASES THAT ARE NOT NEEDED
TDB_TCFE9: @@
TDB_TCFE9: rej ph * all
GAS:G          LIQUID:L        BCC_A2
FCC_A1         HCP_A3          CBCC_A12
CUB_A13        DIAMOND_FCC_A4 GRAPHITE
CEMENTITE      M23C6          M7C3
M6C            M5C2           KSI_CARBIDE
Z_PHASE        FE4N_LP1        FECN_CHI
SIGMA          MU_PHASE       LAVES_PHASE_C14
G_PHASE        CR3SI          NBNi3-
AL5FE4 REJECTED
TDB_TCFE9: res ph fcc bcc grap
FCC_A1         BCC_A2          GRAPHITE
RESTORED
TDB_TCFE9: @@
TDB_TCFE9: @@
TDB_TCFE9: @@ RETRIEVE DATA FROM THE DATABASE FILE
TDB_TCFE9: @@
TDB_TCFE9: get
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
Creating a new composition set FCC_A1#2
PARAMETERS ...
FUNCTIONS ...

List of references for assessed data

'A. 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, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
    volumes'
'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
'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'
'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
'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'
'B.-J. Lee, Metall. Mater. Trans. A, 32A (2001) 2423-39'
'S. Canderyd, Report IM-2005-109, Stockholm, Sweden; Fe-Nb-C'
'W. Huang, Z. Metallkd., 6 (1990) 397-404; Fe-Nb-C'
-OK-
TDB_TCFE9: @@
TDB_TCFE9: @@
TDB_TCFE9: @@ NOW APPEND A SSUB DATABASE FROM WHICH WE READ THE THERMODYNAMIC
TDB_TCFE9: @@ DESCRIPTION OF NIOBIUM CARBIDE
```

```

TDB_TCFE9: @@
TDB_TCFE9:
TDB_TCFE9: app SSUB6
Current database: SGTE Substances v6.0

VA DEFINED
APP: def-sys fe c nb
FE C NB
DEFINED
APP: rej ph *
GAS:G C0_749NB1_S C0_877NB1_S
C0_98NB1_S C_S C_L
DIAMOND C1FE3_S C1NB1_S
C1NB2_S C60_S FE_S
FE_S2 FE_S3 FE_L
FE2NB1_S NB_S NB_L
REJECTED
APP: rest ph c1nb1_s
C1NB1_S RESTORED
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS .....

List of references for assessed data

C1NB1 I. BARIN 3rd. Edition
C1NB1
Data taken from BARIN 3rd. Ed. (1995)
-OK-
APP:
APP: @@ MOBILITY/DIFFUSIVITY DATA ARE STORED IN A SEPARATE DATABASE FILE.
APP: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE THE DATA
APP: @@ app mobfe4
Current database: Steels/Fe-Alloys Mobility v4.0

VA DEFINED
B2_BCC REJECTED
APP: def-sys fe c nb
FE C NB
DEFINED
APP: rej ph * all
BCC_A2 CEMENTITE FCC_A1
FE4N_LP1 HCP_A3 LIQUID:L
REJECTED
APP: res ph fcc bcc
FCC_A1 BCC_A2 RESTORED
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS .....

List of references for assessed data

'This parameter has not been assessed'
'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'
'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
-Ni'
'J. Geise and Ch. Herzog, Z. Metallkd. 76(1985)622.; Impurity diffusion of
Nb in fcc Fe.'
'Assessed from data presented by B. B. Yu and R. F. Davis J. Phys. Chem.
Solids 40(1979)997.; C Self-Diff in NbC.'
'B. Jonsson: Z. Metallkunde 85(1994)498-501; C and N diffusion in bcc Cr
-Fe-Ni'
'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
in bcc Fe'
'R. F. Peart, Acta Metall. 10(1962)519.; Impurity diffusion of Fe in bcc
Nb.'
'Assessed from data presented in Landolt-Bornstein, Vol. 26, ed. H.
Mehrer, Springer (1990); Impurity diff of Nb in bcc Fe.'
'R. E. Einziger et al., Phys. Rev. B 17(1978)440.; self-diffusion of Nb in
bcc Nb.'

-OK-
APP:
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP
APP: @@
APP: go d-m
NO TIME STEP DEFINED
*** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
*** ENTERING C1NB1_S AS A DIFFUSION NONE PHASE
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T 0 1073.15; * N
DIC>
DIC> @@
DIC> @@ ENTER REGIONS ferr AND aus
DIC> @@
DIC> enter-region
REGION NAME : ferr
DIC>
DIC> ent-reg
REGION NAME : aus
ATTACH TO REGION NAMED /FERR/: ferr
ATTACHED TO THE RIGHT OF FERR /YES/: n
DIC>
DIC> @@
DIC> @@ ENTER GRIDS INTO REGIONS
DIC> @@
DIC> enter-grid
REGION NAME : /AUS/: ferr
WIDTH OF REGION /1/: 2.499999e-3
TYPE /LINEAR/: AUTO
DIC>

```

```

DIC>
DIC> enter-grid
REGION NAME : /AUS/: aus
WIDTH OF REGION /1/: 1e-9
TYPE /LINEAR/: AUTO
DIC>
DIC>
DIC> @@
DIC> @@ ENTER active PHASES INTO REGIONS
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /AUS/: ferr
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: bcc
DIC>
DIC>
DIC> en-ph
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /AUS/: ferr
PHASE TYPE /MATRIX/: sph
PHASE NAME: /NONE/: c1nb1_s
INFO: EQUILIBRIUM COMPOSITION AND FRACTION OF SPHEROID PHASES USED AS DEFAULT
DIC>
DIC>
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /AUS/: aus
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC>
DIC> en-ph
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /AUS/: aus
PHASE TYPE /MATRIX/: sph
PHASE NAME: /NONE/: c1nb1_s
INFO: EQUILIBRIUM COMPOSITION AND FRACTION OF SPHEROID PHASES USED AS DEFAULT
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITIONS OF THE PHASES
DIC> @@
DIC> enter-composition
REGION NAME : /AUS/: ferr
PHASE NAME: /BCC_A2/: bcc
DEPENDENT COMPONENT ? /NB/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: C
TYPE /LINEAR/: lin
VALUE OF FIRST POINT : 1e-3
VALUE OF LAST POINT : /1E-3/: 1e-3
PROFILE FOR /NB/: nb
TYPE /LINEAR/: lin
VALUE OF FIRST POINT : 0.28
VALUE OF LAST POINT : /0.28/: 0.28
DIC>
DIC> en-co
REGION NAME : /AUS/: ferr
PHASE NAME: /BCC_A2/: c1nb1_s
USE EQUILIBRIUM VALUE /Y/: y
DIC>
DIC> enter-composition
REGION NAME : /AUS/: aus
PHASE NAME: /FCC_A1#1/: fcc#1
DEPENDENT COMPONENT ? /NB/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: C
TYPE /LINEAR/: lin
VALUE OF FIRST POINT : 0.89
VALUE OF LAST POINT : /0.89/: 0.89
PROFILE FOR /NB/: nb
TYPE /LINEAR/: lin
VALUE OF FIRST POINT : 0.28
VALUE OF LAST POINT : /0.28/: 0.28
DIC>
DIC> en-co
REGION NAME : /AUS/: aus
PHASE NAME: /FCC_A1#1/: c1nb1_s
USE EQUILIBRIUM VALUE /Y/: y
DIC>
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 32400
AUTOMATIC TIMESTEP CONTROL /YES/: y
MAX TIMESTEP DURING INTEGRATION /3240/: 3240
INITIAL TIMESTEP : /1E-07/: 1e-8
SMALLEST ACCEPTABLE TIMESTEP : /1E-08/: 1e-15
DIC>
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ SET THE REFERENCE PHASE OF CARBON AS GRAPHITE
DIC> @@
DIC> s-ref
Component: c
Reference state: grap
Temperature /*/: *
Pressure /100000/: 1e5
DIC>
DIC> @@
DIC> @@ SET THE BOUNDARY CONDITION.
DIC> @@ THE CARBON ACTIVITY IS THE ONE ON THE BOUNDARY
DIC> @@
DIC> s-cond
GLOBAL OR BOUNDARY CONDITION /GLOBAL/: bound
BOUNDARY /LOWER/: low

```

```
CONDITION TYPE /CLOSED_SYSTEM/: mix
Dependent substitutional element:FE
Dependent interstitial element:VA
TYPE OF CONDITION FOR COMPONENT C /ZERO_FLUX/: act
LOW TIME LIMIT /0/: 0
ACR(C) (TIME)= 1.0;
HIGH TIME LIMIT /*/: *
ANY MORE RANGES /N/: N
TYPE OF CONDITION FOR COMPONENT NB /ZERO_FLUX/: zero
DIC>
DIC> @@ 
DIC> @@ ENABLE THE HOMOGENIZATION MODEL
DIC> @@ 
DIC> ho y y
INFO: HOMOGENIZATION MODEL ENABLED
DIC>
DIC>
DIC>
DIC>
DIC> @@ 
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@ 
DIC> save exb7 Y
DIC>
DIC>
DIC> set-inter
--OK---
DIC>
```

**exb7-run**

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exb7\run.DCM"
DIC> @@
DIC> @@ READ THE SET UP FROM FILE AND START THE SIMULATION
DIC> @@
DIC>
DIC> go d-m
TIME STEP AT TIME 0.00000E+00
*** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
*** ENTERING C1NB1_S AS A DIFFUSION NONE PHASE
DIC> read exb7
OK
DIC> sim yes
Region: AUS
double geometric
dense at outer boundaries, coarse at 0.50000E-09
lower part 1.0800 16
upper part 0.92593 16
Region: FERR
single geometric dense at 0.0000
1.0800 114
DEGREE OF IMPLICITY SET TO EULER BACKWARD
STARTING SIMULATION USING HOMOGENIZATION MODEL
-----
WARNING: ELEMENT C
IS BOTH INTERSTITIAL AND SUBSTITUTIONAL
AND RESULTS MUST BE INTERPRETED WITH CARE
INFO: PHASE WITH LIMITED SOLUBILITY OF ELEMENT(S) EXIST
A FALBACK PHASE ZZDICTRA GHOST WILL BE DEFINED
ALONG WITH THE FOLLOWING PARAMETERS:
G(ZZDICTRA_GHOST,C;0)-H298(GRAPHITE,C;0)
G(ZZDICTRA_GHOST,FE;0)-H298(BCC_A2,FE;0)
G(ZZDICTRA_GHOST,NB;0)-H298(BCC_A2,NB;0)
L(ZZDICTRA_GHOST,C,FE;0)
L(ZZDICTRA_GHOST,C,NB;0)
L(ZZDICTRA_GHOST,FE,NB;0)
INFO: FCC_A1#2 is stable but not entered in the simulation
WARNING:C1NB1_S HAS NO VOLUME FRACTION, CREATING ONE
WARNING:C1NB1_S HAS NO VOLUME FRACTION, CREATING ONE
Starting time-step t0= 0.000000 dt= 0.1000000E-07
Error 408
Error 408
Starting time-step t0= 0.48828125E-11 dt= 0.48828125E-11
Starting time-step t0= 0.97656250E-11 dt= 0.97656250E-11
Starting time-step t0= 0.19531250E-10 dt= 0.19531250E-10
Starting time-step t0= 0.39062500E-10 dt= 0.39062500E-10
Starting time-step t0= 0.78125000E-10 dt= 0.78125000E-10
Starting time-step t0= 0.15625000E-09 dt= 0.15625000E-09
Starting time-step t0= 0.31250000E-09 dt= 0.15625000E-09
Starting time-step t0= 0.46875000E-09 dt= 0.31250000E-09
Starting time-step t0= 0.78125000E-09 dt= 0.31250000E-09
Starting time-step t0= 0.10937500E-08 dt= 0.31250000E-09
Starting time-step t0= 0.14062500E-08 dt= 0.31250000E-09
Starting time-step t0= 0.17187500E-08 dt= 0.62500000E-09
Starting time-step t0= 0.23437500E-08 dt= 0.62500000E-09
Starting time-step t0= 0.29687500E-08 dt= 0.12500000E-08
Starting time-step t0= 0.42187500E-08 dt= 0.25000000E-08
Starting time-step t0= 0.67187500E-08 dt= 0.50000000E-08
Starting time-step t0= 0.11718750E-07 dt= 0.10000000E-07
Starting time-step t0= 0.21718750E-07 dt= 0.10000000E-07
Starting time-step t0= 0.31718750E-07 dt= 0.10000000E-07
Starting time-step t0= 0.41718750E-07 dt= 0.10000000E-07
Starting time-step t0= 0.51718750E-07 dt= 0.20000000E-07
Starting time-step t0= 0.71718750E-07 dt= 0.20000000E-07
Starting time-step t0= 0.91718750E-07 dt= 0.20000000E-07
Starting time-step t0= 0.11171875E-06 dt= 0.40000000E-07
Starting time-step t0= 0.15171875E-06 dt= 0.40000000E-07
Starting time-step t0= 0.19171875E-06 dt= 0.80000000E-07
Starting time-step t0= 0.27171875E-06 dt= 0.80000000E-07
Starting time-step t0= 0.35171875E-06 dt= 0.16000000E-06
Starting time-step t0= 0.51171875E-06 dt= 0.32000000E-06
Starting time-step t0= 0.83171875E-06 dt= 0.64000000E-06
Starting time-step t0= 0.14717187E-05 dt= 0.12800000E-05
Starting time-step t0= 0.27517187E-05 dt= 0.25600000E-05
Starting time-step t0= 0.53117187E-05 dt= 0.51200000E-05
Starting time-step t0= 0.10431719E-04 dt= 0.10240000E-04
Starting time-step t0= 0.20671719E-04 dt= 0.20480000E-04
Starting time-step t0= 0.41151719E-04 dt= 0.40960000E-04
Starting time-step t0= 0.82111719E-04 dt= 0.81920000E-04
Starting time-step t0= 0.16403172E-03 dt= 0.16384000E-03
Starting time-step t0= 0.32787172E-03 dt= 0.32768000E-03
Starting time-step t0= 0.65555172E-03 dt= 0.65536000E-03
Starting time-step t0= 0.13109117E-02 dt= 0.13107200E-02
Starting time-step t0= 0.26216317E-02 dt= 0.26214400E-02
Starting time-step t0= 0.52430717E-02 dt= 0.52428800E-02
Starting time-step t0= 0.10485952E-01 dt= 0.10485760E-01
Starting time-step t0= 0.20971712E-01 dt= 0.20971520E-01
Starting time-step t0= 0.41943232E-01 dt= 0.41943040E-01
Starting time-step t0= 0.83886272E-01 dt= 0.41943040E-01
Starting time-step t0= 0.12582931 dt= 0.41943040E-01
Starting time-step t0= 0.16777235 dt= 0.83886080E-01
Starting time-step t0= 0.18874387 dt= 0.20971520E-01
Error 408
Error 408
Starting time-step t0= 0.18907155 dt= 0.32768000E-03
Starting time-step t0= 0.18939923 dt= 0.32768000E-03
Starting time-step t0= 0.18972691 dt= 0.32768000E-03
Starting time-step t0= 0.19005459 dt= 0.32768000E-03
Starting time-step t0= 0.19038227 dt= 0.32768000E-03
Starting time-step t0= 0.19070995 dt= 0.32768000E-03
Starting time-step t0= 0.19103763 dt= 0.32768000E-03
Starting time-step t0= 0.19136531 dt= 0.32768000E-03
Starting time-step t0= 0.19169299 dt= 0.32768000E-03
Starting time-step t0= 0.19202067 dt= 0.65536000E-03
Starting time-step t0= 0.19267603 dt= 0.65536000E-03
Starting time-step t0= 0.19333139 dt= 0.65536000E-03
Starting time-step t0= 0.19398675 dt= 0.65536000E-03
Starting time-step t0= 0.19464211 dt= 0.65536000E-03
Starting time-step t0= 0.19529747 dt= 0.65536000E-03
Starting time-step t0= 0.19595283 dt= 0.13107200E-02
Starting time-step t0= 0.19726355 dt= 0.13107200E-02
```

```
Starting time-step t0= 0.19857427 dt= 0.13107200E-02
Starting time-step t0= 0.19988499 dt= 0.13107200E-02
Starting time-step t0= 0.20119571 dt= 0.13107200E-02
Starting time-step t0= 0.20250643 dt= 0.26214400E-02
Starting time-step t0= 0.20512787 dt= 0.26214400E-02
Starting time-step t0= 0.20774931 dt= 0.52428800E-02
Starting time-step t0= 0.21299219 dt= 0.52428800E-02
Starting time-step t0= 0.21823507 dt= 0.52428800E-02
Starting time-step t0= 0.22347795 dt= 0.10485760E-01
Starting time-step t0= 0.23396371 dt= 0.10485760E-01
Starting time-step t0= 0.24444947 dt= 0.10485760E-01
Starting time-step t0= 0.25493523 dt= 0.10485760E-01
Starting time-step t0= 0.26542099 dt= 0.10485760E-01
Starting time-step t0= 0.27590675 dt= 0.20971520E-01
Starting time-step t0= 0.29687827 dt= 0.20971520E-01
Starting time-step t0= 0.31784979 dt= 0.20971520E-01
Starting time-step t0= 0.33882131 dt= 0.20971520E-01
Starting time-step t0= 0.35979283 dt= 0.20971520E-01
Starting time-step t0= 0.38076435 dt= 0.20971520E-01
Starting time-step t0= 0.40173587 dt= 0.20971520E-01
Starting time-step t0= 0.42270739 dt= 0.20971520E-01
Starting time-step t0= 0.44367891 dt= 0.20971520E-01
Starting time-step t0= 0.46465043 dt= 0.20971520E-01
Starting time-step t0= 0.48562195 dt= 0.20971520E-01
Starting time-step t0= 0.50659347 dt= 0.41943040E-01
```

output ignored...

... output resumed

```
DELETING TIME-RECORD FOR TIME 26712.141
DELETING TIME-RECORD FOR TIME 26755.091
DELETING TIME-RECORD FOR TIME 26798.041
DELETING TIME-RECORD FOR TIME 26851.728
DELETING TIME-RECORD FOR TIME 26916.152
DELETING TIME-RECORD FOR TIME 26959.102
DELETING TIME-RECORD FOR TIME 27002.052
DELETING TIME-RECORD FOR TIME 27045.001
DELETING TIME-RECORD FOR TIME 27087.951
DELETING TIME-RECORD FOR TIME 27130.901
DELETING TIME-RECORD FOR TIME 27173.850
DELETING TIME-RECORD FOR TIME 27216.800
DELETING TIME-RECORD FOR TIME 27259.750
DELETING TIME-RECORD FOR TIME 27302.699
DELETING TIME-RECORD FOR TIME 27345.649
DELETING TIME-RECORD FOR TIME 27388.599
DELETING TIME-RECORD FOR TIME 27431.548
DELETING TIME-RECORD FOR TIME 27474.498
DELETING TIME-RECORD FOR TIME 27517.448
DELETING TIME-RECORD FOR TIME 27560.397
DELETING TIME-RECORD FOR TIME 27603.347
DELETING TIME-RECORD FOR TIME 27646.297
DELETING TIME-RECORD FOR TIME 27689.246
DELETING TIME-RECORD FOR TIME 27764.408
DELETING TIME-RECORD FOR TIME 27807.358
DELETING TIME-RECORD FOR TIME 27850.308
DELETING TIME-RECORD FOR TIME 27893.257
DELETING TIME-RECORD FOR TIME 27957.682
DELETING TIME-RECORD FOR TIME 28000.632
DELETING TIME-RECORD FOR TIME 28043.581
DELETING TIME-RECORD FOR TIME 28086.531
DELETING TIME-RECORD FOR TIME 28129.481
DELETING TIME-RECORD FOR TIME 28172.430
DELETING TIME-RECORD FOR TIME 28215.380
DELETING TIME-RECORD FOR TIME 28258.330
DELETING TIME-RECORD FOR TIME 28301.279
DELETING TIME-RECORD FOR TIME 28344.229
DELETING TIME-RECORD FOR TIME 28387.179
DELETING TIME-RECORD FOR TIME 28430.128
DELETING TIME-RECORD FOR TIME 28473.078
DELETING TIME-RECORD FOR TIME 28516.028
DELETING TIME-RECORD FOR TIME 28558.977
DELETING TIME-RECORD FOR TIME 28601.927
DELETING TIME-RECORD FOR TIME 28644.877
DELETING TIME-RECORD FOR TIME 28687.826
DELETING TIME-RECORD FOR TIME 28730.776
DELETING TIME-RECORD FOR TIME 28773.726
DELETING TIME-RECORD FOR TIME 28848.888
DELETING TIME-RECORD FOR TIME 28891.837
DELETING TIME-RECORD FOR TIME 28945.524
DELETING TIME-RECORD FOR TIME 28988.474
DELETING TIME-RECORD FOR TIME 29052.899
DELETING TIME-RECORD FOR TIME 29095.848
DELETING TIME-RECORD FOR TIME 29138.798
DELETING TIME-RECORD FOR TIME 29181.748
DELETING TIME-RECORD FOR TIME 29224.697
DELETING TIME-RECORD FOR TIME 29267.647
DELETING TIME-RECORD FOR TIME 29310.597
DELETING TIME-RECORD FOR TIME 29353.546
DELETING TIME-RECORD FOR TIME 29396.496
DELETING TIME-RECORD FOR TIME 29439.446
DELETING TIME-RECORD FOR TIME 29482.395
DELETING TIME-RECORD FOR TIME 29536.082
DELETING TIME-RECORD FOR TIME 29579.032
DELETING TIME-RECORD FOR TIME 29621.982
DELETING TIME-RECORD FOR TIME 29664.931
DELETING TIME-RECORD FOR TIME 29707.881
DELETING TIME-RECORD FOR TIME 29750.831
DELETING TIME-RECORD FOR TIME 29793.780
DELETING TIME-RECORD FOR TIME 29836.730
DELETING TIME-RECORD FOR TIME 29879.680
DELETING TIME-RECORD FOR TIME 29922.629
DELETING TIME-RECORD FOR TIME 29965.579
DELETING TIME-RECORD FOR TIME 30008.529
DELETING TIME-RECORD FOR TIME 30051.478
DELETING TIME-RECORD FOR TIME 30094.428
DELETING TIME-RECORD FOR TIME 30137.378
DELETING TIME-RECORD FOR TIME 30180.327
DELETING TIME-RECORD FOR TIME 30223.277
DELETING TIME-RECORD FOR TIME 30266.227
DELETING TIME-RECORD FOR TIME 30309.176
DELETING TIME-RECORD FOR TIME 30352.126
DELETING TIME-RECORD FOR TIME 30395.076
```

DELETING TIME-RECORD FOR TIME 30438.025  
DELETING TIME-RECORD FOR TIME 30480.975  
DELETING TIME-RECORD FOR TIME 30523.925  
DELETING TIME-RECORD FOR TIME 30588.349  
DELETING TIME-RECORD FOR TIME 30631.299  
DELETING TIME-RECORD FOR TIME 30674.249  
DELETING TIME-RECORD FOR TIME 30738.673  
DELETING TIME-RECORD FOR TIME 30781.623  
DELETING TIME-RECORD FOR TIME 30824.573  
DELETING TIME-RECORD FOR TIME 30867.522  
DELETING TIME-RECORD FOR TIME 30910.472  
DELETING TIME-RECORD FOR TIME 30953.422  
DELETING TIME-RECORD FOR TIME 30996.371  
DELETING TIME-RECORD FOR TIME 31039.321  
DELETING TIME-RECORD FOR TIME 31082.271  
DELETING TIME-RECORD FOR TIME 31125.220  
DELETING TIME-RECORD FOR TIME 31178.907  
DELETING TIME-RECORD FOR TIME 31221.857  
DELETING TIME-RECORD FOR TIME 31264.807  
DELETING TIME-RECORD FOR TIME 31307.756  
DELETING TIME-RECORD FOR TIME 31350.706  
DELETING TIME-RECORD FOR TIME 31393.656  
DELETING TIME-RECORD FOR TIME 31436.605  
DELETING TIME-RECORD FOR TIME 31479.555  
DELETING TIME-RECORD FOR TIME 31522.505  
DELETING TIME-RECORD FOR TIME 31565.454  
DELETING TIME-RECORD FOR TIME 31608.404  
DELETING TIME-RECORD FOR TIME 31651.354  
DELETING TIME-RECORD FOR TIME 31694.303  
DELETING TIME-RECORD FOR TIME 31737.253  
DELETING TIME-RECORD FOR TIME 31780.203  
DELETING TIME-RECORD FOR TIME 31823.152  
DELETING TIME-RECORD FOR TIME 31866.102  
DELETING TIME-RECORD FOR TIME 31909.052  
DELETING TIME-RECORD FOR TIME 31952.001  
DELETING TIME-RECORD FOR TIME 31994.951  
DELETING TIME-RECORD FOR TIME 32037.901  
DELETING TIME-RECORD FOR TIME 32080.850  
DELETING TIME-RECORD FOR TIME 32123.800  
DELETING TIME-RECORD FOR TIME 32166.750  
DELETING TIME-RECORD FOR TIME 32209.699  
DELETING TIME-RECORD FOR TIME 32252.649  
DELETING TIME-RECORD FOR TIME 32295.599  
DELETING TIME-RECORD FOR TIME 32338.548

KEEPING TIME-RECORD FOR TIME 32381.498  
AND FOR TIME 32400.000  
WORKSPACE RECLAIMED

-----  
INTERPOLATION SCHEME USED THIS FRACTION OF  
THE ALLOCATED MEMORY: 1.00000000000000  
EFFICIENCY FACTOR: 14.9663819050254  
MEMORY FRACTION USAGE PER BRANCH:  
1.00000000000000  
1.00000000000000  
1.00000000000000

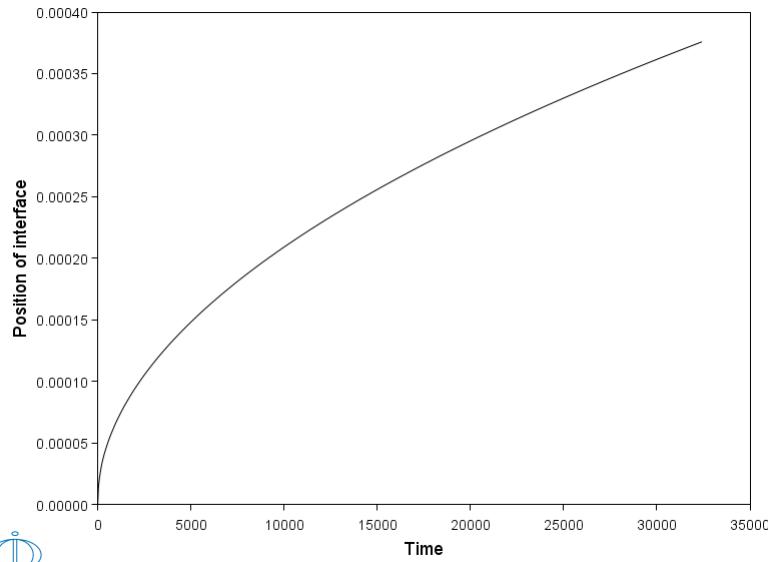
-----  
DEALLOCATING

-----  
TIMESTEP AT 32400.0000 SELECTED

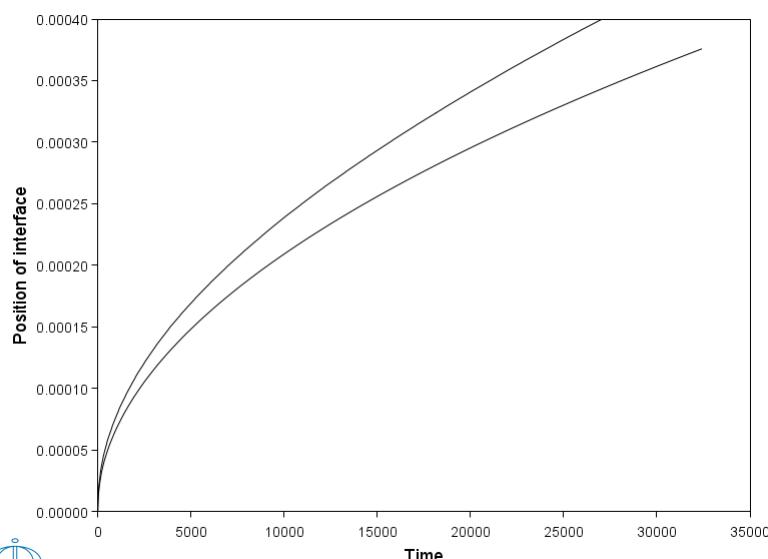
DIC>  
DIC> set-inter  
--OK--  
DIC>

**exb7-plot**

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exb7\plot.DCM"
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 3.24000E+04
*** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
*** ENTERING C1NB1_S AS A DIFFUSION NONE PHASE
DIC> read exb7
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1: @@
POST-1: @@ PLOT THE INTERFACE POSITION AS A FUNCTION OF TIME
POST-1: @@
POST-1: s-d-a x time
INFO: Time is set as independent variable
POST-1: s-d-a y po-o-in aus upp
POST-1:
POST-1: plot
```



```
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ APPEND DATA FROM A CORRESPONDING SIMULATION
POST-1: @@ WITHOUT NIOBIUM
POST-1: @@
POST-1:
POST-1: app y fec.exp 0
DATASET NUMBER(s): /-1/: 1
POST-1:
POST-1: plot
```



POST-1:

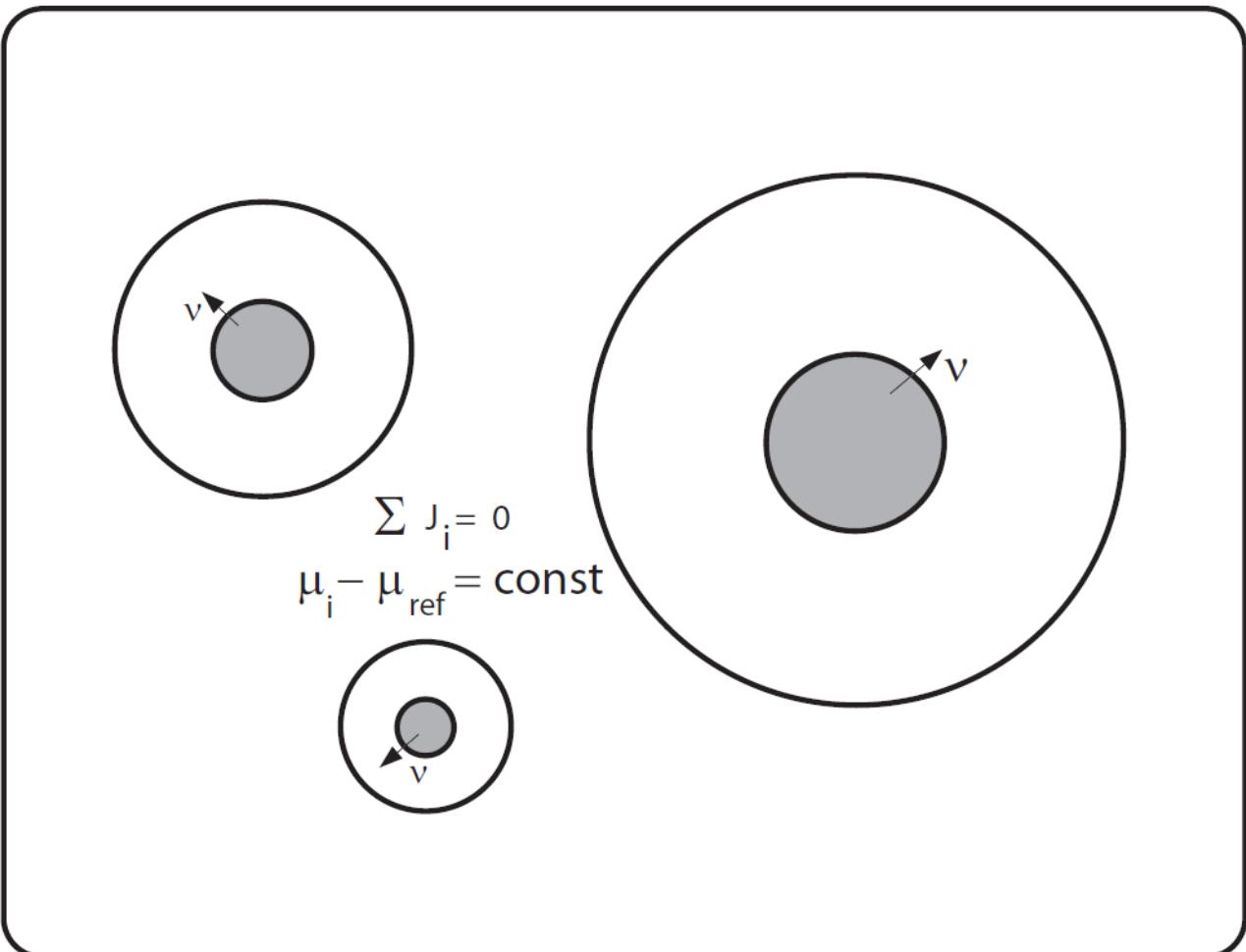
**POST-1:** set-inter

--OK---

**POST-1:**



## Cell Calculations



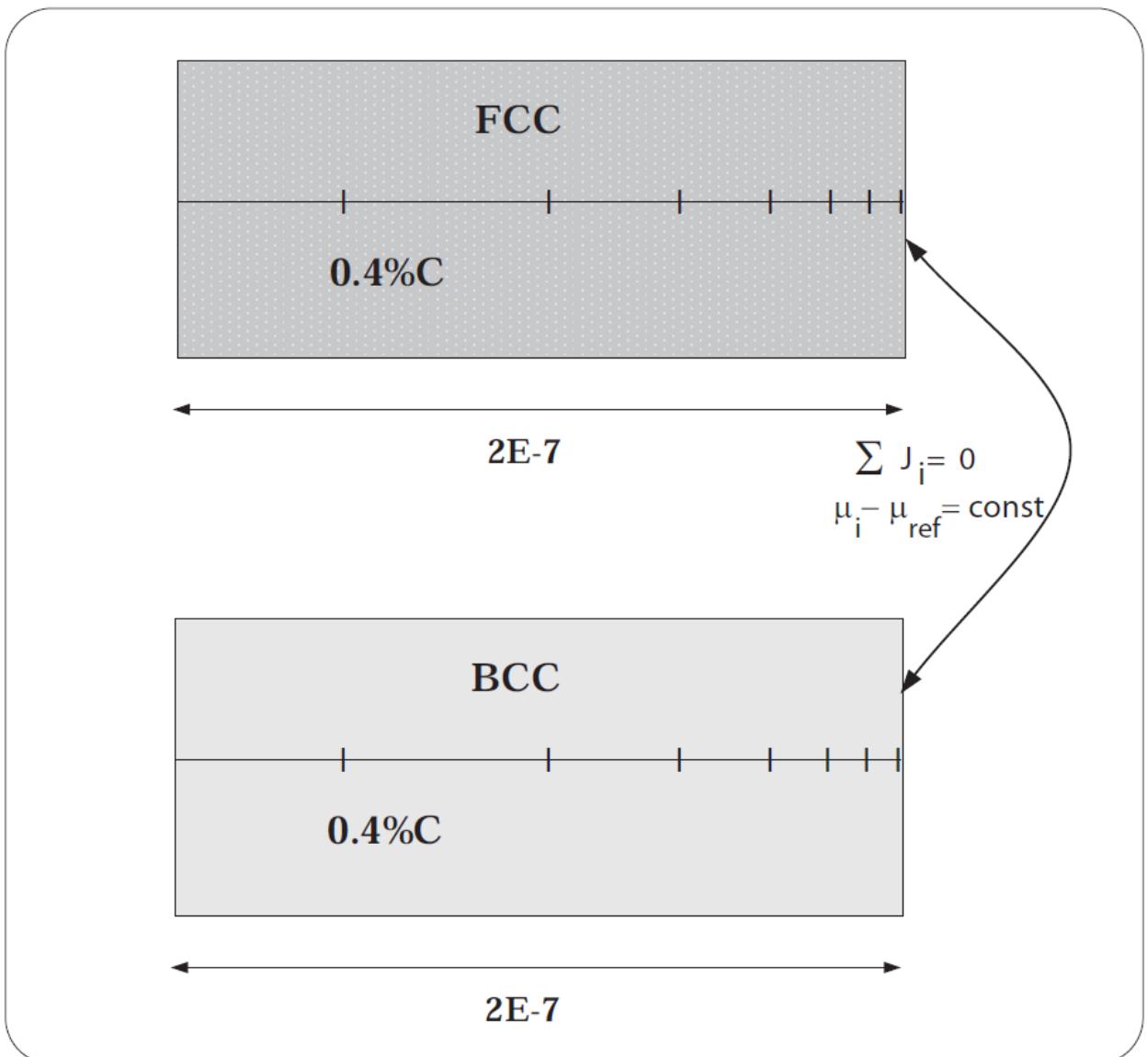


## Example exc1

### 'Carbon cannon' in $\alpha/\gamma$ Fe-C system: Two-cell calculation

This example simulates what happens to a ferrite plate that has inherited the carbon content of its parent austenite. The ferrite plate formed is embedded in an austenite matrix. This setup corresponds to a proposed mechanism for formation of Widmannstätten ferrite or for the ferrite phase of the bainite structure. It is assumed that the phase boundary between ferrite and austenite is immobile, this is achieved in the simulation by putting the ferrite and the austenite in two different cells. See also M. Hillert, L. Höglund and J. Ågren: Acta Metall. Mater. 41 (1993), pp.1951-1957.

$T = 673\text{K}$



**excl-setup****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\_dictra\_console\_examples\examples\excl\setup.DCM"**  
**SYS: i>\_@@**  
NO SUCH COMMAND, USE HELP  
**SYS: @@ Cell calculation.**  
**SYS: @@ Carbon cannon in ferrite/austenite: Fe-C system, 2-cell calculation**  
**SYS: @@ This example simulates what happens to a ferrite plate that has**  
**SYS: @@ inherited the carbon content of its parent austenite. The ferrite**  
**SYS: @@ plate formed is embedded in an austenite matrix. This setup**  
**SYS: @@ corresponds to a proposed mechanism for formation of Widmannst tten**  
**SYS: @@ ferrite or for the ferrite phase of the bainite structure. It is**  
**SYS: @@ assumed that the phase boundary between ferrite and austenite is**  
**SYS: @@ immobile, this is achieved in the simulation by putting the ferrite**  
**SYS: @@ and the austenite in two different cells. See also M. Hillert,**  
**SYS: @@ L. H glund and J.  gren: Acta Metall. Mater. 41 (1993), pp.1951-1957.**  
**SYS: -----**  
NO SUCH COMMAND, USE HELP  
**SYS:**  
**SYS: @@ excl\_setup.DCM**  
**SYS:**  
**SYS: @@**  
**SYS: @@ RETRIEVE DATA FROM THE DATABASE**  
**SYS: @@**  
**SYS: go da**  
THERMODYNAMIC DATABASE module  
Database folder:  
C:\jenkins\workspace\generate\_dictra\_console\_examples\databases\data  
Current database: Steels/Fe-Alloys v12.0  
  
VA                   /- DEFINED  
DICTRA\_FCC\_A1 REJECTED  
**TDB\_TCFE12:**  
**TDB\_TCFE12: @@**  
**TDB\_TCFE12: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA**  
**TDB\_TCFE12: @@**  
**TDB\_TCFE12: sw fedemo**  
Current database: Iron Demo Database v4.0  
  
VA                   /- DEFINED  
**TDB\_FEDEMO: def-sys fe c**                   C DEFINED  
**FE**  
**TDB\_FEDEMO: rej ph \* all**  
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,bcc**  
FCC\_A1                BCC\_A2 RESTORED  
**TDB\_FEDEMO: get**  
17:22:41,996 [Thread-0] INFO JavaWrapper: \*\*\* Invoking Gibbs Energy System v6 \*\*\*  
REINITIATING GES ....  
ELEMENTS ....  
SPECIES ....  
PHASES ....  
PARAMETERS ...  
FUNCTIONS ....  
  
List of references for assessed data  
  
'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'  
'X.G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'  
'A.T. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'  
'X.G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar  
volumes'  
-OK-  
**TDB\_FEDEMO:**  
**TDB\_FEDEMO: @@**  
**TDB\_FEDEMO: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE DATA**  
**TDB\_FEDEMO: @@**  
**TDB\_FEDEMO: app mfdemo**  
Current database: Fe-Alloys Mobility demo database v2.0  
  
VA   DEFINED  
**APP: def-sys fe c**                   C DEFINED  
**FE**  
**APP: rej ph \* all**  
BCC\_A2                FCC\_A1                   CEMENTITE  
REJECTED  
**APP: res ph fcc,bcc**  
FCC\_A1                BCC\_A2 RESTORED  
**APP: get**  
ELEMENTS ....  
SPECIES ....  
PHASES ....  
PARAMETERS ...  
FUNCTIONS ....  
  
List of references for assessed data  
  
'This parameter has not been assessed'  
'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'  
'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe  
-Ni'  
'B. Jonsson: Z. Metallkunde 85(1994)498-501; C and N diffusion in bcc Cr  
-Fe-Ni'

```

'B. Jonsson: Z. Metallkunde 83(1992) 349-355; Cr, Co, Fe and Ni diffusion
in bcc Fe'
-OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR
APP: @@
APP: go d-m
NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 673; * N
DIC>
DIC> @@
DIC> @@ IN THE FIRST CELL
DIC> @@
DIC> @@ ENTER REGION aus CONTAINING AUSTENITE
DIC> @@ ENTER A GEOMETRICAL GRID INTO THAT REGION
DIC> @@ ENTER THE INITIAL COMPOSITION INTO THE AUSTENITE
DIC> @@
DIC> enter-region aus
DIC> enter-grid aus 0.2e-6 AUTO
DIC> enter-phase act aus matrix fcc_a1#1
DIC>
DIC> enter-composition
REGION NAME : /AUS/: aus
PHASE NAME: /FCC_A1/: fcc_a1#1
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: c
TYPE /LINEAR/: lin 0.4 0.4
DIC>
DIC> @@
DIC> @@ IN THE SECOND CELL
DIC> @@
DIC> create-new-cell
CELL DISTRIBUTION FACTOR /1/: 1
CREATING NEW CELL, NUMBER: 2
CELL 2 SELECTED
DIC-2>
DIC-2> @@
DIC-2> @@ ENTER REGION fer CONTAINING FERRITE
DIC-2> @@ ENTER A GEOMETRICAL GRID INTO THAT REGION
DIC-2> @@ ENTER THE INITIAL COMPOSITION INTO THE FERRITE
DIC-2> @@
DIC-2> enter-region fer
DIC-2>
DIC-2>
DIC-2>
DIC-2> enter-grid fer 0.2e-6 AUTO
DIC-2> enter-phase act fer matrix bcc_a2#1
DIC-2>
DIC-2> enter-composition
REGION NAME : /FER/: fer
PHASE NAME: /BCC_A2/: bcc_a2#1
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: c
TYPE /LINEAR/: lin 0.4 0.4
DIC-2>
DIC-2> @@
DIC-2> @@ SET THE SIMULATION TIME AND OTHER SIMULATION PARAMETERS
DIC-2> @@
DIC-2> set-simulation-time
END TIME FOR INTEGRATION /1/: 0.5
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /.05/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC-2>
DIC-2>
DIC-2>
DIC-2> @@
DIC-2> @@ USE IMPLICIT (1) TIME INTEGRATION
DIC-2> @@
DIC-2> set-simulation-cond
NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA Timesteps IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /AUTO/:
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPURITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -> 1): /AUTO/: 1.0
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/:
DIC-2> @@
DIC-2> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC-2> @@
DIC-2> save excl Y
DIC-2>
DIC-2> set-inter
--OK--
DIC-2>

```

**excl-run**

**DIC-2>About**  
NO SUCH COMMAND, USE HELP  
**DIC-2>MACRO "c:\jenkins\workspace\generate\_dictra\_console\_examples\examples\excl\run.DCM"**  
**DIC-2>**  
**DIC-2>**  
**DIC-2> @@ excl\_run.DCM**  
**DIC-2>**  
**DIC-2> @@**  
**DIC-2> @@ READ THE WORKSPACE AND START THE SIMULATION**  
**DIC-2> @@**  
**DIC-2> go d-m**  
TIME STEP AT TIME 0.00000E+00  
**DIC-2> read excl**  
OK  
**DIC> sim**  
Region: AUS  
single geometric dense at 0.20000E-06  
0.89105 93  
Region: FER  
single geometric dense at 0.20000E-06  
0.96940 72  
U-FRACTION IN SYSTEM: C = .018673311178274 FE = 1  
TOTAL SIZE OF SYSTEM: 4E-07 [m]  
U-FRACTION IN SYSTEM: C = .018673311178274 FE = 1  
TOTAL SIZE OF SYSTEM: 4E-07 [m]  
3022366.53202598 3022336.86631278 1735392.18031433 149154.115966157 3651.34991637126 12.4109488545443  
004 1.957148939937855E-010 TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.19571489E-09  
U-FRACTION IN SYSTEM: C = .0186733111782041 FE = 1  
TOTAL SIZE OF SYSTEM: 4E-07 [m]  
CPU time used in timestep 1 seconds  
1814486.15812001 1814519.61740202 113680.512392189 13139.2196003164 263.258095353916 0.890537790423686  
005 1.930362611600870E-011 TIME = 0.30000000E-06 DT = 0.20000000E-06 SUM OF SQUARES = 0.19303626E-10  
U-FRACTION IN SYSTEM: C = .018673311178248 FE = 1  
TOTAL SIZE OF SYSTEM: 4E-07 [m]  
CPU time used in timestep 1 seconds  
1558906.22556555 1558854.13308717 41004.9888267953 706.088982006915 0.233116547950608 1.390124392924976  
006 2.719872370249612E-015 TIME = 0.70000000E-06 DT = 0.40000000E-06 SUM OF SQUARES = 0.27198724E-14  
U-FRACTION IN SYSTEM: C = .0186733111782479 FE = 1  
TOTAL SIZE OF SYSTEM: 4E-07 [m]  
CPU time used in timestep 0 seconds  
182151.641165161 182136.128729327 681.534988758122 2.17357413136748 2.249148600722316E-  
005 7.484968022000849E-013 TIME = 0.15000000E-05 DT = 0.80000000E-06 SUM OF SQUARES = 0.74849680E-12  
U-FRACTION IN SYSTEM: C = .0186733111782513 FE = 1  
TOTAL SIZE OF SYSTEM: 4E-07 [m]  
CPU time used in timestep 1 seconds  
114803.082215015 114794.284557097 535.629211999917 2.09054264187956 3.251711490430699E-  
005 1.994532585527895E-012 TIME = 0.31000000E-05 DT = 0.16000000E-05 SUM OF SQUARES = 0.19945326E-11  
U-FRACTION IN SYSTEM: C = .0186733111782626 FE = 1  
TOTAL SIZE OF SYSTEM: 4E-07 [m]  
CPU time used in timestep 0 seconds  
47193.8044168227 47189.7170892627 171.508338580425 0.531420271947279 5.019724074894749E-  
006 1.536995814763826E-013 TIME = 0.63000000E-05 DT = 0.32000000E-05 SUM OF SQUARES = 0.15369958E-12  
U-FRACTION IN SYSTEM: C = .0186733111782689 FE = 1  
TOTAL SIZE OF SYSTEM: 4E-07 [m]  
CPU time used in timestep 0 seconds  
22346.2532073365 22344.2496709177 75.7208924550623 0.220392109960369 1.896529433439926E-  
006 4.786257108323287E-014 TIME = 0.12700000E-04 DT = 0.64000000E-05 SUM OF SQUARES = 0.47862571E-13  
U-FRACTION IN SYSTEM: C = .0186733111782759 FE = 1  
TOTAL SIZE OF SYSTEM: 4E-07 [m]  
CPU time used in timestep 1 seconds  
10866.6882301055 10865.6969202408 35.5540442495738 0.100188511165689 8.076953072686729E-  
007 1.849452868890216E-014 TIME = 0.25500000E-04 DT = 0.12800000E-04 SUM OF SQUARES = 0.18494529E-13  
U-FRACTION IN SYSTEM: C = .0186733111782846 FE = 1  
TOTAL SIZE OF SYSTEM: 4E-07 [m]  
CPU time used in timestep 0 seconds  
536671.350368755 536622.009292725 1728.15341270339 4.79830296942944 3.754842818380691E-  
005 8.218682415982446E-013 TIME = 0.51100000E-04 DT = 0.25600000E-04 SUM OF SQUARES = 0.82186824E-12  
output ignored...  
  
... output resumed  
  
9.865591999308139E-007 3.054564315893198E-016 TIME = 0.19893903 DT = 0.25600018E-01 SUM OF SQUARES = 0.30545643E-15  
U-FRACTION IN SYSTEM: C = .0186733111789807 FE = 1  
TOTAL SIZE OF SYSTEM: 4E-07 [m]  
CPU time used in timestep 0 seconds  
7273.32538790891 7280.14414801364 0.123623698242520 3.258005416709585E-006 1.456409338832062E-  
015 TIME = 0.22719739 DT = 0.28258357E-01 SUM OF SQUARES = 0.14564093E-14  
U-FRACTION IN SYSTEM: C = .0186733111789858 FE = 1  
TOTAL SIZE OF SYSTEM: 4E-07 [m]  
CPU time used in timestep 1 seconds  
9378.54841814586 9385.00538933242 0.29353434705986 1.320353071526355E-005 1.646242354950508E-  
014 TIME = 0.25952755 DT = 0.32330166E-01 SUM OF SQUARES = 0.16462424E-13  
U-FRACTION IN SYSTEM: C = .0186733111790062 FE = 1  
TOTAL SIZE OF SYSTEM: 4E-07 [m]  
CPU time used in timestep 0 seconds  
1362089.89161252 1362721.94800038 95.6844441598809 8.452188909772557E-003 4.656121692276779E-  
011 TIME = 0.29855549 DT = 0.39027939E-01 SUM OF SQUARES = 0.46561217E-10  
U-FRACTION IN SYSTEM: C = .0186733111791391 FE = 1  
TOTAL SIZE OF SYSTEM: 4E-07 [m]  
CPU time used in timestep 1 seconds  
1869123.51503498 1869705.74182169 277.331026181688 5.142508584836265E-002 1.274826707926147E-  
009 5.626621956997655E-017 TIME = 0.34855549 DT = 0.50000000E-01 SUM OF SQUARES = 0.56266220E-16  
U-FRACTION IN SYSTEM: C = .0186733111791394 FE = 1  
TOTAL SIZE OF SYSTEM: 4E-07 [m]  
CPU time used in timestep 0 seconds  
196909.337453844 197075.193775145 3.23544555957744 8.584623154585336E-005 2.600497307300055E-  
014 TIME = 0.39855549 DT = 0.50000000E-01 SUM OF SQUARES = 0.26004973E-13  
U-FRACTION IN SYSTEM: C = .0186733111791429 FE = 1  
TOTAL SIZE OF SYSTEM: 4E-07 [m]  
CPU time used in timestep 1 seconds  
17885.2431957863 17840.3484180469 5.698180485068682E-002 6.947732428740355E-008 2.675973518237133E-  
016 TIME = 0.44855549 DT = 0.50000000E-01 SUM OF SQUARES = 0.26759735E-15  
U-FRACTION IN SYSTEM: C = .0186733111791428 FE = 1  
TOTAL SIZE OF SYSTEM: 4E-07 [m]  
CPU time used in timestep 0 seconds  
263417.737397379 263260.024574074 10.9493242321257 4.599674423101631E-004 2.951154733882774E-  
010 2.419639926017883E-002 4.75143377025745E-017 TIME = 0.49855549 DT = 0.50000000E-01  
01 SUM OF SQUARES = 0.47514338E-16  
U-FRACTION IN SYSTEM: C = .0186733111791426 FE = 1

TOTAL SIZE OF SYSTEM: 4E-07 [m]  
CPU time used in timestep 1 seconds  
2919561.84607003 2919279.86387583 4211.80264988287 5.33099541741210 1.007567401794366E-  
005 1.337715021830897E-014 TIME = 0.50000000 DT = 0.14445092E-02 SUM OF SQUARES = 0.13377150E-13  
U-FRACTION IN SYSTEM: C = .0186733111791434 FE = 1  
TOTAL SIZE OF SYSTEM: 4E-07 [m]  
MUST SAVE WORKSPACE ON FILE  
WORKSPACE SAVED ON FILE  
RECLAIMING WORKSPACE  
DELETING TIME-RECORD FOR TIME 0.0000000  
DELETING TIME-RECORD FOR TIME 0.10000000E-06  
DELETING TIME-RECORD FOR TIME 0.30000000E-06  
DELETING TIME-RECORD FOR TIME 0.70000000E-06  
DELETING TIME-RECORD FOR TIME 0.15000000E-05  
DELETING TIME-RECORD FOR TIME 0.31000000E-05  
DELETING TIME-RECORD FOR TIME 0.63000000E-05  
DELETING TIME-RECORD FOR TIME 0.12700000E-04  
DELETING TIME-RECORD FOR TIME 0.25500000E-04  
DELETING TIME-RECORD FOR TIME 0.51100000E-04  
DELETING TIME-RECORD FOR TIME 0.10230000E-03  
DELETING TIME-RECORD FOR TIME 0.20470000E-03  
DELETING TIME-RECORD FOR TIME 0.40950000E-03  
DELETING TIME-RECORD FOR TIME 0.81910000E-03  
DELETING TIME-RECORD FOR TIME 0.16383000E-02  
DELETING TIME-RECORD FOR TIME 0.32767000E-02  
DELETING TIME-RECORD FOR TIME 0.65535000E-02  
DELETING TIME-RECORD FOR TIME 0.13107100E-01  
DELETING TIME-RECORD FOR TIME 0.26214300E-01  
DELETING TIME-RECORD FOR TIME 0.45264232E-01  
DELETING TIME-RECORD FOR TIME 0.64872172E-01  
DELETING TIME-RECORD FOR TIME 0.84957979E-01  
DELETING TIME-RECORD FOR TIME 0.10565621  
DELETING TIME-RECORD FOR TIME 0.12712011  
DELETING TIME-RECORD FOR TIME 0.14957043  
DELETING TIME-RECORD FOR TIME 0.17333901  
DELETING TIME-RECORD FOR TIME 0.19893903  
DELETING TIME-RECORD FOR TIME 0.22719739  
DELETING TIME-RECORD FOR TIME 0.25952755  
DELETING TIME-RECORD FOR TIME 0.29855549  
DELETING TIME-RECORD FOR TIME 0.34855549  
DELETING TIME-RECORD FOR TIME 0.39855549  
DELETING TIME-RECORD FOR TIME 0.44855549  
  
KEEPING TIME-RECORD FOR TIME 0.49855549  
AND FOR TIME 0.50000000  
WORKSPACE RECLAIMED

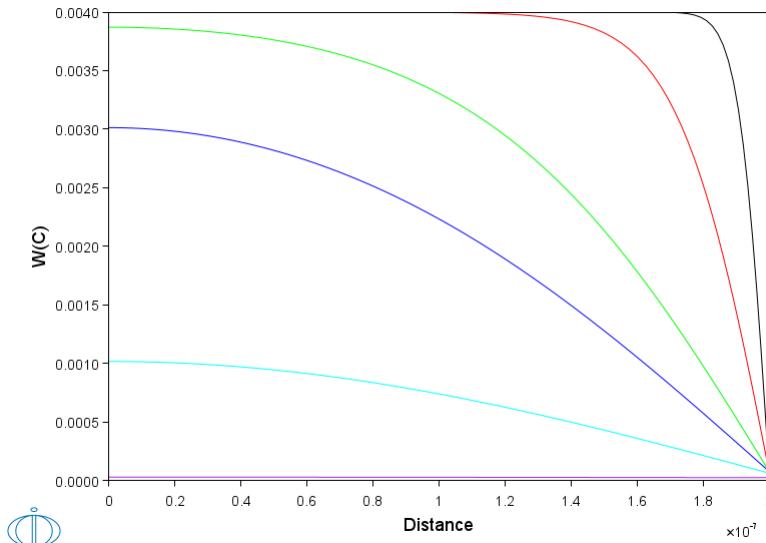
TIMESTEP AT 0.500000000 SELECTED

DIC>  
DIC>  
DIC>  
DIC> set-inter  
--OK---  
DIC>

```
excl-plot
```

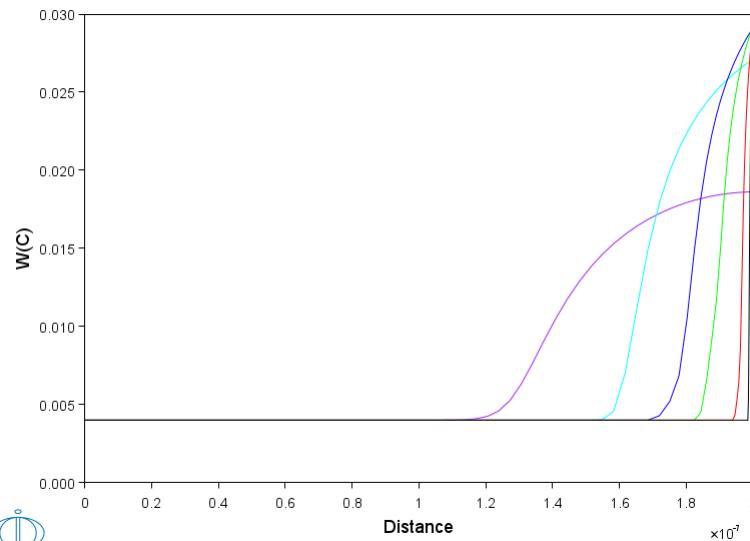
```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\excl\plot.DCM"
DIC>
DIC>
DIC> @@ excl_plot.DCM
DIC>
DIC> @@
DIC> FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE c1
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 5.00000E-01
DIC> read excl
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1: @@
POST-1: @@ FIRST PLOT CARBON CONCENTRATION PROFILES IN FERRITE (CELL-2)
POST-1: @@ THEN SET THE DISTANCE AS X-AXIS (NOT THAT DISTANCE IS SET INDEPENDENT
POST-1: @@ VARIABLE AUTOMATICALLY) AND W-FRACTION CARBON AS Y-AXIS
POST-1: @@ REMEMBER THAT THE PLOT CONDITION ALSO MUST BE SET.
POST-1: @@
POST-1: select-cell
Number /NEXT/: 2
CELL 2 SELECTED
POST-2:
POST-2: @@
POST-2: @@ NOTICE THAT THE PROMPT INCLUDES THE CURRENT CELL NUMBER
POST-2: @@
POST-2: s-d-a x dist glo
INFO: Distance is set as independent variable
POST-2: s-d-a y w(c)
POST-2: s-p-c time .0001 .001 .01 .03 .1 .5
POST-2:
POST-2: @@
POST-2: @@ SET THE TITLE ON THE PLOTS
POST-2: @@
POST-2: set-title Figure c1.1
POST-2: plot
```

Figure c1.1



```
POST-2:
POST-2:
POST-2:
POST-2:@?<_hit_return_to_continue_>
POST-2:
POST-2: @@
POST-2: @@ DO THE SAME THING FOR THE AUSTENITE (CELL-1)
POST-2: @@
POST-2: select-cell
Number /NEXT/: 1
CELL 1 SELECTED
POST-1: set-title Figure c1.2
POST-1: plot
```

**Figure c1.2**

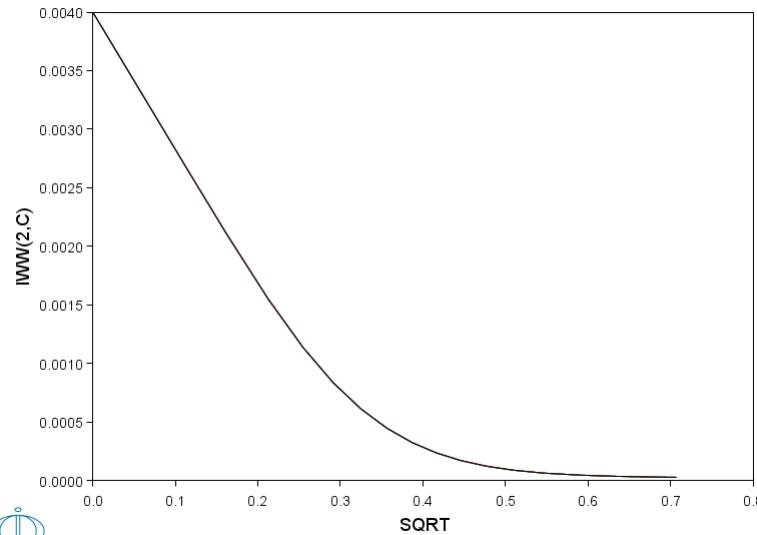


```

 $\odot$ 
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: @@
POST-1: sel-cell 2
CELL 2 SELECTED
POST-2: enter func sqrt=sqrt(time);
POST-2: s-d-a x sqrt
POST-2: s-d-a y iww(2,c)
POST-2: s-i-v time
POST-2: set-title Figure c1.3
POST-2: plot

```

**Figure c1.3**

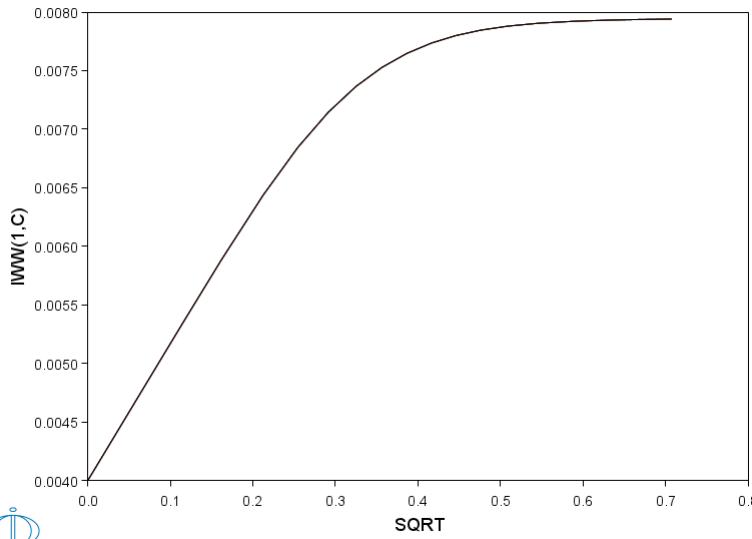


```

 $\odot$ 
POST-2:
POST-2:
POST-2:
POST-2:@?<_hit_return_to_continue_>
POST-2:
POST-2: @@
POST-2: sel-cell 1
CELL 1 SELECTED
POST-1: s-d-a y iww(1,c)
POST-1: set-title Figure c1.4
POST-1: plot

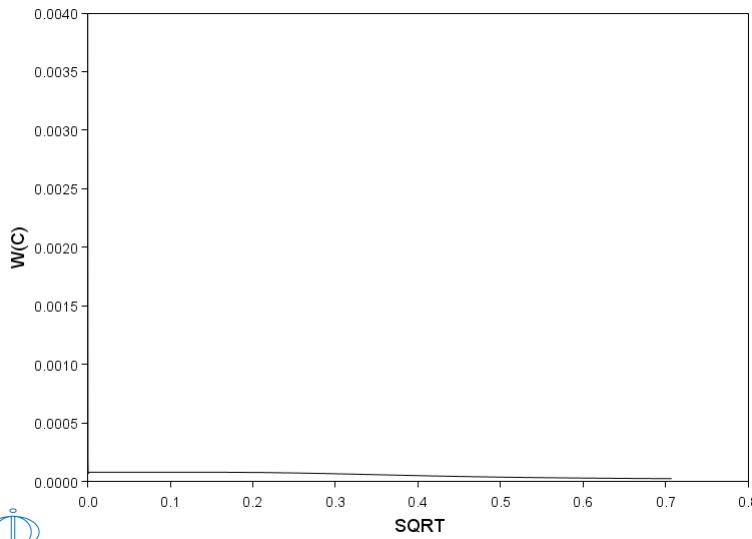
```

**Figure c1.4**



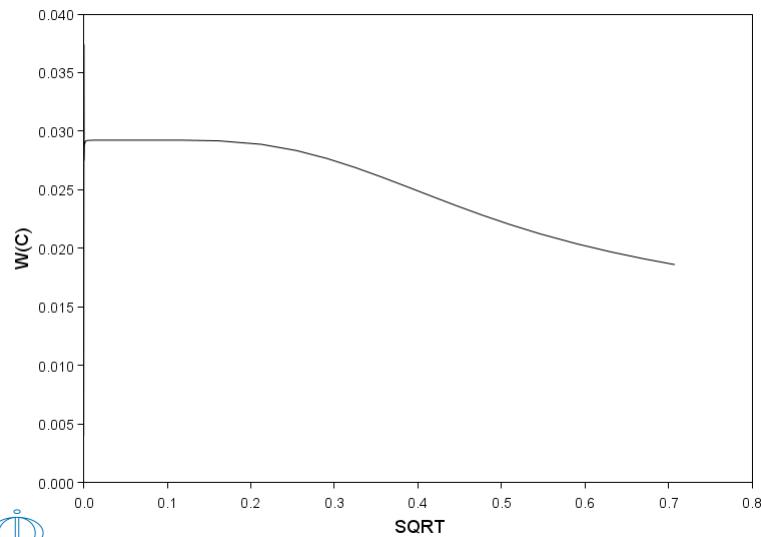
```
POST-1:  
POST-1:  
POST-1:  
POST-1:@?<_hit_return_to_continue_>  
POST-1:  
POST-1: @@  
POST-1: @@ PLOT HOW THE CONCENTRATION IN FERRITE AT THE FERRITE/AUSTENITE BOUNDARY  
POST-1: @@ V.S SQUARE ROOT OF TIME. THE FERRITE/AUSTENITE BOUNDARY IS REPRESENTED  
POST-1: @@ BY THE CELL BOUNDARY I.E. THE "LAST" INTERFACE.  
POST-1: @@  
POST-1: sel-cell 2  
CELL 2 SELECTED  
POST-2: s-d-a y w(c)  
POST-2: s-p-c interface last  
POST-2: set-title Figure c1.5  
POST-2: plot
```

**Figure c1.5**



```
POST-2:  
POST-2:  
POST-2:  
POST-2:@?<_hit_return_to_continue_>  
POST-2:  
POST-2: @@  
POST-2: @@ DO THE SAME THING FOR THE AUSTENITE  
POST-2: @@  
POST-2: sel-cell 1  
CELL 1 SELECTED  
POST-1: set-title Figure c1.6  
POST-1: plot
```

**Figure c1.6**



POST-1:  
POST-1:  
POST-1:  
POST-1:@?<\_hit\_return\_to\_continue\_>  
POST-1:  
POST-1: set-inter  
---OK---  
POST-1:

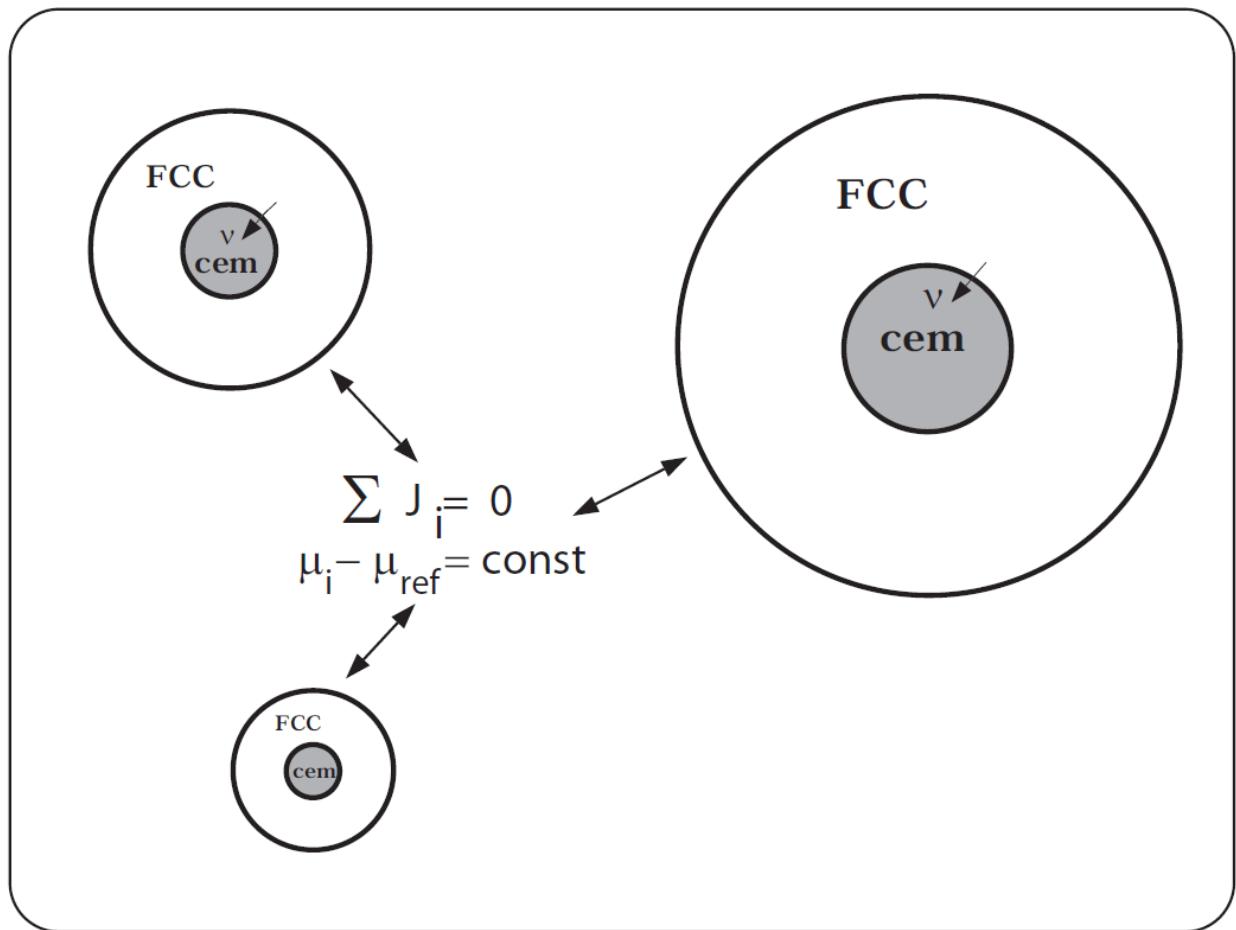


## Example exc2

### Cementite dissolution in an Fe-Cr-C alloy: Three particle sizes and three different cells

This example calculates the dissolution of cementite particles in an austenite matrix. This is the same as exc1 except that there are three particle sizes. Altogether six particles are considered using three different cells. This is to be able to represent some size distribution among the cementite particles. See also Z.-K. Liu, L. Höglund, B. Jönsson and J. Ågren: Metall.Trans.A, v. 22A (1991), pp. 1745-1752.

$$T = 118\text{K}$$



**exc2-setup****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\_dictra\_console\_examples\examples\exc2\setup.DCM"**  
**SYS: i>@@**  
NO SUCH COMMAND, USE HELP  
**SYS: @@ Cell calculation.**  
**SYS: @@ Cementite dissolution in an Fe-Cr-C alloy: Three particle sizes and**  
**SYS: @@ three different cells**  
**SYS: @@ This example calculates the dissolution of cementite particles**  
**SYS: @@ in an austenite matrix. This example is the same as exc1 but**  
**SYS: @@ instead there are three particle sizes. A total of six**  
**SYS: @@ particles are considered using three different cells. This is to**  
**SYS: @@ represent some size distribution among the cementite particles.**  
**SYS: @@ See also Z.-K. Liu, L. Håglund, B. Jähnsson and J. Ågren:**  
**SYS: @@ Metall.Trans.A, v. 22A (1991), pp. 1745-1752.**  
**SYS: -----**  
NO SUCH COMMAND, USE HELP  
**SYS:**  
**SYS: @@ exc2\_setup.DCM**  
**SYS:**  
**SYS: @@**  
**SYS: @@ RETRIEVE DATA FROM THE DATABASE**  
**SYS: @@**  
**SYS: go da**  
THERMODYNAMIC DATABASE module  
Database folder:  
C:\jenkins\workspace\generate\_dictra\_console\_examples\databases\data  
Current database: Steels/Fe-Alloys v12.0  
  
VA                           /- DEFINED  
DICTRA\_FCC\_A1 REJECTED  
**TDB\_TCFE12: @@**  
**TDB\_TCFE12: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA**  
**TDB\_TCFE12: @@**  
**TDB\_TCFE12: switch fedemo**  
Current database: Iron Demo Database v4.0  
  
VA                           /- DEFINED  
**TDB\_FEDEMO: def-sys fe cr c**  
FE                           CR                           C  
DEFINED  
**TDB\_FEDEMO: rej ph \* all**  
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: res ph fcc cementite**  
FCC\_A1                   CEMENTITE RESTORED  
**TDB\_FEDEMO: get**  
17:26:15,875 [Thread-0] INFO JavaWrapper: \*\*\* Invoking Gibbs Energy System v6 \*\*\*  
REINITIATING GES ....  
ELEMENTS ....  
SPECIES ....  
PHASES ....  
Creating a new composition set FCC\_A1#2  
PARAMETERS ...  
FUNCTIONS ....  
  
List of references for assessed data  
  
'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'  
'X.G. Lu, Thermo-Calc Software AB, Sweden, 2006; 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'  
'A.V. Khvan, B. Hallstedt, C. Broeckmann, CALPHAD, 46, 24 -33(2014); Cr-Fe -C'  
'J. Bratberg, Z. Metallkd., 96 (2005) 335-344; Fe-Cr-Mo-C'  
'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'  
'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'  
'A.T. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'  
'X.G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar volumes'  
'R. Naraghi, Thermo-Calc Software AB, Sweden, 2016; FCC Fe-Cr-C and C-Cr-Ni'  
'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270 (1986); CR-FE'  
-OK-  
**TDB\_FEDEMO: @@**  
**TDB\_FEDEMO: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE MOBILITY DATA**  
**TDB\_FEDEMO: @@**  
**TDB\_FEDEMO: app mobfe4**  
Current database: Steels/Fe-Alloys Mobility v4.0  
  
VA    DEFINED  
B2\_BCC REJECTED  
**APP: def-sys fe cr c**  
FE                           CR                           C  
DEFINED  
**APP: rej ph \* all**  
BCC\_A2                   CEMENTITE                   FCC\_A1  
FE4N\_LP1                  HCP\_A3                   LIQUID:L  
REJECTED

```

APP: res ph fcc cementite
FCC A1 CEMENTITE RESTORED
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS .....

List of references for assessed data

'This parameter has not been assessed'
'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'
'B. Jonsson: Z. Metallkunde 85(1994)502-509; C diffusion in fcc Cr-Fe-Ni'
'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Fe diffusion fcc Cr-Fe'
'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
-Ni'
'This parameter has been estimated'
-OK-
APP:
APP: @@ ENTER THE DICTRA MONITOR
APP: @@
APP: go d-m
NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob t 0 1183; * n
DIC>
DIC> @@
DIC> @@ CELL NUMBER ONE
DIC> @@
DIC> @@
DIC> @@
DIC> @@ ENTER REGIONS carb AND aus
DIC> @@
DIC> enter-region carb
DIC> enter-region aus
ATTACH TO REGION NAMED /CARB/:
ATTACHED TO THE RIGHT OF CARB /YES/:
DIC> @@
DIC> @@ ENTER GEOMTRICAL GRIDS INTO THE REGIONS
DIC> @@
DIC>
DIC> @@
DIC> @@ THE SIZE OF THE CEMENTITE PARTICLES ARE KNOWN AS WE ASSUME
DIC> @@ IT HAS BEEN MEASURED.
DIC> @@
DIC> enter-grid
REGION NAME : /CARB/: carb
WIDTH OF REGION /1/: 0.700000e-6
TYPE /LINEAR/: AUTO
DIC>
DIC> @@
DIC> @@ THE SIZE OF THE FCC REGION CAN BE CALCULATED FROM A MASS BALANCE
DIC> @@ AFTER ESTIMATING THE INITIAL COMPOSITIONS IN THE TWO PHASES.
DIC> @@
DIC> enter-grid
REGION NAME : /AUS/: aus
WIDTH OF REGION /1/: 7.1832993E-7
TYPE /LINEAR/: AUTO
DIC>
DIC> @@
DIC> @@ ENTER PHASES INTO REGIONS
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /CARB/: carb
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: cementite
DIC>
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /AUS/: aus
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#
DIC>
DIC> @@
DIC> @@ ENTER INITIAL VALUES FOR THE COMPOSITIONS IN THE PHASES
DIC> @@
DIC> enter-composition carb cementite w-f
PROFILE FOR /CR/: cr lin 0.12423326 0.12423326
DIC>
DIC> enter-composition aus fcc#1 fe w-f
PROFILE FOR /C/: cr lin 4.6615447E-3 4.6615447E-3
PROFILE FOR /CR/: c lin 1.5135207E-4 1.5135207E-4
DIC>
DIC> @@
DIC> @@ CELL NUMBER TWO
DIC> @@
DIC> create-new-cell
CELL DISTRIBUTION FACTOR /1/: 2
CREATING NEW CELL, NUMBER: 2
CELL 2 SELECTED
DIC-2>
DIC-2> @@
DIC-2> @@ ENTER REGIONS carb AND aus
DIC-2> @@
DIC-2> enter-region carb
DIC-2> enter-region aus
ATTACH TO REGION NAMED /CARB/:
ATTACHED TO THE RIGHT OF CARB /YES/:
DIC-2> @@
DIC-2> @@ ENTER GEOMTRICAL GRIDS INTO THE REGIONS
DIC-2> @@
DIC-2> enter-grid carb 0.300000e-6 AUTO
DIC-2> enter-grid aus 3.0785568E-7 AUTO
DIC-2>
DIC-2> @@

```

```

DIC-2> @@ ENTER PHASES INTO THE REGIONS
DIC-2> @@
DIC-2> enter-phase act carb matrix cementite
DIC-2> enter-phase act aus matrix fcc#1
DIC-2> @@
DIC-2> @@
DIC-2> enter-composition carb cementite w-f
PROFILE FOR /CR/: cr lin 0.12423326 0.12423326
DIC-2>
DIC-2> enter-composition aus fcc#1 fe w-f
PROFILE FOR /C/: cr lin 4.6615447E-3 4.6615447E-3
PROFILE FOR /CR/: c lin 1.5135207E-4 1.5135207E-4
DIC-2>
DIC-2> @-----@-----
DIC-2> @@ CELL NUMBER THREE
DIC-2> @-----@-----
DIC-2> create-new-cell
CELL DISTRIBUTION FACTOR /1/: 3
CREATING NEW CELL, NUMBER: 3
CELL 3 SELECTED
DIC-3>
DIC-3> @@
DIC-3> @@ ENTER REGIONS carb AND aus
DIC-3> @@
DIC-3> enter-region carb
DIC-3> enter-region aus
ATTACH TO REGION NAMED /CARB/:
ATTACHED TO THE RIGHT OF CARB /YES/:
DIC-3> @@
DIC-3> @@ ENTER GEOMTRICAL GRIDS INTO THE REGIONS
DIC-3> @@
DIC-3> enter-grid carb 0.525500e-6 AUTO
DIC-3> enter-grid aus 5.3926054E-7 AUTO
DIC-3>
DIC-3> @@
DIC-3> @@ ENTER PHASES INTO REGIONS
DIC-3> @@
DIC-3> enter-phase act carb matrix cementite
DIC-3> enter-phase act aus matrix fcc#1
DIC-3>
DIC-3> @@
DIC-3> @@ ENTER INITIAL VALUES FOR THE COMPOSITIONS IN THE PHASES
DIC-3> @@
DIC-3> enter-composition carb cementite w-f
PROFILE FOR /CR/: cr lin 0.12423326 0.12423326
DIC-3>
DIC-3> enter-composition aus fcc#1 fe w-f
PROFILE FOR /C/: cr lin 4.6615447E-3 4.6615447E-3
PROFILE FOR /CR/: c lin 1.5135207E-4 1.5135207E-4
DIC-3>
DIC-3> @-----@-----
DIC-3> @@ GLOBAL CONDITIONS
DIC-3> @-----@-----
DIC-3> @@
DIC-3> @@ SET TO A SPHERICAL GEOMETRY
DIC-3> @@
DIC-3> enter-geo 2
DIC-3>
DIC-3> @s-n-1
's-n-1' is not recognized as an internal or external command,
operable program or batch file.
DIC-3> @
DIC-3> @1E-3
'1E-3' is not recognized as an internal or external command,
operable program or batch file.
DIC-3>
DIC-3>
DIC-3>
DIC-3>
DIC-3>
DIC-3> @@
DIC-3> @@ SET THE SIMULATION TIME
DIC-3> @@
DIC-3> set-simulation-time
END TIME FOR INTEGRATION /.1/: 10000
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /1000/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC-3>
DIC-3> @@
DIC-3> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC-3> @@
DIC-3> save exc2 Y
DIC-3>
DIC-3>
DIC-3> set-inter
--OK--
DIC-3>

```

**exc2-run**

**DIC-3>About**  
NO SUCH COMMAND, USE HELP  
**DIC-3>DIC-3>MACRO "c:\jenkins\workspace\generate\_dictra\_console\_examples\examples\exc2\run.DCM"**  
**DIC-3>**  
**DIC-3>**  
**DIC-3> @@ exc2\_run.DCM**  
**DIC-3>**  
**DIC-3> @@**  
**DIC-3> @@ READ THE SET UP FROM FILE AND START THE SIMULATION**  
**DIC-3> @@**  
**DIC-3>**  
**DIC-3> go d-m**  
TIME STEP AT TIME 0.00000E+00  
**DIC-3> read exc2**  
OK  
**DIC> sim yes**  
Region: CARB  
single geometric dense at 0.70000E-06  
0.84611 96  
Region: AUS  
double geometric  
dense at outer boundaries, coarse at 0.35916E-06  
lower part 1.0486 22  
upper part 0.95367 22  
Region: CARB  
single geometric dense at 0.30000E-06  
0.86023 95  
Region: AUS  
double geometric  
dense at outer boundaries, coarse at 0.15393E-06  
lower part 1.0067 22  
upper part 0.99334 22  
Region: CARB  
single geometric dense at 0.52550E-06  
0.85084 96  
Region: AUS  
double geometric  
dense at outer boundaries, coarse at 0.26963E-06  
lower part 1.0222 22  
upper part 0.97828 22  
DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE  
Trying old scheme 4  
GENERATING STARTING VALUES FOR CELL # 1 INTERFACE # 2  
DETERMINING INITIAL EQUILIBRIUM VALUES  
CALCULATING STARTING VALUES: 9 EQUILIBRIUM CALCULATIONS DONE 6 OUT OF 9  
04  
Trying old scheme 4  
GENERATING STARTING VALUES FOR CELL # 2 INTERFACE # 2  
DETERMINING INITIAL EQUILIBRIUM VALUES  
CALCULATING STARTING VALUES: 9 EQUILIBRIUM CALCULATIONS DONE 6 OUT OF 9  
04  
Trying old scheme 4  
GENERATING STARTING VALUES FOR CELL # 3 INTERFACE # 2  
DETERMINING INITIAL EQUILIBRIUM VALUES  
CALCULATING STARTING VALUES: 9 EQUILIBRIUM CALCULATIONS DONE 6 OUT OF 9  
04  
U-FRACTION IN SYSTEM: C = .0406910187346776 CR = .0214382352304608  
FE = .978561764900046  
TOTAL SIZE OF SYSTEM: 2.90023192349E-17 [m^3]  
U-FRACTION IN SYSTEM: C = .0406910187346776 CR = .0214382352304608  
FE = .978561764900046  
TOTAL SIZE OF SYSTEM: 2.90023192349E-17 [m^3]  
0.564508261918361 0.564544652017531 0.564567155686083 0.564549543177645 0.564508311768280 0.564508332797992  
002 3.181938772210079E-002 1.197624989906678E-002 1.087476773577146E-004 1.496546201470204E- 1.496546201470204E-  
005 1.899360933178584E-006 1.101408779082102E-005 2.337281895113248E-006 1.904890740536010E- 1.904890740536010E-  
006 1.885755017252722E-006 1.818420616634765E-006 1.864191007396391E-006 1.866972995572343E- 1.866972995572343E-  
006 1.868924665486775E-006 1.235466348956339E-004 1.744312549290258E-003 1.887159023269607E- 1.887159023269607E-  
006 1.869895780653598E-006 1.867139672723058E-006 1.867038385947053E-006 1.865715571719955E- 1.865715571719955E-  
006 1.867094529899203E-006 1.865068389442216E-006 1.864692936248489E-006 1.869035370120004E- 1.869035370120004E-  
006 1.864470845830077E-006 1.797050922567852E-006 1.864346005406620E-006 1.864272246875833E- 1.864272246875833E-  
006 1.864231612832792E-006 1.235466348143361E-004 1.744312548941861E-003 1.887157340316358E- 1.887157340316358E-  
006 1.864214727810508E-006 1.864214800342696E-006 1.867045636240818E-006 1.864214710607443E- 1.864214710607443E-  
006 1.867003737924303E-006 1.8641799609596423E-006 1.864168665158705E-006 1.868937371064565E- 1.868937371064565E-  
006 1.864151283274751E-006 1.796944620177879E-006 1.864127991963316E-006 1.864087358692110E- 1.864087358692110E-  
006 1.864028878464661E-006 1.235201706629520E-004 1.744300465038222E-003 1.886993317249269E-006  
  
output ignored...  
  
... output resumed  
  
CPU time used in timestep 3 seconds  
3.174160612216668E-002 3.174160627348922E-002 3.174160622491674E-002 3.174292785622747E-002 3.174378595740940E-  
002 3.173728154323313E-002 3.174071169524840E-002 2.325307847876008E-003 4.138453357929722E-  
006 1.469327414593945E-009 7.541037038792365E-014 6.236619628119008E- 1.871752405327534E-  
017 TIME = 7842.2057 DT = 1000.0000 SUM OF SQUARES = 0.28643023E-20  
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.11200670E-10 AND -0.11200670E-10  
POSITION OF INTERFACE CARB / AUS IS 0.41731540E-06  
CELL # 3 VELOCITY AT INTERFACE # 2 IS -0.12021570E-10 AND -0.12021570E-10  
POSITION OF INTERFACE CARB / AUS IS 0.24028603E-06  
U-FRACTION IN SYSTEM: C = .0407687535885158 CR = .0216079279382246  
FE = .978392072192282  
TOTAL SIZE OF SYSTEM: 2.90023192349E-17 [m^3]  
2 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: AUS  
  
CPU time used in timestep 4 seconds  
4.017879301972773E-002 4.017879312068801E-002 4.017879306385644E-002 4.018020970835798E-002 4.018108579144634E-  
002 4.017412802651951E-002 4.017770559553085E-002 3.021156710334854E-003 4.589696833002638E-  
006 1.962538881039879E-009 1.598220372474940E-013 1.871752405327534E- 1.871752405327534E-  
016 TIME = 8842.2057 DT = 1000.0000 SUM OF SQUARES = 0.45027256E-17  
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.99661216E-11 AND -0.99661216E-11  
POSITION OF INTERFACE CARB / AUS IS 0.40734928E-06  
CELL # 3 VELOCITY AT INTERFACE # 2 IS -0.11438353E-10 AND -0.11438353E-10  
POSITION OF INTERFACE CARB / AUS IS 0.22884768E-06  
U-FRACTION IN SYSTEM: C = .0407688032171921 CR = .0216077309969347  
FE = .978392269133572  
TOTAL SIZE OF SYSTEM: 2.90023192349E-17 [m^3]  
CPU time used in timestep 3 seconds  
4.195891540311342E-002 4.195891547666201E-002 4.195891541934767E-002 4.196027812217858E-002 4.196107794861525E-  
002 4.195438638429647E-002 4.195766408809014E-002 3.666657467043039E-003 5.829299438319438E-  
006 2.448899262439677E-009 4.685996915054967E-013 1.591976841459803E-

```

016      TIME =  9842.2057    DT =  1000.0000    SUM OF SQUARES =  0.21475656E-18
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.89910239E-11 AND -0.89910239E-11
POSITION OF INTERFACE CARB / AUS IS 0.39835825E-06
CELL # 3 VELOCITY AT INTERFACE # 2 IS -0.11212703E-10 AND -0.11212703E-10
POSITION OF INTERFACE CARB / AUS IS 0.21763497E-06
U-FRACTION IN SYSTEM: C = .0407688355332858 CR = .0216075892181081
FE = .978392410912399
TOTAL SIZE OF SYSTEM: 2.90023192349E-17 [m^3]
CPU time used in timestep          4 seconds
0.214243288265598   0.214243288414991   0.214243288580334   0.214244858971621   0.214245730046770   0.214234669411837
003   1.018997041516797E-005   5.577913583701030E-009   2.438776735966604E-013   3.089540817684289E-
016      TIME = 10000.0000    DT = 157.79433    SUM OF SQUARES = 0.30840169E-15
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.72903630E-11 AND -0.72903630E-11
POSITION OF INTERFACE CARB / AUS IS 0.39720788E-06
CELL # 3 VELOCITY AT INTERFACE # 2 IS -0.82035957E-11 AND -0.82035957E-11
POSITION OF INTERFACE CARB / AUS IS 0.21634049E-06
U-FRACTION IN SYSTEM: C = .0407688569472806 CR = .0216075637360842
FE = .978392436394423
TOTAL SIZE OF SYSTEM: 2.90023192349E-17 [m^3]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 3334.6788
DELETING TIME-RECORD FOR TIME 3500.0284
DELETING TIME-RECORD FOR TIME 3500.0284
DELETING TIME-RECORD FOR TIME 3500.0284
DELETING TIME-RECORD FOR TIME 3500.0285
DELETING TIME-RECORD FOR TIME 3500.0285
DELETING TIME-RECORD FOR TIME 3500.0287
DELETING TIME-RECORD FOR TIME 3500.0290
DELETING TIME-RECORD FOR TIME 3500.0297
DELETING TIME-RECORD FOR TIME 3500.0309
DELETING TIME-RECORD FOR TIME 3500.0335
DELETING TIME-RECORD FOR TIME 3500.0386
DELETING TIME-RECORD FOR TIME 3500.0489
DELETING TIME-RECORD FOR TIME 3500.0693
DELETING TIME-RECORD FOR TIME 3500.1103
DELETING TIME-RECORD FOR TIME 3500.1922
DELETING TIME-RECORD FOR TIME 3500.3561
DELETING TIME-RECORD FOR TIME 3500.6837
DELETING TIME-RECORD FOR TIME 3501.3391
DELETING TIME-RECORD FOR TIME 3502.6498
DELETING TIME-RECORD FOR TIME 3505.2713
DELETING TIME-RECORD FOR TIME 3510.5141
DELETING TIME-RECORD FOR TIME 3520.9999
DELETING TIME-RECORD FOR TIME 3541.9714
DELETING TIME-RECORD FOR TIME 3583.9145
DELETING TIME-RECORD FOR TIME 3667.8005
DELETING TIME-RECORD FOR TIME 3835.5727
DELETING TIME-RECORD FOR TIME 4171.1170
DELETING TIME-RECORD FOR TIME 4842.2057
DELETING TIME-RECORD FOR TIME 5842.2057
DELETING TIME-RECORD FOR TIME 6842.2057
DELETING TIME-RECORD FOR TIME 7842.2057
DELETING TIME-RECORD FOR TIME 8842.2057

KEEPING TIME-RECORD FOR TIME 9842.2057
AND FOR TIME 10000.0000
WORKSPACE RECLAIMED

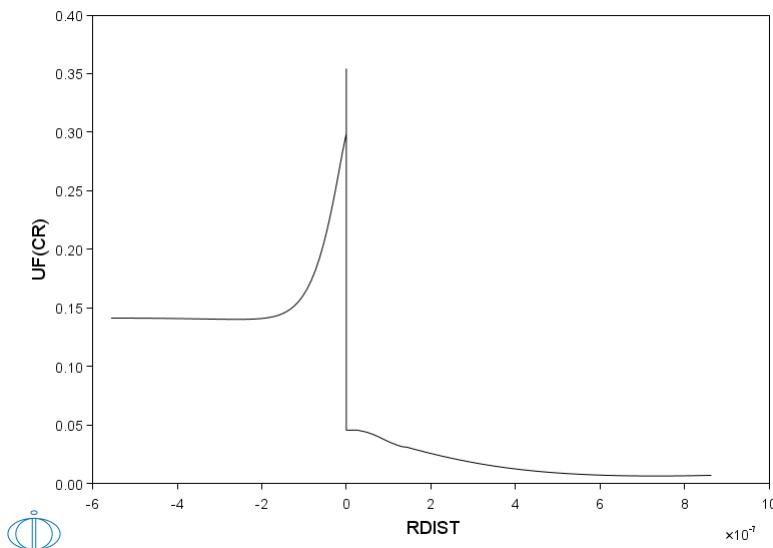
TIMESTEP AT 10000.0000 SELECTED

DIC>
DIC>
DIC>
DIC>
DIC>
DIC> set-inter
--OK--
DIC>
```

## exc2-plot

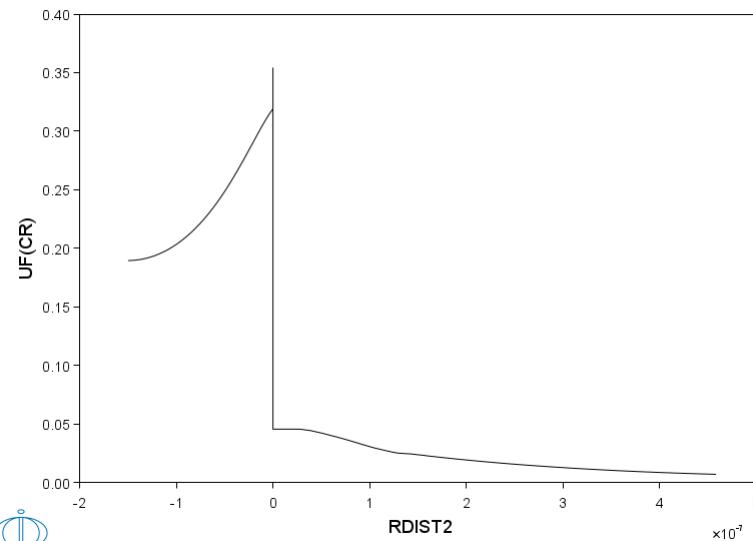
```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exc2\plot.DCM"
DIC>
DIC>
DIC> @@ exc2_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE c2
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 1.00000E+04
DIC> read exc2
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1: @@
POST-1: @@ PLOT THE CHROMIUM CONCENTRATION PROFILES IN THE SAME WAY AS IN exb2
POST-1: @@ BUT NOW FOR EACH PARTICLE. LET US LOOK AT THE PROFILES AFTER 1000s.
POST-1: @@
POST-1: @@
POST-1: @@ FIRST CELL
POST-1: @@
POST-1: enter-symb
Function or table /FUNCTION/: func
NAME: rdist
FUNCTION: gd-poi(carb,u);
POST-1:
POST-1: s-d-a x rdist
POST-1:
POST-1: s-d-a y uf(cr)
POST-1:
POST-1: s-i-v
VARIABLE /TIME/: dist
DISTANCE : /GLOBAL/: glo
POST-1:
POST-1: s-p-c time 1000
POST-1:
POST-1: @@
POST-1: @@ SET THE TITLE ON THE PLOT
POST-1: @@
POST-1: set-title Figure C2.1
POST-1: plot
```

Figure C2.1



```
POST-1:
POST-1:
POST-1:
POST-1:@<_hit_return_to_continue_>
POST-1:
POST-1: @@
POST-1: @@ SELECT CELL 2
POST-1: @@
POST-1: select-cell
Number /NEXT/: 2
CELL 2 SELECTED
POST-2:
POST-2: enter-symb
Function or table /FUNCTION/: func
NAME: rdist2
FUNCTION: gd-poi(carb,u);
POST-2:
POST-2: s-d-a x rdist2
POST-2:
POST-2: set-title Figure C2.2
POST-2: plot
```

**Figure C2.2**

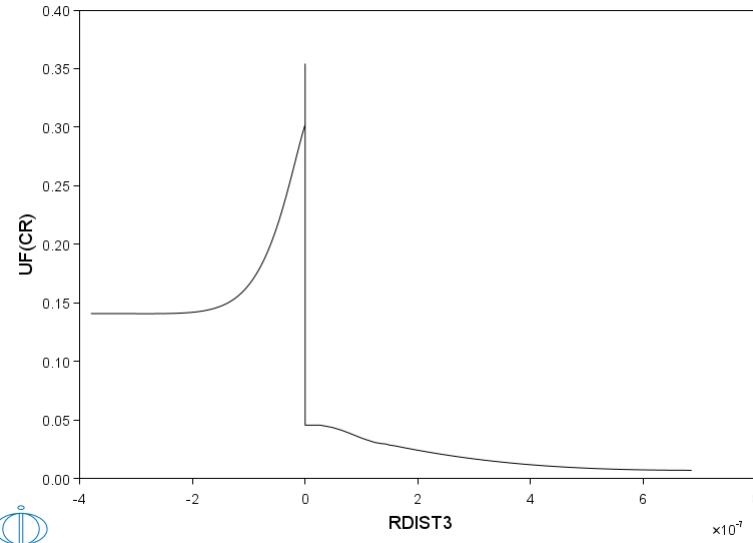


```

POST-2:
POST-2:
POST-2:
POST-2:@?<_hit_return_to_continue_>
POST-2:
POST-2: @@
POST-2: @@ SELECT CELL 3
POST-2: @@
POST-2: select-cell 3
CELL 3 SELECTED
POST-3:
POST-3: enter-symb
Function or table /FUNCTION/: func
NAME: rdist3
FUNCTION: gd-poi(carb,u);
POST-3:
POST-3: s-d-a x rdist3
POST-3:
POST-3: set-title Figure C2.3
POST-3: plot

```

**Figure C2.3**



```

POST-3:
POST-3:
POST-3:
POST-3:
POST-3:@?<_hit_return_to_continue_>
POST-3:
POST-3:
POST-3: @@
POST-3: @@ ALSO PLOT HOW THE DIAMETER OF THE CEMENTITE PARTICLE VARIES
POST-3: @@ WITH TIME IN THE THREE CELLS
POST-3: @@
POST-3:
POST-3: @@
POST-3: @@ SELECT THE FIRST CELL
POST-3: @@
POST-3: sel-cell 1
CELL 1 SELECTED
POST-1:
POST-1: s-d-a x time
INFO: Time is set as independent variable
POST-1: s-s-s x n .01 10000
POST-1: set-axis-type x log
POST-1:
POST-1: enter func diam1=2*poi(carb,u);
POST-1: s-d-a y diam1
POST-1: s-s-s y n 0 1.5e-6
POST-1:

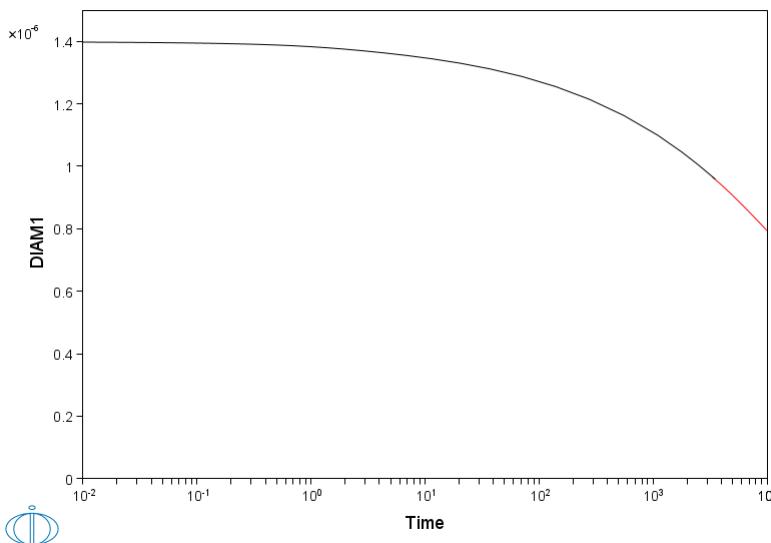
```

```

POST-1: s-p-c interf carb upp
POST-1:
POST-1: app n
POST-1: set-title Figure C2.4
POST-1: plot

```

Figure C2.4

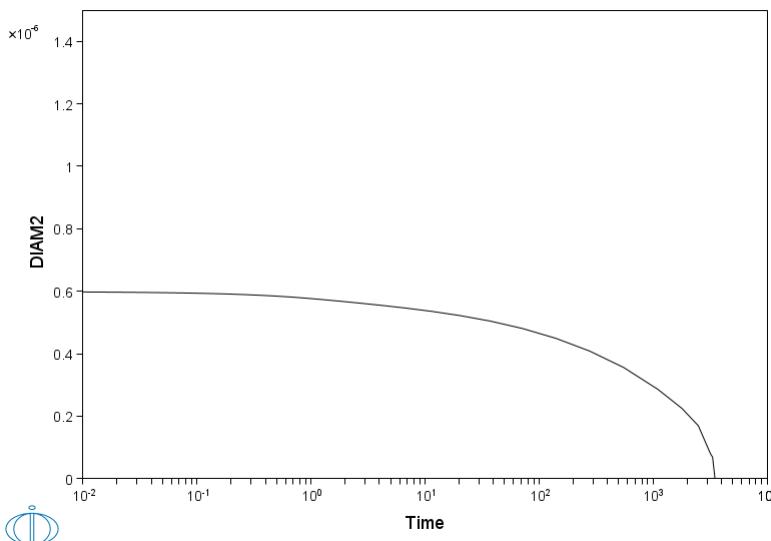


```

POST-1:
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1:
POST-1: @@
POST-1: @@ SELECT CELL 2
POST-1: @@
POST-1: sel-cell 2
CELL 2 SELECTED
POST-2:
POST-2: enter func diam2=2*poi(carb,u);
POST-2: s-d-a y diam2
POST-2: s-s-s y n 0 1.5e-6
POST-2:
POST-2: s-p-c interf carb upp
POST-2:
POST-2: set-title Figure C2.5
POST-2: plot

```

Figure C2.5

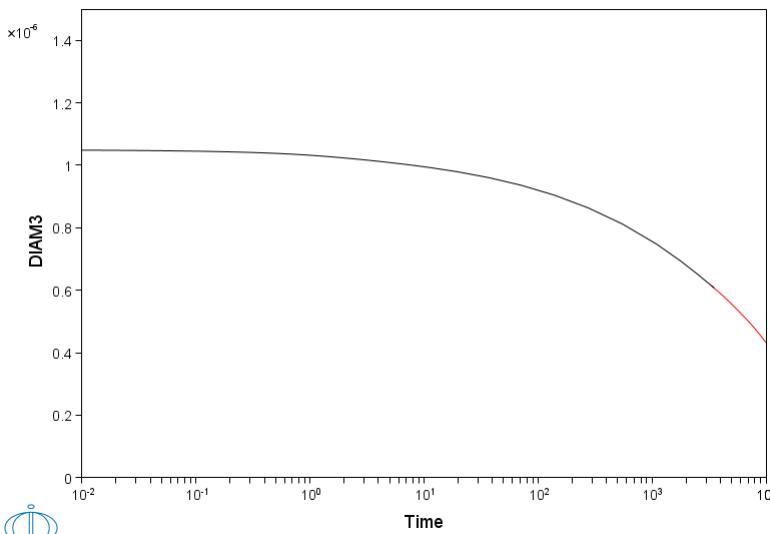


```

POST-2:
POST-2:
POST-2:
POST-2:
POST-2:@?<_hit_return_to_continue_>
POST-2:
POST-2: @@
POST-2: @@ SELECT CELL 3
POST-2: @@
POST-2: sel-cell 3
CELL 3 SELECTED
POST-3:
POST-3: enter func diam3=2*poi(carb,u);
POST-3: s-d-a y diam3
POST-3: s-s-s y n 0 1.5e-6
POST-3:
POST-3: s-p-c interf carb upp
POST-3:
POST-3: set-title Figure C2.6
POST-3: plot

```

**Figure C2.6**

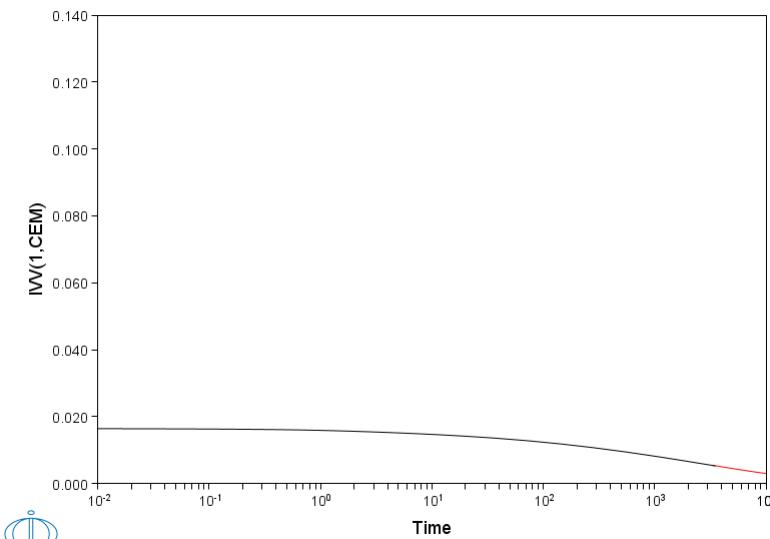


```

POST-3:
POST-3:
POST-3:
POST-3:
POST-3:@?<_hit_return_to_continue_>
POST-3:
POST-3: @@
POST-3: @@ NOW PLOT THE VOLUME FRACTION OF CEMENTITE IN THE THREE CELLS
POST-3: @@
POST-3: s-d-a x time
INFO: Time is set as independent variable
POST-3: s-s-s x n .01 10000
POST-3: set-axis-type x log
POST-3:
POST-3: @@
POST-3: @@ CELL 1
POST-3: @@
POST-3: s-d-a y ivv(1,cem)
POST-3: s-s-s y n 0 0.14
POST-3:
POST-3: s-p-c integral
POST-3:
POST-3: set-title Figure C2.7
POST-3: plot

```

**Figure C2.7**

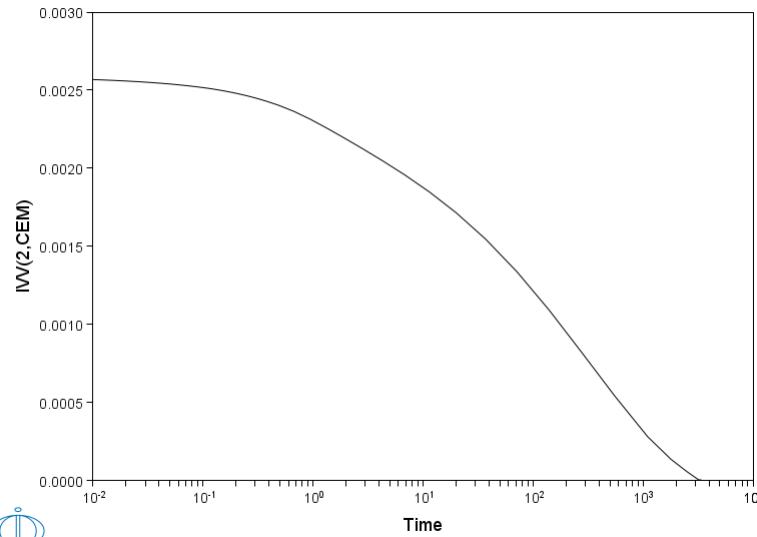


```

POST-3:
POST-3:
POST-3:
POST-3:
POST-3:@?<_hit_return_to_continue_>
POST-3:
POST-3: @@
POST-3: @@ CELL 2
POST-3: @@
POST-3: s-d-a y ivv(2,cem)
POST-3:
POST-3: set-title Figure C2.8
POST-3: plot

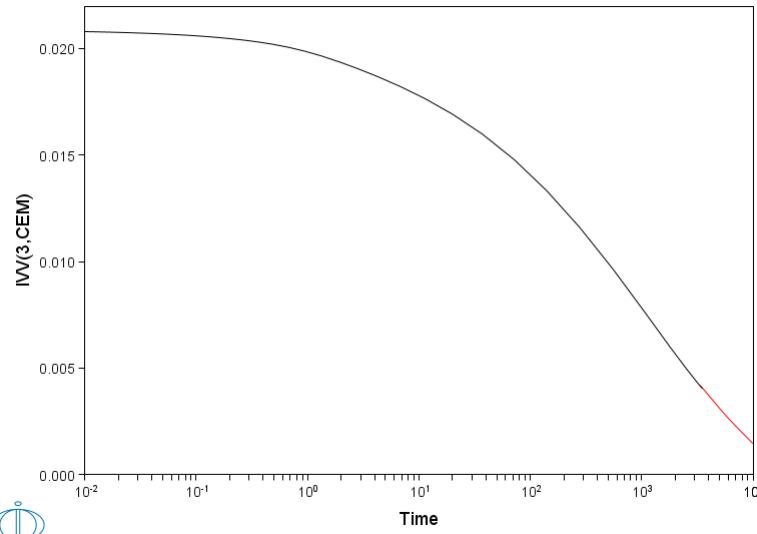
```

**Figure C2.8**



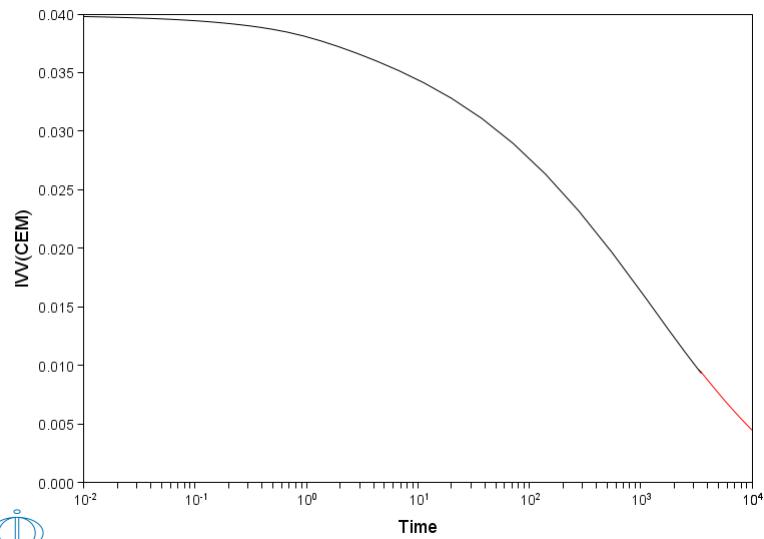
```
POST-3:  
POST-3:  
POST-3:  
POST-3:  
POST-3:@?<_hit_return_to_continue_>  
POST-3:  
POST-3:  
POST-3: @@  
POST-3: @@ CELL 3  
POST-3: @@  
POST-3: s-d-a y ivv(3,cem)  
POST-3:  
POST-3: set-title Figure C2.9  
POST-3: plot
```

**Figure C2.9**



```
POST-3:  
POST-3:  
POST-3:  
POST-3:  
POST-3:@?<_hit_return_to_continue_>  
POST-3:  
POST-3:  
POST-3: @@  
POST-3: @@ FINALLY, PLOT HOW THE TOTAL VOLUME FRACTION OF CEMENTITE  
POST-3: @@ VARIES WITH TIME.  
POST-3: @@  
POST-3: s-d-a y ivv(cem)  
POST-3:  
POST-3: set-title Figure C2.10  
POST-3: plot
```

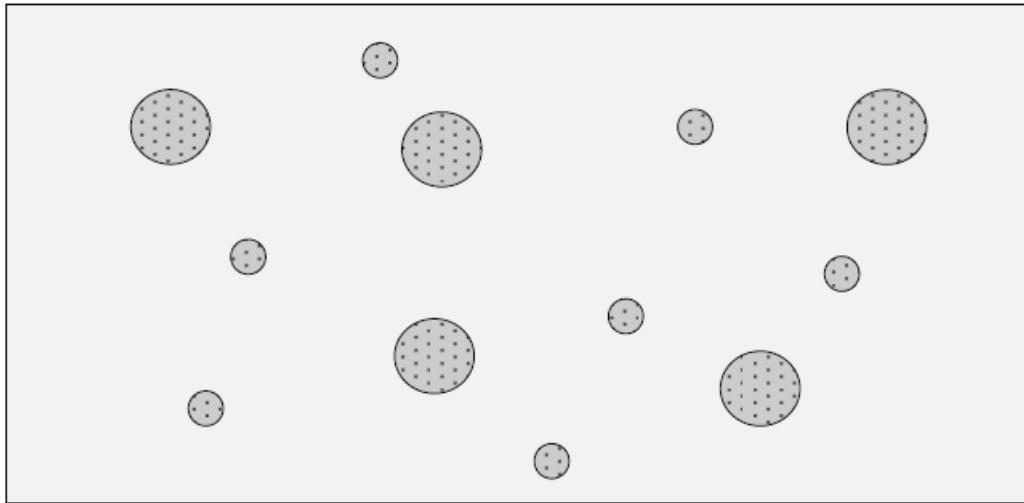
**Figure C2.10**



POST-3:  
POST-3:  
POST-3:  
POST-3:  
POST-3:@?<\_hit\_return\_to\_continue\_>  
POST-3:  
**POST-3:** set-inter  
--OK---  
**POST-3:**



## Diffusion in Dispersed Systems



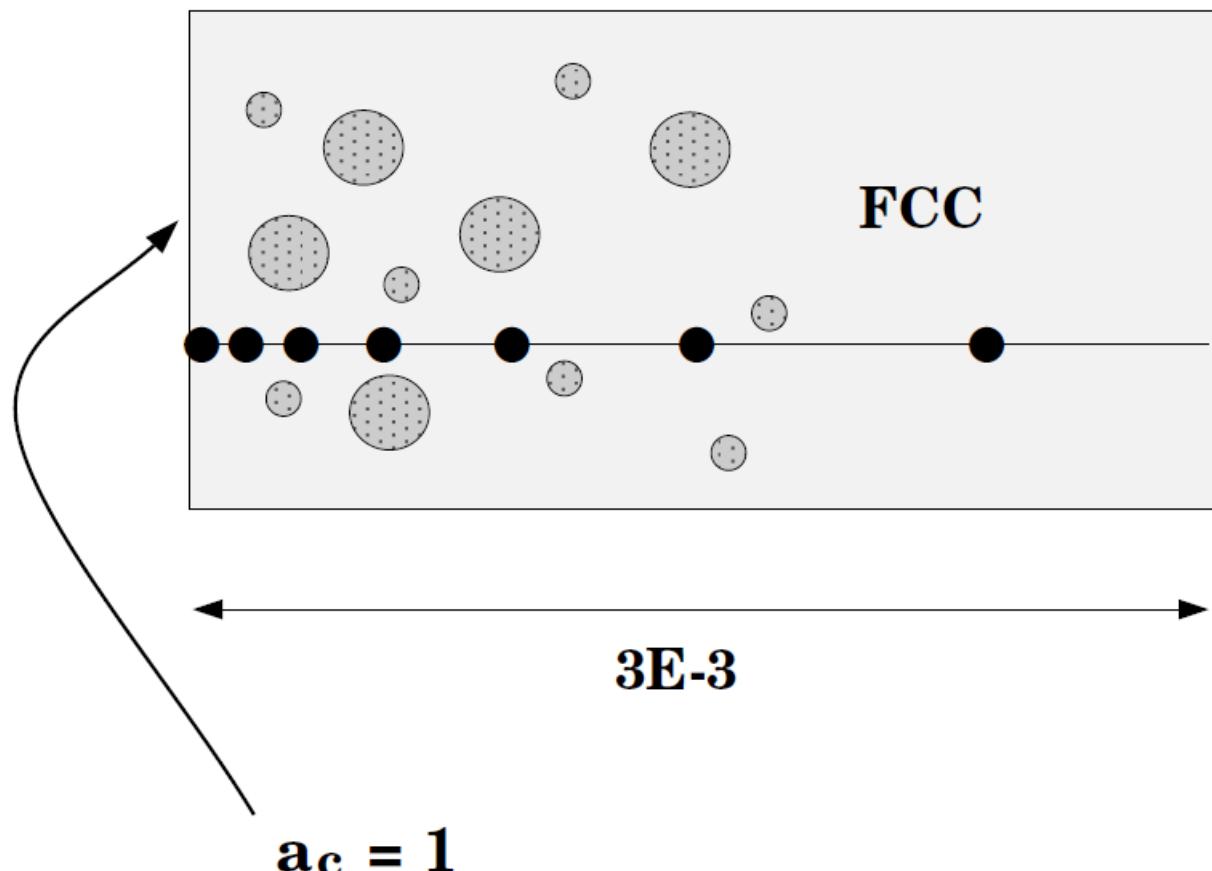


## Example exd1a

### Carburization of a Ni-25% Cr alloy: Dispersed system model

This example is about carburization of a Ni-25Cr alloy. In this case the M<sub>3</sub>C<sub>2</sub> and M<sub>7</sub>C<sub>3</sub> carbides are entered as spheroid phases in a FCC matrix. In this example the DISPERSED SYSTEM MODEL is used. This case is from A. Engström, L. Höglund and J. Ågren: Metall.Trans.A v. 25A (1994), pp. 1127-1134.

$$T = 1123 \text{ K}$$



**exdla-setup****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\_dictra\_console\_examples\examples\exdla\setup.DCM"**  
**SYS: @@**  
**SYS: @@ Diffusion in dispersed systems.**  
**SYS: @@ Carburization of Ni-25%Cr alloy: Dispersed system model**  
**SYS: @@ This example is about carburization of a Ni-25Cr alloy.**  
**SYS: @@ In this case the M3C2 and M7C3 carbides are entered as**  
**SYS: @@ spheroid phases in a FCC matrix. This simulation can be run**  
**SYS: @@ with either the DISPERSED SYSTEM MODEL or the HOMOGENIZATION MODEL.**  
**SYS: @@ In this example the DISPERSED SYSTEM MODEL is used, which requires**  
**SYS: @@ that the default HOMOGENIZATION MODEL is disabled.**  
**SYS: @@ With the DISPERSED SYSTEM MODEL the command**  
**SYS: @@ ENTER\_LABYRINTH\_FUNCTION is used to take into account the**  
**SYS: @@ impeding effect of dispersed phases on long-range diffusion.**  
**SYS: @@ For the HOMOGENIZATION MODEL the command**  
**SYS: @@ ENTER\_HOMOGENIZATION\_FUNCTION should be used.**  
**SYS: @@ This case is from A. Engström, L. Häglund and J. Ågren:**  
**SYS: @@ Metall.Trans.A v. 25A (1994), pp. 1127-1134.**  
**SYS: -----**  
NO SUCH COMMAND, USE HELP  
**SYS:**  
**SYS: @@ exd1\_setup.DCM**  
**SYS:**  
**SYS: @@**  
**SYS: @@ RETRIEVE DATA FROM THE DATABASE**  
**SYS: @@**  
**SYS: go da**  
THERMODYNAMIC DATABASE module  
Database folder:  
C:\jenkins\workspace\generate\_dictra\_console\_examples\databases\data  
Current database: Steels/Fe-Alloys v12.0  
  
VA                   /- DEFINED  
DICTRA\_FCC\_A1 REJECTED  
**TDB\_TCFE12:**  
**TDB\_TCFE12: @@**  
**TDB\_TCFE12: @@ USE THE SSOL DATABASE FOR THERMODYNAMIC DATA**  
**TDB\_TCFE12: @@**  
**TDB\_TCFE12: sw fedemo**  
Current database: Iron Demo Database v4.0  
  
VA                   /- DEFINED  
**TDB\_FEDEMO: def-sys ni cr c**  
NI                   CR                   C  
DEFINED  
**TDB\_FEDEMO: rej ph \* all**  
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  
M7C3               SIGMA            REJECTED  
**TDB\_FEDEMO: res ph fcc,m7c3,m3c2,grap**  
FCC\_A1             M7C3             M3C2  
GRAPHITE RESTORED  
**TDB\_FEDEMO: get**  
18:15:54,891 [Thread-0] INFO JavaWrapper: \*\*\* Invoking Gibbs Energy System v6 \*\*\*  
REINITIATING GES ....  
ELEMENTS ....  
SPECIES ....  
PHASES ....  
Creating a new composition set FCC\_A1#2  
PARAMETERS ...  
FUNCTIONS ....  
  
List of references for assessed data  
  
'J. Bratberg, Z. Metallkd., 96 (2005) 335-344; Fe-Cr-Mo-C'  
'X.G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'  
'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'  
'B.J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'  
'A. Gabriel, C. Chatillon, and I. Ansara, published in High Temp. Sci.  
(Parameters listed in CALPHAD, 11 (1987) 203-218); C-Ni'  
'A.T. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'  
'X.G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar  
volumes'  
'R. Naraghi, Thermo-Calc Software AB, Sweden, 2016; FCC Fe-Cr-C and C-Cr-Ni'  
'NPL, unpublished work (1989); C-Cr-Ni'  
'A.T. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); CR -Ni'  
'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121 -127; Molar  
volumes'  
'P. Villars, L.D. Calvert. Pearson's handbook of crystallographic data for  
intermetallic phases, Metals park, Ohio 1985: American society for  
metals'  
'A.F. Guillermet and G. Grimvall, J. Phys. Chem. Solids, 1992, 53, 105-125;  
Molar volumes'  
-OK-  
**TDB\_FEDEMO: @@**  
**TDB\_FEDEMO: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE MOBILITY DATA**  
**TDB\_FEDEMO: @@**  
**TDB\_FEDEMO: app mfdemo**  
Current database: Fe-Alloys Mobility demo database v2.0  
  
VA   DEFINED  
**APP: def-sys ni c cr**  
NI                   CR  
C

```

DEFINED
APP: rej ph * all
BCC A2           FCC_A1
REJECTED
CEMENTITE
APP: res ph fcc,m7c3,m3c2,grap
*** ERROR M7C3 INPUT IGNORED
*** ERROR M3C2 INPUT IGNORED
*** ERROR GRAP INPUT IGNORED
FCC A1 RESTORED
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
Creating a new composition set FCC_A1#3
PARAMETERS ...
FUNCTIONS .....

List of references for assessed data

'This parameter has not been assessed'
'B. Jonsson: Z. Metallkunde 85(1994)502-509; C diffusion in fcc Cr-Fe-Ni'
'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Fe diffusion fcc Cr-Fe'
'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Ni diffusion fcc Cr-Ni'
'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Ni self-diffusion'

-OK-
APP:
APP: @
APP: @@ ENTER THE DICTRA MONITOR
APP: @@
APP: go d-m
NO TIME STEP DEFINED
*** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
*** ENTERING M3C2 AS A DIFFUSION NONE PHASE
*** ENTERING M7C3 AS A DIFFUSION NONE PHASE
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 1123; * N
DIC>
DIC> @@
DIC> @@ SET THE REFERENCE STATE FOR CARBON
DIC> @@
DIC> set-reference-state
Component: C
Reference state: grap
Temperature /*/: *
Pressure /100000/: 101325
DIC>
DIC> @@
DIC> @@ ENTER THE REGION aus
DIC> @@
DIC> enter-region aus
DIC>
DIC> @@
DIC> @@ ENTER A GEOMETRICAL GRID INTO THE REGION
DIC> @@
DIC> enter-grid aus 3e-3 geo 100 1.02
DIC>
DIC> @@
DIC> @@ ENTER A MATRIX PHASE IN THE REGION
DIC> @@
DIC> enter-phase act aus matrix fcc_a1#1
DIC>
DIC> @@
DIC> @@ ENTER THE START COMPOSITION FOR THE MATRIX PHASE
DIC> @@
DIC> enter-composition
REGION NAME : /AUS/: aus
PHASE NAME: /FCC_A1#1/: fcc#1
DEPENDENT COMPONENT ? /NI/: ni
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: cr
TYPE /LINEAR/: lin 25 25
PROFILE FOR /CR/: c
TYPE /LINEAR/: lin 1e-4 1e-4
DIC>
DIC> @@
DIC> @@ ENTER SPHEROIDAL PHASES IN THE REGION
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /AUS/: aus
PHASE TYPE /MATRIX/: sph
PHASE NAME: /NONE/: m7c3
INFO: EQUILIBRIUM COMPOSITION AND FRACTION OF SPHEROID PHASES USED AS DEFAULT
DIC>
DIC> @@
DIC> @@ ENTER A STOICHIOMETRIC SPHEROIDAL PHASE IN THE REGION
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /AUS/: aus
PHASE TYPE /MATRIX/: sph
PHASE NAME: /NONE/: m3c2
INFO: EQUILIBRIUM COMPOSITION AND FRACTION OF SPHEROID PHASES USED AS DEFAULT
DIC>
DIC>
DIC> @@
DIC> @@ ENTER A START COMPOSITION FOR THE SPHEROIDAL PHASES
DIC> @@
DIC> enter-composition
REGION NAME : /AUS/: aus
PHASE NAME: /FCC_A1#1/: m7c3
USE EQUILIBRIUM VALUE /Y/: Y
DIC> enter-composition
REGION NAME : /AUS/: aus
PHASE NAME: /FCC_A1#1/: m3c2
USE EQUILIBRIUM VALUE /Y/: Y
DIC>
DIC> @@

```

```

DIC> @@ SET THE BOUNDARY CONDITION
DIC> @@
DIC> set-cond
GLOBAL OR BOUNDARY CONDITION /GLOBAL/: boundary
BOUNDARY /LOWER/: lower
CONDITION TYPE /CLOSED_SYSTEM/: mixed
Dependent substitutional element:NI
Dependent interstitial element:VA
TYPE OF CONDITION FOR COMPONENT C /ZERO_FLUX/: activity
LOW TIME LIMIT /0/: 0
ACR(C) (TIME)= 1;
HIGH TIME LIMIT /*/: *
ANY MORE RANGES /N/: N
TYPE OF CONDITION FOR COMPONENT CR /ZERO_FLUX/: zero-flux
DIC> @@
DIC> @@ ENTER THE LABYRINTH FACTOR
DIC> @@
DIC> enter-lab
REGION NAME : aus
f(T,P,VOLFR,X)= volfr**2;
DIC> @@
DIC> @@ SET THE SIMULATION TIME. REMEMBER TO BE CAREFUL WITH THE
DIC> @@ Timestep WHEN THERE ARE SPHEROIDAL PHASES PRESENT. IN THIS CASE
DIC> @@ THE Timestep IS NOT ALLOWED TO BE LARGER THAN 1800s.
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 3600000
AUTOMATIC Timestep CONTROL /YES/: YES
MAX Timestep DURING INTEGRATION /360000/: 1800
INITIAL Timestep : /1E-07/:
SMALLEST ACCEPTABLE Timestep : /1E-07/:
DIC> @@
DIC> @@
DIC> @@ IN ORDER SO SAVE SOME SPACE ON THE DISK THE RESULT IS STORED
DIC> @@ SELECTIVELY. OTHERWISE THE STORE-RESULT-FILE FROM THIS EXAMPLE
DIC> @@ WOULD BE VERY LARGE.
DIC> @@
DIC> set-simulation-condition
NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA Timesteps IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /AUTO/:
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/: 99
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -> 1): /AUTO/:
MAX Timestep CHANGE PER Timestep : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/:
DIC> @@
DIC> @@ BY DEFAULT THE "HOMOGENIZATION MODEL" IS USED WHEN MULTIPLE PHASES
DIC> @@ ARE ENTERED IN A SINGLE REGION. FOR THIS EXAMPLE THE HOMOGENIZATION
DIC> @@ MODEL IS DISABLED.
DIC> ho n
    HOMOGENIZATION DISABLED
DIC> @@
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exd1.y
DIC> @@
DIC> set-inter
--OK---
DIC>

```

**exdla-run**

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exdla\run.DCM"
DIC>
DIC>
DIC> @@ exd1_run.DCM
DIC>
DIC> @@
DIC> @@ READ THE SETUP FILE AND START THE SIMULATION
DIC> @@
DIC> go d-m
TIME STEP AT TIME 0.00000E+00
*** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
*** ENTERING M3C2 AS A DIFFUSION NONE PHASE
*** ENTERING M7C3 AS A DIFFUSION NONE PHASE
DIC> read exd1
OK
DIC> sim
DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
U-FRACTION IN SYSTEM: C = 4.73399450059566E-06 CR = .273386452547573
NI = .726613547452427
TOTAL SIZE OF SYSTEM: .003 [m]
WARNING:M7C3 HAS NO VOLUME FRACTION, CREATING ONE
WARNING:M3C2 HAS NO VOLUME FRACTION, CREATING ONE
U-FRACTION IN SYSTEM: C = 4.73399450059566E-06 CR = .273386452547573
NI = .726613547452427
TOTAL SIZE OF SYSTEM: .003 [m]
TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = 8.32233829951615E-05 CR = .273386452547572
NI = .726613547452428
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 0.10010000E-03 DT = 0.10000000E-03 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = 1.14491977930612E-04 CR = .273386452547544
NI = .726613547452456
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 0.40010010 DT = 0.40000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = 1.3439753194935E-04 CR = .273386452541228
NI = .726613547458772
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 61.226617 DT = 60.826517 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = 1.7323419086632E-04 CR = .273386451404806
NI = .726613548595194
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 1 seconds
TIME = 136.73132 DT = 75.504702 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = 2.15195361346137E-04 CR = .273386450378639
NI = .726613549621361
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 246.77986 DT = 110.04854 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = 2.65132773423408E-04 CR = .273386449367933
NI = .726613550632066
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 417.73078 DT = 170.95092 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = 3.26703519714745E-04 CR = .27338644842744
NI = .72661355157256
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 700.87762 DT = 283.14684 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = 4.03852183677251E-04 CR = .273386447458974
NI = .726613552541026
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 1196.7621 DT = 495.88443 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = 5.03958315340988E-04 CR = .273386446322885
NI = .726613553677116
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 2136.4660 DT = 939.70399 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = 6.43012086810225E-04 CR = .273386444988436
NI = .726613555011564
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 3936.4660 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = 8.38519749163075E-04 CR = .273386443511134
NI = .726613556488866
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 5736.4660 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0010173697033215 CR = .273386442681224
NI = .726613557318776
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 1 seconds
TIME = 7536.4660 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00118296902880158 CR = .273386442066141
NI = .726613557933858
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 9336.4660 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00133879540957735 CR = .273386441011293
NI = .726613558988707
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 11136.466 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00148538430057558 CR = .273386439279029
NI = .726613560720971
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 12936.466 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00162329996141555 CR = .273386436825667
NI = .726613563174333
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 14736.466 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00175666371078121 CR = .273386434544897
NI = .726613565455102
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
```

```

TIME = 16509.560 DT = 1773.0939 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00188419698676039 CR = .273386432317815
NI = .726613567682185
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 1 seconds
TIME = 18202.529 DT = 1692.9692 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00200374370728573 CR = .273386430131716
NI = .726613569868284
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 19871.496 DT = 1668.9668 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00212043403493914 CR = .273386427985689
NI = .726613572014311
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 21585.287 DT = 1713.7913 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00223651041851037 CR = .273386426227075
NI = .726613573772925
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 23385.287 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00235302551823151 CR = .273386424970864

```

output ignored...

... output resumed

```

CPU time used in timestep 0 seconds
TIME = 3563985.3 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0314537983526267 CR = .273386325210631
NI = .726613674789369
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 3565785.3 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0314617329030149 CR = .273386325190174
NI = .726613674809826
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 3567585.3 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0314696650642582 CR = .2733863251695
NI = .7266136748305
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 3569385.3 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0314775948480468 CR = .273386325148608
NI = .726613674851392
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 3571185.3 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0314855222664732 CR = .273386325127499
NI = .726613674872501
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 1 seconds
TIME = 3572985.3 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0314934473320117 CR = .273386325106172
NI = .726613674893828
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 3574785.3 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0315013700574986 CR = .273386325084627
NI = .726613674915374
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 3576585.3 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0315092904561121 CR = .273386325062864
NI = .726613674937136
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 3578385.3 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0315172085413539 CR = .273386325040883
NI = .726613674959117
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 3580185.3 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0315251243270302 CR = .273386325018683
NI = .726613674981316
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 3581985.3 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0315330378272334 CR = .273386324996266
NI = .726613675003734
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 3583785.3 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0315409490563253 CR = .273386324973629
NI = .726613675026371
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 1 seconds
TIME = 3585585.3 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0315488580289196 CR = .273386324950774
NI = .726613675049226
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 3587385.3 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0315567647598653 CR = .273386324927699
NI = .7266136750723
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 3589185.3 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .031564669264231 CR = .273386324904406
NI = .726613675095594
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 3590985.3 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0315725715572893 CR = .273386324880893
NI = .726613675119107
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 3592785.3 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0315804716545019 CR = .27338632485716
NI = .72661367514284
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds

```

```

TIME = 3594585.3 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0315883695715048 CR = .273386324833207
NI = .726613675166793
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 3596385.3 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .031596265324095 CR = .273386324809035
NI = .726613675190965
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 3598185.3 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0316041589282162 CR = .273386324784642
NI = .726613675215358
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 1 seconds
TIME = 3599985.3 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0316120503999463 CR = .273386324760028
NI = .726613675239971
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 3600000.0 DT = 14.712794 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0316121157454989 CR = .273386324759817
NI = .726613675240183
TOTAL SIZE OF SYSTEM: .003 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 0.0000000
DELETING TIME-RECORD FOR TIME 0.1000000E-06
DELETING TIME-RECORD FOR TIME 0.1001000E-03
DELETING TIME-RECORD FOR TIME 163785.29
DELETING TIME-RECORD FOR TIME 341985.29
DELETING TIME-RECORD FOR TIME 520185.29
DELETING TIME-RECORD FOR TIME 698385.29
DELETING TIME-RECORD FOR TIME 876585.29
DELETING TIME-RECORD FOR TIME 1054785.3
DELETING TIME-RECORD FOR TIME 1232985.3
DELETING TIME-RECORD FOR TIME 1411185.3
DELETING TIME-RECORD FOR TIME 1589385.3
DELETING TIME-RECORD FOR TIME 1767585.3
DELETING TIME-RECORD FOR TIME 1945785.3
DELETING TIME-RECORD FOR TIME 2123985.3
DELETING TIME-RECORD FOR TIME 2302185.3
DELETING TIME-RECORD FOR TIME 2480385.3
DELETING TIME-RECORD FOR TIME 2658585.3
DELETING TIME-RECORD FOR TIME 2836785.3
DELETING TIME-RECORD FOR TIME 3014985.3
DELETING TIME-RECORD FOR TIME 3193185.3
DELETING TIME-RECORD FOR TIME 3371385.3
DELETING TIME-RECORD FOR TIME 3549585.3
DELETING TIME-RECORD FOR TIME 3596385.3
DELETING TIME-RECORD FOR TIME 3598185.3

KEEPING TIME-RECORD FOR TIME 3599985.3
AND FOR TIME 3600000.0
WORKSPACE RECLAIMED
```

TIMESTEP AT 3600000.00 SELECTED

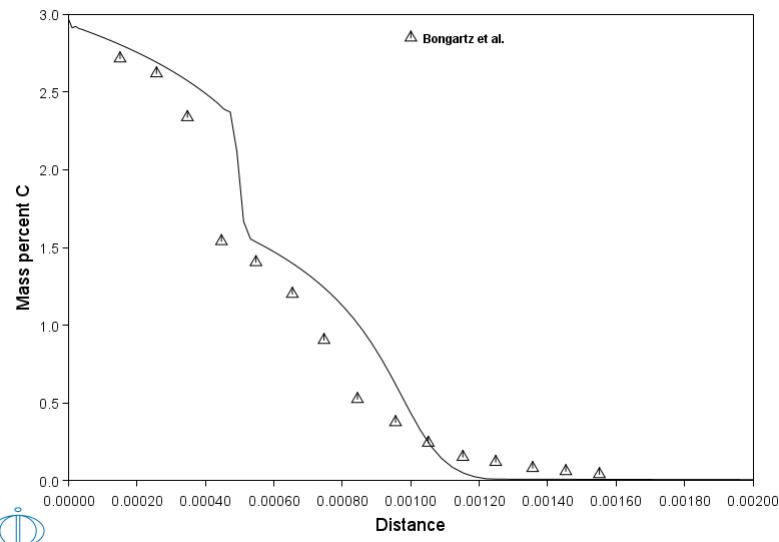
```

DIC>
DIC> set-inter
--OK--
DIC>
```

**exd1a-plot**

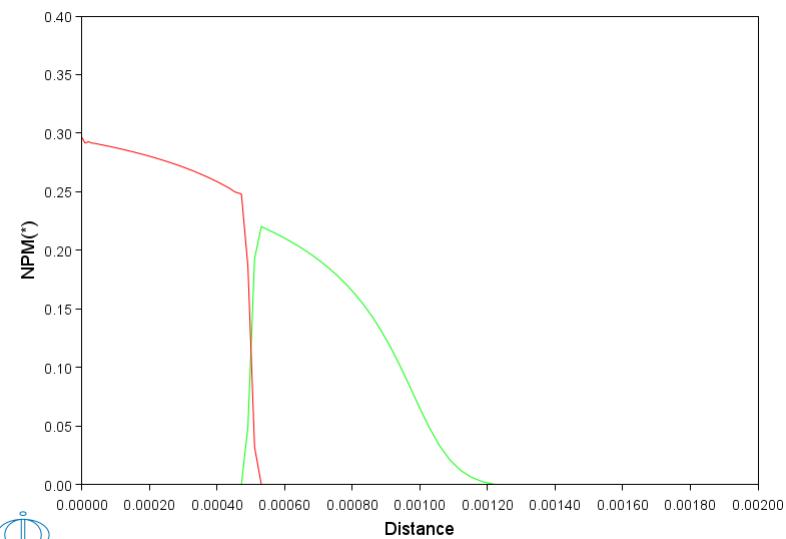
```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exd1a\plot.DCM"
DIC>
DIC>
DIC> @@ exd1_plot.DCM
DIC>
DIC> @@
DIC> @@ FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE exd1
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 3.60000E+06
*** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
*** ENTERING M3C2 AS A DIFFUSION NONE PHASE
*** ENTERING M7C3 AS A DIFFUSION NONE PHASE
DIC> read exd1
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
POST-1:
POST-1: @@ LOT THE TOTAL CARBON CONCENTRATION PROFILE
POST-1: @@
POST-1: s-d-a y w-p c
POST-1: s-d-a x distance global
INFO: Distance is set as independent variable
POST-1: s-s-s x n 0 2e-3
POST-1: s-p-c time 3600000
POST-1:
POST-1: app y exd1.exp
PROLOGUE NUMBER: /0/: 1
DATASET NUMBER(s): /-1/: 1
POST-1:
POST-1: @@
POST-1: @@ SET THE TITLE ON THE PLOT
POST-1: @@
POST-1: set-tit d1.1
POST-1:
POST-1: plot
```

d1.1



```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: @@
POST-1: @@ NOW PLOT THE AMOUNT OF CARBIDES FORMED
POST-1: @@
POST-1: s-d-a y npm(*)
POST-1: s-s-s y n 0 0.4
POST-1: app n
POST-1:
POST-1: set-tit d1.2
POST-1: plot
```

d1.2



```
POST-1:  
POST-1:  
POST-1:  
POST-1:@?<_hit_return_to_continue_>  
POST-1:  
POST-1: set-inter  
---OK---  
POST-1:
```

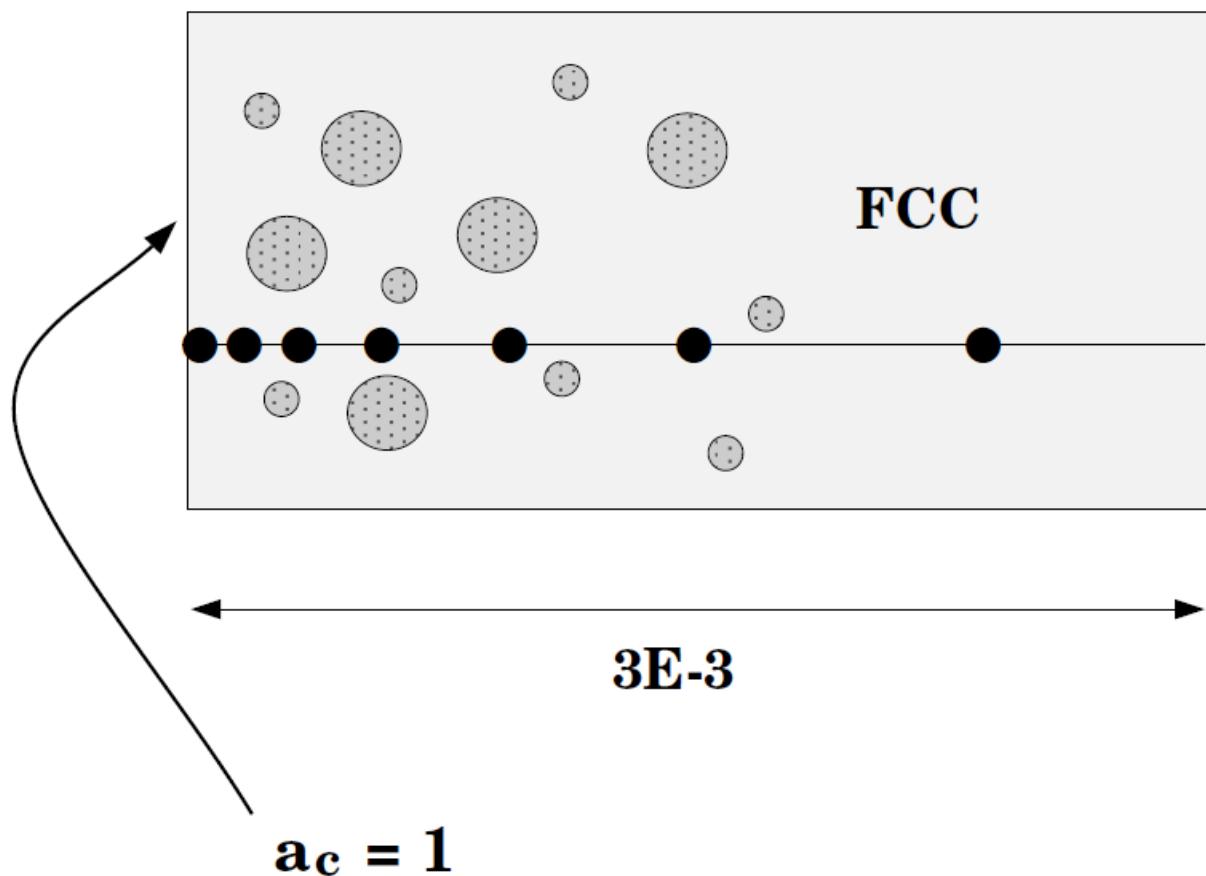


## Example exd1b

### Carburization of a Ni-25% Cr alloy: Homogenization model

This example is about carburization of a Ni-25Cr alloy. In this case the M<sub>3</sub>C<sub>2</sub> and M<sub>7</sub>C<sub>3</sub> carbides are entered as spheroid phases in a FCC matrix. It is similar to exd1a except the default HOMOGENIZATION MODEL is used and then ENTER\_HOMOGENIZATION\_FUNCTION should be used instead of ENTER\_LABYRINTH\_FUNCTION. This case is from A. Engström, L. Höglund and J. Ågren: Metall. Trans. A, v.25A (1994), pp. 1127-1134.

$$T = 1123 \text{ K}$$



**exd1b-setup****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\_dictra\_console\_examples\examples\exd1b\setup.DCM"**  
**SYS: i>@@**  
NO SUCH COMMAND, USE HELP  
**SYS: @@ Diffusion in dispersed systems.**  
**SYS: @@ Carburization of Ni-25%Cr alloy: Homogenization model**  
**SYS: @@ This example is about carburization of a Ni-25Cr alloy.**  
**SYS: @@ In this case the M3C2 and M7C3 carbides are entered as**  
**SYS: @@ spheroid phases in a FCC matrix. This case is from**  
**SYS: @@ A. Engström, L. Häglund and J. Ångren: Metall.Trans. A,**  
**SYS: @@ v.25A (1994), pp. 1127-1134.**  
**SYS: @@ This simulation can be run with the DISPERSED SYSTEM MODEL or**  
**SYS: @@ HOMOGENIZATION MODEL. The default HOMOGENIZATION MODEL is used**  
**SYS: @@ and then ENTER\_HOMOGENIZATION\_FUNCTION should be used instead of**  
**SYS: @@ ENTER\_LABYRINTH\_FUNCTION.**  
**SYS: -----**  
NO SUCH COMMAND, USE HELP  
**SYS:**  
**SYS: @@ exd1b\_setup.DCM**  
**SYS:**  
**SYS: @@**  
**SYS: @@ RETRIEVE DATA FROM THE DATABASE**  
**SYS: @@**  
**SYS: @@**  
**SYS: @@ This example modifies the database interactively, which is not**  
**SYS: @@ yet supported by GES6. Therefore, we enforce the use of GES5.**  
**SYS: set-ges-version 5**  
**SYS:**  
**SYS: go da**  
THERMODYNAMIC DATABASE module  
Database folder:  
C:\jenkins\workspace\generate\_dictra\_console\_examples\databases\data  
Current database: Steels/Fe-Alloys v12.0  
  
VA    /- DEFINED  
DICTRA\_FCC\_A1    REJECTED  
**TDB\_TCFE12: @@**  
**TDB\_TCFE12: @@ USE THE SSOL DATABASE FOR THERMODYNAMIC DATA**  
**TDB\_TCFE12: @@**  
**TDB\_TCFE12: sw fedemo**  
Current database: Iron Demo Database v4.0  
  
VA    /- DEFINED  
**TDB\_FEDEMO: def-sys ni cr c**  
NI    CR    C  
      DEFINED  
**TDB\_FEDEMO: rej ph \* all**  
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  
M7C3    SIGMA                                    REJECTED  
**TDB\_FEDEMO: res ph fcc,m7c3,m3c2,grap**  
FCC\_A1    M7C3    M3C2  
GRAPHITE    RESTORED  
**TDB\_FEDEMO: get**  
REINITIATING GES ....  
ELEMENTS ....  
SPECIES ....  
PHASES ....  
Creating a new composition set FCC\_A1#2  
PARAMETERS ...  
FUNCTIONS ....  
  
List of references for assessed data  
  
'J. Bratberg, Z. Metallkd., 96 (2005) 335-344; Fe-Cr-Mo-C'  
'X.G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'  
'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'  
'B.J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'  
'A. Gabriel, C. Chatillon, and I. Ansara, published in High Temp. Sci.  
(Parameters listed in CALPHAD, 11 (1987) 203-218); C-Ni'  
'A.T. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'  
'X.G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar  
volumes'  
'R. Naraghi, Thermo-Calc Software AB, Sweden, 2016; FCC Fe-Cr-C and C-Cr-Ni'  
'NPL, unpublished work (1989); C-Cr-Ni'  
'A.T. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); CR -Ni'  
'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121 -127; Molar  
volumes'  
'P. Villars, L.D. Calvert. Pearson's handbook of crystallographic data for  
intermetallic phases, Metals park, Ohio 1985: American society for  
metals'  
'A.F. Guillermet and G. Grimvall, J. Phys. Chem. Solids, 1992, 53, 105-125;  
Molar volumes'  
-OK-  
**TDB\_FEDEMO: @@**  
**TDB\_FEDEMO: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE MOBILITY DATA**  
**TDB\_FEDEMO: @@**  
**TDB\_FEDEMO: app mfdemo**  
Current database: Fe-Alloys Mobility demo database v2.0  
  
VA    DEFINED  
**APP: def-sys ni c cr**

```

NI                               C                               CR
      DEFINED
APP: rej ph * all           FCC_A1
BCC_A2                         CEMENTITE
      REJECTED
APP: res ph fcc,m7c3,m3c2,grap
*** ERROR M7C3 INPUT IGNORED
*** ERROR M3C2 INPUT IGNORED
*** ERROR GRAP INPUT IGNORED
FCC_A1 RESTORED
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
Creating a new composition set FCC_A1#3
PARAMETERS ...
FUNCTIONS .....

List of references for assessed data

'This parameter has not been assessed'
'B. Jonsson: Z. Metallkunde 85(1994)502-509; C diffusion in fcc Cr-Fe-Ni'
'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Fe diffusion fcc Cr-Fe'
'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Ni diffusion fcc Cr-Ni'
'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Ni self-diffusion'

-OK-
APP:
APP: @@ ENTER THE DICTRA MONITOR
APP: @@ go d-m
NO TIME STEP DEFINED
*** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
*** ENTERING M3C2 AS A DIFFUSION NONE PHASE
*** ENTERING M7C3 AS A DIFFUSION NONE PHASE
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 1123; * N
DIC>
DIC> @@
DIC> @@ SET THE REFERENCE STATE FOR CARBON
DIC> @@
DIC> set-reference-state
Component: C
Reference state: grap
Temperature /*/: *
Pressure /100000/: 101325
DIC>
DIC> @@
DIC> @@ ENTER THE REGION aus
DIC> @@
DIC> enter-region aus
DIC>
DIC> @@
DIC> @@ ENTER A GEOMETRICAL GRID INTO THE REGION
DIC> @@
DIC> enter-grid aus 3e-3 geo 100 1.02
DIC>
DIC> @@
DIC> @@ ENTER A MATRIX PHASE IN THE REGION
DIC> @@
DIC> enter-phase act aus matrix fcc_a1#1
DIC>
DIC> @@
DIC> @@ ENTER THE START COMPOSITION FOR THE MATRIX PHASE
DIC> @@
DIC> enter-composition
REGION NAME : /AUS/: aus
PHASE NAME: /FCC_A1#1/: fcc#1
DEPENDENT COMPONENT ? /NI/: ni
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: cr
TYPE /LINEAR/: lin 25 25
PROFILE FOR /CR/: c
TYPE /LINEAR/: lin 1e-4 1e-4
DIC>
DIC> @@
DIC> @@ ENTER SPHEROIDAL PHASES IN THE REGION
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /AUS/: aus
PHASE TYPE /MATRIX/: sph
PHASE NAME: /NONE/: m7c3
INFO: EQUILIBRIUM COMPOSITION AND FRACTION OF SPHEROID PHASES USED AS DEFAULT
DIC>
DIC> @@
DIC> @@ ENTER A STOICHIOMETRIC SPHEROIDAL PHASE IN THE REGION
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /AUS/: aus
PHASE TYPE /MATRIX/: sph
PHASE NAME: /NONE/: m3c2
INFO: EQUILIBRIUM COMPOSITION AND FRACTION OF SPHEROID PHASES USED AS DEFAULT
DIC>
DIC> @@
DIC> @@ ENTER A START COMPOSITION FOR THE SPHEROIDAL PHASES
DIC> @@
DIC> enter-composition
REGION NAME : /AUS/: aus
PHASE NAME: /FCC_A1#1/: m7c3
USE EQUILIBRIUM VALUE /Y/: Y
DIC> enter-composition
REGION NAME : /AUS/: aus
PHASE NAME: /FCC_A1#1/: m3c2
USE EQUILIBRIUM VALUE /Y/: Y
DIC>

```

```

DIC> @@
DIC> @@ SET THE BOUNDARY CONDITION
DIC> @@
DIC> set-cond
GLOBAL OR BOUNDARY CONDITION /GLOBAL/: boundary
BOUNDARY /LOWER/: lower
CONDITION TYPE /CLOSED_SYSTEM/: mixed
Dependent substitutional element:NI
Dependent interstitial element:VA
TYPE OF CONDITION FOR COMPONENT C /ZERO_FLUX/: activity
LOW TIME LIMIT /0/: 0
ACR(C) (TIME)= 1;
HIGH TIME LIMIT /*/: *
ANY MORE RANGES /N/: N
TYPE OF CONDITION FOR COMPONENT CR /ZERO_FLUX/: zero-flux
DIC>
DIC> @@
DIC> @@ SELECT THE HOMOGENIZATION FUNCTION
DIC> @@
DIC> enter-homo
ENTER HOMOGENIZATION FUNCTION # /5/: 8
SELECTED FUNCTION IS LABYRINTH FACTOR f**2 WITH PRESCRIBED MATRIX PHASE
PHASE NAME: fcc#1
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME. REMEMBER TO BE CAREFUL WITH THE
DIC> @@ Timestep WHEN SPHEROIDAL PHASES ARE PRESENT. IN THIS CASE
DIC> @@ THE Timestep IS NOT ALLOWED TO BE LARGER THAN 1800s.
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 3600000
AUTOMATIC Timestep CONTROL /YES/: YES
MAX Timestep DURING INTEGRATION /360000/:
INITIAL Timestep : /1E-07/:
SMALLEST ACCEPTABLE Timestep : /1E-07/:
DIC>
DIC>
DIC> @@
DIC> @@ TO SAVE SOME SPACE ON THE DISK THE RESULTS ARE STORED SELECTIVELY,
DIC> @@ OTHERWISE THE STORE-RESULT-FILE FROM THIS EXAMPLE WOULD BE
DIC> @@ VERY LARGE.
DIC> @@
DIC> set-simulation-condition
NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA Timesteps IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /AUTO/:
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/: 99
DEGREE OF IMPLICITY WHEN INTEGRATING PDES (AUTO, 0 -> 0.5 -> 1): /AUTO/:
MAX Timestep CHANGE PER Timestep : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/:
DIC>
DIC> @@
DIC> @@ SAVE THE SETUP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exd1.y
DIC>
DIC> set-inter
--OK---
DIC>

```

**exd1b-run**

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exd1b\run.DCM"
DIC>
DIC>
DIC> @@ exd1_run.DCM
DIC>
DIC> @@
DIC> @@ READ THE SETUP FILE AND START THE SIMULATION
DIC> @@
DIC> go d-m
TIME STEP AT TIME 0.00000E+00
*** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
*** ENTERING M3C2 AS A DIFFUSION NONE PHASE
*** ENTERING M7C3 AS A DIFFUSION NONE PHASE
DIC> read exd1
OK
DIC> sim
DEGREE OF IMPLICITY SET TO EULER BACKWARD
STARTING SIMULATION USING HOMOGENIZATION MODEL
-----
INFO: PHASE WITH LIMITED SOLUBILITY OF ELEMENT(S) EXIST
A FALLBACK PHASE ZZDICTRA_GHOST WILL BE DEFINED
ALONG WITH THE FOLLOWING PARAMETERS:
G(ZZDICTRA_GHOST,C;0)-H298(GRAPHITE,C;0)
G(ZZDICTRA_GHOST,CR;0)-H298(BCC_A2,CR;0)
G(ZZDICTRA_GHOST,NI;0)-H298(FCC_A1,NI;0)
L(ZZDICTRA_GHOST,C,CR;0)
L(ZZDICTRA_GHOST,C,NI;0)
L(ZZDICTRA_GHOST,CR,NI;0)
WARNING:M7C3 HAS NO VOLUME FRACTION, CREATING ONE
WARNING:M3C2 HAS NO VOLUME FRACTION, CREATING ONE
Starting time-step t0= 0.000000 dt= 0.10000000E-06
Starting time-step t0= 0.10000000E-06 dt= 0.20000000E-06
Starting time-step t0= 0.30000000E-06 dt= 0.40000000E-06
Starting time-step t0= 0.70000000E-06 dt= 0.80000000E-06
Starting time-step t0= 0.15000000E-05 dt= 0.16000000E-05
Starting time-step t0= 0.31000000E-05 dt= 0.32000000E-05
Starting time-step t0= 0.63000000E-05 dt= 0.64000000E-05
Starting time-step t0= 0.12700000E-04 dt= 0.12800000E-04
Starting time-step t0= 0.25500000E-04 dt= 0.25600000E-04
Starting time-step t0= 0.51100000E-04 dt= 0.51200000E-04
Starting time-step t0= 0.10230000E-03 dt= 0.10240000E-03
Starting time-step t0= 0.20470000E-03 dt= 0.20480000E-03
Starting time-step t0= 0.40950000E-03 dt= 0.40960000E-03
Starting time-step t0= 0.81910000E-03 dt= 0.81920000E-03
Starting time-step t0= 0.16383000E-02 dt= 0.16384000E-02
Starting time-step t0= 0.32767000E-02 dt= 0.32768000E-02
Starting time-step t0= 0.65535000E-02 dt= 0.65536000E-02
Starting time-step t0= 0.13107100E-01 dt= 0.13107200E-01
Starting time-step t0= 0.26214300E-01 dt= 0.26214400E-01
Starting time-step t0= 0.52428700E-01 dt= 0.52428800E-01
Starting time-step t0= 0.10485750 dt= 0.52428800E-01
Starting time-step t0= 0.15728630 dt= 0.52428800E-01
Starting time-step t0= 0.20971510 dt= 0.52428800E-01
Starting time-step t0= 0.26214390 dt= 0.52428800E-01
Starting time-step t0= 0.31457270 dt= 0.52428800E-01
Starting time-step t0= 0.36700150 dt= 0.10485760
Starting time-step t0= 0.47185910 dt= 0.20971520
Starting time-step t0= 0.68157430 dt= 0.41943040
Starting time-step t0= 1.1010047 dt= 0.41943040
Starting time-step t0= 1.5204351 dt= 0.83886080
Starting time-step t0= 2.3592959 dt= 0.83886080
Starting time-step t0= 3.1981567 dt= 0.83886080
Starting time-step t0= 4.0370175 dt= 0.83886080
Starting time-step t0= 4.8758783 dt= 0.83886080
Starting time-step t0= 5.7147391 dt= 0.83886080
Starting time-step t0= 6.5535999 dt= 0.83886080
Starting time-step t0= 7.3924607 dt= 0.83886080
Starting time-step t0= 8.2313215 dt= 0.83886080
Starting time-step t0= 9.0701823 dt= 0.83886080
Starting time-step t0= 9.9090431 dt= 0.83886080
Starting time-step t0= 10.747904 dt= 0.83886080
Starting time-step t0= 11.586765 dt= 0.83886080
Starting time-step t0= 12.425625 dt= 0.83886080
Starting time-step t0= 13.264486 dt= 0.83886080
Starting time-step t0= 14.103347 dt= 0.83886080
Starting time-step t0= 14.942208 dt= 0.83886080
Starting time-step t0= 15.781069 dt= 0.83886080
Starting time-step t0= 16.619929 dt= 0.83886080
Starting time-step t0= 17.458790 dt= 0.83886080
Starting time-step t0= 18.297651 dt= 0.83886080
Starting time-step t0= 19.136512 dt= 0.83886080
Starting time-step t0= 19.975373 dt= 0.83886080
Starting time-step t0= 20.814233 dt= 0.83886080
Starting time-step t0= 21.653094 dt= 0.83886080
Starting time-step t0= 22.491955 dt= 0.83886080
Starting time-step t0= 23.330816 dt= 0.83886080
Starting time-step t0= 24.169677 dt= 0.83886080
Starting time-step t0= 25.008537 dt= 0.83886080
Starting time-step t0= 25.847398 dt= 0.83886080
Starting time-step t0= 26.686259 dt= 0.83886080
Starting time-step t0= 27.525120 dt= 0.83886080
Starting time-step t0= 28.363981 dt= 0.83886080
Starting time-step t0= 29.202841 dt= 0.83886080
Starting time-step t0= 30.041702 dt= 0.83886080
Starting time-step t0= 30.880563 dt= 0.83886080
Starting time-step t0= 31.719424 dt= 0.83886080
Starting time-step t0= 32.558285 dt= 0.83886080
Starting time-step t0= 33.397145 dt= 0.83886080
Starting time-step t0= 34.236006 dt= 0.83886080
Starting time-step t0= 35.074867 dt= 0.83886080
Starting time-step t0= 35.913728 dt= 0.83886080
Starting time-step t0= 36.752589 dt= 0.83886080
Starting time-step t0= 37.591449 dt= 0.83886080
Starting time-step t0= 38.430310 dt= 1.6777216
Starting time-step t0= 40.108032 dt= 1.6777216
Starting time-step t0= 41.785753 dt= 1.6777216
Starting time-step t0= 43.463475 dt= 1.6777216
Starting time-step t0= 45.141197 dt= 1.6777216
Starting time-step t0= 46.818918 dt= 1.6777216
Starting time-step t0= 48.496640 dt= 1.6777216
```

```
Starting time-step t0= 50.174361 dt= 1.6777216
Starting time-step t0= 51.852083 dt= 1.6777216
Starting time-step t0= 53.529805 dt= 1.6777216
Starting time-step t0= 55.207526 dt= 1.6777216
Starting time-step t0= 56.885248 dt= 1.6777216
Starting time-step t0= 58.562969 dt= 1.6777216
Starting time-step t0= 60.240691 dt= 1.6777216
Starting time-step t0= 61.918413 dt= 1.6777216
Starting time-step t0= 63.596134 dt= 1.6777216
Starting time-step t0= 65.273856 dt= 1.6777216
Starting time-step t0= 66.951577 dt= 1.6777216
Starting time-step t0= 68.629299 dt= 1.6777216
Starting time-step t0= 70.307021 dt= 1.6777216
Starting time-step t0= 71.984742 dt= 1.6777216
Starting time-step t0= 73.662464 dt= 1.6777216
Starting time-step t0= 75.340185 dt= 1.6777216
Starting time-step t0= 77.017907 dt= 3.3554432
Starting time-step t0= 80.373350 dt= 3.3554432
Starting time-step t0= 83.728793 dt= 3.3554432
Starting time-step t0= 87.084237 dt= 3.3554432
Starting time-step t0= 90.439680 dt= 3.3554432
Starting time-step t0= 93.795123 dt= 3.3554432
```

output ignored...

... output resumed

```
DELETING TIME-RECORD FOR TIME 2273980.3
DELETING TIME-RECORD FOR TIME 2280852.3
DELETING TIME-RECORD FOR TIME 2287724.2
DELETING TIME-RECORD FOR TIME 2294596.2
DELETING TIME-RECORD FOR TIME 2301468.1
DELETING TIME-RECORD FOR TIME 2308340.1
DELETING TIME-RECORD FOR TIME 2315212.0
DELETING TIME-RECORD FOR TIME 2322084.0
DELETING TIME-RECORD FOR TIME 2328955.9
DELETING TIME-RECORD FOR TIME 2335827.9
DELETING TIME-RECORD FOR TIME 2342699.8
DELETING TIME-RECORD FOR TIME 2349571.8
DELETING TIME-RECORD FOR TIME 2356443.7
DELETING TIME-RECORD FOR TIME 2363315.7
DELETING TIME-RECORD FOR TIME 2370187.6
DELETING TIME-RECORD FOR TIME 2377059.6
DELETING TIME-RECORD FOR TIME 2383931.5
DELETING TIME-RECORD FOR TIME 2390803.5
DELETING TIME-RECORD FOR TIME 2397675.4
DELETING TIME-RECORD FOR TIME 2404547.3
DELETING TIME-RECORD FOR TIME 2411419.3
DELETING TIME-RECORD FOR TIME 2418291.2
DELETING TIME-RECORD FOR TIME 2425163.2
DELETING TIME-RECORD FOR TIME 2432035.1
DELETING TIME-RECORD FOR TIME 2438907.1
DELETING TIME-RECORD FOR TIME 2445779.0
DELETING TIME-RECORD FOR TIME 2452651.0
DELETING TIME-RECORD FOR TIME 2459522.9
DELETING TIME-RECORD FOR TIME 2466394.9
DELETING TIME-RECORD FOR TIME 2473266.8
DELETING TIME-RECORD FOR TIME 2480138.8
DELETING TIME-RECORD FOR TIME 2487010.7
DELETING TIME-RECORD FOR TIME 2493882.7
DELETING TIME-RECORD FOR TIME 2500754.6
DELETING TIME-RECORD FOR TIME 2507626.6
DELETING TIME-RECORD FOR TIME 2514498.5
DELETING TIME-RECORD FOR TIME 2521370.5
DELETING TIME-RECORD FOR TIME 2528242.4
DELETING TIME-RECORD FOR TIME 2535114.4
DELETING TIME-RECORD FOR TIME 2541986.3
DELETING TIME-RECORD FOR TIME 2548858.3
DELETING TIME-RECORD FOR TIME 2555730.2
DELETING TIME-RECORD FOR TIME 2562602.1
DELETING TIME-RECORD FOR TIME 2569474.1
DELETING TIME-RECORD FOR TIME 2576346.0
DELETING TIME-RECORD FOR TIME 2583218.0
DELETING TIME-RECORD FOR TIME 2593525.9
DELETING TIME-RECORD FOR TIME 2600397.9
DELETING TIME-RECORD FOR TIME 2607269.8
DELETING TIME-RECORD FOR TIME 2614141.8
DELETING TIME-RECORD FOR TIME 2621013.7
DELETING TIME-RECORD FOR TIME 2627885.6
DELETING TIME-RECORD FOR TIME 2634757.6
DELETING TIME-RECORD FOR TIME 2641629.5
DELETING TIME-RECORD FOR TIME 2648501.5
DELETING TIME-RECORD FOR TIME 2655373.4
DELETING TIME-RECORD FOR TIME 2662245.4
DELETING TIME-RECORD FOR TIME 2669117.3
DELETING TIME-RECORD FOR TIME 2675989.3
DELETING TIME-RECORD FOR TIME 2682861.2
DELETING TIME-RECORD FOR TIME 2689733.2
DELETING TIME-RECORD FOR TIME 2696605.1
DELETING TIME-RECORD FOR TIME 2703477.1
DELETING TIME-RECORD FOR TIME 2710349.0
DELETING TIME-RECORD FOR TIME 2717221.0
DELETING TIME-RECORD FOR TIME 2724092.9
DELETING TIME-RECORD FOR TIME 2730964.9
DELETING TIME-RECORD FOR TIME 2737836.8
DELETING TIME-RECORD FOR TIME 2744708.8
DELETING TIME-RECORD FOR TIME 2758452.7
DELETING TIME-RECORD FOR TIME 2772196.6
DELETING TIME-RECORD FOR TIME 2785940.4
DELETING TIME-RECORD FOR TIME 2799684.3
DELETING TIME-RECORD FOR TIME 2813428.2
DELETING TIME-RECORD FOR TIME 2827172.1
DELETING TIME-RECORD FOR TIME 2840916.0
DELETING TIME-RECORD FOR TIME 2854659.9
DELETING TIME-RECORD FOR TIME 2868403.8
DELETING TIME-RECORD FOR TIME 2875275.8
DELETING TIME-RECORD FOR TIME 2882147.7
DELETING TIME-RECORD FOR TIME 2895891.6
DELETING TIME-RECORD FOR TIME 2909635.5
DELETING TIME-RECORD FOR TIME 2923379.4
DELETING TIME-RECORD FOR TIME 2937123.3
DELETING TIME-RECORD FOR TIME 2950867.2
DELETING TIME-RECORD FOR TIME 2964611.1
```

DELETING TIME-RECORD FOR TIME 2978355.0  
DELETING TIME-RECORD FOR TIME 2992098.9  
DELETING TIME-RECORD FOR TIME 3005842.8  
DELETING TIME-RECORD FOR TIME 3019586.7  
DELETING TIME-RECORD FOR TIME 3033330.6  
DELETING TIME-RECORD FOR TIME 3047074.5  
DELETING TIME-RECORD FOR TIME 3060818.4  
DELETING TIME-RECORD FOR TIME 3074562.2  
DELETING TIME-RECORD FOR TIME 3088306.1  
DELETING TIME-RECORD FOR TIME 3102050.0  
DELETING TIME-RECORD FOR TIME 3115793.9  
DELETING TIME-RECORD FOR TIME 3129537.8  
DELETING TIME-RECORD FOR TIME 3143281.7  
DELETING TIME-RECORD FOR TIME 3157025.6  
DELETING TIME-RECORD FOR TIME 3170769.5  
DELETING TIME-RECORD FOR TIME 3184513.4  
DELETING TIME-RECORD FOR TIME 3198257.3  
DELETING TIME-RECORD FOR TIME 3212001.2  
DELETING TIME-RECORD FOR TIME 3225745.1  
DELETING TIME-RECORD FOR TIME 3239489.0  
DELETING TIME-RECORD FOR TIME 3253232.9  
DELETING TIME-RECORD FOR TIME 3266976.8  
DELETING TIME-RECORD FOR TIME 3280720.7  
DELETING TIME-RECORD FOR TIME 3294464.6  
DELETING TIME-RECORD FOR TIME 3308208.5  
DELETING TIME-RECORD FOR TIME 3321952.4  
DELETING TIME-RECORD FOR TIME 3335696.3  
DELETING TIME-RECORD FOR TIME 3349440.2  
DELETING TIME-RECORD FOR TIME 3363184.1  
DELETING TIME-RECORD FOR TIME 3376927.9  
DELETING TIME-RECORD FOR TIME 3390671.8  
DELETING TIME-RECORD FOR TIME 3404415.7  
DELETING TIME-RECORD FOR TIME 3418159.6  
DELETING TIME-RECORD FOR TIME 3431903.5  
DELETING TIME-RECORD FOR TIME 3445647.4  
DELETING TIME-RECORD FOR TIME 3459391.3  
DELETING TIME-RECORD FOR TIME 3473135.2  
DELETING TIME-RECORD FOR TIME 3486879.1  
DELETING TIME-RECORD FOR TIME 3500623.0  
DELETING TIME-RECORD FOR TIME 3514366.9  
DELETING TIME-RECORD FOR TIME 3528110.8  
DELETING TIME-RECORD FOR TIME 3541854.7  
DELETING TIME-RECORD FOR TIME 3555598.6  
DELETING TIME-RECORD FOR TIME 3562470.5  
DELETING TIME-RECORD FOR TIME 3572778.5

KEEPING TIME-RECORD FOR TIME 3586522.3  
AND FOR TIME 3600000.0  
WORKSPACE RECLAIMED

-----  
INTERPOLATION SCHEME USED THIS FRACTION OF  
THE ALLOCATED MEMORY: 1.00000000000000  
EFFICIENCY FACTOR: 6.14323613304541

-----  
DEALLOCATING

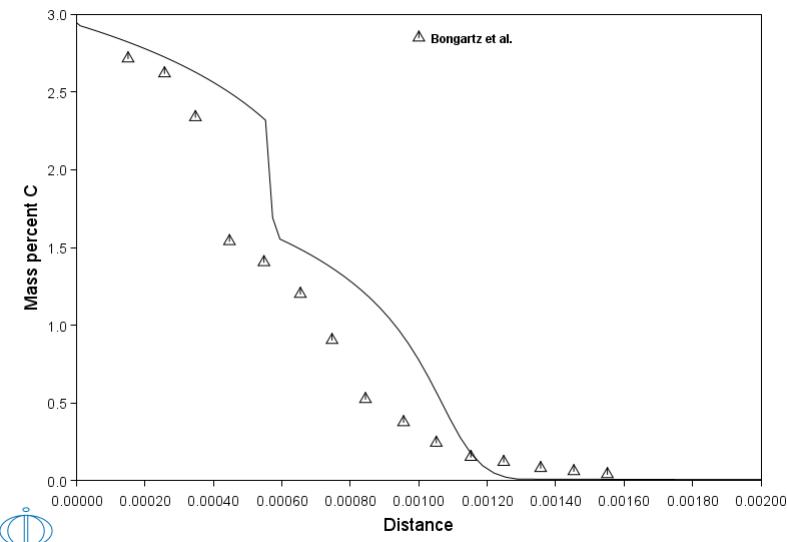
-----  
TIMESTEP AT 3600000.00 SELECTED

DIC>  
DIC> set-inter  
--OK---  
DIC>

**exd1b-plot**

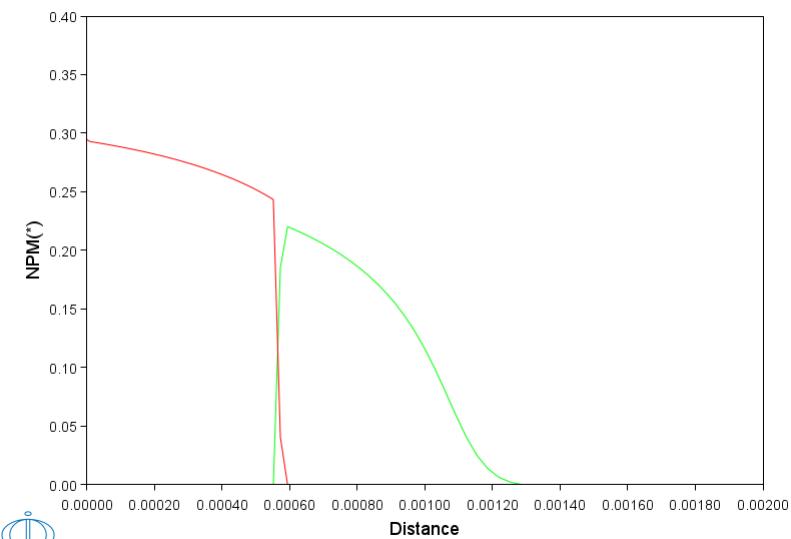
```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exd1b\plot.DCM"
DIC>
DIC>
DIC> @@ exd1_plot.DCM
DIC>
DIC> @@
DIC> @@ FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE exd1b
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 3.60000E+06
*** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
*** ENTERING M3C2 AS A DIFFUSION NONE PHASE
*** ENTERING M7C3 AS A DIFFUSION NONE PHASE
DIC> read exd1
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
POST-1:
POST-1: @@ PLOT THE TOTAL CARBON CONCENTRATION PROFILE
POST-1: @@
POST-1: s-d-a y w-p c
POST-1: s-d-a x distance global
INFO: Distance is set as independent variable
POST-1: s-s-s x n 0 2e-3
POST-1: s-p-c time 3600000
POST-1:
POST-1: app y exd1.exp
PROLOGUE NUMBER: /0/: 1
DATASET NUMBER(s): /-1/: 1
POST-1:
POST-1: @@
POST-1: @@ SET A TITLE ON THE PLOT
POST-1: @@
POST-1: set-tit d1.1
POST-1:
POST-1: plot
```

d1.1



```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: @@
POST-1: @@ PLOT THE AMOUNT OF CARBIDES FORMED
POST-1: @@
POST-1: s-d-a y npm(*)
POST-1: s-s-s y n 0 0.4
POST-1: app n
POST-1:
POST-1: set-tit d1.2
POST-1: plot
```

d1.2



POST-1:  
POST-1:  
POST-1:  
POST-1:@?<\_hit\_return\_to\_continue\_>  
POST-1:  
POST-1: set-inter  
---OK---  
POST-1:



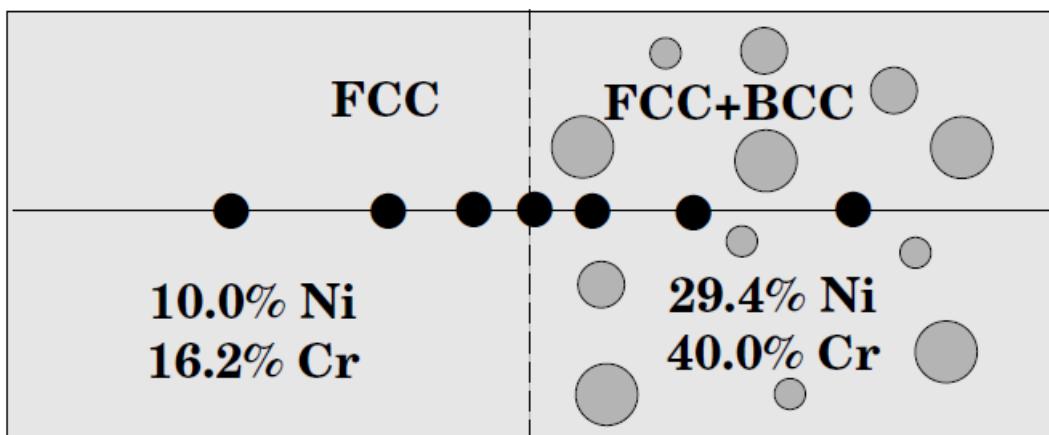
## Example exd2a

### Diffusion couple of Fe-Ni-Cr alloys: Step-profile

This example calculates the interdiffusion in a diffusion couple between a two-phase (FCC+BCC) and a single-phase (FCC) Fe-Ni-Cr alloy. Initially it uses a step profile. This simulation can be run with either the DISPERSED SYSTEM MODEL or the HOMOGENIZATION MODEL. In this example the DISPERSED SYSTEM MODEL is used.

This case is from A. Engström: Scand. J. Met., vol. 24, 1995, pp.12-20.

**T = 1473 K**



**4E-3**



```

'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
-Ni'
'Xia, C. H. et al. JAC, 2021, 853, 157165.'
'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Ni self-diffusion'
'B. Jonsson: ISIJ International, 35(1995)1415-1421; Cr, Fe and Ni
diffusion bcc Cr-Fe-Ni'
'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
in bcc Fe'
-OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR
APP: @@
APP: go d-m
NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 1473; * N
DIC>
DIC> @@
DIC> @@ ENTER THE REGION fer
DIC> @@
DIC> enter-region fer
DIC>
DIC>
DIC> @@
DIC> @@ ENTER A DOUBLE GEOMETRICAL GRID INTO THE REGION
DIC> @@ THIS GIVES A SHORT DISTANCE BETWEEN THE GRIDPOINTS
DIC> @@ IN THE MIDDLE OF THE REGION WHERE THE INITIAL INTERFACE IS
DIC> @@
DIC> enter-grid fer
WIDTH OF REGION /1/: 4e-3
TYPE /LINEAR/: double
NUMBER OF POINTS /50/: 200
VALUE OF R IN THE GEOMETRICAL SERIE FOR LOWER PART OF REGION: 0.97
VALUE OF R IN THE GEOMETRICAL SERIE FOR UPPER PART OF REGION: 1.03093
DIC>
DIC> @@
DIC> @@ ENTER A MATRIX PHASE IN THE REGION
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act fer matrix fcc
DIC>
DIC> @@
DIC> @@ ENTER THE START COMPOSITION FOR THE MATRIX PHASE FROM FILES
DIC> @@
DIC> enter-composition
REGION NAME : /FER/: fer
PHASE NAME: /FCC_A1/: fcc
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /CR/: cr
TYPE /LINEAR/: read d2cr.dat
PROFILE FOR /NI/: ni
TYPE /LINEAR/: read d2ni.dat
DIC>
DIC> @@
DIC> @@ ENTER FERRITE AS THE SPHEROIDAL PHASE IN THE REGION.
DIC> @@ SINCE THE FRACTION OF FERRITE IS SMALL, AND THESE APPEAR
DIC> @@ AS ISOLATED PARTICLES, FERRITE IS ENTERED AS A SPHEROIDAL PHASE
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /FER/: fer
PHASE TYPE /MATRIX/: sph
PHASE NAME: /NONE/: bcc
INFO: EQUILIBRIUM COMPOSITION AND FRACTION OF SPHEROID PHASES USED AS DEFAULT
DIC>
DIC> @@
DIC> @@ ENTER A COMPOSITION FOR THE SPHEROIDAL PHASE
DIC> @@ USE THE EQUILIBRIUM VALUE
DIC> @@
DIC> enter-composition
REGION NAME : /FER/: fer
PHASE NAME: /FCC_A1/: bcc
USE EQUILIBRIUM VALUE /Y/: y
DIC>
DIC>
DIC> @@
DIC> @@ ENTER A LABYRINTH FACTOR
DIC> @@ IN THIS CASE THE LOW DIFFUSIVITY PHASE IS THE MATRIX AND THE
DIC> @@ "EFFECTIVE" DIFFUSIVITY IN THE AUSTENITE+FERRITE TWO-PHASE
DIC> @@ REGION IS EXPECTED TO BE HIGHER THAN THE DIFFUSIVITY IN THE
DIC> @@ AUSTENITE.
DIC> enter-lab
REGION NAME : fer
f(T,P,VOLFR,X)= 1+3*(1-volfr)/volfr;
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME AND OTHER SIMULATION PARAMETERS
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /1/: 720000
AUTOMATIC TIMESTEP CONTROL /YES/: YES
MAX TIMESTEP DURING INTEGRATION /72000/: 5000
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC> set-simulation-condition
NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA Timesteps IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /AUTO/:
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/: 99
DEGREE OF IMPLICITY WHEN INTEGRATING PDES (AUTO, 0 -> 0.5 -> 1): /AUTO/:
MAX TIMESTEP CHANGE PER Timestep : /2/:

```

```
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/:
DIC> @@ BY DEFAULT THE "HOMOGENIZATION MODEL" IS USED WHEN MULTIPLE PHASES
DIC> @@ ARE ENTERED IN A SINGLE REGION. THE HOMOGENIZATION MODEL NEEDS TO BE
DIC> @@ DISABLED FOR THIS EXAMPLE.
DIC> ho n
    HOMOGENIZATION DISABLED
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC>
DIC>
DIC> save exd2 y
DIC>
DIC> set-inter
--OK--
DIC>
```

**exd2a-run**

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exd2a\run.DCM"
DIC>
DIC>
DIC> @@ exd2_run.DCM
DIC>
DIC> @@
DIC> FILE FOR RUNNING THE SIMULATION OF EXAMPLE D2
DIC> @@
DIC>
DIC> @@
DIC> READ THE SETUP FROM FILE AND START THE SIMULATION
DIC> @@
DIC>
DIC>
DIC> go d-m
TIME STEP AT TIME 0.00000E+00
DIC> read exd2
OK
DIC> sim
DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
U-FRACTION IN SYSTEM: CR = .297842647391913 FE = .517227320517284
NI = .184930032090802
TOTAL SIZE OF SYSTEM: .004 [m]
WARNING:BCC_A2 HAS NO VOLUME FRACTION, CREATING ONE
U-FRACTION IN SYSTEM: CR = .297842647391914 FE = .517227320517284
NI = .184930032090802
TOTAL SIZE OF SYSTEM: .004 [m]
TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .29784264735407 FE = .517227320607451
NI = .184930032038479
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep 0 seconds
TIME = 0.10010000E-03 DT = 0.10000000E-03 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297842648053525 FE = .517227318940911
NI = .18493003033005564
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep 0 seconds
TIME = 0.40010010 DT = 0.40000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297842678638828 FE = .517227246207374
NI = .184930075153799
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep 0 seconds
TIME = 271.76911 DT = 271.36901 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297847794798546 FE = .517216242027371
NI = .184935963174084
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep 0 seconds
TIME = 814.50713 DT = 542.73802 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297849638675562 FE = .517212918093924
NI = .184937443230514
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep 0 seconds
TIME = 1899.9832 DT = 1085.4760 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297850567158238 FE = .517211425470574
NI = .184938007371188
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep 1 seconds
TIME = 4070.9352 DT = 2170.9521 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297851129171679 FE = .517210587693033
NI = .184938283135287
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep 0 seconds
TIME = 8412.8394 DT = 4341.9041 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .29785149969426 FE = .517210052591395
NI = .184938447714345
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep 0 seconds
TIME = 13412.839 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297851736277664 FE = .5172097762816
NI = .184938487440737
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep 0 seconds
TIME = 18412.839 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297851886389189 FE = .517209625134759
NI = .184938488476053
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep 1 seconds
TIME = 23412.839 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297851977810746 FE = .517209529647086
NI = .184938492542168
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep 0 seconds
TIME = 28412.839 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297852026379766 FE = .517209463568761
NI = .184938510051473
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep 0 seconds
TIME = 33412.839 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297852041681698 FE = .517209416146609
NI = .184938542171693
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep 0 seconds
TIME = 38412.839 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297852041389975 FE = .517209383196795
NI = .18493857541323
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep 0 seconds
TIME = 43412.839 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297852052526349 FE = .517209358156199
NI = .184938589317452
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep 0 seconds
TIME = 48412.839 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297852064292856 FE = .517209339699238
NI = .184938596007907
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep 0 seconds
TIME = 53412.839 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297852067221178 FE = .517209327191934
NI = .184938605586888
TOTAL SIZE OF SYSTEM: .004 [m]
```

```

CPU time used in timestep          1 seconds
TIME = 58412.839 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297852077918747 FE = .517209313440073
NI = .18493860864118
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep          0 seconds
TIME = 63412.839 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297852087375306 FE = .517209300663091
NI = .184938611961603
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep          0 seconds
TIME = 68412.839 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297852090713848 FE = .517209289909762
NI = .184938611937639
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep          0 seconds
TIME = 73412.839 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .2978520917332989
NI = .184938768595729
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep          0 seconds
TIME = 608412.84 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297852058074382 FE = .51720917332989
NI = .184938768595729
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep          0 seconds
TIME = 613412.84 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297852061397466 FE = .517209173243017
NI = .184938765359517
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep          0 seconds
TIME = 618412.84 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297852063461482 FE = .517209173629272
NI = .184938762909247
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep          0 seconds
TIME = 623412.84 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297852064114503 FE = .517209174567714
NI = .184938761317783
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep          1 seconds
TIME = 628412.84 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .29785206329007 FE = .517209176074386
NI = .184938760635544
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep          0 seconds
TIME = 633412.84 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297852061694184 FE = .517209175615138
NI = .184938762690677
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep          0 seconds
TIME = 638412.84 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297852058476794 FE = .517209175852083
NI = .184938765671123
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep          0 seconds
TIME = 643412.84 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297852053635252 FE = .517209176702648
NI = .1849387696621
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep          0 seconds
TIME = 648412.84 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297852047155237 FE = .517209178126126
NI = .184938774718637
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep          0 seconds
TIME = 653412.84 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297852039017383 FE = .517209180103967
NI = .18493878087865
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep          1 seconds
TIME = 658412.84 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297852029199774 FE = .517209182629548
NI = .184938788170678
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep          0 seconds
TIME = 663412.84 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297852024085671 FE = .517209184240835
NI = .184938791673494
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep          0 seconds
TIME = 668412.84 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297852026954386 FE = .517209184349836
NI = .184938788695778
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep          0 seconds
TIME = 673412.84 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297852032474423 FE = .517209184195858
NI = .184938783329718
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep          0 seconds
TIME = 678412.84 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297852039415593 FE = .517209181872031
NI = .184938778712376
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep          0 seconds
TIME = 683412.84 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297852046164319 FE = .517209179958987
NI = .184938773876693
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep          0 seconds
TIME = 688412.84 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297852052278893 FE = .517209178466725
NI = .184938769254381
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep          1 seconds
TIME = 693412.84 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297852057499371 FE = .517209177402725

```

```

NI = .184938765097904
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep          0 seconds
TIME = 698412.84      DT = 5000.0000      SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297852061660633  FE = .517209176774778
NI = .184938761564589
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep          0 seconds
TIME = 703412.84      DT = 5000.0000      SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297852064650768  FE = .517209176591475
NI = .184938758757758
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep          0 seconds
TIME = 708412.84      DT = 5000.0000      SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297852066389347  FE = .517209176862002
NI = .184938756748651
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep          0 seconds
TIME = 713412.84      DT = 5000.0000      SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297852066815454  FE = .517209177596162
NI = .184938755588384
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep          0 seconds
TIME = 718412.84      DT = 5000.0000      SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297852065944414  FE = .517209178741792
NI = .184938755313795
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep          1 seconds
TIME = 720000.00      DT = 1587.1606      SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297852062299952  FE = .517209179928752
NI = .184938757771296
TOTAL SIZE OF SYSTEM: .004 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME    0.0000000
DELETING TIME-RECORD FOR TIME    0.10000000E-06
DELETING TIME-RECORD FOR TIME    0.10010000E-03
DELETING TIME-RECORD FOR TIME    468412.84
DELETING TIME-RECORD FOR TIME    708412.84
DELETING TIME-RECORD FOR TIME    713412.84

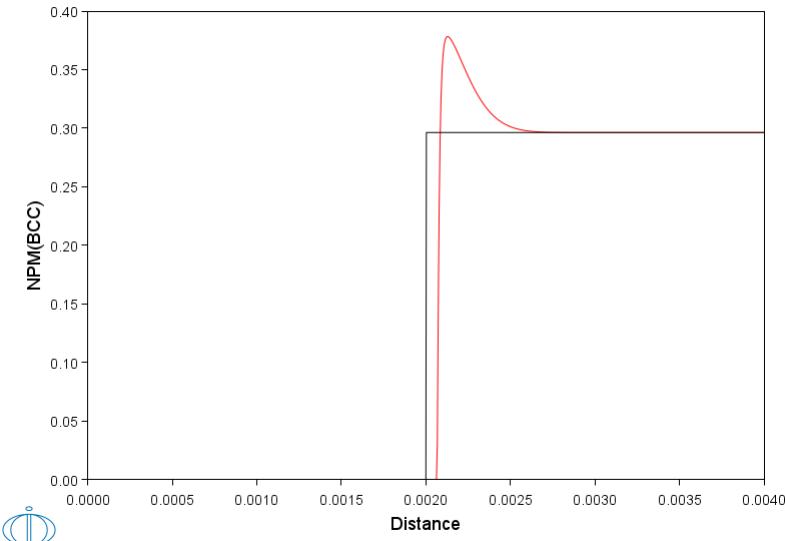
KEEPING TIME-RECORD FOR TIME    718412.84
AND FOR TIME                   720000.00
WORKSPACE RECLAIMED

TIMESTEP AT      720000.000      SELECTED

DIC>
DIC>
DIC>
DIC>
DIC> set-inter
--OK---
DIC>
```

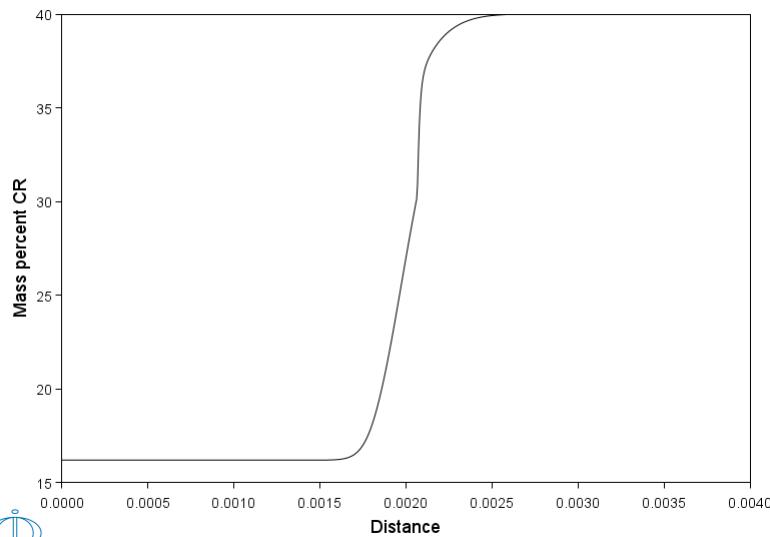
**exd2a-plot**

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exd2a\plot.DCM"
DIC>
DIC>
DIC> @@ exd2_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE D2
DIC> @@
DIC> @@ ENTER THE DICTRA MODULE AND SPECIFY THE STORE-RESULT FILE
DIC> @@
DIC>
DIC>
DIC> go d-m
TIME STEP AT TIME 7.20000E+05
DIC> read exd2
OK
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA POST PROCESSOR
DIC> @@
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1:
POST-1: @@
POST-1: @@ LET US SEE HOW THE FRACTION OF FERRITE HAS CHANGED
POST-1: @@ AS A RESULT OF THE DIFFUSION
POST-1: @@
POST-1: s-d-a y npm(bcc)
POST-1: s-d-a x distance global
INFO: Distance is set as independent variable
POST-1: s-p-c time 0 720000
POST-1: set-tit Figure D2.1
POST-1: plot
```

**Figure D2.1**

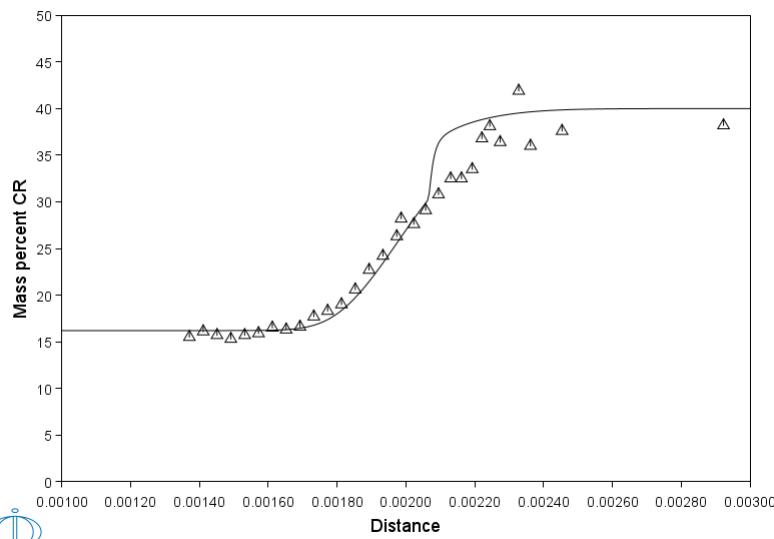
```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1: @@
POST-1: @@ NOW PLOT HOW THE AVERAGE Cr-CONCENTRATION VARIES WITH DISTANCE
POST-1: @@
POST-1: s-d-a y w-p cr
POST-1: s-p-c time last
POST-1: set-tit Figure D2.2
POST-1: plot
```

Figure D2.2



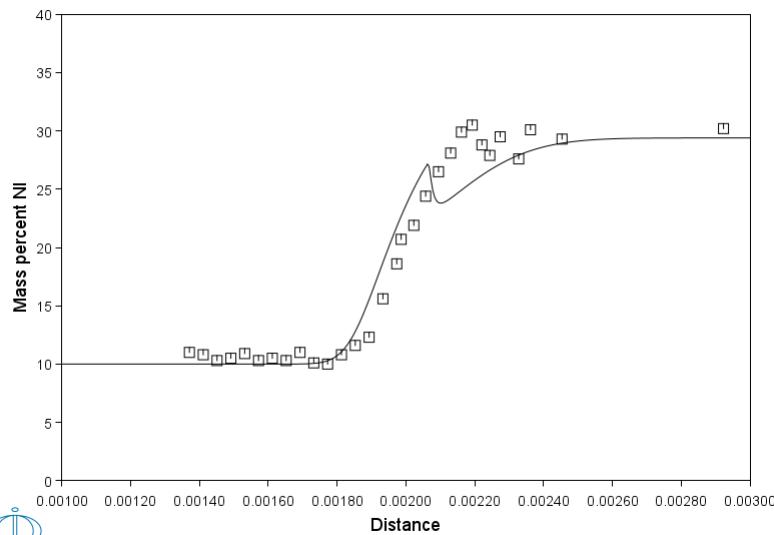
```
POST-1:  
POST-1:  
POST-1:  
POST-1:@?<_hit_return_to_continue_>  
POST-1: @@  
POST-1: @@ NOW SELECT A BETTER SCALING AND APPEND THE EXPERIMENTAL DATA  
POST-1: @@  
POST-1:  
POST-1: app y exd2.exp  
PROLOGUE NUMBER: /0/: 1  
DATASET NUMBER(s): /-1/: 4  
POST-1:  
POST-1: s-s-s y n 0 50  
POST-1: s-s-s x n 10e-4 30e-4  
POST-1:  
POST-1: set-tit Figure D2.3  
POST-1: plot
```

Figure D2.3



```
POST-1:  
POST-1:  
POST-1:  
POST-1:@?<_hit_return_to_continue_>  
POST-1: @@  
POST-1: @@ NOW WE DO THE SAME FOR NICKEL  
POST-1: @@  
POST-1:  
POST-1: s-d-a y w-p ni  
POST-1:  
POST-1: app y exd2.exp  
PROLOGUE NUMBER: /1/: 1  
DATASET NUMBER(s): /-1/: 5  
POST-1:  
POST-1: s-s-s x n 10e-4 30e-4  
POST-1: s-s-s y n 0 40  
POST-1:  
POST-1: set-tit Figure D2.4  
POST-1: plot
```

**Figure D2.4**

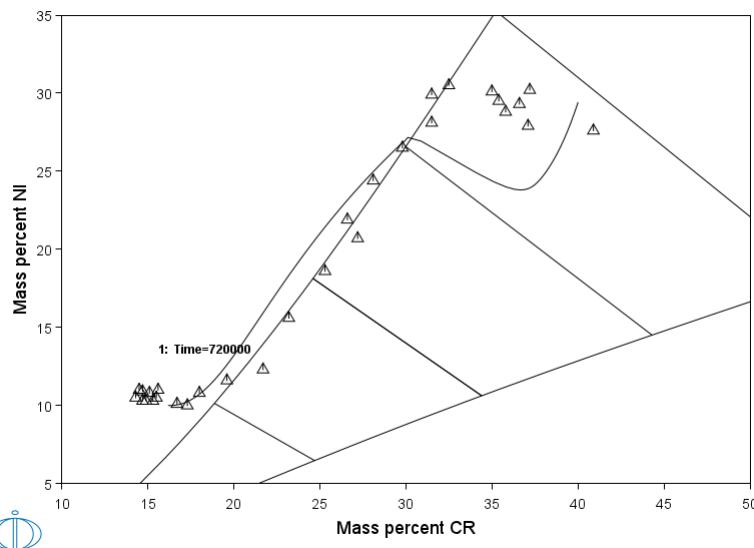


```

POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1: @@
POST-1: @@ LET US PLOT THE DIFFUSION PATH FOR THE COUPLE.
POST-1: @@ WE APPEND THE TERNARY PHASE-DIAGRAM CALCULATED IN THERMO-CALC
POST-1: @@ AND THE EXPERIMENTAL DATA
POST-1: @@
POST-1: s-d-a x w-p cr
POST-1: s-d-a y w-p ni
POST-1: s-i-v dis gl
POST-1: s-p-c time last
POST-1: 
POST-1: app y exd2.exp
PROLOGUE NUMBER: /1/: 1
DATASET NUMBER(s): /-1/: 6 7 8
POST-1:
POST-1: s-s-s x n 10 50
POST-1: s-s-s y n 5 35
POST-1:
POST-1: set-tit Figure D2.5
POST-1: plot

```

**Figure D2.5**



```

POST-1:
POST-1:
POST-1:
POST-1:
POST-1: set-interactive
--OK---
POST-1:

```

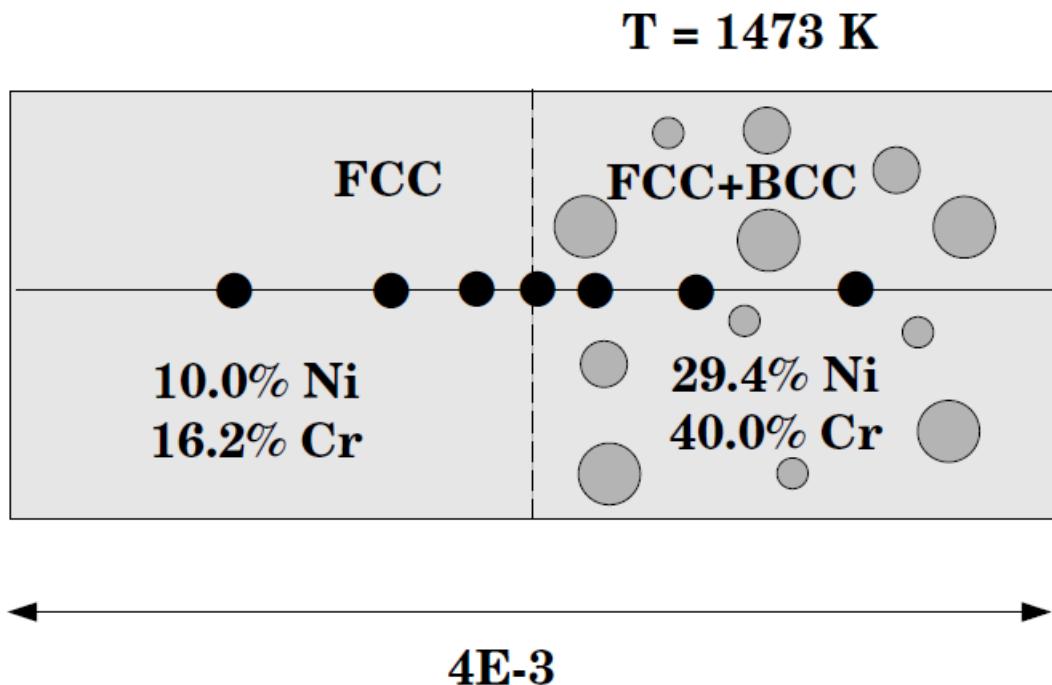


## Example exd2b

### Diffusion couple of Fe-Ni-Cr alloys: Homogenization model

This example calculates the interdiffusion in a diffusion couple between a two-phase (FCC+BCC) and a single-phase (FCC) Fe-Ni-Cr alloy. Initially it has a step profile. It is similar to exd2a except the default HOMOGENIZATION MODEL is used and then ENTER\_HOMOGENIZATION\_FUNCTION is used instead of ENTER\_LABYRINTH\_FUNCTION.

This case is from A. Engström: Scand. J. Met., vol. 24, 1995, pp.12-20.



**exd2b-setup****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\_dictra\_console\_examples\examples\exd2b\setup.DCM"**

**SYS: i>\_@@**  
NO SUCH COMMAND, USE HELP  
**SYS: @@ Diffusion in dispersed systems.**  
**SYS: @@ Diffusion couple of Fe-Cr-Ni alloys: Homogenization model**  
**SYS: @@ This example calculates the interdiffusion in a diffusion**  
**SYS: @@ couple between a two-phase (FCC+BCC) and a single-phase (FCC)**  
**SYS: @@ Fe-Ni-Cr alloy. This case is from A. Engström: Scand. J. Met.,**  
**SYS: @@ v. 24, 1995, pp.12-20. This simulation can be run with either**  
**SYS: @@ the DISPERSED SYSTEM MODEL or the HOMOGENIZATION MODEL.**  
**SYS: @@ Here the default HOMOGENIZATION MODEL is used and then**  
**SYS: @@ ENTER\_HOMOGENIZATION\_FUNCTION should be used instead of**  
**SYS: @@ ENTER\_LABYRINTH\_FUNCTION.**

**SYS: -----**  
NO SUCH COMMAND, USE HELP  
**SYS:**  
**SYS: @@**  
**SYS: @@ RETRIEVE DATA FROM THE DATABASE**  
**SYS: @@**  
**SYS: go da**  
THERMODYNAMIC DATABASE module  
Database folder:  
C:\jenkins\workspace\generate\_dictra\_console\_examples\databases\data  
Current database: Steels/Fe-Alloys v12.0

VA /- DEFINED  
DICTRA\_FCC\_A1 REJECTED  
**TDB\_TCFE12: sw fedemo**  
Current database: Iron Demo Database v4.0  
  
VA /- DEFINED  
**TDB\_FEDEMO: def-sys fe ni cr**  
FE NI CR  
DEFINED  
**TDB\_FEDEMO: rej ph \* all**  
LIQUID:L BCC\_A2 LAVES\_PHASE\_C14  
CBCC\_A12 CHI\_A12 CUB\_A13  
FCC\_A1 HCP\_A3 SIGMA  
REJECTED  
**TDB\_FEDEMO: res ph fcc,bcc**  
FCC\_A1 BCC\_A2 RESTORED  
**TDB\_FEDEMO: get**  
18:36:52,321 [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, SGT Data for Pure Elements, CALPHAD, 15 (1991) 317-425'  
'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'  
'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'  
'A.T. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); CR -NI'  
'A.T. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); FE-NI'  
-OK-

**TDB\_FEDEMO:**  
**TDB\_FEDEMO: @@**  
**TDB\_FEDEMO: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE MOBILITY DATA**  
**TDB\_FEDEMO: @@**  
**TDB\_FEDEMO: app mfdemo**  
Current database: Fe-Alloys Mobility demo database v2.0

VA DEFINED  
**APP: def-sys fe ni cr**  
FE NI CR  
DEFINED  
**APP: rej ph \* all**  
BCC\_A2 FCC\_A1 REJECTED  
**APP: res ph fcc,bcc**  
FCC\_A1 BCC\_A2 RESTORED  
**APP: get**  
ELEMENTS ....  
SPECIES ....  
PHASES ....  
PARAMETERS ...  
FUNCTIONS ....

List of references for assessed data

'This parameter has not been assessed'  
'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Fe diffusion fcc Cr-Fe'  
'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Ni diffusion fcc Cr-Ni'  
'B. Jonsson: Z. Metallkunde 86(1995)686-692; Cr, Fe and Ni diffusion fcc  
Cr-Fe-Ni'  
'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe  
-Ni'  
'Xia, C. H. et al. JAC, 2021, 853, 157165.'  
'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Ni self-diffusion'  
'B. Jonsson: ISIJ International, 35(1995)1415-1421; Cr, Fe and Ni'

```

diffusion bcc Cr-Fe-Ni'
'B. Jonsson: Z. Metallkunde 83(1992) 349-355; Cr, Co, Fe and Ni diffusion
in bcc Fe'

-OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR
APP: @@
APP: go d-m
NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 1473; * N
DIC>
DIC> @@
DIC> @@ ENTER THE REGION fer
DIC> @@
DIC> enter-region fer
DIC>
DIC>
DIC> @@
DIC> @@ ENTER A DOUBLE-GEOMETRICAL GRID INTO THE REGION
DIC> @@ THIS GIVES A SHORT DISTANCE BETWEEN THE GRIDPOINTS
DIC> @@ IN THE MIDDLE OF THE REGION WHERE THE INITIAL INTERFACE IS
DIC> @@
DIC> enter-grid fer
WIDTH OF REGION /1/: 4e-3
TYPE /LINEAR/: double
NUMBER OF POINTS /50/: 200
VALUE OF R IN THE GEOMETRICAL SERIE FOR LOWER PART OF REGION: 0.97
VALUE OF R IN THE GEOMETRICAL SERIE FOR UPPER PART OF REGION: 1.03093
DIC>
DIC> @@
DIC> @@ ENTER A MATRIX PHASE IN THE REGION
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act fer matrix fcc
DIC>
DIC> @@
DIC> @@ ENTER THE START COMPOSITION FOR THE MATRIX PHASE FROM FILES
DIC> @@
DIC> enter-composition
REGION NAME : /FER/: fer
PHASE NAME: /FCC_A1/: fcc
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /CR/: cr
TYPE /LINEAR/: read d2cr.dat
PROFILE FOR /NI/: ni
TYPE /LINEAR/: read d2ni.dat
DIC>
DIC> @@
DIC> @@ ENTER FERRITE AS THE SPHEROIDAL PHASE IN THE REGION
DIC> @@ SINCE THE FRACTION OF FERRITE IS SMALL, AND THESE APPEAR
DIC> @@ AS ISOLATED PARTICLES, FERRITE IS ENTERED AS A SPHEROIDAL PHASE
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /FER/: fer
PHASE TYPE /MATRIX/: sph
PHASE NAME: /NONE/: bcc
INFO: EQUILIBRIUM COMPOSITION AND FRACTION OF SPHEROID PHASES USED AS DEFAULT
DIC>
DIC> @@
DIC> @@ ENTER THE COMPOSITION FOR THE SPHEROIDAL PHASE
DIC> @@ USE THE EQUILIBRIUM VALUE
DIC> @@
DIC> enter-composition
REGION NAME : /FER/: fer
PHASE NAME: /FCC_A1/: bcc
USE EQUILIBRIUM VALUE /Y/: y
DIC>
DIC> @@ SELECT A HOMOGENIZATION FUNCTION
DIC> @@ IN THIS CASE THE LOWER HASHIN-SHTRIKMAN BOUND
DIC> en-ho 1
SELECTED FUNCTION IS HASHIN-SHTRIKMAN BOUND: GENERAL LOWER
DIC>
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME AND OTHER SIMULATION PARAMETERS
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 720000
AUTOMATIC TIMESTEP CONTROL /YES/: YES
MAX TIMESTEP DURING INTEGRATION /72000/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC> set-simulation-condition
NSO1A PRINT CONTROL : /0/: 0
FLUX CORRECTION FACTOR : /1/: 1
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/: 2
CHECK INTERFACE POSITION /AUTO/: n
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/: act
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/: y
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/: 99
DEGREE OF IMPLICITY WHEN INTEGRATING PDES (AUTO, 0 -> 0.5 -> 1) : /AUTO/: 1
MAX TIMESTEP CHANGE PER TIMESTEP : /2/: 2
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/: n
ALWAYS CALCULATE STIFFNESS MATRIX IN MULDIF /YES/: y
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/: n
DIC>
DIC>
DIC> @@
DIC> @@ SAVE THE SETUP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC>
DIC> save exd2 y

```

**DIC>**  
**DIC> set-inter**  
--OK---  
**DIC>**

**exd2b-run**

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exd2b\run.DCM"
DIC>
DIC>
DIC> @@ exd2_run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING THE SIMULATION OF EXAMPLE D2
DIC> @@
DIC>
DIC>
DIC> @@
DIC> @@ READ THE SETUP FROM FILE AND START THE SIMULATION
DIC> @@
DIC>
DIC>
DIC> go d-m
TIME STEP AT TIME 0.00000E+00
DIC> read exd2
OK
DIC> sim
STARTING SIMULATION USING HOMOGENIZATION MODEL
-----
WARNING:BCC_A2 HAS NO VOLUME FRACTION, CREATING ONE
Starting time-step t0= 0.0000000 dt= 0.10000000E-06
Starting time-step t0= 0.10000000E-06 dt= 0.20000000E-06
Starting time-step t0= 0.30000000E-06 dt= 0.40000000E-06
Starting time-step t0= 0.70000000E-06 dt= 0.80000000E-06
Starting time-step t0= 0.15000000E-05 dt= 0.16000000E-05
Starting time-step t0= 0.31000000E-05 dt= 0.32000000E-05
Starting time-step t0= 0.63000000E-05 dt= 0.64000000E-05
Starting time-step t0= 0.12700000E-04 dt= 0.12800000E-04
Starting time-step t0= 0.25500000E-04 dt= 0.25600000E-04
Starting time-step t0= 0.51100000E-04 dt= 0.51200000E-04
Starting time-step t0= 0.10230000E-03 dt= 0.10240000E-03
Starting time-step t0= 0.20470000E-03 dt= 0.20480000E-03
Starting time-step t0= 0.40950000E-03 dt= 0.40960000E-03
Starting time-step t0= 0.81910000E-03 dt= 0.81920000E-03
Starting time-step t0= 0.16383000E-02 dt= 0.16384000E-02
Starting time-step t0= 0.32767000E-02 dt= 0.32768000E-02
Starting time-step t0= 0.65535000E-02 dt= 0.65536000E-02
Starting time-step t0= 0.13107100E-01 dt= 0.13107200E-01
Starting time-step t0= 0.26214300E-01 dt= 0.26214400E-01
Starting time-step t0= 0.52428700E-01 dt= 0.52428800E-01
Starting time-step t0= 0.10485750 dt= 0.10485760
Starting time-step t0= 0.20971510 dt= 0.20971520
Starting time-step t0= 0.41943030 dt= 0.41943040
Starting time-step t0= 0.83886070 dt= 0.83886080
Starting time-step t0= 1.6777215 dt= 1.6777216
Starting time-step t0= 3.3554431 dt= 3.3554432
Starting time-step t0= 6.7108863 dt= 6.7108864
Starting time-step t0= 13.421773 dt= 13.421773
Starting time-step t0= 26.843545 dt= 26.843546
Starting time-step t0= 53.687091 dt= 26.843546
Starting time-step t0= 80.530637 dt= 26.843546
Starting time-step t0= 107.37418 dt= 26.843546
Starting time-step t0= 134.21773 dt= 26.843546
Starting time-step t0= 161.06127 dt= 26.843546
Starting time-step t0= 187.90482 dt= 26.843546
Starting time-step t0= 214.74836 dt= 53.687091
Starting time-step t0= 268.43546 dt= 53.687091
Starting time-step t0= 322.12255 dt= 53.687091
Starting time-step t0= 375.80964 dt= 53.687091
Starting time-step t0= 429.49673 dt= 53.687091
Starting time-step t0= 483.18382 dt= 53.687091
Starting time-step t0= 536.87091 dt= 53.687091
Starting time-step t0= 590.55800 dt= 107.37418
Starting time-step t0= 697.93219 dt= 107.37418
Starting time-step t0= 805.30637 dt= 107.37418
Starting time-step t0= 912.68055 dt= 107.37418
Starting time-step t0= 1020.0547 dt= 107.37418
Starting time-step t0= 1127.4289 dt= 214.74836
Starting time-step t0= 1342.1773 dt= 214.74836
Starting time-step t0= 1556.9256 dt= 214.74836
Starting time-step t0= 1771.6740 dt= 214.74836
Starting time-step t0= 1986.4224 dt= 214.74836
Starting time-step t0= 2201.1707 dt= 214.74836
Starting time-step t0= 2415.9191 dt= 214.74836
Starting time-step t0= 2630.6675 dt= 429.49673
Starting time-step t0= 3060.1642 dt= 429.49673
Starting time-step t0= 3489.6609 dt= 429.49673
Starting time-step t0= 3919.1577 dt= 429.49673
Starting time-step t0= 4348.6544 dt= 429.49673
Starting time-step t0= 4778.1511 dt= 429.49673
Starting time-step t0= 5207.6478 dt= 858.99346
Starting time-step t0= 6066.6413 dt= 858.99346
Starting time-step t0= 6925.6348 dt= 858.99346
Starting time-step t0= 7784.6282 dt= 858.99346
Starting time-step t0= 8643.6217 dt= 858.99346
Starting time-step t0= 9502.6151 dt= 858.99346
Starting time-step t0= 10361.609 dt= 858.99346
Starting time-step t0= 11220.602 dt= 858.99346
Starting time-step t0= 12079.596 dt= 1717.9869
Starting time-step t0= 13797.582 dt= 1717.9869
Starting time-step t0= 15515.569 dt= 1717.9869
Starting time-step t0= 17233.556 dt= 1717.9869
Starting time-step t0= 18951.543 dt= 1717.9869
Starting time-step t0= 20669.530 dt= 1717.9869
Starting time-step t0= 22387.517 dt= 3435.9738
Starting time-step t0= 25823.491 dt= 3435.9738
Starting time-step t0= 29259.465 dt= 3435.9738
Starting time-step t0= 32695.439 dt= 3435.9738
Starting time-step t0= 36131.412 dt= 3435.9738
Starting time-step t0= 39567.386 dt= 3435.9738
Starting time-step t0= 43003.360 dt= 3435.9738
Starting time-step t0= 46439.334 dt= 6871.9477
Starting time-step t0= 53311.282 dt= 6871.9477
Starting time-step t0= 60183.229 dt= 6871.9477
Starting time-step t0= 67055.177 dt= 6871.9477
Starting time-step t0= 73927.125 dt= 6871.9477
Starting time-step t0= 80799.072 dt= 6871.9477
Starting time-step t0= 87671.020 dt= 6871.9477
Starting time-step t0= 94542.968 dt= 6871.9477
```

```

Starting time-step t0= 101414.92 dt= 13743.895
Starting time-step t0= 115158.81 dt= 13743.895
Starting time-step t0= 122030.76 dt= 6871.9477
Starting time-step t0= 128902.71 dt= 13743.895
Starting time-step t0= 142646.60 dt= 13743.895
Starting time-step t0= 149518.55 dt= 13743.895
Starting time-step t0= 163262.44 dt= 13743.895
Starting time-step t0= 177006.34 dt= 13743.895
Starting time-step t0= 183878.29 dt= 13743.895
Starting time-step t0= 197622.18 dt= 13743.895
Starting time-step t0= 211366.08 dt= 27487.791
Starting time-step t0= 238853.87 dt= 27487.791
Starting time-step t0= 266341.66 dt= 27487.791
Starting time-step t0= 293829.45 dt= 27487.791
Starting time-step t0= 321317.24 dt= 27487.791
Starting time-step t0= 335061.14 dt= 27487.791
Starting time-step t0= 348805.03 dt= 13743.895
Starting time-step t0= 362548.93 dt= 27487.791
Starting time-step t0= 390036.72 dt= 27487.791
Starting time-step t0= 396908.67 dt= 13743.895
Starting time-step t0= 410652.56 dt= 13743.895
Starting time-step t0= 424396.46 dt= 27487.791
Starting time-step t0= 451884.25 dt= 27487.791
Starting time-step t0= 465628.14 dt= 27487.791
Starting time-step t0= 479372.04 dt= 13743.895
Starting time-step t0= 493115.93 dt= 27487.791
Starting time-step t0= 520603.72 dt= 54975.581
Starting time-step t0= 548091.51 dt= 27487.791
Starting time-step t0= 575579.30 dt= 54975.581
Starting time-step t0= 630554.89 dt= 54975.581
Starting time-step t0= 658042.68 dt= 27487.791
Starting time-step t0= 685530.47 dt= 34469.532

MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 0.0000000
DELETING TIME-RECORD FOR TIME 0.10000000E-06
DELETING TIME-RECORD FOR TIME 805.3037
DELETING TIME-RECORD FOR TIME 1556.9256
DELETING TIME-RECORD FOR TIME 2415.9191
DELETING TIME-RECORD FOR TIME 3489.6609
DELETING TIME-RECORD FOR TIME 4348.6544
DELETING TIME-RECORD FOR TIME 5207.6478
DELETING TIME-RECORD FOR TIME 6066.6413
DELETING TIME-RECORD FOR TIME 6925.6348
DELETING TIME-RECORD FOR TIME 7784.6282
DELETING TIME-RECORD FOR TIME 8643.6217
DELETING TIME-RECORD FOR TIME 9502.6151
DELETING TIME-RECORD FOR TIME 10361.609
DELETING TIME-RECORD FOR TIME 11220.602
DELETING TIME-RECORD FOR TIME 12079.596
DELETING TIME-RECORD FOR TIME 13797.582
DELETING TIME-RECORD FOR TIME 15515.569
DELETING TIME-RECORD FOR TIME 17233.556
DELETING TIME-RECORD FOR TIME 18951.543
DELETING TIME-RECORD FOR TIME 20669.530
DELETING TIME-RECORD FOR TIME 22387.517
DELETING TIME-RECORD FOR TIME 25823.491
DELETING TIME-RECORD FOR TIME 29259.465
DELETING TIME-RECORD FOR TIME 32695.439
DELETING TIME-RECORD FOR TIME 36131.412
DELETING TIME-RECORD FOR TIME 39567.386
DELETING TIME-RECORD FOR TIME 43003.360
DELETING TIME-RECORD FOR TIME 46439.334
DELETING TIME-RECORD FOR TIME 53311.282
DELETING TIME-RECORD FOR TIME 60183.229
DELETING TIME-RECORD FOR TIME 67055.177
DELETING TIME-RECORD FOR TIME 73927.125
DELETING TIME-RECORD FOR TIME 80799.072
DELETING TIME-RECORD FOR TIME 87671.020
DELETING TIME-RECORD FOR TIME 94542.968
DELETING TIME-RECORD FOR TIME 101414.92
DELETING TIME-RECORD FOR TIME 115158.81
DELETING TIME-RECORD FOR TIME 122030.76
DELETING TIME-RECORD FOR TIME 128902.71
DELETING TIME-RECORD FOR TIME 142646.60
DELETING TIME-RECORD FOR TIME 149518.55
DELETING TIME-RECORD FOR TIME 163262.44
DELETING TIME-RECORD FOR TIME 177006.34
DELETING TIME-RECORD FOR TIME 183878.29
DELETING TIME-RECORD FOR TIME 197622.18
DELETING TIME-RECORD FOR TIME 211366.08
DELETING TIME-RECORD FOR TIME 238853.87
DELETING TIME-RECORD FOR TIME 266341.66
DELETING TIME-RECORD FOR TIME 293829.45
DELETING TIME-RECORD FOR TIME 321317.24
DELETING TIME-RECORD FOR TIME 335061.14
DELETING TIME-RECORD FOR TIME 348805.03
DELETING TIME-RECORD FOR TIME 362548.93
DELETING TIME-RECORD FOR TIME 390036.72
DELETING TIME-RECORD FOR TIME 396908.67
DELETING TIME-RECORD FOR TIME 410652.56
DELETING TIME-RECORD FOR TIME 424396.46
DELETING TIME-RECORD FOR TIME 451884.25
DELETING TIME-RECORD FOR TIME 465628.14
DELETING TIME-RECORD FOR TIME 479372.04
DELETING TIME-RECORD FOR TIME 493115.93
DELETING TIME-RECORD FOR TIME 520603.72
DELETING TIME-RECORD FOR TIME 548091.51
DELETING TIME-RECORD FOR TIME 575579.30
DELETING TIME-RECORD FOR TIME 630554.89
DELETING TIME-RECORD FOR TIME 658042.68

KEEPING TIME-RECORD FOR TIME 685530.47
AND FOR TIME 720000.00
WORKSPACE RECLAIMED
-----
```

```

INTERPOLATION SCHEME USED THIS FRACTION OF
THE ALLOCATED MEMORY: 1.00000000000000
EFFICIENCY FACTOR: 1.97948863714510
-----
```

```

DEALLOCATING
-----
```

```

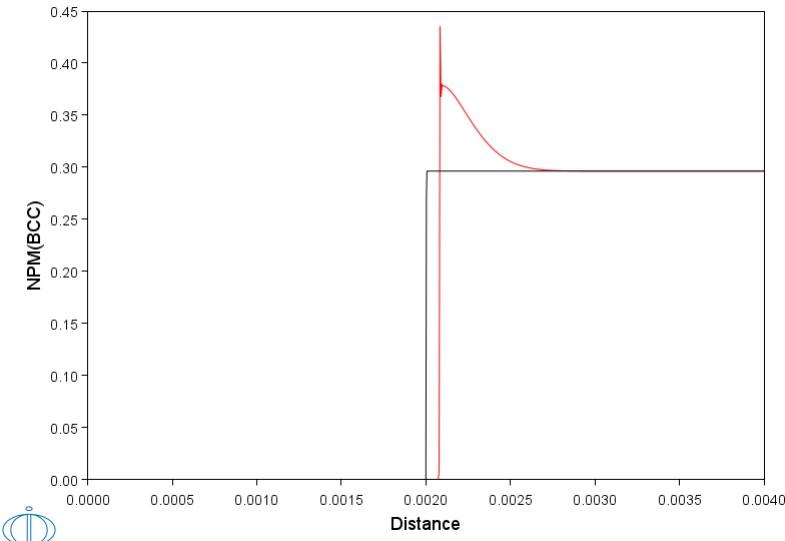
TIMESTEP AT 720000.000 SELECTED
```

```
DIC>
DIC>
DIC>
DIC>
DIC> set-inter
--OK---
DIC>
```

## exd2b-plot

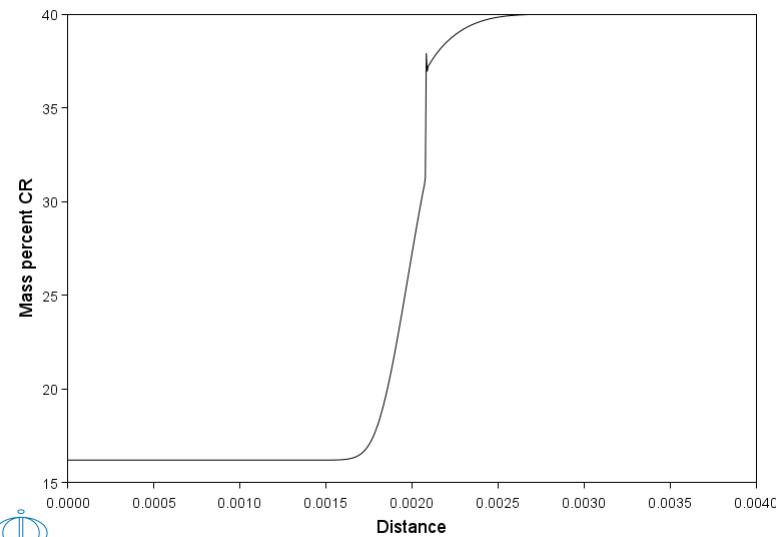
```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exd2b\plot.DCM"
DIC>
DIC>
DIC> @@ exd2_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE D2
DIC> @@
DIC> @@ ENTER THE DICTRA MODULE AND SPECIFY THE STORE-RESULT FILE
DIC> @@
DIC>
DIC>
DIC> go d-m
TIME STEP AT TIME 7.20000E+05
DIC> read exd2
OK
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA POST PROCESSOR
DIC> @@
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1:
POST-1: @@
POST-1: @@ LET US FIRST SEE HOW THE FRACTION OF FERRITE HAS CHANGED
POST-1: @@ AS A RESULT OF THE DIFFUSION
POST-1: @@
POST-1: s-d-a y npm(bcc)
POST-1: s-d-a x distance global
INFO: Distance is set as independent variable
POST-1: s-p-c time 0 720000
POST-1: set-tit Figure D2.1
POST-1: plot
```

Figure D2.1



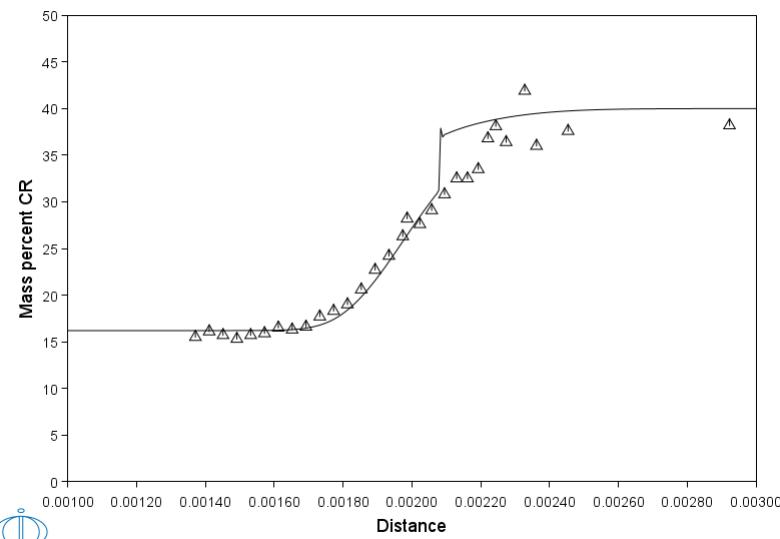
```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1: @@
POST-1: @@ LET US NOW PLOT HOW THE AVERAGE CR-CONCENTRATION VARIES WITH DISTANCE
POST-1: @@
POST-1: s-d-a y w-p cr
POST-1: s-p-c time last
POST-1: set-tit Figure D2.2
POST-1: plot
```

**Figure D2.2**



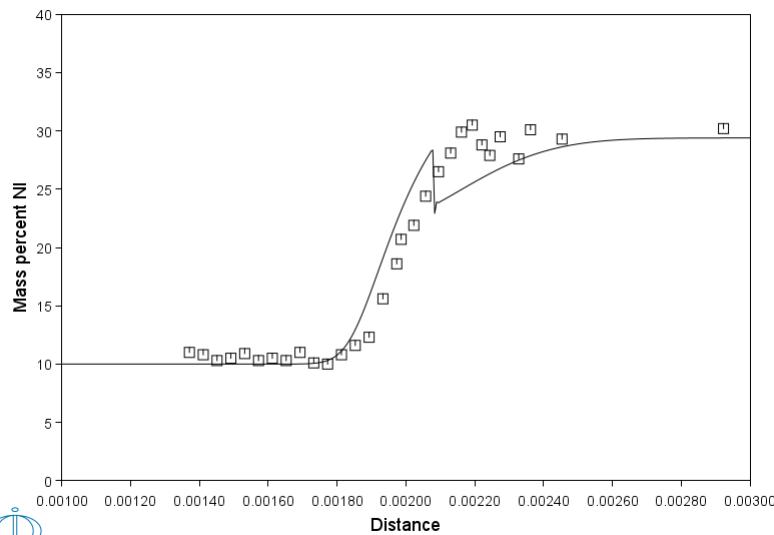
```
POST-1:  
POST-1:  
POST-1:  
POST-1:@?<_hit_return_to_continue_>  
POST-1: @@  
POST-1: @@ WE SELECT A BETTER SCALING AND APPEND EXPERIMENTAL DATA  
POST-1: @@  
POST-1:  
POST-1: app y exd2.exp  
PROLOGUE NUMBER: /0/: 1  
DATASET NUMBER(s): /-1/: 4  
POST-1:  
POST-1: s-s-s y n 0 50  
POST-1: s-s-s x n 10e-4 30e-4  
POST-1:  
POST-1: set-tit Figure D2.3  
POST-1: plot
```

**Figure D2.3**



```
POST-1:  
POST-1:  
POST-1:  
POST-1:@?<_hit_return_to_continue_>  
POST-1: @@  
POST-1: @@ NOW WE DO THE SAME FOR NICKEL  
POST-1: @@  
POST-1:  
POST-1: s-d-a y w-p ni  
POST-1:  
POST-1: app y exd2.exp  
PROLOGUE NUMBER: /1/: 1  
DATASET NUMBER(s): /-1/: 5  
POST-1:  
POST-1: s-s-s x n 10e-4 30e-4  
POST-1: s-s-s y n 0 40  
POST-1:  
POST-1: set-tit Figure D2.4  
POST-1: plot
```

**Figure D2.4**

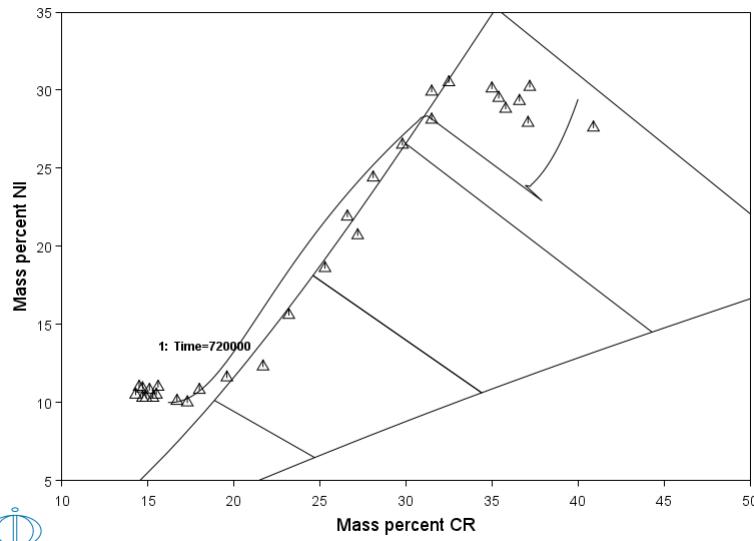


```

POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1: @@
POST-1: @@ LET US PLOT THE DIFFUSION PATH FOR THE COUPLE
POST-1: @@ WE APPEND THE TERNARY PHASE-DIAGRAM CALCULATED IN THERMO-CALC
POST-1: @@ AND THE EXPERIMENTAL DATA
POST-1: @@
POST-1: s-d-a x w-p cr
POST-1: s-d-a y w-p ni
POST-1: s-i-v dis gl
POST-1: s-p-c time last
POST-1: 
POST-1: app y exd2.exp
PROLOGUE NUMBER: /1/: 1
DATASET NUMBER(s): /-1/: 6 7 8
POST-1:
POST-1: s-s-s x n 10 50
POST-1: s-s-s y n 5 35
POST-1:
POST-1: set-tit Figure D2.5
POST-1: plot

```

**Figure D2.5**



```

POST-1:
POST-1:
POST-1:
POST-1:
POST-1: set-interactive
--OK---
POST-1:

```

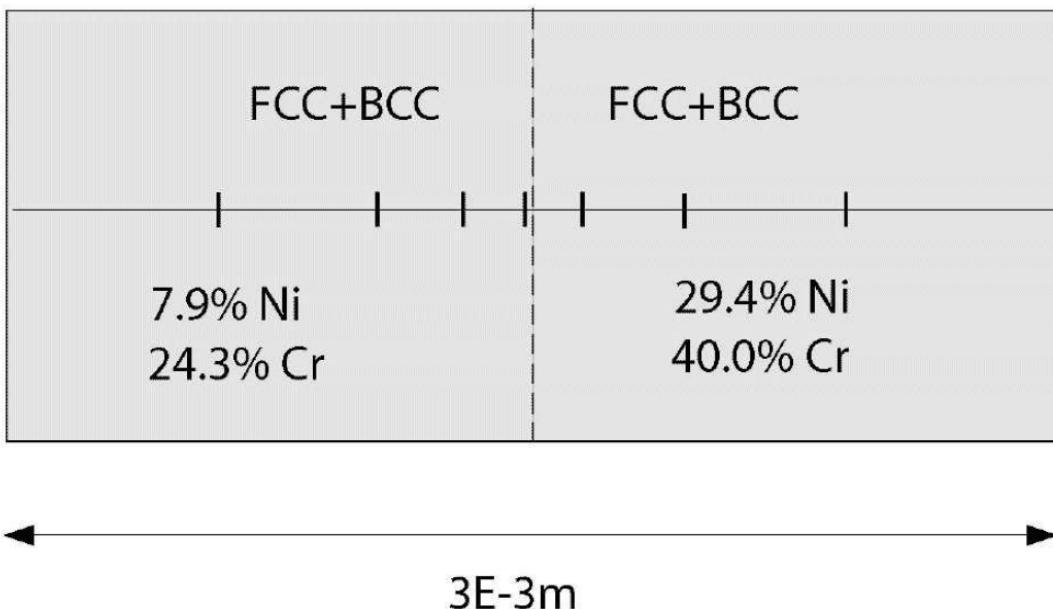


## Example exd3

### Diffusion couple of Fe-Ni-Cr alloys: Homogenization Model

This example shows the use of the homogenization model. It is taken from H. Larsson and A. Engström, Acta. Mater. v.54 (2006), pp. 2431-2439. Experimental data from A. Engström, Scand J Metall, v.243 (1995), p.12. The homogenization model can be used for multiphase simulations like the dispersed system model, but unlike the dispersed system model there is no need to have a single continuous matrix phase and, furthermore, there is no need to limit the size of time-steps. The set-up is performed in the same manner as for the dispersed system model, which means that a certain phase is entered as the matrix phase and the other phases are entered as spheroidal, but the choice of matrix phase will not affect the simulation.

$T = 1373 \text{ K}$



**exd3-setup****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\_dictra\_console\_examples\examples\exd3\setup.DCM.test"**

**SYS:** i>@  
NO SUCH COMMAND, USE HELP  
**SYS:** @@ Diffusion in dispersed systems.  
**SYS:** @@ Diffusion couple of Fe-Cr-Ni alloys: Homogenization model  
**SYS:** @@ This example uses the homogenization model. It is taken from  
**SYS:** @@ H. Larsson and A. Engström, Acta. Mater. v.54 (2006), pp. 2431-2439.  
**SYS:** @@ Experimental data from A. Engström, Scand J Metall, v.243 (1995), p.12.  
**SYS:** @@ The homogenization model can be used for multiphase simulations  
**SYS:** @@ like the dispersed system model, but unlike the dispersed system model  
**SYS:** @@ there is no need to have a single continuous matrix phase and, furthermore,  
**SYS:** @@ there is no need to limit the size of time-steps.  
**SYS:** @@ The set-up is performed in the same manner as for the dispersed system  
**SYS:** @@ model, which means that a certain phase is entered as the matrix phase  
**SYS:** @@ and the other phases are entered as spheroidal, but the choice of matrix  
**SYS:** @@ phase will not affect the simulation.

**SYS:** -----  
NO SUCH COMMAND, USE HELP

**SYS:**  
**SYS:** @@ exd3\_setup.DCM  
**SYS:**  
**SYS:**

**SYS:** go da

THERMODYNAMIC DATABASE module  
Database folder:  
C:\jenkins\workspace\generate\_dictra\_console\_examples\databases\data  
Current database: Steels/Fe-Alloys v12.0

VA /- DEFINED

DICTRA\_FCC\_A1 REJECTED

**TDB\_TCFE12:** sw fedemo

Current database: Iron Demo Database v4.0

VA /- DEFINED

**TDB\_FEDEMO:** def-sys fe cr ni

FE CR NI

DEFINED

**TDB\_FEDEMO:** rej-ph \*

LIQUID:L BCC\_A2 LAVES\_PHASE\_C14  
CBCC\_A12 CHI\_A12 CUB\_A13  
FCC\_A1 HCP\_A3 SIGMA

REJECTED

**TDB\_FEDEMO:** rest-ph bcc,fcc

BCC\_A2 FCC\_A1 RESTORED

**TDB\_FEDEMO:** get

18:41:36,356 [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'  
'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'  
'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'  
'A.T. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); CR -NI'  
'A.T. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); FE-NI'

-OK-

**TDB\_FEDEMO:**

**TDB\_FEDEMO:** app mfdemo

Current database: Fe-Alloys Mobility demo database v2.0

VA DEFINED

**APP:** def-sys fe cr ni

FE CR NI

DEFINED

**APP:** rej-ph \*

BCC\_A2 FCC\_A1 REJECTED

**APP:** rest-ph bcc,fcc

BCC\_A2 FCC\_A1 RESTORED

**APP:** get

ELEMENTS .....

SPECIES .....

PHASES .....

PARAMETERS ...

FUNCTIONS ....

List of references for assessed data

'This parameter has not been assessed'  
'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Fe diffusion fcc Cr-Fe'  
'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Ni diffusion fcc Cr-Ni'  
'B. Jonsson: Z. Metallkunde 86(1995)686-692; Cr, Fe and Ni diffusion fcc  
Cr-Fe-Ni'  
'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe  
-Ni'  
'Xia, C. H. et al. JAC, 2021, 853, 157165.'  
'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Ni self-diffusion'  
'B. Jonsson: ISIJ International, 35(1995)1415-1421; Cr, Fe and Ni

```

diffusion bcc Cr-Fe-Ni'
'B. Jonsson: Z. Metallkunde 83(1992) 349-355; Cr, Co, Fe and Ni diffusion
in bcc Fe'
-OK-
APP:
APP: go -m
NO TIME STEP DEFINED
DIC>
DIC> set-cond glob T 0 1373.15; * N
DIC>
DIC> ent-geo 0
DIC>
DIC> ent-reg
REGION NAME : fecrni
DIC>
DIC> ent-grid
REGION NAME : /FECRNI/: fecrni
WIDTH OF REGION /1/: 3e-3
TYPE /LINEAR/: double
NUMBER OF POINTS /50/: 60
VALUE OF R IN THE GEOMETRICAL SERIE FOR LOWER PART OF REGION: 0.85
VALUE OF R IN THE GEOMETRICAL SERIE FOR UPPER PART OF REGION: 1.15
DIC>
DIC> ent-ph
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /FECRNI/: fecrni
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC> ent-ph
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /FECRNI/: fecrni
PHASE TYPE /MATRIX/: sph
PHASE NAME: /NONE/: bcc
INFO: EQUILIBRIUM COMPOSITION AND FRACTION OF SPHEROID PHASES USED AS DEFAULT
DIC>
DIC> ent-comp
REGION NAME : /FECRNI/: fecrni
PHASE NAME: /FCC_A1/: fcc#1
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: m-f
PROFILE FOR /CR/: cr
TYPE /LINEAR/: read cr.dat
PROFILE FOR /NI/: ni
TYPE /LINEAR/: read ni.dat
DIC>
DIC> ent-comp
REGION NAME : /FECRNI/: fecrni
PHASE NAME: /FCC_A1/: bcc
USE EQUILIBRIUM VALUE /Y/: y
DIC>
DIC> se-si-ti
END TIME FOR INTEGRATION /.1/: 3.6e5
AUTOMATIC TIMESTEP CONTROL /YES/: yes
MAX TIMESTEP DURING INTEGRATION /36000/: 3.6e4
INITIAL TIMESTEP : /1E-07/: 1
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/: 1e-7
DIC>
DIC> @@ SIMULATIONS ARE FASTER WHEN THE RESULTS ARE NOT SAVED
DIC> @@ FOR EVERY TIME STEP
DIC> s-s-c
NSOIA PRINT CONTROL : /0/: 0
FLUX CORRECTION FACTOR : /1/: 1
NUMBER OF DELTA Timesteps IN CALLING MULDIF: /2/: 2
CHECK INTERFACE POSITION /AUTO/: n
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/: act
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/: y
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/: 99
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -> 1): /AUTO/: .5
MAX TIMESTEP CHANGE PER Timestep : /2/: 2
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/: n
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/: y
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/:
DIC>
DIC> @@ There are a several options available for the homogenization
DIC> @@ model. There is also an interpolation scheme that may reduce
DIC> @@ simulation times. However, for this example, the default settings
DIC> @@ are kept and the interpolation scheme is turned off.
DIC> @@
DIC> homogen yes yes
INFO: HOMOGENIZATION MODEL ENABLED
DIC>
DIC> @@ There are a large number of homogenization functions
DIC> @@ available. These determine how the average kinetics
DIC> @@ of the multiphase mixture is evaluated. For this example
DIC> @@ the General lower Hashin-Shtrikman bound is a good choice.
DIC> en-ho
ENTER HOMOGENIZATION FUNCTION # /5/: 1
SELECTED FUNCTION IS HASHIN-SHTRIKMAN BOUND: GENERAL LOWER
DIC>
DIC>
DIC>
DIC> save exd3 Y
DIC>
DIC>
DIC> set-inter
--OK--
DIC>
```

**exd3-run**

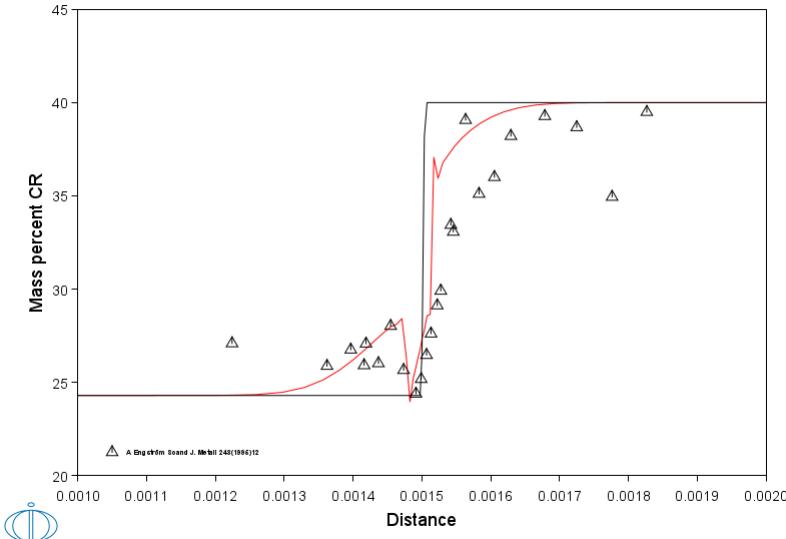
```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exd3\run.DCM.test"
DIC>
DIC>
DIC> @@ exd3_run.DCM
DIC>
DIC> @@
DIC> @@ READ THE SETUP FROM FILE AND START THE SIMULATION
DIC> @@
DIC>
DIC>
DIC> go d-m
TIME STEP AT TIME 0.00000E+00
DIC> read exd3
OK
DIC>
DIC> sim
STARTING SIMULATION USING HOMOGENIZATION MODEL
-----
WARNING:BCC_A2 HAS NO VOLUME FRACTION, CREATING ONE
Starting time-step t0= 0.0000000 dt= 1.0000000
Starting time-step t0= 1.0000000 dt= 2.0000000
Starting time-step t0= 3.0000000 dt= 4.0000000
Starting time-step t0= 7.0000000 dt= 8.0000000
Starting time-step t0= 15.0000000 dt= 16.0000000
Starting time-step t0= 31.0000000 dt= 32.0000000
Starting time-step t0= 63.0000000 dt= 64.0000000
Starting time-step t0= 127.0000000 dt= 128.0000000
Starting time-step t0= 255.0000000 dt= 256.0000000
Starting time-step t0= 511.0000000 dt= 256.0000000
Starting time-step t0= 767.0000000 dt= 256.0000000
Starting time-step t0= 1023.0000000 dt= 512.0000000
Starting time-step t0= 1535.0000000 dt= 512.0000000
Starting time-step t0= 2047.0000000 dt= 1024.0000000
Starting time-step t0= 3071.0000000 dt= 1024.0000000
Starting time-step t0= 4095.0000000 dt= 2048.0000000
Starting time-step t0= 6143.0000000 dt= 2048.0000000
Starting time-step t0= 8191.0000000 dt= 4096.0000000
Starting time-step t0= 12287.0000000 dt= 4096.0000000
Starting time-step t0= 16383.0000000 dt= 8192.0000000
Starting time-step t0= 24575.0000000 dt= 8192.0000000
Starting time-step t0= 32767.0000000 dt= 8192.0000000
Starting time-step t0= 40959.0000000 dt= 8192.0000000
Starting time-step t0= 49151.0000000 dt= 8192.0000000
Starting time-step t0= 57343.0000000 dt= 8192.0000000
Starting time-step t0= 65535.0000000 dt= 8192.0000000
Starting time-step t0= 73727.0000000 dt= 16384.0000000
Starting time-step t0= 90111.0000000 dt= 32768.0000000
Starting time-step t0= 122879.0000000 dt= 32768.0000000
Starting time-step t0= 155647.0000000 dt= 32768.0000000
Starting time-step t0= 188415.0000000 dt= 32768.0000000
Starting time-step t0= 221183.0000000 dt= 32768.0000000
Starting time-step t0= 253951.0000000 dt= 32768.0000000
Starting time-step t0= 286719.0000000 dt= 32768.0000000
Starting time-step t0= 319487.0000000 dt= 32768.0000000
Starting time-step t0= 352255.0000000 dt= 7745.0000000
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 0.0000000
DELETING TIME-RECORD FOR TIME 1.0000000
DELETING TIME-RECORD FOR TIME 511.0000000
DELETING TIME-RECORD FOR TIME 1023.0000000
DELETING TIME-RECORD FOR TIME 1535.0000000
DELETING TIME-RECORD FOR TIME 2047.0000000
DELETING TIME-RECORD FOR TIME 3071.0000000
DELETING TIME-RECORD FOR TIME 4095.0000000
DELETING TIME-RECORD FOR TIME 6143.0000000
DELETING TIME-RECORD FOR TIME 8191.0000000
DELETING TIME-RECORD FOR TIME 12287.0000000
DELETING TIME-RECORD FOR TIME 16383.0000000
DELETING TIME-RECORD FOR TIME 24575.0000000
DELETING TIME-RECORD FOR TIME 32767.0000000
DELETING TIME-RECORD FOR TIME 40959.0000000
DELETING TIME-RECORD FOR TIME 49151.0000000
DELETING TIME-RECORD FOR TIME 57343.0000000
DELETING TIME-RECORD FOR TIME 65535.0000000
DELETING TIME-RECORD FOR TIME 73727.0000000
DELETING TIME-RECORD FOR TIME 90111.0000000
DELETING TIME-RECORD FOR TIME 122879.0000000
DELETING TIME-RECORD FOR TIME 155647.0000000
DELETING TIME-RECORD FOR TIME 188415.0000000
DELETING TIME-RECORD FOR TIME 221183.0000000
DELETING TIME-RECORD FOR TIME 253951.0000000
DELETING TIME-RECORD FOR TIME 286719.0000000
DELETING TIME-RECORD FOR TIME 319487.0000000
KEEPING TIME-RECORD FOR TIME 352255.0000000
AND FOR TIME 360000.0000000
WORKSPACE RECLAIMED
-----
INTERPOLATION SCHEME USED THIS FRACTION OF
THE ALLOCATED MEMORY: 1.000000000000000
EFFICIENCY FACTOR: 3.57603859304014
-----
DEALLOCATING
-----
TIMESTEP AT 360000.0000000 SELECTED

DIC>
DIC>
DIC> set-inter
--OK--
DIC>
```

**exd3-plot**

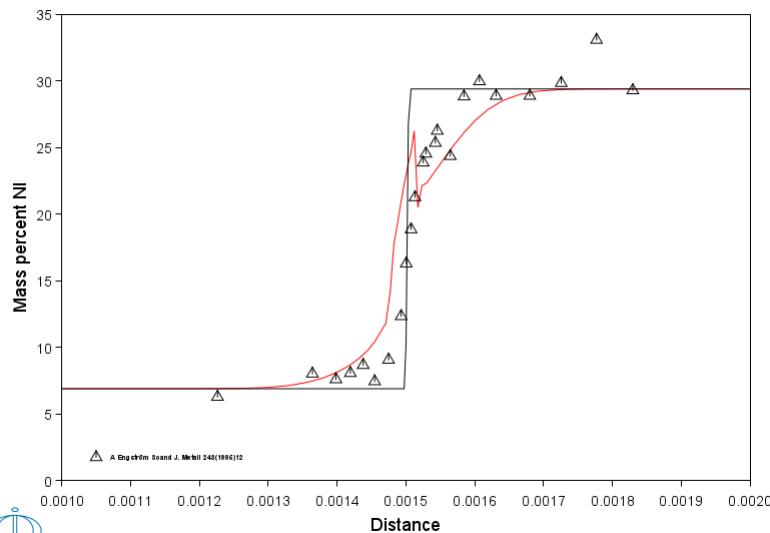
```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exd3\plot.DCM.test"
DIC>
DIC>
DIC> @@ exd3_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE d3
DIC> @@
DIC> @@ ENTER THE DICTRA MODULE AND SPECIFY THE STORE-RESULT FILE
DIC> @@
DIC>
DIC>
DIC> go d-m
TIME STEP AT TIME 3.60000E+05
DIC> read exd3
OK
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA POST PROCESSOR
DIC> @@
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1:
POST-1: @@
POST-1: @@ First study the composition profiles of Cr and Ni
POST-1: @@
POST-1: s-d-a x distance global
INFO: Distance is set as independent variable
POST-1: s-d-a y w-p Cr
POST-1: s-p-c time 0 360000
POST-1: set-tit Figure D3.1
POST-1:
POST-1: app yes k5k7cr.exp 0; 1
POST-1:
POST-1: s-s-s x n 1e-3 2e-3
POST-1:
POST-1: s-s-s y n 20 45
POST-1:
POST-1: SET_EXP_FILE_FORMAT 3
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

Figure D3.1



```
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1: s-d-a y w-p Ni
POST-1: set-tit Figure D3.2
POST-1:
POST-1: app yes k5k7ni.exp 0; 1
POST-1:
POST-1: s-s-s y n 0 35
POST-1:
POST-1: SET_EXP_FILE_FORMAT 3
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

**Figure D3.2**



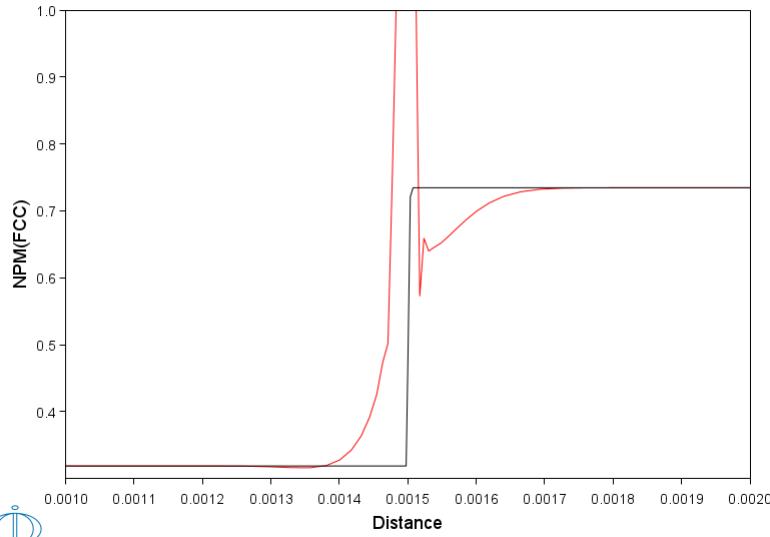
 A Engström *Scand J Metall* 24(1995)12

```

POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1: @@
POST-1: @@ Then study the amount of FCC and BCC
POST-1: @@
POST-1: app no
POST-1: s-d-a y npm(fcc)
POST-1: set-tit Figure D3.3
POST-1:
POST-1: SET_EXP_FILE_FORMAT 3
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

```

**Figure D3.3**



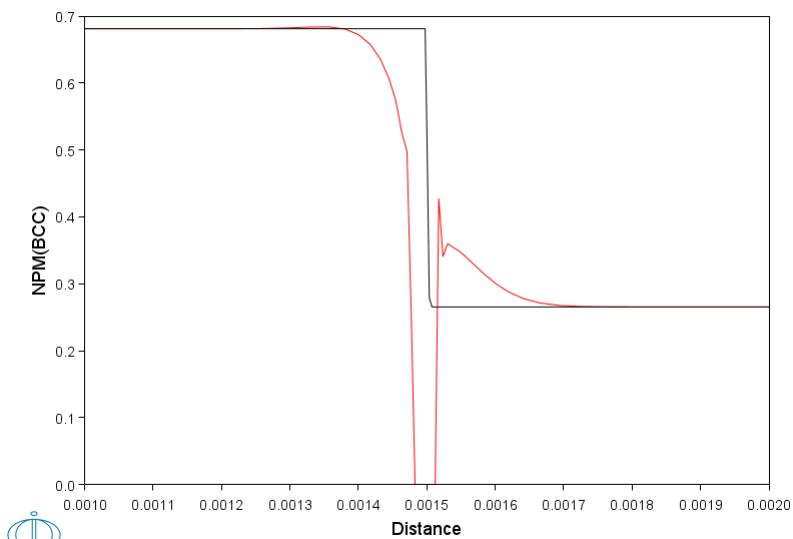
 A Engström *Scand J Metall* 24(1995)12

```

POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1: @@
POST-1: @@ Then study the amount of FCC and BCC
POST-1: @@
POST-1: app no
POST-1: s-d-a y npm(bcc)
POST-1: set-tit Figure D3.4
POST-1:
POST-1: SET_EXP_FILE_FORMAT 3
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

```

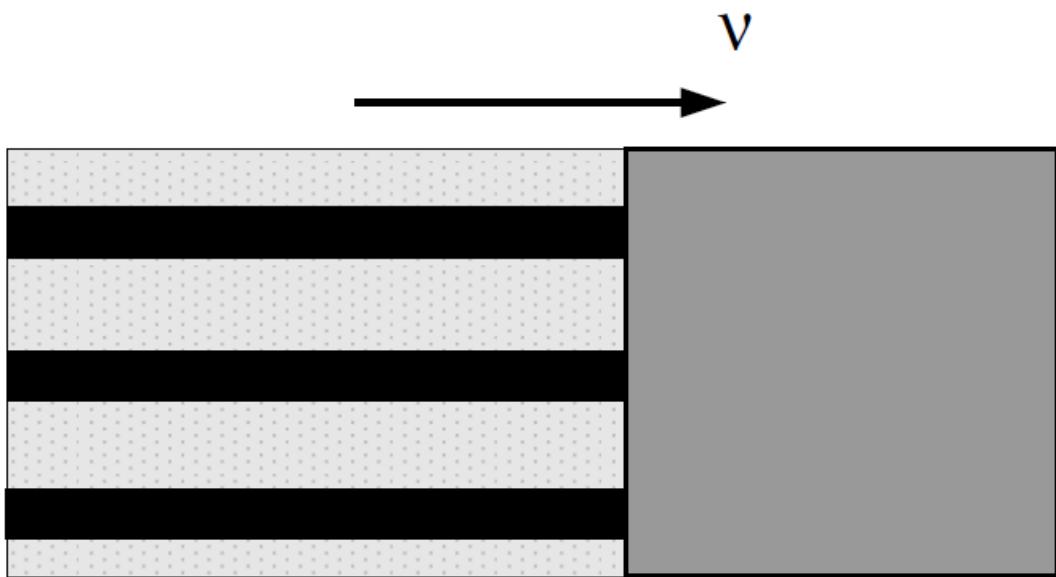
**Figure D3.4**



**POST-1:**  
**POST-1:**  
**POST-1:** set-interactive  
--OK---  
**POST-1:**



## Cooperative Growth



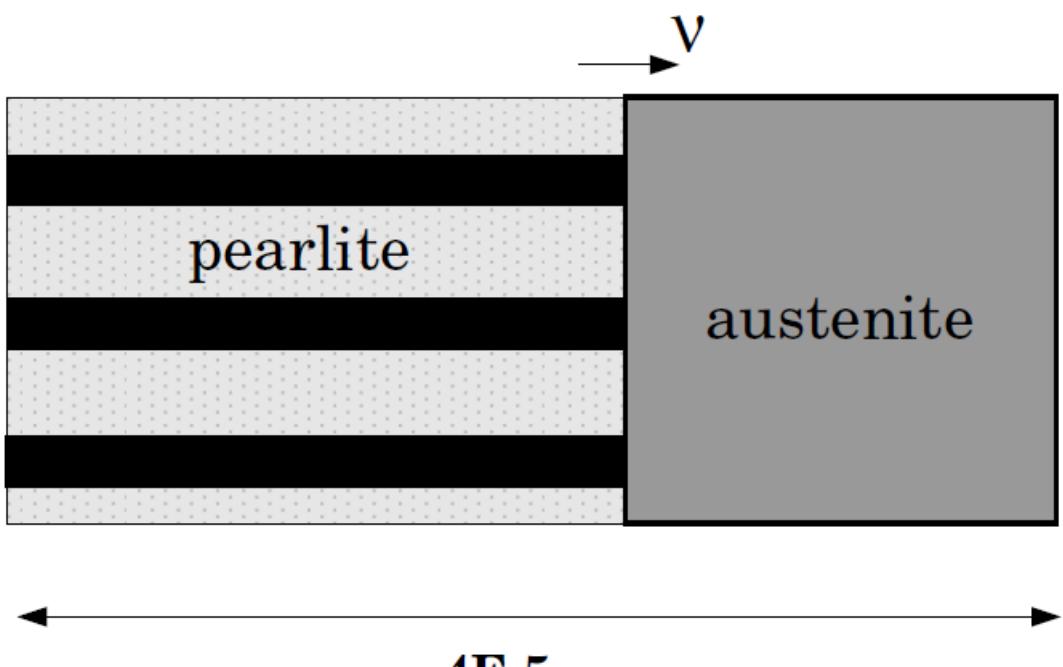


## Example exe1

### Growth of pearlite in an Fe-Mn-C alloy

This is an example of pearlite growth in an Fe-0.50wt%C - 0.91wt%Mn steel.

$$T = 900 - \text{Time} * 10$$





```

BCC_A2          CEMENTITE          FCC_A1
FE4N_LP1        HCP_A3            LIQUID:L
REJECTED
APP: rest-ph bcc,fcc,cem
BCC_A2          FCC_A1           CEMENTITE
RESTORED
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS .....

List of references for assessed data

'This parameter has not been assessed'
'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'
'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
-Ni'
'Y. Liu, L. Zhang, et al. CALPHAD 33(2009)614-23; Fe-Mn-C (fcc)'
'B. Jonsson: Z. Metallkunde 85(1994)498-501; C and N diffusion in bcc Cr
-Fe-Ni'
'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
in bcc Fe'
'S. Deng, et al., CALPHAD, 56 (2017) 230-240.'
'Assessed from data presented in Landolt-Bornstein, Vol. 26, ed. H.
Mehrer, Springer (1990); Impurity diff of Mn in bcc Fe.'
-OK-
APP:
APP: @@
APP: @@ ALL THE THERMODYNAMIC AND KINETIC DATA HAVE BEEN RETRIEVED.
APP: @@ GO TO THE DICTRA MONITOR TO SET UP YOUR PROBLEM.
APP: @@
DIC>
DIC> @@
DIC> @@ SET THE CONDITION FOR TEMPERATURE
DIC> @@
DIC> set-cond glob t 0 900-time*10; * n
DIC>
DIC> @@
DIC> @@ ENTER A REGION
DIC> @@
DIC> enter-reg pearlite
DIC>
DIC> @@
DIC> @@ ENTER A SMALL INITIAL SIZE OF THE GRID IN THE 'PEARLITE' REGION
DIC> @@
DIC> enter-grid pearlite 5e-10 lin 5
DIC>
DIC> @@
DIC> @@ ENTER INTO THE 'PEARLITE' REGION THE PHASES 'BCC' AND 'CEM' AND SPECIFY
DIC> @@ THAT ARE PRESENT IN THE FORM OF A 'LAMELLAR AGGREGATE. SET THE STATUS
DIC> @@ TO 'ACTIVE'. SEVERAL PROMPTS FOLLOW ABOUT THE VALUES OF THE PARAMETERS
DIC> @@ IN THE PEARLITE GROWTH MODEL, FOR EXAMPLE AS SURFACE TENSION, OPTIMUM
DIC> @@ GROWTH RATE FACTOR, AND BOUNDARY DIFFUSION COEFFICIENTS.
DIC> @@
DIC> @@ CARBON(C) IS TREATED IN A SPECIAL WAY. IF 'AUTOMATIC' IS ENTERED
DIC> @@ THE DIFFUSION OF C IS CALCULATED ACCORDING TO AN EQUATION FOR
DIC> @@ MIXED BOUNDARY AND VOLUME DIFFUSION. YOU CAN CHOOSE BETWEEN
DIC> @@ MANUAL OR AUTOMATIC START VALUES FOR ALL VARIABLES EXCEPT THE GROWTH
DIC> @@ RATE. IN THIS EXAMPLE WE WILL TRY 1E-6
DIC> @@
DIC> @@ FOR MORE INFORMATION ABOUT THE PEARLITE GROWTH MODEL SEE
DIC> @@ B. JÄNSSON: TRITA-MAC-0478, 1992 (ROYAL INSTITUTE OF TECHNOLOGY)
DIC> @@ STOCKHOLM, SWEDEN, 1992.
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /PEARLITE/: pearlite
PHASE TYPE /MATRIX/: lam
    Eutectoid reaction is "GAMMA" ==> "ALPHA" + "BETA"
Enter name of "ALPHA" phase /BCC_A2/: bcc_a2
Enter name of "BETA" phase /CEMENTITE/: cementite
Enter name of "GAMMA" phase /FCC_A1/: fcc_a1
Enter "ALPHA"/"BETA" surface tension
LOW TIME LIMIT /0/: 0
    Surface tension(T,P,TIME)= 1;
HIGH TIME LIMIT /*/: 1000
ANY MORE RANGES /N/: N
Enter "ALPHA"/"GAMMA" surface tension
LOW TIME LIMIT /0/: 0
    Surface tension(T,P,TIME)= 1;
HIGH TIME LIMIT /*/: 1000
ANY MORE RANGES /N/: N
Enter "BETA"/"GAMMA" surface tension
LOW TIME LIMIT /0/: 0
    Surface tension(T,P,TIME)= 1;
HIGH TIME LIMIT /*/: 1000
ANY MORE RANGES /N/: N
Optimum growth condition factor /2/: 2
Name of dependent element /FE/: fe
INPUT OF DIFFUSION DATA
    Growth model (VOLUME/BOUNDARY/KIRKALDY) for element C /BOUNDARY/: boundary
    DF(C) = /value/AUTOMATIC/MIXED/: auto
    Growth model (VOLUME/BOUNDARY/KIRKALDY) for element MN /BOUNDARY/: boundary
    DF(MN) = /value/MIXED/: 5.4e-14
    DQ(MN): 155000
Automatic start values for the S0 determination /Y/: Y
Growth rate V: 1E-6
Automatic start values on other variables /Y/: Y
DIC>
DIC> @@
DIC> @@ INITIATE THE COMPOSITION RECORDS FOR THE 'PEARLITE'
DIC> @@
DIC> enter-composition
REGION NAME : /PEARLITE/: pearlite
DIC>
DIC> @@
DIC> @@ NOW CONTINUE BY DEFINING A MATRIX PHASE INTO WHICH THE PEARLITE

```

```
DIC> @@ WILL GROW. START BY ENTERING A REGION NAME, 'AUSTENITE'
DIC> @@
DIC> enter-region austenite
ATTACH TO REGION NAMED /PEARLITE/:
ATTACHED TO THE RIGHT OF PEARLITE /YES/:
DIC> @@
DIC> @@ SPECIFY WHAT PHASE 'FCC' WILL BE PRESENT IN THE 'AUSTENITE' REGION
DIC> @@ AND WHAT TYPE OF PHASE 'MATRIX' IT IS AND ITS INITIAL STATE 'ACTIVE'
DIC> @@
DIC> enter-phase act austenite matrix fcc
DIC>
DIC> @@
DIC> @@ WE ALSO NEED TO HAVE A SPATIAL GRID IN THE 'AUSTENITE' REGION.
DIC> @@ CHOSE SIZE '4E-5' GRIDTYPE 'GEOMETRICAL', '30' GRIDPOINTS AND '1.5'
DIC> @@ AS VALUES FOR THE GEOMETRICAL FACTOR OF THE GRID.
DIC> @@
DIC> enter-grid austenite 4e-5 geo 30 1.5
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL CONCENTRATION PROFILES IN THE 'FCC' PHASE OF THE
DIC> @@ 'AUSTENITE' REGION. CONCENTRATIONS MUST BE GIVEN IN Y-FRACTIONS.
DIC> @@
DIC> enter-composition
REGION NAME : /AUSTENITE/: austenite
PHASE NAME: /FCC_A1/: fcc
DEPENDENT COMPONENT ? /MN/: fe
COMPOSITION TYPE /MOLE_FRACTION/: site-fraction
PROFILE FOR MN
TYPE /LINEAR/: lin 9.29232973E-3 9.29232973E-3
PROFILE FOR C
TYPE /LINEAR/: lin 2.3384332E-2 2.3384332E-2
DIC>
DIC> @@
DIC> @@ THE MATRIX PHASE IS NOW COMPLETE.
DIC> @@
DIC>
DIC> @@
DIC> @@ SPECIFY A SPHERICAL '2' GEOMETRY
DIC> @@
DIC> enter-geo 2
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 5
AUTOMATIC TIMESTEP CONTROL /YES/: YES
MAX TIMESTEP DURING INTEGRATION /.5/: 0.1
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exel Y
DIC>
DIC> set-inter
--OK--
DIC>
```

**exe1-run**

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exe1\run.DCM.test"
DIC>
DIC>
DIC> @@ exe1_run.DCM
DIC>
DIC> @@
DIC> FILE FOR RUNNING EXAMPLE e1
DIC> @@
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA MONITOR
DIC> @@
DIC> go d-m
TIME STEP AT TIME 0.00000E+00
DIC>
DIC> @@
DIC> @@ READ SETUP FROM FILE
DIC> @@
DIC> read exe1
OK
DIC>
DIC> @@
DIC> @@ START THE SIMULATION
DIC> @@
DIC> simulate
DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
Trying old scheme 4
U-FRACTION IN SYSTEM: C = .0233843320030518 FE = .990707670399293
MN = .0092923297312127
TOTAL SIZE OF SYSTEM: 2.68092626329E-13 [m^3]
U-FRACTION IN SYSTEM: C = .0233843320030518 FE = .990707670399293
MN = .0092923297312127
TOTAL SIZE OF SYSTEM: 2.68092626329E-13 [m^3]
17 GRIDPOINT(S) ADDED TO CELL #1 REGION: AUSTENITE
TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.0000000
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.77954867E-05 AND 0.77954867E-05
POSITION OF INTERFACE PEARLITE / AUSTENITE IS 0.50077955E-09
U-FRACTION IN SYSTEM: C = .0233843320030518 FE = .990707670399294
MN = .00929232973121272
TOTAL SIZE OF SYSTEM: 2.68092626329E-13 [m^3]
10 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: AUSTENITE

CPU time used in timestep 4 seconds
4 GRIDPOINT(S) ADDED TO CELL #1 REGION: AUSTENITE
TIME = 0.10010000E-03 DT = 0.10000000E-03 SUM OF SQUARES = 0.0000000
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.77957274E-05 AND 0.77957274E-05
POSITION OF INTERFACE PEARLITE / AUSTENITE IS 0.12803523E-08
U-FRACTION IN SYSTEM: C = .0233843320030518 FE = .990707670399294
MN = .00929232973121271
TOTAL SIZE OF SYSTEM: 2.68092626329E-13 [m^3]
CPU time used in timestep 0 seconds
1 GRIDPOINT(S) REMOVED FROM CELL# 1 REGION # 1
TIME = 0.13027597E-02 DT = 0.12026597E-02 SUM OF SQUARES = 0.0000000
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.77986225E-05 AND 0.77986225E-05
POSITION OF INTERFACE PEARLITE / AUSTENITE IS 0.10659441E-07
U-FRACTION IN SYSTEM: C = .0233843320030518 FE = .990707670399295
MN = .00929232973121271
TOTAL SIZE OF SYSTEM: 2.68092626329E-13 [m^3]
CPU time used in timestep 0 seconds
2 GRIDPOINT(S) REMOVED FROM CELL# 1 REGION # 1
TIME = 0.37080790E-02 DT = 0.24053193E-02 SUM OF SQUARES = 0.0000000
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.78044138E-05 AND 0.78044138E-05
POSITION OF INTERFACE PEARLITE / AUSTENITE IS 0.29431548E-07
U-FRACTION IN SYSTEM: C = .0233843320030517 FE = .990707670399294
MN = .00929232973121271
TOTAL SIZE OF SYSTEM: 2.68092626329E-13 [m^3]
CPU time used in timestep 0 seconds
1 GRIDPOINT(S) REMOVED FROM CELL# 1 REGION # 1
TIME = 0.85187177E-02 DT = 0.48106387E-02 SUM OF SQUARES = 0.0000000
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.78160011E-05 AND 0.78160011E-05
POSITION OF INTERFACE PEARLITE / AUSTENITE IS 0.67031506E-07
U-FRACTION IN SYSTEM: C = .0233843320030517 FE = .990707670399294
MN = .00929232973121271
TOTAL SIZE OF SYSTEM: 2.68092626329E-13 [m^3]
CPU time used in timestep 1 seconds
1 GRIDPOINT(S) REMOVED FROM CELL# 1 REGION # 1
TIME = 0.18139995E-01 DT = 0.96212773E-02 SUM OF SQUARES = 0.0000000
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.78391945E-05 AND 0.78391945E-05
POSITION OF INTERFACE PEARLITE / AUSTENITE IS 0.14245457E-06
U-FRACTION IN SYSTEM: C = .0233843320030517 FE = .990707670399295
MN = .00929232973121269
TOTAL SIZE OF SYSTEM: 2.68092626329E-13 [m^3]
CPU time used in timestep 0 seconds
TIME = 0.37382550E-01 DT = 0.19242555E-01 SUM OF SQUARES = 0.0000000
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.78856562E-05 AND 0.78856562E-05
POSITION OF INTERFACE PEARLITE / AUSTENITE IS 0.29419474E-06
U-FRACTION IN SYSTEM: C = .0233843320030516 FE = .990707670399294
MN = .00929232973121268
TOTAL SIZE OF SYSTEM: 2.68092626329E-13 [m^3]
CPU time used in timestep 0 seconds
TIME = 0.75867659E-01 DT = 0.38485109E-01 SUM OF SQUARES = 0.0000000
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.79788762E-05 AND 0.79788762E-05
POSITION OF INTERFACE PEARLITE / AUSTENITE IS 0.60126266E-06
U-FRACTION IN SYSTEM: C = .0233843320030516 FE = .990707670399294
MN = .00929232973121267
TOTAL SIZE OF SYSTEM: 2.68092626329E-13 [m^3]
CPU time used in timestep 0 seconds
1 GRIDPOINT(S) REMOVED FROM CELL# 1 REGION # 1
TIME = 0.15283788 DT = 0.76970219E-01 SUM OF SQUARES = 0.0000000
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.81664857E-05 AND 0.81664857E-05
POSITION OF INTERFACE PEARLITE / AUSTENITE IS 0.12298389E-05
U-FRACTION IN SYSTEM: C = .0233843320030516 FE = .990707670399294
MN = .00929232973121267
TOTAL SIZE OF SYSTEM: 2.68092626329E-13 [m^3]
CPU time used in timestep 0 seconds
TIME = 0.25283788 DT = 0.10000000 SUM OF SQUARES = 0.0000000
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.84125012E-05 AND 0.84125012E-05
POSITION OF INTERFACE PEARLITE / AUSTENITE IS 0.20710890E-05
U-FRACTION IN SYSTEM: C = .0233843320030516 FE = .990707670399294
```

```

        MN = .00929232973121268
TOTAL SIZE OF SYSTEM: 2.68092626329E-13 [m^3]
CPU time used in timestep          0 seconds
1 GRIDPOINT(S) REMOVED FROM CELL# 1 REGION # 1
TIME = 0.35283788 DT = 0.10000000 SUM OF SQUARES = 0.0000000
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.86610019E-05 AND 0.86610019E-05
POSITION OF INTERFACE PEARLITE / AUSTENITE IS 0.29371892E-05
U-FRACTION IN SYSTEM: C = .0233843320030515 FE = .990707670399294
MN = .00929232973121272
TOTAL SIZE OF SYSTEM: 2.68092626329E-13 [m^3]
CPU time used in timestep          0 seconds

output ignored...

... output resumed

WORKSPACE RECLAIMED
INFO: CELL 1 REGION AUSTENITE DELETED
U-FRACTION IN SYSTEM: C = .0233843320030516 FE = .990707670399325
MN = .00929232973118255
TOTAL SIZE OF SYSTEM: 2.68089005379E-13 [m^3]
U-FRACTION IN SYSTEM: C = .0233843320030516 FE = .990707670399325
MN = .00929232973118255
TOTAL SIZE OF SYSTEM: 2.68089005379E-13 [m^3]
TIME = 3.2743811 DT = 0.10000000E-04 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0233843320030516 FE = .990707670399325
MN = .00929232973118255
TOTAL SIZE OF SYSTEM: 2.68089005379E-13 [m^3]
CPU time used in timestep          0 seconds
TIME = 3.2843811 DT = 0.10000000E-01 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0233843320030516 FE = .990707670399325
MN = .00929232973118255
TOTAL SIZE OF SYSTEM: 2.68089005379E-13 [m^3]
CPU time used in timestep          0 seconds
TIME = 3.3843811 DT = 0.10000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0233843320030516 FE = .990707670399325
MN = .00929232973118255
TOTAL SIZE OF SYSTEM: 2.68089005379E-13 [m^3]
CPU time used in timestep          0 seconds
TIME = 3.4843811 DT = 0.10000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0233843320030516 FE = .990707670399325
MN = .00929232973118255
TOTAL SIZE OF SYSTEM: 2.68089005379E-13 [m^3]
CPU time used in timestep          0 seconds
TIME = 3.5843811 DT = 0.10000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0233843320030516 FE = .990707670399325
MN = .00929232973118255
TOTAL SIZE OF SYSTEM: 2.68089005379E-13 [m^3]
CPU time used in timestep          0 seconds
TIME = 3.6843811 DT = 0.10000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0233843320030516 FE = .990707670399325
MN = .00929232973118255
TOTAL SIZE OF SYSTEM: 2.68089005379E-13 [m^3]
CPU time used in timestep          0 seconds
TIME = 3.7843811 DT = 0.10000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0233843320030516 FE = .990707670399325
MN = .00929232973118255
TOTAL SIZE OF SYSTEM: 2.68089005379E-13 [m^3]
CPU time used in timestep          0 seconds
TIME = 3.8843811 DT = 0.10000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0233843320030516 FE = .990707670399325
MN = .00929232973118255
TOTAL SIZE OF SYSTEM: 2.68089005379E-13 [m^3]
CPU time used in timestep          0 seconds
TIME = 3.9843811 DT = 0.10000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0233843320030516 FE = .990707670399325
MN = .00929232973118255
TOTAL SIZE OF SYSTEM: 2.68089005379E-13 [m^3]
CPU time used in timestep          0 seconds
TIME = 4.0843811 DT = 0.10000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0233843320030516 FE = .990707670399325
MN = .00929232973118255
TOTAL SIZE OF SYSTEM: 2.68089005379E-13 [m^3]
CPU time used in timestep          0 seconds
TIME = 4.1843811 DT = 0.10000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0233843320030516 FE = .990707670399325
MN = .00929232973118255
TOTAL SIZE OF SYSTEM: 2.68089005379E-13 [m^3]
CPU time used in timestep          0 seconds
TIME = 4.2843811 DT = 0.10000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0233843320030516 FE = .990707670399325
MN = .00929232973118255
TOTAL SIZE OF SYSTEM: 2.68089005379E-13 [m^3]
CPU time used in timestep          0 seconds
TIME = 4.3843811 DT = 0.10000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0233843320030516 FE = .990707670399325
MN = .00929232973118255
TOTAL SIZE OF SYSTEM: 2.68089005379E-13 [m^3]
CPU time used in timestep          0 seconds
TIME = 4.4843811 DT = 0.10000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0233843320030516 FE = .990707670399325
MN = .00929232973118255
TOTAL SIZE OF SYSTEM: 2.68089005379E-13 [m^3]
CPU time used in timestep          0 seconds
TIME = 4.5843811 DT = 0.10000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0233843320030516 FE = .990707670399325
MN = .00929232973118255
TOTAL SIZE OF SYSTEM: 2.68089005379E-13 [m^3]
CPU time used in timestep          0 seconds
TIME = 4.6843811 DT = 0.10000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0233843320030516 FE = .990707670399325
MN = .00929232973118255
TOTAL SIZE OF SYSTEM: 2.68089005379E-13 [m^3]
CPU time used in timestep          0 seconds
TIME = 4.7843811 DT = 0.10000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0233843320030516 FE = .990707670399325
MN = .00929232973118255
TOTAL SIZE OF SYSTEM: 2.68089005379E-13 [m^3]
CPU time used in timestep          0 seconds
TIME = 4.8843811 DT = 0.10000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0233843320030516 FE = .990707670399325
MN = .00929232973118255
TOTAL SIZE OF SYSTEM: 2.68089005379E-13 [m^3]
```

```

CPU time used in timestep          0 seconds
TIME = 4.9843811      DT = 0.10000000    SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0233843320030516  FE = .990707670399325
MN = .00929232973118255
TOTAL SIZE OF SYSTEM: 2.68089005379E-13 [m^3]
CPU time used in timestep          0 seconds
TIME = 5.0000000     DT = 0.15618919E-01 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0233843320030516  FE = .990707670399325
MN = .00929232973118255
TOTAL SIZE OF SYSTEM: 2.68089005379E-13 [m^3]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME    3.2528379
DELETING TIME-RECORD FOR TIME    3.2743711
DELETING TIME-RECORD FOR TIME    3.2743811
DELETING TIME-RECORD FOR TIME    3.2843811
DELETING TIME-RECORD FOR TIME    3.3843811
DELETING TIME-RECORD FOR TIME    3.4843811
DELETING TIME-RECORD FOR TIME    3.5843811
DELETING TIME-RECORD FOR TIME    3.6843811
DELETING TIME-RECORD FOR TIME    3.7843811
DELETING TIME-RECORD FOR TIME    3.8843811
DELETING TIME-RECORD FOR TIME    3.9843811
DELETING TIME-RECORD FOR TIME    4.0843811
DELETING TIME-RECORD FOR TIME    4.1843811
DELETING TIME-RECORD FOR TIME    4.2843811
DELETING TIME-RECORD FOR TIME    4.3843811
DELETING TIME-RECORD FOR TIME    4.4843811
DELETING TIME-RECORD FOR TIME    4.5843811
DELETING TIME-RECORD FOR TIME    4.6843811
DELETING TIME-RECORD FOR TIME    4.7843811
DELETING TIME-RECORD FOR TIME    4.8843811

KEEPING TIME-RECORD FOR TIME    4.9843811
AND FOR TIME                   5.0000000
WORKSPACE RECLAIMED

TIMESTEP AT      5.00000000      SELECTED

```

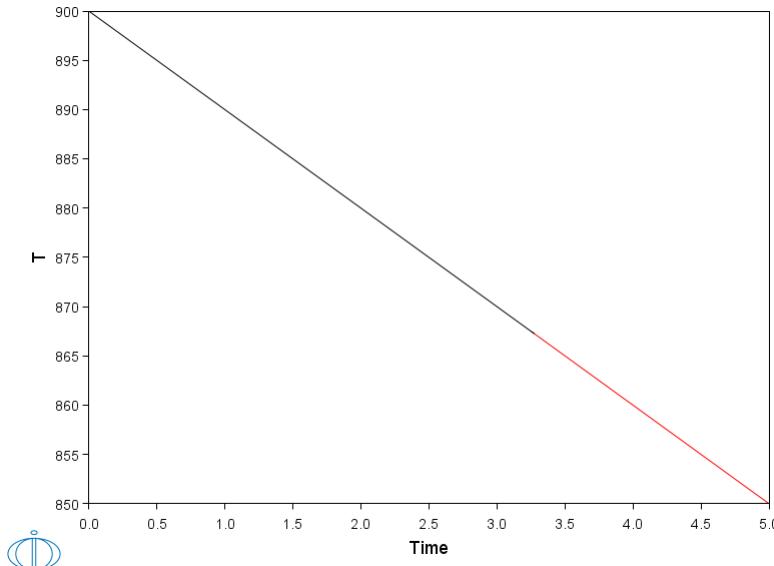
```

DIC>
DIC> @@
DIC> @@ THE SIMULATION IS FINISHED
DIC> @@
DIC>
DIC> set-inter
--OK---
DIC>

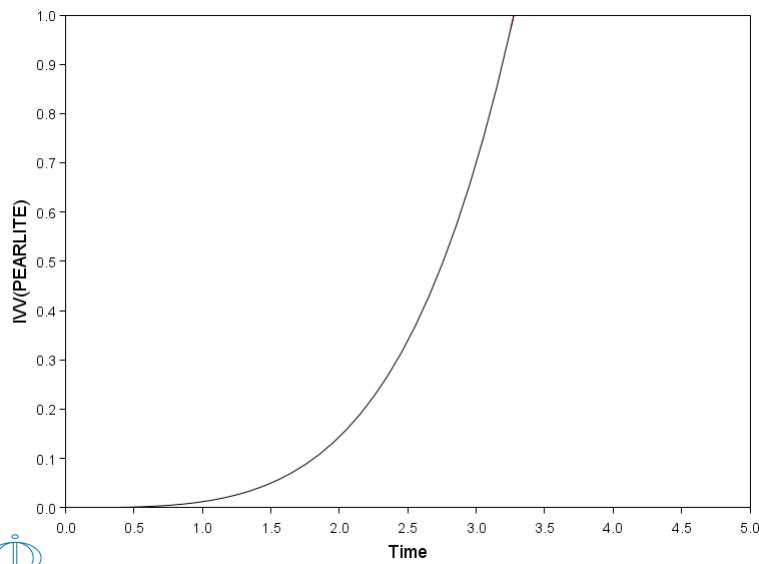
```

**exe1-plot**

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exe1\plot.DCM.test"
DIC>
DIC>
DIC> @@ exe1_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE e1
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 5.00000E+00
DIC> read exe1
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1: @@
POST-1: @@ PLOT THE TEMPERATURE AS A FUNCTION OF TIME
POST-1: @@
POST-1: s-d-a x time
INFO: Time is set as independent variable
POST-1: s-d-a y t
POST-1: s-p-c interface first
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 3
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
ORKING ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```



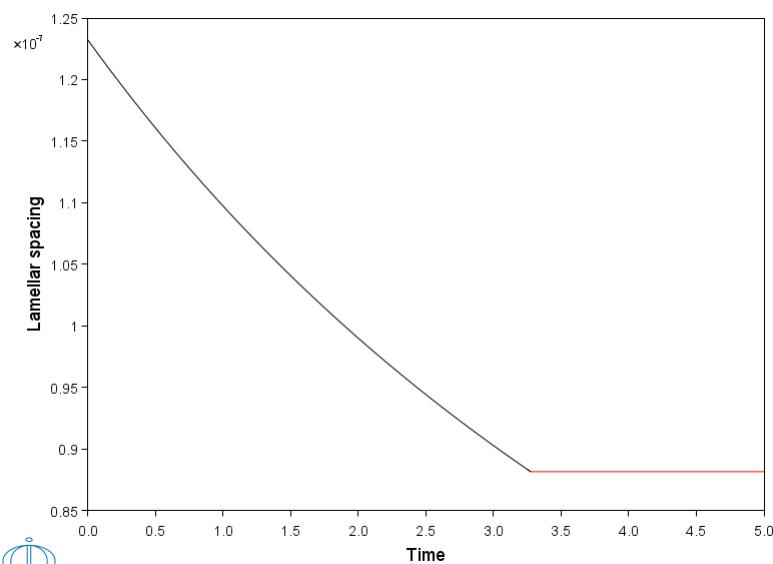
```
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ NOW PLOT THE FRACTION OF PEARLITE VS. TIME
POST-1: @@
POST-1: s-d-a y ivv(pearlite)
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 3
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
ORKING ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```



```

POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ PLOT THE LAMELLAR SPACING AS A FUNCTION OF TIME
POST-1: @@
POST-1: s-d-a
AXIS (X, Y OR Z) : y
VARIABLE : lamellar-sp
IN REGION: /*/: pearlite
POST-1:
POST-1: s-p-c
CONDITION /INTEGRAL/: interface
INTERFACE : pearlite
UPPER OR LOWER INTERFACE OF REGION PEARLITE#1 /LOWER/: upper
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 3
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
ORKING ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

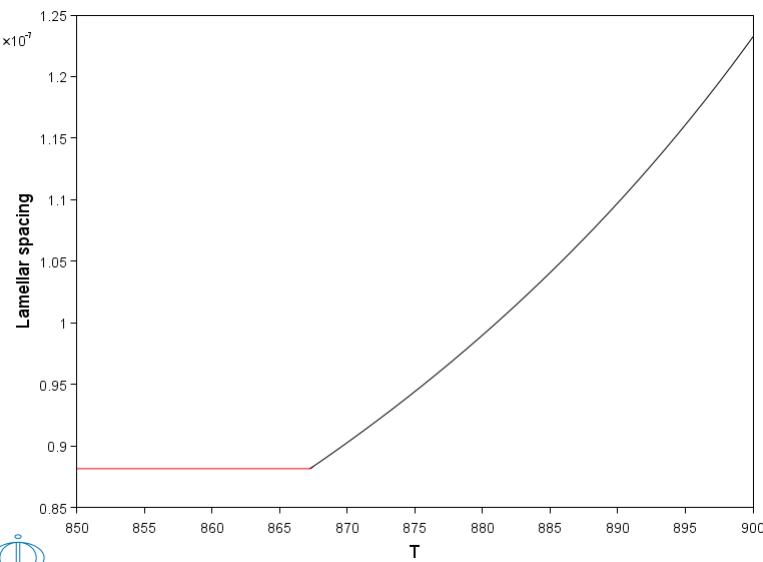
```



```

POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ LET'S LOOK AT THE LAMELLAR SPACING VS. TEMPERATURE INSTEAD
POST-1: @@
POST-1: s-d-a x t
POST-1:
POST-1: s-p-c interface pearlite upper
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 3
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
ORKING ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

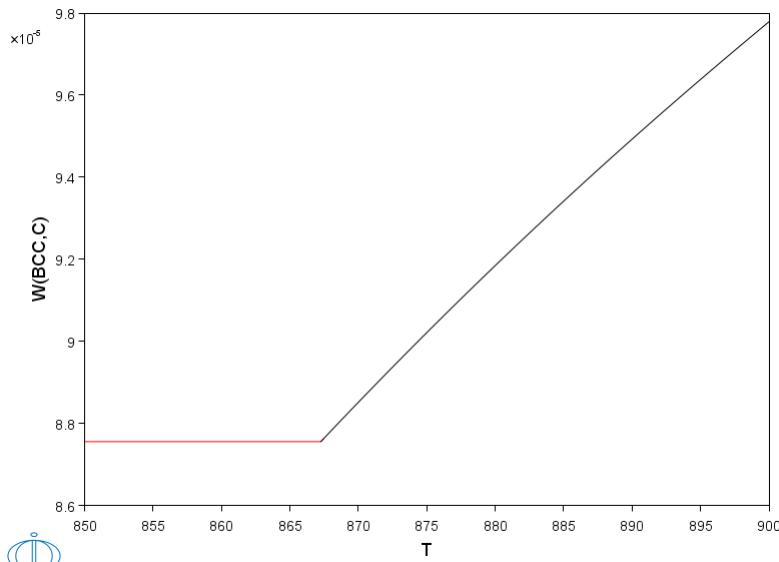
```



```

POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ AND THE C COMPOSITION IN THE FERRITE VS. TEMP
POST-1: @@
POST-1: s-d-a y w(bcc,c)
POST-1:
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 3
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
ORKING ...
OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

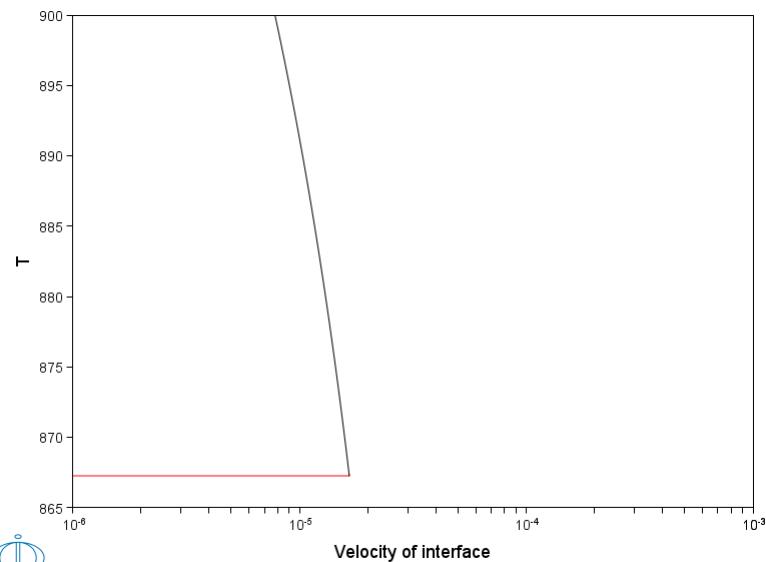
```



```

POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ FINALLY, LET'S LOOK AT THE VELOCITY OF THE INTERFACE VS. TEMP
POST-1: @@
POST-1: s-d-a y t
POST-1: s-d-a x velocity
INTERFACE : pearlite
UPPER OR LOWER INTERFACE OF REGION PEARLITE#1 /LOWER/: upper
POST-1: set-ax-ty x log
POST-1: s-s-s x n 1e-6 1e-4
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 3
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
ORKING ...
OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

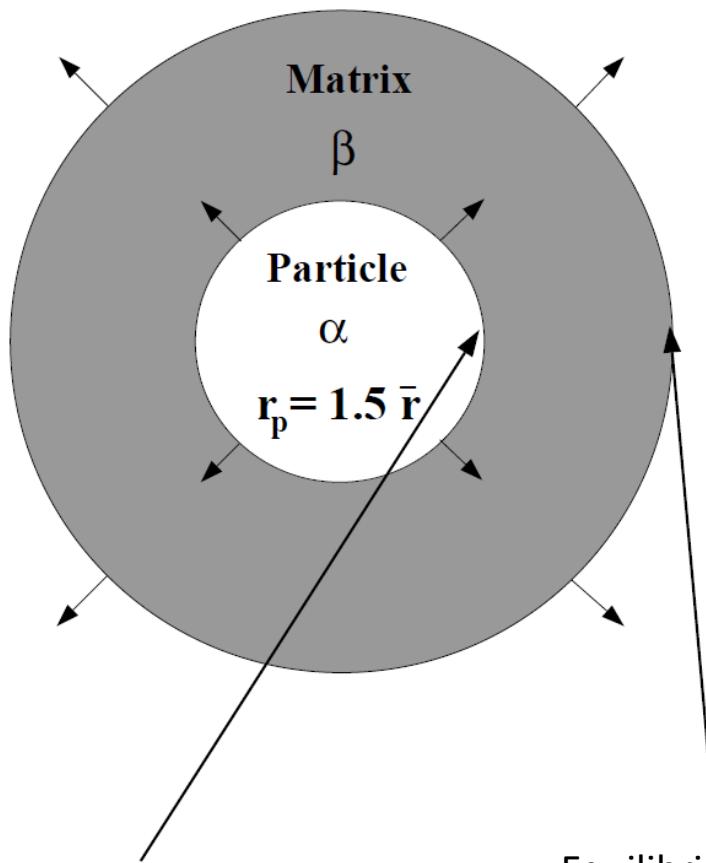
```



```
POST-1:  
POST-1:  
POST-1:  
POST-1:Hit RETURN to continue  
POST-1:  
POST-1:  
POST-1:  
POST-1: set-inter  
--OK---  
POST-1:
```



## Coarsening



Moving phase interface  
with  $\alpha$  and  $\beta$  in local  
equilibrium.

$\frac{2\sigma V_m}{r}$  Interfacial energy  
contribution for  $\alpha$  phase

Equilibrium as defined by  
the average composition  
in the system.

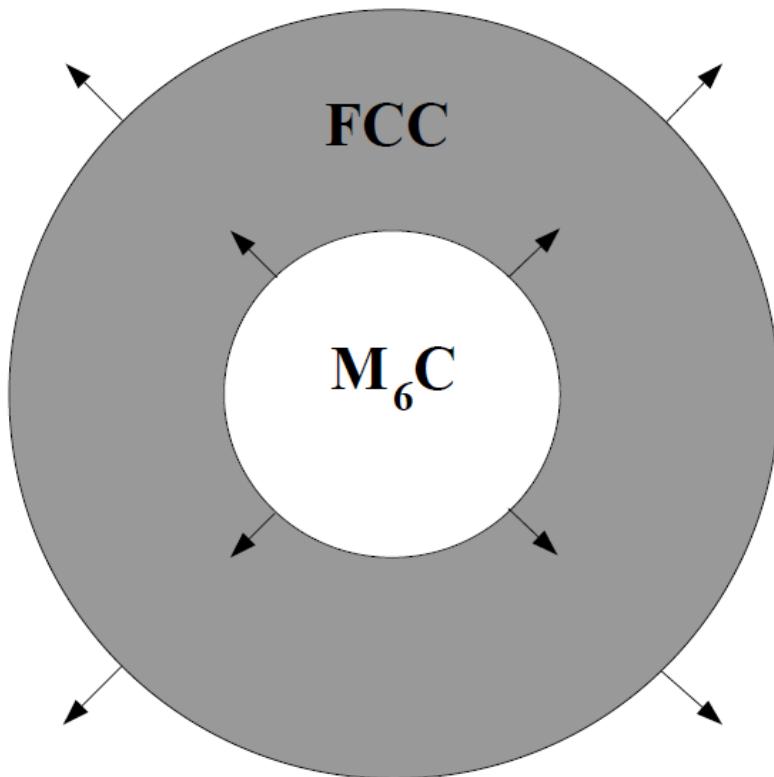
$\frac{2\sigma V_m}{r_p}$  Interfacial energy  
contribution for  $\alpha$  phase



## Example exf1

### Coarsening of an $M_6C$ precipitate in an Fe-Mo-C alloy

This example calculates the Ostwald-ripening of a spherical  $M_6C$  carbide in an austenite matrix.



$$T = 1173\text{K}$$

$$r_p = 0.228 \mu\text{m}$$

**exf1-setup****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\_dictra\_console\_examples\examples\exf1\setup.DCM.test"**

**SYS: @@**  
**SYS: @@** Coarsening problem.  
**SYS: @@** Coarsening of M6C precipitate in an Fe-Mo-C alloy  
**SYS: @@** This example calculates the Ostwald-ripening of a spherical  
**SYS: @@** M6C carbide in an austenite matrix.

**SYS: -----**

NO SUCH COMMAND, USE HELP

**SYS: @@**  
**SYS: @@** RETRIEVE DATA FROM THE DATABASES  
**SYS: @@**  
**SYS: go da**

THERMODYNAMIC DATABASE module

Database folder:

C:\jenkins\workspace\generate\_dictra\_console\_examples\databases\data

Current database: Steels/Fe-Alloys v12.0

VA /- DEFINED

DICTRA\_FCC\_A1 REJECTED

**TDB\_TCFE12:** switch TCFE9

Current database: Steels/Fe-Alloys v9.3

VA /- DEFINED  
L12\_FCC B2\_BCC DICTRA\_FCC\_A1

REJECTED

**TDB\_TCFE9:** def-sys fe mo c  
FE MO C

DEFINED  
**TDB\_TCFE9:** rej ph \* all  
GAS:G LIQUID:L BCC\_A2  
FCC\_A1 HCP\_A3 CBCC\_A12  
CUB\_A13 DIAMOND\_FCC\_A4 GRAPHITE  
CEMENTITE M23C6 M7C3  
M6C M5C2 M3C2  
MC\_ETA MC\_SHP KSI\_CARBIDE  
Z\_PHASE FE4N\_LP1 FECN\_CHI  
SIGMA MU\_PHASE P\_PHASE  
R\_PHASE CHI\_A12 LAVES\_PHASE\_C14  
AL5FE4 M2O3C:I REJECTED

**TDB\_TCFE9:** res ph fcc m6c  
FCC\_A1 M6C RESTORED

**TDB\_TCFE9:** get

18:48:19,722 [Thread-0] INFO JavaWrapper: \*\*\* Invoking Gibbs Energy System v6 \*\*\*  
REINITIATING GES ....  
ELEMENTS .....  
SPECIES .....  
PHASES .....  
PARAMETERS ...  
FUNCTIONS ....

List of references for assessed data

'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'  
'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'  
'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'  
'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'  
'J-O. Andersson, CALPHAD, 12 (1988) 1-8; TRITA 0317 (1986); C-MO'  
'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'  
'A. Fernandez Guillermet, CALPHAD, 6 (1982) 127-140; (sigma phase revised  
1986); TRITA-MAC 200 (1982); FE-MO'  
'J-O. Andersson, CALPHAD, 12 (1988) 9-23; TRITA 0321 (1986); C-FE-MO'  
'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'

-OK-

**TDB\_TCFE9:**

**TDB\_TCFE9:** @@

**TDB\_TCFE9:** @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE MOBILITY DATA

**TDB\_TCFE9:** @@

**TDB\_TCFE9:** app

Use one of these databases

TCFE12 = Steels/Fe-Alloys v12.0  
TCFE9 = Steels/Fe-Alloys v9.3  
SSUB6 = SGTE Substances v6.0  
FEDEMO = Iron Demo Database v4.0  
MOB2 = Alloys Mobility v2.7  
MOBF2 = Steels/Fe-Alloys Mobility v2.0  
MOBF4 = Steels/Fe-Alloys Mobility v4.0  
MOBF7 = Steels/Fe-Alloys Mobility v7.1  
MFEDEMO = Fe-Alloys Mobility demo database v2.0  
USER = User defined Database

**DATABASE NAME /TCFE9:** mobfe4

Current database: Steels/Fe-Alloys Mobility v4.0

VA DEFINED  
B2\_BCC REJECTED  
**APP:** def-sys fe mo c  
FE MO C  
DEFINED  
**APP:** rej ph \* all  
BCC\_A2 CEMENTITE FCC\_A1  
FE4N\_LP1 HCP\_A3 LIQUID:L

```

REJECTED
APP: res ph fcc m6c
*** ERROR M6C INPUT IGNORED
FCC_A1 RESTORED
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS .....
FUNCTIONS .....

List of references for assessed data

'This parameter has not been assessed'
'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'
'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
-Ni'
'Y. Liu et al., Calphad 34(2010)253-262; fcc Cu-Fe.'
'W. Zheng, et al., Metall Mater Trans, 48 (2017) 536-550; Fe-Mn-Mo (fcc
and bcc)'

-OK-
APP:
APP:
APP: @@ ENTER THE DICTRA MONITOR
APP: @@ go d-m
NO TIME STEP DEFINED
*** ENTERING M6C AS A DIFFUSION NONE PHASE
DIC>
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> s-cond glob t 0 1173; * N
DIC>
DIC> @@
DIC> @@ ENTER REGIONS part AND aus
DIC> @@
DIC> enter-region
REGION NAME : part
DIC> enter-region aus
ATTACH TO REGION NAMED /PART/:
ATTACHED TO THE RIGHT OF PART /YES/:
DIC> @@
DIC> @@ ENTER GEOMTRICAL GRIDS INTO THE REGIONS
DIC> @@
DIC> @@
DIC> @@
DIC> @@ THE INITIAL SIZE OF THE CARBIDE PARTICLE IS ASSUMED TO BE KNOWN
DIC> @@ (IN THIS CASE THE VALUE IS FROM NISHIZAWA ET. AL.). THE
DIC> @@ AVERAGE PARTICLE SIZE IS ASSUMED TO BE 0.152E-6 METERS. HOWEVER, THE
DIC> @@ CALCULATIONS ARE PERFORMED ON A MAXIMUM SIZE PARTICLE, WHICH IS ASSUMED
DIC> @@ TO BE 1.5 TIMES THE AVERAGE SIZE. THE SURROUNDING AUSTENITIC MATRIX
DIC> @@ SIZE IS CHOOSEN TO MAINTAIN THE AVERAGE COMPOSITION.
DIC> @@
DIC> enter-grid
REGION NAME : /PART/: part
WIDTH OF REGION /1/: 0.228E-6
TYPE /LINEAR/: AUTO
DIC>
DIC> enter-grid
REGION NAME : /AUS/: aus
WIDTH OF REGION /1/: 4.53147041E-7
TYPE /LINEAR/: AUTO
DIC>
DIC> @@
DIC> @@ ENTER PHASES INTO REGIONS
DIC> @@
DIC> enter-phase active part matrix m6c
DIC>
DIC> enter-phase active aus matrix fcc#1
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITIONS IN THE PHASES
DIC> @@
DIC> enter-composition
REGION NAME : /PART/: part
PHASE NAME: /M6C/: m6c
DEPENDENT COMPONENT ? /MO/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-f
PROFILE FOR /MO/: mo lin 6.20117E-01 6.20117E-01
DIC>
DIC> ent-composition
REGION NAME : /AUS/: aus
PHASE NAME: /FCC_A1/: fcc#1
DEPENDENT COMPONENT ? /MO/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-f
PROFILE FOR /C/: mo lin 1.82099E-02 1.82099E-02
PROFILE FOR /MO/: c lin 2.83351E-03 2.83351E-03
DIC>
DIC>
DIC> @@
DIC> @@ SET A SPHERICAL GEOMETRY
DIC> @@
DIC> ent-geo 2
DIC>
DIC> @@
DIC> @@ ENTER THE SURFACE TENSION ENERGY CONTRIBUTION AS A FUNCTION OF
DIC> @@ THE INTERFACE POSITION (THE RADIUS OF THE PARTICLE).
DIC> @@ ALSO ENTER THE MOLAR VOLUME OF THE PHASE CORRECTED TO BE THE
DIC> @@ MOLAR VOLUME PER SUBSTITUTIONAL ATOM.
DIC> @@
DIC> @@ THE SURFACE TENSION IS 0.7, THE MOLAR VOLUME IS 0.71 AND THE
DIC> @@ TRANSFORMATION TO MOLAR VOLUME PER SUBSTITUTIONAL ATOM IS 7/6.
DIC> @@
DIC> set-surf 2*0.7*0.71*(7/6)/X;
ENTERED FUNCTION :2*.7*.71*7/6/X FOR CELL #1
DIC>
DIC>
DIC> @@

```

```
DIC> @@ ENABLE THE SIMPLIFIED MODEL FOR THE COARSENING (OSTWALD-RIPENING)
DIC> @@
DIC> coarse YES
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME AND OTHER SIMULATION PARAMETERS
DIC> @@
DIC> set-simulation-time 1E6
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /100000/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exf1 Y
DIC>
DIC> set-inter
--OK--
DIC>
```

**exf1-run**

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exf1\run.DCM.test"
DIC> @@ exf1_run.DCM
DIC>
DIC> @@
DIC> @@ READ THE SETUP FROM FILE AND START THE SIMULATION
DIC> @@
DIC>
DIC> go d-m
TIME STEP AT TIME 0.00000E+00
*** ENTERING M6C AS A DIFFUSION NONE PHASE
DIC> read exf1
OK
DIC> sim
Region: PART
single geometric dense at 0.22800E-06
0.80000 64
Region: AUS
single geometric dense at 0.0000
1.00600 63
DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
Trying old scheme 4
GENERATING STARTING VALUES FOR CELL # 1 INTERFACE # 2
DETERMINING INITIAL EQUILIBRIUM VALUES
CALCULATING STARTING VALUES: 9 EQUILIBRIUM CALCULATIONS DONE 6 OUT OF 9
U-FRACTION IN SYSTEM: C = .0190652843033664 FE = .970761291162784
MO = .0292387089677228
TOTAL SIZE OF SYSTEM: 1.32376603026E-18 [m^3]
U-FRACTION IN SYSTEM: C = .0190652843033664 FE = .970761291162784
MO = .0292387089677228
TOTAL SIZE OF SYSTEM: 1.32376603026E-18 [m^3]
0.610222970497625 0.610391048253360 0.610222911134902 2.564830792704480E-002 2.191933775609301E-
003 1.266865150888817E-004 1.096501654713504E-003 1.278319049399803E-004 4.432656450601522E-
007 1.566395317892607E-009 1.947833765313978E-009 3.659996125120900E-009 1.418022110198698E-
009 1.309139507131020E-009 1.103984934282495E-009 3.800021059935427E-009 7.446660066835133E-
010 2.344008708335402E-010 1.080152259465027E-013 1.867047546680927E-018 TIME = 0.1000000E-06 DT = 0.1000000E-
06 SUM OF SQUARES = 0.15190630E-17
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.50349408E-05 AND -0.50349408E-05
POSITION OF INTERFACE PART / AUS IS 0.22799950E-06
U-FRACTION IN SYSTEM: C = .0190659317665348 FE = .97075948763499
MO = .0292405124955171
TOTAL SIZE OF SYSTEM: 1.32375726043E-18 [m^3]
6 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: PART

CPU time used in timestep 1 seconds
5.960103082661315E-005 5.961330244477064E-005 5.959458009987109E-005 3.934421751033465E-007 1.790908700287879E-
012 8.025303437845193E-020 SWITCHING ACTIVITIES FOR INTERFACE #2, CELL #1
FROM: C TO: MO
TIME = 0.254446964E-05 DT = 0.244446964E-05 SUM OF SQUARES = 0.80119136E-19
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.39293667E-08 AND -0.39293667E-08
POSITION OF INTERFACE PART / AUS IS 0.22799949E-06
U-FRACTION IN SYSTEM: C = .0190664790756638 FE = .970759484159471
MO = .029240515971036
TOTAL SIZE OF SYSTEM: 1.32375709311E-18 [m^3]
CPU time used in timestep 0 seconds
2.51515852968503E-008 2.515761992652319E-008 2.499573886069665E-008 2.005534172058944E-008 1.975331989336378E-
008 1.917061703504815E-008 1.798309031228442E-008 1.798198228999587E-008 1.576453639540498E-
008 1.173116059611238E-008 5.468961563766386E-009 5.475061906690870E-009 2.640249636669288E-
011 1.077666851477393E-019 TIME = 0.74340891E-05 DT = 0.48893927E-05 SUM OF SQUARES = 0.10181449E-18
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.56129636E-09 AND -0.56129636E-09
POSITION OF INTERFACE PART / AUS IS 0.22799948E-06
U-FRACTION IN SYSTEM: C = .0190671017629171 FE = .970759483986865
MO = .0292405161436416
TOTAL SIZE OF SYSTEM: 1.32375704531E-18 [m^3]
CPU time used in timestep 0 seconds
4.333438087398587E-010 4.334345197563670E-010 4.419215189297320E-010 4.026611773882563E-010 4.018893334371022E-
010 4.003483969890692E-010 3.972574074743073E-010 3.977091085443222E-010 3.911287935104968E-
010 3.789974357867931E-010 3.553242205200265E-010 3.55979648331291E-010 3.102532494486979E-
010 2.292896951167527E-010 1.040111356100155E-010 1.045003432102073E-010 9.69062436076466E-
014 4.713884980308892E-024 TIME = 0.17212874E-04 DT = 0.97787854E-05 SUM OF SQUARES = 0.46486834E-23
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.11440105E-09 AND -0.11440105E-09
POSITION OF INTERFACE PART / AUS IS 0.22799948E-06
U-FRACTION IN SYSTEM: C = .0190679130516543 FE = .970759484521662
MO = .0293075024612657
TOTAL SIZE OF SYSTEM: 1.32375702582E-18 [m^3]
CPU time used in timestep 1 seconds

output ignored...

... output resumed

2.171297261534317E-011 9.341085436010698E-013 1.185632317509854E-013 1.157575007606943E-
022 TIME = 667998.25 DT = 100000.00 SUM OF SQUARES = 0.87275999E-22
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.22669488E-13 AND 0.22669488E-13
POSITION OF INTERFACE PART / AUS IS 0.24398484E-06
U-FRACTION IN SYSTEM: C = .019556197188195 FE = .970692497669241
MO = .0293075024612657
TOTAL SIZE OF SYSTEM: 1.62216577705E-18 [m^3]
29 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: PART
29 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: AUS

CPU time used in timestep 0 seconds
8.463229105648878E-012 8.732923810174576E-012 1.10630567858858E-011 1.671261465075374E-012 8.083191454220552E-
013 2.031412919309583E-015 4.756793755048421E-
025 TIME = 767998.25 DT = 100000.00 SUM OF SQUARES = 0.39675494E-26
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.22252996E-13 AND 0.22252996E-13
POSITION OF INTERFACE PART / AUS IS 0.24621014E-06
U-FRACTION IN SYSTEM: C = .0195587075255164 FE = .970694293020122
MO = .0293057071103851
TOTAL SIZE OF SYSTEM: 1.66695743697E-18 [m^3]
16 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: PART
16 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: AUS

CPU time used in timestep 0 seconds
4.716189843803081E-012 4.737893940451163E-012 6.250071127630892E-012 2.547264388925926E-012 1.906488084462803E-
012 8.178986810072403E-013 4.518673827601144E-
022 TIME = 867998.25 DT = 100000.00 SUM OF SQUARES = 0.18485018E-23
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.21855116E-13 AND 0.21855116E-13
```

POSITION OF INTERFACE PART / AUS IS 0.24839565E-06  
 U-FRACTION IN SYSTEM: C = .0195611435099161 FE = .970696048456853  
 MO = .0293039516736542  
 TOTAL SIZE OF SYSTEM: 1.71174343902E-18 [m^3]  
 25 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: PART  
 25 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: AUS

CPU time used in timestep 0 seconds  
 3.96324298439393E-012 3.789984632754622E-012 4.665295441188398E-012 3.497963869501466E-012 3.136690178437880E-012  
 012 2.396321761152848E-012 1.082065602964671E-012 1.796670475822717E-015 5.709761494322691E-025  
 TIME = 967998.25 DT = 100000.00 SUM OF SQUARES = 0.75033670E-26  
 CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.21474553E-13 AND 0.21474553E-13  
 POSITION OF INTERFACE PART / AUS IS 0.25054311E-06  
 U-FRACTION IN SYSTEM: C = .019563510079962 FE = .970697758696434  
 MO = .0293022414340732  
 TOTAL SIZE OF SYSTEM: 1.756523973737E-18 [m^3]  
 13 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: PART  
 13 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: AUS

CPU time used in timestep 1 seconds  
 3.163580379550386E-010 3.128551215447078E-010 3.018312582226520E-010 3.724165375968103E-011 1.354264012443001E-011  
 011 1.037102048003190E-019 TIME = 1000000.0 DT = 32001.746 SUM OF SQUARES = 0.86048866E-19  
 CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.21247167E-13 AND 0.21247167E-13  
 POSITION OF INTERFACE PART / AUS IS 0.25122306E-06  
 U-FRACTION IN SYSTEM: C = .0195660575765671 FE = .9706988317476  
 MO = .0293011683829064  
 TOTAL SIZE OF SYSTEM: 1.77086385838E-18 [m^3]  
 MUST SAVE WORKSPACE ON FILE  
 WORKSPACE SAVED ON FILE  
 RECLAIMING WORKSPACE  
 DELETING TIME-RECORD FOR TIME 0.0000000  
 DELETING TIME-RECORD FOR TIME 0.10000000E-06  
 DELETING TIME-RECORD FOR TIME 0.25446964E-05  
 DELETING TIME-RECORD FOR TIME 0.74340891E-05  
 DELETING TIME-RECORD FOR TIME 0.17212874E-04  
 DELETING TIME-RECORD FOR TIME 0.36770445E-04  
 DELETING TIME-RECORD FOR TIME 0.75885587E-04  
 DELETING TIME-RECORD FOR TIME 0.15411587E-03  
 DELETING TIME-RECORD FOR TIME 0.31057644E-03  
 DELETING TIME-RECORD FOR TIME 0.62349757E-03  
 DELETING TIME-RECORD FOR TIME 0.12493398E-02  
 DELETING TIME-RECORD FOR TIME 0.25010244E-02  
 DELETING TIME-RECORD FOR TIME 0.50043934E-02  
 DELETING TIME-RECORD FOR TIME 0.10011132E-01  
 DELETING TIME-RECORD FOR TIME 0.20024608E-01  
 DELETING TIME-RECORD FOR TIME 0.40051560E-01  
 DELETING TIME-RECORD FOR TIME 0.80105465E-01  
 DELETING TIME-RECORD FOR TIME 0.16021328  
 DELETING TIME-RECORD FOR TIME 0.32042890  
 DELETING TIME-RECORD FOR TIME 0.64086014  
 DELETING TIME-RECORD FOR TIME 1.2817226  
 DELETING TIME-RECORD FOR TIME 2.5634476  
 DELETING TIME-RECORD FOR TIME 5.1268975  
 DELETING TIME-RECORD FOR TIME 10.253797  
 DELETING TIME-RECORD FOR TIME 20.507597  
 DELETING TIME-RECORD FOR TIME 41.015196  
 DELETING TIME-RECORD FOR TIME 82.030395  
 DELETING TIME-RECORD FOR TIME 164.06079  
 DELETING TIME-RECORD FOR TIME 328.12159  
 DELETING TIME-RECORD FOR TIME 656.24318  
 DELETING TIME-RECORD FOR TIME 1312.4864  
 DELETING TIME-RECORD FOR TIME 2624.9727  
 DELETING TIME-RECORD FOR TIME 5249.9454  
 DELETING TIME-RECORD FOR TIME 10499.891  
 DELETING TIME-RECORD FOR TIME 20999.782  
 DELETING TIME-RECORD FOR TIME 41999.564  
 DELETING TIME-RECORD FOR TIME 83999.127  
 DELETING TIME-RECORD FOR TIME 167998.25  
 DELETING TIME-RECORD FOR TIME 267998.25  
 DELETING TIME-RECORD FOR TIME 367998.25  
 DELETING TIME-RECORD FOR TIME 467998.25  
 DELETING TIME-RECORD FOR TIME 567998.25  
 DELETING TIME-RECORD FOR TIME 667998.25  
 DELETING TIME-RECORD FOR TIME 767998.25  
 DELETING TIME-RECORD FOR TIME 867998.25

KEEPING TIME-RECORD FOR TIME 967998.25  
 AND FOR TIME 1000000.0  
 WORKSPACE RECLAIMED

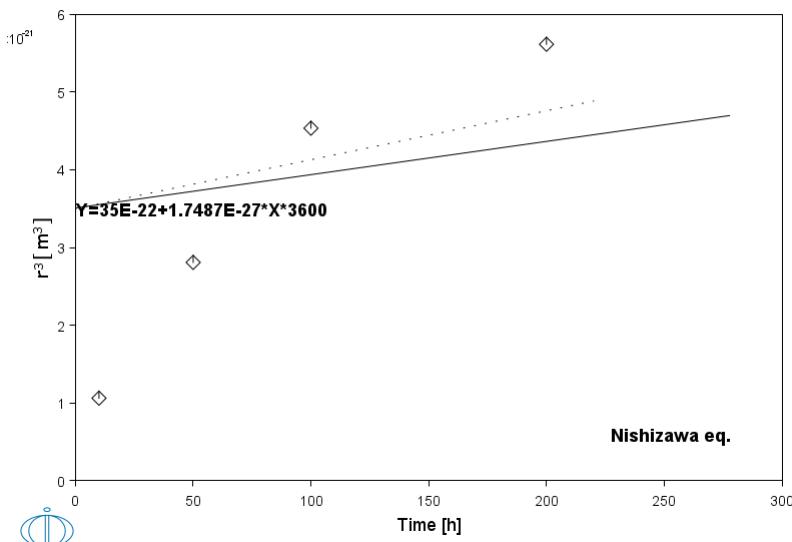
TIMESTEP AT 1000000.00 SELECTED

**DIC>**  
**DIC>**  
**DIC> set-inter**  
**--OK--**  
**DIC>**

**exf1-plot**

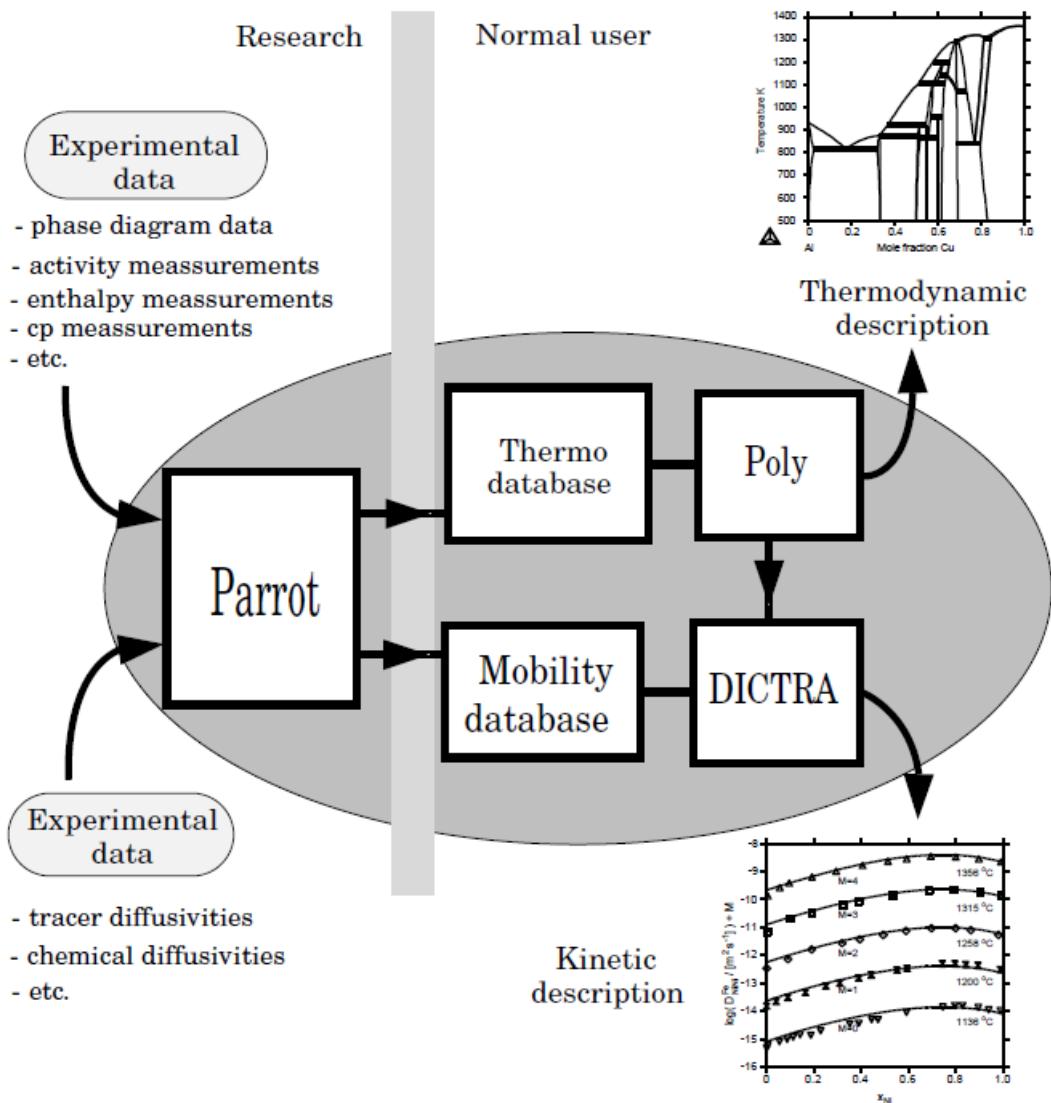
```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exf1\plot.DCM.test"
DIC> @@ exf1_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE f1
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 1.00000E+06
*** ENTERING M6C AS A DIFFUSION NONE PHASE
DIC> read exf1
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1: @@
POST-1: @@ PLOT THE AVERAGE PARTICLE SIZE (CUBED) AS THIS ASSUMED TO
POST-1: @@ SCALE LINEARLY WITH TIME. THEN A FUNCTION IS ENTERED SO
POST-1: @@ THIS QUANTITY CAN BE ACCESSED. WE ALSO WANT TO PLOT THIS
POST-1: @@ QUANTITY VERSUS TIME (IN HOURS) SO A FUNCTION IS ENTERED.
POST-1: @@
POST-1: enter-symbol func rr3=(poi(part,u)/1.5)**3;
POST-1: enter-symbol func hours=time/3600;
POST-1: s-d-a x hours
POST-1: s-d-a y rr3
POST-1: @@
POST-1: @@ AS WE ARE PLOTTING FUNCTIONS ON BOTH AXES WE MUST EXPLICITLY
POST-1: @@ DEFINE THE INDEPENDENT VARIABLE AND THE PLOT CONDITION
POST-1: @@
POST-1: s-ind time
POST-1: s-p-c inter
INTERFACE : part upper
POST-1:
POST-1:
POST-1: set-axis-text-status x n
AXIS TEXT : Time [h]
POST-1:
POST-1: @@
POST-1: @@ WHEN THIS IS PLOTTED, THIS AXIS TEXT NOTATION WORKS WELL FOR
POST-1: @@ THE AVERAGE RADIUS CUBED. FOR MORE INFORMATION ABOUT HOW TO
POST-1: @@ ADJUST TEXT IN THE POST PROCESSOR USING THE DATAPLOT LANGUAGE,
POST-1: @@ SEARCH THE ONLINE HELP (FROM THE MAIN MENU -> HELP > ONLINE HELP)
POST-1:
POST-1:
POST-1: set-axis-text-status y n
AXIS TEXT : \ latex r^3\, [m^3]
POST-1:
POST-1:
POST-1: @@
POST-1: @@ COMPARE WITH EXPERIMENTAL DATA FROM NISHIZAWA ET AL.
POST-1: @@ TRANS. JPN. INST. MET. VOL. 22 1981 PP. 733-742.
POST-1: @@
POST-1: @@
POST-1: app y exf1
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 1
POST-1:
POST-1: s-s-s y n 0 6e-21
POST-1:
POST-1: @@
POST-1: @@ SET A TITLE ON THE PLOT
POST-1: @@
POST-1: set-title Figure f1.1
POST-1:
POST-1: @@ SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
      OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

**Figure f1.1**





## Kinetic Data

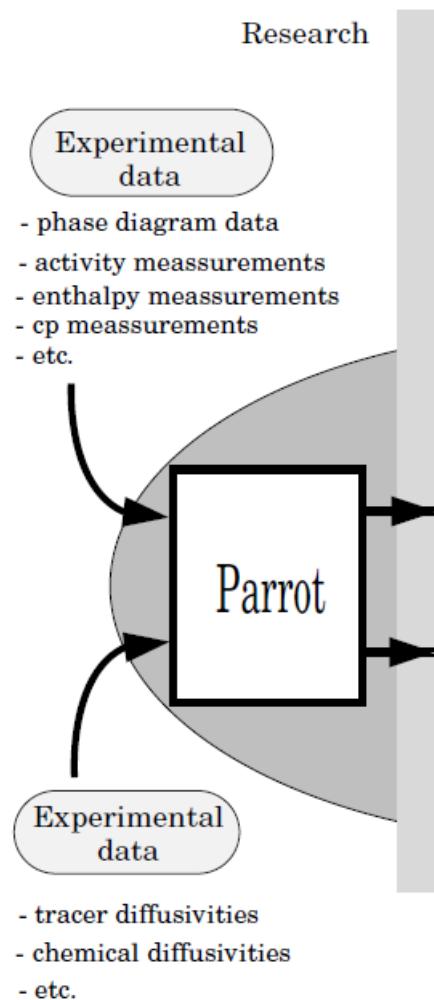




## Example exg2

### Optimization of mobilities in Ni-Al fcc alloys

A file for reading thermodynamic data and setting up the kinetic parameters which are needed for an optimization of the FCC phase in the binary Ni-Al system. See also A. Engström and J. Ågren: ("Assessment of Diffusional Mobilities in Face-Centered Cubic Ni-Cr-Al Alloys" in Z. METALLKUNDE, Feb. 1996).

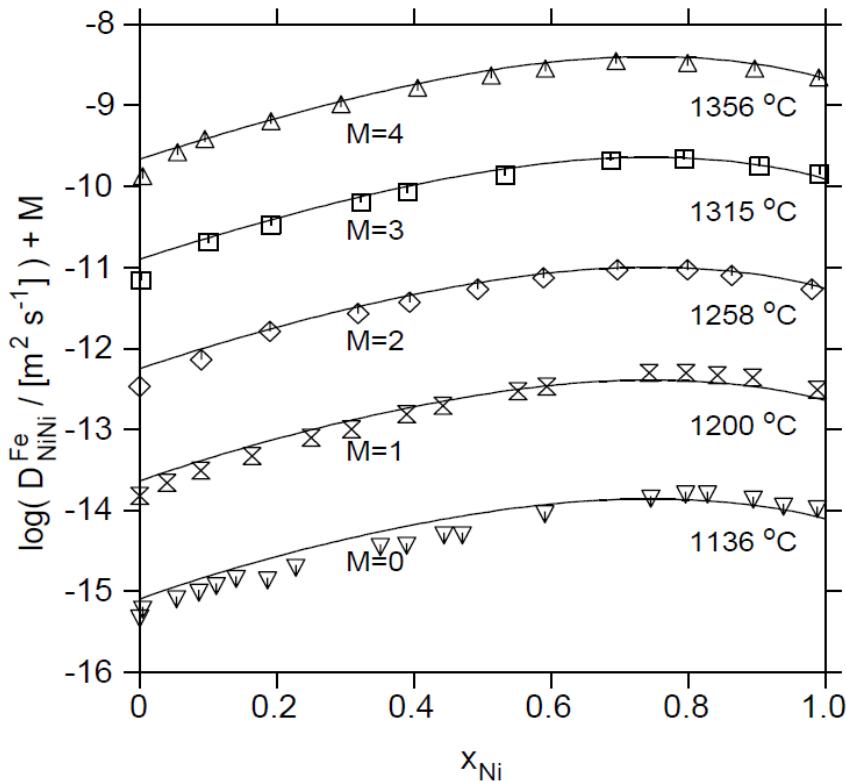




## Example exg1

### Checking diffusivities in an Fe-Ni alloy

This is an example file to check the mobilities and diffusivities in an Fe-Ni alloy.



**exgl-setup****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_dictra_console_examples\examples\exgl\setup.DCM.test"
SYS: @@
SYS: @@ Kinetic data example.
SYS: @@ Checking mobilities and diffusivities in an Fe-Ni alloy
SYS: @@ This is an example file to check the mobilities and diffusivities
SYS: @@ in an Fe-Ni alloy.
SYS: -----
NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exgl_setup.DCM
SYS:
SYS: @@
SYS: @@ START BY GOING TO THE DATABASE MODULE
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\generate_dictra_console_examples\databases\data
Current database: Steels/Fe-Alloys v12.0

VA          /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE12:
TDB_TCFE12: @@
TDB_TCFE12: @@ SELECT A DATABASE FOR THERMODYNAMIC DATA
TDB_TCFE12: @@
TDB_TCFE12: sw fedemo
Current database: Iron Demo Database v4.0

VA          /- DEFINED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ DEFINE THE SYSTEM TO WORK WITH
TDB_FEDEMO: @@
TDB_FEDEMO: def-sys fe ni
FE          NI DEFINED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ EXCLUDE THE THERMODYNAMIC DATA FOR THE PHASES THAT ARE NOT NEEDED
TDB_FEDEMO: @@
TDB_FEDEMO: rej ph * all
LIQUID:L           BCC_A2           LAVES_PHASE_C14
CBCC_A12          CUB_A13          FCC_A1
HCP_A3             REJECTED
TDB_FEDEMO: res ph fcc
FCC_A1             RESTORED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ RETRIEVE DATA FROM THE DATABASE FILE
TDB_FEDEMO: @@
TDB_FEDEMO: get
18:51:46,940 [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'
'X.G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
    volumes'
'A.T. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); FE-NI'
'X.G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
-OK-
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ MOBILITY/DIFFUSIVITY DATA ARE STORED IN A SEPARATE DATABASE FILE.
TDB_FEDEMO: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE DATA
TDB_FEDEMO: @@
TDB_FEDEMO: app
Use one of these databases

TCFE12 = Steels/Fe-Alloys v12.0
TCFE9 = Steels/Fe-Alloys v9.3
SSUB6 = SGTE Substances v6.0
FEDEMO = Iron Demo Database v4.0
MOB2 = Alloys Mobility v2.7
MOBFE2 = Steels/Fe-Alloys Mobility v2.0
MOBFE4 = Steels/Fe-Alloys Mobility v4.0
MOBFE7 = Steels/Fe-Alloys Mobility v7.1
MFEDEMO = Fe-Alloys Mobility demo database v2.0
USER = User defined Database

DATABASE NAME /FEDEMO/: mfedemo
Current database: Fe-Alloys Mobility demo database v2.0

VA  DEFINED
APP: def-sys fe ni
FE          NI DEFINED
APP: rej ph * all
BCC_A2           FCC_A1 REJECTED
APP: res ph fcc
FCC_A1           RESTORED
```

```

APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS .....
FUNCTIONS .....

List of references for assessed data

'This parameter has not been assessed'
'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
-Ni'
'Xia, C. H. et al. JAC, 2021, 853, 157165.'
'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Ni self-diffusion'
-OK-
APP:
APP: @@ 
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP
APP: @@ 
APP: go d-m
NO TIME STEP DEFINED
DIC>
DIC> @@ 
DIC> @@ CHECK THE DIFFUSIVITIES
DIC> @@ 
DIC> check-diffusion-matrix
OUTPUT TO SCREEN OR FILE /SCREEN/:
PHASE NAME : fcc
DEPENDENT COMPONENT ? /NI/: fe
CONCENTRATION OF NI IN U-FRACTION /1/: 0.3
Pressure /100000/: 101325
Temperature /298.15/: 1409
OPTION ( dlpbmx0ez or * ) /D/: dl

Dkj (reduced n=FE)
k / j NI
NI +4.86136E-15
L0kj = Uk*Mvak IF (kES) ELSE Uk*Yva*Mvak
k / j FE NI
FE +1.00113E-19
NI +1.00113E-19

Volume = 1.000000000000000E-005

DIC>
DIC>
DIC>@?<Hit_return_to_continue>
DIC>
DIC> @@ 
DIC> @@ USE STEPPING IN POLY-3 TO CALCULATE THE DIFFUSIVITIES VS. COMPOSITION
DIC> @@ 
DIC> go p-3
POLY: s-c t=1409,p=101325,n=1,x(ni)=0.3
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: s-a-v
Axis number: /1/: 1
Condition /NONE/: x(ni)
Min value /0/: 0
Max value /1/: 1
Increment /.025/: 1e-3
POLY:
POLY: step
Option? /NORMAL/: normal
No initial equilibrium, using default
Step will start from axis value 0.300000
...OK

Phase Region from 0.300000 for:
FCC_A1
Global test at 3.08000E-01 .... OK
Global test at 3.18000E-01 .... OK
Global test at 3.28000E-01 .... OK
Global test at 3.38000E-01 .... OK
Global test at 3.48000E-01 .... OK
Global test at 3.58000E-01 .... OK
Global test at 3.68000E-01 .... OK
Global test at 3.78000E-01 .... OK
Global test at 3.88000E-01 .... OK
Global test at 3.98000E-01 .... OK
Global test at 4.08000E-01 .... OK
Global test at 4.18000E-01 .... OK
Global test at 4.28000E-01 .... OK
Global test at 4.38000E-01 .... OK
Global test at 4.48000E-01 .... OK
Global test at 4.58000E-01 .... OK
Global test at 4.68000E-01 .... OK
Global test at 4.78000E-01 .... OK
Global test at 4.88000E-01 .... OK
Global test at 4.98000E-01 .... OK
Global test at 5.08000E-01 .... OK
Global test at 5.18000E-01 .... OK
Global test at 5.28000E-01 .... OK
Global test at 5.38000E-01 .... OK
Global test at 5.48000E-01 .... OK
Global test at 5.58000E-01 .... OK
Global test at 5.68000E-01 .... OK
Global test at 5.78000E-01 .... OK
Global test at 5.88000E-01 .... OK
Global test at 5.98000E-01 .... OK
Global test at 6.08000E-01 .... OK
Global test at 6.18000E-01 .... OK
Global test at 6.28000E-01 .... OK
Global test at 6.38000E-01 .... OK
Global test at 6.48000E-01 .... OK
Global test at 6.58000E-01 .... OK
Global test at 6.68000E-01 .... OK
Global test at 6.78000E-01 .... OK

```

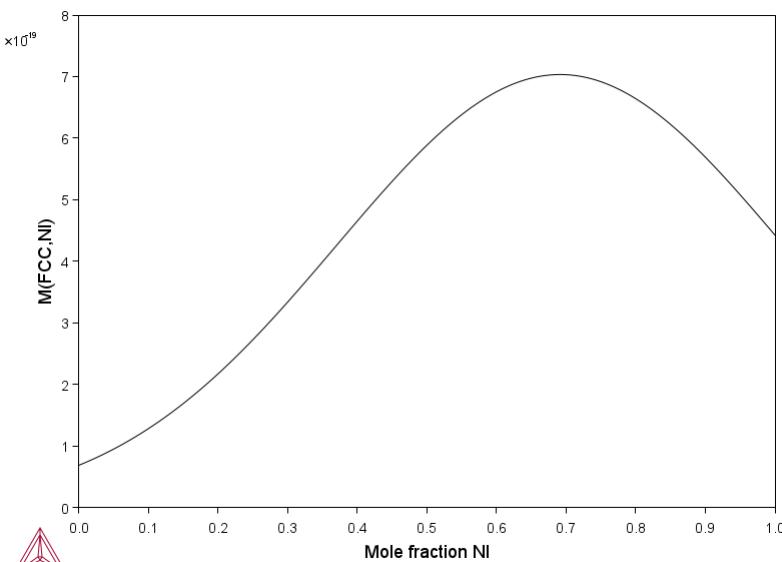
```

Global test at 6.88000E-01 .... OK
Global test at 6.98000E-01 .... OK
Global test at 7.08000E-01 .... OK
Global test at 7.18000E-01 .... OK
Global test at 7.28000E-01 .... OK
Global test at 7.38000E-01 .... OK
Global test at 7.48000E-01 .... OK
Global test at 7.58000E-01 .... OK
Global test at 7.68000E-01 .... OK
Global test at 7.78000E-01 .... OK
Global test at 7.88000E-01 .... OK
Global test at 7.98000E-01 .... OK
Global test at 8.08000E-01 .... OK
Global test at 8.18000E-01 .... OK
Global test at 8.28000E-01 .... OK
Global test at 8.38000E-01 .... OK
Global test at 8.48000E-01 .... OK
Global test at 8.58000E-01 .... OK
Global test at 8.68000E-01 .... OK
Global test at 8.78000E-01 .... OK
Global test at 8.88000E-01 .... OK
Global test at 8.98000E-01 .... OK
Global test at 9.08000E-01 .... OK
Global test at 9.18000E-01 .... OK
Global test at 9.28000E-01 .... OK
Global test at 9.38000E-01 .... OK
Global test at 9.48000E-01 .... OK
Global test at 9.58000E-01 .... OK
Global test at 9.68000E-01 .... OK
Global test at 9.78000E-01 .... OK
Global test at 9.88000E-01 .... OK
Global test at 9.98000E-01 .... OK
Terminating at 1.00000
Calculated 703 equilibria

Phase Region from 0.300000 for:
FCC_A1
Global test at 2.92000E-01 .... OK
Global test at 2.82000E-01 .... OK
Global test at 2.72000E-01 .... OK
Global test at 2.62000E-01 .... OK
Global test at 2.52000E-01 .... OK
Global test at 2.42000E-01 .... OK
Global test at 2.32000E-01 .... OK
Global test at 2.22000E-01 .... OK
Global test at 2.12000E-01 .... OK
Global test at 2.02000E-01 .... OK
Global test at 1.92000E-01 .... OK
Global test at 1.82000E-01 .... OK
Global test at 1.72000E-01 .... OK
Global test at 1.62000E-01 .... OK
Global test at 1.52000E-01 .... OK
Global test at 1.42000E-01 .... OK
Global test at 1.32000E-01 .... OK
Global test at 1.22000E-01 .... OK
Global test at 1.12000E-01 .... OK
Global test at 1.02000E-01 .... OK
Global test at 9.20000E-02 .... OK
Global test at 8.20000E-02 .... OK
Global test at 7.20000E-02 .... OK
Global test at 6.20000E-02 .... OK
Global test at 5.20000E-02 .... OK
Global test at 4.20000E-02 .... OK
Global test at 3.20000E-02 .... OK
Global test at 2.20000E-02 .... OK
Global test at 1.20000E-02 .... OK
Global test at 2.00000E-03 .... OK
Terminating at 0.100000E-11
Calculated 303 equilibria
*** Buffer saved on file: C:\Users\azureuser\AppData\Local\Temp\RESULT_002.POLY3

POLY:
POLY: @@
POLY: @@ ENTER THE POST PROCESSOR AND PLOT THE RESULT
POLY: @@
POLY: post
    POLY-3 POSTPROCESSOR VERSION 3.2
POST:
POST:
POST:
POST: @@
POST: @@ PLOT THE MOBILITY OF Ni VS. X(Ni)
POST: @@
POST: s-d-a y m(fcc,ni)
POST: s-d-a x m-f ni
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_dictra_console_examples/unite/distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot

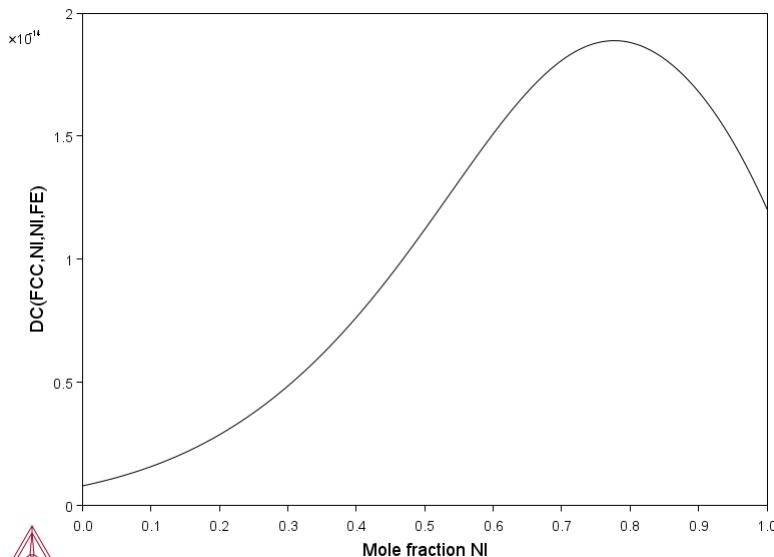
```



```

POST:
POST:
POST:
POST:@?<Hit_return_to_continue>
POST:
POST: @@
POST: @@ THEN PLOT THE DIFFUSIVITY OF Ni VS. X(Ni)
POST: @@
POST: s-d-a y dc(fcc,ni,ni,fe)
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_dictra_console_examples/unite/distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot

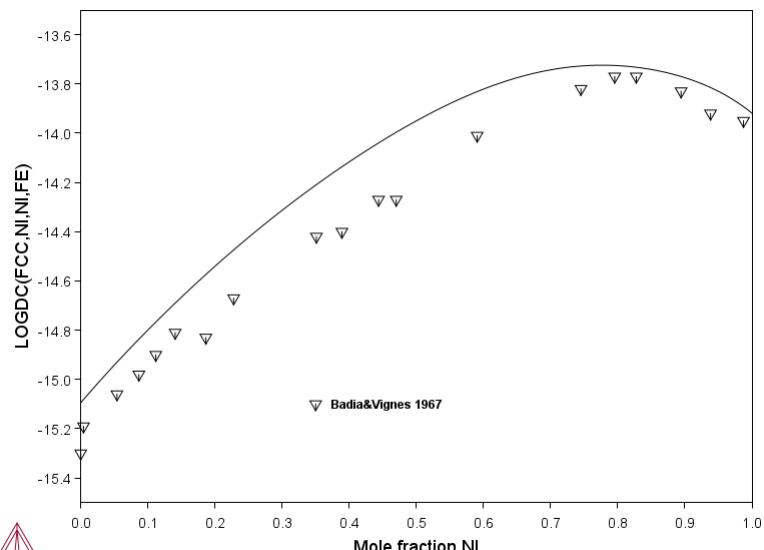
```



```

POST:
POST:
POST:@?<Hit_return_to_continue>
POST:
POST: @@
POST: @@ PLOT THE LOGARITHM OF DC AND APPEND THE EXPERIMENTAL DATA
POST: @@
POST: s-d-a y logdc(fcc,ni,ni,fe)
POST:
POST: app y feni.exp
PROLOGUE NUMBER: /0/: 1
DATASET NUMBER(s): /-1/: 1
POST:
POST: s-s-s y n -15.5 -13.5
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_dictra_console_examples/unite/distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot

```



```

POST:
POST:
POST:<?<Hit_return_to_continue>
POST:
POST: set-inter
POST:

```

**exg2-setup****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_dictra_console_examples\examples\exg2\setup.DCM.test"
SYS: i>_@_
NO SUCH COMMAND, USE HELP
SYS: @@ Kinetic data example.
SYS: @@ Optimization of mobilities in Ni-Al fcc alloys
SYS: @@ A file for reading thermodynamic data and setting up the kinetic
SYS: @@ parameters that are needed for an optimization of the FCC phase
SYS: @@ in the binary Ni-Al system.
SYS: @@ See also A. Engström and J. Ågren: ("Assessment of Diffusional
SYS: @@ Mobilities in Face-Centered Cubic Ni-Cr-Al Alloys" in
SYS: @@ Z. Metallkunde, Feb. 1996).
SYS: -----
NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exg2_setup.DCM
SYS:
SYS:
SYS: @@
SYS: @@ EXPLICITLY SELECTING GES VERSION 5 BECAUSE PARAMETER OPTIMIZATION
SYS: @@ IS NOT SUPPORTED IN GES VERSION 6
SYS: @@
SYS: set ges-version 5
SYS:
SYS: @@
SYS: @@ RETRIEVE THERMODYNAMIC DATA FROM A USER-DEFINED DATABASE
SYS: @@
SYS: go data
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\generate_dictra_console_examples\databases\data
Current database: Steels/Fe-Alloys v12.0

VA           /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE12: sw us tdata.TDB
Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

VA DEFINED
TDB_USER: def-sys al ni
AL           NI   DEFINED
TDB_USER: rej ph *
LIQUID          B2_BCC          BCC_A2
FCC_A1          GAMMA_PRIME    REJECTED
TDB_USER: rest ph fcc_a1
FCC_A1 RESTORED
TDB_USER: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS .....
-OK-
TDB_USER:
TDB_USER: @@
TDB_USER: @@ APPEND THE KINETIC DATA FROM THE MOBILITY DATABASE IN ORDER TO
TDB_USER: @@ HAVE SOME DUMMY PARAMETERS.
TDB_USER: @@
TDB_USER: app mob2
Current database: Alloys Mobility v2.7

VA DEFINED
GAS:G REJECTED
APP: def-sys al ni
AL           NI   DEFINED
APP: rej ph *
BCC_A2          FCC_A1          M4N
HCP_A3          LIQUID:L    REJECTED
APP: res ph fcc_a1
FCC_A1 RESTORED
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS .....

List of references for assessed data

'This parameter has not been assessed'
'A. Engstrom and J. Agren: Z. Metallkunde 87(1996) 92-97;
  Al, Cr and Ni diffusion in fcc Al-Cr-Ni'
'B. Jonsson: Scand. J. Metall. 24(1995) 21-27;
  Ni self-diffusion'
-OK-
APP:
APP: @@
APP: @@ GO TO THE DICTRA MODULE AND DEFINE THE KINETIC PARAMETERS. THE
APP: @@ VARIABLES V1,V2,V3 AND V4 ARE TO BE OPTIMIZED. NOTE THAT IF
APP: @@ YOU ARE OPTIMIZING PARAMETERS FOR A PHASE WITH MAGNETIC
APP: @@ CONTRIBUTION. I.E. USING BOTH MF- AND MQ-PARAMETERS, YOU
APP: @@ MIGHT HAVE TO ENTER THE PARROT MODULE AND GO BACK BEFORE
APP: @@ ENTERING PARAMETERS CONTAINING VARIABLES.
APP: @@
APP: go dic_par
PARROT VERSION 5.3d RUNNING ON PC/WINDOWS NT
```

Developed at the Division of Physical Metallurgy  
Royal Institute of Technology Stockholm, Sweden

**PARROT:**  
**PARROT:**  
**PARROT:** go d-m  
NO TIME STEP DEFINED  
**DIC>**  
**DIC>** @@ MOBILITY OF Al IN Al  
**DIC>** ENTER-MOB-DATA  
**PARAMETER:** MQ(FCC\_A1&AL,AL:VA) 298.15 -142000+R\*T\*LN(1.71E-4); 6000 N  
MQ(FCC\_A1&AL#1,AL:VA;0)  
**DIC>**  
**DIC>** @@ MOBILITY OF Al IN Ni  
**DIC>** ENTER-MOB-DATA  
**PARAMETER:** MQ(FCC\_A1&AL,NI:VA) 298.15 -284000+R\*T\*LN(7.5E-4); 6000 N  
MQ(FCC\_A1&AL#1,NI:VA;0)  
**DIC>**  
**DIC>** @@ MOBILITY OF Al INTERACTION BETWEEN Al AND Ni  
**DIC>** ENTER-MOB-DATA  
**PARAMETER:** MQ(FCC\_A1&AL,AL,NI:VA;0) 298.15 V1+V2\*T; 6000 N  
MQ(FCC\_A1&AL#1,AL,NI:VA;0)  
**DIC>**  
**DIC>** @@ MOBILITY OF Ni IN Al  
**DIC>** ENTER-MOB-DATA  
**PARAMETER:** MQ(FCC\_A1&NI,AL:VA) 298.15 -145900+R\*T\*LN(4.4E-4); 6000 N  
MQ(FCC\_A1&NI#1,AL:VA;0)  
**DIC>**  
**DIC>** @@ MOBILITY OF Ni INTERACTION BETWEEN Ni AND Al  
**DIC>** ENTER-MOB-DATA  
**PARAMETER:** MQ(FCC\_A1&NI,NI,AL:VA;0) 298.15 V3+V4\*T; 6000 N  
MQ(FCC\_A1&NI#1,NI,AL:VA;0)  
**DIC>**  
**DIC>** @@  
**DIC>** @@ GO TO PARROT AND SAVE THE SET UP TO FILE  
**DIC>** @@  
**DIC>** go dic\_parrot  
PARROT VERSION 5.3d RUNNING ON PC/WINDOWS NT  
**PARROT:** create-new-store-file opt  
**PARROT:**  
**PARROT:** set-inter  
--OK--  
**PARROT:**

**exg2-run**

```
PARROT:About
NO SUCH COMMAND, USE HELP
PARROT:PARROT:MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exg2\run.DCM.test"
PARROT: @@ exg2_run.DCM
PARROT:
PARROT: -----
PARROT: @@ FILE FOR DOING THE OPTIMIZATION IN PARROT
PARROT: -----
PARROT:
PARROT: @@
PARROT: @@ GO TO PARROT AND READ THE SETUP
PARROT: @@
PARROT: go dic_parrot
PARROT: VERSION 5.3d RUNNING ON PC/WINDOWS NT
PARROT: set-store-file opt
PARROT:
PARROT:
PARROT: @@
PARROT: @@ COMPILE THE EXPERIMENTAL DATA IN exp.DOP INTO STRUCTURED BINARY DATA.
PARROT: @@
PARROT: compile-experiments exp
OUTPUT TO SCREEN OR FILE /SCREEN/:
INITIATE STORE FILE: /Y/:

-----+
$ DOP-FILE CONTAINING EXPERIMENTAL INFORMATION USED DURING THE
$ OPTIMIZATION IN PARROT (COMPARE WITH POP-FILE USED WHEN EVALUATING
$ THERMODYNAMIC DATA). THE EXPERIMENTAL DATA HERE STEAM FROM A STUDY BY
$ YAMAMOTO ET AL. TRANS. JPN. INST. MET. VOL. 21, NO. 9 (1980), P. 601.
$ CONSULT THE THERMO-CALC USER'S GUIDE TO LEARN MORE ABOUT SYNTAXES
$ FOR OPTIMIZATION OF THERMODYNAMIC DATA.
$-----+


ENTER CONST P0=101325

TABLE_HEAD 10
CREATE_NEW 0010,1
C-S PH FCC=ENT 1
S-C T=1573,N=1,P=P0
S-C X(AL)=.01055
EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.6:.1
CREATE_NEW 0011,1
C-S PH FCC=ENT 1
S-C T=1573,N=1,P=P0
S-C X(AL)=.02032
EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.56:.1
CREATE_NEW 0012,1
C-S PH FCC=ENT 1
S-C T=1573,N=1,P=P0
S-C X(AL)=.02957
EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.65:.1
CREATE_NEW 0013,1
C-S PH FCC=ENT 1
S-C T=1573,N=1,P=P0
S-C X(AL)=.03884
EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.52:.1
CREATE_NEW 0014,1
C-S PH FCC=ENT 1
S-C T=1573,N=1,P=P0
S-C X(AL)=.03884
EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.52:.1
CREATE_NEW 0015,1
C-S PH FCC=ENT 1
S-C T=1573,N=1,P=P0
S-C X(AL)=.04927
EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.48:.1
CREATE_NEW 0016,1
C-S PH FCC=ENT 1
S-C T=1573,N=1,P=P0
S-C X(AL)=.06062
EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.43:.1
CREATE_NEW 0017,1
C-S PH FCC=ENT 1
S-C T=1573,N=1,P=P0
S-C X(AL)=.07029
EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.41:.1
CREATE_NEW 0018,1
C-S PH FCC=ENT 1
S-C T=1573,N=1,P=P0
S-C X(AL)=.08113
EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.37:.1
CREATE_NEW 0019,1
C-S PH FCC=ENT 1
S-C T=1573,N=1,P=P0
S-C X(AL)=.09166
EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.32:.1
CREATE_NEW 0020,1
C-S PH FCC=ENT 1
S-C T=1573,N=1,P=P0
S-C X(AL)=.09945
EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.28:.1
CREATE_NEW 0021,1
C-S PH FCC=ENT 1
S-C T=1573,N=1,P=P0
S-C X(AL)=.1099
EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.24:.1
CREATE_NEW 0022,1
C-S PH FCC=ENT 1
S-C T=1573,N=1,P=P0
S-C X(AL)=.1207
EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.2:.1
CREATE_NEW 0023,1
C-S PH FCC=ENT 1
S-C T=1573,N=1,P=P0
S-C X(AL)=.129
EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.18:.1
CREATE_NEW 0024,1
C-S PH FCC=ENT 1
S-C T=1573,N=1,P=P0
S-C X(AL)=.1392
EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.16:.1
```

```

CREATE_NEW 0025,1
C-S PH FCC=ENT 1
S-C T=1573,N=1,P=P0
S-C X(AL)=.1503
EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.1:.
CREATE_NEW 0026,1
C-S PH FCC=ENT 1
S-C T=1573,N=1,P=P0
S-C X(AL)=.1589
EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.08:.
CREATE_NEW 0027,1
C-S PH FCC=ENT 1
S-C T=1573,N=1,P=P0

```

output ignored...

... output resumed

V3	-1.32972463E+05	-1.32959167E+05	-1.32959167E+05	3.97449919E+00	3.97449919E+00
	3.97449919E+00	3.97449919E+00	3.97449919E+00	3.97449919E+00	3.97449919E+00
	3.97449919E+00	3.97449919E+00	3.97449919E+00	3.97449919E+00	3.97449919E+00
	3.97449919E+00	3.97449919E+00	3.97449919E+00	3.97449919E+00	3.97449919E+00
V4	7.81857805E+01	7.81857805E+01	7.81857805E+01	4.46532140E+00	4.46532140E+00
	4.46532140E+00	4.46532140E+00	4.46532140E+00	4.46532140E+00	4.46532140E+00
	4.46532140E+00	4.46532140E+00	4.46532140E+00	4.46532140E+00	4.46532140E+00
	4.46532140E+00	4.46532140E+00	4.46532140E+00	4.46532140E+00	4.46532140E+00

NUMBER OF OPTIMIZING VARIABLES : 4  
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO  
THE SUM OF SQUARES HAS CHANGED FROM 2.02977003E+01 TO 2.02976923E+01  
DEGREES OF FREEDOM 113. REDUCED SUM OF SQUARES 1.79625595E-01

Sorry, LIST-DATA disabled for this database

===== BLOCK NUMBER 1

DEFINED CONSTANTS					
P0=101325					
10 LOGDC(F...,AL,NI)=-12.6	-12.56	0.10	4.3827E-02	0.4383	
11 LOGDC(F...,AL,NI)=-12.56	-12.55	0.10	1.2341E-02	0.1234	
12 LOGDC(F...,AL,NI)=-12.65	-12.53	0.10	0.1167	1.167	
13 LOGDC(F...,AL,NI)=-12.52	-12.51	0.10	5.8843E-03	5.8843E-02	
14 LOGDC(F...,AL,NI)=-12.52	-12.51	0.10	5.8843E-03	5.8843E-02	
15 LOGDC(F...,AL,NI)=-12.48	-12.49	0.10	-8.4123E-03	-8.4123E-02	
16 LOGDC(F...,AL,NI)=-12.43	-12.46	0.10	-2.6851E-02	-0.2685	
17 LOGDC(F...,AL,NI)=-12.41	-12.43	0.10	-1.7821E-02	-0.1782	
18 LOGDC(F...,AL,NI)=-12.37	-12.39	0.10	-2.3493E-02	-0.2349	
19 LOGDC(F...,AL,NI)=-12.32	-12.36	0.10	-3.8626E-02	-0.3863	
20 LOGDC(F...,AL,NI)=-12.28	-12.33	0.10	-5.1933E-02	-0.5193	
21 LOGDC(F...,AL,NI)=-12.24	-12.29	0.10	-5.4919E-02	-0.5492	
22 LOGDC(F...,AL,NI)=-12.2	-12.26	0.10	-5.5128E-02	-0.5513	
23 LOGDC(F...,AL,NI)=-12.18	-12.22	0.10	-4.3400E-02	-0.4340	
24 LOGDC(F...,AL,NI)=-12.16	-12.18	0.10	-2.2927E-02	-0.2293	
25 LOGDC(F...,AL,NI)=-12.1	-12.14	0.10	-3.6888E-02	-0.3689	
26 LOGDC(F...,AL,NI)=-12.08	-12.10	0.10	-1.9703E-02	-0.1970	
27 LOGDC(F...,AL,NI)=-12.02	-12.04	0.10	-2.2272E-02	-0.2227	
28 LOGDC(F...,AL,NI)=-11.98	-11.99	0.10	-9.0917E-03	-9.0917E-02	
29 LOGDC(F...,AL,NI)=-11.94	-11.95	0.10	-9.1618E-03	-9.1618E-02	
30 LOGDC(F...,AL,NI)=-13	-12.86	0.10	0.1360	1.360	
31 LOGDC(F...,AL,NI)=-12.96	-12.85	0.10	0.1059	1.059	
32 LOGDC(F...,AL,NI)=-12.92	-12.84	0.10	8.4799E-02	0.8480	
33 LOGDC(F...,AL,NI)=-12.9	-12.82	0.10	8.2549E-02	0.8255	
34 LOGDC(F...,AL,NI)=-12.77	-12.79	0.10	-1.5173E-02	-0.1517	
35 LOGDC(F...,AL,NI)=-12.74	-12.75	0.10	-1.1192E-02	-0.1119	
36 LOGDC(F...,AL,NI)=-12.82	-12.72	0.10	9.5223E-02	0.9522	
37 LOGDC(F...,AL,NI)=-12.82	-12.72	0.10	9.5223E-02	0.9522	
38 LOGDC(F...,AL,NI)=-12.69	-12.68	0.10	5.7856E-03	5.7856E-02	
39 LOGDC(F...,AL,NI)=-12.65	-12.65	0.10	2.6229E-03	2.6229E-02	
40 LOGDC(F...,AL,NI)=-12.64	-12.62	0.10	1.9222E-02	0.1922	
41 LOGDC(F...,AL,NI)=-12.61	-12.58	0.10	2.8492E-02	0.2849	
42 LOGDC(F...,AL,NI)=-12.55	-12.54	0.10	9.2091E-03	9.2091E-02	
43 LOGDC(F...,AL,NI)=-12.53	-12.51	0.10	2.1034E-02	0.2103	
44 LOGDC(F...,AL,NI)=-12.47	-12.47	0.10	2.0402E-03	2.0402E-02	
45 LOGDC(F...,AL,NI)=-12.41	-12.42	0.10	-1.0621E-02	-0.1062	
46 LOGDC(F...,AL,NI)=-12.38	-12.38	0.10	-1.6323E-04	-1.6323E-03	
47 LOGDC(F...,AL,NI)=-12.36	-12.32	0.10	3.6256E-02	0.3626	
48 LOGDC(F...,AL,NI)=-12.36	-12.32	0.10	3.6256E-02	0.3626	
49 LOGDC(F...,AL,NI)=-12.3	-12.27	0.10	3.0494E-02	0.3049	
50 LOGDC(F...,AL,NI)=-13.23	-13.19	0.10	3.8416E-02	0.3842	
51 LOGDC(F...,AL,NI)=-13.23	-13.19	0.10	3.8416E-02	0.3842	
52 LOGDC(F...,AL,NI)=-13.19	-13.18	0.10	1.3209E-02	0.1321	
53 LOGDC(F...,AL,NI)=-13.15	-13.16	0.10	-5.5530E-03	-5.5530E-02	
54 LOGDC(F...,AL,NI)=-13.12	-13.13	0.10	-1.4736E-02	-0.1474	
55 LOGDC(F...,AL,NI)=-13.09	-13.10	0.10	-1.2913E-02	-0.1291	
56 LOGDC(F...,AL,NI)=-13.06	-13.07	0.10	-6.9397E-03	-6.9397E-02	
57 LOGDC(F...,AL,NI)=-13.02	-13.04	0.10	-1.5971E-02	-0.1597	
58 LOGDC(F...,AL,NI)=-12.99	-13.00	0.10	-1.0672E-02	-0.1067	
59 LOGDC(F...,AL,NI)=-12.96	-12.96	0.10	8.0069E-04	8.0069E-03	
60 LOGDC(F...,AL,NI)=-12.91	-12.93	0.10	-2.0470E-02	-0.2047	
61 LOGDC(F...,AL,NI)=-12.88	-12.89	0.10	-7.3947E-03	-7.3947E-02	
62 LOGDC(F...,AL,NI)=-12.86	-12.85	0.10	1.4312E-02	0.1431	
63 LOGDC(F...,AL,NI)=-12.86	-12.85	0.10	1.4312E-02	0.1431	
64 LOGDC(F...,AL,NI)=-12.83	-12.81	0.10	1.7076E-02	0.1708	
65 LOGDC(F...,AL,NI)=-12.8	-12.77	0.10	2.9558E-02	0.2956	
66 LOGDC(F...,AL,NI)=-12.75	-12.72	0.10	2.5293E-02	0.2529	
67 LOGDC(F...,AL,NI)=-12.71	-12.68	0.10	2.6861E-02	0.2686	
68 LOGDC(F...,AL,NI)=-12.67	-12.63	0.10	4.4033E-02	0.4403	
70 LOGDC(F...,AL,NI)=-13.5	-13.54	0.10	-4.2456E-02	-0.4246	
71 LOGDC(F...,AL,NI)=-13.47	-13.53	0.10	-5.5160E-02	-0.5516	
72 LOGDC(F...,AL,NI)=-13.45	-13.50	0.10	-5.0384E-02	-0.5038	
73 LOGDC(F...,AL,NI)=-13.42	-13.48	0.10	-5.6139E-02	-0.5614	
74 LOGDC(F...,AL,NI)=-13.39	-13.44	0.10	-5.3034E-02	-0.5303	
75 LOGDC(F...,AL,NI)=-13.36	-13.40	0.10	-4.3865E-02	-0.4386	
76 LOGDC(F...,AL,NI)=-13.34	-13.37	0.10	-3.0943E-02	-0.3094	
77 LOGDC(F...,AL,NI)=-13.31	-13.33	0.10	-2.0539E-02	-0.2054	
78 LOGDC(F...,AL,NI)=-13.24	-13.29	0.10	-5.0311E-02	-0.5031	
79 LOGDC(F...,AL,NI)=-13.22	-13.26	0.10	-4.1318E-02	-0.4132	
80 LOGDC(F...,AL,NI)=-13.19	-13.22	0.10	-2.6230E-02	-0.2623	
81 LOGDC(F...,AL,NI)=-13.13	-13.17	0.10	-4.3098E-02	-0.4310	
82 LOGDC(F...,AL,NI)=-13.12	-13.14	0.10	-1.9773E-02	-0.1977	

83	LOGDC(F...,AL,NI)=-13.08	-13.09	0.10	-1.4457E-02	-0.1446
84	LOGDC(F...,AL,NI)=-13.04	-13.05	0.10	-9.4618E-03	-9.4618E-02
85	LOGDC(F...,AL,NI)=-13.03	-13.01	0.10	2.2404E-02	0.2240
90	LOGDC(F...,AL,NI)=-13.97	-13.92	0.10	5.1241E-02	0.5124
91	LOGDC(F...,AL,NI)=-13.92	-13.90	0.10	2.0497E-02	0.2050
92	LOGDC(F...,AL,NI)=-13.88	-13.87	0.10	9.3920E-03	9.3920E-02
93	LOGDC(F...,AL,NI)=-13.85	-13.84	0.10	5.2264E-03	5.2264E-02
94	LOGDC(F...,AL,NI)=-13.82	-13.81	0.10	1.1044E-02	0.1104
95	LOGDC(F...,AL,NI)=-13.78	-13.77	0.10	1.3352E-02	0.1335
96	LOGDC(F...,AL,NI)=-13.9	-13.74	0.10	0.1640	1.640
97	LOGDC(F...,AL,NI)=-13.85	-13.69	0.10	0.1576	1.576
98	LOGDC(F...,AL,NI)=-13.65	-13.65	0.10	1.5604E-03	1.5604E-02
99	LOGDC(F...,AL,NI)=-13.62	-13.62	0.10	4.9052E-03	4.9052E-02
100	LOGDC(F...,AL,NI)=-13.57	-13.57	0.10	-9.5589E-04	-9.5589E-03
101	LOGDC(F...,AL,NI)=-13.52	-13.53	0.10	-5.4819E-03	-5.4819E-02
102	LOGDC(F...,AL,NI)=-13.47	-13.49	0.10	-2.0262E-02	-0.2026
103	LOGDC(F...,AL,NI)=-13.45	-13.45	0.10	4.9628E-03	4.9628E-02
104	LOGDC(F...,AL,NI)=-13.4	-13.40	0.10	2.8073E-03	2.8073E-02
110	LOGDC(F...,AL,NI)=-14.32	-14.32	0.10	-3.9760E-03	-3.9760E-02
111	LOGDC(F...,AL,NI)=-14.32	-14.30	0.10	1.9307E-02	0.1931
112	LOGDC(F...,AL,NI)=-14.28	-14.27	0.10	1.0664E-02	0.1066
113	LOGDC(F...,AL,NI)=-14.25	-14.24	0.10	8.9412E-03	8.9412E-02
114	LOGDC(F...,AL,NI)=-14.22	-14.20	0.10	1.8329E-02	0.1833
115	LOGDC(F...,AL,NI)=-14.17	-14.16	0.10	1.2994E-02	0.1299
116	LOGDC(F...,AL,NI)=-14.15	-14.12	0.10	3.0489E-02	0.3049
117	LOGDC(F...,AL,NI)=-14.1	-14.07	0.10	2.5593E-02	0.2559
118	LOGDC(F...,AL,NI)=-14.03	-14.03	0.10	-1.4483E-03	-1.4483E-02
119	LOGDC(F...,AL,NI)=-14	-14.00	0.10	2.7074E-03	2.7074E-02
120	LOGDC(F...,AL,NI)=-13.95	-13.95	0.10	-1.9282E-03	-1.9282E-02
121	LOGDC(F...,AL,NI)=-13.9	-13.91	0.10	-5.2349E-03	-5.2349E-02
122	LOGDC(F...,AL,NI)=-13.85	-13.87	0.10	-1.6645E-02	-0.1665
130	LOGDC(F...,AL,NI)=-14.73	-14.76	0.10	-3.0493E-02	-0.3049
131	LOGDC(F...,AL,NI)=-14.71	-14.73	0.10	-2.3757E-02	-0.2376
132	LOGDC(F...,AL,NI)=-14.68	-14.70	0.10	-1.9446E-02	-0.1945
133	LOGDC(F...,AL,NI)=-14.66	-14.67	0.10	-8.5997E-03	-8.5997E-02
134	LOGDC(F...,AL,NI)=-14.61	-14.63	0.10	-1.5314E-02	-0.1531
135	LOGDC(F...,AL,NI)=-14.61	-14.63	0.10	-1.5314E-02	-0.1531
136	LOGDC(F...,AL,NI)=-14.58	-14.58	0.10	3.4408E-03	3.4408E-02
137	LOGDC(F...,AL,NI)=-14.54	-14.54	0.10	3.3897E-03	3.3897E-02
138	LOGDC(F...,AL,NI)=-14.5	-14.49	0.10	9.2113E-03	9.2113E-02
139	LOGDC(F...,AL,NI)=-14.46	-14.44	0.10	1.5390E-02	0.1539
140	LOGDC(F...,AL,NI)=-14.41	-14.41	0.10	1.6005E-03	1.6005E-02
141	LOGDC(F...,AL,NI)=-14.35	-14.36	0.10	-1.1351E-02	-0.1135
142	LOGDC(F...,AL,NI)=-14.27	-14.31	0.10	-4.1487E-02	-0.4149
143	LOGDC(F...,AL,NI)=-14.2	-14.27	0.10	-7.4774E-02	-0.7477

PARROT:  
PARROT:  
PARROT: set-inter  
--OK--  
PARROT:

**exg2-plot**

```
PARROT:About
NO SUCH COMMAND, USE HELP
PARROT:PARROT:MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exg2\plot.DCM.test"
PARROT: @@ exg2_plot.DCM
PARROT:
PARROT: @@-----
PARROT: @@ FILE FOR PLOTTING THE RESULT AFTER THE OPTIMIZATION. HERE
PARROT: @@ DIFFUSIVITIES CALCULATED FROM THE OPTIMIZED VARIABLES ARE
PARROT: @@ COMPARED WITH EXPERIMENTALLY MEASURED ONES.
PARROT: @@-----
PARROT:
PARROT: @@-----  
PARROT: @@ GO TO PARROT AND READ THE FILE CONTAINING THE RESULT FROM
PARROT: @@ THE OPTIMIZATION.
PARROT: @@-----  
PARROT:  
PARROT: go dic_parrot
PARROT VERSION 5.3d RUNNING ON PC/WINDOWS NT
PARROT: set-store-file opt
PARROT:
PARROT: @@-----  
PARROT: @@ GO TO POLY3 AND STEP IN X(AL)
PARROT: @@-----  
PARROT: go p-3
POLY: s-c n=1,p=101325,t=1573
POLY: s-c x(al)=.1
POLY: c-e,,,
Using global minimization procedure
Calculated          209 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: add,
POLY:  
  
POLY: s-a-v 1 x(al) 0.0001 .20 0.001,,,
POLY: step
Option? /NORMAL/:
Step will start from axis value 0.100000
...OK  
  
Phase Region from 0.100000 for:
FCC_A1
Global test at 1.08000E-01 .... OK
Global test at 1.18000E-01 .... OK
Global test at 1.28000E-01 .... OK
Global test at 1.38000E-01 .... OK
Global test at 1.48000E-01 .... OK
Global test at 1.58000E-01 .... OK
Global test at 1.68000E-01 .... OK
Global test at 1.78000E-01 .... OK
Global test at 1.88000E-01 .... OK
Global test at 1.98000E-01 .... OK
Terminating at 0.200000
Calculated 103 equilibria  
  
Phase Region from 0.100000 for:
FCC_A1
Global test at 9.20000E-02 .... OK
Global test at 8.20000E-02 .... OK
Global test at 7.20000E-02 .... OK
Global test at 6.20000E-02 .... OK
Global test at 5.20000E-02 .... OK
Global test at 4.20000E-02 .... OK
Global test at 3.20000E-02 .... OK
Global test at 2.20000E-02 .... OK
Global test at 1.20000E-02 .... OK
Global test at 2.00000E-03 .... OK
Terminating at 0.100000E-03
Calculated 103 equilibria
*** Buffer saved on file: C:\Users\azureuser\AppData\Local\Temp\RESULT_002.POLY3
POLY: @@-----  
POLY: @@ REPEAT THE PROCEDURE FOR SOME OTHER TEMPERATURES
POLY: @@-----  
POLY: s-c t=1523,x(al)=.1
POLY: c-e,,,
Using global minimization procedure
Calculated          209 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 x(al) 0.0001 .20 0.001,,,
POLY: step
Option? /NORMAL/:
Step will start from axis value 0.100000
...OK  
  
Phase Region from 0.100000 for:
FCC_A1
Global test at 1.08000E-01 .... OK
Global test at 1.18000E-01 .... OK
Global test at 1.28000E-01 .... OK
Global test at 1.38000E-01 .... OK
Global test at 1.48000E-01 .... OK
Global test at 1.58000E-01 .... OK
Global test at 1.68000E-01 .... OK
Global test at 1.78000E-01 .... OK
Global test at 1.88000E-01 .... OK
Global test at 1.98000E-01 .... OK
Terminating at 0.200000
Calculated 103 equilibria  
  
Phase Region from 0.100000 for:
FCC_A1
Global test at 9.20000E-02 .... OK
Global test at 8.20000E-02 .... OK
Global test at 7.20000E-02 .... OK
Global test at 6.20000E-02 .... OK
Global test at 5.20000E-02 .... OK
Global test at 4.20000E-02 .... OK
Global test at 3.20000E-02 .... OK
Global test at 2.20000E-02 .... OK
Global test at 1.20000E-02 .... OK
Global test at 2.00000E-03 .... OK
```

```

Terminating at 0.100000E-03
Calculated 103 equilibria
*** Buffer saved on file: C:\Users\azureuser\AppData\Local\Temp\RESULT_002.POLY3
POLY: s-c t=1473,x(al)=1
POLY: c-e,,,,,
Using global minimization procedure
Calculated 209 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 x(al) 0.0001 .20 0.001,,,
POLY: step
Option? /NORMAL/:
Step will start from axis value 0.100000
...OK

Phase Region from 0.100000 for:
FCC_A1
Global test at 1.08000E-01 .... OK
Global test at 1.18000E-01 .... OK
Global test at 1.28000E-01 .... OK
Global test at 1.38000E-01 .... OK
Global test at 1.48000E-01 .... OK
Global test at 1.58000E-01 .... OK
Global test at 1.68000E-01 .... OK
Global test at 1.78000E-01 .... OK
Global test at 1.88000E-01 .... OK
Global test at 1.98000E-01 .... OK
Terminating at 0.200000
Calculated 103 equilibria

Phase Region from 0.100000 for:
FCC_A1
Global test at 9.20000E-02 .... OK
Global test at 8.20000E-02 .... OK
Global test at 7.20000E-02 .... OK
Global test at 6.20000E-02 .... OK
Global test at 5.20000E-02 .... OK
Global test at 4.20000E-02 .... OK
Global test at 3.20000E-02 .... OK
Global test at 2.20000E-02 .... OK
Global test at 1.20000E-02 .... OK
Global test at 2.00000E-03 .... OK
Terminating at 0.100000E-03
Calculated 103 equilibria
*** Buffer saved on file: C:\Users\azureuser\AppData\Local\Temp\RESULT_002.POLY3
POLY: s-c t=1423,x(al)=1
POLY: c-e,,,,,
Using global minimization procedure
Calculated 209 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 x(al) 0.0001 .20 0.001,,,
POLY: step
Option? /NORMAL/:
Step will start from axis value 0.100000
...OK

Phase Region from 0.100000 for:
FCC_A1
Global test at 1.08000E-01 .... OK
Global test at 1.18000E-01 .... OK
Global test at 1.28000E-01 .... OK
Global test at 1.38000E-01 .... OK
Global test at 1.48000E-01 .... OK
Global test at 1.58000E-01 .... OK
Global test at 1.68000E-01 .... OK
Global test at 1.78000E-01 .... OK
Global test at 1.88000E-01 .... OK
Global test at 1.98000E-01 .... OK
Terminating at 0.200000
Calculated 103 equilibria

Phase Region from 0.100000 for:
FCC_A1
Global test at 9.20000E-02 .... OK
Global test at 8.20000E-02 .... OK
Global test at 7.20000E-02 .... OK
Global test at 6.20000E-02 .... OK
Global test at 5.20000E-02 .... OK
Global test at 4.20000E-02 .... OK
Global test at 3.20000E-02 .... OK
Global test at 2.20000E-02 .... OK
Global test at 1.20000E-02 .... OK
Global test at 2.00000E-03 .... OK
Terminating at 0.100000E-03
Calculated 103 equilibria
*** Buffer saved on file: C:\Users\azureuser\AppData\Local\Temp\RESULT_002.POLY3
POLY: s-c t=1373,x(al)=1
POLY: c-e,,,,,
Using global minimization procedure
Calculated 209 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 x(al) 0.0001 .20 0.001,,,
POLY: step
Option? /NORMAL/:
Step will start from axis value 0.100000
...OK

Phase Region from 0.100000 for:
FCC_A1
Global test at 1.08000E-01 .... OK
Global test at 1.18000E-01 .... OK
Global test at 1.28000E-01 .... OK
Global test at 1.38000E-01 .... OK
Global test at 1.48000E-01 .... OK
Global test at 1.58000E-01 .... OK
Global test at 1.68000E-01 .... OK
Global test at 1.78000E-01 .... OK
Global test at 1.88000E-01 .... OK
Global test at 1.98000E-01 .... OK
Terminating at 0.200000
Calculated 103 equilibria

Phase Region from 0.100000 for:

```

```

FCC_A1
Global test at 9.20000E-02 .... OK
Global test at 8.20000E-02 .... OK
Global test at 7.20000E-02 .... OK
Global test at 6.20000E-02 .... OK
Global test at 5.20000E-02 .... OK
Global test at 4.20000E-02 .... OK
Global test at 3.20000E-02 .... OK
Global test at 2.20000E-02 .... OK
Global test at 1.20000E-02 .... OK
Global test at 2.00000E-03 .... OK
Terminating at 0.10000E-03
Calculated 103 equilibria
*** Buffer saved on file: C:\Users\azureuser\AppData\Local\Temp\RESULT_002.POLY3
POLY: s-c t=1323,x(al)=.1
POLY: c-e,,,
Using global minimization procedure
Calculated 209 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 x(al) 0.0001 .20 0.001,,
POLY: step
Option? /NORMAL/:
Step will start from axis value 0.100000
...OK

Phase Region from 0.100000 for:
FCC_A1
Global test at 1.08000E-01 .... OK
Global test at 1.18000E-01 .... OK
Global test at 1.28000E-01 .... OK
Global test at 1.38000E-01 .... OK
Global test at 1.48000E-01 .... OK
Global test at 1.58000E-01 .... OK
Global test at 1.68000E-01 .... OK
Global test at 1.78000E-01 .... OK
Global test at 1.88000E-01 .... OK
Global test at 1.98000E-01 .... OK
Terminating at 0.200000
Calculated 103 equilibria

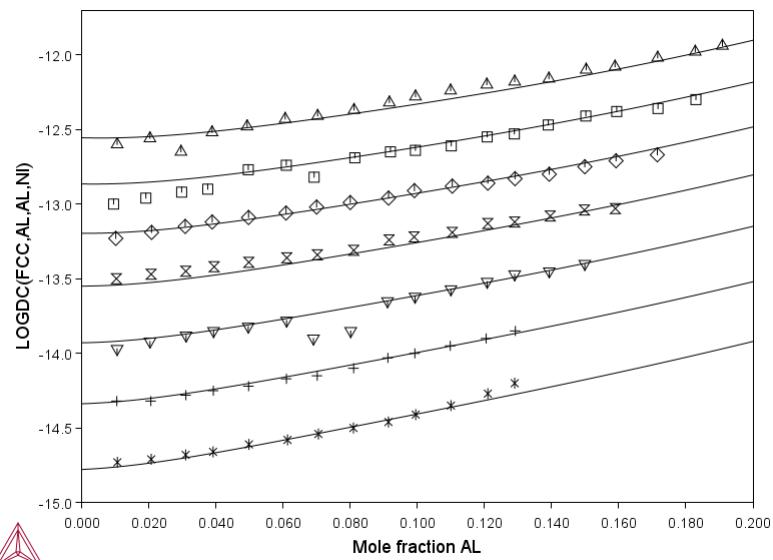
Phase Region from 0.100000 for:
FCC_A1
Global test at 9.20000E-02 .... OK
Global test at 8.20000E-02 .... OK
Global test at 7.20000E-02 .... OK
Global test at 6.20000E-02 .... OK
Global test at 5.20000E-02 .... OK
Global test at 4.20000E-02 .... OK
Global test at 3.20000E-02 .... OK
Global test at 2.20000E-02 .... OK
Global test at 1.20000E-02 .... OK
Global test at 2.00000E-03 .... OK
Terminating at 0.10000E-03
Calculated 103 equilibria
*** Buffer saved on file: C:\Users\azureuser\AppData\Local\Temp\RESULT_002.POLY3
POLY: s-c t=1273,x(al)=.1
POLY: c-e,,,
Using global minimization procedure
Calculated 209 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 x(al) 0.0001 .20 0.001,,
POLY: step
Option? /NORMAL/:
Step will start from axis value 0.100000
...OK

Phase Region from 0.100000 for:
FCC_A1
Global test at 1.08000E-01 .... OK
Global test at 1.18000E-01 .... OK
Global test at 1.28000E-01 .... OK
Global test at 1.38000E-01 .... OK
Global test at 1.48000E-01 .... OK
Global test at 1.58000E-01 .... OK
Global test at 1.68000E-01 .... OK
Global test at 1.78000E-01 .... OK
Global test at 1.88000E-01 .... OK
Global test at 1.98000E-01 .... OK
Terminating at 0.200000
Calculated 103 equilibria

Phase Region from 0.100000 for:
FCC_A1
Global test at 9.20000E-02 .... OK
Global test at 8.20000E-02 .... OK
Global test at 7.20000E-02 .... OK
Global test at 6.20000E-02 .... OK
Global test at 5.20000E-02 .... OK
Global test at 4.20000E-02 .... OK
Global test at 3.20000E-02 .... OK
Global test at 2.20000E-02 .... OK
Global test at 1.20000E-02 .... OK
Global test at 2.00000E-03 .... OK
Terminating at 0.10000E-03
Calculated 103 equilibria
*** Buffer saved on file: C:\Users\azureuser\AppData\Local\Temp\RESULT_002.POLY3
POLY: @@
POLY: @@ ENTER THE POST MODULE, PLOT THE DIFFUSIVITY ON THE Y-AXIS
POLY: @@ AND MOLE-FRACTION Al ON THE X-AXIS.
POLY: @@
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2
POST:
POST: s-d-a x m-f al
POST: s-d-a y logdc(fcc,al,al,ni)
POST:
POST: app y yama.exp
PROLOGUE NUMBER: /0/: 1
DATASET NUMBER(s): /-1/: 1 2 3 4 5 6 7
POST:
POST:
POST: s-t-m-s y

```

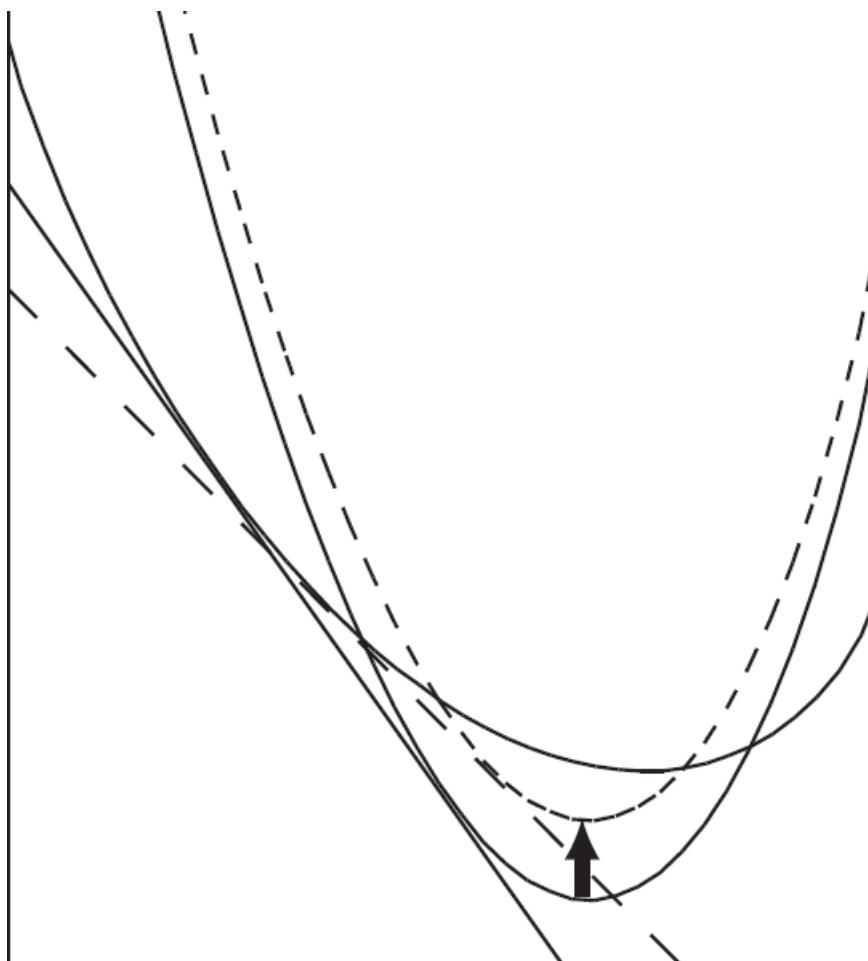
```
COMMAND NOT SUPPORTED IN THIS PLOT DRIVER
POST: s-s-s y n -15 -11.7
POST: s-t-m-s y
COMMAND NOT SUPPORTED IN THIS PLOT DRIVER
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\generate_dictra_console_examples/unite/distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
```



```
POST:
POST:@?<Hit_return_to_continue>
POST:
POST: set-inter
POST:
```



## Deviation From Local Equilibrium

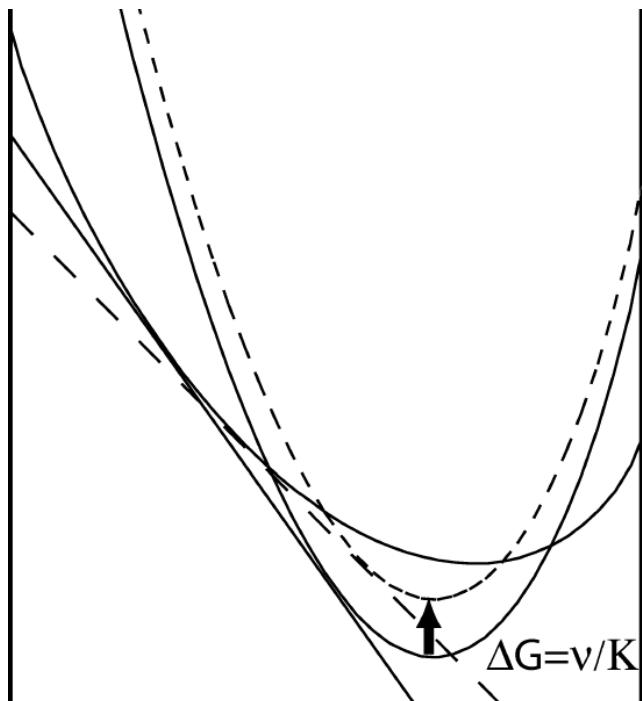




## Example exh1

### $\sigma/\gamma$ diffusion couple with limited interface mobility

This example calculates the growth of ferrite ( $\alpha$ ) into austenite ( $\gamma$ ) with a limited interface mobility. This is achieved by adding a Gibbs-energy contribution to the ferrite using the SET-SURFACE-ENERGY command.



**exh1-setup****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\_dictra\_console\_examples\examples\exh1\setup.DCM.test"**  
**SYS: @@**  
**SYS: @@ Deviation from local equilibrium.**  
**SYS: @@ Ferrite/austenite diffusion couple with interface mobility**  
**SYS: @@ This example calculates the growth of ferrite into austenite with**  
**SYS: @@ a limited interface mobility. this is done by adding a Gibbs-energy**  
**SYS: @@ contribution to the ferrite using the SET-SURFACE-ENERGY command.**  
**SYS: -----**  
NO SUCH COMMAND, USE HELP  
**SYS:**  
**SYS: @@**  
**SYS: @@ RETRIEVE DATA FROM THE DATABASE**  
**SYS: @@**  
**SYS: go da**  
THERMODYNAMIC DATABASE module  
Database folder:  
C:\jenkins\workspace\generate\_dictra\_console\_examples\databases\data  
Current database: Steels/Fe-Alloys v12.0  
  
VA                           /- DEFINED  
DICTRA\_FCC\_A1 REJECTED  
**TDB\_TCFE12:**  
**TDB\_TCFE12: @@**  
**TDB\_TCFE12: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE THE DATA**  
**TDB\_TCFE12: @@**  
**TDB\_TCFE12: sw FEDEMO**  
Current database: Iron Demo Database v4.0  
  
VA                           /- DEFINED  
**TDB\_FEDEMO: def-sys fe c**                           C DEFINED  
**TDB\_FEDEMO: rej ph \* all**  
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 bcc fcc**  
BCC\_A2                     FCC\_A1 RESTORED  
**TDB\_FEDEMO: get**  
18:56:20,809 [Thread-0] INFO JavaWrapper: \*\*\* Invoking Gibbs Energy System v6 \*\*\*  
REINITIATING GES ....  
ELEMENTS ....  
SPECIES ....  
PHASES ....  
PARAMETERS ....  
FUNCTIONS ....  
  
List of references for assessed data  
  
'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'  
'P. Gustafsson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'  
'X.G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'  
'A.T. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'  
'X.G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar  
volumes'  
-OK-  
**TDB\_FEDEMO:**  
**TDB\_FEDEMO: @@**  
**TDB\_FEDEMO: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE MOBILITY DATA**  
**TDB\_FEDEMO: @@**  
**TDB\_FEDEMO: app mfdemo**  
Current database: Fe-Alloys Mobility demo database v2.0  
  
VA    DEFINED  
**APP: def-sys fe c**                           C DEFINED  
FE                            C  
**APP: rej ph \* all**  
BCC\_A2                     FCC\_A1                   CEMENTITE  
REJECTED  
**APP: res ph bcc fcc**  
BCC\_A2                     FCC\_A1 RESTORED  
**APP: get**  
ELEMENTS ....  
SPECIES ....  
PHASES ....  
PARAMETERS ...  
FUNCTIONS ....  
  
List of references for assessed data  
  
'This parameter has not been assessed'  
'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'  
'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe  
-Ni'  
'B. Jonsson: Z. Metallkunde 85(1994)498-501; C and N diffusion in bcc Cr  
-Fe-Ni'  
'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion  
in bcc Fe'  
-OK-  
**APP: @@**  
**APP: @@ ENTER THE DICTRA MONITOR**  
**APP: @@**  
**APP: go d-m**  
NO TIME STEP DEFINED

```

DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 1000; * N
DIC>
DIC> @@
DIC> @@ START BY ENTERING THE REGIONS ferrite AND austenite WHERE
DIC> @@ THE BCC AND FCC PHASES ARE PUT, RESPECTIVELY. THE FERRITE REGION IS
DIC> @@ ASSUMED INITIALLY TO BE VERY THIN, 1E-9 METERS.
DIC> @@
DIC> enter-region
REGION NAME : ferrite
DIC>
DIC> enter-region
REGION NAME : austenite
ATTACH TO REGION NAMED /FERRITE/:
ATTACHED TO THE RIGHT OF FERRITE /YES/:
DIC>
DIC> @@
DIC> @@ ENTER GRIDS INTO THE REGIONS
DIC> @@
DIC> enter-grid
REGION NAME : /FERRITE/: ferrite
WIDTH OF REGION /1/: 1e-9
TYPE /LINEAR/: AUTO
DIC>
DIC> enter-grid austenite
WIDTH OF REGION /1/: 0.999e-6
TYPE /LINEAR/: AUTO
DIC>
DIC> @@
DIC> @@ ENTER THE active PHASES INTO THE REGIONS
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /FERRITE/: ferrite
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: bcc
DIC>
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /AUSTENITE/: austenite
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITION INTO BCC
DIC> @@
DIC> enter-composition
REGION NAME : /FERRITE/: ferrite
PHASE NAME: /BCC_A2/: bcc
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: C
TYPE /LINEAR/: linear
VALUE OF FIRST POINT : 0.019091893
VALUE OF LAST POINT : /1.9091893E-2/: 0.019091893
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITION INTO FCC
DIC> @@
DIC> enter-composition
REGION NAME : /AUSTENITE/: austenite
PHASE NAME: /FCC_A1/: fcc#1
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: C
TYPE /LINEAR/: linear
VALUE OF FIRST POINT : 0.0191
VALUE OF LAST POINT : /1.91E-2/: 0.0191
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exhl.y
DIC>
DIC> set-inter
--OK--
DIC>

```

**exh1-run**

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exh1\run.DCM.test"
DIC>
DIC>
DIC> @@
DIC> @@ READ THE SETUP FROM FILE AND START THE SIMULATION
DIC> @@
DIC>
DIC> go d-m
TIME STEP AT TIME 0.00000E+00
DIC>
DIC> read exh1
OK
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-sim-time
END TIME FOR INTEGRATION /1/: 2.5E-3
AUTOMATIC TIMESTEP CONTROL /YES/: YES
MAX TIMESTEP DURING INTEGRATION /2.5E-04/:
INITIAL TIMESTEP : /1E-07/: 1E-7
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/: 1E-7
DIC>
DIC>
DIC> @@
DIC> @@ START THE SIMULATION
DIC> @@
DIC> sim
Region: FERRITE
single geometric dense at 0.10000E-08
0.99998 24
Region: AUSTENITE
single geometric dense at 0.0000
1.0666 84
DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
Trying old scheme 3
U-FRACTION IN SYSTEM: C = 8.8825328568563E-04 FE = 1
TOTAL SIZE OF SYSTEM: 1E-06 [m]
U-FRACTION IN SYSTEM: C = 8.8825328568563E-04 FE = 1
TOTAL SIZE OF SYSTEM: 1E-06 [m]
2.137709938543949E-004 2.137625593783627E-004 13.8289494082011 2.120998911035789E-004 2.112667987438772E-004
2.108508673179424E-004 2.106430552934355E-004 2.104353457279473E-004 2.101948159848891E-004
2.097141691265310E-004 2.087545259209826E-004 2.068418415541200E-004 2.030428809977812E-004
1.955505925945084E-004 1.80985466255661E-004 1.535545780378763E-004 1.054471342636204E-004
3.627422031933180E-005 13.8289493973143 3.615700659637290E-005 3.609847086651284E-005
3.606922078447431E-005 3.60546018916993E-005 3.603998255771458E-005 3.602477866736845E-005

ERROR RETURN FROM NS01A BECAUSE THERE HAVE BEEN 25 CALLS OF CALFUN
RESCALING
3.883944143922924E-007 3.882539150545330E-007 0.138289494549039 3.870958777913919E-007 3.864474248777306E-007
3.861234022677696E-007 3.859614419240409E-007 3.85799515551698E-007 3.856306041286111E-007
3.852928922295713E-007 3.846179122468376E-007 3.832697275449583E-007 3.805804591934837E-007
3.7529303266987117E-007 3.646436785436601E-007 3.439248495707180E-007 3.043050609751792E-007
2.323369611824800E-007 1.174866711920061E-007 8.677377375815751E-002 1.172648822508408E-007
007 1.171540663584507E-007 1.170769077778130E-007 1.169997746143189E-007 1.169226668677405E-007

ERROR RETURN FROM NS01A BECAUSE THERE HAVE BEEN 25 CALLS OF CALFUN
** ERROR 1890 IN DCNS01: ERROR RETURN FROM NS01A
1.169226668677405E-007 1.169226525134302E-007 1.169226668677405E-007 0.138291370392232 1.169226668677405E-007
007 1.167079409303351E-007 1.167079265859497E-007 1.167079409303351E-007 1.166006519683773E-007
007 1.166006519683773E-007 1.163862220574208E-007 1.163862220574208E-007 1.159579542887088E-007

output ignored...

... output resumed

TIME = 0.24974219E-02 DT = 0.18906543E-05 SUM OF SQUARES = 0.88471153E-22
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.83026409E-03 AND 0.83026409E-03
POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.93685846E-06
U-FRACTION IN SYSTEM: C = 8.98896995185644E-04 FE = 1
TOTAL SIZE OF SYSTEM: 1E-06 [m]
CPU time used in timestep 0 seconds
7.867968423650945E-008 7.858086700827199E-008 2.896163618344889E-010 1.378865335079752E-012 3.162640407458178E-008
017 TIME = 0.24986188E-02 DT = 0.11968793E-05 SUM OF SQUARES = 0.31626404E-16
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.95217371E-03 AND 0.95217371E-03
POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.93799810E-06
U-FRACTION IN SYSTEM: C = 8.98949653154461E-04 FE = 1
TOTAL SIZE OF SYSTEM: 1E-06 [m]
1 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: FERRITE

CPU time used in timestep 0 seconds
1.221664300962714E-007 1.220136773979831E-007 2.382573136249435E-010 6.480649597822680E-013 4.343406401024631E-007
018 TIME = 0.24993549E-02 DT = 0.73617682E-06 SUM OF SQUARES = 0.43434064E-17
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.10896139E-02 AND 0.10896139E-02
POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.93880024E-06
U-FRACTION IN SYSTEM: C = 8.98990551867659E-04 FE = 1
TOTAL SIZE OF SYSTEM: 1E-06 [m]
CPU time used in timestep 0 seconds
3.067772851428954E-007 3.064723216583984E-007 3.258591432650207E-010 5.434030609685222E-013 1.322954334308893E-007
018 TIME = 0.24997403E-02 DT = 0.38533755E-06 SUM OF SQUARES = 0.13229543E-17
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.12901467E-02 AND 0.12901467E-02
POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.93929739E-06
U-FRACTION IN SYSTEM: C = 8.99048032536186E-04 FE = 1
TOTAL SIZE OF SYSTEM: 1E-06 [m]
1 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: FERRITE

CPU time used in timestep 0 seconds
3.533106209108938E-007 3.528981709400178E-007 1.629527128729134E-010 8.176156478808468E-014 2.097394977859221E-007
020 TIME = 0.24999374E-02 DT = 0.19708476E-06 SUM OF SQUARES = 0.20973950E-19
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.14857531E-02 AND 0.14857531E-02
POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.93959021E-06
U-FRACTION IN SYSTEM: C = 8.99106406246185E-04 FE = 1
TOTAL SIZE OF SYSTEM: 1E-06 [m]
CPU time used in timestep 0 seconds
```

1.376922464050572E-006 1.375921904429487E-006 1.880066284182330E-010 1.124790659796382E-014 4.737871704746039E-  
 022 TIME = 0.25000000E-02 DT = 0.62635582E-07 SUM OF SQUARES = 0.47378717E-21  
 CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.18520473E-02 AND 0.18520473E-02  
 POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.93970621E-06  
 U-FRACTION IN SYSTEM: C = 8.99167266914905E-04 FE = 1  
 TOTAL SIZE OF SYSTEM: 1E-06 [m]  
 MUST SAVE WORKSPACE ON FILE  
 WORKSPACE SAVED ON FILE  
 RECLAIMING WORKSPACE  
 DELETING TIME-RECORD FOR TIME 0.0000000  
 DELETING TIME-RECORD FOR TIME 0.10000000E-06  
 DELETING TIME-RECORD FOR TIME 0.30000000E-06  
 DELETING TIME-RECORD FOR TIME 0.70000000E-06  
 DELETING TIME-RECORD FOR TIME 0.15000000E-05  
 DELETING TIME-RECORD FOR TIME 0.28565078E-05  
 DELETING TIME-RECORD FOR TIME 0.52014932E-05  
 DELETING TIME-RECORD FOR TIME 0.98914639E-05  
 DELETING TIME-RECORD FOR TIME 0.19271406E-04  
 DELETING TIME-RECORD FOR TIME 0.33686773E-04  
 DELETING TIME-RECORD FOR TIME 0.53416545E-04  
 DELETING TIME-RECORD FOR TIME 0.78652588E-04  
 DELETING TIME-RECORD FOR TIME 0.10952599E-03  
 DELETING TIME-RECORD FOR TIME 0.14612624E-03  
 DELETING TIME-RECORD FOR TIME 0.18852383E-03  
 DELETING TIME-RECORD FOR TIME 0.23678901E-03  
 DELETING TIME-RECORD FOR TIME 0.29103504E-03  
 DELETING TIME-RECORD FOR TIME 0.35143593E-03  
 DELETING TIME-RECORD FOR TIME 0.41821144E-03  
 DELETING TIME-RECORD FOR TIME 0.48720815E-03  
 DELETING TIME-RECORD FOR TIME 0.55626110E-03  
 DELETING TIME-RECORD FOR TIME 0.62543509E-03  
 DELETING TIME-RECORD FOR TIME 0.69478360E-03  
 DELETING TIME-RECORD FOR TIME 0.76435016E-03  
 DELETING TIME-RECORD FOR TIME 0.83416447E-03  
 DELETING TIME-RECORD FOR TIME 0.90422644E-03  
 DELETING TIME-RECORD FOR TIME 0.97470459E-03  
 DELETING TIME-RECORD FOR TIME 0.10456240E-02  
 DELETING TIME-RECORD FOR TIME 0.11169644E-02  
 DELETING TIME-RECORD FOR TIME 0.11887516E-02  
 DELETING TIME-RECORD FOR TIME 0.12609316E-02  
 DELETING TIME-RECORD FOR TIME 0.13331372E-02  
 DELETING TIME-RECORD FOR TIME 0.14055753E-02  
 DELETING TIME-RECORD FOR TIME 0.14782433E-02  
 DELETING TIME-RECORD FOR TIME 0.15510762E-02  
 DELETING TIME-RECORD FOR TIME 0.16239552E-02  
 DELETING TIME-RECORD FOR TIME 0.16973277E-02  
 DELETING TIME-RECORD FOR TIME 0.17713800E-02  
 DELETING TIME-RECORD FOR TIME 0.18458976E-02  
 DELETING TIME-RECORD FOR TIME 0.19207879E-02  
 DELETING TIME-RECORD FOR TIME 0.19960404E-02  
 DELETING TIME-RECORD FOR TIME 0.20715254E-02  
 DELETING TIME-RECORD FOR TIME 0.21477511E-02  
 DELETING TIME-RECORD FOR TIME 0.22245013E-02  
 DELETING TIME-RECORD FOR TIME 0.23020429E-02  
 DELETING TIME-RECORD FOR TIME 0.23637224E-02  
 DELETING TIME-RECORD FOR TIME 0.24065959E-02  
 DELETING TIME-RECORD FOR TIME 0.24364873E-02  
 DELETING TIME-RECORD FOR TIME 0.24572307E-02  
 DELETING TIME-RECORD FOR TIME 0.24715931E-02  
 DELETING TIME-RECORD FOR TIME 0.24814530E-02  
 DELETING TIME-RECORD FOR TIME 0.24881120E-02  
 DELETING TIME-RECORD FOR TIME 0.24925851E-02  
 DELETING TIME-RECORD FOR TIME 0.24955312E-02  
 DELETING TIME-RECORD FOR TIME 0.24974219E-02  
 DELETING TIME-RECORD FOR TIME 0.24986188E-02  
 DELETING TIME-RECORD FOR TIME 0.24993549E-02  
 DELETING TIME-RECORD FOR TIME 0.24997403E-02  
  
 KEEPING TIME-RECORD FOR TIME 0.24999374E-02  
 AND FOR TIME 0.25000000E-02  
 WORKSPACE RECLAIMED

TIMESTEP AT 0.25000000E-02 SELECTED

```

DIC>
DIC>
DIC> set-inter
--OK--
DIC>

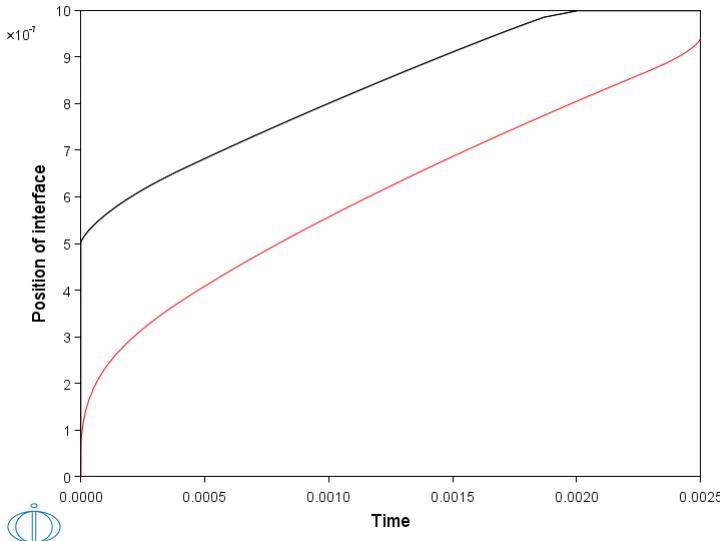
```

**exh1-plot**

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exh1\plot.DCM.test"
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 2.50000E-03
DIC>
DIC> read exh1
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1: @@
POST-1: @@ SET THE DATA APPENDED FROM THE "EXP" FILE TO BE READ
POST-1: @@
POST-1: set-col for for red
COMMAND NOT SUPPORTED IN THIS PLOT DRIVER
POST-1:
POST-1: @@
POST-1: @@ COMPARE THE POSITION OF THE INTERFACE AS A FUNCTION OF TIME
POST-1: @@
POST-1: s-d-a x time
INFO: Time is set as independent variable
POST-1: s-d-a y posi aus low
POST-1:
POST-1: @@
POST-1: @@ APPEND THE SIMULATION (WITHOUT THE ENERGY CONTRIBUTION) FROM FILE
POST-1: @@
POST-1: app y noadd.exp 1; 1
POST-1:
POST-1: @@
POST-1: @@ SET A TITLE ON THE PLOT
POST-1: @@
POST-1: set-title Figure h1
POST-1:
POST-1: @@
POST-1: @@ PLOT THE RESULTS
POST-1: @@
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
ORKING ...
OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

**Figure h1**

CELL # 1



```
POST-1:
POST-1:
POST-1: set-inter
--OK---
POST-1:
```

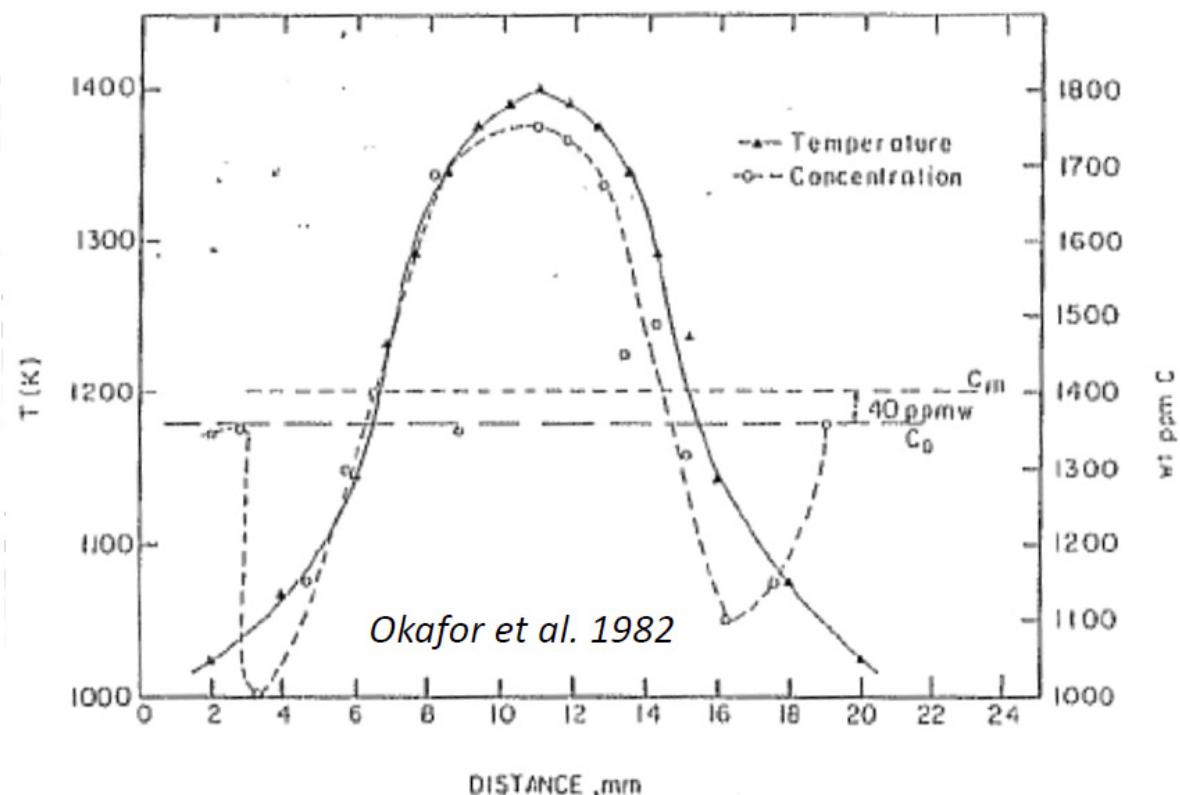


## Example exh3

### Diffusion induced by a temperature gradient (thermomigration)

This calculation shows how a temperature gradient induces diffusion.

$$J_C = -\frac{u_C}{V_s} y_{Va} M_{CVa} \left( \frac{\partial \mu_C}{\partial x} + \frac{Q_C^*}{T} \frac{\partial T}{\partial x} \right)$$

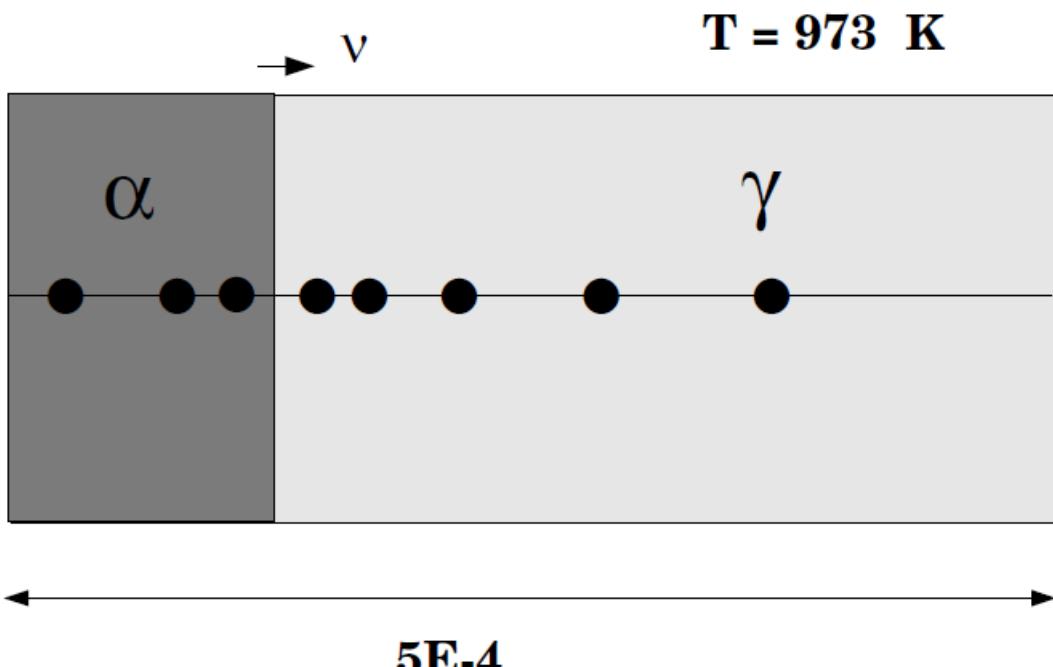




## Example exh2

### $\sigma/\gamma$ para-equilibrium in an Fe-Ni-C alloy

This example calculates the growth of ferrite ( $\alpha$ ) into austenite ( $\gamma$ ) in an Fe-2.02%Ni-0.0885%C alloy using the para-equilibrium model. The results are compared with experimental information from Hutchinson, C. R., A. Fuchsmann, and Yves Brechet. "The diffusional formation of ferrite from austenite in Fe-C-Ni alloys." Met. Mat. Trans A 35.4 (2004): 1211-1221.



**exh2-setup****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_dictra_console_examples\examples\exh2\setup.DCM.test"
SYS: @@
SYS: @@ Deviation from local equilibrium.
SYS: @@ Ferrite/austenite para-equilibrium in an Fe-Ni-C alloy
SYS: @@ This example calculates the growth of ferrite into austenite
SYS: @@ in an Fe-2.02%Ni-0.0885%C alloy using the para-equilibrium model.
SYS: @@ The results are compared with experimental information from
SYS: @@ Hutchinson, C. R., A. Fuchsmann, and Yves Brechet. "The diffusional
SYS: @@ formation of ferrite from austenite in Fe-C-Ni alloys." Metall.
SYS: @@ Mat. Trans. A 35.4 (2004): 1211-1221.
SYS: -----
NO SUCH COMMAND, USE HELP
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASE
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\generate_dictra_console_examples\databases\data
Current database: Steels/Fe-Alloys v12.0

VA          /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE12: @@
TDB_TCFE12: @@ SELECT A DATABASE FOR THERMODYNAMIC DATA
TDB_TCFE12: @@
TDB_TCFE12: sw fedemo
Current database: Iron Demo Database v4.0

VA          /- DEFINED
TDB_FEDEMO: def-sys fe ni c
FE           NI           C
DEFINED
TDB_FEDEMO: rej ph * all
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 bcc fcc
BCC_A2          FCC_A1 RESTORED
TDB_FEDEMO: get
18:59:58,819 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS .....

List of references for assessed data

'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'
'X.G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
'A. Gabriel, C. Chatillon, and I. Ansara, published in High Temp. Sci.
(Parameters listed in CALPHAD, 11 (1987) 203-218); C-NI'
'A.T. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
'X.G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
volumes'
'A. Gabriel, P. Gustafson, and I. Ansara, CALPHAD, 11 (1987) 203 -218;
TRITA-MAC 285 (1986); C-FE-NI'
'A.T. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); FE-NI'
'B.J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
-OK-
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE MOBILITY DATA
TDB_FEDEMO: @@
TDB_FEDEMO: app mfdemo
Current database: Fe-Alloys Mobility demo database v2.0

VA DEFINED
APP: def-sys fe ni c
FE           NI           C
DEFINED
APP: rej ph * all
BCC_A2          FCC_A1 RESTORED
REJECTED
APP: res ph bcc fcc
BCC_A2          FCC_A1 RESTORED
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS .....

List of references for assessed data

'This parameter has not been assessed'
'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'
'B. Jonsson: Z. Metallkunde 85(1994)502-509; C diffusion in fcc Cr-Fe-Ni'
```

```

'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
-Ni'
'Xia, C. H. et al. JAC, 2021, 853, 157165.'
'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Ni self-diffusion'
'B. Jonsson: Z. Metallkunde 85(1994)498-501; C and N diffusion in bcc Cr
-Fe-Ni'
'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
in bcc Fe'
'B. Jonsson: ISIJ International, 35(1995)1415-1421; Cr, Fe and Ni
diffusion bcc Cr-Fe-Ni'

--OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR
APP: @@
APP: go d-m
NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 973; * N
DIC>
DIC> @@
DIC> @@ START BY ENTERING THE REGIONS ferrite AND austenite WHERE THE
DIC> @@ BCC AND FCC PHASES ARE PUT, RESPECTIVELY. THE FERRITE REGION IS
DIC> @@ ASSUMED INITIALLY TO BE VERY THIN, 1E-9 METERS.
DIC> @@
DIC> enter-region
REGION NAME : ferrite
DIC>
DIC> enter-region
REGION NAME : austenite
ATTACH TO REGION NAMED /FERRITE/:
ATTACHED TO THE RIGHT OF FERRITE /YES/:
DIC>
DIC> @@
DIC> @@ ENTER GRIDS INTO THE REGIONS
DIC> @@
DIC> enter-grid
REGION NAME : /FERRITE/: ferrite
WIDTH OF REGION /1/: 1e-9
TYPE /LINEAR/: AUTO
DIC>
DIC> enter-grid austenite
WIDTH OF REGION /1/: 50e-6
TYPE /LINEAR/: AUTO
DIC>
DIC> @@
DIC> @@ ENTER active PHASES INTO THE REGIONS
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /FERRITE/: ferrite
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: bcc
DIC>
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /AUSTENITE/: austenite
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITION INTO BCC
DIC> @@
DIC> enter-composition
REGION NAME : /FERRITE/: ferrite
PHASE NAME: /BCC_A2/: bcc
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: c
TYPE /LINEAR/: linear
VALUE OF FIRST POINT : 0.0885
VALUE OF LAST POINT : /8.85E-2/: 0.0885
PROFILE FOR /NI/: ni
TYPE /LINEAR/: linear
VALUE OF FIRST POINT : 2.02
VALUE OF LAST POINT : /2.02/: 2.02
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITION INTO FCC
DIC> @@
DIC> enter-composition
REGION NAME : /AUSTENITE/: austenite
PHASE NAME: /FCC_A1/: fcc#1
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: c
TYPE /LINEAR/: linear
VALUE OF FIRST POINT : 0.0885
VALUE OF LAST POINT : /8.85E-2/: 0.0885
PROFILE FOR /NI/: ni
TYPE /LINEAR/: linear
VALUE OF FIRST POINT : 2.02
VALUE OF LAST POINT : /2.02/: 2.02
DIC>
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exh2 y
DIC>
DIC> set-inter
--OK--
DIC>
```

**exh2-run**

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exh2\run.DCM.test"
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ FILE TO RUN EXAMPLE exh2
DIC> @@
DIC>
DIC> @@
DIC> @@ READ THE SETUP FROM FILE
DIC> @@
DIC>
DIC>
DIC> go d-m
TIME STEP AT TIME 0.00000E+00
DIC>
DIC> read exh2
OK
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-sim-time 50,,,
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ ENABLE THE PARA-EQUILIBRIUM MODEL
DIC> @@
DIC> para
ENABLE PARAEQ : /NO/: YES
U-FRACTION OF COMPONENT FE /AUTO/: AUTO
U-FRACTION OF COMPONENT NI /AUTO/: AUTO
DIC>
DIC> @@
DIC> @@ START THE SIMULATION
DIC> @@
DIC> sim
Region: FERRITE
single geometric dense at 0.10000E-08
0.99997 24
Region: AUSTENITE
single geometric dense at 0.0000
1.1602 98
DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
Trying old scheme 4
GENERATING STARTING VALUES FOR CELL # 1 INTERFACE # 2
DETERMINING INITIAL EQUILIBRIUM VALUES
CALCULATING STARTING VALUES: 9 EQUILIBRIUM CALCULATIONS DONE 6 OUT OF 9
DETERMINED ACTIVITIES ACR(C) .161541295585
UNABLE TO OBTAIN GOOD STARTING VALUE USING THE OLD SCHEME
USE NEW SCHEME /YES/:
Trying new scheme
GENERATING STARTING VALUES FOR CELL # 1 INTERFACE # 2
DETERMINING INITIAL EQUILIBRIUM VALUES
CALCULATING STARTING VALUES: 18 EQUILIBRIUM CALCULATIONS DONE 1 OUT OF 18
U-FRACTION IN SYSTEM: C = .00412262676333 FE = .980742621143594
NI = .0192573788564064
TOTAL SIZE OF SYSTEM: 5.0001E-05 [m]
U-FRACTION IN SYSTEM: C = .00412262676333 FE = .980742621143594
NI = .0192573788564064
TOTAL SIZE OF SYSTEM: 5.0001E-05 [m]
2232.10931280664 2232.10931281204 2228.18551830805 2.32383619747326 1.947806789673184E-
003 8.416187481247426E-003 7.623215840702783E-006 1.892250162170694E-003 5.168572767775522E-
006 2.142557862886661E-006 3.440441261060793E-013 TIME = 0.1000000E-06 DT = 0.1000000E-
06 SUM OF SQUARES = 0.17152417E-19
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.20272106E-01 AND 0.20272106E-01
POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.30272106E-08
U-FRACTION IN SYSTEM: C = .00412273631313628 FE = .980742621143594
NI = .0192573788564064
TOTAL SIZE OF SYSTEM: 5.0001E-05 [m]
11 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: AUSTENITE
CPU time used in timestep 1 seconds
2189.02035753886 2189.02035754035 2185.12779966696 2.22490243110584 1.816590401838329E-
003 7.875020867328213E-003 7.030645470386523E-007 1.892093522491090E-003
output ignored...
... output resumed
1.035878360336796E-006 4.070485716170575E-010 2.083957705860817E-003 2.977850872345636E-
019 TIME = 39.294678 DT = 4.0585213 SUM OF SQUARES = 0.29778502E-18
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.19678982E-06 AND 0.19678982E-06
POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.12958007E-04
U-FRACTION IN SYSTEM: C = .00412955173352621 FE = .980742621143594
NI = .0192573788564067
TOTAL SIZE OF SYSTEM: 5.0001E-05 [m]
18 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: FERRITE
CPU time used in timestep 1 seconds
1039.08650681154 1039.08650681441 1036.25652818197 0.435769080849054 1.582425627600989E-
004 9.540441846200684E-007 3.683313609770359E-010 2.086872290624549E-003 2.520452856195749E-
019 TIME = 43.471006 DT = 4.1763285 SUM OF SQUARES = 0.25204524E-18
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.18739200E-06 AND 0.18739200E-06
POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.13740618E-04
U-FRACTION IN SYSTEM: C = .00413007208773368 FE = .980742621143594
NI = .0192573788564067
TOTAL SIZE OF SYSTEM: 5.0001E-05 [m]
10 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: FERRITE
CPU time used in timestep 1 seconds
1018.81026652885 1018.81026652886 1016.00487583637 0.417681858566207 1.485067582194666E-
004 8.663986179629915E-007 3.298391462430085E-010 2.089741151576187E-003 2.376457022230289E-
019 TIME = 47.752801 DT = 4.2817943 SUM OF SQUARES = 0.23764568E-18
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.17907231E-06 AND 0.17907231E-06
POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.14507369E-04
U-FRACTION IN SYSTEM: C = .00413054997255924 FE = .980742621143593
```

NI = .0192573788564067  
 TOTAL SIZE OF SYSTEM: 5.000E-05 [m]  
 13 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: FERRITE

CPU time used in timestep 1 seconds  
 998.925416406910 998.925416407378 996.144440719064 0.400354341744198  
 004 2.022498947386798E-004 8.988128259110068E-010 2.089216887434514E-003  
 013 TIME = 49.893698 DT = 2.1408972 SUM OF SQUARES = 0.13918475E-12  
 CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.20276693E-06 AND 0.20276693E-06  
 POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.14941472E-04  
 U-FRACTION IN SYSTEM: C = .00413164822661486 FE = .980742621143593  
 NI = .0192573788564067

TOTAL SIZE OF SYSTEM: 5.000E-05 [m]  
 5 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: FERRITE

CPU time used in timestep 1 seconds  
 979.424536431009 979.424536431920 976.667803135423 0.383754222070973  
 004 5.518608566587773E-004 1.410273832322884E-008 2.084196758114002E-003  
 009 1.192064516431363E-009 3.530517560542321E-010 8.502194385026583E-  
 015 TIME = 50.000000 DT = 0.10630230 SUM OF SQUARES = 0.13234890E-20  
 CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.39308726E-06 AND 0.39308726E-06  
 POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.14983258E-04  
 U-FRACTION IN SYSTEM: C = .00413198331504803 FE = .980742621143593  
 NI = .0192573788564067

TOTAL SIZE OF SYSTEM: 5.000E-05 [m]  
 MUST SAVE WORKSPACE ON FILE  
 WORKSPACE SAVED ON FILE  
 RECLAIMING WORKSPACE

DELETING TIME-RECORD FOR TIME 0.0000000  
 DELETING TIME-RECORD FOR TIME 0.10000000E-06  
 DELETING TIME-RECORD FOR TIME 0.20000000E-06  
 DELETING TIME-RECORD FOR TIME 0.40000000E-06  
 DELETING TIME-RECORD FOR TIME 0.80000000E-06  
 DELETING TIME-RECORD FOR TIME 0.16000000E-05  
 DELETING TIME-RECORD FOR TIME 0.32000000E-05  
 DELETING TIME-RECORD FOR TIME 0.64000000E-05  
 DELETING TIME-RECORD FOR TIME 0.12800000E-04  
 DELETING TIME-RECORD FOR TIME 0.25600000E-04  
 DELETING TIME-RECORD FOR TIME 0.48352395E-04  
 DELETING TIME-RECORD FOR TIME 0.79491360E-04  
 DELETING TIME-RECORD FOR TIME 0.12664729E-03  
 DELETING TIME-RECORD FOR TIME 0.21423275E-03  
 DELETING TIME-RECORD FOR TIME 0.38940367E-03  
 DELETING TIME-RECORD FOR TIME 0.73974551E-03  
 DELETING TIME-RECORD FOR TIME 0.14404292E-02  
 DELETING TIME-RECORD FOR TIME 0.27785191E-02  
 DELETING TIME-RECORD FOR TIME 0.54207495E-02  
 DELETING TIME-RECORD FOR TIME 0.10705210E-01  
 DELETING TIME-RECORD FOR TIME 0.21274132E-01  
 DELETING TIME-RECORD FOR TIME 0.42411975E-01  
 DELETING TIME-RECORD FOR TIME 0.84687661E-01  
 DELETING TIME-RECORD FOR TIME 0.16923903  
 DELETING TIME-RECORD FOR TIME 0.33834178  
 DELETING TIME-RECORD FOR TIME 0.67654726  
 DELETING TIME-RECORD FOR TIME 1.3529582  
 DELETING TIME-RECORD FOR TIME 2.7057802  
 DELETING TIME-RECORD FOR TIME 5.2358091  
 DELETING TIME-RECORD FOR TIME 7.8217420  
 DELETING TIME-RECORD FOR TIME 10.658634  
 DELETING TIME-RECORD FOR TIME 13.690757  
 DELETING TIME-RECORD FOR TIME 16.905149  
 DELETING TIME-RECORD FOR TIME 20.286260  
 DELETING TIME-RECORD FOR TIME 23.819574  
 DELETING TIME-RECORD FOR TIME 27.493141  
 DELETING TIME-RECORD FOR TIME 31.300679  
 DELETING TIME-RECORD FOR TIME 35.236156  
 DELETING TIME-RECORD FOR TIME 39.294678  
 DELETING TIME-RECORD FOR TIME 43.471006  
 DELETING TIME-RECORD FOR TIME 47.752801

KEEPING TIME-RECORD FOR TIME 49.893698  
 AND FOR TIME 50.000000  
 WORKSPACE RECLAIMED

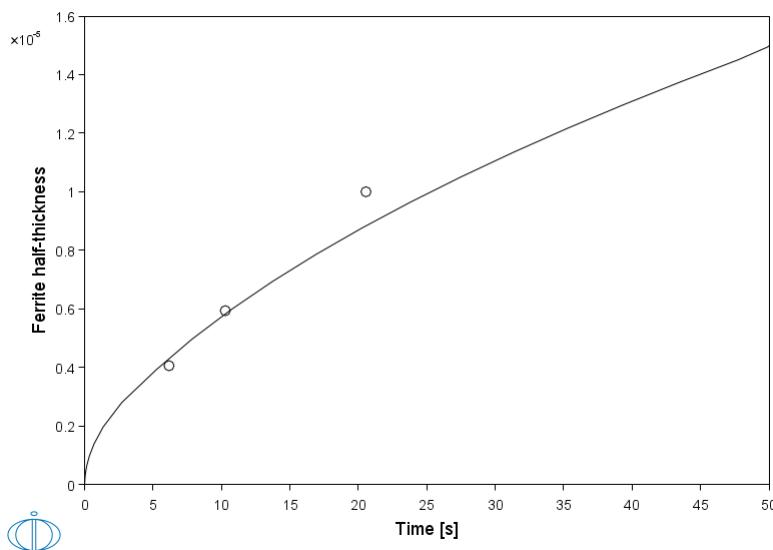
TIMESTEP AT 50.0000000 SELECTED

**DIC>**  
**DIC> set-inter**  
**--OK--**  
**DIC>**

## exh2-plot

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exh2\plot.DCM.test"
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 5.00000E+01
DIC>
DIC> read exh2
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1: @@
POST-1: @@ WE WANT TO PLOT THE POSITION OF THE INTERFACE AS A FUNCTION OF TIME
POST-1: @@ I.E. THE FERRITE HALF-THICKNESS
POST-1: @@
POST-1: s-d-a x time
INFO: Time is set as independent variable
POST-1: s-d-a y posi aus low
POST-1: @@
POST-1: @@ APPEND THE EXPERIMENTAL INFORMATION
POST-1: @@
POST-1: app y exh2.exp 1; 1
POST-1: @@
POST-1: @@ SET A TITLE ON THE PLOT
POST-1: @@
POST-1: set-title Figure h2
POST-1: @@
POST-1: @@ RENAME THE AXIS LABELS
POST-1: @@
POST-1: set-axis-text-status
AXIS (X, Y OR Z) : x
AUTOMATIC AXIS TEXT (Y OR N) /N/: NO
AXIS TEXT : Time [s]
POST-1: @@
POST-1: set-axis-text-status
AXIS (X, Y OR Z) : y
AUTOMATIC AXIS TEXT (Y OR N) /N/: NO
AXIS TEXT : Ferrite half-thickness
POST-1: @@
POST-1: @@
POST-1: @@ PLOT THE RESULTS
POST-1: @@
POST-1: @@ PLOT THE RESULTS
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

Figure h2



```
POST-1:
POST-1:
POST-1:
POST-1: set-inter
--OK--
POST-1:
```

**exh3-setup****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\_dictra\_console\_examples\examples\exh3\setup.DCM.test"**

**SYS: @@**

**SYS: @@ Deviation from local equilibrium.**

**SYS: @@ Diffusion induced by a temperature gradient (thermomigration)**

**SYS: @@ This calculation shows how a temperature gradient induces**

**SYS: @@ diffusion.**

**SYS: -----**

NO SUCH COMMAND, USE HELP

**SYS:**

**SYS: go da**

  THERMODYNAMIC DATABASE module

  Database folder:

  C:\jenkins\workspace\generate\_dictra\_console\_examples\databases\data

  Current database: Steels/Fe-Alloys v12.0

  VA                           /- DEFINED

  DICTRA\_FCC\_A1 REJECTED

**TDB\_TCFE12: sw fedemo**

  Current database: Iron Demo Database v4.0

  VA                           /- DEFINED

**TDB\_FEDEMO: def-sys fe ni c**

  FE                           NI                           C

  DEFINED

**TDB\_FEDEMO: rej ph \* all**

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 graph**

  FCC\_A1                   GRAPHITE RESTORED

**TDB\_FEDEMO: get**

19:03:54,804 [Thread-0] INFO JavaWrapper: \*\*\* Invoking Gibbs Energy System v6 \*\*\*

REINITIATING GES ....

ELEMENTS ....

SPECIES ....

PHASES ....

PARAMETERS ...

FUNCTIONS ....

List of references for assessed data

'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'  
'X.G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'  
'B.J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'  
'A. Gabriel, C. Chatillon, and I. Ansara, published in High Temp. Sci.  
(Parameters listed in CALPHAD, 11 (1987) 203-218); C-Ni'  
'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'  
'A.T. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'  
'X.G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar  
volumes'  
'A. Gabriel, P. Gustafson, and I. Ansara, CALPHAD, 11 (1987) 203 -218;  
TRITA-MAC 285 (1986); C-FE-NI'  
'A.T. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); FE-NI'  
'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121 -127; Molar  
volumes'

-OK-

**TDB\_FEDEMO: app mfdemo**

  Current database: Fe-Alloys Mobility demo database v2.0

  VA DEFINED

**APP: def-sys fe ni c**

  FE                           NI                           C

  DEFINED

**APP: rej ph \* all**

  BCC\_A2                   FCC\_A1                           CEMENTITE

  REJECTED

**APP: res ph fcc**

  FCC\_A1 RESTORED

**APP: get**

ELEMENTS ....

SPECIES ....

PHASES ....

PARAMETERS ...

FUNCTIONS ....

List of references for assessed data

'This parameter has not been assessed'  
'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'  
'B. Jonsson: Z. Metallkunde 85(1994)502-509; C diffusion in fcc Cr-Fe-Ni'  
'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe  
-Ni'  
'Xia, C. H. et al. JAC, 2021, 853, 157165.'  
'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Ni self-diffusion'

-OK-

**APP:**

**APP: go d-m**

  NO TIME STEP DEFINED

  \*\*\* ENTERING GRAPHITE AS A DIFFUSION NONE PHASE

**DIC>**

**DIC> @@ ENTER A GAUSSIAN-SHAPED TEMPERATURE GRADIENT**

**DIC> set-cond glob T 0 1000+400\*exp(-3.35074E4\*(x-11e-3)\*\*2); \* N**

**DIC>**

**DIC> set-ref C grap,.....,**

```
DIC>
DIC> ent-reg aus,,,
DIC> ent-grid aus 25e-3 auto
DIC>
DIC> ent-phd act aus matrix fcc#1
DIC>
DIC> ent-comp aus fcc#1 fe w-p
PROFILE FOR /C/: c lin 0.14 0.14
PROFILE FOR /NI/: ni lin 32.5 32.5
DIC>
DIC> s-s-time 5E7,,,
DIC>
DIC> @@ ENTER THE HEAT OF TRANSFER PARAMETER FOR CARBON
DIC> ent-heat-tra-p
HEAT TRANSFER PARAMETER FOR PHASE: fcc
ELEMENT: C
PARAMETER /0/: -42000
DIC>
DIC>
DIC> save exh3 y
DIC>
DIC> set-inter
--OK--
DIC>
```

**exh3-run**

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exh3\run.DCM.test"
DIC>
DIC> go d-m
TIME STEP AT TIME  0.00000E+00
*** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
DIC>
DIC> read exh3
OK
DIC>
DIC> sim
Region: AUS
linear grid  75
DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
U-FRACTION IN SYSTEM: C = .00662305741857946 FE = .68534915460493
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
U-FRACTION IN SYSTEM: C = .00662305741857946 FE = .68534915460493
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741857945 FE = .68534915460493
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep          0 seconds
TIME = 0.10010000E-03 DT = 0.10000000E-03 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741857945 FE = .68534915460493
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep          0 seconds
TIME = 0.40010010 DT = 0.40000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741857945 FE = .685349154604931
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep          0 seconds
TIME = 1600.4001 DT = 1600.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741857936 FE = .68534915460493
NI = .314650845395069
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep          0 seconds
TIME = 75402.174 DT = 73801.774 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741847484 FE = .685349154604931
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep          1 seconds
TIME = 223005.72 DT = 147603.55 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741807354 FE = .685349154604931
NI = .314650845395069
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep          0 seconds
TIME = 518212.82 DT = 295207.10 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741807247 FE = .68534915460493
NI = .314650845395069
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep          0 seconds
TIME = 1108627.0 DT = 590414.19 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741807065 FE = .685349154604931
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep          1 seconds
TIME = 2289455.4 DT = 1180828.4 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741802882 FE = .685349154604931
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep          0 seconds
TIME = 4651112.2 DT = 2361656.8 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741803467 FE = .685349154604931
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep          0 seconds
TIME = 7580409.9 DT = 2929297.8 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741804455 FE = .68534915460493
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep          0 seconds
TIME = 10062302. DT = 2481892.5 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741804834 FE = .68534915460493
NI = .31465084539509
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep          1 seconds
TIME = 12331236. DT = 2268933.5 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741805146 FE = .68534915460493
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep          0 seconds
TIME = 14490786. DT = 2159549.7 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0066230574180534 FE = .685349154604931
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep          0 seconds
TIME = 16584412. DT = 2093626.7 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741805514 FE = .685349154604931
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep          1 seconds
TIME = 18634814. DT = 2050401.2 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741762449 FE = .68534915460493
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep          0 seconds
TIME = 20655269. DT = 2020455.8 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0066230574168603 FE = .68534915460493
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep          0 seconds
TIME = 22654113. DT = 1998843.7 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0066230574162096 FE = .68534915460493
NI = .314650845395069
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep          0 seconds
TIME = 24636840. DT = 1982726.6 SUM OF SQUARES = 0.0000000
```

```

U-FRACTION IN SYSTEM: C = .00662305741564917 FE = .68534915460493
NI = .314650845395069
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep 1 seconds
TIME = 26607198. DT = 1970358.7 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741516077 FE = .68534915460493
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep 0 seconds
TIME = 28567826. DT = 1960628.1 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741473552 FE = .68534915460493
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep 0 seconds
TIME = 30520626. DT = 1952799.8 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741436302 FE = .68534915460493
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep 0 seconds
TIME = 32467004. DT = 1946377.7 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741403512 FE = .68534915460493
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep 1 seconds
TIME = 34408025. DT = 1941021.2 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741374738 FE = .68534915460493
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep 0 seconds
TIME = 36344516. DT = 1936491.3 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741349365 FE = .68534915460493
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep 0 seconds
TIME = 38277133. DT = 1932617.0 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741327036 FE = .68534915460493
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep 0 seconds
TIME = 40206407. DT = 1929273.4 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741307241 FE = .68534915460493
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep 0 seconds
TIME = 42132775. DT = 1926367.8 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741289557 FE = .685349154604931
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep 1 seconds
TIME = 44056603. DT = 1923828.8 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741273927 FE = .68534915460493
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep 0 seconds
TIME = 45978204. DT = 1921600.3 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0066230574125992 FE = .68534915460493
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep 0 seconds
TIME = 47618063. DT = 1639858.9 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741249883 FE = .68534915460493
NI = .314650845395069
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep 0 seconds
TIME = 48913601. DT = 1295538.8 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741243379 FE = .685349154604931
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep 1 seconds
TIME = 49750910. DT = 837308.31 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741240292 FE = .68534915460493
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep 0 seconds
TIME = 50000000. DT = 249090.24 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741240173 FE = .685349154604931
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 0.0000000
DELETING TIME-RECORD FOR TIME 0.10000000E-06
DELETING TIME-RECORD FOR TIME 0.10010000E-03
DELETING TIME-RECORD FOR TIME 0.40010010
DELETING TIME-RECORD FOR TIME 1600.4001
DELETING TIME-RECORD FOR TIME 75402.174
DELETING TIME-RECORD FOR TIME 223005.72
DELETING TIME-RECORD FOR TIME 518212.82
DELETING TIME-RECORD FOR TIME 1108627.0
DELETING TIME-RECORD FOR TIME 2289455.4
DELETING TIME-RECORD FOR TIME 4651112.2
DELETING TIME-RECORD FOR TIME 7580409.9
DELETING TIME-RECORD FOR TIME 10062302.
DELETING TIME-RECORD FOR TIME 12331236.
DELETING TIME-RECORD FOR TIME 14490786.
DELETING TIME-RECORD FOR TIME 16584412.
DELETING TIME-RECORD FOR TIME 18634814.
DELETING TIME-RECORD FOR TIME 20655269.
DELETING TIME-RECORD FOR TIME 22654113.
DELETING TIME-RECORD FOR TIME 24636840.
DELETING TIME-RECORD FOR TIME 26607198.
DELETING TIME-RECORD FOR TIME 285567826.
DELETING TIME-RECORD FOR TIME 30520626.
DELETING TIME-RECORD FOR TIME 32467004.
DELETING TIME-RECORD FOR TIME 34408025.
DELETING TIME-RECORD FOR TIME 36344516.
DELETING TIME-RECORD FOR TIME 38277133.
DELETING TIME-RECORD FOR TIME 40206407.
DELETING TIME-RECORD FOR TIME 42132775.
DELETING TIME-RECORD FOR TIME 44056603.
DELETING TIME-RECORD FOR TIME 45978204.
DELETING TIME-RECORD FOR TIME 47618063.
DELETING TIME-RECORD FOR TIME 48913601.

```

KEEPING TIME-RECORD FOR TIME 49750910.

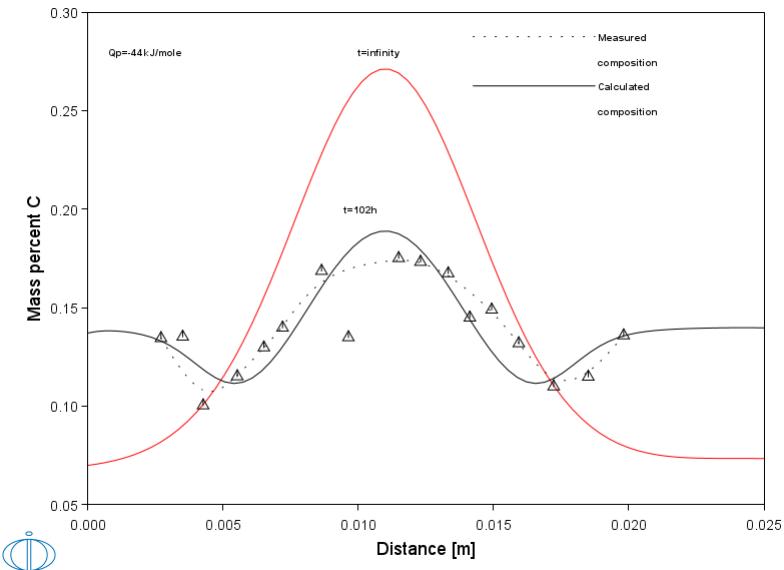
AND FOR TIME 50000000.  
WORKSPACE RECLAIMED

TIMESTEP AT 50000000.0 SELECTED

**DIC>**  
**DIC>** set-inter  
--OK---  
**DIC>**

**exh3-plot**

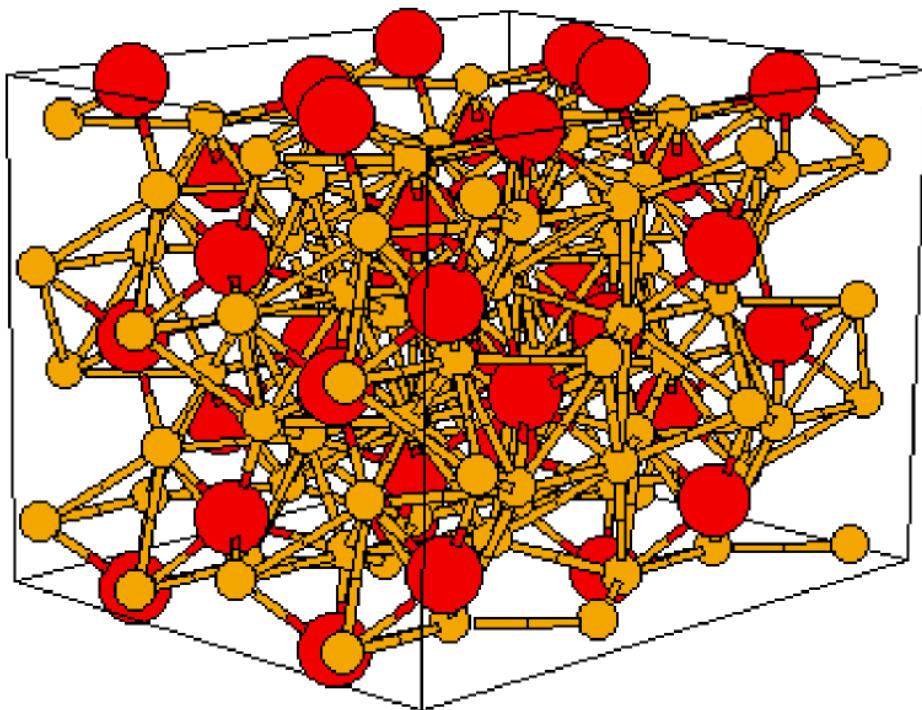
```
DIC>About  
NO SUCH COMMAND, USE HELP  
DIC>DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exh3\plot.DCM.test"  
DIC> go d-m  
TIME STEP AT TIME 5.00000E+07  
*** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE  
DIC>  
DIC>  
DIC> read exh3  
OK  
DIC>  
DIC> post  
POST PROCESSOR VERSION 1.7  
Implemented by Bjorn Jonsson  
POST-1: s-d-a x dist glob  
INFO: Distance is set as independent variable  
POST-1: s-d-a y w-p c  
POST-1: s-p-c time 367200 SE7  
POST-1: s-s-s y n 0.1 0.18  
POST-1: s-s-s Y Y  
POST-1: app y exh3.exp 0; 1 3;  
POST-1: s-p-o n y y n y n n,,,...,  
POST-1:  
POST-1: set-ax-text-st x  
AUTOMATIC AXIS TEXT (Y OR N) /N/: n  
AXIS TEXT : Distance [m]  
POST-1:  
POST-1: set-ax-text-st y  
AUTOMATIC AXIS TEXT (Y OR N) /N/: n  
AXIS TEXT : Mass percent C  
POST-1:  
POST-1:  
POST-1: SET_EXP_FILE_FORMAT 5  
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y  
POST-1: SET_EXP_FILE_FORMAT 10  
POST-1:  
POST-1: plot
```



```
POST-1:  
POST-1:  
POST-1:  
POST-1:  
POST-1: set-inter  
---OK---  
POST-1:
```



## Diffusion in Complex Phases

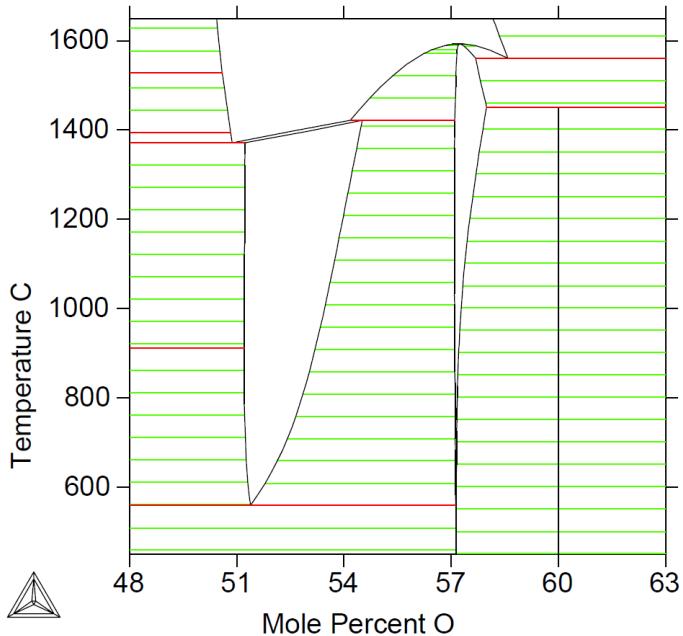




## Example exi3a

### Diffusion in iron oxide (FeO)

This example shows the oxidation of an iron sample and the consequent growth of an oxide layer using the grain boundary diffusion contribution model.





## Example exi2

### Diffusion of carbon in cementite

This example demonstrates the use of the model for calculation of diffusion through a stoichiometric phase. The flux of a component in the stoichiometric phase is assumed to be proportional to the difference in chemical potential at each side of the stoichiometric phase multiplied with the mobility for the component in the phase. The mobility is assessed from experimental information and is basically the tracer diffusivity for the component. This calculation is compared with experimental data where a sample of pure iron has been exposed to a gas atmosphere with a certain carbon activity. The weight gain is then measured as a function of time. The experimental data is obtained from Ozturk B., Fearing V. L., Ruth A. Jr. and Simkovich G., Met. Trans A, vol 13A (1982), pp. 1871-1873.

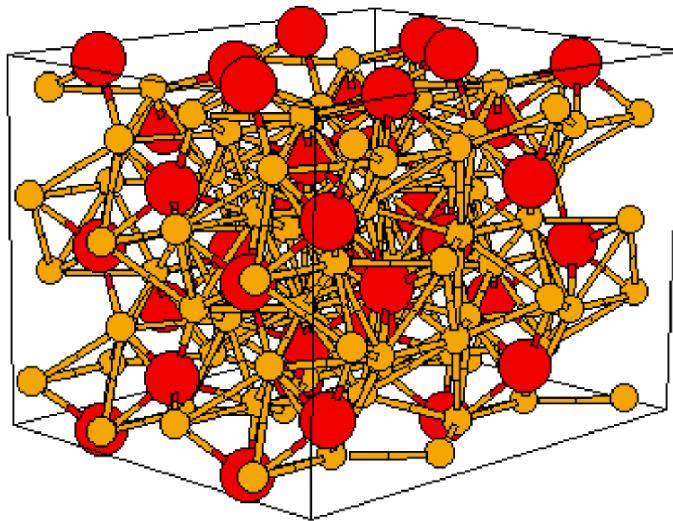
$$J \sim \Delta\mu$$



## Example exi1

### Diffusion in system with B2 ordering

Diffusion in including effects from chemical ordering. In this example folder, there is also a datafile AlFeNi-data.TDB, which contains both a thermodynamic and kinetic description for the ordered and disordered bcc.



**exil-setup**

**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_dictra_console_examples\examples\exil\setup.DCM.test"
SYS: @@
SYS: @@ Diffusion in complex phases.
SYS: @@ Diffusion in a system with B2 ordering
SYS: @@ This example shows diffusion in a system with B2 ordering.
SYS: @@ The datafile AlFeNi-data.TDB contains both a thermodynamic
SYS: @@ and kinetic description for the ordered and disordered BCC.
SYS: -----
NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exil_setup.DCM
SYS:
SYS:
SYS: go da
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\generate_dictra_console_examples\databases\data
Current database: Steels/Fe-Alloys v12.0

VA DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFC12: sw user AlFeNi-data.TDB
Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

VA DEFINED
19:07:15,962 [Thread-0] INFO TDBFileParser: USER_1737920627_14, number of lines read: 609
19:07:16,216 [Thread-0] INFO DatabaseUtils: Parsing of USER_1737920627_14 completed in 305 ms
TDB_USER: def-sys fe al ni
    FE           AL           NI
    DEFINED
TDB_USER: rej ph *
    B2_BCC          BCC_DIS          B2_ORD
    REJECTED
TDB_USER: res ph bcc_dis b2_ord
    BCC_DIS          B2_ORD  RESTORED
TDB_USER: get
19:07:16,332 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS .....
INFO: Forcing option USE_POLY3 for complex phase B2_ORD
-OK-
TDB_USER: go -m
NO TIME STEP DEFINED
DIC> set-cond glob T 0 1277; * N
DIC>
DIC> enter-region beta
DIC>
DIC> enter-grid beta
WIDTH OF REGION /1/: 2e-3
TYPE /LINEAR/: double
NUMBER OF POINTS /50/: 50
VALUE OF R IN THE GEOMETRICAL SERIE FOR LOWER PART OF REGION: 0.85
VALUE OF R IN THE GEOMETRICAL SERIE FOR UPPER PART OF REGION: 1.1765
DIC>
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /BETA/: beta
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: b2_ord
DIC>
DIC> enter-composition
REGION NAME : /BETA/: beta
PHASE NAME: /B2_ORD/: b2_ord
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: mole-fraction
PROFILE FOR /AL/: ni
TYPE /LINEAR/: function
Function F(X)= 0.28-0.277*erf((x-1e-3)/3e-6);
PROFILE FOR /NI/: al
TYPE /LINEAR/: function
Function F(X)= 0.4295-0.0105*erf((x-1e-3)/3e-6);
19:07:16,933 [Thread-0] INFO Database: Preparing system for use: USER_1737920627_14
19:07:17,770 [Thread-0] INFO Phase: Preparing phase for use: B2_ORD
19:07:18,265 [Thread-0] INFO Phase: Preparing phase for use: BCC_DIS
DIC>
DIC> set-simulation-time
END TIME FOR INTEGRATION ./1/: 345600
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /34560/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC> s-a-s-v
AUTOMATIC STARTING VALUES FOR PHASE COMPOSITIONS /YES/: no
START VALUES FOR PHASES IN REGION BETA
PHASE: B2_ORD
MAJOR CONSTITUENTS IN PHASE B2_ORD: NI;AL
DIC>
DIC>
DIC>
DIC>
DIC>
```

```
DIC> save exil yes
DIC>
DIC> set-inter
--OK---
DIC>
```

**exil-run**

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exil\run.DCM.test"
DIC>
DIC>
DIC> @@ exil_run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING EXAMPLE i1
DIC> @@
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 0.00000E+00
DIC> read exil
OK
DIC>
DIC> @@
DIC> @@ START THE SIMULATION
DIC> @@
DIC> sim
DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
INFO: FORCED STARTING VALUES TURNED ON
U-FRACTION IN SYSTEM: AL = .429499345639258 FE = .290517917020317
NI = .279982737340425
TOTAL SIZE OF SYSTEM: .002 [m]
U-FRACTION IN SYSTEM: AL = .429499345639258 FE = .290517917020317
NI = .279982737340425
TOTAL SIZE OF SYSTEM: .002 [m]
6 GRIDPOINT(S) ADDED TO CELL #1 REGION: BETA
TIME = 0.1000000E-06 DT = 0.1000000E-06 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: AL = .429499345639258 FE = .290517917020317
NI = .279982737340425
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 4 seconds
TIME = 0.1001000E-03 DT = 0.1000000E-03 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: AL = .429499345639258 FE = .290517917020317
NI = .279982737340425
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 0 seconds
TIME = 0.40010010 DT = 0.40000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: AL = .429499345639258 FE = .290517917020317
NI = .279982737340425
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 1 seconds
TIME = 513.08856 DT = 512.68846 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: AL = .429499345639248 FE = .290517917020327
NI = .279982737340426
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 1 seconds
TIME = 1538.4655 DT = 1025.3769 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: AL = .429499345639234 FE = .290517917020342
NI = .279982737340425
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 1 seconds
TIME = 3589.2193 DT = 2050.7538 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: AL = .429499345639231 FE = .290517917020345
NI = .279982737340424
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 0 seconds
TIME = 7690.7270 DT = 4101.5077 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: AL = .429499345639227 FE = .290517917020345
NI = .279982737340428
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 1 seconds
TIME = 15893.742 DT = 8203.0154 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: AL = .429499345639233 FE = .290517917020342
NI = .279982737340425
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 2 seconds
TIME = 32299.773 DT = 16406.031 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: AL = .429499345639211 FE = .290517917020362
NI = .279982737340427
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 1 seconds
TIME = 65111.835 DT = 32812.062 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: AL = .429499345639174 FE = .290517917020382
NI = .279982737340444
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 1 seconds
TIME = 99671.835 DT = 34560.000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: AL = .429499345639089 FE = .290517917020496
NI = .279982737340415
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 2 seconds
TIME = 134231.83 DT = 34560.000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: AL = .429499345639132 FE = .290517917020483
NI = .279982737340386
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 1 seconds
TIME = 168791.83 DT = 34560.000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: AL = .429499345639167 FE = .290517917020446
NI = .279982737340387
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 1 seconds
TIME = 203351.83 DT = 34560.000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: AL = .429499345639157 FE = .290517917020456
NI = .279982737340387
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 1 seconds
TIME = 237911.83 DT = 34560.000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: AL = .429499345639151 FE = .290517917020441
NI = .279982737340408
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 1 seconds
TIME = 272471.83 DT = 34560.000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: AL = .429499345639152 FE = .290517917020425
NI = .279982737340423
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 1 seconds
```

```
TIME = 307031.83 DT = 34560.000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: AL = .42949934563916 FE = .290517917020412
NI = .279982737340428
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 1 seconds
TIME = 341591.83 DT = 34560.000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: AL = .429499345639172 FE = .290517917020402
NI = .279982737340425
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 1 seconds
TIME = 345600.00 DT = 4008.1652 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: AL = .429499345639173 FE = .290517917020401
NI = .279982737340426
TOTAL SIZE OF SYSTEM: .002 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 0.0000000
DELETING TIME-RECORD FOR TIME 0.1000000E-06
DELETING TIME-RECORD FOR TIME 0.10010000E-03
DELETING TIME-RECORD FOR TIME 0.40010010
DELETING TIME-RECORD FOR TIME 513.08856
DELETING TIME-RECORD FOR TIME 1538.4655
DELETING TIME-RECORD FOR TIME 3589.2193
DELETING TIME-RECORD FOR TIME 7690.7270
DELETING TIME-RECORD FOR TIME 15893.742
DELETING TIME-RECORD FOR TIME 32299.773
DELETING TIME-RECORD FOR TIME 65111.835
DELETING TIME-RECORD FOR TIME 99671.835
DELETING TIME-RECORD FOR TIME 134231.83
DELETING TIME-RECORD FOR TIME 168791.83
DELETING TIME-RECORD FOR TIME 203351.83
DELETING TIME-RECORD FOR TIME 237911.83
DELETING TIME-RECORD FOR TIME 272471.83
DELETING TIME-RECORD FOR TIME 307031.83

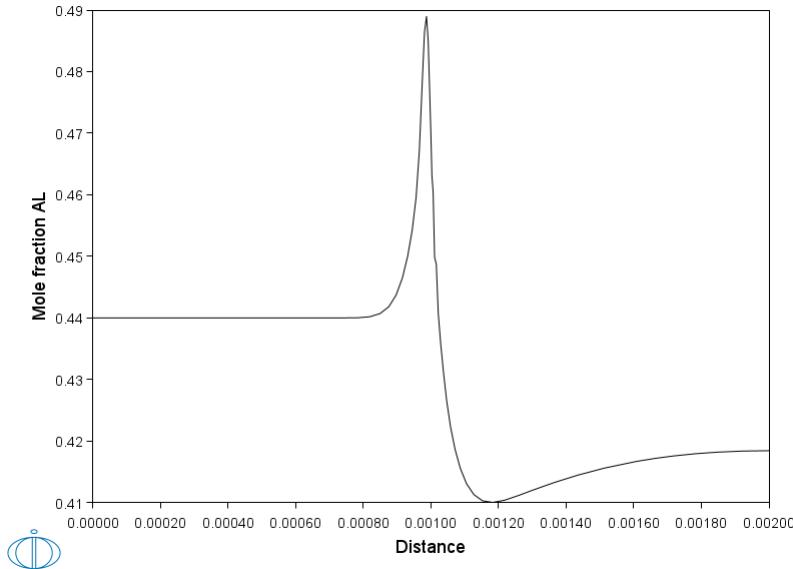
KEEPING TIME-RECORD FOR TIME 341591.83
AND FOR TIME 345600.00
WORKSPACE RECLAIMED
```

TIMESTEP AT 345600.000 SELECTED

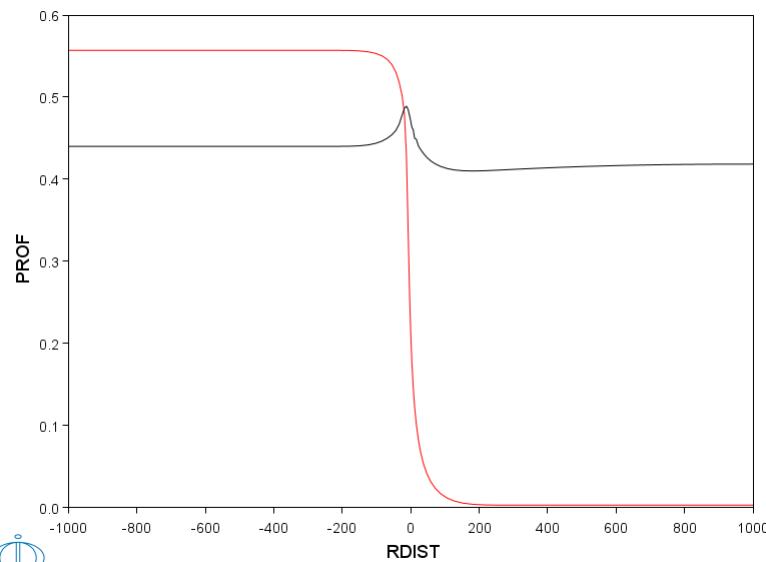
DIC>
DIC> set-inter
--OK---
DIC>

## exil-plot

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exil\plot.DCM.test"
DIC>
DIC> @@ exil_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE i1
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 3.45600E+05
DIC> read exil
OK
DIC>
DIC> @@
DIC> @@ ENTER THE POST PROCESSOR
DIC> @@
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1: s-d-a x dist glob
INFO: Distance is set as independent variable
POST-1:
POST-1: s-d-a y m-f al
POST-1:
POST-1: s-p-c time last
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```



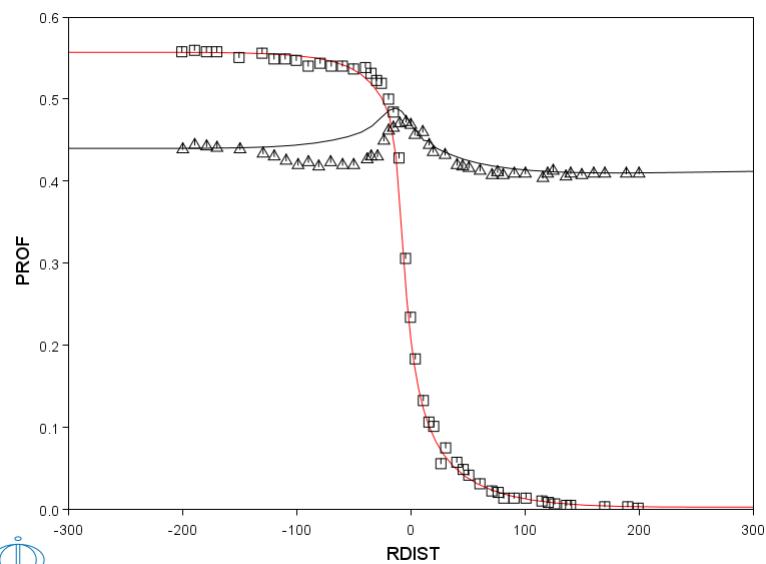
```
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: ent tab prof
Variable(s) x(al) x(ni)
POST-1:
POST-1: ent fun rdist
FUNCTION: 1e6*(gd-10e-4)
&
POST-1: s-d-a y prof
COLUMN NUMBER /*/: 1 2
POST-1:
POST-1: s-d-a x rdist
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```



```

POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: app y exil.exp
PROLOGUE NUMBER: /0/: 1
DATASET NUMBER(s): /-1/: 1
POST-1:
POST-1: s-s-s x n -300 300
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

```



```

POST-1:
POST-1:
POST-1: set-inter
--OK--
POST-1:

```

**exi2-setup****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_dictra_console_examples\examples\exi2\setup.DCM.test"
SYS: @@
SYS: @@ Diffusion in complex phases.
SYS: @@ Diffusion of carbon in cementite
SYS: @@ This example demonstrates the use of the model for calculation of
SYS: @@ diffusion through a stoichiometric phase. The flux of a component in
SYS: @@ the stoichiometric phase is assumed to be proportional to the
SYS: @@ difference in chemical potential at each side of the stoichiometric
SYS: @@ phase multiplied with the mobility for the component in the phase. The
SYS: @@ mobility is assessed from experimental information and is basically
SYS: @@ the tracer diffusivity for the component.
SYS: @@
SYS: @@ This calculation is compared with experimental data where a sample of
SYS: @@ pure iron has been exposed to a gas atmosphere with a certain carbon
SYS: @@ activity. The weight gain is then measured as a function of time.
SYS: @@ The experimental data is obtained from Ozturk B., Fearing V. L.,
SYS: @@ Ruth A. Jr. and Simkovich G., Met. Trans A, vol 13A (1982), pp. 1871-1873.
SYS: -----
NO SUCH COMMAND, USE HELP
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASES
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\generate_dictra_console_examples\databases\data
Current database: Steels/Fe-Alloys v12.0

VA           /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE12: @@
TDB_TCFE12: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA
TDB_TCFE12: @@
TDB_TCFE12: switch FEDEMO
Current database: Iron Demo Database v4.0

VA           /- DEFINED
TDB_FEDEMO: def-sys fe c           C DEFINED
TDB_FEDEMO: rej ph * all
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 bcc fcc cementite grap
BCC_A2          FCC_A1           CEMENTITE
GRAPHITE RESTORED
TDB_FEDEMO: get
19:10:51,598 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS .....
FUNCTIONS .....

List of references for assessed data

'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'
'X.G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
'A.T. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
'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'
'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121 -127; Molar
volumes'
-OK-
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE MOBILITY DATA
TDB_FEDEMO: @@
TDB_FEDEMO: app user cembccstoik.TDB
Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

VA DEFINED
19:10:51,796 [Thread-0] INFO TDBfileParser: USER_529217061_14, number of lines read: 51
19:10:51,854 [Thread-0] INFO DatabaseUtils: Parsing of USER_529217061_14 completed in 85 ms
TDB_APP: def-sys fe c           C DEFINED
TDB_APP: rej ph * all
BCC_A2          CEMENTITE REJECTED
TDB_APP: res ph fcc bcc cementite
*** ERROR FCC INPUT IGNORED
BCC_A2          CEMENTITE RESTORED
TDB_APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
```

```

FUNCTIONS ....
-OK-
TDB_APP:
TDE_APP: @@
TDE_APP: @@ ENTER THE DICTRA MONITOR
TDB_APP: @@
TDE_APP: go d-m
NO TIME STEP DEFINED
*** ENTERING FCC_A1 AS A DIFFUSION NONE PHASE
*** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
DIC>
DIC> set-ref c grap,.....
19:10:52,410 [Thread-0] INFO Database: Preparing system for use: USER_529217061_14
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob t 0 723; * n
DIC>
DIC> @@
DIC> @@ ENTER THE REGIONS carb AND fer
DIC> @@
DIC> enter-region
REGION NAME : fer
DIC>
DIC> enter-region
REGION NAME : carb
ATTACH TO REGION NAMED /FER/:
ATTACHED TO THE RIGHT OF FER /YES/:
DIC> @@
DIC> @@ ENTER LINEAR GRIDS INTO THE REGIONS
DIC> @@
DIC>
DIC> @@
DIC> @@ ENTER A SIZE FOR THE FERRITE
DIC> @@
DIC> enter-grid
REGION NAME : /FER/: fer
WIDTH OF REGION /1/: 3.3E-6
TYPE /LINEAR/: AUTO
DIC>
DIC> @@
DIC> @@ ENTER A SIZE (VERY SMALL) FOR THE CEMENTITE LAYER
DIC> @@
DIC> @@
DIC> enter-grid
REGION NAME : /CARB/: carb
WIDTH OF REGION /1/: 1E-12
TYPE /LINEAR/: AUTO
DIC>
DIC>
DIC> @@
DIC> @@ ENTER PHASES INTO THE REGIONS
DIC> @@
DIC> enter-phase act carb matrix cementite
COMPOSITION RECORD FOR STOICHIOMETRIC PHASE CEMENTITE IN REGION CARB CREATED
DIC> enter-phase act fer matrix bcc#1
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITIONS IN THE PHASES
DIC> @@
DIC> enter-composition
REGION NAME : /FER/: carb
PHASE NAME: /CEMENTITE/: cementite
DIC>
DIC> enter-composition
REGION NAME : /FER/: fer
PHASE NAME: /BCC_A2/: bcc#1
COMPOSITION TYPE /MOLE_FRACTION/: weig-fraction
PROFILE FOR /C/: C lin 1E-5 1E-5
19:10:53,378 [Thread-0] INFO Phase: Preparing phase for use: BCC_A2
DIC>
DIC> set-cond bound upp
CONDITION TYPE /CLOSED_SYSTEM/: mix
Dependent substitutional element:FE
Dependent interstitial element:VA
LOW TIME LIMIT /0/: 0
ACR(C)(TIME)= 9;
HIGH TIME LIMIT /*/: *
ANY MORE RANGES /N/: N
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ SIMULATE FOR 150 MINUTES
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 9000
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /900/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exi2 Y
DIC>
DIC> set-inter
--OK---
DIC>
```

**exi2-run**

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exi2\run.DCM.test"
DIC>
DIC>
DIC> @@ exi2_run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING EXAMPLE i2
DIC> @@
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 0.00000E+00
*** ENTERING FCC_A1 AS A DIFFUSION NONE PHASE
*** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
DIC> read exi2
OK
DIC>
DIC> @@
DIC> @@ START THE SIMULATION
DIC> @@
DIC> sim
Region: FER
single geometric dense at 0.33000E-05
0.91945 87
Region: CARB
double geometric
dense at outer boundaries, coarse at 0.50000E-12
lower part 1.2500 9
upper part 0.80000 9
DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
Trying old scheme 3
U-FRACTION IN SYSTEM: C = 4.6598005784384E-05 FE = 1
TOTAL SIZE OF SYSTEM: 3.300001E-06 [m]
U-FRACTION IN SYSTEM: C = 4.6598005784384E-05 FE = 1
TOTAL SIZE OF SYSTEM: 3.300001E-06 [m]
19:11:49,153 [Thread-0] INFO Phase: Preparing phase for use: CEMENTITE
0.111094107740055 0.111116327660160 1.168933545268372E-022 TIME = 0.10000000E-06 DT = 0.10000000E-06
06 SUM OF SQUARES = 0.11689335E-21
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.55732855E-06 AND -0.55732855E-06
POSITION OF INTERFACE FER / CARB IS 0.32999999E-05
U-FRACTION IN SYSTEM: C = 4.65969237107415E-05 FE = 1
TOTAL SIZE OF SYSTEM: 3.300001E-06 [m]
2 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: FER

CPU time used in timestep 0 seconds
1.985503622653896E-006 1.986016682715921E-006 8.569006692077880E-023 TIME = 0.25999666E-05 DT = 0.24999666E-05
05 SUM OF SQUARES = 0.85690067E-22
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.12341808E-06 AND -0.12341808E-06
POSITION OF INTERFACE FER / CARB IS 0.32999996E-05
U-FRACTION IN SYSTEM: C = 4.66223850218017E-05 FE = 1
TOTAL SIZE OF SYSTEM: 3.300001E-06 [m]
CPU time used in timestep 0 seconds
9.632817666939915E-007 9.640732404382838E-007 1.188386949892457E-025 TIME = 0.75998999E-05 DT = 0.49999333E-05
05 SUM OF SQUARES = 0.11883869E-24
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.91502734E-07 AND -0.91502734E-07
POSITION OF INTERFACE FER / CARB IS 0.32999992E-05
U-FRACTION IN SYSTEM: C = 4.66617913784151E-05 FE = 1
TOTAL SIZE OF SYSTEM: 3.300001E-06 [m]
CPU time used in timestep 0 seconds
5.520598281728859E-007 5.525040595679611E-007 1.288882881968142E-026 TIME = 0.17599767E-04 DT = 0.99998666E-04
05 SUM OF SQUARES = 0.12888829E-25
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.67380405E-07 AND -0.67380405E-07
POSITION OF INTERFACE FER / CARB IS 0.32999985E-05
U-FRACTION IN SYSTEM: C = 4.67208116371187E-05 FE = 1
TOTAL SIZE OF SYSTEM: 3.300001E-06 [m]
CPU time used in timestep 1 seconds
3.294904029785889E-007 3.297431202262135E-007 1.295444436331959E-026 TIME = 0.37599500E-04 DT = 0.19999733E-04
04 SUM OF SQUARES = 0.12954444E-25
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.48810906E-07 AND -0.48810906E-07
POSITION OF INTERFACE FER / CARB IS 0.32999975E-05
U-FRACTION IN SYSTEM: C = 4.68069809139129E-05 FE = 1
TOTAL SIZE OF SYSTEM: 3.300001E-06 [m]
CPU time used in timestep 0 seconds
1.842051604944532E-007 1.843420424822769E-007 2.883351411658548E-025 TIME = 0.77598966E-04 DT = 0.39999466E-04
04 SUM OF SQUARES = 0.28833514E-24
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.34957854E-07 AND -0.34957854E-07
POSITION OF INTERFACE FER / CARB IS 0.32999961E-05
U-FRACTION IN SYSTEM: C = 4.69308608646657E-05 FE = 1
TOTAL SIZE OF SYSTEM: 3.300001E-06 [m]
14 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: CARB

CPU time used in timestep 0 seconds
9.778279834954450E-008 9.785422397002206E-008 4.591163632256574E-026 TIME = 0.15759790E-03 DT = 0.79998933E-03
04 SUM OF SQUARES = 0.45911636E-25
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.24876846E-07 AND -0.24876846E-07
POSITION OF INTERFACE FER / CARB IS 0.32999941E-05
U-FRACTION IN SYSTEM: C = 4.7107484088289E-05 FE = 1
TOTAL SIZE OF SYSTEM: 3.300001E-06 [m]
49 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: CARB

CPU time used in timestep 0 seconds
5.038045607978919E-006 5.041694023512990E-006

output ignored...

... output resumed

TIME = 3142.1594 DT = 900.00000 SUM OF SQUARES = 0.30569333E-26
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.44854482E-11 AND -0.44854482E-11
POSITION OF INTERFACE FER / CARB IS 0.32722305E-05
U-FRACTION IN SYSTEM: C = .00283057618776268 FE = 1
TOTAL SIZE OF SYSTEM: 3.300001E-06 [m]
55 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: CARB

CPU time used in timestep 0 seconds
3.512901236232409E-008 3.518395504427621E-008 9.883740367838172E-
```

029 TIME = 4042.1594 DT = 900.00000 SUM OF SQUARES = 0.98837404E-28  
 CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.38334138E-11 AND -0.38334138E-11  
 POSITION OF INTERFACE FER / CARB IS 0.32687804E-05  
 U-FRACTION IN SYSTEM: C = .00317904137490982 FE = 1  
 TOTAL SIZE OF SYSTEM: 3.300001E-06 [m]  
 9 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: CARB

CPU time used in timestep 0 seconds  
 1.337273691247514E-008 1.340171249957068E-008 1.438479107187262E-  
 026 TIME = 4942.1594 DT = 900.00000 SUM OF SQUARES = 0.14384791E-25  
 CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.34097971E-11 AND -0.34097971E-11  
 POSITION OF INTERFACE FER / CARB IS 0.32657116E-05  
 U-FRACTION IN SYSTEM: C = .00348899893656291 FE = 1  
 TOTAL SIZE OF SYSTEM: 3.300001E-06 [m]  
 9 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: CARB

CPU time used in timestep 0 seconds  
 6.238597392600730E-009 6.256204152659696E-009 5.094464669698199E-  
 030 TIME = 5842.1594 DT = 900.00000 SUM OF SQUARES = 0.50944647E-29  
 CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.31046285E-11 AND -0.31046285E-11  
 POSITION OF INTERFACE FER / CARB IS 0.32629174E-05  
 U-FRACTION IN SYSTEM: C = .00377121604704377 FE = 1  
 TOTAL SIZE OF SYSTEM: 3.300001E-06 [m]  
 20 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: CARB

CPU time used in timestep 0 seconds  
 3.280281446311425E-009 3.291907995787571E-009 1.615191351151320E-  
 030 TIME = 6742.1594 DT = 900.00000 SUM OF SQUARES = 0.16151914E-29  
 CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.28707015E-11 AND -0.28707015E-11  
 POSITION OF INTERFACE FER / CARB IS 0.32603338E-05  
 U-FRACTION IN SYSTEM: C = .00403216870914809 FE = 1  
 TOTAL SIZE OF SYSTEM: 3.300001E-06 [m]  
 6 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: CARB

CPU time used in timestep 0 seconds  
 1.864873577374436E-007 1.872981046725814E-007 2.114851935796025E-  
 029 TIME = 7642.1594 DT = 900.00000 SUM OF SQUARES = 0.21148519E-28  
 CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.26837249E-11 AND -0.26837249E-11  
 POSITION OF INTERFACE FER / CARB IS 0.32579185E-05  
 U-FRACTION IN SYSTEM: C = .00427612481768566 FE = 1  
 TOTAL SIZE OF SYSTEM: 3.300001E-06 [m]  
 7 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: CARB

CPU time used in timestep 0 seconds  
 1.118941665778596E-007 1.124814013230816E-007 5.830945499626795E-  
 030 TIME = 8542.1594 DT = 900.00000 SUM OF SQUARES = 0.58309455E-29  
 CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.25296909E-11 AND -0.25296909E-11  
 POSITION OF INTERFACE FER / CARB IS 0.32556417E-05  
 U-FRACTION IN SYSTEM: C = .00450607892012324 FE = 1  
 TOTAL SIZE OF SYSTEM: 3.300001E-06 [m]  
 6 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: CARB

CPU time used in timestep 0 seconds  
 6.975845442326852E-008 7.019562008375879E-008 9.016845897022004E-  
 030 TIME = 9000.0000 DT = 457.84063 SUM OF SQUARES = 0.90168459E-29  
 CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.23998555E-11 AND -0.23998555E-11  
 POSITION OF INTERFACE FER / CARB IS 0.32545430E-05  
 U-FRACTION IN SYSTEM: C = .00461705531635743 FE = 1  
 TOTAL SIZE OF SYSTEM: 3.300001E-06 [m]  
 MUST SAVE WORKSPACE ON FILE  
 WORKSPACE SAVED ON FILE  
 RECLAIMING WORKSPACE  
 DELETING TIME-RECORD FOR TIME 0.0000000  
 DELETING TIME-RECORD FOR TIME 0.10000000E-06  
 DELETING TIME-RECORD FOR TIME 0.25999666E-05  
 DELETING TIME-RECORD FOR TIME 0.75998999E-05  
 DELETING TIME-RECORD FOR TIME 0.17599767E-04  
 DELETING TIME-RECORD FOR TIME 0.37599500E-04  
 DELETING TIME-RECORD FOR TIME 0.77598966E-04  
 DELETING TIME-RECORD FOR TIME 0.15759790E-03  
 DELETING TIME-RECORD FOR TIME 0.31759576E-03  
 DELETING TIME-RECORD FOR TIME 0.63759149E-03  
 DELETING TIME-RECORD FOR TIME 0.12775830E-02  
 DELETING TIME-RECORD FOR TIME 0.25575659E-02  
 DELETING TIME-RECORD FOR TIME 0.51175317E-02  
 DELETING TIME-RECORD FOR TIME 0.10237463E-01  
 DELETING TIME-RECORD FOR TIME 0.20477327E-01  
 DELETING TIME-RECORD FOR TIME 0.40957054E-01  
 DELETING TIME-RECORD FOR TIME 0.81916507E-01  
 DELETING TIME-RECORD FOR TIME 0.16383541  
 DELETING TIME-RECORD FOR TIME 0.32767323  
 DELETING TIME-RECORD FOR TIME 0.65534886  
 DELETING TIME-RECORD FOR TIME 1.3107001  
 DELETING TIME-RECORD FOR TIME 2.6214026  
 DELETING TIME-RECORD FOR TIME 5.2428076  
 DELETING TIME-RECORD FOR TIME 10.485618  
 DELETING TIME-RECORD FOR TIME 20.971238  
 DELETING TIME-RECORD FOR TIME 41.942478  
 DELETING TIME-RECORD FOR TIME 83.884958  
 DELETING TIME-RECORD FOR TIME 167.76992  
 DELETING TIME-RECORD FOR TIME 335.53984  
 DELETING TIME-RECORD FOR TIME 671.07968  
 DELETING TIME-RECORD FOR TIME 1342.1594  
 DELETING TIME-RECORD FOR TIME 2242.1594  
 DELETING TIME-RECORD FOR TIME 3142.1594  
 DELETING TIME-RECORD FOR TIME 4042.1594  
 DELETING TIME-RECORD FOR TIME 4942.1594  
 DELETING TIME-RECORD FOR TIME 5842.1594  
 DELETING TIME-RECORD FOR TIME 6742.1594  
 DELETING TIME-RECORD FOR TIME 7642.1594

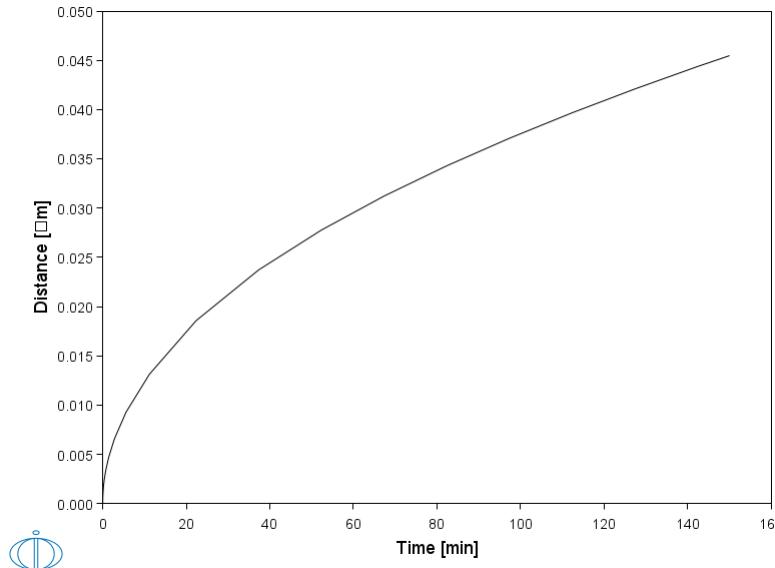
KEEPING TIME-RECORD FOR TIME 8542.1594  
 AND FOR TIME 9000.0000  
 WORKSPACE RECLAIMED

TIMESTEP AT 9000.00000 SELECTED

**DIC>**  
**DIC> set-inter**  
**--OK--**  
**DIC>**

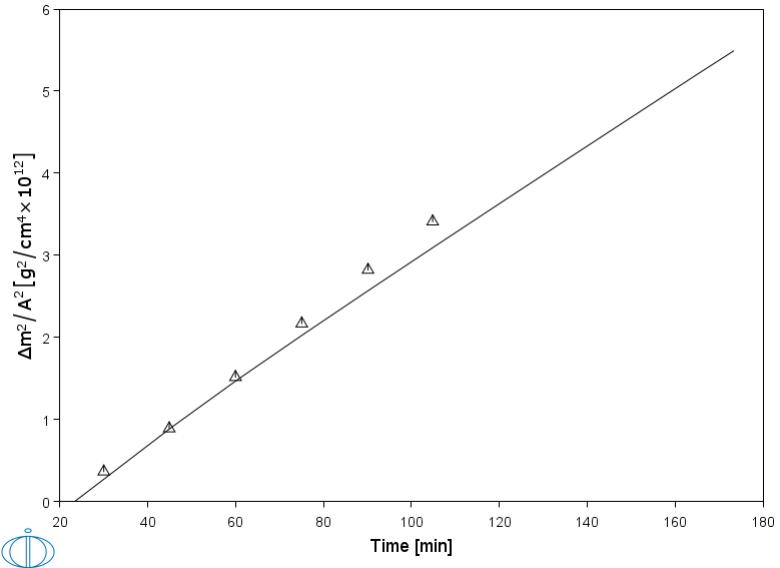
## exi2-plot

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exi2\plot.DCM.test"
DIC>
DIC> @@ exi2_plot.DCM
DIC>
DIC> @@
DIC> FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE i2
DIC> @@
DIC>
DIC> @@
DIC> GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 9.00000E+03
*** ENTERING FCC_A1 AS A DIFFUSION NONE PHASE
*** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
DIC>
DIC>
DIC> read exi2 Y
OK
DIC>
DIC>
DIC> @@
DIC> @@ PLOT THE SIZE OF THE CEMENTITE LAYER AS A FUNCTION OF TIME
DIC> @@
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1: ent-symb func csize
FUNCTION: 1e6*(poi(car,u)-poi(car,l));
POST-1:
POST-1: ent-symb func minutes
FUNCTION: time/60;
POST-1:
POST-1: s-d-a x minutes
POST-1: s-d-a y csize
POST-1:
POST-1: s-p-c inter first
POST-1:
POST-1: s-a-t-s x n Time [min]
POST-1: s-a-t-s y n Distance [ $\mu$ m]
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```



```
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1:
POST-1: @@
POST-1: @@ ASSUME A CERTAIN TIME FOR NUCLEATION OF THE CEMENTITE LAYER
POST-1: @@
POST-1: ent-symb func cortim
FUNCTION: (time+1400)/60;
POST-1:
POST-1: @@
POST-1: @@ PLOT THE WEIGHT GAIN AS A FUNCTION OF TIME
POST-1: @@
POST-1: ent-symb func cwei
FUNCTION: 1e12*((poi(car,u)-poi(car,l)-1E-12)*12.01/2.33E-5*1e-4)**2;
POST-1:
POST-1:
POST-1: s-d-a x cortim
POST-1: s-d-a y cwei
POST-1:
POST-1: @@
POST-1: @@ COMPARE WITH EXPERIMENTAL DATA
POST-1: @@
POST-1: app y exi2.exp 0; 1
POST-1:
POST-1:
```

```
POST-1: s-a-t-s x n Time [min]
POST-1: s-a-t-s y n \Delta m^2/A^2, [g^2/cm^4\times 10^{12}]
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```



```
POST-1:
POST-1:
POST-1: set-inter
--OK---
POST-1:
```

**exi3a-setup****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_dictra_console_examples\examples\exi3a\setup.DCM.test"
SYS: @@
SYS: @@ Diffusion in complex phases.
SYS: @@ Diffusion in iron oxide (FeO)
SYS: @@ This example shows the oxidation of an iron sample and the
SYS: @@ consequent growth of an oxide layer.
SYS: -----
NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exi3_setup.DCM
SYS:
SYS: @@
SYS: @@ START BY GOING TO THE DATABASE MODULE
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\generate_dictra_console_examples\databases\data
Current database: Steels/Fe-Alloys v12.0

VA          /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE12: @@
TDB_TCFE12: @@ SELECT A USER DATABASE FOR READING THE THERMODYNAMIC DATA
TDB_TCFE12: @@
TDB_TCFE12: sw user FeO.TDB
Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

VA          /- DEFINED
19:14:08,077 [Thread-0] INFO  TDBfileParser: USER_1296293566_14, number of lines read: 217
19:14:08,241 [Thread-0] INFO  DatabaseUtils: Parsing of USER_1296293566_14 completed in 213 ms
TDB_USER: def-sys fe o
FE          O DEFINED
TDB_USER: rej sp *
/-           VA          FE
O            FE+2        FE+3
FE+4         FE2O3       FEO
FEO3/2       O-2         O2
REJECTED
TDB_USER: res sp fe fe+2 fe+3 o o2 o-2 va
FE          FE+2        FE+3
O            O2          O-2
VA RESTORED
TDB_USER: rej ph * all
GAS:G        BCC_A2      SPINEL:I
REJECTED
TDB_USER: res ph bcc spinel gas
BCC_A2      SPINEL:I      GAS:G
RESTORED
TDB_USER:
TDB_USER: get
19:14:08,317 [Thread-0] INFO  JavaWrapper: *** Invoking Gibbs Energy System v6 ***
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ...

List of references for assessed data

'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317 -425'
'M. Kowalski and P.J. Spencer, Calphad, 19 (1995), 229-243; Cr-O, Fe-O and
Ni-O'
'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'
'B. Sundman, J. Phase Equil., 12 (1991), 127-140; Fe-O'
-OK-
*** WARNING: One or more elements have been rejected only as species but not as elements. This is not allowed with GES6, temporarily reverting

TDB_USER:
TDB_USER: @@
TDB_USER: @@ SWITCH TO A USER-DEFINED MOBILITY DATABASE TO RETRIEVE MOBILITY DATA
TDB_USER: @@
TDB_USER: app user FeOmob.TDB
Current database: User defined Database
test database

VA          /-          O
DEFINED
19:14:08,370 [Thread-0] INFO  TDBfileParser: USER_866996310_14, number of lines read: 129
19:14:08,395 [Thread-0] INFO  DatabaseUtils: Parsing of USER_866996310_14 completed in 26 ms
TDB_APP: def-sys fe o
FE          O DEFINED
TDB_APP: rej sp *
/-           VA          FE
O            FE+2        FE+3
FE2O3        FEO         FEO3/2
O-2          O2          O-2
REJECTED
TDB_APP: res sp fe fe+2 fe+3 o o2 o-2 va
FE          FE+2        FE+3
O            O2          O-2
VA RESTORED
TDB_APP: rej ph * all
```

```

SPINEL:I           GAS:G          BCC_A2
REJECTED
TDB_APP: res ph bcc spinel gas      SPINEL:I          GAS:G
BCC_A2
RESTORED
TDB_APP:
TDB_APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
*** ERROR 2018 IN DESHPH: DIFFUSION DATA NOT POSSIBLE FOR GAS PHASE
*** ERROR 2018 IN DESHPH: DIFFUSION DATA NOT POSSIBLE FOR GAS PHASE
FUNCTIONS .....
-OK-
TDB_APP:
TDB_APP:
TDB_APP: @@ @
TDB_APP: @@ ENTER THE DICTRA MONITOR
TDB_APP: @@
TDB_APP: go d-m
NO TIME STEP DEFINED
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 823; * N
DIC>
DIC>
DIC> @@
DIC> @@ SET THE REFERENCE STATE FOR O TO O2 (GAS)
DIC> @@
DIC> set-ref o gas,,,,,,,
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE REGIONS fer AND sp
DIC> @@
DIC> ent-reg fer
DIC> ent-reg sp,,,,,,,
DIC>
DIC>
DIC> @@
DIC> @@ ENTER PHASES INTO THE REGIONS
DIC> @@
DIC> ent-phase act fer matrix bcc#1
DIC> ent-phase act sp matrix spinel
DIC>
DIC>
DIC> @@
DIC> @@ ENTER GRIDS INTO THE REGIONS
DIC> @@
DIC>
DIC> @@
DIC> @@ ENTER A SIZE FOR THE FERRITE
DIC> @@
DIC> ent-grid fer 4.99999e-3 AUTO
DIC>
DIC> @@
DIC> @@ ENTER A THIN INITIAL SIZE FOR THE OXIDE
DIC> @@
DIC> ent-grid sp 1.00e-10 AUTO
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITIONS IN BCC
DIC> @@
DIC> ent-comp fer bcc#1 m-f
PROFILE FOR /O/: o lin 1e-9 1e-9
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITIONS IN THE OXIDE
DIC> @@
DIC> ent-comp sp spinel m-f
this is a phase with charged species
with more than 2 sublattices
PROFILE FOR /FE/: FE lin 4.28771E-01 4.28549E-01
DIC>
DIC>
DIC> @@
DIC> @@ ENTER A BOUNDARY CONDITION "GAS" ON THE UPPER (RIGHT-MOST) INTERFACE
DIC> @@ OF THE OXIDE. THIS ALLOWS THE SYSTEM TO EXPAND AND THE OXIDE LAYER
DIC> @@ TO GROW EXTERNALLY. FOR THIS EXAMPLE AN OXYGEN ACTIVITY IS SPECIFIED
DIC> @@ THAT IS LOW ENOUGH NOT TO FORM CORUNDUM (FE2O3). WE ALSO SPECIFY
DIC> @@ THAT THERE IS NO FLUX OF Fe ACROSS THIS INTERFACE, I.E. NO Fe
DIC> @@ IS ALLOWED TO ENTER OR LEAVE THE SYSTEM.
DIC> @@
DIC> set-cond boundary upper gas
TYPE OF CONDITION FOR COMPONENT FE /ZERO_FLUX/: zero-flux
TYPE OF CONDITION FOR COMPONENT O /ZERO_FLUX/: act
LOW TIME LIMIT /0/: 0 4.5e-4; * N
DIC>
DIC>
DIC> @@
DIC> @@ ENTER START VALUES FOR THE INITIAL INTERFACE VELOCITIES
DIC> @@
DIC> s-a-s-v -1e-5 1e-5 yes
STARTING VALUES WILL BE TAKEN FROM PROFILES
DIC>
DIC>
DIC> @@
DIC> @@ SIMULATE FOR 24 HOURS
DIC> @@
DIC> s-s-time 86400,,
SMALLEST ACCEPTABLE Timestep : /1E-07/:
DIC>
DIC> @@

```

```
DIC> @@ SPECIFY THAT POTENTIALS AND NOT ACTIVITIES ARE VARIED AT THE PHASE
DIC> @@ INTERFACE. ALSO USE A FULLY IMPLICIT SCHEME FOR TIME INTEGRATION.
DIC> @@
DIC> s-s-c 0 1 1 YES POT YES YES 1 2.....,,
RELEASING OLD STARTING VALUES
DIC>
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exi3.DIC Y
DIC>
DIC> set-inter
--OK--
DIC>
```

exi3a-run

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exi3a\run.DCM.test"
DIC>
DIC>
DIC> @@ exi3_run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING EXAMPLE i3
DIC> @@
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 0.00000E+00
DIC> read exi3
OK
DIC>
DIC> @@
DIC> @@ START THE SIMULATION
DIC> @@
DIC> sim y
Region: FER
single geometric dense at 0.50000E-02
0.87701      95
Region: SP
double geometric
dense at outer boundaries, coarse at 0.50000E-10
lower part 1.2500      9
upper part 0.80000      9
Trying old scheme
U-FRACTION IN SYSTEM: FE = 0.99999999500542 O = 2.10000395011622E-08
TOTAL SIZE OF SYSTEM: .0049999901 [m]
U-FRACTION IN SYSTEM: FE = 0.99999999500542 O = 2.10000395011622E-08
TOTAL SIZE OF SYSTEM: .0049999901 [m]
0.347387301619801      0.347386528699714      0.347386701354949      4.618089872758388E-002      1.115613915594681E-
022    TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.89824625E-22
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.39646054E-03 AND 0.0000000
POSITION OF INTERFACE FER / SP IS 0.49999900E-02
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.66982674E-03 AND 0.0000000
POSITION OF INTERFACE SP / gas interface IS 0.49999901E-02
U-FRACTION IN SYSTEM: FE = 0.99999998954903 O = 3.44025119032269E-08
TOTAL SIZE OF SYSTEM: .0049999012734 [m]
9 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: FER

CPU time used in timestep          3 seconds
1.507552605991796E-005      1.507739146468342E-005      1.507822847288494E-005      2.226308397653058E-007      1.429909696475841E-
030    TIME = 0.30000000E-06 DT = 0.20000000E-06 SUM OF SQUARES = 0.13914844E-29
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.14849229E-03 AND 0.0000000
POSITION OF INTERFACE FER / SP IS 0.49999989E-02
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.20393047E-03 AND 0.0000000
POSITION OF INTERFACE SP / gas interface IS 0.49999901E-02
U-FRACTION IN SYSTEM: FE = 0.99999998713864 O = 4.25594164341045E-08
TOTAL SIZE OF SYSTEM: .0049999013842 [m]
CPU time used in timestep          0 seconds
1.398975101990497E-008      1.397926495092157E-008      1.395940586855521E-008      3.137487098349537E-011      2.138929520756234E-
033    TIME = 0.70000000E-06 DT = 0.40000000E-06 SUM OF SQUARES = 0.21332401E-32
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.14913262E-03 AND 0.0000000
POSITION OF INTERFACE FER / SP IS 0.49999989E-02
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.21655229E-03 AND 0.0000000
POSITION OF INTERFACE SP / gas interface IS 0.49999902E-02
U-FRACTION IN SYSTEM: FE = 0.99999998167656 O = 5.98849352760284E-08
TOTAL SIZE OF SYSTEM: .0049999016539 [m]
CPU time used in timestep          1 seconds
5.609742547833871E-007      5.611234846494888E-007      5.611264634780973E-007      2.444637653773242E-010      4.760752120830264E-
033    TIME = 0.15000000E-05 DT = 0.80000000E-06 SUM OF SQUARES = 0.46655371E-32
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.93393028E-04 AND 0.0000000
POSITION OF INTERFACE FER / SP IS 0.49999989E-02
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.13339356E-03 AND 0.0000000
POSITION OF INTERFACE SP / gas interface IS 0.49999902E-02
U-FRACTION IN SYSTEM: FE = 0.99999997507588 O = 8.12308039073763E-08
TOTAL SIZE OF SYSTEM: .0049999019739 [m]
23 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: SP

CPU time used in timestep          0 seconds
8.108701238761151E-006      8.112502966933972E-006      8.112138099331446E-006      1.121067578687688E-008      1.024782809510141E-
031    TIME = 0.31000000E-05 DT = 0.16000000E-05 SUM OF SQUARES = 0.99678912E-31
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.70760985E-04 AND 0.0000000
POSITION OF INTERFACE FER / SP IS 0.499999897E-02
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.10183290E-03 AND 0.0000000
POSITION OF INTERFACE SP / gas interface IS 0.49999902E-02
U-FRACTION IN SYSTEM: FE = 0.99999996490465 O = 1.13822384430487E-07
TOTAL SIZE OF SYSTEM: .0049999024711 [m]
35 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: SP

CPU time used in timestep          0 seconds
8.100481734384663E-006      8.103302413524720E-006      8.103162850445104E-006      7.195354225979485E-009      2.092379944463672E-
031    TIME = 0.63000000E-05 DT = 0.32000000E-05 SUM OF SQUARES = 0.20735720E-30
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.49011444E-04 AND 0.0000000

output ignored...

... output resumed

POSITION OF INTERFACE FER / SP IS 0.49497263E-02
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.85406534E-09 AND 0.0000000
POSITION OF INTERFACE SP / gas interface IS 0.50216007E-02
U-FRACTION IN SYSTEM: FE = .995601423066389 O = .0143132204530773
TOTAL SIZE OF SYSTEM: .005021600735 [m]
23 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: SP

CPU time used in timestep          0 seconds
2.789556770989041E-007      2.794057583234963E-007      2.793655766044823E-007      3.800585454066780E-010      4.890056499420716E-
034    TIME = 56943.895 DT = 8640.0000 SUM OF SQUARES = 0.21741944E-33
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.54743813E-09 AND 0.0000000
POSITION OF INTERFACE FER / SP IS 0.49449965E-02
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.78319309E-09 AND 0.0000000
POSITION OF INTERFACE SP / gas interface IS 0.50236377E-02
```

U-FRACTION IN SYSTEM: FE = .995194725257642 O = .0156544064678572  
 TOTAL SIZE OF SYSTEM: .00502363765793 [m]  
 8 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: SP

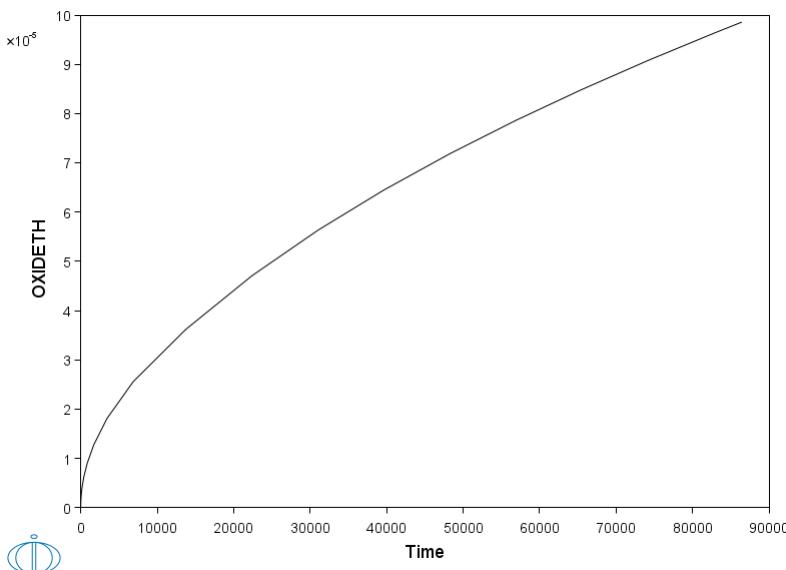
	CPU time used in timestep	0 seconds		
1.595105700626305E-007	1.598217866680118E-007	1.597953811596246E-007	2.020602968610680E-010	1.504632769052528E-
034 TIME = 65583.895 DT = 8640.0000	SUM OF SQUARES = 0.14745401E-33			
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.50751127E-09 AND 0.0000000				
POSITION OF INTERFACE FER / SP IS 0.49406116E-02				
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.72677808E-09 AND 0.0000000				
POSITION OF INTERFACE SP / gas interface IS 0.50255321E-02				
U-FRACTION IN SYSTEM: FE = .994817249745994 O = .0168979971924619				
TOTAL SIZE OF SYSTEM: .0050255321232 [m]				
7 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: SP				
CPU time used in timestep 0 seconds				
9.568367499961301E-008	9.590684464762445E-008	9.588874683500770E-008	1.147888046655320E-010	8.200248591336278E-
034 TIME = 74223.895 DT = 8640.0000	SUM OF SQUARES = 0.81927254E-33			
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.47495053E-09 AND 0.0000000				
POSITION OF INTERFACE FER / SP IS 0.49365080E-02				
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.68062878E-09 AND 0.0000000				
POSITION OF INTERFACE SP / gas interface IS 0.50273092E-02				
U-FRACTION IN SYSTEM: FE = .994463754813103 O = .0180617615442039				
TOTAL SIZE OF SYSTEM: .00502730918328 [m]				
10 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: SP				
CPU time used in timestep 0 seconds				
5.962030960627459E-008	5.978502100811573E-008	5.977212459374164E-008	6.869420013217193E-011	6.394689268473244E-
034 TIME = 82863.895 DT = 8640.0000	SUM OF SQUARES = 0.54843864E-33			
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.44778107E-09 AND 0.0000000				
POSITION OF INTERFACE FER / SP IS 0.49326392E-02				
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.64203085E-09 AND 0.0000000				
POSITION OF INTERFACE SP / gas interface IS 0.50289875E-02				
U-FRACTION IN SYSTEM: FE = .994130359456925 O = .0191587681410554				
TOTAL SIZE OF SYSTEM: .00502898750134 [m]				
8 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: SP				
CPU time used in timestep 0 seconds				
9.162180973783613E-009	9.108164932134297E-009	9.224421744015108E-009	1.011580317788514E-011	3.671303956488168E-
034 TIME = 86400.000 DT = 3536.1047	SUM OF SQUARES = 0.36412113E-33			
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.44500201E-09 AND 0.0000000				
POSITION OF INTERFACE FER / SP IS 0.49310656E-02				
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.61834793E-09 AND 0.0000000				
POSITION OF INTERFACE SP / gas interface IS 0.50296005E-02				
U-FRACTION IN SYSTEM: FE = .994008758985561 O = .0195911680901968				
TOTAL SIZE OF SYSTEM: .00502960047066 [m]				
MUST SAVE WORKSPACE ON FILE				
WORKSPACE SAVED ON FILE				
RECLAIMING WORKSPACE				
DELETING TIME-RECORD FOR TIME 0.0000000				
DELETING TIME-RECORD FOR TIME 0.10000000E-06				
DELETING TIME-RECORD FOR TIME 0.30000000E-06				
DELETING TIME-RECORD FOR TIME 0.70000000E-06				
DELETING TIME-RECORD FOR TIME 0.15000000E-05				
DELETING TIME-RECORD FOR TIME 0.31000000E-05				
DELETING TIME-RECORD FOR TIME 0.63000000E-05				
DELETING TIME-RECORD FOR TIME 0.12700000E-04				
DELETING TIME-RECORD FOR TIME 0.25500000E-04				
DELETING TIME-RECORD FOR TIME 0.51100000E-04				
DELETING TIME-RECORD FOR TIME 0.10230000E-03				
DELETING TIME-RECORD FOR TIME 0.20470000E-03				
DELETING TIME-RECORD FOR TIME 0.40950000E-03				
DELETING TIME-RECORD FOR TIME 0.81910000E-03				
DELETING TIME-RECORD FOR TIME 0.16383000E-02				
DELETING TIME-RECORD FOR TIME 0.32767000E-02				
DELETING TIME-RECORD FOR TIME 0.65535000E-02				
DELETING TIME-RECORD FOR TIME 0.13107100E-01				
DELETING TIME-RECORD FOR TIME 0.26214300E-01				
DELETING TIME-RECORD FOR TIME 0.52428700E-01				
DELETING TIME-RECORD FOR TIME 0.10485750				
DELETING TIME-RECORD FOR TIME 0.20971510				
DELETING TIME-RECORD FOR TIME 0.41943030				
DELETING TIME-RECORD FOR TIME 0.83886070				
DELETING TIME-RECORD FOR TIME 1.6777215				
DELETING TIME-RECORD FOR TIME 3.3554431				
DELETING TIME-RECORD FOR TIME 6.7108863				
DELETING TIME-RECORD FOR TIME 13.421773				
DELETING TIME-RECORD FOR TIME 26.843545				
DELETING TIME-RECORD FOR TIME 53.687091				
DELETING TIME-RECORD FOR TIME 107.37418				
DELETING TIME-RECORD FOR TIME 214.74836				
DELETING TIME-RECORD FOR TIME 429.49673				
DELETING TIME-RECORD FOR TIME 858.99346				
DELETING TIME-RECORD FOR TIME 1717.98669				
DELETING TIME-RECORD FOR TIME 3435.9738				
DELETING TIME-RECORD FOR TIME 6871.9477				
DELETING TIME-RECORD FOR TIME 13743.895				
DELETING TIME-RECORD FOR TIME 22383.895				
DELETING TIME-RECORD FOR TIME 31023.895				
DELETING TIME-RECORD FOR TIME 39663.895				
DELETING TIME-RECORD FOR TIME 48303.895				
DELETING TIME-RECORD FOR TIME 56943.895				
DELETING TIME-RECORD FOR TIME 65583.895				
DELETING TIME-RECORD FOR TIME 74223.895				
KEEPING TIME-RECORD FOR TIME 82863.895				
AND FOR TIME 86400.000				
WORKSPACE RECLAIMED				

TIMESTEP AT 86400.0000 SELECTED

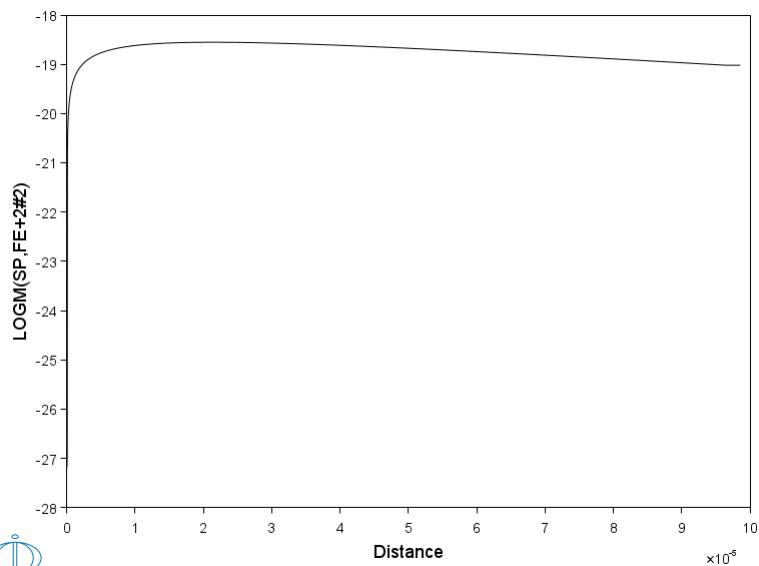
**DIC>**  
**DIC> set-inter**  
**--OK--**  
**DIC>**

### exi3a-plot

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exi3a\plot.DCM.test"
DIC>
DIC> @@ exi3_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE i3
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 8.64000E+04
DIC> read exi3
OK
DIC>
DIC> @@
DIC> @@ ENTER THE POST PROCESSOR
DIC> @@
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1: @@
POST-1: @@ PLOT THE THICKNESS OF THE OXIDE LAYER GROWING AT THE SURFACE.
POST-1: @@ FOR THIS WE NEED TO ENTER A FUNCTION ACCORDING TO THE FOLLOWING.
POST-1: ent func oxideth
FUNCTION: poi(sp,upper)-poi(sp,lower)
&
POST-1: @@
POST-1: @@ PUT THIS FUNCTION ON THE Y-AXIS
POST-1: @@
POST-1: s-d-a y oxideth
POST-1: @@
POST-1: @@
POST-1: @@ AND PLOT THE OXIDE THICKNESS VERSUS TIME
POST-1: @@
POST-1: s-d-a x time
INFO: Time is set as independent variable
POST-1:
POST-1: @@
POST-1: @@ SINCE WE ARE PLOTTING A FUNCTION, SPECIFY A PLOT CONDITION
POST-1: @@
POST-1: s-p-c interface sp upper
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```



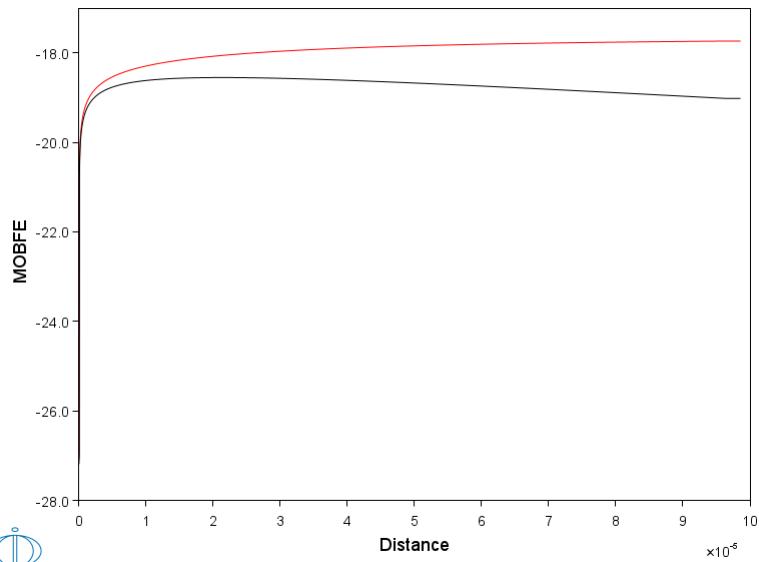
```
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: @@
POST-1: @@ NOW PLOT THE MOBILITY IN A SPINEL FOR Fe+2 ON THE SECOND SUBLATTICE
POST-1: @@
POST-1: s-d-a y logm(sp,fe+2#2)
POST-1:
POST-1: @@
POST-1: @@ LIMIT THE PLOT TO THE SPINEL PHASE
POST-1: @@
POST-1: s-d-a x dis local sp
INFO: Distance is set as independent variable
POST-1:
POST-1: s-p-c time 86400
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```



```

 $\odot$ 
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: @@
POST-1: @@ COMPARE MOBILITIES IN A SPINEL FOR Fe+2 AND Fe+3 SPECIES PRESENT ON THE
POST-1: @@ SECOND SUBLATTICE. FOR THIS WE NEED TO ENTER A TABLE.
POST-1: @@
POST-1: ent table mobfe
Variable(s) logm(sp,fe+2#2) logm(sp,fe+3#2)
POST-1:
POST-1: s-d-a y mobfe
COLUMN NUMBER /*/
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

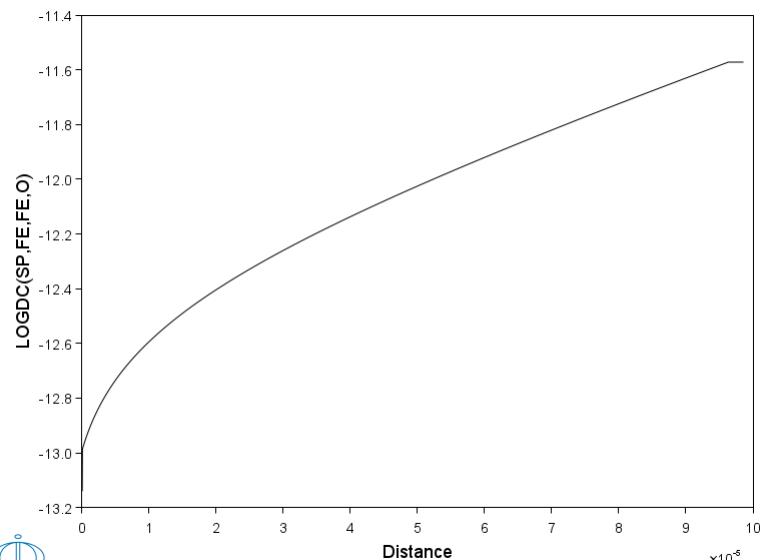
```



```

 $\odot$ 
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: @@
POST-1: @@ NOW PLOT THE INTERDIFFUSION COEFFICIENT OF Fe IN A SPINEL
POST-1: @@
POST-1: s-d-a y logdc(sp,fe,fe,o)
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

```



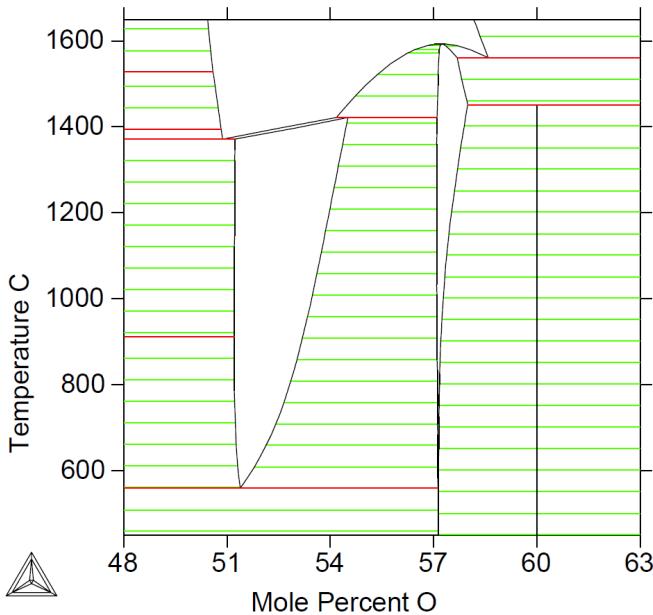
POST-1:  
POST-1:  
POST-1: set-inter  
--OK---  
POST-1:



## Example i3b

### Diffusion in iron oxide (FeO) with grain boundary contribution

Oxidation of iron sample and consequent growth of an oxide layer using the grain boundary diffusion contribution model.



**exi3b-setup****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\_dictra\_console\_examples\examples\exi3b\setup.DCM.test"**

**SYS:** @@  
**SYS:** @@ Diffusion in complex phases.  
**SYS:** @@ Diffusion in iron oxide (FeO) with a grain boundary contribution  
**SYS:** @@ This example shows the oxidation of an iron sample and consequent  
**SYS:** @@ growth of an oxide layer using the grain boundary diffusion  
**SYS:** @@ contribution model.

**SYS:** -----  
NO SUCH COMMAND, USE HELP

**SYS:**  
**SYS:** @@ exi3\_setup.DCM

**SYS:** @@  
**SYS:** @@ START BY GOING TO THE DATABASE MODULE

**SYS:** @@

**SYS:** go da

  THERMODYNAMIC DATABASE module

  Database folder:

  C:\jenkins\workspace\generate\_dictra\_console\_examples\databases\data  
  Current database: Steels/Fe-Alloys v12.0

  VA                   /- DEFINED

  DICTRA\_FCC\_A1   REJECTED

**TDB\_TCFE12:**

**TDB\_TCFE12:** @@

**TDB\_TCFE12:** @@ SELECT A USER DATABASE TO READ THE THERMODYNAMIC DATA

**TDB\_TCFE12:** @@

**TDB\_TCFE12:** sw user FeO.TDB

  Current database: User defined Database

This database does not support the DATABASE\_INFORMATION command

  VA                   /- DEFINED

19:17:32,796 [Thread-0] INFO TDBfileParser: USER\_511160897\_14, number of lines read: 217

19:17:32,956 [Thread-0] INFO DatabaseUtils: Parsing of USER\_511160897\_14 completed in 211 ms

**TDB\_USER:** def-sys fe o

  FE                   O DEFINED

**TDB\_USER:** rej sp \*

  /-                  VA                   FE

  O                   FE+2               FE+3

  FE+4               FE2O3              FE0

  FEO3/2             O-2               O2

  REJECTED

**TDB\_USER:** res sp fe fe+2 fe+3 o o2 o-2 va

  FE                   FE+2               FE+3

  O                   O2                 O-2

  VA RESTORED

**TDB\_USER:** rej ph \* all

  GAS:G               BCC\_A2           SPINEL:I

  REJECTED

**TDB\_USER:** res ph bcc spinel gas

  BCC\_A2              SPINEL:I        GAS:G

  RESTORED

**TDB\_USER:**

**TDB\_USER:** get

19:17:33,037 [Thread-0] INFO JavaWrapper: \*\*\* Invoking Gibbs Energy System v6 \*\*\*

ELEMENTS .....

SPECIES .....

PHASES .....

PARAMETERS ....

FUNCTIONS ....

List of references for assessed data

'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317 -425'

'M. Kowalski and P.J. Spencer, Calphad, 19 (1995), 229-243; Cr-O, Fe-O and Ni-O'

'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'

'B. Sundman, J. Phase Equil., 12 (1991), 127-140; Fe-O'

-OK-

\*\*\* WARNING: One or more elements have been rejected only as species but not as elements. This is not allowed with GES6, temporarily reverting

**TDB\_USER:**

**TDB\_USER:** @@

**TDB\_USER:** @@ SWITCH TO A USER-DEFINED MOBILITY DATABASE TO RETRIEVE MOBILITY DATA

**TDB\_USER:** @@

**TDB\_USER:** app user FeOmob.TDB

  Current database: User defined Database

  test database

  VA                   /-               O

  DEFINED

19:17:33,088 [Thread-0] INFO TDBfileParser: USER\_737913591\_14, number of lines read: 128

19:17:33,117 [Thread-0] INFO DatabaseUtils: Parsing of USER\_737913591\_14 completed in 29 ms

**TDB\_APP:** def-sys fe o

  FE DEFINED

**TDB\_APP:** rej sp \*

  /-                  VA                FE

  O                   FE+2              FE+3

  FE2O3              FEO              FEO3/2

  O-2                O2                O2 REJECTED

**TDB\_APP:** res sp fe fe+2 fe+3 o o2 o-2 va

  FE                   FE+2               FE+3

  O                   O2                 O-2

  VA RESTORED

```

TDB_APP: rej ph * all
SPINEL:I           GAS:G          BCC_A2
REJECTED
TDB_APP: res ph bcc spinel gas
BCC_A2           SPINEL:I        GAS:G
RESTORED
TDB_APP:
TDB_APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS .....
*** ERROR 2018 IN DESHPH: DIFFUSION DATA NOT POSSIBLE FOR GAS PHASE
*** ERROR 2018 IN DESHPH: DIFFUSION DATA NOT POSSIBLE FOR GAS PHASE
FUNCTIONS .....
-OK-
TDB_APP:
TDB_APP:
TDB_APP: @@ 
TDB_APP: @@ ENTER THE DICTRA MONITOR
TDB_APP: @@ 
TDB_APP: go d-m
NO TIME STEP DEFINED
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 823; * N
DIC>
DIC>
DIC> @@
DIC> @@ SET THE REFERENCE STATE FOR O TO O2 (GAS)
DIC> @@
DIC> set-ref o gas,,,,,,,
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE REGIONS fer AND sp
DIC> @@
DIC> ent-reg fer
DIC> ent-reg sp,,,,,,,
DIC>
DIC>
DIC> @@
DIC> @@ ENTER PHASES INTO THE REGIONS
DIC> @@
DIC> ent-phase act fer matrix bcc#1
DIC> ent-phase act sp matrix spinel
DIC>
DIC>
DIC> @@
DIC> @@ ENTER GRIDS INTO THE REGIONS
DIC> @@
DIC>
DIC> @@
DIC> @@ ENTER A SIZE FOR THE FERRITE
DIC> @@
DIC> @@
DIC> ent-grid fer 4.99999e-3 AUTO
DIC>
DIC> @@
DIC> @@ ENTER A THIN INITIAL SIZE FOR THE OXIDE
DIC> @@
DIC> @@
DIC> ent-grid sp 1.00e-10 AUTO
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITIONS IN BCC
DIC> @@
DIC> ent-comp fer bcc#1 m-f
PROFILE FOR /O/: o lin 1e-9 1e-9
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITIONS IN THE OXIDE
DIC> @@
DIC> ent-comp sp spinel m-f
this is a phase with charged species
with more than 2 sublattices
PROFILE FOR /FE/: FE lin 4.28771E-01 4.28549E-01
DIC>
DIC>
DIC> @@
DIC> @@ ENTER A BOUNDARY CONDITION "GAS" ON THE UPPER (RIGHT-MOST) INTERFACE
DIC> @@ OF THE OXIDE. THIS ALLOWS THE SYSTEM TO EXPAND AND THE OXIDE LAYER
DIC> @@ TO GROW EXTERNALLY. FOR THIS EXAMPLE AN OXYGEN ACTIVITY IS SPECIFIED
DIC> @@ THAT IS LOW ENOUGH NOT TO FORM CORUNDUM (FE2O3). ALSO SPECIFY THAT
DIC> @@ THERE IS NO FLUX OF Fe ACROSS THIS INTERFACE, I.E. NO Fe IS
DIC> @@ ALLOWED TO ENTER OR LEAVE THE SYSTEM.
DIC> @@
DIC> set-cond boundary upper gas
TYPE OF CONDITION FOR COMPONENT FE /ZERO_FLUX/: zero-flux
TYPE OF CONDITION FOR COMPONENT O /ZERO_FLUX/: act
LOW TIME LIMIT /0/: 0 4.5e-4; * N
DIC>
DIC>
DIC> @@
DIC> @@ ENTER START VALUES FOR THE INITIAL INTERFACE VELOCITIES
DIC> @@
DIC> s-a-s-v -1e-5 1e-5 yes
STARTING VALUES WILL BE TAKEN FROM PROFILES
DIC>
DIC>
DIC> @@
DIC> @@ SIMULATE FOR 24 HOURS
DIC> @@
DIC> s-s-time 86400,,
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>

```

```
DIC> @@
DIC> @@ SPECIFY THAT POTENTIALS AND NOT ACTIVITIES ARE VARIED AT THE PHASE
DIC> @@ INTERFACE. ALSO USE A FULLY IMPLICIT SCHEME FOR TIME INTEGRATION.
DIC> @@
DIC> s-s-c 0 1 1 YES POT YES YES 1 2,.....
RELEASING OLD STARTING VALUES
DIC>
DIC>
DIC> @@ ENABLE THE GRAIN BOUNDARY DIFFUSION CONTRIBUTION MODEL
DIC> GB
REGION NAME : /SP/: SP
PHASE NAME: /SPINEL/: SPINEL
Enable model for grainboundary contribution to diffusion /YES/: YES
Grainboundary thickness /5E-10/: 5e-10
Grainsize(T,P,TIME)= 10.0e-6;
Bulkdiffusion activation energy multiplier /.5/: 0.333333
Enable model for dislocation contribution to diffusion /YES/: NO
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exi3b.DIC Y
DIC>
DIC>
DIC>
DIC> set-inter
--OK--
DIC>
```

**exi3b-run**

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exi3b\run.DCM.test"
DIC>
DIC>
DIC> @@ exi3_run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING EXAMPLE i3
DIC> @@
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 0.00000E+00
DIC> read exi3b
OK
DIC>
DIC> @@
DIC> @@ START THE SIMULATION
DIC> @@
DIC> sim y
Region: FER
single geometric dense at 0.50000E-02
0.87701      95
Region: SP
double geometric
dense at outer boundaries, coarse at 0.50000E-10
lower part 1.2500      9
upper part 0.80000      9
Trying old scheme
U-FRACTION IN SYSTEM: FE = 0.99999999500542 O = 2.10000395011622E-08
TOTAL SIZE OF SYSTEM: .0049999901 [m]
U-FRACTION IN SYSTEM: FE = 0.99999999500542 O = 2.10000395011622E-08
TOTAL SIZE OF SYSTEM: .0049999901 [m]
6.14108503765165E-002   6.141055227761509E-002   6.141059649120947E-002   8.444695307336839E-003   1.457812889792273E-
024 TIME = 0.1000000E-06 DT = 0.1000000E-06 SUM OF SQUARES = 0.14517775E-23
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.16338052E-03 AND 0.0000000
POSITION OF INTERFACE FER / SP IS 0.49999900E-02
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.29859816E-03 AND 0.0000000
POSITION OF INTERFACE SP / gas interface IS 0.49999901E-02
U-FRACTION IN SYSTEM: FE = 0.99999999230858 O = 2.69779255762996E-08
TOTAL SIZE OF SYSTEM: .0049999011352 [m]
9 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: FER

CPU time used in timestep          0 seconds
8.109385106269871E-006   8.108697705670329E-006   8.108646583145077E-006   3.429164871688112E-007   5.443979530183559E-
031 TIME = 0.3000000E-06 DT = 0.2000000E-06 SUM OF SQUARES = 0.26903135E-30
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.37478212E-03 AND 0.0000000
POSITION OF INTERFACE FER / SP IS 0.49999989E-02
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.57006070E-03 AND 0.0000000
POSITION OF INTERFACE SP / gas interface IS 0.49999902E-02
U-FRACTION IN SYSTEM: FE = 0.99999998461782 O = 4.97800676096266E-08
TOTAL SIZE OF SYSTEM: .0049999015258 [m]
CPU time used in timestep          0 seconds
8.244192928749400E-006   8.245597661116344E-006   8.245807164019650E-006   5.265202845644101E-009   2.950288635535600E-
032 TIME = 0.7000000E-06 DT = 0.4000000E-06 SUM OF SQUARES = 0.28314179E-31
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.17607368E-03 AND 0.0000000
POSITION OF INTERFACE FER / SP IS 0.49999989E-02
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.24106853E-03 AND 0.0000000
POSITION OF INTERFACE SP / gas interface IS 0.49999902E-02
U-FRACTION IN SYSTEM: FE = 0.9999997890226 O = 6.9066888819746E-08
TOTAL SIZE OF SYSTEM: .0049999017858 [m]
CPU time used in timestep          0 seconds
1.134925725903101E-007   1.135900229911682E-007   1.135511870615491E-007   5.608728337076656E-010   2.264331258101956E-
033 TIME = 0.1500000E-05 DT = 0.8000000E-06 SUM OF SQUARES = 0.22551154E-32
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.14432289E-03 AND 0.0000000
POSITION OF INTERFACE FER / SP IS 0.49999897E-02
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.20898647E-03 AND 0.0000000
POSITION OF INTERFACE SP / gas interface IS 0.49999902E-02
U-FRACTION IN SYSTEM: FE = 0.99999996836327 O = 1.02507646839312E-07
TOTAL SIZE OF SYSTEM: .0049999023031 [m]
8 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: SP

CPU time used in timestep          1 seconds
4.495109847370196E-007   4.496446010596877E-007   4.496424689401166E-007   2.514742727557657E-010   1.443342493600654E-
033 TIME = 0.3100000E-05 DT = 0.1600000E-05 SUM OF SQUARES = 0.12878834E-32
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.94208038E-04 AND 0.0000000
POSITION OF INTERFACE FER / SP IS 0.49999896E-02
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.13424765E-03 AND 0.0000000
POSITION OF INTERFACE SP / gas interface IS 0.49999903E-02
U-FRACTION IN SYSTEM: FE = 0.9999999509026 O = 1.45471966758E-07
TOTAL SIZE OF SYSTEM: .0049999029437 [m]
32 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: SP

CPU time used in timestep          0 seconds
1.153180642284307E-005   1.153636959819412E-005   1.153594127740359E-005   1.797714957772355E-008   4.232148297988653E-
031 TIME = 0.6300000E-05 DT = 0.3200000E-05 SUM OF SQUARES = 0.42317797E-30
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.67615627E-04 AND 0.0000000

output ignored...

... output resumed

POSITION OF INTERFACE FER / SP IS 0.49333470E-02
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.11009831E-08 AND 0.0000000
POSITION OF INTERFACE SP / gas interface IS 0.50286092E-02
U-FRACTION IN SYSTEM: FE = .994180844256236 O = .0189442386268419
TOTAL SIZE OF SYSTEM: .00502860924769 [m]
21 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: SP

CPU time used in timestep          1 seconds
5.273123767838843E-007   5.281052804184015E-007   5.280434168127061E-007   7.076352497325021E-010   5.535995347174966E-
032 TIME = 56943.895 DT = 8640.0000 SUM OF SQUARES = 0.54438366E-31
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.70247279E-09 AND 0.0000000
POSITION OF INTERFACE FER / SP IS 0.49272776E-02
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.10045406E-08 AND 0.0000000
POSITION OF INTERFACE SP / gas interface IS 0.50312191E-02
```

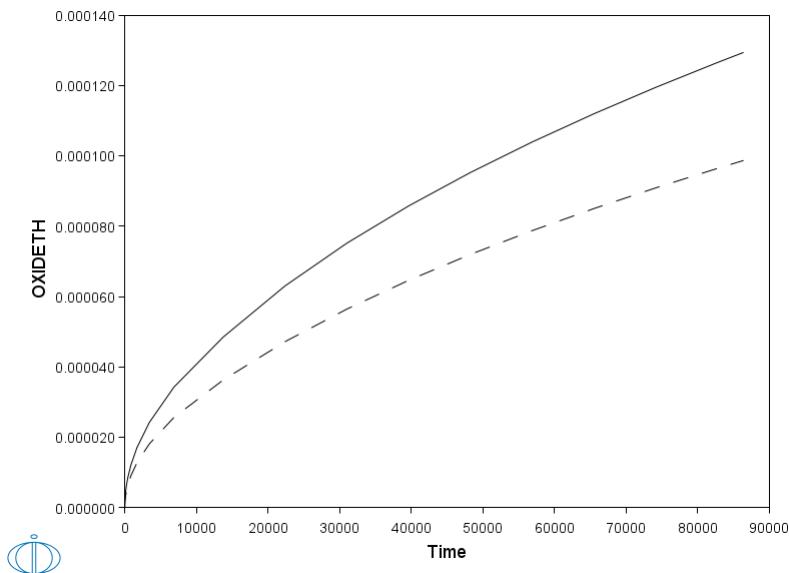
U-FRACTION IN SYSTEM: FE = .993661317146276 O = .0206594864095021  
 TOTAL SIZE OF SYSTEM: .00503121911318 [m]  
 9 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: SP

	CPU time used in timestep	0 seconds		
2.946684369965207E-007	2.952124445708061E-007	2.951636472770453E-007	3.823703016289697E-010	2.362273447412469E-
034 TIME = 65583.895 DT = 8640.0000 SUM OF SQUARES = 0.21741944E-33				
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.64894663E-09 AND 0.0000000				
POSITION OF INTERFACE FER / SP IS 0.49216707E-02				
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.92920436E-09 AND 0.0000000				
POSITION OF INTERFACE SP / gas interface IS 0.50336405E-02				
U-FRACTION IN SYSTEM: FE = .993180429204049 O = .0222444822395802				
TOTAL SIZE OF SYSTEM: .00503364053996 [m]				
8 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: SP				
CPU time used in timestep 0 seconds				
1.646051457260130E-007	1.649797488548725E-007	1.649486900573763E-007	1.988149803887363E-010	2.711348249832655E-
033 TIME = 74223.895 DT = 8640.0000 SUM OF SQUARES = 0.27083390E-32				
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.60654807E-09 AND 0.0000000				
POSITION OF INTERFACE FER / SP IS 0.49164301E-02				
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.86919599E-09 AND 0.0000000				
POSITION OF INTERFACE SP / gas interface IS 0.50359098E-02				
U-FRACTION IN SYSTEM: FE = .992730593208195 O = .023725718750502				
TOTAL SIZE OF SYSTEM: .00503590981794 [m]				
11 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: SP				
CPU time used in timestep 1 seconds				
1.056445773902876E-007	1.059232611576854E-007	1.059039581621122E-007	1.220605088849088E-010	1.504632769052528E-
035 TIME = 82863.895 DT = 8640.0000 SUM OF SQUARES = 0.30092655E-35				
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.57100506E-09 AND 0.0000000				
POSITION OF INTERFACE FER / SP IS 0.49114966E-02				
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.81838274E-09 AND 0.0000000				
POSITION OF INTERFACE SP / gas interface IS 0.50380472E-02				
U-FRACTION IN SYSTEM: FE = .992307543396601 O = .0251191388071113				
TOTAL SIZE OF SYSTEM: .00503804716102 [m]				
7 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: SP				
CPU time used in timestep 0 seconds				
1.518629947825178E-008	1.512783804441976E-008	1.530719582875733E-008	1.085105168628729E-011	1.271414689849386E-
034 TIME = 86400.000 DT = 3536.1047 SUM OF SQUARES = 0.12714147E-33				
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.56483658E-09 AND 0.0000000				
POSITION OF INTERFACE FER / SP IS 0.49094993E-02				
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.78548538E-09 AND 0.0000000				
POSITION OF INTERFACE SP / gas interface IS 0.50388274E-02				
U-FRACTION IN SYSTEM: FE = .992153350395529 O = .025666480290727				
TOTAL SIZE OF SYSTEM: .00503882739826 [m]				
MUST SAVE WORKSPACE ON FILE				
WORKSPACE SAVED ON FILE				
RECLAIMING WORKSPACE				
DELETING TIME-RECORD FOR TIME 0.0000000				
DELETING TIME-RECORD FOR TIME 0.10000000E-06				
DELETING TIME-RECORD FOR TIME 0.30000000E-06				
DELETING TIME-RECORD FOR TIME 0.70000000E-06				
DELETING TIME-RECORD FOR TIME 0.15000000E-05				
DELETING TIME-RECORD FOR TIME 0.31000000E-05				
DELETING TIME-RECORD FOR TIME 0.63000000E-05				
DELETING TIME-RECORD FOR TIME 0.12700000E-04				
DELETING TIME-RECORD FOR TIME 0.25500000E-04				
DELETING TIME-RECORD FOR TIME 0.51100000E-04				
DELETING TIME-RECORD FOR TIME 0.10230000E-03				
DELETING TIME-RECORD FOR TIME 0.20470000E-03				
DELETING TIME-RECORD FOR TIME 0.40950000E-03				
DELETING TIME-RECORD FOR TIME 0.81910000E-03				
DELETING TIME-RECORD FOR TIME 0.16383000E-02				
DELETING TIME-RECORD FOR TIME 0.32767000E-02				
DELETING TIME-RECORD FOR TIME 0.65535000E-02				
DELETING TIME-RECORD FOR TIME 0.13107100E-01				
DELETING TIME-RECORD FOR TIME 0.26214300E-01				
DELETING TIME-RECORD FOR TIME 0.52428700E-01				
DELETING TIME-RECORD FOR TIME 0.10485750				
DELETING TIME-RECORD FOR TIME 0.20971510				
DELETING TIME-RECORD FOR TIME 0.41943030				
DELETING TIME-RECORD FOR TIME 0.83886070				
DELETING TIME-RECORD FOR TIME 1.6777215				
DELETING TIME-RECORD FOR TIME 3.3554431				
DELETING TIME-RECORD FOR TIME 6.7108863				
DELETING TIME-RECORD FOR TIME 13.421773				
DELETING TIME-RECORD FOR TIME 26.843545				
DELETING TIME-RECORD FOR TIME 53.687091				
DELETING TIME-RECORD FOR TIME 107.37418				
DELETING TIME-RECORD FOR TIME 214.74836				
DELETING TIME-RECORD FOR TIME 429.49673				
DELETING TIME-RECORD FOR TIME 858.99346				
DELETING TIME-RECORD FOR TIME 1717.98669				
DELETING TIME-RECORD FOR TIME 3435.9738				
DELETING TIME-RECORD FOR TIME 6871.9477				
DELETING TIME-RECORD FOR TIME 13743.895				
DELETING TIME-RECORD FOR TIME 22383.895				
DELETING TIME-RECORD FOR TIME 31023.895				
DELETING TIME-RECORD FOR TIME 39663.895				
DELETING TIME-RECORD FOR TIME 48303.895				
DELETING TIME-RECORD FOR TIME 56943.895				
DELETING TIME-RECORD FOR TIME 65583.895				
DELETING TIME-RECORD FOR TIME 74223.895				
KEEPING TIME-RECORD FOR TIME 82863.895				
AND FOR TIME 86400.000				
WORKSPACE RECLAIMED				
TIMESTEP AT 86400.0000 SELECTED				

**DIC>**  
**DIC> set-inter**  
**--OK--**  
**DIC>**

**exi3b-plot**

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>MACRO "c:\jenkins\workspace\generate_dictra_console_examples\examples\exi3b\plot.DCM.test"
DIC>
DIC> @@ exi3_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE i3
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 8.64000E+04
DIC> read exi3b
OK
DIC>
DIC> @@
DIC> @@ ENTER THE POST PROCESSOR
DIC> @@
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1: @@
POST-1: @@ PLOT THE THICKNESS OF THE OXIDE LAYER GROWING AT THE SURFACE.
POST-1: @@ FOR THIS WE NEED TO ENTER A FUNCTION ACCORDING TO THE FOLLOWING.
POST-1: ent func oxideth
FUNCTION: poi(sp,upper)-poi(sp,lower)
&
POST-1: @@
POST-1: @@ PUT THIS FUNCTION ON THE Y-AXIS
POST-1: @@
POST-1: s-d-a y oxideth
POST-1: @@
POST-1: @@
POST-1: @@ AND PLOT THE OXIDE THICKNESS VERSUS TIME
POST-1: @@
POST-1: s-d-a x time
INFO: Time is set as independent variable
POST-1:
POST-1: @@
POST-1: @@ SINCE WE ARE PLOTTING A FUNCTION, SPECIFY A PLOT CONDITION
POST-1: @@
POST-1: s-p-c interface sp upper
POST-1:
POST-1: app y exi3a.exp 0; 1;
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 4
POST-1: MAKE c:\jenkins\workspace\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
      OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```



```
POST-1:
POST-1:
POST-1: set-inter
--OK---
POST-1:
```

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