

**THERIAK-DOMINO**

**User’s Guide   
Vers. 11.03.2020  
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"Si quis laetali serpentis, saucius, ictu  
Cepit, et ignara, toxica saeva, manu,  
Nec mora pro degustato, tactoque veneno,  
Laeta propinabis pocula Theriacae,  
Ista dabit vigili, Caesar, medicina soporem,  
Atque medela gravis sumpta doloris erit,  
Hactenus exposui vires, nunc tempora dicam,  
Vipera cum certo sit capienda modo."  
  
Galenos: Libellus de Theriaca ad Pisonem (cited from: Daniëls ,1911)

# Introduction

## What does the theriak/domino suite?

The **theriak/domino suite** includes several programs for thermodynamic calculations and plotting of results in PostScript® format. These programs are:

**theriak**, the heart of the suite, calculates the stable mineral assemblage and phase compositions for a given rock (bulk composition) at specified P, T conditions or along a specified PT-path.

**domino** may calculate

* Equilibrium assemblage phase diagrams for selectable axes (P, T, components activities etc.)
* Pseudo-binary or pseudo-ternary phase diagrams.
* Pixelmaps for all thermodynamic variables.
* Isolines of several thermodynamic properties for bulk rock, non-solution and solution phases.

**therbin** calculates binary phase diagrams at constant P or T.

**therter** calculates ternary phase diagrams at constant P and T.

**thalia** calculates phase thermodynamic parameters as functions of T or P or (binary) composition.

**thermo** calculates thermodynamic parameters at T and P and tables of V and G.

**guzzler** uses the output graphics files produced by theriak, domino or thalia as input and cleans up labels, making graphics information more readable.

**explot** transforms files containing graphics information from the above programs to “ready to use” PostScript files that can be seen on screen or printed to a hard copy.

**makemap** uses the pixelmap information from domino and incorporates a grey pixelmap image of any variable into a PostScript® file and a portable grey map-file (pgm).

**plotxy** prepares plots of XY diagrams by selecting as axes among the numerous thermodynamic variables involved in a multi-step calculation done by theriak.

The theriak/domino suite is written in standard FORTRAN; it is developing and made available to the scientific community since 1987 by C. De Capitani. Executable files for the most common operating systems (Unix and derivates; Mac-OS X; Windows) have been created by using the gfortran compilers under the GNU Public Licence. The current version (11.03.2020) promises to add more convenience to the user:

* On-line help, besides a reworked user guide.
* Tailoring file names as well as installation and working directories according to user preferences.
* Scheduling time-consuming, unattended runs.
* Compatibility with currently available thermodynamic databases (Standard data and activity models).

## Why use the theriak/domino suite?

Results calculated by theriak/domino suite are not better or worse than results calculated by other comparable programs. The quality of results depends merely on the quality of the thermodynamic data used as well as to user personal (subjective) choices rather than on any modern software package. Based on its approach to equilibrium by Gibbs free energy minimization (c.f. de Capitani & Brown, 1987) rather, than solving complex and large equation systems, the theriak/domino software is exceptionally fast. The various types of phase diagrams are calculated and plotted without user intervention that might be a source of serious errors.

Fig. 1 demonstrates these properties for a complex equilibrium assemblage diagram including 185 stable reactions. Calculation and plot of this “ready-to-use” diagram has been carried out with a 1.4 GHz Notebook running Windows XP in less than 30 minutes!

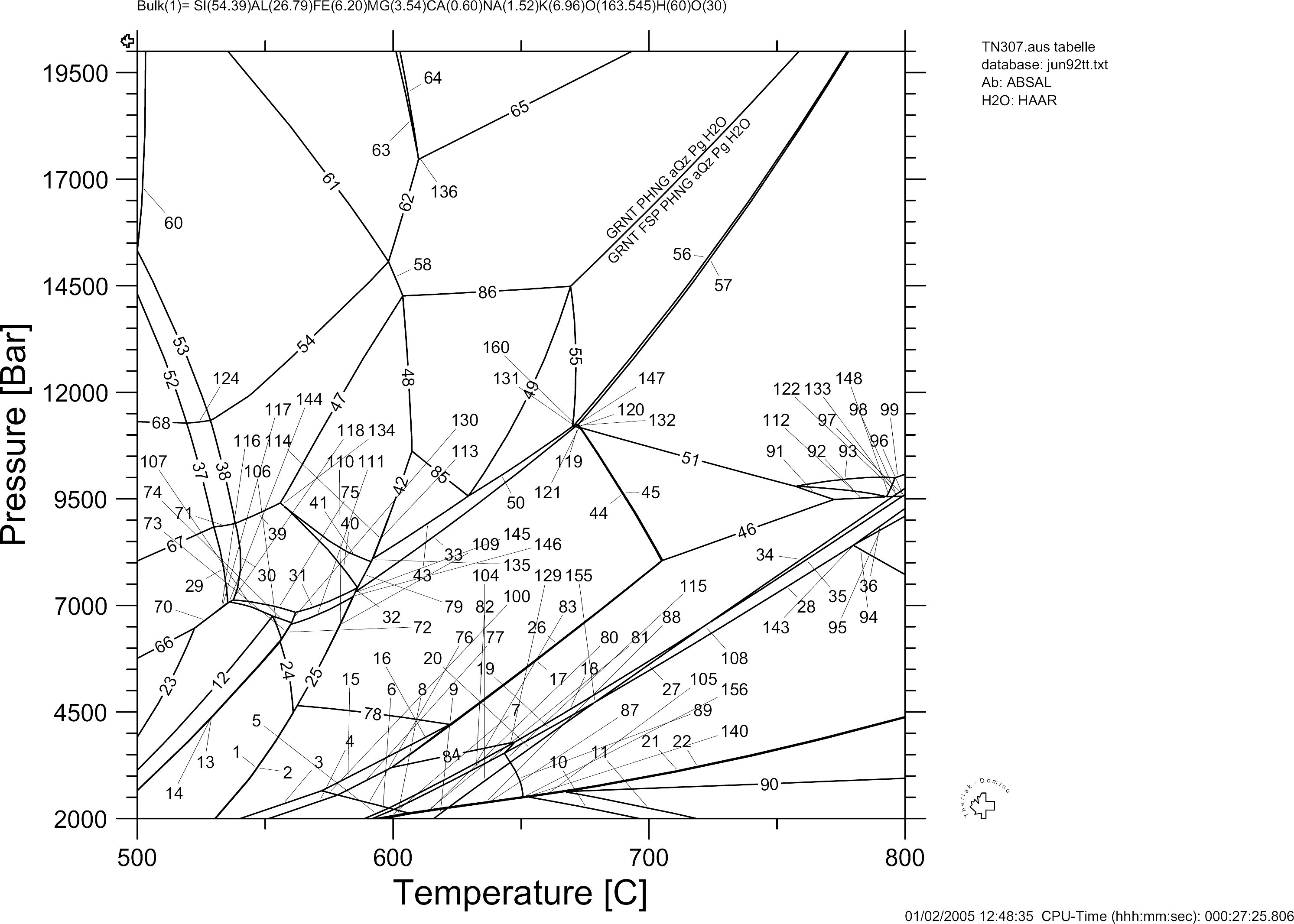


Fig. 1: Equilibrium assemblage diagram for bulk composition TN307 from Nagel (2002), Metamorphic and structural history of the southern Adula nappe (Graubünden, Switzerland), Table 2. PhD thesis Basel,

## Terms of use

The executable files of the theriak/domino suite as well as the source code for programmers and developers are available for free download and use for non-commercial purposes. The use and modification of the theriak/domino suite underlies solely the responsibility of the user. The source developer and distributor C. de Capitani does not undertake any responsibility for any results produced by the user. By using or modifying the theriak/domino suite, the user implicitly agrees, that he or she has accepted these terms of use.

## Download THERIAK-DOMINO software.

Download the software: http://titan.minpet.unibas.ch/minpet/theriak/theruser.html

Site maintained by C. de Capitani.

**for Mac OS X and UNIX**

TheriakDominoMAC/Programs.zip : Programs.

[TheriakDominoMAC/Working.zip](https://titan.minpet.unibas.ch/minpet/theriak/prog190309/TheriakDominoMAC/Working.zip) : Example of Working directory with databases.

[TheriakDominoMAC/Documentation.zip](https://titan.minpet.unibas.ch/minpet/theriak/prog190309/TheriakDominoMAC/documentation.zip) : Documentation.

[TheriakDominoMAC/Examples.zip](https://titan.minpet.unibas.ch/minpet/theriak/prog190309/TheriakDominoMACexamples.zip) : Examples.

**for Windows**

TheriakDominoWIN/Programs.zip : Programs.

[TheriakDominoWIN/Working.zip](https://titan.minpet.unibas.ch/minpet/theriak/prog190309/TheriakDominoWIN/Working.zip) : Example of Working directory with databases.

[TheriakDominoWIN/Documentation.zip](https://titan.minpet.unibas.ch/minpet/theriak/prog190309/TheriakDominoWIN/Documentation.zip) : Documentation.

[TheriakDominoWIN/Examples.zip](https://titan.minpet.unibas.ch/minpet/theriak/prog190309/TheriakDominoWIN/Examples.zip) : Examples.

Download the zipped folders and expand them. (double-clicking should work, else download a free unzip/expander software)

Information on installing and running are in the “readme” file.

# Getting started

## Getting started with theriak

Consider a bulk composition of 10 moles of muscovite, 10 moles of paragonite with excess SiO2 and water. Calculate the equilibrium assemblage at 600 oC and 4000 Bar.

Write the following two lines at the top (not counting the comment lines) of the dat-file:

600 4000

0 SI(60)AL(60)NA(10)K(10)SI(100)H(100)O(?) \*

**start theriak.**

database **JUN92.bs**

type of calculation **no**

The result will be a Feldspar coexisting with white mica, quartz and water.

Feldspar: Ab0.94An0.04

Mica: Mu0.70Pg0

For more detailed information, see also the commented run of theriak in commented\_theriak.pdf

With the same composition do multiple calculations between 650 and 800 oC at 4000 Bar.

**start theriak**

database **JUN92.bs**

type of calculation **loop**

Temperature and Pressure **650 4000**

Temperature and Pressure **700 4000**

Temperature and Pressure **800 4000**

Temperature and Pressure (CR)

## Getting started with domino

Consider a bulk composition of 10 moles of muscovite, 10 moles of paragonite with excess SiO2 and water.

Calculate a P-T equilibrium assemblage diagram, using the database JUN92.bs

Temperature range: 500 - 900 oC

Pressure range: 1000 - 13000 Bar

Write the following two lines at the top (not counting the comment lines) of the dat-file:

600 4000

0 SI(60)AL(60)NA(10)K(10)SI(100)H(100)O(?) \*

**start domino.**

database **JUN92.bs**

X-axis **TC 500 900**

Y-axis **P 1000 13000**

Calculation type **.**

labeling of reactions **1**

For the X- and Y-axis insert several blank between the parameters.

As calculation type enter "." (dot)

Domino produces a graphics file (plt-file, usually called coplot). In order to label the curves with the assemblages, this must be processed by the program guzzler.

**start guzzler**

graphics file name **coplot**

size of labels **(CR)**

option **(CR)**

(CR) ("Carriage return", or "enter"): Use the default values

Guzzler produces a new graphics file (cln-file, usually called clean). this can be translated to plot-files, usually called plot.ps and plot.svg

**start explot**

graphics file name **clean**

The resulting plot-files can be displayed (and modified) e.g. with ghostview, Adobe Illustrator, Corel Draw, Inkscape etc.

## Getting started with therter

The program therter calculates ternary phase diagrams. The system must be strictly ternary, i.e. all phases must be linear combinations of the three ternary endmembers.

Once the three ternary endmembers are defined, therter will automatically exclude all phases outside this ternary.

We will calculate the phase relations of the K-feldspar-Albite-Anorthite ternary.

The bulk composition must contain at least all elements needed for the ternary system. Use e.g. the same dat-file as in the previous examples, and add Calcium.

600 4000

0 CA(1)SI(60)AL(60)NA(10)K(10)SI(100)H(100)O(?) \*

**start therter**

database **JUN92.bs**

endmember 1 **Ab**

endmember 1 **An**

endmember 2 **Kfs**

Temperature and pressure **800 2000**

number of seeds  **(CR)**

X-scan-density…. **(CR)**

Therter produces a graphics file (plt-file, usually called plot). **This cannot be processed by guzzler.** It can be translated to a plot-file by explot.

**start explot**

graphics file **plot**

The resulting plot-files can be displayed (and modified) e.g. with ghostview, Adobe Illustrator, Corel Draw, Inkscape etc.

## Getting started with therbin

The program therbin calculates binary phase diagrams. The system must be strictly binary, i.e. all phases must be linear combinations of the two binary endmembers.

Once the two binary endmembers are defined, therbin will automatically exclude all phases outside this binary.

We will calculate the phase relations of the K-feldspar-Albite binary.

The bulk composition must contain at least all elements needed for the binary system. Use e.g. the same dat-file as in the previous examples:

600 4000

0 SI(60)AL(60)NA(10)K(10)SI(100)H(100)O(?) \*

**start therbin**

database **JUN92.bs**

endmember 1 **Kfs**

endmember 2 **Ab**

Y-variable **TC 200 800**

pressure **2000**

X-scan-density…. **(CR)**

Therbin produces a graphics file (plt-file, usually called plot). **This cannot be processed by guzzler.** It can be translated to a plot-file file by explot.

**start explot**

graphics file **plot**

The resulting plot-files can be displayed (and modified) e.g. with ghostview, Adobe Illustrator, Corel Draw, Inkscape etc.

## Getting started with thermo

For a given p and T, THERMO calculates ∆G (apparent Gibbs free energy, = ∆H - T.S), ∆H, S, Cp and V. Also, for each thermodynamic function (Cp, volume, disorder, lambda transition) its contribution to the total ∆G, ∆H.

The bulk composition is not used by thermo. However, the dat-file must be present. Use any composition e.g.:

600 4000

0 SI(60)AL(60)NA(10)K(10)SI(100)H(100)O(?) \*

**start thermo**

phases **And Ky Si**

phases **v**

phases **end**

## Getting started with thalia

THALIA plots thermodynamic functions versus T or P, or ∆G (total, configurational, excess or mixing), the chemical potential, or the activity of a phase along a binary link of a solution phase.

The bulk composition is not used by thermo. However, the dat-file is must be present. Use any composition.

**start thalia**

database **JUN92.bs**

X-variable ….. **X**

solution-name **FSP**

endmember1 **1 0 0**

endmember2 **0 1 0**

Y-variable **GMIX**

temperature and pressure **600 2000**

temperature and pressure **end**

Thalia produces a graphics file (plt-file, usually called thplot). This can be processed by guzzler and explot.

**start guzzler**

graphics file **thplot**

size of labels **(CR)**

option **(CR)**

**start explot**

graphics file **clean**

The resulting plot-files can be displayed (and modified) e.g. with ghostview, Adobe Illustrator, Corel Draw, Inkscape etc.

## Making "pixel maps" with domino

Consider a bulk composition of 10 moles of muscovite, 10 moles of paragonite with excess SiO2 and water.

Temperature range: 500 - 900 oC

Pressure range: 1000 - 13000 Bar

Write the following two lines at the top (not counting the comment lines) of the dat-file:

600 4000

0 SI(60)AL(60)NA(10)K(10)SI(100)H(100)O(?) \*

**Start domino.**

database **JUN92.bs**

X-axis **TC 500 900**

Y-axis **P 1000 13000**

Calculation type **pix 100 100**

For the X- and Y-axis insert several blank between the parameters.

domino will create a new folder called "\_pixelmaps". If this folder already exists, you can enter a new name or overwrite the existing folder. In this folder the information for each available variable needed for pixelmaps is stored. This can be visualized with the program makemap

**start makemap**

folderNr **1**

functionNr **40**

This example will produce a grey map (100 x 100) of "vol\_solids" in folder "\_pixelmaps/".

The file created is a plot-file (usually called plot.ps and plot.svg) and can be displayed e.g. with ghostview, Adobe Illustrator, Corel Draw, Inkscape etc.

## Calculations along a PT-path with theriak

Consider a bulk composition of 10 moles of muscovite, 10 moles of paragonite with excess SiO2 and water.

Make a table with all amounts, compositions, activities and much more along a PT-path from 500 oC/3500 Bar to 800 oC/6000 Bar.

Use the following composition in the dat-file (usually THERIN):

600 4000

0 SI(60)AL(60)NA(10)K(10)SI(100)H(100)O(?) \*

Create a text file (e.g. **ptpath**) with the following directives:

TP 500 3500

TP 800 6000 50

**start theriak**

database **JUN92.bs**

type of calculations **ptpath**

Theriak writes a (sometimes very large), comma delimited table to the tab- and tcp-files. (usually named loop.table and loop.tecplt). For simple X-Y-plots these tables can be processed by the program plotxy.

**start plotxy**

filename **loop.table**

X-axis **3**

Y-axis **54,55,56,57,58+59**

X-min X-max **<CR>**

Y-min Y-max **<CR>**

plotxy produces a graphics file (plt-file, usually called xyplot). This can be processed by guzzler and explot.

**start guzzler**

graphics file **xyplot**

size of labels **<CR>**

option **<CR>**

**start explot**

graphics file **clean**

The resulting plot-files can be displayed (and modified) e.g. with ghostview, Adobe Illustrator, Corel Draw, Inkscape etc.

## Defining a specific activity for water

In some calculations, specially at higher pressures it may be desired to calculate equilibria or phase diagram with water having a reduced activity. A reduced water activity at HP conditions in magnesian metapelites has e.g. been shown by Chopin C. (1984): Coesite and pure pyrope in high-grade blueschists of the Western Alps: a first record and some consequences. Contrib Mineral Petrol 86:107–118

**defining a reduced activity**

In the database (dbs-file) we insert a new phase (e.g. STEAM06) after the definition of STEAM. (Note: The name refers to JUN92 database and may be different in others)

STEAM06 H(2)O(1) H2Oa na

ST

CP1

COM STEAM[1] 0.6

In the above example, the activity is set to 0.6. The name and the abbreviation are chosen to be different from any others in the database. The ST and CP1 lines are empty (or all zeroes) but must be included.

If sufficient H2O is in the bulk composition, then STEAM06 instead of STEAM will become stable and the activity of STEAM will be 0.6.

**Don't forget to remove (or comment out) the newly defined phase before you proceed to "normal" calculations. Alternatively, you could give the phase a special code, as is usually done with buffers.**

## Defining a buffer

Buffers are often used in experimental petrology to control the oxygen activity. These simple buffers are probably not controlling the O2 activity in nature, but calculations with a buffer may give some insights into more complex processes.

**defining a buffer phase**

As an example, we will consider the hematite-magnetite buffer. This means, that we want to force an equilibrium between hematite and magnetite according to the reaction:

6 hematite = 4 magnetite + O2

We achieve this equilibrium by defining a new phase with the composition O2, having for each pressure and temperature a ∆aG of 6∆aG(hematite)-4∆aG(magnetite).

In the database (dbs-file) we insert this new phase (e.g. OHM-Buffer) after the definition of HEMATITE and MAGNETITE. (Note: The names refer to JUN92 database and may be different in others)

OHM-BUFFER O(2) OHM \*OHM

ST 0.000 000000.000 000.000000 0.000000

CP1 0.000000 0.00000 0.00 0.0

COM HEMATITE[6]MAGNETITE[-4] 0 HEMATITE

Important: The code (4th parameter in the first line) must begin with "\*" (star) and defines the name of the buffer. The ST and CP1 lines are empty (or all zeroes) but must be included.

The last line defines the thermodynamic properties of the buffer. The activity variable is set to zero (=not used) and HEMATITE will be excluded from any equilibrium.

For the case, that not sufficient O2 is present in the bulk, we add an additional negative buffer:

-OHM-BUFFER O(-2) -OHM \*OHM

ST 0.000 000000.000 000.000000 0.000000

CP1 0.000000 0.00000 0.00 0.0

COM OHM-BUFFER[-1]

The code (\*OHM) is the same as for the positive buffer.

To use this buffer, the 'use'-variable in the dat-file must contain ",OHM" (Comma, buffer name), Example:

600 4000

1 FE(1)O(1) \*,OHM

**Note: buffer phases can stay in the database. They are only used when called for through the 'use'-variable.**

# Description of programs

## theriak

Theriak is a program that calculates the equilibrium assemblage for a given bulk composition with data from a thermodynamic database. Most programs that attempt this calculation, fail if one or more solution phases are highly non-ideal and show miscibility gaps. A more detailed discussion on why this happens and how this can be avoided, with additional references can be found in de Capitani and Brown (1987). The strategy of THERIAK is a linear programming method designed to produce the correct answer even in extremely complex, non-ideal systems. As a consequence, the program is sometimes rather slow with simple ideal systems. Because there is no absolutely infallible method to solve a nonlinear program, there is no guarantee that the result produced by THERIAK is indeed the chemical equilibrium. So far, however, no indications for any serious misbehavior of THERIAK have been reported.

### Filenames associated with Theriak

|  |  |  |  |
| --- | --- | --- | --- |
| **I/O unit** | **type** | **file name** | **Description** |
| 01 | ini | theriak.ini (\*) | Program initialization data file |
| 02 | hlp | thhelp.txt (\*) | Help file |
| 05 | kbd | Keyboard (\*) | Keyboard (standard input) |
| 06 | scr | Screen (\*) | Screen (standard output) |
| 07 | dat | THERIN | User's general input file |
| 08 | dbs | Run-time defined | Thermodynamic database |
| 09 | log | theriak.last | User responses during last run |
| 10 | out | OUT | Calculation results to print or view on screen |
| 11 | bin | binout | Graphic data for "pseudo-binary system" calculations |
| 12 | drv | Run-time defined | "Special calculations" directives to run program |
| 13 | tab | loop.table | Table of variable values; input to spreadsheet programs |
| 14 | tcp | loop.tecplt | Table of variable values; input to program "TecPlot" |
| 25 | inf | loop\_info | info for tables of variable values |
| 39 | ifnr |  | Interactive input-file, passed as argument |
| 41,42 |  |  | Used for some experiments on subduction |

(\*) Hard-coded file names (cannot be changed)

### Theriak Input files

Theriak can be invoked with a command line argument which is the file name containing the interactive input. Used e.g. by the program “dbcheck” to plot functions (fun++), pseudo-binaries (bin++) or reactions (rea++)

**Theriak.ini**

This file is read at the beginning and contains information on file names and calculation parameters. If this file is present in the working directory, this will be used, else the file in the program directory is taken. To make changes, copy the file to the working directory and edit its content. The most important items one might change are:

$GHELP=0 (reduces the comments at the start of the programs)

and the following list with the names of input and output files used by THERIAK.

$THERIAK-FILES

dat=THERIN #User's chemical input to program

dbs=Run-time-defined #Thermodynamic data base to be used

log=theriak.last #User's responses during last run of program

out=OUT #Calculation information to be printed or viewed on screen

bin=binout #Graphics data for "pseudo-binary system" calculations

drv=Run-time-defined #"Special calculation" directives for running the program

tab=loop\_table #Table of variable values; input to a spreadsheet program

tcp=loop\_tecplt #Table of variable values; input to "TechPlot"

inf=loop\_info #info for Table of variable values

use the keyword "files" in the interactive input to print all file names defined.

**thhelp.txt**

is located in the program directory and contains the text printed if the user enters a "?" in the interactive input.

**dat-file**

usually called THERIN or THERIN.txt. This file must be present in the working directory and contains the user input for one T and P and the chemical compositions. E.g.:

600 4000

0 SI(60)AL(60)NA(10)K(10)SI(100)H(100)O(?) \*

**dbs-file**

This is the thermodynamic database used for the calculations. The name is entered by the user in the interactive input. The file must be in the working directory. E.g.: JUN92.bs

**drv-file**

In the working directory. File containing information for repeated calculations. E.g. on a line between two PT points or changes in bulk composition. Enter "?" in the interactive input for more information.

**log-file**

In the working directory. Contains the interactive input from the last run. All input that remains the same (e.g. the name of the database) can be used again with CR. (carriage return)

**Terminal input**

Is the interactive input through the keyboard

### Theriak output files

**Terminal output**

Is the text output of the program to the screen. This is the dialog, help comments, error messages and the calculated equilibria.

**out-file**

In the working directory. Usually called "OUT". Most of the above "Terminal output" is also written to this file.

**bin-file**

In the working directory. Usually called "binout". This is a special output file produced in pseudo-binary calculations. (Keyword "bin" in interactive input). It contains the graphics information for the (∆Grel - X) diagram.

∆Grel is ∆G relative to a straight line between the first and last composition calculated. This is useful to visualize ∆Gmix of complex solutions, with a reduced database (containing just one solution).

The bin-file has a similar format as the DOMINO graphics output and can be converted to a PostScript file with EXPLOT. (It cannot be used as input to GUZZLER)

**tab-file**

In the working directory. Usually called "loop.table". This file is produced either in pseudo-binary calculations. (Keyword "bin" in interactive input), or when doing multiple calculations with a drv-file. It is a large table with one row for each calculation and columns for (almost) every variable calculated: Bulk composition, total ∆G, density of solids, wt% of H2O in solids, amounts, volumes, molar volumes of all phases, concentrations and activities of endmembers and much more.

This table (comma-delimited) can be read by most spreadsheet programs (e.g. Excel), or statistics software (e.g. StatView).

**tcp-file**

In the working directory. Usually called "loop.tecplt". This file is contains the same information as the tab-file, but is specially tailored as input to the program "Tecplot".

### Interactive input for THERIAK

This information is also available by entering "?" in the program dialogue.

#### database definition

CR accept <last input> (if any) and continue.

"files" to see the default names, types and descriptions of files associated with the program. You may change these defaults by editing file theriak.ini with a common text editor.

database filename file name of database to be used (dbs-file).

database phase1 phase2 etc. file name of database to be used followed by names of phases to  
include in calculations.

#### type of calculations

CR Accept the last run entry enclosed in < >.

"no" Do no special calculations, just calculate with T and P values defined in your dat-file.

"bin" s s1 Calculate a pseudo-binary in "s" steps (default = 100) using the 'endmember' bulk compositions defined in your dat-file. In this case, a table with all variables is written into the tab- and tcp-file (see note below). Grel (Gtot relative to a straight line between the first and last composition calculated) is written into the bin-file  
if s1 not zero (or blank): calculate only loop s1 (for testing purposes)

"loop" Prompts for new T and P values after each calculation.

file name: If the input is not recognized as one of the keywords above, it is interpreted as the name of a drv-file. This file drives equilibria calculations, e. g., along a given PT-path. The format of the drv-file is as follows:

“check” Used to test the subroutine “GETVAL”. After equilibrium calculation you can enter   
phase var (Phase name and variable name) repeatedly. (see program “prtcal.f90”)

#### format of the drv-file

Each line defines one "action" of Theriak:

"REF" t1 p2 defines the equilibrium assemblage at the reference t1, p2. This is the "reference assemblage" adding the variable "G\_overstep" to the files of type "tab" and "tcp".  
Example:  
REF 650 4500

"COMP" formula use Defines the bulk composition for further calculations. Example:  
COMP SI(3)AL(1)MG(3)K(1)O(12)H(2) \*

"ADD" formula Adds the given formula to the current bulk composition. The amounts may be negative, but only so much will be subtracted that all components remain >= 0. Example:  
ADD H(20)O(10)

"REMOVE" phase p After each of the following calculations, the composition of stable "phase" will be (partly) removed from the bulk. "p" is the percentage of "phase" that is to be removed. Example:  
REMOVE GARNET 100

"TP" t2 p2 s Calculates equilibria along a linear TP-path. T and P change between the current values t1,p1 and t2,p2. The current values t1,p1 are either the input from the dat-file or from a preceding TP-directive within the drv-file. "s" is the number of calculation steps (default= 1) along the path. All variable values for each step are written into the tab- and tcp-files. Example:  
TP 800 5000 10

#### Temperature and Pressure

If the input to "type of calculation" was "loop", T and P can be entered repeatedly.

"end" Same as CR.

T(C) P(bar) start a new equilibrium calculation with new T and P values.

## domino

DOMINO calculates almost any type of equilibrium assemblage phase diagram. The user defines two independent variables which may be P, T, activity of a component or a pseudo-binary system. (or, as special case, a pseudo-ternary system). The calculation may be a phase diagram, mapping the stable assemblages, isopleths of mineral compositions, isolines for amounts, densities, volumes of single phases or rock bulk parameters and much more.

the output is a graphics file (plt-file) that may be cleaned and translated to PostScript with the programs GUZZLER and EXPLOT. Optionally the output may also consist of pixmaps for all variables with a fixed grid.

Multiple diagram calculations can be defined with scripts and run as batch-jobs.

### Filenames associated with Domino

|  |  |  |  |
| --- | --- | --- | --- |
| **I/O unit** | **type** | **file name** | **Description** |
| 01 | ini | theriak.ini (\*) | Program initialization data file |
| 02 | hlp | thhelp.txt (\*) | Help file |
| 03 | spt | script | Domino default script file name |
| 04 | job | domjob | Domino default batch job file |
| 05 | kbd | Keyboard (\*) | Keyboard (standard input) |
| 06 | scr | Screen (\*) | Screen (standard output) |
| 07 | dat | THERIN | User's general input file |
| 08 | dbs | Run-time defined | Thermodynamic database |
| 09 | log | domino.last | User responses during last run |
| 10 | out | OUT | Calculation results to print or view on screen |
| 15 | plt | coplot | Graphics data; input to GUZZLER or EXPLOT |
| 16 | cln | clean | Labeling reactions in graphics files; input to EXPLOT |
| 19 | pst | plot.ps | Graphics file in PostScript format |
| 20 | fig | pixelmaps | Directory name for pixelmaps (no filename extension) |
| 39 | ifnr |  | Interactive input-file, passed as argument |

(\*) Hard-coded file names (cannot be changed)

### Domino Input files

Domino can be invoked with a command line argument, which is the file name of a script-file. See below.

**Theriak.ini**

This file is read at the beginning and contains information on file names and calculation parameters. If this file is present in the working directory, this will be used, else the file in the program directory is taken. To make changes, copy the file to the working directory and edit its content. The most important items one might change are:

$GHELP=0 (reduces the comments at the start of the programs)

and the following list with the names of input and output files used by Domino.

$DOMINO-FILES

dat=xxxx #User's chemical input to program

dbs=Run time-defined #Thermodynamic data base to be used

log=xxxx #User's responses during last run of program

out=xxxx #Calculation information to be printed or viewed on screen

plt=xxxx #Graphics data (e.g. input to GUZZLER)

cln=xxxx #Graphics data after label arranging and cleaning (e.g. input to  
 EXPLOT)

pst=xxxx #Graphics file in PostScript format

fig=xxxx #Directory name for pixelmaps (no filename extension!)

$END

use the keyword "files" in the interactive input to print all file names defined.

**thhelp.txt**

is located in the program directory and contains the text printed if the user enters a "?" in the interactive input.

**dat-file**

usually called THERIN or therin.txt. This file must be present in the working directory and contains the user input for one T and P and the chemical compositions. E.g.:

600 4000

0 SI(60)AL(60)NA(10)K(10)SI(100)H(100)O(?) \*

**dbs-file**

This is the thermodynamic database used for the calculations. The name is entered by the user in the interactive input. The file must be in the working directory. E.g.: JUN92.bs

**script file**

Script files may be produced by DOMINO (Keyword "script"). These are then used instead of the interactive input. The first line of script files begin with "script.". A single script may be run with the command:

domino < scriptname (Input Redirection

domino scriptname (Command Line Argument)

**log-file**

In the working directory. Contains the interactive input from the last run. All input that remains the same (e.g. the name of the database) can be used again with CR. (carriage return)

**Terminal input**

Is the interactive input through the keyboard

### Domino output files

**Terminal output**

Is the text output of the program to the screen. This is the dialog, help comments, error messages and a short summary of calculation progress.

**out-file**

In the working directory. Usually called "OUT". Most of the above "Terminal output" is also written to this file.

**plt-file**

In the working directory. Usually called "coplot". This file contains the graphics information computed by Domino. (Its format is almost identical to the graphics output of TWQ.) A description of the format can be found in the Explot users guide, keyword "NPLOIG".

The graphics file is usually first run through GUZZLER, which formats the labels on the curves and writes a cln-file, which can be translated to a PostScript file by EXPLOT.

**spt-file**

Written to the working directory. Script files produced by DOMINO (Keyword "script"). These contain all necessary information for a single Domino run.

**job-file**

Written to the working directory by DOMINO (Keyword "script"). Contains the commands to run DOMINO with script files.

**pixelmaps folder**

This folder is created if the keyword "pix" is used as calculation type, and contains files with graymap information for all variables. Phase diagram information is written to "datetime" and " pixinfo". The folder name begins with a "\_" to be recognized by the program Makemap that crates Postscript and pgm (portable graymap) images.

### Interactive input for DOMINO

This information is also available by entering "?" in the program dialogue.

#### database definition

CR to use the thermodynamic database used in the last run and run DOMINO interactively.

"files" to see the default names, types and descriptions of files associated with the program. You may change these defaults by editing file theriak.ini with a common text editor.

database filename file name of database to be used (dbs-file).

database phase1 phase2 etc.: file name of database to be used followed by names of phases to include in calculations.

"script" to start creating script files (file type "spt") that are used to run DOMINO unattended (e.g. over-night). For more information about scripting, see below.

#### domino-scripting

DOMINO can be instructed to calculate many different phase diagrams non-interactively, for example overnight. For each of these phase diagrams, the input normally needed by DOMINO, e.g. name of the database, definition of X and Y axis, calculation parameters etc., must be prepared and saved in a SCRIPT file (spt-file) beforehand. The names of script files may be defined individually, or are generated by default as files named "scriptXX.spt", where XX is an integer between 01 and 99. Each of the script files substitutes for the keyboard, i.e. for your responses to questions that DOMINO normally asks you. So, you may let DOMINO do its job unattended without you being present and answering the questions. The script files may be executed by means of an executable BATCH JOB file.

##### Structure of the executable batch files

The default name (domjob) of this file is given in "theriak.ini". For DOS-Win it has usually the extension ".bat", which makes it executable. For Unix/Linux/Mac one has to set this attribute before execution, with.  
"chmod u+x domjob"

job-file and spt-file names may be defined individually during execution. The following default names are however proposed by the program:

|  |  |
| --- | --- |
| job name | Script names |
| default: **domjob** | script001.txt, script002.txt, script003.txt etc |
| user defined (e.g.): **myplot** | myplot001.txt, myplot002.txt, myplot003.txt etc. |

The name of the pixelmap folder (if needed) is always "\_(script name)\_pix"

If the chosen names exist, job-files are always appended and spt-files always overwritten.

The executable BATCH JOB file "myplot.bat" (DOS, Windows) or "myplot" (Unix and derivates) will contain the following records:

domino < myplot001.spt

guzzler myplot001.plt myplot001.cln myplot001.rxn

explot myplot001.cln myplot001.ps

domino < myplot002.spt

guzzler myplot002.plt myplot002.cln myplot002.rxn

explot myplot002.cln myplot002.ps

etc.

The first of these records calls DOMINO and instructs it that the information it needs for calculation of phase diagram myplot001 is provided by script file "myplot001.txt". The graphics data will be written into a plt-file having the name myplot001.plt. This is given as input argument to program GUZZLER in the second line. GUZZLER will create appropriately named files that, again, are input arguments to program EXPLOT in the third line. The final result will be a PostScript file named myplot001.ps.

NOTE: BATCH JOB files may be edited (carefully) with any text editor!

##### Structure of SCRIPT files

Each script file contains records with the following information needed by DOMINO. Text in parentheses are comments.

|  |  |
| --- | --- |
| script.script001.txt | (keyword "script." is diagnostic, don't change!) |
| script001.txt | (graphics output file name) |
| jun92bs.txt | (name of database |
| 1.0 350 0.01 0.1E-08 0.1E-06 0.1E+01 0.1E-04 25 15 100 | (calculation parameters) |
| 0 AL(2)SI(1)O(?) \* calculates the triple point | (1 to 6 lines of chemical information) |
|  | (2-6 are often empty) |
|  | (empty) |
|  | (empty) |
|  | (empty) |
|  | (empty) |
| TC 300 1000 | (definition of X-axis variable) |
| P 1 10000 | (definition of Y-axis variable) |
| . | (type of calculation) |
| 1 | (choice of labels) |
| 0.0000000E+00 0.0000000E+00 | (T and P if constant) |
| \_script01\_pix\ | (folder name for pixel map information) |

NOTE: SCRIPT files may be edited carefully with any text editor!

#### definition of X-axis

"list" Prints an alphabetically ordered list of all considered phases and their abbreviations.

X-variable: "TC" Temperature in deg. C.

"TK" Temperature in K

"P" Pressure in bar.

"A(Abc)" Activity of phase Abc. (phase name abbreviation)

"LNA(Abc)" Natural logarithm of activity for phase Abc (phase name abbreviation).

"LOGA(Abc)" Logarithm of activity for phase Abc (phase name abbreviation).

"BIN" Binary (compositions read from input file (dat-file)).

"TER" Ternary (compositions read from input file (dat-file)).

NOTE: "Abc" is the abbreviation of a phase referred in the thermodynamic database.  
 (The phase is usually an endmember of a solution, but may be any non-solution phase)

X-min X-max Defines the value-range of the X-variable.

Grid\_Points (optional) Number of grid points along the X-axis (default=10).

width (optional) Width (cm) of diagram (default=15).

IF X-variable = "TER", no X-min, X-max and definition of Y-axis is necessary.

**Examples:**

TC 400 800

LNA(Ab) 0.5 1.2

#### 

#### definition of Y-axis

"list" Prints an alphabetically ordered list of all considered phases and their abbreviations.

Y-variable: "TC" Temperature in deg. C.

"TK" Temperature in K

"P" Pressure in bar.

"PT" special function: Temperature in oC. P defined along "gradient":  
 P = 1062.091685 + 2.567123·TC + 0.01085·TC2

“THG” thgr Gradient defined as P = (TC-25.0D0)\*thgr+1.0D0

"A(Abc)" Activity of phase Abc. (phase name abbreviation)

"LNA(Abc)" Natural logarithm of activity for phase Abc (phase name abbreviation).

"LOGA(Abc)" Logarithm of activity for phase Abc (phase name abbreviation).

"BIN" Binary (compositions read from input file (dat-file)).

NOTE: "Abc" is the abbreviation of a phase referred in the thermodynamic database.  
 (The phase is usually an endmember of a solution, but may be any non-solution phase)

Y-min Y-max Defines the value-range of the Y-variable.

Grid\_Points (optional) Number of grid points along the Y-axis (default=10).

height (optional) Height (cm) of diagram (default=15).

**Examples:**

P 1000 20000

A(H2O) 0 1

Some checking is made, that X-axis and Y-axis is not the same variable.

#### calculation type

"list" Prints an alphabetically ordered list of all considered phases and their abbreviations, and a list of solutions, endmembers and site occupancies.

"." (dot) calculates an equilibrium assemblage phase diagram

"pix" ix iy Calculates equilibria on an ix by iy grid and stores all results for graymap images.  
(see below for more details)

"I" Provides a simplified input for isolines calculations.

(Phase) Key (Nr) min max step Isolines calculation (see below)

##### isolines calculation

(Phase) Key (Nr) min max step

**1. for bulk rock properties**

Enter: key min max step

key is one of the following keywords:

"volsol" Volume of solids [ccm]

"wtsol" Weight of solids [g]

"rhosol" Density of solids [g/ccm]

"gtot" Total Gibbs Free Energy [J]

"%h2o.sol" Wt% of H2O in solids

min max step minimum, maximum and step values for the isolines.

The maximum number of isolines calculated is 50.

**Example: plot Wt% of H2O in solids between 0 and 10 in steps of 0.5**

%h2o.sol 0 10 0.5

**1. for non-solution phases**

Enter: Name key min max step

Name is the name (not abbreviation) of a phase

Key is one of the following keywords:

"mol" Amount of phase [mol]

"vol" Volume of phase [ccm]

"mvol" Molar volume of phase [ccm]

"wt" Weight of phase [g]

"mwt" Molar weight of phase [g]

"rho" Density of phase [g/ccm]

"vol%" Volume% of phase (% of solids)

min max step minimum, maximum and step values for the isolines.

The maximum number of isolines calculated is 50.

**Example: plot iso-density lines of quartz between 2.5 and 2.7 in steps of 0.02**

A-QUARTZ rho 2.5 2.7 0.02

**1. for solution phases**

Enter: Name Key Nr min max step

Name is the name of a solution phase

Nr: If more than one phase of the same solution is stable, the phase with the highest concentration of the first endmember is numbered 1, the next lower is numbered 2 and so on. This is for most cases sufficient to distinguish the different phases. Nr. must be at least = 1.

Key is one of the following keywords:

endmember abbreviation of endmember, isopleths will be calculated.

El(site) Site occupancies, isopleths will be calculated.

"mol" Amount of solution phase [mol]

"vol" Volume of solution phase [ccm]

"mvol" Molar volume of solution phase [ccm]

"wt" Weight of solution phase [g]

"mwt" Molar weight of phase [g]

"rho" Density of solution phase [g/ccm]

"vol%" Volume% of solution phase (% of solids)

"Mg#" Ratio Mg/(Mg+Fe) of solution phase.

min max step minimum, maximum and step values for the isolines.

The maximum number of isolines calculated is 50.

**Example: Plot grossular isopleths in garnet between 0.3 and 0.6 in steps of 0.02**

GARNET Grs 1 0.3 0.6 0.02

**Example: plot iso-density lines of feldspar between 2.5 and 2.7 in steps of 0.02**

FSP rho 1 2.5 2.7 0.02

Note: Valid endmembers and site occupancies can be printed with "list"

##### pixelmap calculations

"pix" ix iy Calculates equilibria on a ix by iy grid and stores all results for graymap images.

reasonable values for ix and iy are 50-200.

The information stored is the assemblage and most variables available for isolines calculation. For each variable a file is created. The information on the diagram dimension, the X- and Y-axes and the names of all variables are written to the file "pixinfo", the date and time to "datetime" These files are later used by the program MAKEMAP to reconstruct graymaps for any variable. All files are stored in a folder with a name that begins with '\_'. If no such folder exists, the program will create a folder "\_pixelmaps". If that name exists already, the user is asked to either enter a new name or to overwrite the folder.

#### labeling of reactions

(only if calculation type is not "pix")

Label Is "1", "2" or "3".  
"1" For labeling reactions on each side with the stable assemblage.

E.g.: A B C = A B D

"2" For labeling reactions only by new phases produced.

E.g.: (C) = (D)

"3" For labeling reactions with a balanced equation.

E.g. A + 2 B + C = 3 D

(If more than one reaction is involved, the coefficients are omitted.

E.g.: A B C = D)

"prec" Optional, precision in cm, (default=0.005).

"smooth" Optional, smoothness in cm, (default=0.04).

The most useful option is "1", because the labels will contain the maximum information on assemblages.

During calculation, DOMINO prints comments on progress. Some are explained in commented\_domino.pdf.

### Interpretation of phase diagrams produced by DOMINO

Once the calculation is finished. the plt-file should be cleaned with GUZZLER (use label-size 0.2 or smaller, no special options), translated by EXPLOT and printed.

Also print the rxn-file (table) that contains a numbered list of all curves.

Because the phase diagram may consist of many curves, it is not always easy to understand. The following suggestions may help:

1. use THERIAK to get detailed information of single points in the diagram.
2. trace important curves (e.g. the stability fields of staurolite, garnet, plagioclase etc. ) with colored pencils.
3. Consider calculating a simplified diagram with less components, or some phases deleted from the database.

## therbin

The core of THERBIN is the equilibrium calculation program THERIAK. This approach is chosen in order to calculate very complex and non-ideal binary phase diagrams automatically, without human interference (or almost). The strategy of the program is to scan the T-x (or P-x) surface is for two-phase regions. Once one is found, it is mapped and a search for new two-phase regions is initiated adjacent to it. When all interconnected regions are found, the scanning is resumed, but only outside the already mapped areas. For THERBIN, all considered phases have to be part of a binary sub-system.

### Filenames associated with Therbin

|  |  |  |  |
| --- | --- | --- | --- |
| **I/O unit** | **type** | **file name** | **Description** |
| 01 | ini | theriak.ini (\*) | Program initialization data file |
| 02 | hlp | thhelp.txt (\*) | Help file |
| 05 | kbd | Keyboard (\*) | Keyboard (standard input) |
| 06 | scr | Screen (\*) | Screen (standard output) |
| 07 | dat | THERIN | User's general input file |
| 08 | dbs | Run-time defined | Thermodynamic database |
| 09 | log | therbin.last | User responses during last run |
| 10 | out | OUT | Calculation results to print or view on screen |
| 15 | plt | plot | Graphics data; input to EXPLOT |

(\*) Hard-coded file names (cannot be changed)

### Therbin Input files

Therbin can be invoked with a command line argument which is the file name containing the interactive input.

**Theriak.ini**

This file is read at the beginning and contains information on file names and calculation parameters. If this file is present in the working directory, this will be used, else the file in the program directory is taken. To make changes, copy the file to the working directory and edit its content. The most important items one might change are:

$GHELP=0 (reduces the comments at the start of the programs)

and the following list with the names of input and output files used by THERBIN.

$THERBIN-FILES

dat=THERIN #User's chemical input to program

log=therbin.last #User's responses during last run of program

dbs=Run time-defined #Thermodynamic data base to be used

plt=plot #Graphics data input (e.g. from DOMINO)

out=OUT #Calculation information to be printed or viewed on screen

$END

use the keyword "files" in the interactive input to print all file names defined.

**thhelp.txt**

is located in the program directory and contains the text printed if the user enters a "?" in the interactive input.

**dat-file**

usually called THERIN or therin.txt. This file must be present in the working directory and contains the user input for one T and P and the chemical compositions. e.g.:

400 2000

1 K(0.5)NA(0.5)AL(3)SI(3)O(12)H(2) SI(10)O(20) H(20)O(10) \*

**dbs-file**

This is the thermodynamic database used for the calculations. The name is entered by the user in the interactive input. The file must be in the working directory. E.g.: JUN92.bs

**log-file**

In the working directory. Contains the interactive input from the last run. All input that remains the same (e.g. the name of the database) can be used again with CR. (carriage return)

**Terminal input**

Is the interactive input through the keyboard

### Therbin Output files

**Terminal output**

Is the text output of the program to the screen. This is the dialog, help comments, error messages and a short summary of calculation progress.

**out-file**

In the working directory. Usually called "OUT". Most of the above "Terminal output" is also written to this file.

**plt-file**

In the working directory. Usually called "plot". This file contains the graphics information computed by Therbin. A description of the format can be found in the Explot users guide, keyword "NPLOIG".

The graphics file can be translated to a PostScript file by EXPLOT. It cannot be read by GUZZLER.

### Interactive input for THERBIN

This information is also available by entering "?" in the program dialogue.

#### database definition

"files" to see the default names, types and descriptions of files associated with the program. You may change these defaults by editing file theriak.ini with a common text editor.

database filename file name of database to be used (dbs-file).

#### endmembers:

"list" Prints an alphabetically ordered list of abbreviations of all considered phases.

endmember 1 Abbreviation of phase defining the composition to the left side of the diagram.

formula 1 Optional if endmember 1 is a one of the phases considered. Else the composition may be entered in the same format as the bulk is written in the dat-file.

**Exemples:**

aQz

phaseX SI(1)AL(0.5)

endmember 2, formula2:

same as above, but defining the composition ro the right side of the diagram.

#### Y-variable

Y-variable may be one or the following:

"TC" Temperature in (C)

"TK" Temperature in (K)

"P" Pressure in (Bar)

ymin, ymax minimal and maximal values for the Y-axis of the binary diagram.

If the Y-variable was Temperature you have to enter the constant pressure for the diagram.

If the Y-variable was Pressure you have to enter the constant temperature for the diagram.

#### seeds

Usually=0.

Seeds are points in the diagram that will be searched for two-phase regions, besides the grid points. If one suspects, that a small two-phase region might be overlooked several "seeds" may be entered manually. The program will ask the coordinates for each point

#### scan density and tolerance

Usually suggested values are OK

X-scan-density Number of grid points in X-direction (program always suggests 10)

Y-scan-density Number of grid points in Y-direction (program always suggests 10)

tolerance Precision of calculation in [cm] (program always suggests 0.02)

Before performing any calculation, the program excludes all phases that are not within the defined binary system. (Phases must be a linear combination of the two given compositions)

The graphics input is written to the plt-file which can be converted to PostScript with EXPLOT.

## therter

The core of THERTER is the equilibrium calculation program THERIAK. This approach is chosen in order to calculate very complex and non-ideal ternary phase diagrams automatically, without human interference (or almost). The strategy of the program is to scan the ternary composition surface for two-phase regions and three-phase regions. Once one is found, it is mapped and a search for new multi-phase regions is initiated adjacent to it. When all interconnected regions are found, the scanning is resumed, but only outside the already mapped areas. For THERTER, all considered phases have to be part of a ternary sub-system.

### Filenames associated with Therter

|  |  |  |  |
| --- | --- | --- | --- |
| **I/O unit** | **type** | **file name** | **Description** |
| 01 | ini | theriak.ini (\*) | Program initialization data file |
| 02 | hlp | thhelp.txt (\*) | Help file |
| 05 | kbd | Keyboard (\*) | Keyboard (standard input) |
| 06 | scr | Screen (\*) | Screen (standard output) |
| 07 | dat | THERIN | User's general input file |
| 08 | dbs | Run-time defined | Thermodynamic database |
| 09 | log | therter.last | User responses during last run |
| 10 | out | OUT | Calculation results to print or view on screen |
| 15 | plt | plot | Graphics data; input to EXPLOT |

(\*) Hard-coded file names (cannot be changed)

### Therter Input files

Therter can be invoked with a command line argument which is the file name containing the interactive input.

**Theriak.ini**

This file is read at the beginning and contains information on file names and calculation parameters. If this file is present in the working directory, this will be used, else the file in the program directory is taken. To make changes, copy the file to the working directory and edit its content. The most important items one might change are:

$GHELP=0 (reduces the comments at the start of the programs)

and the following list with the names of input and output files used by THERTER.

$THERTER-FILES

dat=THERIN #User's chemical input to program

log=therbin.last #User's responses during last run of program

dbs=Run time-defined #Thermodynamic data base to be used

plt=plot #Graphics data input (e.g. from DOMINO)

out=OUT #Calculation information to be printed or viewed on screen

$END

use the keyword "files" in the interactive input to print all file names defined.

**thhelp.txt**

is located in the program directory and contains the text printed if the user enters a "?" in the interactive input.

**dat-file**

usually called THERIN or therin.txt. This file must be present in the working directory and contains the user input for one T and P and the chemical compositions. E.g.:

400 2000

1 K(0.5)NA(0.5)AL(3)SI(3)O(12)H(2) SI(10)O(20) H(20)O(10) \*

**dbs-file**

This is the thermodynamic database used for the calculations. The name is entered by the user in the interactive input. The file must be in the working directory. E.g.: JUN92.bs

**log-file**

In the working directory. Contains the interactive input from the last run. All input that remains the same (e.g. the name of the database) can be used again with <CR>. (carriage return)

**Terminal input**

Is the interactive input through the keyboard

### Therter Output files

**Terminal output**

Is the text output of the program to the screen. This is the dialog, help comments, error messages and a short summary of calculation progress.

**out-file**

In the working directory. Usually called "OUT". Most of the above "Terminal output" is also written to this file.

**plt-file**

In the working directory. Usually called "plot". This file contains the graphics information computed by Therter. A description of the format can be found in the Explot users guide, keyword "NPLOIG".

The graphics file can be translated to a PostScript file by EXPLOT. It cannot be read by GUZZLER.

### Interactive input for THERTER

This information is also available by entering "?" in the program dialogue.

#### database definition

"files" to see the default names, types and descriptions of files associated with the program. You may change these defaults by editing file theriak.ini with a common text editor.

database filename file name of database to be used (dbs-file).

#### endmembers

"list" Prints an alphabetically ordered list of abbreviations of all considered phases.

endmember 1 Abbreviation of phase defining the composition in the left lower corner of the diagram.

formula 1 Optional if endmember 1 is a one of the phases considered. Else the composition may be entered in the same format as the bulk is written in the dat-file.

**Exemples:**

Gr

phaseX SI(1)AL(0.5)

**endmember 2, formula 2**

same as above, but defining the composition in the right lower corner of the diagram.

**endmember 3, formula 3**

same as above, but defining the composition in the top corner of the diagram.

#### Temperature and Pressure

T(C) Temperature in deg. C

P(Bar) Pressure in Bar

#### seeds

Usually=0.

Seeds are points in the diagram that will be searched for two-phase regions, besides the grid points. If one suspects, that a small two-phase region might be overlooked several "seeds" may be entered manually. The program will ask the coordinates for each point.

#### scan density and tolerance

Usually suggested values are OK

scan-density Number of grid points for each side (program always suggests 11)

tolerance Precision of calculation in [cm] (program always suggests 0.02)

Before performing any calculation, the program excludes all phases that are not within the defined ternary system. (Phases must be a linear combination of the three given compositions)

The graphics input is written to the plt-file which can be converted to PostScript with EXPLOT.

## thalia

THALIA plots thermodynamic functions versus T or P, or ∆G (total, configurational, excess or mixing), the chemical potential, or the activity of a phase along a binary link of a solution phase. THALIA does not do any equilibrium calculations and is mostly useful to visualize the variation of thermodynamic functions and to check the database for typing errors.

### Filenames associated with Thalia

|  |  |  |  |
| --- | --- | --- | --- |
| **I/O unit** | **type** | **file name** | **Description** |
| 01 | ini | theriak.ini (\*) | Program initialization data file |
| 02 | hlp | thhelp.txt (\*) | Help file |
| 05 | kbd | Keyboard (\*) | Keyboard (standard input) |
| 06 | scr | Screen (\*) | Screen (standard output) |
| 07 | dat | THERIN | User's general input file |
| 08 | dbs | Run-time defined | Thermodynamic database |
| 09 | log | thalia.last | User responses during last run |
| 10 | out | OUT | Calculation results to print or view on screen |
| 15 | plt | thplot | Graphics data; input to GUZZLER and EXPLOT |
| 21 | lpl | thaliaplot | Graphics data (long format); input to GUZZLER and EXPLOT |

(\*) Hard-coded file names (cannot be changed)

### Thalia Input files

Thalia can be invoked with a command line argument which is the file name containing the interactive input.

**Theriak.ini**

This file is read at the beginning and contains information on file names and calculation parameters. If this file is present in the working directory, this will be used, else the file in the program directory is taken. To make changes, copy the file to the working directory and edit its content. The most important items one might change are:

$GHELP=0 (reduces the comments at the start of the programs)

and the following list with the names of input and output files used by THALIA.

$THALIA-FILES

dat=THERIN #User's chemical input to program

log=thalia.last #User's responses during last run of program

dbs=Run time-defined #Thermodynamic data base to be used

out=OUT #Calculation information to be printed or viewed on screen

plt=thplot #Graphics data input

lpl=thaliaplot #Graphics data input

$END

use the keyword "files" in the interactive input to print all file names defined.

**thhelp.txt**

is located in the program directory and contains the text printed if the user enters a "?" in the interactive input.

**dat-file**

usually called THERIN or therin.txt. This file must be present in the working directory and contains the user input for one T and P and the chemical compositions. E.g.:

400 2000

1 K(0.5)NA(0.5)AL(3)SI(3)O(12)H(2) SI(10)O(20) H(20)O(10) \*

**dbs-file**

This is the thermodynamic database used for the calculations. The name is entered by the user in the interactive input. The file must be in the working directory. E.g.: JUN92.bs

**log-file**

In the working directory. Contains the interactive input from the last run. All input that remains the same (e.g. the name of the database) can be used again with CR. (carriage return)

**Terminal input**

Is the interactive input through the keyboard

### Thalia Output files

**Terminal output**

Is the text output of the program to the screen. This is the dialog, help comments, error messages and the calculation results.

**out-file**

In the working directory. Usually called "OUT". Most of the above "Terminal output" is also written to this file.

**plt-file**

In the working directory. Usually called "thplot". This file contains the graphics information computed by Thalia. (Its format is almost identical to the graphics output of TWQ.) A description of the format can be found in the Explot users guide, keyword "NPLOIG".

The graphics file is usually first run through GUZZLER, which formats the labels on the curves and writes a cln-file, which can be translated to a PostScript file by EXPLOT.

**lpl-file**

In the working directory. Usually called "thaliaplot". This file contains the graphics information computed by Thalia. The difference to the plt-file is, that all numbers are in the format:   
(0PE20.12) instead of F10.4.

This is because for some plots with large numbers (e.g. ∆G versus T) the number of digits in the plt-file is not sufficient and produces steps in the curve.

### Interactive input for THALIA

This information is also available by entering "?" in the program dialogue.

#### database definition

"files" to see the default names, types and descriptions of files associated with the program. You may change these defaults by editing file theriak.ini with a common text editor.

database filename file name of database to be used (dbs-file).

#### X-variable definition

X-variable "TC" Temperature in deg. C  
"TK" Temperature in K  
"1000/T" (1000/T) Temperature in K  
"P" Pressure in Bar

xmin, xmax minimal and maximal values for the X-axis.

"X" to plot G-X, µ-X or a-X diagrams (see below)

#### Y-variable definition (X-variable is TC, TK, 1000/T or P)

"B" back one step (in this case: stop the program)

"end" Stop the program

Y-var the Y-variable may be one of the following:

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| G | V | CP | H | S | LNK | LOGK | K | Basic thermodynamic functions |
| G-G0 | V-V0 | CP-CP0 | H-H0 | S-S0 |  |  |  | Difference between T/P and 25 C/1Bar |
| G.CP |  | CP.CP | H.CP | S.CP |  |  |  | Contribution from the Cp-function |
| G.DIS | V.DIS | CP.DIS | H.DIS | S.DIS |  |  |  | Contribution from the disorder function |
| G.TR | V.TR | CP.TR | H.TR | S.TR |  |  |  | Contribution from lambda transitions |
| G.VOL | V.VOL |  |  |  |  |  |  | Contribution from the volume function |
| G.GAS | V.GAS |  |  |  |  |  |  | Contribution from the Gas function (Van der Waal, Redlich-Kwong) |

#### Formula definition (X-variable is TC, TK, 1000/T or P)

"B" back to Y-variable definition: This allows to draw several thermodynamic functions on the same plot.

"end" Stop the program

"list" Prints an alphabetically ordered list of abbreviations of all considered phases.

formula the abbreviation of a single phase  
or a formula like: n1 A + n2 B + C - n4 D - E  
A, B, C etc: abbreviations of phases  
n1, n2, etc. coefficients, may be omitted if =1)  
all items are separated by one blank.

#### Pressure or Temperature

"B" Back to formula definition. This allows to draw thermodynamic functions for different phases (or formulas).

"end" Stop the program

P Pressure in Bar. If the X-variable was P, the program asks for T.

After this dialogue a Diagram is calculated and the question is repeated. Thus, you may enter a new pressure (or temperature), go back one step or stop the program.

#### Solution definition (X-variable is "X")

The program will always print a list of all solution phases.

"B" back one step (in this case: stop the program)

"end" Stop the program

solution name Name of the solution.

#### Composition definition (X-variable is "X")

Define "binary endmembers" as linear combination of the endmembers of the solution

"B" Back to solution definition. This allows to draw different solutions on the same plot.

"end" Stop the program

binary endmember1 Definition of the left side of the diagram in terms of endmember concentrations.  
As an example with FSP as solution phase, Ab would be (1 0 0), Kfs is (0 1 0) and An is (0 0 1). One could also define a mixture e.g. (1 1 0), which would lie in the middle between Ab and Kfs. (Note: the concentrations are normalized to a sum of one by the program)

**binary endmember2**

same as above for the second composition, defining the right side of the diagram.

#### Y-variable definition (X-variable is "X")

"B" Back to composition definition. This allows to draw different binary links on the same plot.

"end" Stop the program

Y-variable The Y-variable may be:  
"G" Total Gibbs Free Energy ∆G  
"GCON" Configurational Contribution to ∆G  
"GEX" Excess contribution to ∆G  
"MUE" n Chemical potential of n'th endmember  
"ACT" n Activity of n'th endmember

#### Temperature and Pressure

"B" Back to composition definition. This allows to draw different thermodynamic functions on the same plot.

"end" Stop the program

temperature pressure Temperature in deg. C and pressure in Bar.

After this dialogue a Diagram is calculated and the question is repeated. Thus you may enter a new pressure (or temperature), go back one step or stop the program.

The graphics input is written to the plt- and lpl-file which can be cleaned with GUZZLER and converted to PostScript with EXPLOT.

## thermo

For a given p and T, THERMO calculates ∆G (apparent Gibbs free energy, = ∆H - T.S), ∆H, S, Cp and V. Also, for each thermodynamic function (Cp, volume, disorder, lambda transition) its contribution to the total ∆G, ∆H. The main application of THERMO is to check the calculations for programming errors and to check the database for typing errors. Further it prints tables of ∆G and Volume for comparing different databases or equations of state.

### Filenames associated with Thermo

|  |  |  |  |
| --- | --- | --- | --- |
| **I/O unit** | **type** | **file name** | **Description** |
| 01 | ini | theriak.ini (\*) | Program initialization data file |
| 02 | hlp | thhelp.txt (\*) | Help file |
| 05 | kbd | Keyboard (\*) | Keyboard (standard input) |
| 06 | scr | Screen (\*) | Screen (standard output) |
| 07 | dat | THERIN | User's general input file |
| 08 | dbs | Run-time defined | Thermodynamic database |
| 09 | log | thermo.last | User responses during last run |
| 10 | out | OUT | Calculation results to print or view on screen |
| 13 | tab | stat.table | Table of variable values; input to spreadsheet programs |

(\*) Hard-coded file names (cannot be changed)

### Thermo Input files

Thermo can be invoked with a command line argument which is the file name containing the interactive input.

**Theriak.ini**

This file is read at the beginning and contains information on file names and calculation parameters. If this file is present in the working directory, this will be used, else the file in the program directory is taken. To make changes, copy the file to the working directory and edit its content. The most important items one might change are:

$GHELP=0 (reduces the comments at the start of the programs)

and the following list with the names of input and output files used by THERMO.

$THERMO-FILES

dat=THERIN #User's chemical input to program

log=thermo.last #User's responses during last run of program

dbs=Run time-defined #Thermodynamic data base to be used

out=OUT #Calculation information to be printed or viewed on screen

tab=stat.table #Table of variable values; input to a spreadsheet program

$END

use the keyword "files" in the interactive input to print all file names defined.

**thhelp.txt**

is located in the program directory and contains the text printed if the user enters a "?" in the interactive input.

**dat-file**

usually called THERIN or therin.txt. This file must be present in the working directory and contains the user input for one T and P and the chemical compositions (not used by Thermo). E.g.:

400 2000

1 K(0.5)NA(0.5)AL(3)SI(3)O(12)H(2) SI(10)O(20) H(20)O(10) \*

**dbs-file**

This is the thermodynamic database used for the calculations. The name is entered by the user in the interactive input. The file must be in the working directory. E.g.: JUN92.bs

**log-file**

In the working directory. Contains the interactive input from the last run. All input that remains the same (e.g. the name of the database) can be used again with CR. (carriage return)

**Terminal input**

Is the interactive input through the keyboard

### Thermo Output files

**Terminal output**

Is the text output of the program to the screen. This is the dialog, help comments, error messages and the calculation results.

**out-file**

In the working directory. Usually called "OUT". Most of the above "Terminal output" is also written to this file.

### Interactive input for THERMO

#### database definition

"files" to see the default names, types and descriptions of files associated with the program. You may change these defaults by editing file theriak.ini with a common text editor.

database filename file name of database to be used (dbs-file).

#### phase definition

"list" Prints an alphabetically ordered list of abbreviations of all considered phases.  
Independently on the chemical composition given in the dat-file, these are all phases in the database.

"end" Stop the program.

"TP" t p Set the Temperature (C) and Pressure (Bar) (Initially set to the values from the dat-file)

"g" Calculate a table of G-values (for previously defined phases)

"v" Calculate a table of Vol-values (for previously defined phases)

phases may be a single phase (one abbreviation)  
or a list of phases, each item separated by two blanks  
or the keyword "all"

## GUZZLER

GUZZLER is a program that distributes the labels on the curves, avoiding overlaps. The input file to GUZZLER is a graphics file (plt-file) produced by DOMINO, or THALIA. Because TWQ uses the same file format, GUZZLER may also be used to clean up the plot.dat files from TWQ.  
The plt-files from DOMINO have initially a label-size of zero. Translating them with EXPLOT to PostScript and printing will show no labels. GUZZLER assigns a size and distributes the labels. Four cases are distinguished:

1) Full label is written

2) Only the number of the label is written on the curve.

3) The number is written somewhere close, with a fine line pointing to the reaction.

4) The curve is not labeled at all

Like all software that appears to do some "thinking", GUZZLER is quite straight forward and does not do any thinking at all.

### Filenames associated with Guzzler

|  |  |  |  |
| --- | --- | --- | --- |
| **I/O unit** | **type** | **file name** | **Description** |
| 01 | ini | theriak.ini (\*) | Program initialization data file |
| 02 | hlp | thhelp.txt (\*) | Help file |
| 05 | kbd | Keyboard (\*) | Keyboard (standard input) |
| 06 | scr | Screen (\*) | Screen (standard output) |
| 12 | log | guzzler.last | User responses during last run |
| 13 | cln | clean | Labeling reactions in graphics files; input to EXPLOT |
| 14 | plt | Run-time defined | Graphics data; input to GUZZLER |
| 15 | rxn | table | List of reactions and assemblages |
| 16 | grd | gitter | File used for bookkeeping. |

(\*) Hard-coded file names (cannot be changed)

### Guzzler Input files

Guzzler can be invoked with three command line arguments which are the file name of the graphics file (e.g. plot), the name of the cleaned file (e.g. clean) and the name of the reaction list (e.g. table)

.

**Theriak.ini**

Only used in the "kguzzler" version. See comments inTheriakDominoGuide.doc.

This file is read at the beginning and contains information on file names and calculation parameters. If this file is present in the working directory, this will be used, else the file in the program directory is taken. To make changes, copy the file to the working directory and edit its content. The most important items one might change are:

$GHELP=0 (reduces the comments at the start of the programs)

and the following list with the names of input and output files used by GUZZLER.

$GUZZLER-FILES

log=guzzler.last #User's responses during last run of program

cln=clean #Graphics data after label arranging and cleaning (e.g. input to EXPLOT)

plt=Run time-defined #Graphics data input (e.g. from DOMINO)

rxn=table #Reaction/assemblage list

grd=gitter #Grid information for graphics file

$END

use the keyword "files" in the interactive input to print all file names defined.

**thhelp.txt**

is located in the program directory and contains the text printed if the user enters a "?" in the interactive input.

**plt-file**

In the working directory. This file contains the graphics information computed e.g. by Domino. (Its format is almost identical to the graphics output of TWQ.) A description of the format can be found in the Explot users guide, keyword "NPLOIG".

**log-file**

In the working directory. Contains the interactive input from the last run. All input that remains the same (e.g. the name of the database) can be used again with CR. (carriage return)

**Terminal input**

Is the interactive input through the keyboard

### Guzzler output files

**Terminal output**

Is the text output of the program to the screen. This is the dialog, help comments and error messages

**cln-file**

In the working directory. Usually called "clean". This file contains the graphics information of the "cleaned-up" plot. This may be translated to PostScript by EXPLOT.

**rxn-file**

In the working directory. Usually called "table". This is a numbered list of all curves defined in the graphics file.

**grd-file**

In the working directory. Usually called "gitter". This file is used by Guzzler to keep track of space available for labeling. For the user this file is of no interest.

### Interactive input for GUZZLER

This information is also available by entering "?" in the program dialogue.

#### graphics file

Enter [ "?" | CR | graphics file name ] <coplot>?

graphics file name name of a graphics file to be used as input.

#### Size of labels

size of labels label-size in cm. with no log-file the program will suggest 0.2

After this input, a numbered list of all curves is printed on the screen.

#### Labeling

option choose one of the options (see below) (default=-3)

min\_length define the minimum length of a curve for labeling (default=0.02 cm)

##### options

-3 (default) Write full labels, if possible, else try numbers on lines or offset numbers.

3 Force full text-labels on every curve. This may be useful, if few lines are present and the overlapping labels are still readable.

-2 Use only numbers (no text-labels). The numbers may be either on the curve or offset.

2 Force the reaction numbers to be written on each curve.

-1 (use offset numbers only, option not recommended)

1 (force offset numbers, option not recommended)

0 Do not label curves. This option removes all labels and produces a clean diagram which can be labeled and colored manually.

4 Label all curves with either full text-labels or with numbers on line

5 No offset numbers. This option produces a nice readable diagram. Short lines will not be labeled.

### run GUZZLER with no interactive input

This option is normally used with DOMINO scripts, doing multiple phase diagram calculations. In this case GUZZLER is run with command line arguments:

**guzzler plt-file [cln-file rxn-file]**

where plt-file Name of graphics input file

cln-file Name of "cleaned" output file (if not given, default name is taken)

rxn-file Name of file with table of reactions (if not given, default name is taken)

GUZZLER will use the default labeling method and 0.2 for label-size or the value given in the log-file.

## EXPLOT

Explot is a simple general-purpose plot program. The input is a command language, similar to the plot commands used by many computer languages. The output is a PostScript file that may be sent to a printer or viewed at a console. A detailed description of the input options is given in ExplotGuide.doc.

One of the options for input is the format used by DOMINO and other software for the graphics output file.

### Filenames associated with Explot

|  |  |  |  |
| --- | --- | --- | --- |
| **I/O unit** | **type** | **file name** | **Description** |
| 01 | ini | theriak.ini (\*) | Program initialization data file |
| 02 | hlp | thhelp.txt (\*) | Help file |
| 05 | kbd | Keyboard (\*) | Keyboard (standard input) |
| 06 | scr | Screen (\*) | Screen (standard output) |
| 12 | log | explot.last | User responses during last run |
| 13 | cln | clean | Labeling reactions in graphics files; input to EXPLOT |
| 14 | plt | Run-time defined | Graphics data; input to GUZZLER |
| 15 | rxn | table | List of reactions and assemblages |
| 16 | grd | gitter | File used for bookkeeping. |
| 17 | pst | plot.ps | Graphics in PostScript format |

(\*) Hard-coded file names (cannot be changed)

### Explot Input files

**Theriak.ini**

Only used in the "kexplot" version. See comments inTheriakDominoGuide.doc.

This file is read at the beginning and contains information on file names and calculation parameters. If this file is present in the working directory, this will be used, else the file in the program directory is taken. To make changes, copy the file to the working directory and edit its content. The most important items one might change are:

$GHELP=0 (reduces the comments at the start of the programs)

and the following list with the names of input and output files used by EXPLOT.

$EXPLOT-FILES

log=explot.last #User's responses during last run of program

cln=Run time-defined #Graphics data (input)

pst=plot.ps #Graphics file in PostScript format

$END

use the keyword "files" in the interactive input to print all file names defined.

**thhelp.txt**

is located in the program directory and contains the text printed if the user enters a "?" in the interactive input.

**cln-file**

In the working directory. This file contains the graphics information computed e.g. by DOMINO or GUZZLER or a general EXPLOT input file. A description of the format can be found in the Explot users guide, keyword "NPLOIG".

### Explot output files

Explot can be invoked with two command line argument which are the file name of the graphics file (e.g. clean) and the name of the plot file (e.g. plot.ps). (Note that a second plot file (plot.svg) will also be produced.)

**Terminal output**

Is the text output of the program to the screen. This is the dialog, help comments and error messages

**pst-file**

In the working directory. Usually called "plot.ps". This is a PostScript file and may be viewed (and even modified) by several programs, e.g. Adobe Illustrator, Corel Draw, PreView or ghostview (UNIX).

### Interactive input for EXPLOT

This information is also available by entering "?" in the program dialogue.

graphics file name Name of input file.

### run EXPLOT with no interactive input

This option is normally used with DOMINO scripts, doing multiple phase diagram calculations. In this case EXPLOT is run with command line arguments:

**explot cln-file [pst-file]**

where cln-file Name of EXPLOT input file

pst-file Name of PostScript file produced by EXPLOT. (Usually with the extension ".ps")  
 (if not given, default name is taken)

## makemap

MAKEMAP makes graymap images from the information stored by DOMINO in the pixelmap folder. (Calculation type "pix"). MAKEMAP searches in the working directory for folder names beginning with "\_". These are assumed to contain the files "pixinfo", "datetime" and one file for each variable. The files produced are a pst-file (image in PostScript format) and a pgm-file (image as 'portable gray map').

### Filenames associated with Makemap

|  |  |  |  |
| --- | --- | --- | --- |
| **I/O unit** | **type** | **file name** | **Description** |
| 01 | ini | theriak.ini (\*) | Program initialization data file |
| 02 | hlp | thhelp.txt (\*) | Help file |
| 05 | kbd | Keyboard (\*) | Keyboard (standard input) |
| 06 | scr | Screen (\*) | Screen (standard output) |
| 09 | log | makemap.last | User responses during last run |
| 10 | out | OUT | Error messages to print or view on screen |
| 19 | pst | pixel.ps | Image file in PostScript format |
| 24 | pgm | pixels.pgm | Pixelmap file in pgm format (Portable Gray Map) |
| 30 |  | pixinfo (\*) | Diagram information for graymaps |
| 32 |  | datetime (\*) | Date and time of diagram calculation |
| 33 |  | names read from pixinfo | graymap info for each variable |

(\*) Hard-coded file names (cannot be changed)

### Makemap Input files

Makemap can be invoked with a command line argument which is the file name containing the interactive input.

**Theriak.ini**

This file is read at the beginning and contains information on file names and calculation parameters. If this file is present in the working directory, this will be used, else the file in the program directory is taken. To make changes, copy the file to the working directory and edit its content. The most important items one might change are:

$GHELP=0 (reduces the comments at the start of the programs)

and the following list with the names of input and output files used by MAKEMAP.

$MAKEMAP-FILES

log=makemap.last #User's responses during last run of program

pgm=pixels.pgm # ascii-image of pixel map

pst=pixel.ps # Pixel map (PostScript file) (old unit 20)

$END

use the keyword "files" in the interactive input to print all file names defined.

**thhelp.txt**

is located in the program directory and contains the text printed if the user enters a "?" in the interactive input.

**log-file**

In the working directory. Contains the interactive input from the last run. All input that remains the same (e.g. the name of the database) can be used again with CR. (carriage return)

**Terminal input**

Is the interactive input through the keyboard

**pixelmap folder**

Folder containing the information for graymaps. Folder name must begin with "\_".

**file "pixinfo"**

Inside pixelmap folder. Contains;

* label for X-axis
* label for Y-axis
* lower and upper limits for X- and Y-axis
* height and width of diagram in cm
* number of grid points in X and Y direction and a code for xy or triangle plots.
* number of comment lines, followed by this amount of comments.
* number of composition lines followed by this amount of compositions.
* one line for each variable name.

**file "datetime"**

Inside pixelmap folder. Contains one line with date, time and calculation time.

**files with graymap information**

Inside pixelmap folder. The names of these files were created by domino. A list is included in "pixinfo".

### Makemap output files

**Terminal output**

Is the text output of the program to the screen. This is the dialog, help comments and error messages

**pgm-file**

graymap image in "portable graymap' format. This may be used as raw data for some programs for coloring and enhancing. File contains only the grayscale information.

**pst-file**

PostSript image. Contains the axes, comments and a scale of gray values.

### Interactive input for MAKEMAP

This information is also available by entering "?" in the program dialogue.

#### pixelmap folder

The program prints a numbered list of folders containing pixel map information.

"files" to see the default names, types and descriptions of files associated with the program. You may change these defaults by editing file theriak.ini with a common text editor.

folderNr Choose from the above list which folder to use. (enter the folder number)

#### function number

The program prints a numbered list of functions available for mapping.

"list" to print the numbered list of all available functions for mapping.

functionNr the number corresponding to the desired function.

key optional key for special mapping  
"x1" map the first derivative of the chosen function f with respect to the  
 X-variable of the diagram (df/dX)  
y1" map the first derivative of the chosen function f with respect to the  
 Y-variable of the diagram (df/dY).  
"alpha" map (1/f)\*(df/dX)  
"beta" map -(1/f)\*(df/dY)

The keys "alpha" and "beta" are primarily defined having in mind the volume function (corresponding to thermal expansion coefficient and isothermal compressibility coefficient, respectively). However, they may be used for any other function too.

## plotxy

This program makes simple X-Y-plots from the tables (tab- and tcp-files) produced by theriak. One axis is always restricted to one variable, the other may have up to 20 variables. Plotting the sum of variables is also possible. Note: the tables can also be analyzed with some statistical software or e.g. Excel.

### Filenames associated with plotxy

|  |  |  |  |
| --- | --- | --- | --- |
| **I/O unit** | **type** | **file name** | **Description** |
| 01 | \*ini | theriak.ini | Program initialization data file |
| 02 | \*hlp | thhelp.txt | Help file |
| 05 | \*kbd | Keyboard | Keyboard (standard input) |
| 06 | \*scr | Screen | Screen (standard output) |
| 08 | dbs | Run-time defined | Table of thermodynamic variables |
| 09 | log | plotxy.last | User responses during last run |
| 10 | out | OUT | Calculation results to print or view on screen |
| 15 | plt | xyplot | Graphics data; input to GUZZLER or EXPLOT |

\*: Hard-coded file names (cannot be changed)!

### plotxy Input files

Plotxy can be invoked with a command line argument which is the file name containing the interactive input.

**theriak.ini**

This file is read at the beginning and contains information on file names and calculation parameters. If this file is present in the working directory, this will be used, else the file in the program directory is taken. To make changes, copy the file to the working directory and edit its content. The most important items one might change are:

$GHELP=0 (reduces the comments at the start of the programs)

and the following list with the names of input and output files used by PLOTXY.

$PLOTXY-FILES

log=plotxy.last #User's responses during last run of program

out=OUT #Calculation information to be printed or viewed on screen

dbs=Run time-defined #table to be used

plt=xyplot #Graphics data (e.g. input to GUZZLER)

$END

**thhelp.txt**

is located in the program directory and contains the text printed if the user enters a "?" in the interactive input.

**dbs-file**

This is the table of thermodynamic variables. The name is entered by the user in the interactive input. The file must be in the working directory. E.g.: loop.table

**log-file**

In the working directory. Contains the interactive input from the last run. All input that remains the same (e.g. the name of the table) can be used again with <CR>. (carriage return)

**Terminal input**

Is the interactive input through the keyboard

### plotxy Output files

**Terminal output**

Is the text output of the program to the screen. This is the dialog, help comments, error messages and a short summary of calculation progress.

**out-file**

In the working directory. Usually called "OUT". Most of the above "Terminal output" is also written to this file.

**plt-file**

In the working directory. Usually called "xyplot". This file contains the graphics information computed by plotxy. A description of the format can be found in the Explot users guide, keyword "NPLOIG".

The graphics file is usually first run through GUZZLER, which formats the labels on the curves and writes a cln-file, which can be translated to a PostScript file by EXPLOT.

### Interactive input for PLOTXY

This information is also available by entering "?" in the program dialogue.

#### table filename

"files" to see the files associated with the program.

filename name of a file containing a table of thermodynamic variables corresponding to an theriak output tab-file.

#### X-axis and Y-axis:

number(s) list of variable numbers or variable expressions separated by commas. A variable expression has the format: var1+var2+var3 ...  
Each variable may be the sum of several variables.  
Note: One of the axes must have only one variable number or expression.  
 EXAMPLE:  
 For X: 1  
 For Y: 3, 5, 6+7, 8+9

#### X-min X-max and Y-min Y-max

The minimum and maximum values for the axis are printed. Enter different values if desired.

At the end the program prints the labels of the X- and Y-axis, and all for all plotted lines.

# Description of input files

## The Initialization file theriak.ini

The name of this file is hard-coded and should not be changed. It contains all appropriate information need by the programs on start. The following information describes the format of theriak.ini; it is included also in this file.

Significant records in theriak.ini start with $ at position1 have the following forms:

$Variable=value

or

$Block-Identifier

key1=val1 #Description1

key2=val2 #Description2

.....................................

$END

The former defines the numerical value of a program control variable (e.g. $Clear=0); the latter defines a data block. Note that in either case no space is allowed before and after the equal sign.

A data block starts with a block-identifier that is hard-coded and should not be changed, e.g. $THERIAK-FILES. Each record within a block starts at position 1 with a 3-character long keyword that is hard-coded and should not be changed. This keyword is followed by = and then by a value, e.g.dat=THERIN. A # character signifies an optional comment within the record. Within a block, those records that are empty or start at position 1 with ! are ignored. The block ends with $END.

### Control variables

The following control variables are currently implemented.

$Clear=1

It defines if the screen will be cleared (value=1) or not (value <>1) before printing help information.

$GHELP=1

It controls if the first help after program start will be printed or not. Valid values are 1 (print) or 0 (don't print)

$BATCH=1

It controls if DOMINO plot files created with the help of script files are immediately processed with the programs GUZZLER and EXPLOT. Valid values are 0 (do not proceed) or 1 (proceed).

### Data blocks

The following data blocks are currently implemented.

#### Calculation parameters

$CALC-PARAMS  
TEST=1E-9 LO1MAX=300 GCMAX=500 DELXSTAR=1E-4 STEPSTAR=25   
EQUALX=1E-2 DELXSCAN=1.0 STEPMAX=25 DELXMIN=1E-9

$END

This block contains one or more statements in the form: **parameter=value** separated by at least two blanks. For parameters that are not assigned a value in the ini-file, the default value is used. In general, these values may be changed, but if this is not done carefully, the results may be unpredictable. It is suggested not to change these parameters.

|  |  |  |
| --- | --- | --- |
| **Parameter** | **Default** | **Description** |
| LO1MAX | 80 | Maximum number of iterations for the calculation. If LO1MAX < 0 then the number of iterations will be exactly |LO1MAX|. |
| TEST | 10E-8 | The calculation will stop, if the absolute sum of all non-positive Gi after the linear programming step is smaller than |TEST|.If TEST < 0 then the program prints a short summary for each iteration. (For testing the program). |
| EQUALX | 10E-5 | Two phases of the same solution are considered equal if |Xi| < EQUALX. |
| DELXMIN | 10E-7 | Smallest possible stepsize = precision for calculating Xi's in a non-ideal solution. |
| DELXSCAN | 1 | Grid width for scanning non-ideal solution phases for initial guess. DELXSCAN cannot be smaller than 0.001 or bigger than 1. |
| DELXSTAR | 0.02 | Initial stepsize. |
| STEPSTAR | 2 | Maximum number of steps, if initial guess results from a scan. |
| STEPMAX | 3 | Maximum number of steps if initial guess is a previous minimum. |
| GCMAX | 100 | Maximum number of G-function calls per step (= maximum m in stepsize procedure). |

#### File data blocks

In these blocks the user may define the default filenames for each program. Note that there are no default filenames, so the user must define them. There are as many blocks as programs. Each program is associated with a number of files that have certain contents. For example, the program THERIAK is associated with at least the following file types:

|  |  |
| --- | --- |
| **Type** | **Description** |
| dbs | Thermodynamic data |
| dat | User data, chemical composition of system |
| out | Calculation results |
| log | User input from the previous run |

Depending on the nature of contents, these files are assigned a **filetype** that is a hard-coded, 3 characters long **keyword**, as shown above. The default filenames defined by the user for each program are actually associated with the filetypes needed by this program. For all programs, some filenames are hard-coded and cannot be changed by the user. These include:

|  |  |  |  |
| --- | --- | --- | --- |
| **Type** | **Filename** | **Status** | **Description** |
| ini | theriak.ini | Should always exist | Program initialization data file |
| hlp | thhelp.txt | Should always exist | Help file |
| kbd | keyboard | System | Interactive input from user (standard input) |
| scr | screen | System | Output to the screen (standard output) |

For the Windows operating system, file domjob will automatically become domjob.bat. The names of all other files for each program may be defined by the user in **program-files blocks** (see below). The file types implemented in the current versions are the following:

|  |  |  |  |
| --- | --- | --- | --- |
| **Type** | Description | **Type** | **Description** |
| ini | Program initialization data file | tab | Table of variable values; input to a spreadsheet program |
| hlp | Help file | tcp | Table of variable values; input to "TechPlot" |
| spt | DOMINO script file (default: scriptXXX[.txt]) | plt | Graphics data (input to GUZZLER and EXPLOT) |
| job | DOMINO batch job file (default: domjob[.bat]) | cln | Graphics data after arranging labels and cleaning (input to EXPLOT) |
| kbd | Keyboard, standard input | rxn | Reaction/assemblage list |
| scr | Screen, standard output | grd | Grid information for GUZZLER |
| dat | User data, chemical composition of system | pst | Graphics file in PostScript format |
| dbs | Thermodynamic data base | fig | Directory name for pixelmaps |
| log | User's responses during last run of program | lpl | Graphics data; long format. |
| out | Calculation results to print or view on screen | lbk | (reserved for future use) |
| bin | Graphic data for "pseudo-binary system" calculations | ibk | (reserved for future use) |
| drv | Special calculation directives to run THERIAK | pgm | Pixelmap file in pgm format (Portable Gray Map) |

#### File name conventions and assignments

Note: Unix and derivate operating systems need case sensitive file names!

A filename can be as long as 30 characters. In case the default filenames contain period(s), the program will consider the character string immediately following the left-most period as a file extension, i.e. as filename.extension. In this case filename should not exceed 20 characters and extension (including the period) 10 characters. If the default filenames do not contain period(s) only the first 20 chars will be assigned to filename, whereas the extension will be empty. There are two methods to assign the default filenames for each program.

**Method 1: Fixed default filenames.** This method becomes obvious by the example of the $THERIAK-FILES block.

$THERIAK-FILES

dat=THERIN #User's chemical input to program

dbs=Run-time-defined #Thermodynamic data base to be used

log=theriak.last #User's responses during last run of program

out=OUT #Calculation information to be printed or viewed on screen

bin=binout #Graphics data for "pseudo-binary system" calculations

drv=Run-time-defined #"Special calculation" directives for running the program

tab=loop\_table #Table of variable values; input to a spreadsheet program

tcp=loop\_tecplt #Table of variable values; input to "TechPlot"

inf=loop\_info # Table of variable values; additional information

$END

For the Windows operating system all files are usually defined with the extension .txt, so they can be double-clicked on any File Manager window and get opened with the default text editor NOTEPAD. Note that all files of the programs are ordinary text files that can be viewed and modified by any text editor of your choice. For Unix and derivate operating systems, the file/program-to-open associations follow different rules that are not only related to file extension. Note that the number of files for each program is fixed by the number of file types. Note also that more that one programs produce output information (file type out). For some users It may be convenient to distinguish among the various out-files, e.g. ThkOut.txt could be a THERIAK out-file whereas ThbOut.ixt is a THERBIN out-file.

**Method 2: Run-time-defined file names.** This method allows for file naming at run time. It is active in case you set the filename of type dat to a single question mark. For the example above, this looks like this:

$THERIAK-FILES

dat=? #User's chemical input to program

.....................................................

$END

In this case, the information following the dat-record is ignored and the program will state on start that

Filename for file type dat not defined in theriak.ini

Enter file name:

Now you enter the name of file type dat that contains the chemical input for your calculation, e.g.

mydata

Then, the files that will be created by the program will be named automatically to

mydata-plt.txt

mydata-cln.txt

mydata-tab.txt

etc.

In this example, the contents of the associated files become evident by appending the file type to the input string “mydata”. How each program names its files can be checked at program’s first prompt by entering the keyword "files" (see on-line help).

## User Input (dat-file)

The dat-file contains information on pressure, temperature as well as bulk chemical composition of the system. Although this information is not always used, this file must be present in the working directory, because it is read by all thermodynamic programs.

### File format

Comments in this file start with ! at position 1. The structure of input data includes two parts of information:

1. External conditions for calculation (e.g. T and P) and
2. Bulk system composition given as element amounts

The **first significant line** should contain the external conditions as follows in the following form:

**temperature(deg C) pressure(bar) optional-[PGAS]-ratio**

where

**[PGAS]-ratio** = (fluid pressure)/(total pressure)

This line should be followed by **at least** one bulk composition line have the following form:

**print-code bulk-formula use-code optional-comment**

The arguments should be **separated by at least two blanks (no tabs!)**. Their significance and format are as follows:

**print-code** should start at position 1 and may take the following values:

< -1: Print information about selected or rejected phases; no equilibrium calculation.

-1: Print composition, considered phases and solution models; no equilibrium calculation.

0: Short output of stable assemblage calculation.

1: Long output of stable assemblage calculation including information about composition, considered phases, solution models, and activities of all phases.

**bulk-formula** is the element bulk composition written as follows.

**COMP1(A1)COMP2(A2).....**

where **COMP1, COMP2** ... are the components that are defined in the database file (see dbs-file, Components) and **A1, A2**, .... their amounts enclosed in parentheses. Usually, the components are the **elements**. For the **total oxygen** of the bulk-formula, the input **O(?)** instructs the program to assign the exact stoichiometric oxygen amount to the other input elements. The amounts may be any numbers, but should be positive to avoid unpredictable results. The maximum length of **bulk-formula** is 170 characters; it may contain single blanks and must be separated from **print-code** and **use-code** by at least two blanks.

**use-code** controls if some or all phases included in the database and matching the given bulk composition should be taken in consideration. In the normal case, an asterisk **\*** includes all matching phases. How to work with the **use-code** is further explained in paragraph .

**optional-comment** may describe shortly the bulk composition. This information will be printed into the final diagram.

For the most typical case, only one chemical input line is needed. Any subsequent lines will be ignored. If a pseudo-binary (or pseudo-ternary) diagram is to be calculated (in THERIAK: keyword "bin"; in DOMINO: keywords **"BIN"** or **"TER"**) two (or three) **additional** composition lines are needed that define the endmember compositions of the binary (or ternary) sub-system. Accordingly, if both axes in a DOMINO calculation should be pseudo-binary systems, two pairs of composition lines (a total of four) are required. Note that the second and further composition lines should not contain elements that are not already included in the first one.

### Examples of dat-files

Example 1

700 3000

0 NA(0.5)K(0.5)AL(1.0)SI(3.0)O(8.0) SI(10)O(20) H(20)O(10) \*

This is a typical input for a simple equilibrium calculation. The temperature is 700 C, the Pressure 3000 bar. The bulk composition corresponds to 0.5 K-Feldspar + 0.5 Albite, with "excess" (10 mole) SiO2 and H2O. The Zero at the beginning of the second line produces a short output (only the basic results) and the star "\*" at the end means, that all matching phases in the database are to be considered.

Exemple 2

700 3000

0 NA(0.5)K(0.5)AL(1.0)SI(3.0)O(8.0) SI(10)O(20) H(20)O(10) \*

0 K(1)AL(1)SI(3)O(8) SI(10)O(20) H(20)O(10) \*

0 NA(1)AL(1)SI(3)O(8) SI(10)O(20) H(20)O(10) \*

DOMINO may use this input to calculate, for example, a binary T-X phase diagram along the K-Feldspar - Albite joint. Note that the first composition line defines the whole system completely whereas the following lines define the endmembers of the binary.

Exemple 3

0 A(1)B(1)X(1)Y(1) \*

0 A(1) \*

0 B(1) \*

0 X(1) \*

0 Y(1) \*

This example demonstrates how DOMINO can handle a hypothetical reciprocal solution system by defining both diagram axes (x and y) as binary sub-systems by means of the keyword "BIN" entered at run-time. Provided that the database contains thermodynamic properties for AX, AY, BX, BY as well as an appropriate solution model, isopleths for the total Gibbs free energy may be calculated and plotted.

## Directives for theriak (drv-file)

The drv-file drives equilibria calculations, e. g., along a given PT-path. The drv-file is a text file created with any editor and saved as text only if necessary. It contains commands for theriak which are executed in order.

### File format

Each line contains a command and some parameters.

Initially the temperature, pressure and composition are read from the dat-file (usually THERIN). These values can be re-defined in the drv-file.

|  |  |  |
| --- | --- | --- |
| Command | Parameters | Description |
| REF | t1 t2 | defines the equilibrium assemblage at the reference t1, p2. This is the "reference assemblage" adding the variable "G\_overstep" to the tab- and tcp-files. |
| COMP | formula use | Defines new bulk composition for further calculations. Initially the composition is read from the dat-file. It can be changed several times during one run. Example: COMP SI(3)AL(1)MG(3)K(1)O(12)H(2) \* |
| ADD | formula | Adds the given formula to the current bulk composition. The amounts may be negative, but only so much will be subtracted that all components remain >= 0 Example: ADD H(20)O(10) |
| REMOVE | phase p | After each of the following calculations, the composition of stable phase will be (partly) removed from the bulk. p is the percentage of phase that is to be removed. Example: REMOVE GARNET 100 |
| TP | t2 p2 s | Calculates equilibria along a linear PT-path from t1 and p1 to t2 and p2  The current values t1, p1 are input   1. either from the dat-file  2. or from a preceding "TP" or "REF" directive "s" is the number of calculation steps (default= 1) along the path. All variable values for each step are written into the tab- and tcp-file. Example: TP 800 5000 10 |

## The database (dbs-file)

### General structure

The format of the database follows closely the one used by E.H. Perkins, R.G. Berman and T.H. Brown for the calculation of phase diagrams. The first few lines of the database define the components to be used. The rest of the database is organized in sections. Each section begins with a line having the string \*\*\* as the first three non-blank characters. The rest of that line is scanned for a string identifying the section. The sections recognized by THERIAK are:

\*\*\* ... MINERAL DATA ...

\*\*\* ... GAS DATA ...

These two sections are treated identically. They contain the phase definitions and the information to calculate G for variable pressures and temperatures.

\*\*\* ... SOLUTION DATA ...

Definitions of solutions and solution models.

\*\*\* ... MARGULES ...

This section contains Margules parameters for non-ideal solution phases.

\*\*\* ... FIXED PHASES ...

Section containing solution phases with fixed compositions

Other sections (e.g. \*\*\* ... COMMENTS ...) will be skipped by the program. Principally the sections can be in any order and may appear more than once. It is obvious that if we define a solution phase, its endmembers must have been read-in previously. Similarly the Margules parameters for a solution can only be assigned properly after the solution phase is defined.

Any line that is empty or begins with a '!' is considered a comment line and is skipped.

### Components information

The database always begins with the definition of all components (usually elements), their atomic weight and the number of oxygens associated with them:

NC [R]

COMPN(1) COMPN(2) ... ... CMPN(7) ...

COMPN(X) COMPN(Y) ... ... CMPN(NC)

MOLWT(1) MOLWT(2) ... ... MOLWT(7) ...

MOLWT(X) MOLWT(Y) ... ... MOLWT(NC)

OXYNR(1) OXYNR (2) ... ... OXYNR(7) ...

OXYNR(X) OXYNR(Y) ... ... OXYNR(NC)

where

**NC**: Number of components used in the database

**R:** Optional input of gas constant [J/mol] (default: 8.3143).

**COMPN(i):** Components (Format = 7A10)

**MOLWT(i):** Atomic weights. (Format = 7F10.2)

**OXYNR(i):** Standard number of oxygens for the corresponding component. (Format = 7F10.2)

Example

25  
 O AL BA C CA CL CO  
 CU F FE H K MN MG  
 NA NI P S SI SR TI  
 ZN ZR B E  
 15.99940 26.98154 137.32700 12.01100 40.07800 35.45270 58.93320  
 63.54600 18.99840 55.84700 1.00794 39.09830 54.93085 24.30500  
 22.98977 58.69000 30.97362 32.06600 28.08550 87.62000 47.88000  
 65.39000 91.22400 10.81000 1.00000  
 0.0 1.5 1.0 2.0 1.0 0.0 1.0  
 1.0 0.0 1.0 0.5 0.5 1.0 1.0  
 0.5 1.0 1.0 0.0 2.0 1.0 2.0  
 1.0 2.0 0.0 0.0

### Section \*\*\* ... MINERAL DATA ...

Each phase is defined with one phase definition line and a variable number of data lines. The phase definition line contains the name and the chemical composition; the data lines contain the parameters used to calculate the thermodynamic properties of the phase. Different equations of state are implemented in the code. Unusual or very complex equations (e.g. the properties of H2O according to Haar et al., 1983) are programmed as external subroutines. (See paragraph )

#### Phase definition line

NAME FORMULA ABBREV [CODE]

The four strings are separated by at least two blanks and may contain single blanks.

**NAME** is the name of the phase (maximum 16 characters).  
Special case: If the name begins with a '$' (dollar sign), the phase will not be considered for an equilibrium. However, if a table or pixelmap is produced its chemical potential is recorded as G\_name and Gneg\_name.

**FORMULA** is the chemical formula of the phase in the form described earlier, i.e.

**COMP1(A1)COMP2(A2).....**

where **COMP1, COMP2 ...** are the components that are defined in the database file and A1, A2, .... their amounts enclosed in parentheses. Note that here **A1, A2, ....** may be negative.

**ABBREV** is a suitable abbreviation for the phase name (maximum 8 characters)

**CODE** is optional and may be composed of **less than 16 characters**, each of them defining a **group** that the phase belongs to. Phases belonging to the same group, i.e. having the same character in their code may be addressed by the use-code discussed earlier. Examples of using code and use-code are discussed in the chapter " USE and CODE (selecting phases)". If the first character in code is an asterisk \* then the phase is considered as "**special**", e.g. a buffer.

A line within this section is recognized to be a phase definition line if it contains at least one '(' (left parenthesis) and is not a comment line.

**Example**

HIGH ALBITE NA(1)AL(1)SI(3)O(8) halb n

#### Data lines

The general equation to calculate the ***apparent Gibbs Free Energy*** of a phase is:



where

*T* = the temperature in Kelvin

*P* = the pressure in bar

*To* and *Po* are 25 oC and 1 bar, respectively.

*∆aGT,P* [J/mol] = the molar "***apparent" Gibbs Free Energy***

*∆fHTo,Po* [J/mol] = the Enthalpy of formation from the elements at *T0* and *P0*.

*STo,Po* [J/(K mol)] = the molar entropy at *T0* and *P0*.*.*

*Cp* [J/(K mol)] = the heat capacity function *Cp(T)* at *P0*.

*V* [J/(Bar mol)] is the molar volume function *V(T,P)*

The thermodynamic data lines for each phase follow the phase definition line in **any order**. They have the general format

**Cod |Number-field01|Number-field02|Number-field03|Number-field04|Number-field05|**

corresponding to the Fortran format (A5,5F15.4). The three consecutive non-blank characters **cod** identify the content of the data line. They must lie **within the first five** characters of the data line. The rest of the data line (character 6 to 80) may contain at most five 15-characters-wide numerical fields. The currently implemented data lines are discussed below.

##### Standard state (25°C, 1 bar) information, cod = ST

**ST** G0 H0 S0 V0

G0 = *∆aGo* [J/mol] is the molar "apparent" Gibbs Free Energy. It is commonly not used and this field may me empty.

H0 = *∆fHo* [J/mol] is the Enthalpy of formation from the elements.

S0 = *So* [J/(K mol)] is the molar entropy.

V0 = *Vo* [J/(Bar mol)] is the molar volume.

**Example** (Albite)

ST -3701276.00 -3921618.20 224.4120 10.083 1.00000

##### Heat capacity information, cod = Cn

**C1** k1 k4 k3 k8

**C2** k6 k2 k5 k7 k9

**C3** k1 k2 k3 k4

**C1** corresponds to the *Cp*-function according to Berman & Brown, 1984

**C3** corresponds to the Maier-Kelly equation

For all nine parameters, the implemented *Cp*-function at 1 bar has the following general form. In most cases only three or four parameters are used.



The two integrals needed for the Gibbs Free Energy function become:





**Example (Albite)**

C1 393.63574 -2415.498 -7892826.000 1070636032. 0.00000

##### Van der Waals Equation of state for real and ideal gases, cod = VDW

**VDW** a0 a1 b0 b1

The Van der Waals equation is 

Implemented is a linear temperature dependency of the parameters a and b:

a = a0 + a1·T [J/mol]

b = b0 + b1·T [cm3]



This equation is solved for Vo and V (at Po and P), then



Exempel: (ideal gas)

VDW 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00

In this example, an ideal gas is defined by setting all parameters zero.

##### Redlich-Kwong Equation of state for gases, cod = R-K

**R-K** a0 a1 b0 b1

The Redlich-Kwong equation is:

Redlich-Kwong: 

Implemented is a linear temperature dependency of the parameters a and b:

a = a0 + a1·T [J/mol]

b = b0 + b1·T [cm3]



This equation is solved for Vo and V (at Po and P), then



**Exempel** (Oxygen):

R-K 1.73888400E+07 0.00000000E+00 2.20990000E+01 0.00000000E+00

##### Simple volume function for solids. (as in TWQ), cod = V1

V1 v1\*1E5 v2\*1E5 v3\*1E5 v4\*1E8

Note that for the equation below, **v1, v2** and **v3** must be divided by 105, and **v4** by 108

The simple volume function as used in TWQ is:





where VTa = v1·V0 VTb = v2·V0 VPa = v3·V0 VPb = v4·V0

Example (Albite)

V1 2.63072032 0.00032407 -0.19446932 0.00048611 0.00000000

##### Another Simple Volume function for solids. (with alpha (=f(T) and beta (=const.)), cod = V2

**V2** aa ab b

 and 

The volume function used is:





##### Volume function for solids as used by Holland and Powell (1998), cod = VHP and VH2

VHP a0 K Tcr0 Smax Vmax

VH2 a2 Ks dkdt

Note: here Q is Q2 of Holland and Powell (1998)

PK = P/1000 = pressure in Kilobar

According to Holland and Powell (1998):

a2 = 10 (set constant in formula below)

Ks = 4 (set constant in formula below)

dkdt = - 1.5•10-4







The additional contribution of the transition to the Gibbs Free Energy becomes:



Example (Gehlenite)

VHP 0.000041700 1080.0 700.0000 11.00 0.09700

VH2 10.0000 4.0000 -0.000162000

##### 

##### Volume function as used by Holland and Powell (2011), cod = V11

V11 a0 k0 k0’ k0’’ L Θ

α0 : thermal expansion at T0P0

k0 : bulk modulus at T0P0

ko’ and ko’’ : first and second derivative of k0

L : flag 0: no additional transition

1: phase transition described via Landau theory

2: phase transition described via Bragg-Williams theory

3: phase is an aqueous species

4: phase is a melt end-member

(For following equations, P is in KBar)

(Θ may be input, just in case it becomes another adjustable parameter)

if Θ = 0 then

Einstein temperature of phase i

where Si = molar entropy of phase i (at T0P0 ??)

ni = number of atoms in phase i

function defined for α.k = n.ζ

where u = Θ/T

u0 = Θ/T0

thermal pressure term

volume

where

Gibbs Free Energy

note: (P-P0)V0 .. etc. etc. used

**Example** (Forsterite)

V11 0.000028500 1285.00 3.8400 -0.003000 0.00

##### Landau order function as used by Holland and Powell (2011), cod = LA1 (must be used with above volume function, cod = V11)

LA1 Tcr0 Smax Vmax

(For following equations, P is in KBar)

Q defined as in Holland and Powell (1998)

Tcr0 : Critical temperature at 1 Bar

Smax : entropy of ordering at Tcr

Vmax : volume of ordering at Tcr

k0 : bulk modulus at T0P0 (from volume function, cod = V11)

α0 : thermal expansion at T0P0 (from volume function, cod = V11)

**Example** (Sphene)

LA1 485.00 0.4000 0.00500

##### Bragg-Williams order function as used by Holland and Powell (2011), cod = BW1

BW1 ∆HBW ∆VBW WH Wv n fac

##### Note: all units in [J] not [KJ]

##### ∆HBW : Enthalpy of disordering

∆VBW : Volume of disordering

WH and WV : Interaction terms used in W = WH + P.WV

n : number of Si disordering with each Al

fac : mystical factor

W = WH + P.WV

A = ∆HBW – W + P.∆VBW

B = 2.W

(W, A and B are divided by fac)

Q = ordering parameter

At equilibrium:

Solve iteratively for Q then:

**Exemple** (Albite)

BW1 14000.00 0.04200 13000.00 0.04200 3.0 0.9000

##### Lambda transitions 1.

T1 Totr Toref l1 l2 ∆Htr  
T2 Tq ∆Vtr (dV/dT) (dV/dP)

According to Berman and Brown, 1985, Contributions to Mineralogy and Petrology, 89, 168-183

Between the limits Tref and Ttr a Cp-like function is added.



It is assumed, that Ttr (transition) is a linear function of P with slope Tq.

∆T = (P-P0)·Tq Tref = T0ref + ∆T, Ttr = T0tr + ∆T,

V and ∆G is adjusted for ∆Htr, ∆Vtr, (dV/dT) and (dV/dP) for low T polymorph.

For T<Ttr:





For T>Ttr:



One phase may have more than one transition.

**Exemple** (Quartz)

T1 848.00 373.00 -0.09186959 0.00024607 0.00  
T2 0.023743 0.000000 0.0000000000 0.0000000000 0.00000

##### Cp and Lambda transitions 2.

**CSK** a b c TTr0 ∆Htr ∆Vtr Tslop

According to Helgesson et al., 1978, Amer. Jour. Sci., v. 278A, 229 p. (as used in SUPCRT)

The Cp-function is divided into n (up to four) temperature ranges:

T0 < T < Ttr0(1): 

Ttr0(1) < T < Ttr0(2): 

...

Ttr0(n-1) < T: 

**Exemple** (Quartz)

CSK 46.94448 0.0343088 -1129680.0 848.000 1213.36 0.3720 38.5000

CSK 60.29144 0.0081170 0.0 0.000 0.00 0.0000 0.0000

##### Disorder contributions

**D1** d1 d4 d3 d8 d6  
**D2** d2 d5 To Td Vad

Disorder contributions to G can be approximated by adding a cp-like function between the limits To and Td.



The volume is taken from the shape of the enthalpy function and is scaled to the data by the variable Vad.



The total contribution to the Gibbs Free Energy becomes:



**Example** (Gehlenite)

D1 -221.74000 0.00000 17291280.00000 0.00000 0.00000  
D2 0.36950 -0.00015 698.15000 1600.00000 0.00000

##### Special phases:

**SPC** keyword

If the equation of state cannot be expressed with the above keywords, G at P and T may calculated in an external subroutine (fsol.f). All other data lines will be ignored. Used e.g. to calculate G for water and steam according to Haar et al. (1982). The maximum length of the keyword is 10 characters.

In the file fsol.f, the following equations of state are present and reasonably tested:

Keyword description

HAAR equation of state for water and steam, according to Haar et al. (1982)

ABSAL compute thermodynamic properties of albite ordering relative to low albite standard state.

Function of Salje (1985), used with albite from database of Berman et al. (1992)

CK&J CO2 according to Kerrick and Jacobs (1981)

WK&J H2O according to Kerrick and Jacobs (1981)

CHP98 CO2 according to Holland and Powell (1998)

HHP98 H2O according to Holland and Powell (1998)

**Example** (H2O)

SPC HAAR

##### Combination of phases:

**COM** name[value] name[value]... activity Rname

To the ∆G defined by the standard state, Cp's etc. we can add any combination of previously calculated ∆G's. This is also useful e.g. for polymorphs or buffers. The thermodynamic parameters calculated are ∆aG and Volume.

name name of phase. (must be in the database before the com-line)

value amount of phase used in the combination (the value may be a fraction, like 1/3)

activity (optional) activity of phase. Note that S0 is set to -R·ln(a). (overwrites existing S0)  
 A value of zero means no activity correction (Useful if Rname is used)

Rname (optional) name of phase that should not be included in calculation of stable assemblage.(This may be important for buffers where ∆rG (buffer = phases) is zero, which results in an indifferent, non-unique equilibrium)

**Example** (Buffer)

COM MAGNETITE[2] STEAM[1] HEMATITE[-3] 0 HEMATITE

### USE and CODE (selecting phases)

The phases in the database may be divided into different groups. Each group is coded as one character (e.g. A, B, C, D). The variable "CODE" in the database (optional) defines for each phase to which groups it belongs. When the program is run we can specify in the variable "USE" all groups that should be considered. If USE = '\*' then all groups are considered, including those with no CODE defined.

#### special phases:

If the first character of CODE is a '\*' then the phase is "special" (e.g. a buffer) and does not belong to a specific group. It will only be considered if mentioned in USE after a comma. The first comma in USE is a delimiter between the group names and the special phases.

If the first character of CODE is a '+' then G of this phase will be calculated even if its composition is outside the compositional space. In that case this phase can still be used to define G of other phases, but will itself not be considered for the equilibrium assemblage.

If the first character of CODE is a '-' then the phase will be excluded from becoming stable.

In general a phase will be considered if:

* The group code is matching
* No phase with identical name is already considered.
* Its components are a subsystem of the bulk components.
* Enough data to calculate G is provided. (Standard state and Cp line)

#### Examples for USE and CODE

CODE USE Considered phases  
Phase1 A A 1,4  
Phase2 BC B 2  
Phase3 C C 2,3,4  
Phase4 AC AB 1,2,4  
Phase5 AC 1,2,3,4  
Phase6 \*QFM BC 2,3,4  
Phase7 \*CB ABC 1,2,3,4  
 \* 1,2,3,4,5  
 AB,QFM 1,2,4,6  
 AB,QFM,CB 1,2,4,6,7  
 ABC ,CB 1,2,3,4,5,7  
 A,CB 1,4,7

### Section \*\*\* ... SOLUTION DATA ...

A solution phase is defined by one definition line followed by any number of endmember lines.

#### Solution definition line:

SOLNAME (modell)[mul] s1(m1):e11,e12... - s2(m2):e21,... - ...

A line within this section is recognized to be a solution definition line if it contains the string '..(' (blank,blank,left parenthesis) and is not a comment line.

**SOLNAME**: Name of solution phase (maximum 16 characters)

**modell**: This string is scanned for certain keywords:

**SKIP**: the solution phase will not be considered.

**EXCL**: the solution phase will not be considered for an equilibrium, however the chemical potential of the solution with the smallest Gibbs Free Energy will be calculated. If a table or pixelmap is produced this chemical potential is recorded as G\_solname and Gneg\_solname.

**IDEAL**: An ideal solution model is assumed. (ai=ximul). This is also the default. si, mi: and eij are not used to calculate the activities, however the output will include the site occupancies.

**SITE**: An ideal site mixing is used, where:   
 si: name of site i.   
 mi: multiplicity of site i   
 eij: possible elements for site i.

**EXT**: The activities of the endmembers are defined in an external subroutine (e.g. in file fsol.f). Other keywords (except SKIP and MARGULES) are ignored. si, mi: and eij have no influence

**MARGULES**: This keyword states, that there may be Margules parameters defined for this phase. They will only be added if this keyword appears in 'modell'.

**mul**: If a number follows immediately the (modell), then this number is used to calculate multiplicities. The number may be a fraction, like "1/3"

The element names (max. 8 characters) do not have to correspond to a compositional element. They may represent element groups or coupled elements.

NOTE: A site mixing model which is not conform with THERIAK's philosophy will produce nasty warning messages.

For ideal site mixing the following general formula is used to define the activities:

e.g. MÄDER, U.K., PERCIVAL, J.A. & BERMAN, R.G. (1994): Thermobarometry of garnet – clinopyroxene – hornblende granulites from the Kapuskasing structural zone. Can. J. Earth Sci. 31, 1134-1145.



ns = multiplicity of site (s)  
 rm = number of ions (m) on site (s) for phase (j)  
 xm = mole fraction of ions (m) on site (s)

#### Endmember lines:

EMNAME e11,e12,.. - e21,... - 0 T P

**EMNAME**: Name of the endmember. (maximum 16 characters). The endmember will be added to the solution phase if a considered phase with the same name exists.

**eij**: the mi elements occupying site i of the endmember.

**0, T, P**: coefficients for the asymmetric van Laar model, according to Holland and Powell (2002).

i is the van Laar parameter for endmember i.

i = 0 + T\*T + P\*P (T=Temperature, P=Pressure [Bar])

The contribution ∆Gijex to ∆G from a single binary interaction parameter Wij becomes:

 where ne is the number of endmembers in the solution

Examples:

GAS PHASE (IDEAL)  
 CARBON DIOXIDE  
 STEAM  
 OXYGEN  
 CARBON MONOXYDE  
H-FELDSPAR (IDEAL,MARGULES)  
 H-ALBITE  
 H-SANIDINE  
GARNETS (MARGULES,IDEAL)3 M(3):Ca,Mg,Fe  
 GROSSULAR Ca,Ca,Ca  
 PYROPE Mg,Mg,Mg  
 ALMANDINE Fe,Fe,Fe

FSP (MARGULES,IDEAL) M(1):Na,K,Ca

sanidine K 1.0 0 0

high-albite Na 0.643 0 0

anorthiteC1 Ca 1.0 0 0

### Section \*\*\* ... MARGULES ...

The Margules parameters are grouped in subsystems (binary, ternary etc.) Each subsystem is defined by a definition line followed by any number of parameter lines.

#### Margules definition line

EMNANE1 - EMNAME2 - ...

A line within this section is recognized to be a definition line if it contains the string ' - ' (blank, minus, blank).

EMNAMEn: Name of nth endmember in subsystem.

#### parameter lines:

k1k2k3... WH WS WV WCP K

The number of k's defines the degree (p) of the polynomial in the Margules equation. This does not have to be the same for all parameters. The generalized equation used is:



S = sum of different components xj involved in polynomial xk1.xk2....xkp

K = Parameter to extrapolate binary data to higher order systems. This follows the ideas of Kohler (1960) and produces results comparable to the better known Wohl (1964) equation. (See e.g. de Capitani and Kirschen, 1994)

WG = WH + WCP· (T-To)-(WS + ln(T/To) ·WCP) ·T + WV·P

#### Example

\*\*\*\*\* SOLUTION DATA \*\*\*\*\*

H-FELDSPAR (IDEAL,MARGULES)  
 H-ALBITE  
 H-SANIDINE

!

\*\*\*\*\* MARGULES PARAMETERS \*\*\*\*\*  
H-ALBITE - H-SANIDINE   
112 32098.8 16.1356 0.46903 0 0   
122 26470.9 19.3807 0.38702 0 0

### Section \*\*\* ... SITMARG ...

Margules parameters defined for site-mixing

#### Site-Margules definition line

\* SOLNAME

A line within this section is recognized to be a definition line if it contains the string '\* ' (star,blank).

SOLNAME: Name of solution phase to which the site Margules should be applied.

#### parameter lines:

s - el1el2el3... WH WS WV

s : name of the site as defined in the solution definition line.

eli: names of elements for mixing as defined in the solution definition line.

The number of el's defines the degree (p) of the polynomial in the Margules equation. This does not have to be the same for all parameters. The generalized equation used is:



xelis = concentration of element (i) on site (s)

WG = WH - WS·(T-To) + WV·P

#### Example

\*\*\*\*\* SOLUTION DATA \*\*\*\*\*

BIO (-SITE) M2(2):Mg,Fe - M1(1):Mg,Fe,Al - T2(2):Al,Si

PHLOGOPITE Mg,Mg - Mg - Al,Si

ANNITE Fe,Fe - Fe - Al,Si

SIDEROPHYLLITE Fe,Fe - Al - Al,Al

EASTONITE Mg,Mg - Al - Al,Al

!

\*\*\*\*\* SITEMARG \*\*\*\*\*

\* BIO

M2 - Mg,Fe 12769.0 10.200 -.060

M1 - Mg,Fe 6384.6 5.100 -.030

M1 - Mg,Al -6520.0 -18.977 0.000

M1 - Fe,Al 27270.1 29.983 0.000

### Section \*\*\* ... SEEDS ...

Initial guesses for the minimizations

Each line defines one initial guess with the following format:

SOLNAME Em1 x1 Em2 x2 Em3 x3 etc.

SOLNAME: Name of solution phase

Em1: Name of first endmember

X1: Concentration of first endmember

etc.

Each initial guess must be on one single line.

When the print-code in the dat-file (first character in THERIN) is “1” (long output) the result printed at the end of the theriak run can be used as seeds.

#### Exempel

PHNG Muscovite 6.34806424E-01 Celadonite 2.19890500E-01 Fe-Celadonite 8.95907168E-02 Paragonite 5.39715500E-02 Margarite2 1.74080966E-03 FeMusc 8.01769453E-11

ClAMg tremolite 8.17905247E-02 tschermakite2 1.12218622E-01 pargasite2 4.29616696E-01 glaucophane2 3.11389590E-01 cummingtonite 4.98053328E-03 grunerite2 3.00056441E-01 acam -2.43150519E-01 bcam -3.82003419E-02 mgriebekite 0.00000000E+00 kpargasite 2.14781407E-02 ttschermakite 1.98203137E-02

CPXo jadeite 1.00401610E-01 diopside 1.72170370E-03 omphacite 6.32092292E-01 clinoFM 2.65784395E-01 jadacm 0.00000000E+00

CHTD Mg-Chloritoid -4.82160477E-01 Fe-Chloritoid 5.41981319E-01 F3-Chloritoid 9.40179158E-01

### Section \*\*\* ... FIXED PHASES ...

For some specific applications it is useful to include solution phases with fixed compositions to the calculations. These may be included for comparison (calculated equilibria versus measured compositions) or replacing a solution (metastable equilibria).

#### Fixed phase definition line

fcod fname SOLNAM EM1(X1)EM2(X2)...EMne(Xne)

each line in this section defines one fixed solution phase

**fcod**=0 the fixed phase is added for comparison. Equilibrium calculated including solution SOLNAM.

**fcod**=1 The solution phase SOLNAM is not included in the equilibrium calculation. Only the fixed phases are considered.

**fname** name of the fixed composition phase (Max. 16 characters)

**SOLNAM** Name of the solution used to define the fixed composition phase

**EMi(Xi)** Names of the endmembers and their concentrations. One blank optional between items.

Example

\*\*\*\*\* FIXED PHASES \*\*\*\*\*

0 PL1 FSP ALBITE(0.83) ANORTHITE(0.15) K-FELDSPAR(0.02)

0 PL2 FSP ALBITE(0.70) ANORTHITE(0.30) K-FELDSPAR(0.00)

## Calculation of G in an external subroutine

If ∆G is to be calculated in an external subroutine, (data line: SCP keyword), then the program calls a subroutine named GSPEC. The parameters transmitted are: NAME (name of phase), P (pressure), PGAS (pressure of fluid phases), T (temperature), CASE (=keyword), G (∆G) and V (volume). The subroutine calculates G and V, then returns control to the main program.

### Example of GSPEC:

SUBROUTINE GSPEC(NAME,P,PGAS,T,FALL,G,V)  
CHARACTER\*16 NAME  
CHARACTER\*10 CASE  
REAL\*8 P,PGAS,T,G  
G=0.0D0  
IF (CASE.EQ.'HAAR') CALL WHAAR2(NAME,PGAS,T,G,V)  
IF (CASE.EQ.'CK&J') CALL CO2KJ(PGAS,T,G,V)  
IF (CASE.EQ.'HOPO') CALL HOPOH2O(PGAS,T,G,V)  
RETURN  
END

## Calculation of activities in an external subroutine.

If the model of a solution phase contains the string 'EXT' then three subroutines will be called:

**SOLINI**. In this subroutine we define for a given solution phase the number and the names of the endmembers.

**SOLMOD**. This subroutine returns a string to be printed, and which describes the activity according to solution name and endmember number. (optional).

**SOLCAL**. For each endmember the activity is calculated.

The solution has to be defined in the database, but may have fewer endmembers and in a different order than the same solution in the external subroutine.

The calling parameters are relatively complex, but to add a new solution phase to the already existing subroutines, only few lines have to be inserted.

### Examples for using external subroutines:

**in SOLINI:**...  
IF (SOLNAM.EQ.'FELDSPAR') THEN  
N=3  
NAME(1)='ALBITE'  
NAME(2)='POTASSIUM FELDSP'  
NAME(3)='ANORTHITE'  
END IF  
IF (SOLNAM.EQ.'H2O-CO2') THEN  
N=2   
NAME(1)='STEAM'  
NAME(2)='CARBON DIOXIDE'  
END IF

**in SOLMOD:**  
MODELL='NOT EXPLICITLY DEFINED'

...  
IF (SOLNAM.EQ.'FELDSPAR') THEN  
IF (K.EQ.1) MODELL='X(Ab)\*(1-X(An)\*\*2)'  
IF (K.EQ.2) MODELL='X(Or)\*(1-X(An)\*\*2)'  
IF (K.EQ.3) MODELL='(X(An)\*(1+X(An))\*\*2)/4'  
END IF  
IF (SOLNAM.EQ.'H2O-CO2') THEN  
MODELL='See: Kerrick & Jacobs(1981)'  
END IF

**in SOLCAL:**

...  
IF (SOLNAM.EQ.'FELDSPAR') THEN  
A(1)=X(1)\*(1.0D0-(X(3)\*\*2))  
A(2)=X(2)\*(1.0D0-(X(3)\*\*2))  
A(3)=(X(3)\*(1.0D0+X(3))\*\*2)/4.0D0  
RETURN  
END IF  
IF (SOLNAM.EQ.'H2O-CO2') THEN  
XCO2=X(2)  
CALL MIXKJ(T,P,XCO2,F1,F2,A1,A2)  
A(1)=A2  
A(2)=A1  
RETURN  
END IF