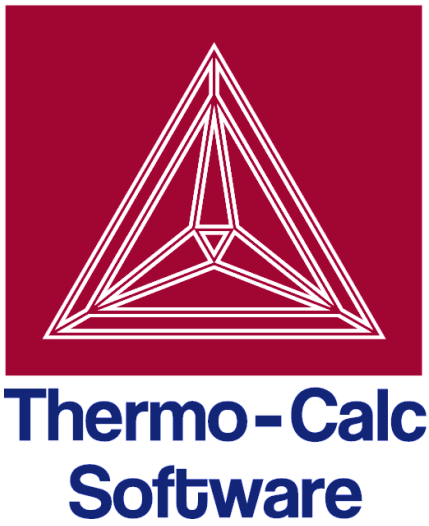

DICTRA Module Command Reference

Thermo-Calc 4.0

Stockholm, Sweden

DICTRA Module Command Reference

Contents

1 Introduction

1.1 Target group

This command reference is aimed at users of the DICTRA module in the Thermo-Calc software package.

1.2 Purpose

Describes the function and syntax of the various commands that are available in the DICTRA module and the POST module of the DICTRA program.

1.3 Content

The Command Reference is divided into two main parts. The first part lists the commands available in the DICTRA module in alphabetical order, while the second part lists the commands that are available in the POST module, also in alphabetical order. For information about commands in other modules, see the *Thermo-Calc Console Command Reference*.

There are also two appendices. The first gives a brief introduction to the DATAPLOT language, while the second appendix contains tables with the available state variables, integral variables and auxiliary variables.

2 DICTRA commands

AMEND_CELL_DISTRIBUTION

Description: This command creates a new cell and attaches it to the list of current existing cell.

Syntax: CELL_DISTRIBUTION_FACTOR

A parameter that determines the weight of the cell, this parameter can be used in order to simulate a distribution of different cell sizes.

AMEND_MOBILITY_DATA

Description: Mobility data may be changed interactively by this command.

Syntax: AMEND_MOBILITY_DATA

BACK

Description: This command gives the control back to the most recent module. From the post-processor one goes back to the DICTRA-MONITOR module.

Syntax: BACK

CHECK_DIFFUSION_MATRIX

Description: This commands enables the user to display the diffusion coefficient matrix for a phase at a given composition, pressure and temperature.

Syntax: CHECK_DIFFUSION_MATRIX <PHASE NAME> <CONCENTRATION OF> <PRESSURE> <TEMPERATURE> <OPTIONS>

Prompt: `phase name`

Name of the phase for which the diffusion coefficient matrix is to be displayed.

`CONCENTRATION OF`

Concentration of the component in U-fraction for which the diffusion coefficient matrix is to be displayed.

`Pressure`

Pressure for which the diffusion coefficient matrix is to be displayed.

`Temperature`

Temperature at which diffusion coefficient matrix is to be displayed.

`Options`

Use one or several of DLPBMX0E

- D: reduced diffusion matrix
- L: L matrix (diagonal)
- P: L' matrix
- B: L" matrix
- M: MU(k) array
- X: dMU(k)/dCj matrix
- 0: unreduced diffusion matrix
- E: eigen values of matrix

COARSENING_MODEL

Description: This command enables or disables the use of the simplified model for coarsening.

The model is based on LSW theory (after Lifshitz and Slyozov Chem Solids 19(1961)35 and Wagner Z Elektrochemie 65(1961)581). The model is also described in *Gustafson et al proc Adv heat resistant steel for power gen Spain 1998 p. 270* and *Björklund et al Acta Met 20(1972)867*.

LSW theory is strictly only valid for low volume fractions of the particle phase. The theory predicts that the normalized particle size distribution will obtain a constant shape where the largest particles have a radius equal to 1.5 times the average particle radius.

The calculations are performed in one cell on a maximum size particle which thus is assumed to be 1.5 times the size of the average particle size. The matrix phase is on one side in contact with the maximum size particle and on the other the matrix phase is in local equilibrium with an average sized particle. The effect of the surface energy will then be such that both the maximum size particle as well as the matrix phase grows.

Syntax: `COARSENING_MODEL <Y/N>`

`ENABLE COARSENING MODEL`

Enables or disables the use of this model by using one of the key words YES or NO.

CREATE_NEW_CELL

Description: This command is used to amend the cell distribution factor of the currently selected cell.

Syntax: CREATE_NEW_CELL

Prompt: CELL DISTRIBUTION FACTOR

A parameter that determines the weight of the cell, this parameter can be used in order to simulate a distribution of different cell sizes.

DEBUGGING

Determines the debugging level. Depending on the value given, different amounts of information are written onto the output device. This can be used to determine what causes the program to crash during a simulation.

DEBUG LEVEL (YES,NO,0,1,2,3,4)

The level of debugging information to be displayed

DELETE_REGION

Description: Use this command to delete a region and all its associated data from the current cell.

Syntax: DELETE_REGION

ENTER_COMPOSITIONS

Description: This command enters the composition into the phases in a region.

Syntax: ENTER_COMPOSITIONS

Prompt: REGION NAME

Name of the region into which the compositions are to be entered.

PHASE NAME

Name of the phase in a region into which the compositions are to be entered.

USE EQUILIBRIUM VALUE

This is only for spheroid phases in simulations with dispersed phases. If this option is used the program will automatically calculate the equilibrium fractions of the spheroid phase and its constitution at the start of the simulation.

DEPENDENT SUBSTITUTIONAL SPECIES

A dependent substitutional species is required in order to be able to determine which species are independent. The program will then only query for the compositions of the independent species. NOTE: Sometimes the dependent species is chosen by the program and thus this question is never given. This maybe due to stoichiometric constraints or to the fact that it has been set already in the kinetics database due to the model selected for the diffusion.

`DEPENDENT INTERSTITIAL SPECIES`

A dependent interstitial species is required in order to be able to determine which species are independent. The program will then only query for the compositions of the independent species. NOTE: vacancies are always regarded as dependent and therefore if vacancies are present in the phase then this question is never given.

`COMPOSITION TYPE`

Type of composition used for the constitution of the phase. Legal alternatives are:

- SITE_FRACTION
- MOLE_FRACTION
- MOLE_PERCENT
- WEIGHT_FRACTION
- WEIGHT_PERCENT
- U_FRACTION

`TYPE`

Type of composition profile to be entered, possible alternatives are:

- LINEAR
- READ_POINT_BY_POINT
- FUNCTION
- GEOMETRIC

If FUNCTION is chosen the composition profile can be given as a function of the global distance denoted X. Some useful functions are the error function denoted erf(X) and the Heaviside step-function denoted hs(X).

For example the function “3+2hs(x-1e-4)” provides a concentration of 3 at the left side and 5 at the right side with a sharp step in the concentration profile at 1e-4m=100μm.

`VALUE OF FIRST POINT`

Composition in the first gridpoint. Values in between are interpolated linearly if a LINEAR type of profile is specified.

`VALUE OF LAST POINT`

Composition for the last gridpoint. Values in between are interpolated linearly if a LINEAR type of profile is specified.

INPUT FILE

The input source from which to read the points when entering values point by point, default is TERMINAL.

VALUE OF POINT

The value of the point when entering values point by point.

VALUE OF R IN THE GEOMETRICAL SERIE

Use the same geometrical factor as for the geometrical grid.

VOLUME FRACTION OF

Initial volume fraction of a spheroid phase.

ENTER_ENHANCEMENT_FACTOR

Description: This command changes the mobility of a specific element in a specific phase. The mobility of the element in the phase is multiplied by a factor which is specified as an argument to the command.

Syntax: ENTER_ENHANCEMENT_FACTOR <PHASE><ELEMENT><FACTOR>

ENTER_GEOMETRICAL_EXPONENT

Description: Enter the geometrical exponent which defines the geometry of the system. The program handles 1-dimensional geometries defined by the geometrical exponent.

These geometries are:

- 0. Planar geometry. This corresponds to an infinitely wide plate of a certain thickness.
- 1. Cylindrical geometry. This corresponds to an infinitely long cylinder of a certain radius.
- 2. Spherical geometry. Sphere with a certain radius.
- Syntax: ENTER_GEOMETRICAL_EXPONENT

Prompt: GEOMETRICAL EXPONENT

An integer value between 0 and 2 is required.

ENTER_GRID_COORDINATES

Description: Enter the size and gridpoint distribution of the grid in each region separately. The size of the region is specified in the units that the diffusion data is entered in. The grid may be of the type LINEAR, READ_POINT_BY_POINT, GEOMETRIC or DOUBLE_GEOMETRIC.

A linear grid will give a equally spaced grid. A geometrical grid will yield a higher number of gridpoints at the lower end of the region if a geometrical factor larger than one is given and a higher number of gridpoints at the upper end of the region if the factor is smaller than one. A double geometrical grid makes it possible to have a high number of gridpoints in the middle or at both ends of a region, two geometrical factors should be entered in this case. A point by point read may be done either from the keyboard or from a predefined file.

Syntax: ENTER_GRID_COORDINATES

Prompt: REGION NAME

Name of the region into which a grid is to be entered.

WIDTH OF REGION

The actual size of the region is entered. Note that the size of the region is specified in units compatible with those of the diffusion data.

TYPE

Type of grid to entered, possible alternatives are

- LINEAR
- READ_POINT_BY_POINT
- GEOMETRIC
- DOUBLE_GEOMETRIC

A linear grid will give an equally spaced grid. A geometrical grid will yield a higher number of gridpoints at the lower end of the region if a geometrical factor larger than one is given and a higher number of gridpoints at the upper end of the region if the factor i smaller than one. A double geometrical grid divides the region in two halves and generates a separate geometrical grid in each half.

NUMBER OF POINTS

The number of points present in the region. Please consider the interspacing of the grid when determining the number of points.

INPUT FILE

The input source from which to read the points when entering values point by point, default is TERMINAL.

VALUE OF POINT

The value of the point when entering values point by point.

VALUE OF R IN THE GEOMETRICAL SERIES

Value in the geometrical factor in the series determining the distribution of the grid points. A geometrical factor larger than one will yield a higher density of gridpoints at the lower end of the region and a factor i smaller than one will yield a higher density of gridpoints at the upper end of the region.

`VALUE OF R IN THE GEOMETRICAL SERIE FOR LOWER PART OF REGION`

The geometrical factor in the series for the lower (left) part of a region in a double geometrical grid

`VALUE OF R IN THE GEOMETRICAL SERIE FOR UPPER PART OF REGION`

The geometrical factor in the series for the upper (right) part of a region in a double geometrical grid.

ENTER_HEAT_TRANSFER_PARAMETER

Description: A model for thermomigration has been implemented to simulate the thermal induced diffusion in temperature gradients. This model requires that the temperature depends on the length coordinate in the system and that the quantuty, "heat of transport" is entered. This quantity "heat of transport", denoted Q* is a entered with this command.

Syntax: `ENTER_HEAT_TRANSFER_PARAMETER`

This parameter is entered separately for each component in each phase. This implementation and functionality of this model is described in the paper: *Simulation of Carbon Diffusion in Steel Driven by a Temperature Gradient, Lars Höglund and John Ågren in Journal of Phase Equilibria and Diffusion. 2010.*

ENTER_HOMOGENIZATION_FUN

Description: This command is only of interest if the homogenization model is enabled. The homogenization model for multiphase simulations is based on the assumption of local equilibrium at each node point, which yields the local chemical potentials at each node point from which the local chemical potential gradients may be estimated. The chemical potential gradients are the driving forces for diffusion. The local kinetics must also be evaluated by some averaging procedure, the choice of which is the purpose of this command. The local kinetics is evaluated by considering the product of mobility times u-fraction for each component in each phase and the volume fraction of each phase. At present, there are 14 different varieties of homogenization functions. The homogenization function to be used is selected by entering a digit between 1 and 14 (default is #5). Depending on function, the user may be prompted for further input. The homogenization functions are the following:

1. General lower Hashin-Shtrikman bound

2. General upper Hashin-Shtrikman bound
3. Hashin-Shtrikman bound with prescribed matrix phase
4. Hashin-Shtrikman bound with majority phase as matrix phase
5. Rule of mixtures (upper Wiener bound)
6. Inverse rule of mixtures (lower Wiener bound)
7. Labyrinth factor f with prescribed matrix phase
8. Labyrinth factor f**2 with prescribed matrix phase
9. General lower Hashin-Shtrikman bound with excluded phase(s)
10. General upper Hashin-Shtrikman bound with excluded phase(s)
11. Hashin-Shtrikman bound with prescribed matrix phase with excluded phase(s)
12. Hashin-Shtrikman bound with majority phase as matrix phase with excluded phase(s)
13. Rule of mixtures (upper Wiener bound) with excluded phase(s)
14. Inverse rule of mixtures (lower Wiener bound) with excluded phase(s)

For the Hashin-Shtrikman bounds, see Z Hashin, S Shtrikman, J Appl Phys 33(1962)3125. The geometrical interpretation of the Hashin-Shtrikman bounds are concentric spherical shells of each phase. For the general lower Hashin-Shtrikman bound the “outermost shell” consists of the phase with the most sluggish kinetics and vice versa for the general upper bound. The geometrical interpretation of the Hashin-Shtrikman bounds suggest further varieties of the bounds, viz. #3 and #4, where the outermost shell consist of a prescribed phase or the phase with highest local volume fraction, respectively.

The geometrical interpretation of the Wiener bounds are continuous layers of each phase either parallell with (upper bound) or orthogonal to (lower bound) the direction of diffusion.

The labyrinth factor functions implies that all diffusion takes place in a single continuous matrix phase. The impeding effect on diffusion by phases dispersed in the matrix phase is taken into account by multiplying the flux with either the volume fraction (#7), or the volume fraction squared (#8), of the matrix phase.

The varieties with “excluded phases” are useful in several respects. First, if a phase is modelled as having zero solubility for a component, the mobility of that component in that phase is undefined, which causes a (non-terminal) error. Setting a phase as “excluded” causes the mobility of all components in that phase to be set to zero. Second, often there are some “major” matrix solid solution phases and some “minor” precipitate phases. If the mobilities in the minor precipitate phases are zero the lower Hashin-Shtrikman bound is useless as it will produce a kinetic coefficient that is zero. However, using homogenization function #9 the excluded phases will not be considered when evaluating which phase has the most sluggish kinetics.

ENTER_LABYRINTH_FUNCTION

Description: Enters a constant value or a function of temperature, pressure, or the volume fraction of the phase where diffusion occurs. This function increase or reduces the diffusion coefficient matrix. This function is primarily used when spheroid phases have been entered into a region. It may also be used for increasing or decreasing all diffusion coefficients in a certain matrix phase by a constant factor. NOTE: This function do not apply to the homogenization model. For the homogenization model the command ENTER_HOMOGENIZATION_FUNCTION should be used.

Syntax: ENTER_LABYRINTH_FUNCTION

ENTER_MOBILITY_DATA

Description: Mobility data may be entered interactively. If there already was a function defined it is deleted.

Syntax: ENTER_MOBILITY_DATA

ENTER_PHASE_IN_REGION

Description: This command enters a phase into an earlier defined region.

Syntax: ENTER_PHASE_IN_REGION

Prompt: ACTIVE OR INACTIVE PHASE

Type of phase entered. An inactive phase is a phase which will not participate in the calculations until has become stable. This is done by regarding the driving force for precipitation of the phase in an equilibrium calculation. The program will then automatically retransform the inactive phase into an active one.

REGION NAME

Name of the region into which the phase is to be entered.

PHASE TYPE

Type of phase entered. Depending on your answer a selected variety of the below sub-prompts will appear. Legal types are:

- MATRIX
- LAMELLAR
- SPHEROID

If the LAMELLAR type of 'phase' is chosen, the pearlite calculation model is invoked. The following text is displayed:

```
Eutectoid reaction is "GAMMA" ==> "ALPHA" + "BETA"
```

This is in order to clarify what we mean with GAMMA, ALPHA and BETA in the specific sub-prompts that will appear, see further below. A SPHEROID type of phase requires that a MATRIX phase has been previously entered.

`PHASE NAME`

Name of the phase that is to be entered. A #-sign and a digit may append the phase name in order to specify the composition set number, e.g. FCC#2.

`COMPOSITION SET`

Number of the composition set. This is needed if the phase has been amended to have more than one composition set and the number was not given directly on the phase name, see above.

`ATTACH TO REGION NAMED`

Enter the name of the region onto which the inactive phase is to be attached.

`ATTACHED TO THE RIGHT OF`

Enter Y to attach the inactive phase on the right side of the region else, enter N to attach on the left side.

`REQUIRED DRIVING FORCE FOR PRECIPITATION`

The required driving force (evaluated as DGM(phase) in POLY-3) to be used for determining whether an inactive phase is stable.

`CONDITION TYPE`

Boundary condition used if the inactive phase becomes stable.

LAMELLAR

Specific subprompts for the lamellar type:

`Enter name of "ALPHA" phase`

Enter the GES phase name for the ALPHA phase of the eutectic/eutectoid decomposition product.

`Enter name of "BETA" phase`

Enter the GES phase name for the BETA phase of the eutectic/eutectoid decomposition product.

`Enter name of "GAMMA" phase`

Enter the GES phase name for the GAMMA matrix phase.

`Enter "ALPHA"/"BETA" surface tension:`

Enter function for the surface tension between the ALPHA and BETA phases, $\sigma^{\alpha/\beta}$

```
Enter "ALPHA"/"GAMMA" surface tension:
```

Enter function for the surface tension between the ALPHA and GAMMA phases, $\sigma^{\alpha/\gamma}$

```
Enter "BETA"/"GAMMA" surface tension:
```

Enter function for the surface tension between the BETA and GAMMA phases, $\sigma^{\beta/\gamma}$

```
Optimum growth condition factor /2/:
```

Enter the 'Optimum-growth-rate-factor'. Due to Zener's maximum growth rate criteria this factor has a value of 2 for volume controlled growth and 3/2 for boundary controlled growth. Due to Kirkaldy's extreme in entropy production criteria the values are 3 and 2, respectively.

```
Name of dependent element
```

Enter the name of the substitutional element to consider as the dependent one.

```
Growth model (VOLUME/BOUNDARY/KIRKALDY) for
element X
```

Select growth model to be used for element X. Choose between:

- Volume diffusion model.
- Boundary diffusion model.
- Kirkaldy's mixed mode diffusion model. Implies MIXED, see below.

```
DF(X) = /value/AUTOMATIC/MIXED/TDB/
```

Either input a numerical value on the pre-exponential factor DF or select one of the key words:

- AUTOMATIC
- MIXED
- TDB

AUTOMATIC is only available for element Carbon. It implies a mixed type of calculation where the volume diffusion part is calculated due to J. Ågren: Scripta Met. 20(1986)1507-1510 (volume diffusion of C in Austenite) and the boundary diffusion part due to J. Ågren: Acta Metall. 20(1982)841-851 (boundary diffusion of C is assumed to be the same as C diffusion in Ferrite). The k' or k'', as appropriate, are given by B. Jönsson: Trita-Mac 478, 1992. MIXED means a mixed mode calculation using an effective diffusioncoefficient, see B. Jönsson: Trita-Mac 478, 1992. Coefficient k' or k'' will be asked for, see below. TDB means calculate the diffusion coefficient for volume diffusion for element X from the parameters stored in the database.

```
DQ(X)=
```

Input a numerical value on the activation energy DQ for element X.

```
k'=
```

```
k''=
```

Input a numerical value on the k coefficient used to calculate the effective diffusion coefficient, use in MIXED mixed mode calculations, see B. Jönsson: Trita-Mac 478, 1992.

```
DF_boundary(X)=
```

Input a numerical value on DF for boundary diffusion of element X in a mixed mode calculation.

```
DQ_boundary(X)=
```

Input a numerical value on DQ for boundary diffusion of element X in a mixed mode calculation.

```
DF_volume(X)=
```

Input a numerical value on DF for volume diffusion of element X in a mixed mode calculation. N.B. key word TDB may also be used, see TDB above.

```
DQ_volume(X)=
```

Input a numerical value on DQ for volume diffusion of element X in a mixed mode calculation.

```
Automatic start values for the S0 determination
/Y/:
```

Enter Y if you want automatic start values for the unknown parameters in the S0 determination else enter N. S0 is the critical lamellar spacing for which the growth rate is zero.

```
Critical thickness of "ALPHA" lamella:
```

If you answered N on the previous question this prompt will appear. The critical thickness of ALPHA is about 0.9 of S0, which in turn is about 1/3 to 1/2 of the observed lamellar spacing S. For binary Fe-C alloys the observed pearlite lamellar spacing is approximately given by

$$S = 1.75 \cdot 10^{-5} (A_{1e} - T)^{-1}$$

The equation may be used as a start value approx. for alloyed steels. However, use the A_{1e} temperature of the steel.

```
Critical thickness of "BETA" lamella:
```

The critical thickness of BETA is about 0.1 of S0, see above.

```
Automatic start values on potentials /Y/:
```

Enter Y if you want automatic start values for the unknown potentials else N.

```
Give potentials for "ALPHA"/"GAMMA" equil.
```

If you answered N on the previous question this prompt will appear. Enter start values for the unknown potentials, MU, at the ALPHA/GAMMA phase boundary.

`Give potentials for "BETA"/"GAMMA" equil.`

Enter start values for the unknown potentials, MU, at the BETA/GAMMA phase boundary.

`Growth rate V:`

Enter a start guess on the growth rate. As a hint on what value to choose we recognize that for binary Fe-C alloys the pearlite growth rate is approximately given by:

$$S = 8 \cdot 10^{-9} (A_{1e} - T)^2$$

The equation may be used as a start value approx. for alloyed steels. However, use the A_{1e} of the steel.

`Automatic start values on other variables /Y/:`

Enter Y if you want automatic start values for the unknowns in the determination of the growth rate else enter N.

`Fraction of "ALPHA" phase:`

Enter a guess on the fraction of the ALPHA phase. For pearlite it is about 0.9.

`Give potentials for "ALPHA"/"GAMMA" equil.`

Enter start values for the unknown potentials, MU, at the ALPHA/GAMMA phase boundary.

`Give potentials for "BETA"/"GAMMA" equil.`

Enter start values for the unknown potentials, MU, at the BETA/GAMMA phase boundary.

ENTER_REGION

Description: This command enters a region into the system. This is the first thing that must be done before entering a grid and any phases.

Syntax: `ENTER_REGION`

`REGION NAME`

Name of a region to be entered. The name of the region can be arbitrarily chosen.

`ATTACH TO REGION NAMED`

Name of a region to which the new region should be attached.

`ATTACHED TO THE RIGHT OF`

Relative position of the new region. To attach the new region to the right of the named region answer YES, to attach to the left answer NO.

EXIT

Description: Terminates the program and returns to the operating system. Unless a SAVE_WORKSPACES command has been given before all data entered by user are lost.

Syntax: `EXIT`

GB_MODEL

Description: Grain-boundary and dislocation assisted diffusion is implemented by assuming that these contributed to the diffusion by using the same frequency factor and a modified bulk activation energy. The grain-boundaries and the dislocations will contribute to the total amount of diffusion according to their weighted fractions.

Syntax: GB_MODEL

The parameters are entered separately for each region in order to different expression for different phases.

The used expressions for the grain-boundary and dislocation contributions are:

$M^{gb}=M_0^{bulk}\cdot\exp(F_{redGB}\cdot Q^{bulk}/R/T)$
$M^{disl}=M_0^{bulk}\cdot\exp(F_{redDisl}\cdot Q^{bulk}/R/T)$

where

- M_0^{bulk}: frequency-factor in the bulk
- Q^{bulk}: activation energy in the bulk
- F_{redGB}: Bulkdiffusion activation energy multiplier (typical value 0.5)
- $F_{redDisl}$: the bulkdiffusion activation energy multiplier (typical value 0.8)

The weighted calculated value for the mobility M^{new} is then evaluated from:

$$M^{new}= \delta/d\cdot M^{gb}+ \rho\cdot b^2\cdot M^{disl}+ (1-\delta/d-\rho\cdot b^2)\cdot M^{bulk}$$

where

δ: the grainboundary thickness (typical value $0.5\cdot10^{10}$)

d: the grainsize as a function of time and temperature (typical value $25\cdot10^{-6}$)

ρ: the dislocation density as a function of time and temperature

b: burgersvector (typical value $1\cdot10^{-10}$)

M^{bulk}: the mobility in the bulk (δ/d being the fraction of grainboundaries in the bulk and $\rho\cdot b^2$ being the fraction of dislocations in the bulk)

These models are activiated by the use of the command GB_MODEL in the dictra monitor where these parameters also are entered.

GOTO_MODULE

Description: The user may select another module by this command.

Syntax: GOTO_MODULE <MODULE NAME>

MODULE NAME

The name of the module must be given. In order to obtain a list of available modules give a return.

HELP

Description: Help can be obtained either as a list of all commands (also by just entering a "?"), or specific help for a command by giving the command (abbreviated).

Syntax: COMMAND

The command for which a description is wanted should be given. If the abbreviation is not unique a list of all matching commands are given.

HOMOGENIZATION_MODEL

Description: This command enables or disables the use of the homogenization model and its default settings. These commands are used to enable the homogenization model in DICTRA. The homogenization model is used for multiphase simulations assuming that local equilibrium holds at each node point. When entering phases into a region one of them is entered as MATRIX phase and all other phases as SPHEROID, but it does not matter which one is entered as matrix phase and it will not affect simulations. Homogenization model simulations differs from all other DICTRA simulations in that it is implemented using an implicit finite volume method in order to increase numerical stability (degree of implicity can be chosen using the SET_SIMULATION_CONDITIONS command). Because of this, and other factors, homogenization model simulations will generally run slower than other comparable DICTRA simulations.

Syntax: HOMOGENIZATION_MODEL

Prompt: ENABLE HOMOGENIZATION

Enter yes to enable the homogenization model.

USE DEFAULT SETTINGS

Enter yes to use default settings for the homogenization model. If no is entered the following sub-prompts appear.

ADD IDEAL FLUX CONTRIBUTION

Enter yes or no. If yes is entered the user is prompted to enter a fractional ideal flux contribution between zero and one. In multiphase regions the system loses degrees of freedom which may cause fluctuations in the composition profiles. This can be amended by adding a small ideal contribution to the fluxes. The ideal flux contribution should normally not be used.

USE INTERPOLATION SCHEME

Enter yes or no. The interpolation scheme may speed up simulations significantly. If yes is entered several sub-prompts appear:

-Enter what is essentially the number of steps in composition space. In the limit where an infinite number of steps are used, exactly the same solution is obtained as without the interpolation scheme. However, excellent results can be obtained with a reasonable discretization.

-The discretisation can be either linear or logarithmic. For the linear discretisation the scheme will not be used at node points where the content of one or more solutes fall below a certain critical value. For such cases, where composition span many orders of magnitude, the logarithmic discretisation can be tried.

-Enter the fraction of free physical memory to be used by the interpolation scheme.

`USE GLOBAL MINIMIZATION`

Enter yes or no whether global minimization should be used in equilibrium calculations. In general, using global minimization will significantly increase the CPU time for a given simulation, but there will also be a significantly reduced risk for non-converged equilibrium calculations.

`REFRESH JACOBIAN EVERY ITERATION`

Entering yes will increase computational demand for each iteration, but may in some cases improve conergence rate

`DEFAULT GRID PARAMETER VALUES`

These settings only affect moving phase boundary simulations where the grid changes during the simulation. Entering 'no' causes the following sub-prompts to appear

- Geometrical coefficient. The geometrical coefficient used in each region.
- Fixed interface width. A value larger than zero makes interface widths fixed to that value.
- Grid fineness away from interface. A value other than one causes the grid away from the interface to be coarser (>1) or finer (<1) than what would be obtained just by the geometrical coefficient.
- Interface width fraction. If the interface width isn't fixed the program aims for a width equal to this factor times the cell width.
- Consecutive critical time-steps to delete region. If the width of a region falls below a certain critical value and shrinks monotonically for this number of time-steps it is deleted.

LIST_CONDITIONS

Description: Lists the conditions set with the SET_CONDITION command.

Syntax: LIST_CONDITIONS

Prompt: OUTPUT FILE

File where the information is to be written.

LIST_MOBILITY_DATA

Description: List the previously entered mobility data.

Syntax: LIST_MOBILITY_DATA

Prompt: OUTPUT FILE

File where the information is to be written.

LIST_PROFILES

Description: Lists profiles in the cell.

Syntax: LIST_PROFILES

Prompt: NAME OF REGION

Name of region(s) in which the profiles are to be listed.

OUTPUT FILE

File where the information is to be written.

COMPOSITION TYPE

Composition type in which the profiles are to be written. Legal composition types are:

- SITE_FRACTION
- MOLE_FRACTION
- WEIGHT_FRACTION
- U_FRACTION

COMPONENTS

The output information may be limited to the specified components.

CONSTITUENTS

The output information may be limited to the specified constituents.

LIST_REGION

Description: List the names of the defined regions, active and inactive phases and the global coordinates of the interfaces.

Syntax: LIST_REGION

Prompt: OUTPUT FILE

File where the information is to be written.

LIST_TIMESTEPS

Description: This command lists timesteps in the workspace and those stored on file during a simulation.

Syntax: LIST_TIMESTEPS

MACRO_FILE_OPEN

Description: Macro is a convenient way of predefining sequences of commands on a file and then executing them by the MACRO command. This is useful when the same calculation is made often with just small changes. One good case for applying this is when calculating diagrams from an assessment. With a macro file all commands can be stored on a file and you just type MACRO <filename>.

The macro file can contain any legal DICTRA commands. The macro must be terminated with EXIT or in the SYS, DICTRA, POLY-3 or POST module with the command SET_INTERACTIVE.

Syntax: MACRO_FILE_OPEN

Prompt: `Macro filename:`

Give the name of the file with the macro commands. Default extension is DCM.

PARA_EQUILIBRIUM_MODEL

Description: This command enables or disables the use of the para-equlibrium model.

Turns on the para-equilibrium model in the DICTRA simulation. This implies that the local equilibrium assumption is no longer valid and that substitutional components are regarded as one composite component. The model is limited to treating only one single moving interface in one cell. The composition of the substitutional components in the phase that is to be dissolved may be chosen in several ways (AUTO, value%, -value and value), see below.

Syntax: PARA_EQUILIBRIUM_MODEL

Prompt: `ENABLE PARAEQ`

Enables or disables the use of this model by using one of the key words YES or NO.

`AUTO`

The value at the far end (upper or lower end) of the region.

`value %`

The value at a certain percentage from the interface in the region.

`- value`

The value at a fixed distance from the interface.

`value`

A specific value.

PATCH

Description: This command is only for those who think they know what they are doing (and that does not even include the author of this program).

Syntax: PATCH

POLY_COMMAND

Description: Sends a command to the POLY-3 module where it is executed.

Syntax: POLY_COMMAND

Prompt: `To Poly`

Command line sent to the POLY-3 module.

POST_PROCESSOR

Description: This command gives control to the post processor which has its own command repertoire.

Syntax: POST_PROCESSOR

READ_WORKSPACES

Description: The DICTRA, POLY-3 and GES5 workspaces can be read from a file where they must have been saved previously with a SAVE command. This file is not printable.

Syntax: READ_WORKSPACES

Prompt: `File name`

Name of the file where the workspaces shall be read from. The default file extension is DIC.

SAVE_WORKSPACES

Description: The workspaces in DICTRA, POLY-3 and GES5 are saved on a file with this command. After a SAVE command the user can always come back to exactly the state he had when he issued the SAVE command by simply give a READ command.

Syntax: SAVE_WORKSPACES

Prompt: `File name`

Name of the file where the workspaces shall be saved on.

The default file extension is DIC.

`Overwrite current file content`

`Proceed with SAVE`

There is already a file with this name and if you answer Y the previous content will be overwritten. Note that results from SIMULATE_REACTION command is destroyed by SAVE. You may append several results by the SIMULATE_REACTION command without destroying the previous results but SAVE will erase them all.

SELECT_CELL

Description: Selects the current cell from the list of existing cells and enables the user to enter and display data into that cell.

Syntax: SELECT_CELL

Prompt: Number

The cell number to be selected. Specify cell number by giving an integer or one of the key words NEXT or PREVIOUS.

SELECT_TIMESTEP

Description: This command selects a timestep from those stored on file during a simulation. The profiles can be listed and simulation can be continued from this timestep.

Syntax: SELECT_TIMESTEP

Prompt: TIMESTEP

The timestep to be selected, legal syntax is:

- FIRST
- LAST
- time
- #nnn
- #?

When selecting a time no interpolation is performed but the timestep closest to the time entered will be selected. #nnn can be obtained from the number given by LIST_TIMESTEPS or by typing #?.

DELETE ALL OTHER TIMESTEPS

Clears the current workspace from all other timesteps except the one selected. This is necessary if the simulation is to be continued from this timestep.

SET_ACCURACY

Description: This command enables the user to enter the accuracy requirements to be used in the determination of the timestep when using the automatic timestep procedure.

Syntax: SET_ACCURACY

Prompt: MAX RELATIVE ERROR

The maximum allowed relative error of the profile during one timestep integration.

MAX ABSOLUTE ERROR

Maximum allowed absolute error of the profile during one timestep integration. This parameter must be chosen with some relation to the smallest concentration in the profiles.

SET_ALL_START_VALUES

Description: This command enables the user to enter starting values for various quantities, such as velocities and potentials.

Syntax: SET_ALL_START_VALUES

Prompt: START VALUE FOR VELOCITY OF INTERFACE

A starting value for velocity at the named interface is required.

START VALUE FOR POTENTIAL

A starting value for a potential at the named interface is required. If an AUTOMATIC value is specified the program will the attempt to determine a starting value and also select a suitable component for which the potential is varied.

VARYING SPECIES IN INTERFACE

The species which potential is treated as unknown.

AUTOMATIC STARTING VALUES FOR PHASE COMPOSITIONS

Compositions used as starting values in the equilibrium calculations using POLY-3. When using automatic starting values the compositions are taken from the entered profiles.

SET_CONDITION

Description: This command defines conditions that reduces the degrees of freedom at equilibrium or define the boundary conditions at the outer rims of the system. This command must be used to set the temperature,pressure or heat extracted from the system.

Conditions can be a function of time and different time-dependent functions can be specified at different time intervals. The syntax for this is approximately the same as used in the GES to specify temperature ranges for thermodynamic parameters.

Syntax: SET_CONDITION

Prompt: GLOBAL OR BOUNDARY CONDITION

Type of condition to be specified. A global condition is either pressure (P), temperature (T) or heat content removal (P) and may be specified as a function of time. Boundary conditions determine how the cell interacts with the world outside the cell.

VARIABLE

Legal variables are pressure (P), temperature (T) or heat extracted (Q) as a function of time (TIME), or time-temperature-pairs (T-T-P) that specifies temperature at a specific time and lets the program calculate the cooling or heating rate. For Q the amount of extracted heat per time unit is normalized and the size of the system is normalized to 1 mole of atoms.

BOUNDARY

Defines on which side of the system the boundary conditions are to be specified. Legal alternatives are UPPER (the rightmost side of the system) and LOWER (the leftmost side of the system).

CONDITION TYPE

Defines the type of boundary condition to be specified. The different alternatives may in most cases be functions of both TIME, T (temperature) and P (pressure). The default is CLOSED_SYSTEM which is equivalent to setting the fluxes of all components to zero at the boundary.

Legal alternatives are:

- FIX_FLUX_VALUE: Enter functions that yield the flux times the molar volume for the independent components. May be a function of time, temperature and pressure.
- STATE_VARIABLE_VALUE: A legal expression in POLY-3 syntax that reduces the degrees of freedom. This type of boundary condition should be used with the uttermost care as no checks are done if it is a legal expression in advance.
- POTENTIAL_FLUX_FUNCTION and ACTIVITY_FLUX_FUNCTION: These types of boundary conditions are used to take into account the finite rate of a surface reaction. The flux for the independent components must be given in the format:
  $J_k = f_k(T,P,TIME) * \left[ACTIVITY_k^N - g_k(T,P,TIME) \right]$
  or
  $J_k = f_k(T,P,TIME) * \left[POTENTIAL_k^N - g_k(T,P,TIME) \right]$
  where f and g may be functions of time (TIME), temperature (T), and pressure (P), and N is an integer. Note that the activities are those with user defined reference states.
- ITERATIVE_ACTIVITY_FLUX_FUNCTION: Same as activity flux function above. However, an iterative scheme is used to determine the flux. This method may be used instead of activity flux function when the latter has problems.
- CLOSED_SYSTEM: Corresponds to a fix flux value, which is set to zero at all times.
- MIXED_ZERO_FLUX_AND_ACTIVITY: The flux of selected components will be set to zero and the activity of others may be set to a prescribed value.

- GAS: The flux of selected components will be set to zero and the activity of others may be set to a prescribed value. This option is used for treating an expanding system, e.g. the growth of an external oxide scale.

LOW TIME LIMIT

The lower time limit to be used when entering a time dependent function.

HIGH TIME LIMIT

The upper time limit to be used when entering a time dependent function. An asterisk "*" will indicate the high limit as infinity.

ANY MORE RANGES

To specify whether any additional time dependent functions exists or not.

TYPE OF CONDITION FOR COMPONENT

The type of condition when setting a boundary condition of the type MIXED. Allowed alternatives are ZERO_FLUX and ACTIVITY.

SET_FIRST_INTERFACE

Description: This command sets the coordinate of the first interface in the cell. The default value is zero

Syntax: SET_FIRST_INTERFACE

Prompt: COORDINATE FOR FIRST INTERFACE

The coordinate to which the first interface is to be set.

SET_INITIAL_TEMPERATURE

Description: This command is only used when the heat removal rate from the system is specified. It yields the initial temperature of the system. How the temperature then varies during the simulation is a result of the heat removed from the system.

Syntax: SET_INITIAL_TEMPERATURE

SET_INTERACTIVE_MODE

Description: This command is useful in demonstration or macro files in order to stop the execution of the command file and pass over input focus to the keyboard. It has no meaning in interactive mode.

Syntax: SET_INTERACTIVE_MODE

SET_NUMERICAL_LIMITS

Description: This command set various parameters used to control the integration, the solution of the flux balance equations, diffusion equations and the equilibrium calculation during the simulation.

Syntax: SET_NUMERICAL_LIMITS

Prompt: REQUIRED SUM OF SQUARES IN NS01A

Required accuracy during the solution of the fluxbalance equations.

MAX NUMBER OF CALLS TO CALFUN OF NS01A

The maximum number of iterations when solving the fluxbalance equations. This number acts as a "safety valve", a moderate choice is 10*(number_of_interfaces *(number_of_components - 1)) but use a larger value if necessary.

STEP USED BY NS01A

A user supplied parameter which is used to calculate the estimates of the partial derivatives numerically when solving the fluxbalance equations.

MAX STEP USED BY NS01A

A parameter which must be set to a generous estimate of the 'distance' between the initial approximation and the required solution of the fluxbalance equations.

MAX NUMBER OF EQUIDISTANT POINTS IN A REGION

The number of equidistant parts in which a region is divided into that is required to describe the profile. This parameter is used by the procedure that removes "unnecessary" gridpoints from the profile during the simulation; the number of gridpoints is normally not allowed to be less than this number if a linear grid is used.

FRACTION OF REGION ASSIGNED TO THE INTERFACE

Fraction of a region at the region border that is to be regarded as part of the interface. This parameter is used by the procedure that removes "unnecessary" gridpoints from the profile during the simulation.

SMALLEST NUMBER USED IN SCALING FLUX EQUATIONS

The fluxbalance equations are scaled by the velocities calculated in the previous timestep. This number may however decrease to such a small value so that convergence may be affected. The scaling factor is therefore not allowed to decrease below this value.

DEFAULT DRIVING FORCE FOR INACTIVE PHASES

Sets the necessary driving force needed before an inactive phase is allowed to start to precipitate.

SET_REFERENCE_STATE

Description: The reference state for a component is important when using activities, chemical potentials and enthalpies. The reference state for a component is determined by the data. For each component the data must be referred to a selected phase, temperature and pressure "the reference state". All data in all phases where this component dissolves must use the same reference state. However, different datasets may use different reference states for the same element. Thus one must mix data from different databases with caution.

By default activities etc. are computed relative to the reference state used by the database and this may thus differ depending on the database. With this command the user may select himself the reference state of a component if the reference state in the database does not suit him.

Syntax: SET_REFERENCE_STATE

Prompt: Component

The name of the component must be given.

Reference state

The name of a phase that must be either entered or dormant must be given. The component must be a constituent of this phase of course.

A subtle problem is if the component exists in several species in the phase, for example oxygen as O, O2 and O3 in a gas. Normally one would like to have the most stable species as reference state of oxygen, i.e. O2 in this case. Therefore the program will calculate the Gibbs energy of all possible states with the phase with the pure component at the current temperature and select the most stable one.

Temperature

One may select the temperature for the reference state. The value * means the temperature used for the calculation.

Pressure

One may select the pressure for the reference state.

SET_SIMULATION_CONDITION

Description: This command sets miscellaneous parameters used to control output and certain parameters during the simulation.

Syntax: SET_SIMULATION_CONDITION

Prompt: NS01A PRINT CONTROL

Determines whether data should be printed about the iterative procedure to solve fluxbalance equations. This parameter is normally set to 0 but can be set to 1 when difficulties with convergence occur. NS01A will then print out the values used in the iterations and the residuals.

FLUX CORRECTION FACTOR

This parameter controls if the flux correction scheme should be used in the calculations. The value should normally always be 1.

NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF

This parameter specifies the number of equally large timesteps that one timestep should be subdivided into.

CHECK INTERFACE POSITION

This parameter determines whether the timestep is to be controlled by the phase interface displacement during the simulation.

VARY POTENTIALS OR ACTIVITIES

Determines whether the program should use the potential or the activity of a component in order to find the correct tieline at the phase interface. The potential or the activity is varied by the program and is set in order to reduce the degrees of freedom at the local equilibrium.

ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT

Determines whether the program is allowed to itself switch the component that is used to reduce the degrees of freedom at the local equilibrium. The scheme used is that of choosing the components which activities or potentials varied most during the previous timestep.

SAVE WORKSPACE ON FILE

This parameter determines whether the workspaces are to be saved on file during the course of the simulation. Legal alternatives are

- yes Always save on file
- NO Never save on file
- ## Save every n:th time on file (## is a integer value ranging from 0 to 99.)

DEGREE OF IMPLICITY WHEN INTEGRATING PDEs

Normally a value of 0.5 (trapezoidal rule) should be used. If however, large fluctuations occur in the profiles it may be necessary to use the value 1.0 (Euler backwards).

- 0.0 Euler forwards
- 0.5 Trapezoidal rule
- 1.0 Euler backwards

MAX TIMESTEP CHANGE PER TIMESTEP

Factor specifying the maximum increase in the timestep taken from one timestep to another. If 2 is given the maximum timestep will be twice as long as the previous timestep taken.

USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION

This command mainly concerns the calculation of the equilibrium when using the disperse model in DICTRA, where the equilibrium calculations sometimes fail due the abrupt changes in the composition over the region. If YES, then these equilibrium calculations will be performed using forced starting values in POLY_3.

ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF

This determines how often the diffusion coefficient matrix is calculated when solving the partial differential equations (PDE) of diffusion problem. The default setting is to calculate the diffusion coefficient matrix, yielding the stiffness matrix, at each iteration. However, when setting this parameter to NO, it is only calculated at the first iteration and a constant stiffness matrix is used to obtain the solution to the PDEs. This will then lead to an implicit solution and therefore the degree of implicity is automatically set to 1.

SET_SIMULATION_TIME

Description: This command enables the user to enter the time specific conditions for a simulation.

Syntax: SET_SIMULATION_TIME

Prompt: END TIME FOR INTEGRATION

The time up to which the simulation is to be carried out.

AUTOMATIC TIMESTEP CONTROL

Determines whether the timestep should be controlled by an automatic procedure or not. If the user answers "NO" to this question the user will then be prompted for the fix timestep to use during the simulation. The timestep determined by the automatic timestep control procedure is controlled by the parameters set by the command SET_ACCURACY.

MAX TIMESTEP DURING INTEGRATION

The maximum timestep allowed during the simulation. This is required when using the automatic procedure to determine the timestep.

TIMESTEP DURING INTEGRATION

Fixed timestep used when the automatic timestep procedure is disabled.

INITIAL TIMESTEP

Timestep used as the initial timestep.

SMALLEST ACCEPTABLE TIMESTEP

The smallest timestep allowed during the simulation. This is required when using the automatic procedure to determine the timestep.

SET_STOICH_FACTOR

SET_SURFACE_TENSION

Description: This command enters a surface energy function which added to the Gibbs Energy expression for the phase located at the lower (left) side of the interface. The expression is multiplied with the volume per mole substitional atoms. This command is also utilized for simulating a limited interfacial mobility control where the energy function is a function of the interface velocity.

The SET_SURFACE_TENSION command is used to enter the surface energy to enable coarsening. However, it can also be utilized for simulating a case with a limited interfacial mobility.

Syntax: SET_SURFACE_TENSION

Prompt: FUNCTION

Function describing how the (surface) energy function varies with the particle radius and/or the interface velocity.

The classical expression for the surface energy contribution has the form of:

$$\frac{2\sigma V_m}{r}$$

The molar volume should be given relative to the molar volume used by default in DICTRA , $1 \cdot 10^{-5}$ (m^3/mole). The volume should also be given per mole of substitutional atoms. For a precipitate of type M_xC_y this means multiplying with a factor (y+x)/x. If we use M_6C as an example with surface tension 0.5 (J/m^2) and molar volume of $0.71 \cdot 10^{-5}$ (m^3/mole), the entered function should be:

2*0.5*0.71*(7/6)/X;

SET_ACCURACY

Description: For many cases it is necessary to change the default accuracy. The accuracy determines which time step is selected when using the automatic time step control. It may also be necessary to modify the parameters to control the removal of grid points and set manual starting values for velocities and potentials at the phase interfaces.

Syntax: SET_ACCURACY

SIMULATE_REACTION

Description: Start the simulation. If given without any argument, the user will be prompted for certain values during simulations where phases appear or disappear.

Syntax: SIMULATE_REACTION

The command can also be given with the argument YES typed on the same line:

```
SIMULATE_REACTION YES
```

With the YES argument, default values will be used during simulation and no user input can be given. This is especially useful when using DICTRA in batch mode.

SWITCH_MODEL

There are two solvers for moving phase boundary problems in DICTRA. One is more robust but also computationally more demanding than the other "classic" solver. By default, DICTRA will try using the classic solver first. If this fails, then DICTRA will try the new solver for a few time-steps before switching back again to the classic solver, and so on.

This command allows the user to select which solver should be tried first and if only one solver should be used.

Syntax: SWITCH_MODEL

Prompt: `Enable automatic switch of model (y/n)`

Determines if one or two solvers should be used.

`Try classic first (y/n)`

Determines which of the two solvers should be tried first.

The new solver has evolved from the implementation of the "homogenization model", which originally only was intended for single region, multi-phase simulations. Certain settings unique for the new solver are therefore selected using the homogenization model commands, viz.

- HOMOGENIZATION_MODEL
- ENTER_HOMOGENIZATION_FUNCTION
- UTILITIES_HOMOGENIZATION

For some selections and set-ups only one of the two solvers is allowed.

TABULATE_MOBILITY_DATA

Description: Tabulate the previously entered mobility data for a phase.

Syntax: TABULATE_MOBILITY_DATA

Prompt: `Phase`

Phase for which the mobility data is to be tabulated.

`Diffusing species`

Independent species for which the mobility data is to be tabulated.

`Pressure`

Pressure at which the mobility data is to be tabulated.

`Low temperature limit`

Lower temperature limit at which the mobility data is to be tabulated.

`High temperature limit`

Upper temperature limit at which the mobility data is to be tabulated.

`Step in temperature`

The step in temperature for which to tabulate the mobility data.

UTILITIES_HOMOGENIZATION

Description: This command is only of interest if the homogenization model is enabled. Under this heading various miscellaneous utilities of the homogenization model are collected.

Syntax: UTILITIES_HOMOGENIZATION

Prompt: SET TEMPERATURE ACCORDING TO SOLIDUS TEMPERATURE

Enabling this setting causes the global temperature to be set such that it strives towards a certain value T_{target}=T_{sol}-X, where X is a value supplied by the user. The rate by which the temperature approaches T_{target} is also supplied by the user. The solidus temperature is determined with a +/- 1 K accuracy. The user is also asked to input guesses of the minimum and maximum temperature to occur during the simulation. This utility can be useful for optimizing homogenisation heat treatments. Note that the liquid phase must be entered into the system in order for this utility to be used.

DUMP RESULTS TO TEXT FILES

Select 'yes' to save simulation results to various text files. The names of these files are fixed and the files will be saved to the current working directory.

READ INITIAL COMPOSITION FROM TEXT FILE

Select 'yes' to read initial composition from a text file "XF.TXT" that must be present in the working directory. The file should contain the mole fractions of all elements, in alphabetical order, starting from the first grid point, in the first region, in the first cell.

ENTER GHOST PHASE

Select 'yes' to force the so-called ghost phase to be created. This phase has full solubility of all components and zero diffusivity. The Gibbs energy surface of the ghost phase will be set above all other phases. The name of this phase is "ZZDICTRA_GHOST". It can be used for numerical reasons. It is created automatically if there is a phase that lack solubility range of one or more components and then used internally by the program, though the user should normally never need to worry about it.

ENTER INACTIVE PHASES INTO ONE REGION

Select yes to make all inactive phases at a given interface to be entered into a single multiphase region when any one of the phases becomes stable.

EXPLICITLY SET SUBSTITUTIONAL/INTERSTITIAL

Select yes to explicitly select for each element whether it should be substitutional or interstitial. There must be at least one substitutional element in each region. These settings only have effect for the homogenization model and results viewed in the post processor must be interpreted with care; use “dump results to text files” to get results corresponding to the settings entered here.

`SAVE AVERAGE FINITE VOLUME COMPOSITION`

Use this setting to save the average finite volume composition instead of a converted piece-wise linear composition.

`SET CONSTANT PHASE ADDITION`

Use this setting to add constant Gibbs energy contributions to phases (in J / mol formula unit).

3 POST PROCESSOR commands

APPEND_EXPERIMENTAL_DATA

Description: This command is typically used for adding experimental data and text on a calculated diagram. This is achieved by placing the experimental data and text on a file prepared according to the syntax of a graphical language called DATAPLOT. The picture generated from the data is superimposed on the ordinary graphical output from the POST PROCESSOR. Such an experimental datafile may be created by an ordinary text editor. Another use of the APPEND_EXPERIMENTAL_DATA command is to superimpose plots from several independent calculations. For this purpose, there is a command MAKE_EXPERIMENTAL_DATAFILE which will dump a calculated diagram on a file according to the DATAPLOT syntax. With the aid of a normal text editor many such files may be merged. Remember to have only one prologue section on the file (see below).

Syntax: `APPEND_EXPERIMENTAL_DATA`

Prompt: `USE EXPERIMENTAL (Y OR N)`

Specify whether the data from an experimental datafile should be included in the next plot. If N, no experimental data will be plotted.

`EXPERIMENTAL DATAFILE:`

Specify the name of the file with the experimental data. Default file extension is exp.

`PROLOGUE NUMBER:`

Select which prologue to use. In a prologue one may e.g. give the scaling of an axis, the axis texts, and so on. -1 gives a list of all prologues on the file. Read more about prologues below.

`DATASET NUMBER(S):`

Select from which dataset(s) data should be read. Several datasets may be given separated with commas or spaces. -1 gives a list of all datasets on the file.

For more information about DATAPLOT, see Appendix 1: A brief introduction to DATAPLOT.

BACK

Description: This command gives the control back to the most recent module. From the POST PROCESSOR one goes back to the DICTRA monitor.

Syntax: BACK

DIFFERENTIATE_VALUES

Description: Differentiate the plotted curve.

Syntax: DIFFERENTIATE_VALUES

DUMP_DIAGRAM

Description: This command is an alternative command for producing plots. Supported graphical formats are PNG,BMP,PDF,JPEG,TIFF. The plot is saved to a file.

Syntax: DUMP_DIAGRAM

Prompt: OUTPUT FORMAT (PNG,BMP,PDF,JPEG,TIFF)

Specifies which graphical format should be used.

RESOLUTION (LOW,MEDIUM,HIGH)

Specifies the resoluion of the plot.

ENTER_SYMBOL

Description: This command defines a symbolic name that represents either a table or an 'arbitrary' function. Legal variables in functions and columns in tables are state variables, auxiliary variables, integral variables or previously defined functions. Functions are a useful feature of the POST PROCESSOR for defining quantities that are convenient for the user.

Syntax: ENTER_SYMBOL

Prompt: Function or table /FUNCTION/:

Select what kind of symbol to enter.

NAME:

Each symbol has a unique name that must start with a letter and can have maximum 8 characters. If one wishes to enter the name and the value on the same line they must be separated with an equal sign "=".

Function:

Functions are evaluated from an expression of state variables, auxiliary variables, integral variables or previously defined functions. The expression is a fortran like expression and operators +, -, *, / and ** can be used (** only with integer powers). Unary functions like LOG, LOG10, EXP, SIN, COS, ABS and ERF can also be used. An expression can be continued on more than one line. An expression should be terminated by a semicolon or an empty line. Examples of functions:

- POI(CEM,U)-POI(CEM,L);
  The thickness of the region named CEMENTITE
- AC(CR)/X(FCC,CR);
  The activity coefficient for Cr in phase FCC
- SQRT(TIME);
  The square root of the simulation time

`&`

This sub-prompt appears if the function was not terminated by a semicolon. It allows the user to continue to write the function on the new line if one line is not enough for the function. If one has finished the function just press return again.

`Variable(s):`

When entering a table, specify what variables are to be in the various columns. Separate the variables with commas or space characters. At present a maximum of 15 columns are allowed. Note that the independent variable is always printed in the first column.

EXIT

Description: Terminates the program and returns to the operating system.

Syntax: EXIT

HELP

Description: Help can be obtained either as a list of all commands (also by just giving a ?), or specific help for a command by giving the command (abbreviated).

Syntax: HELP <COMMAND>

Prompt: `Command`

The command for which a description is wanted should be given. If the abbreviation is not unique all matching commands is listed.

INFORMATION

Description: Some general on-line information about the POST PROCESSOR is given.

Syntax: INFORMATION <SUBJECT>

Prompt: `WHICH SUBJECT`

Select which subject you want additional information about. Type a "?" in order to presents the list below on possible topics.

- PURPOSE
- STATE VARIABLES
- INTEGRAL VARIABLES
- AUXILIARY VARIABLES
- PLOT CONDITION AND INDEPENDENT VARIABLE
- BASIC METHODOLOGY

INTEGRATE_VALUES

Description: Integrate the plotted curve.

Syntax: INTEGRATE_VALUES

LABEL_CURVES

Description: This command toggles the option. Each label is explained with a text to the right of the diagram.

Example: 1. X: X(CR); Y: TIME; PC:3

Read like this. Label 1 is a curve with X(CR) on the x-axis, TIME on the y-axis and plot condition (PC) according to value 3 specified on the plot condition line printed above the diagram.

Syntax: LABEL_CURVES <YES/NO>

Prompt: LABEL CURVES

Toggle the option by giving YES or NO.

LIST_PLOT_SETTINGS

Description: The present values of most parameters specifying the type of diagram to be plotted will be listed on the terminal.

Syntax: LIST_PLOT_SETTINGS

LIST_REGION_NAMES

Description: Lists all region names defined. Note that all region names have got a #-sign and the cell number appended.

Syntax: LIST_REGION_NAMES

LIST_SYMBOLS

Description: Lists a specific or all symbols defined.

Syntax: LIST_SYMBOLS

Prompt: NAME:

Give the name of a symbol or an * to list all defined symbols.

LIST_TIME_STEPS

Description: Lists all integration time steps.

Syntax: LIST_TIME_STEPS

MAKE_EXPERIMENTAL_DATAFILE

Description: This command makes it possible to save graphical information on a file using the DATAPLOT format (see separate documentation or, for a brief introduction, the APPEND_EXPERIMENTAL_DATA command). In order to merge two or more diagrams from separate calculations one may write them out on files with this command and then add them together with a normal text editor.

Syntax: MAKE_EXPERIMENTAL_DATAFILE

Prompt: `Output file`

File where the graphical information will be written. Default file extension is exp.

PLOT_DIAGRAM

Description: The graphical information will be plotted on the specified device using the plot format set by SET_PLOT_FORMAT.

Syntax: PLOT_DIAGRAM

Prompt: `PLOT FILE`

The name of the file or graphical device

PRINT_DIAGRAM (PC/WINDOWS only)

Description: This command prints the diagram using the printers defined in windows.

Syntax: PRINT_DIAGRAM

QUICK_EXPERIMENTAL_PLOT

Description: This command is similar to the APPEND_EXPERIMENTAL_DATA command but can be used when there is no graphical information to be plotted in the DICTRA workspace. It defines a pair of axis, sets the axis labels to "X" and "Y", and scales both x- and y-axis between 0.0 and 1.0 unless a prologue is read from the datafile. See command APPEND_EXPERIMENTAL_DATA for more information about the format of the datafile.

Syntax: QUICK_EXPERIMENTAL_PLOT

REINITIATE_PLOT_SETTINGS

Description: All parameters describing the diagram will be given default values.

Syntax: REINITIATE_PLOT_SETTINGS

SELECT_CELL

Description: One may only plot data from one cell at the time. This command lets the user select for which cell data should be processed. Type “?” in order to get a list of valid cell numbers. N.B. The current cell number is displayed as a part of the POST PROCESSOR prompt.

Syntax: SELECT_CELL

Prompt: `Number`

Number of the cell to be selected. Specify cell number by giving an integer or one of the key words NEXT or PREVIOUS.

`TABULATE`

Tabulate a named table. Note that the independent variable is always printed in the first column.

`Name:`

Give the symbolic name of the table.

`Output file /SCREEN/:`

Select output device/file. Just typing a return gives output on the screen.

SET_AXIS_LENGTH

Description: This command can be used to change the relative length of an axis, i.e. the number of tic-marks on the axis. The default number of tic-marks on an axis is 10 when the relative length is 1. This command has been added due to some idiosyncrasies in the graphical package used. The number of units per tic-mark must be a multiple of 1, 2, or 5 to obtain a reasonable scaling of an axis.

Syntax: `SET_AXIS_LENGTH`

Prompt: `AXIS`

The user must specify for what axis to set the axis length.

`AXIS LENGTH`

The user can specify the relative axis length. The relative length 1 corresponds to 10 tic-marks on the axis.

SET_AXIS_PLOT_STATUS

Description: The user can specify whether a diagram axis is to be plotted or not. This can be used to merge different diagrams on a pen-plotter or to obtain the diagram faster. Default status is that the axis are to be plotted.

Syntax: `SET_AXIS_PLOT_STATUS`

Prompt: `AXIS PLOT (Y OR N)`

The user can specify to plot axis or not.

SET_AXIS_TEXT_STATUS

Description: This command can be used to change the axis text from the automatic text given by the axis specification to a text given by the user.

Syntax: `SET_AXIS_TEXT_STATUS`

Prompt: `AXIS (X, Y OR Z)`

The user must specify for which axis the axis-text status is to be changed (if the axis type (see below) is INVERSE, X2 or Y2 may be used to set the corresponding opposite linear axis text).

```
AUTOMATIC AXIS TEXT  (Y OR N)
```

The user must specify if automatic axis text is to be used or not.

```
AXIS TEXT
```

If automatic axis text has not been chosen, the user will be prompted for his own axis text.

SET_AXIS_TYPE

Description: Allows the user to change between linear, logarithmic and inverse axis.

Syntax: SET_AXIS_TYPE

Prompt:

```
AXIS (X, Y or Z)
```

Specify for which axis you want to change the axis type.

```
AXIS TYPE
```

Specify which axis type to set. Select LINear (default), LOGarithmic or INVerse. Only the three first characters are relevant.

SET_COLOR

Description: On devices that support colors/(line types), one may select different colors/(line types) on the following items:

- Text and axis Color
- Diagram Color
- DATAPLOT Color

Syntax: SET_COLOR

SET_DIAGRAM_AXIS

Description: This command is used for specifying the axis variables of a plot. In order to plot a diagram at least two axis variables (x and y) must be specified.

Syntax: SET_DIAGRAM_AXIS

Prompt:

```
AXIS (X,Y OR Z)
```

Specifies for which axis to set a variable.

```
VARIABLE
```

Specifies which variable to plot along this axis. A variable is specified by its mnemonic or name. The different valid variable mnemonics and names are tabulated and explained in more detail below. However, first a brief listing of possible variable types:

- NONE: Use the word NONE in order to clear an axis setting.

- INTEGRAL VARIABLES: An integral variable is a quantity that has been obtained by integration in space over the whole system or over a specific region. In a planar geometry values are given per unit area, in a cylindrical geometry they are given per unit length, and in a spherical geometry they are absolute values.
- FUNCTIONS: Functions are identified by their names which have been entered with the command ENTER_FUNCTION. Use the LIST_SYMBOLS command to get a list of valid function names.
- AUXILIARY VARIABLES: As a complement to state variables and integral variables the following auxiliary variables have been defined. The variables may also be called by their mnemonic names, which are shown in the rightmost column. These are convenient to use in user defined functions.
- STATE VARIABLES: State variables in the POST module has a similar meaning as those defined in POLY-3. Examples of state variables are temperature, mole fraction, enthalpy etc. In POLY-3 a general notation method based on character mnemonics has been designed for a predefined set of state variables.

For more information about state variables, integral variables and auxiliary variables, see

Appendix 2: State, integral and auxiliary variables.

Depending on your choice of axis variable some of the below additional sub-prompts may appear.

`FOR COMPONENT`

When an activity, flux, mole-, weight- or U-fraction or percent is plotted the name of the component must be supplied.

`IN REGION`

When the lamellar spacing, e.g. for pearlite, is plotted the name of the region must be supplied.

`FOR PHASE`

When the lamellar thickness, e.g. for ferrite in pearlite, is plotted the name of the phase must be supplied.

`INTERFACE`

When the velocity or the position of an interface is plotted the name of the interface must be given. An interface is identified by the name of the region on its upper side.

`TYPE`

When choosing distance as variable one has additionally to specify what type of distance. A distance may be GLOBAL, i.e. counted from the leftmost interface, or LOCAL, i.e. counted from the interface to the left of the region whose name you will be prompted for.

`REGION NAME`

Name of the region wherein the local distance is measured.

SET_DIAGRAM_TYPE

Description: The user can choose between square plot or triangular plot (Gibbs triangle). Default diagram type is square.

Syntax: `SET_DIAGRAM_TYPE`

Prompt: `TRIANGULAR DIAGRAM (Y OR N)`

The user can specify triangular plot by answering Yes. Otherwise square plot will be set.

`PLOT 3:RD AXIS`

If triangular plot is selected the user can specify if a 3:rd axis, connecting the end points of the x- and y-axis is plotted.

`CLIP ALONG THE 3:RD AXIS`

If desired, all lines outside the region limited by a line joining the end points of the X- and Y-axis will be removed.

SET_FONT

Description: The user can select the font to be used for labels and numbers when plotting the diagram. For some devices (e.g PostScript) there may be other fonts available and these are selected by the SET_PLOT_FORMAT command.

Syntax: SET_FONT

Prompt: SELECT FONTNUMBER

Give the number for the font you will select. Type ? to get an on-line list the available fonts.

FONT SIZE

Specify the size of the font. A value around 0.3 is recommended.

SET_INDEPENDENT_VARIABLE

Description: There are two "free" variables after a simulation done by DICTRA. One is the simulation TIME, the other is a DISTANCE in the system. When plotting a diagram you must choose either one to vary along the curve, i.e. the independent variable, the other one is then the plot condition. N.B. When plotting integral quantities TIME should be independent variable.

Syntax: SET_INDEPENDENT_VARIABLE

Prompt: VARIABLE

Select which variable TIME (Integration time) or DISTANCE (Space coordinate) should be treated as the independent variable

TYPE

When choosing distance as independent variable one has additionally to specify what type of distance. A distance may be GLOBAL, i.e. counted from the leftmost interface, or LOCAL, i.e. counted from the interface to the left of the region whose name you will be prompted for.

NAME OF REGION

For a LOCAL distance one has to supply the name of the region within which the distance is measured. Type a “?”, to get an on-line list of valid region names.

SET_INTERACTIVE_MODE

Description: This command is useful in demonstration or macro files in order to stop the execution of the command file and pass over input focus to the keyboard. It has no meaning in interactive mode.

Syntax: SET_INTERACTIVE_MODE

SET_PLOT_CONDITION

Description: There are two "free" variables after a simulation done by DICTRA. One is the simulation TIME, the other one is a DISTANCE in the system. In general, when plotting a diagram you must choose either type as fixed (i.e. the plot condition), the other one is then the independent variable. However, when plotting integral quantities, plot condition is automatically set to INTEGRAL and TIME is chosen as independent variable. N.B. You cannot mix different kinds of plot conditions. However, for TIME and DISTANCE you may supply up to 15 different condition values, see sub-prompt VALUE(S) below. The plot condition chosen is printed on a separate line above the diagram.

Syntax: SET_PLOT_CONDITION

Prompt: CONDITION

One has to specify which type of condition should be set. Valid conditions are:

- NONE: Condition not set.
- TIME: Integration time.
- DISTANCE: Distance in system.
- INTERFACE: At a certain interface.
- INTEGRAL: Value is integrated over the phase/region/system volume
- TIE_LINE: Pair of values from both sides of certain interface.

Depending on which condition you choose, some or none of the following sub-prompts may appear.

INTERFACE

One has to specify at which interface the condition should be set. FIRST and LAST refer to the leftmost and the rightmost interface of the system, respectively. Type ? in order to get an on-line full list of relevant region names.

TYPE

When distance is chosen as plot condition one has to additionally specify the type of distance. A distance may be GLOBAL, i.e. counted from the leftmost interface, or LOCAL, i.e. counted from the interface to the left of the region whose name you will be prompted for.

NAME OF REGION

Give the name of the region within which the distance is measured.

AT UPPER INTERFACE OF REGION

Give the name of the region which upper interface is specified for the TIE_LINE plotting. This plot-condition allows you to plot a certain quantity from both sides of an interface. The typical application is for plotting tie-lines.

`UPPER OR LOWER INTERFACE OF REGION ....`

Specify if the condition is at the LOWER or UPPER interface of a region. The LOWER interface is placed on the left side of a region and the UPPER interface on its right side.

`VALUE(S)`

Supply up to 15 numerical values separated by commas or spaces for the condition set. If plot condition TIME was chosen FIRST, LAST or #n (where n is an integer number) may be specified. "#?" provides a list of time steps.

SET_PLOT_FORMAT

Description: With this command the user can adjust the format of the graphical output to different graphical devices. Usually the default device is a Tektronix-4010 terminal. This default may be altered with the SET_PLOT_ENVIRONMENT command in the SYSTEM MONITOR or by your TC.INI file, see separate documentation.

Syntax: SET_PLOT_FORMAT

Prompt: `Graphic Device number`

Depending on the available hardware different plot formats may be available. These are listed on-line with a ?. With some formats there can be additional sub-prompts asking for e.g. font type and size.

SET_PLOT_OPTIONS

Description: You will be prompted for and may toggle on/off the plotting some option on your diagram.

Syntax: SET_PLOT_OPTIONS

Prompt: `PLOT HEADER`

Toggle the plot of the DICTRA-header text above the diagram.

`PLOT LOGO`

Toggle the plot of the DICTRA logotype at lower-left corner of the diagram.

`PLOT FOOTER`

Toggle the plot of the footer identifier text (only on postscript devices).

`WHITE COUNTOURED PS CHARS`

Toggle the option of having a thin white contour around postscript

characters (only on postscript devices).

PLOT REMOTE EXPONENTS

Toggle the plot of the remote exponents on the axis.

PLOT CELL#

Toggle the plot of the cell number text at the upper-right corner of the diagram.

PLOT-CONDITION STATUS

Toggle the plot of the plot-condition status line above the diagram.

SET_PLOT_SIZE

Description: The user can change the size of the diagram by specifying a relative scale factor. The default value of the scaling factor depends on what output device the user has chosen by the SET_PLOT_FORMAT command. The default plot size is adjusted to the chosen device.

Syntax: SET_PLOT_SIZE

Prompt: RELATIVE PLOT SIZE

Enter the relative scaling factor.

SET_PREFIX_SCALING

Description: When prefix scaling is enabled the remote exponent for an axis is automatically chosen to have a value which is a multiple of three, i.e. ..., -6, -3, 0, 3, 6, ...

Syntax: SET_PREFIX_SCALING

Prompt: AXIS (X OR Y)

The use must specify X or Y axis.

USE PREFIX SCALING

Enables or disables prefix scaling by giving YES or NO.

Give an integer value to select a prefix power of your own.

SET_RASTER_STATUS

Description: It is possible to have a raster plotted in the diagram. Default status is no raster plotted.

Syntax: SET_RASTER_STATUS <YES/NO>

Prompt: RASTER PLOT

Enables or disables the raster plot.

SET_SCALING_STATUS

Description: The user can choose between manual or automatic scaling on a specified axis. If manual scaling is chosen the user must specify a minimum and a maximum value. Manual scaling can be used to magnify interesting parts of a diagram. When an axis variable is selected by the SET_DIAGRAM_AXIS command the scaling status for the axis is always set to automatic scaling.

Syntax: SET_SCALING_STATUS

Prompt: AXIS(X, Y OR Z)

Specify for what axis you want to set the scaling status.

AUTOMATIC SCALING (Y OR N)

You can chose between automatic(Y) and manual(N) scaling.

MIN VALUE

If manual scaling was chosen you must specify the value of the starting point of the specified axis.

MAX VALUE

If manual scaling was chosen you must specify the value of the end point of the specified axis.

SET_TIC_TYPE

Description: You may alter the size of the tic marks as well as their placement on the axis, inside or outside.

Syntax: SET_TIC_TYPE

Prompt: TIC TYPE

Tic markes may be placed on either the inside or the outside of the diagram axis. The absolute value of TIC TYPE determines their length.

- TIC TYPE > 0 ➔ tic marks on the outside of the axis
- TIC TYPE < 0 ➔ tic marks on the inside of the axis

SET_TITLE

Description: The user can specify a title that will appear on all listings and diagrams from the POST PROCESSOR.

Syntax: SET_TITLE

Prompt: TITLE

Enter the title you want to appear on all output. Note that there is a maximum length of about 60 characters.

SET_TRUE_MANUAL_SCALING

Description: The tickmarks on the axis are normally placed in even intervals using the whole axis length. The scaling routine adjusts the given minimum and maximum values slightly to accomplish this. If this behavior is unwanted it can be avoided by using this command. The command works like a toggle. To reset the scaling behavior just repeat the command a second time.

Syntax: SET_TRUE_MANUAL_SCALING

Prompt: AXIS (X or Y)

Specify for what axis you want to toggle between automatic adjustment or avoiding the adjustment of the given maximum and minimum values.

4 Appendix 1: A brief introduction to DATAPLOT

A DATAPLOT file may be divided into two different sections. The prologue section, which contains directives for manipulating the default settings on the diagram layout, and the dataset section, which contains the actual data and possibly any text that is to be plotted in the diagram. The sections may contain multiple PROLOGUE and DATASET statements, respectively.

All prologues *must* be placed before the first DATASET statement.

The below presented syntax must be used for the DATAPLOT file. For a more complete reference, see the *DATAPLOT User's Guide and Examples.*

In general, each line in a DATAPLOT file must consist of a legal keyword plus its parameters or an XY coordinate pair.

An XY coordinate pair is two real numbers and an optional graphical operation code (GOC).

Legal keywords for prologues are:

Keyword	Parameters
PROLOGUE	inumb text
XSCALE	min max
YSCALE	min max
XTEXT	text
YTEXT	text
XTYPE	LIN, LOG or INV
YTYPE	LIN, LOG or INV
XLENGTH	rnumb
YLENGTH	rnumb
DIAGRAM_TYPE	TRIANGULAR or SQUARE
TIC_TYPE	rnumb
TITLE	text

Legal keywords for datasets are:

Keyword	Parameters
DATASET	inumb text
FONT	inumb
CHARSIZE	rnumb
COLOR	inumb
GLOBALSIZE	rnumb
LFSIZE	rnumb
LINETYPE	inumb
BLOCK GOC=C3,DEFGOC; X=C1+273.15; Y=LOG10(C2);	Select one X and one Y variable

BLOCK GOC=C3,DWR; X1=C1+273.15; X2=C1; Y=C1+C2*4.184;	or multiple X and one Y variable
BLOCK GOC=C4,MWAS; X=C1+273.15; Y1=C2*4.184; Y2=C3;	or one X and multiple Y variables
BLOCK GOC=C5,DWA; X1=C1; X2=C4; Y1=C2*4.184; Y2=C3;	or multiple XY pairs
BLOCKEND	
DRAWLINE	x,y x,y ...
TEXT	text or ~name (of a string, see below) If output to a PostScript device and the postscript hardcopy fonts are used, most LTEXT codes will work in text string. Consult your LTEXT or DATAPLOT manual about such codes.
ATTRIBUTE	TOP, CENTER or BOTTOM
STRING	name text The text string may contain text formatting codes namely:^S# to set font size, ^G for greek font, ^F# to set font type, ^U# for positioning the text upwards, ^D# for positioning the text downwards, ^R#for positioning the text to the right, ^L# for positioning the text to the left, and finally ^N for printing without updating current position to the end of the character. These text formatting codes only work for soft fonts not hardcopy postscript fonts.
INCLUDE	filename
CLIP	ON or OFF
SYMBOLSIZE	rnumb
FUNCTION Y=203(X); or X=203(Y);	<start end steps GOC> The < > denotes an optional parameter.
PAINT	<code> <video> <mode> The <> denotes optional parameters.

	Paint the area enclosed by the current path in the current pattern. The current path starts at the last 'moveto' given and includes all subsequent 'draws'. See also PCFUNCTION below. Default is <code>=0, <video>=NORMAL and <mode>=TRANSPARENT. To set a new current pattern supply any or all of the optional parameters. <code> is a single letter 0-9, A-Z or a-t (if <code>=t supply also a number in the range 0.00 - 1.00, e.g. PAINT t 0.25.) <video> is a string reading NORMAL or INVERSE. <mode> is a string reading TRANSPARENT or OPAQUE.
PCFUNCTION Y=203(X); or X=203(Y);	<start end steps GOC> The <> denotes an optional parameter. May be used to add a function to the current path.

The following are the legal GOCs:

W	World coordinates (* DEFAULT)
V	Virtual coordinates
N	Normalized plotbox coordinates (NPC)
M	Move to this XY (*)
D	Draw to this XY
A	XY is absolute values (*)
R	XY are relative values
S	Plot current symbol at XY
B	Apply soft spines on the drawn curve (use only on BLOCK data)
S2	Change current symbol to 2 and plot at XY
'	Plot the following text at XY

Examples:

```
700 2.54
50 1.91 WRDS
1.1 0.9 NS3
100 20'This is a text
BLOCK GOC=C3,MWAS; X=C1+273.15; Y=C2*4.184;
600 -1400 S1'text
700 -1500
BLOCKEND
```

5 Appendix 2: State, integral and auxiliary variables

5.1 State variables

The numerical values of some state variables, e.g. activity, chemical potential, and the Energetic Extensive properties, are given relative to some reference state which has been defined in the thermodynamic database file. Sometimes the user may have specified a reference state of his own, using SET_REFERENCE_STATE. To get numerical values relative to the user defined reference state, append an R to the mnemonic names as defined below.

5.1.1 Intensive properties

Mnemonic	Description
T	temperature
P	pressure
AC(component)	activity
MU(component)	chemical potential

5.1.2 Extensive properties

NORMALIZATION of extensive properties: For all extensive properties a suffix can be added to the mnemonic name to indicate a normalized extensive property.

Mnemonic	Description
Extensive property `Z at each grid point:	
Z	ext. prop. `Z at each grid point.
ZM	ext. prop. `Z per moles of atoms.
ZW	ext. prop. `Z per mass (gram).
ZV	ext. prop. `Z per volume (m3).
Extensive property `Z for a phase at each grid point:	
Z	ext. prop. `Z for the current amount of the phase.
ZM	ext. prop. `Z per mole of atoms of the phase.
ZW	ext. prop. `Z per mass (gram) of the phase.
ZV	ext. prop. `Z per volume (m3) of the phase.
ZF	ext. prop. `Z per mole formula unit of the phase.
Energetic Extensive properties (note: suffixes M, W, V and F can be applied)	
S	entropy
S(phase)	entropy of a phase
V	volume
V(phase)	volume of a phase
G	Gibbs energy

G(phase)	Gibbs energy of a phase
H	enthalpy
H(phase)	enthalpy of a phase
A	Helmholtz energy
A(phase)	Helmholtz energy of a phase
Amount of components (note: suffixes M, W and V can be applied)	
N(component)	Number of moles of a component.
N(phase,component)	Number of moles of a component in a phase.
B(component)	Mass of a component.
B(phase,component)	Mass of a component in a phase.
N	Number of moles
B	Mass (Note that the combination BW is not very interesting as it will always be unity. BV is the density.)
Amount of a phase (note: suffixes M, W and V can be applied) The normalizing properties are calculated at each grid point.	
NP(phase)	Number of moles of a phase.
BP(phase)	Mass of a phase.
VP(phase)	Volume of a phase.
Constitution	
Y(phase,species#sublattice)	site fraction (this quantity is dependent upon the model chosen for the phase)

5.2 Integral variables

The variable mnemonics are constructed in the following way. The first letter is always I for INTEGRAL VARIABLE. The second letter specifies quantity.

Class	Quantity	Description
I	N	for number of moles
I	W	for mass
I	V	for volume
I	U	for number of moles of volume-contributing elements
II	S	for entropy
II	H	for enthalpy
II	G	for Gibbs energy
II	A	for Helmholtz energy

Third letter is OPTIONAL and specifies the normalizing quantity,

Quantity	Description
N	for total number of moles in system
W	for total mass of system

V	for total volume of system
U	for total number of moles of volume-contributing elements in system

Integral quantities of CLASS=I may take 0-3 arguments.

The arguments MUST be given in 'falling' order of significance.

1 Region name
2 Phase name
3 Component name

Integral quantities of CLASS=II may take 0-2 arguments.

The arguments MUST be given in 'falling' order of significance.

1 Region name
2 Phase name

Examples:

- IW(PEARLITE,BCC,CR) is the mass of CR in the BCC phase in region PEARLITE.
- IW(PEARLITE,BCC) is the mass of BCC phase in region PEARLITE. IW is the total mass in the system.

5.3 Auxiliary variables

The following table lists auxiliary variables that are associated with both names and mnemonics.

Interface names are the same as the region names with the addition that you also have to specify if the interface is at the U(pper) or L(ower) end of the regions.

Name	Mnemonic	Argument
ACTIVITY	AC(component)	component
DISTANCE		
FLUX	JV(component)	component
LAMELLAR-SPACING	LS(name)	region name
LAMELLAR-THICKNESS	LT(name)	phase name
MOLE-FRACTION	X(component)	component
MOLE-PERCENT		component
POSITION-OF-INTERFACE	POI(name,U/L)up*)	interface name
TEMPERATURE-KELVIN	T	
TEMPERATURE-CELSIUS -	-	
U-FRACTION	UF(component)	component
VELOCITY-OF-INTERFACE	VOI(name,U/L)up*)	interface name

WEIGHT-FRACTION	W(component)	component
WEIGHT-PERCENT		component

There are also auxiliary variables that are only associated with a mnemonic.

Mnemonic	Description
GD	global distance
LD	local distance
M(phase,J)	mobility coefficient where J=diffusing specie
LOGM(phase,J)	^{10}log of the mobility coefficient
DT(phase,J)	tracer diffusion coefficient where J=diffusing specie
LOGDT(phase,J)	10log of the tracer diffusion coefficient
DC(phase,J,K,N)	chemical diffusion coefficient where K=gradient specie, and N=reference specie
LOGDC(phase,J,K,N)	10log of chemical diffusion coefficient
DI(phase,J,K,N)	intrinsic diffusion coefficient
LOGDI(phase,J,K)	^{10}log of intrinsic diffusion coefficient
JV(phase and/or specie)	flux in volume fixed frame of reference
JL(phase and/or specie)	flux in lattice fixed frame of reference
QC(phase,J,K,N)	Q=R(ln (DC{T1}) - ln (DC{ T1+e}))/(1/(T1+e) - 1/ T1)
QT(phase,J)	Q=R(ln (DT{T1}) - ln (DT{T1+e}))/(1/(T1+e) - 1/ T1)
QI(phase,J,K,N)	Q=R(ln (DI{T1}) - ln (DI{T1+e}))/(1/(T1+e) - 1/T1)
FC(phase,J,K,N)	D0=exp(ln (DC{T1})+Q/R/ T1)
FT(phase,J)	D0=exp(ln (DT{T1})+Q/R/T1)
FI(phase,J,K,N)	D0=exp(ln (DI{T1})+Q/R/T1)