



DICTRA Command Reference

Version 2015b



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2 Introduction to the DICTRA Commands

This guide is for users of DICTRA in the Thermo-Calc software package. It describes the function and syntax of the commands available in DICTRA and the POST module of the DICTRA program.

See [General Commands](#) for a list of common commands, and [DICTRA Commands](#) and [POST PROCESSOR Commands](#) for DICTRA-specific commands listed in alphabetical order. Other commands are described in the Thermo-Calc Console Command Reference. You can find the guide on the Thermo-Calc website <http://www.thermocalc.com/support/documentation/>

There are also two sections with information [About DATAPLOT Files](#) and [State, Integral and Auxiliary Variables](#).



These topics are discussed in this section:

- [Typographical Conventions](#)
- [Help Resources](#)
- [General Commands](#)

2.1 Typographical Conventions

The following conventions are used throughout the documentation:

<i>Convention</i>	<i>Definition</i>
Forward arrow →	The forward arrow → instructs you to select a series of menu items in a specific order. For example, Tools → Options is equivalent to: From the Tools menu, select Options .
Boldface font	A boldface font indicates that the given word(s) are shown that way in on a toolbar button or as a menu selection. For example, if you are told to select a menu item in a particular order, such as Tools → Options , or to click Save .
<i>Italic font</i>	An <i>italic</i> font indicates the introduction of important terminology. Expect to find an explanation in the same paragraph or elsewhere in the guide.
COMMAND	This font and all capital letters indicates that this is a COMMAND used in the Console Mode terminal.
HELP	Text in blue and underline is a link to another section. In this document commands are also sections. Clicking this link will take you to more detail about a particular command.
PROMPT	The ALL CAPS CODE FONT indicates this is a prompt on the terminal asking for input or an option presented on the terminal after a command is entered.
<Enter>	Text with <angle brackets> indicates a keyboard entry. Usually to press Enter (or Return).
SYNTAX	SMALL ALL CAPITALS indicates this is the family of commands, the principles for the information that follows.

<i>Convention</i>	<i>Definition</i>
code and code bold	A code font shows a programming code or code example. The code bold font highlights the entry.
Note	 The information can be of use to you. It is recommended that you read the text or follow the link to more information.
Examples	 Go to the example collection to learn more.

2.2 Help Resources

Online Help

- To access online help, open Thermo-Calc and select **Help → Online Help**.

In Console Mode at the command line prompt, you can access help in these ways:

- For a list of all the available commands in the current module, at the prompt type a question mark (?) and press <Enter>.
- For a description of a specific command, type `Help` followed by the name of the command. You can only get online help about a command related to the current module you are in.
- For general system information type `Information`. Specify the subject or type ? and the available subjects are listed. This subject list is specific to the current module.

PDFs

- On [Thermo-Calc Software's website](http://www.thermocalc.com).
- Wherever the software is installed, folders containing the PDFs versions of the documentation are also downloaded. See the *Thermo-Calc Installation Guide* for details of where these are installed for your operating system.

2.3 General Commands

These commands are universal in the Console Mode for both Thermo-Calc and DICTRA. For convenience they are repeated here.

Other commands are described in the Thermo-Calc Console Command Reference. You can find the guide on the Thermo-Calc website

<http://www.thermocalc.com/support/documentation/>

Command/Syntax	Description and Prompts
BACK	Return to the previous module. From the POST-processor you go back to the DICTRA-MONITOR module.
EXIT	Terminates the program and returns to the operating system. Unless a SAVE_WORKSPACES command has been given before all data entered is lost.
GOTO_MODULE	MODULE NAME Select and go to another module. The name of the module must be given. In order to obtain a list of available modules give a return.

Command/Syntax	Description and Prompts
HELP <COMMAND> ?	<p data-bbox="639 248 1316 353">Enter HELP or ? to either a list of all commands or specific help for a command by giving the command (abbreviated)</p> <p data-bbox="639 371 778 400">COMMAND</p> <p data-bbox="639 423 1302 528">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.</p>

3 DICTRA Commands

- [AMEND_CELL_DISTRIBUTION](#)
- [AMEND_MOBILITY_DATA](#)
- [CHECK_DIFFUSION_MATRIX](#)
- [COARSENING_MODEL](#)
- [CREATE_NEW_CELL](#)
- [DEBUGGING](#)
- [DELETE_REGION](#)
- [ENTER_COMPOSITIONS](#)
- [ENTER_ENHANCEMENT_FACTOR](#)
- [ENTER_GEOMETRICAL_EXPONENT](#)
- [ENTER_GRID_COORDINATES](#)
- [ENTER_HEAT_TRANSFER_PARAMETER](#)
- [ENTER_HOMOGENIZATION_FUN](#)
- [ENTER_INTERFACE_MOBILITY](#)
- [ENTER_LABYRINTH_FUNCTION](#)
- [ENTER_MOBILITY_DATA](#)
- [ENTER_MOBILITY_ESTIMATE](#)
- [ENTER_PHASE_IN_REGION](#)
- [ENTER_REGION](#)
- [GB_MODEL](#)
- [HOMOGENIZATION_MODEL](#)
- [INPUT_SCHEIL_PROFILE](#)
- [LIST_CONDITIONS](#)
- [LIST_MOBILITY_DATA](#)
- [LIST_MOBILITY_ESTIMATES](#)
- [LIST_PROFILES](#)
- [LIST_REGION](#)
- [LIST_TIMESTEPS](#)
- [MACRO_FILE_OPEN](#)
- [PARA_EQUILIBRIUM_MODEL](#)
- [POLY_COMMAND](#)
- [POST_PROCESSOR](#)
- [READ_WORKSPACES](#)
- [SAVE_WORKSPACES](#)
- [SELECT_CELL](#)
- [SELECT_TIMESTEP](#)
- [SET_ACCURACY](#)
- [SET_ALL_START_VALUES](#)
- [SET_CONDITION](#)
- [SET_FIRST_INTERFACE](#)
- [SET_INITIAL_TEMPERATURE](#)
- [SET_INTERACTIVE](#)
- [SET_NUMERICAL_LIMITS](#)
- [SET_REFERENCE_STATE](#)
- [SET_SIMULATION_CONDITION](#)
- [SET_SIMULATION_TIME](#)
- [SET_SURFACE_TENSION](#)
- [SIMULATE_REACTION](#)
- [STORE_HOMOGENIZATION_DATA](#)
- [SWITCH_MODEL](#)
- [UTILITIES_HOMOGENIZATION](#)

3.1 AMEND_CELL_DISTRIBUTION

Use this to amend the cell distribution factor of the currently selected cell.

Syntax	AMEND_CELL_DISTRIBUTION
Prompt	CELL DISTRIBUTION FACTOR /4.446590813-323/ A parameter that determines the weight of the cell, it can be used to simulate a distribution of different cell sizes.

3.2 AMEND_MOBILITY_DATA

Change the mobility data. See [ENTER_MOBILITY_DATA](#) for information about the parameter names and prompts.

Syntax	AMEND_MOBILITY_DATA
Prompt	PARAMETER NAME <IDENTIFIER> (<PHASE>, <COMPONENT ARRAY>; <DIGIT>) Enter ? to get an overview

3.3 CHECK_DIFFUSION_MATRIX

Display the diffusion coefficient matrix for a phase at a given composition, pressure and temperature.

Syntax	CHECK_DIFFUSION_MATRIX
Prompt	OUTPUT TO SCREEN OR FILE /SCREEN/ 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. Use one or several of DLPBMXOE: <ul style="list-style-type: none"> • 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

3.4 COARSENING_MODEL

Enable or disable the use of the simplified model for calculating Ostwald-ripening in multicomponent systems. This must be used together with the SET_SURFACE_TENSION command.

The model is based on LSW theory (after Lifshitz and Slyozov *Chem Solids* 19(1961) p. 35 and Wagner *Z Elektrochemie* 65 (1961) p. 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) p. 867.

LSW theory is strictly only valid for low volume fractions of the particle phase. The theory predicts that the normalized particle size distribution obtains 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 is such that both the maximum size particle as well as the matrix phase grows.



For another example of coarsening, search the online help for *Property Model Calculator* in the *Thermo-Calc User Guide*.

Syntax	COARSENING_MODEL
Prompt	ENABLE COARSENING MODEL /N/ The default is N. Enter Y to enable the use of this model.

3.5 CREATE_NEW_CELL

Create a new cell and attach it to the list of existing cells.

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.

3.6 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.

Syntax	DEBUGGING
Prompt	DEBUG LEVEL (YES,NO,0,1,2,3,4) /NO/ The level of debugging information to be displayed.

3.7 DELETE_REGION

Delete a region and all its associated data from the current cell.

Syntax	DELETE_REGION
Prompt	REGION NAME The region name to delete.

3.8 ENTER_COMPOSITIONS

Enter 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 automatically calculates 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 only queries for the compositions of the independent species. <input checked="" type="checkbox"/> Sometimes the dependent species is chosen by the program and thus this question is never given. This may be 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 only queries for the compositions of the independent species. <input checked="" type="checkbox"/> 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. Options are: <ul style="list-style-type: none"> • SITE_FRACTION

	<ul style="list-style-type: none"> • MOLE_FRACTION • MOLE_PERCENT • WEIGHT_FRACTION • WEIGHT_PERCENT • U_FRACTION <p>TYPE</p> <p>Type of composition profile to be entered, options are:</p> <ul style="list-style-type: none"> • LINEAR • READ_POINT_BY_POINT • FUNCTION • GEOMETRIC <p>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 $hs(X)$.</p> <p>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 $1e-4m=100\mu m$.</p> <p>VALUE OF FIRST POINT</p> <p>Composition in the first gridpoint. Values in between are interpolated linearly if a LINEAR type of profile is specified.</p> <p>VALUE OF LAST POINT</p> <p>Composition for the last gridpoint. Values in between are interpolated linearly if a LINEAR type of profile is specified.</p> <p>INPUT FILE</p> <p>The input source from which to read the points when entering values point by point, default is TERMINAL.</p> <p>VALUE OF POINT</p> <p>The value of the point when entering values point by point.</p> <p>VALUE OF R IN THE GEOMETRICAL SERIE</p> <p>Use the same geometrical factor as for the geometrical grid.</p> <p>VOLUME FRACTION OF</p> <p>Initial volume fraction of a spheroid phase.</p>
--	---

3.9 ENTER_ENHANCEMENT_FACTOR

Change 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
Prompt	MOBILITY ENHANCEMENT FACTOR FOR PHASE

3.10 ENTER_GEOMETRICAL_EXPONENT


Enter the geometrical exponent which defines the geometry of the system. The program handles one-dimensional geometries defined by the geometrical exponent. These geometries are:

- Planar. This corresponds to an infinitely wide plate of a certain thickness.
- Cylindrical. This corresponds to an infinitely long cylinder of a certain radius.
- Spherical. Sphere with a certain radius.

Syntax	ENTER_GEOMETRICAL_EXPONENT
Prompt	GEOMETRICAL EXPONENT Enter an integer value between 0 and 2.

3.11 ENTER_GRID_COORDINATES

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 in a specific region may also be subdivided into several parts, where the type of each part is chosen independently, by first entering SUB_REGION as the overall grid type.

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.  The size of the region is specified in units compatible with those of the diffusion data.

Options	Description
TYPE of grid	<p>TYPE</p> <p>Type of grid to entered, options are:</p> <ul style="list-style-type: none"> • LINEAR: For an equally spaced grid. • READ_POINT_BY_POINT: Can be done either from the keyboard or from a predefined file. • GEOMETRIC: Yields 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. • DOUBLE_GEOMETRIC: Divides the region in two halves and generates a separate geometrical grid in each half. It gives a high number of gridpoints in the middle or at both ends of a region, two geometrical factors should be entered.

Options	Description
SUB_REGION	<p>If SUB_REGION is entered when you are prompted to enter the grid type, then the next prompt is</p> <p>END COORDINATE IN SUB REGION</p> <p>Enter a value equal to or less than the total width of the region. You are then prompted for the number of grid points and the grid type to be used between the left-hand side of the region and the end coordinate. As long as the end coordinate is less than the total width of the region you are prompted for an end coordinate and the grid to be used in the sub region starting at the end of the former sub region. Thus, progressively higher end coordinates must be entered and the final end coordinate must be equal to the total width of the region.</p>
	<p>NUMBER OF POINTS</p> <p>The number of points present in the region. Please consider the interspacing of the grid when determining the number of points.</p> <p>INPUT FILE</p> <p>The input source from which to read the points when entering values point by point, default is TERMINAL.</p> <p>VALUE OF POINT</p> <p>The value of the point when entering values point by point.</p> <p>VALUE OF R IN THE GEOMETRICAL SERIES</p> <p>Value in the geometrical factor in the series determining the distribution of the grid points. A geometrical factor larger than one yields a higher density of gridpoints at the lower end of the region and a factor is smaller than one yields a higher density of gridpoints at the upper end of the region.</p> <p>VALUE OF R IN THE GEOMETRICAL SERIE FOR LOWER PART OF REGION</p> <p>The geometrical factor in the series for the lower (left) part of a region in a double geometrical grid</p> <p>VALUE OF R IN THE GEOMETRICAL SERIE FOR UPPER PART OF REGION</p> <p>The geometrical factor in the series for the upper (right) part of a region in a double geometrical grid.</p>

3.12 ENTER_HEAT_TRANSFER_PARAMETER

A model for thermos-migration simulates the thermal induced diffusion in temperature gradients. This model requires that the temperature depends on the length coordinate in the system and that the quantity `heat of transport (Q*)`, is entered.

Syntax	ENTER_HEAT_TRANSFER_PARAMETER
Prompt	HEAT TRANSFER PARAMETER FOR PHASE

This parameter is entered separately for each component in each phase. The implementation and functionality of this model is described in Höglund, L. & Ågren, J. "Simulation of Carbon Diffusion in Steel Driven by a Temperature Gradient". *J. Phase Equilibria Diffus.* 31, 212–215 (2010).

3.13 ENTER_HOMOGENIZATION_FUN

Use this with the homogenization model for multiphase simulations. The homogenization model 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 determined by 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.

Homogenization Functions

Enter a digit between 1 and 14 (default is #5) to assign the homogenization function then follow the prompts. The homogenization functions are:

No.	Function name
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 Hashin, Z. & Shtrikman, S. "A Variational Approach to the Theory of the Effective Magnetic Permeability of Multiphase Materials". *J. Appl. Phys.* 33, 3125–3131 (1962).

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 parallel 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 produces a kinetic coefficient of zero. However, using homogenization function #9 the excluded phases are not considered when evaluating what phase has the most sluggish kinetics.

Syntax	ENTER_HOMOGENIZATION_FUN
Prompt	ENTER_HOMOGENIZATION_FUNCTION # /5/ Enter a digit between 1 and 14 (default is 5). The options corresponding to the numbers are listed above.


3.14 ENTER_INTERFACE_MOBILITY

Syntax	ENTER_INTERFACE_MOBILITY
Prompt	FUNCTION F (X, V, TIME, T) =

Enter a formula as a FORTRAN statement with the following rules:

- A variable must begin with a letter and a number with a number (not a dot).
- A real number must have a dot or an exponent (E).
- The operators +, -, *, /, ** (exponentiation) can be used and any level of parenthesis.
- SQRT(X) is the square root
- EXP(X) is the exponential
- LOG(X) is the natural logarithm
- LOG10(X) is the base 10 logarithm
- SIN(X), COS(X), ATAN(X)

- SIGN(X)
- ERF(X) is the error function

 These operators must be followed by a (. The statement must be terminated by a semicolon (;)

3.15 ENTER_LABYRINTH_FUNCTION

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.

Syntax	ENTER_LABYRINTH_FUNCTION
Prompt	REGION F (T, P, VOLFR, X) =

3.16 ENTER_MOBILITY_DATA

Enter mobility data. If a function is already defined it is deleted.

A valid parameter should have the general form of:

```
<IDENTIFIER> ( <PHASE NAME> , <COMPONENT ARRAY> ; <DIGIT> )
```

The `identifier` must be followed by an opening parenthesis, a phase name, a comma and a component array. Optionally, the component array can be followed by a semicolon and a digit. The parameter name is terminated by a closing parenthesis.

The following identifiers are legal:

- MQ (activation energy for mobility)
- MF (frequency factor for mobility)
- DQ (activation energy for diffusivity)
- DF (frequency factor for diffusivity)
- OQ (activation energy for mobility, ordered part)
- OF (frequency factor for mobility, ordered part).

The `phase name` must be followed by an & and directly following that the name of the diffusing specie.

The `component array` consists of a list of constituent names. Interaction parameters have two or more constituents separated by a comma. If the phase has sublattices at least one constituent in each sublattice must be specified. The constituents in different sublattices must be given in sublattice order and are separated by a colon.

After the component array a subindex `digit` can be specified after a semicolon. This digit must be in the range 0 to 9. The interpretation of the subindex depends on the excess model used for the phase. If no semicolon and digit is given the subindex value is assumed to be zero.

Examples of parameter names:

- MQ (FCC&C, Fe:Va) Mobility of C in fcc Fe with interstitials.
- MQ (FCC&C, Fe, Cr; 0) The regular parameter for Fe and Cr in fcc.
- MQ (FCC&C, Fe, Cr; 1) The subregular interaction parameter (Redlich-Kister model).

Syntax:	ENTER_MOBILITY_DATA
Prompt	<p>PARAMETER: <PARAMETER NAME></p> <p>As explained above, specify a correct and complete parameter name, which should contain all the necessary parts of the general form:</p> <p><IDENTIFIER> (<PHASE>, <COMPONENT ARRAY>; <DIGIT>)</p> <p>If a parameter name is not acceptable or <Enter>, is pressed, the error message displays:</p> <p>*** ERROR, PLEASE RE-ENTER EACH PART SEPARATELY</p>
Identifier	<p>IDENTIFIER /MQ/ <MQ, MF, DQ, DF, OQ, OF></p> <p>If this command is used one or more times, the previous value on this prompt is set as default. Press <Enter> for the same type identifier or specify a new type.</p>
Phase name	<p>PHASE NAME /FCC&C/</p> <p>Each parameter is valid for a specific phase. The name of that phase must be supplied. The name must not be abbreviated. The phase name must be followed by an '&' and directly following that, the name of the diffusion specie.</p>

3.17 ENTER_MOBILITY_ESTIMATE

Use this command to enter a constant mobility estimate for specific elements in specific phases. Also see [LIST_MOBILITY_ESTIMATES](#).

Syntax	ENTER_MOBILITY_ESTIMATE
Prompt	<p>MOBILITY ESTIMATE FOR PHASE</p> <p>Interactively enter a constant mobility estimate for specific elements in specific phases. This can be used to enter mobility estimates in phases for which there is no assessed data. Estimates entered here override database values.</p>

3.18 ENTER_PHASE_IN_REGION

Enter a phase into an earlier defined region.

Syntax	ENTER_PHASE_IN_REGION
Prompt	ACTIVE OR INACTIVE PHASE

	<p>Type of phase entered. An inactive phase is a phase which does not participate in the calculations until it is stable. This is done by regarding the driving force for precipitation of the phase in an equilibrium calculation. The program then automatically retransforms the inactive phase into an active one.</p> <p>REGION NAME</p> <p>Name of the region into which the phase is to be entered.</p> <p>PHASE TYPE</p> <p>Type of phase entered. Depending on your answer a selected variety of the below sub-prompts display. Legal types are:</p> <ul style="list-style-type: none"> • MATRIX • LAMELLAR • SPHEROID <p>If LAMELLAR is entered, see Lameller Prompts below.</p> <p>A SPHEROID type of phase requires that a MATRIX phase has been previously entered.</p> <p>PHASE NAME</p> <p>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.</p> <p>COMPOSITION SET</p> <p>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.</p> <p>ATTACH TO REGION NAMED</p> <p>Enter the name of the region onto which the inactive phase is to be attached.</p> <p>ATTACHED TO THE RIGHT OF</p> <p>Enter Y to attach the inactive phase on the right side of the region else, enter N to attach on the left side.</p> <p>REQUIRED DRIVING FORCE FOR PRECIPITATION</p> <p>The required driving force (evaluated as DGM (phase) in POLY-3) to be used for determining whether an inactive phase is stable.</p> <p>CONDITION TYPE</p> <p>Boundary condition used if the inactive phase becomes stable.</p>
--	---

3.18.1 Lameller Prompts

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

```
eutectoid reaction is "gamma" ==> "alpha" +
"beta"
```

This is to clarify what is meant with GAMMA, ALPHA and BETA in the specific sub-prompts that display as follows.

Subprompts for LAMELLER	<p>ENTER NAME OF "ALPHA" PHASE</p> <p>Enter the GES phase name for the ALPHA phase of the eutectic/eutectoid decomposition product.</p> <p>ENTER NAME OF "BETA" PHASE</p> <p>Enter the GES phase name for the BETA phase of the eutectic/eutectoid decomposition product.</p> <p>ENTER NAME OF "GAMMA" PHASE</p> <p>Enter the GES phase name for the GAMMA matrix phase.</p> <p>ENTER "ALPHA"/"BETA" SURFACE TENSION:</p> <p>Enter function for the surface tension between the ALPHA and BETA phases, $\sigma^{\alpha\beta}$</p> <p>ENTER "ALPHA"/"GAMMA" SURFACE TENSION:</p> <p>Enter function for the surface tension between the ALPHA and GAMMA phases, $\sigma^{\alpha\gamma}$</p> <p>ENTER "BETA"/"GAMMA" SURFACE TENSION:</p> <p>Enter function for the surface tension between the BETA and GAMMA phases, $\sigma^{\beta\gamma}$</p> <p>OPTIMUM GROWTH CONDITION FACTOR /2/:</p> <p>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.</p> <p>NAME OF DEPENDENT ELEMENT</p> <p>Enter the name of the substitutional element to consider as the dependent one.</p> <p>GROWTH MODEL (VOLUME/BOUNDARY/KIRKALDY) FOR ELEMENT X</p> <p>Select growth model to be used for element X. Choose between:</p> <ul style="list-style-type: none"> • Volume diffusion model • Boundary diffusion model • Kirkaldy's mixed mode diffusion model. Implies MIXED, see below. <p>DF (X) = /VALUE/AUTOMATIC/MIXED/TDB/</p> <p>Either input a numerical value on the pre-exponential factor DF or select one of the keywords:</p> <ul style="list-style-type: none"> • AUTOMATIC • MIXED • TDB
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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 "A revised expression for the diffusivity of carbon in binary Fe-C austenite". *Scr. Metall.* 20, 1507–1510 (1986) (volume diffusion of C in Austenite) and the boundary diffusion part due to J. Ågren "Computer simulations of the austenite/ferrite diffusional transformations in low alloyed steels" *Acta Metall.* 30, 841–851 (1982) (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 "On the Lamellar Growth of Eutectics and Eutectoids in Multicomponent Systems" *Trita-Mac R. Inst. Technol. Stock.* 478, 27 pages (1992). MIXED means a mixed mode calculation using an effective diffusion coefficient. Coefficient k' or k'' is 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 S_0 DETERMINATION /Y/:

Enter Y if you want automatic start values for the unknown parameters in the S_0 determination else enter N. S_0 is the critical lamellar spacing for which the growth rate is zero.

CRITICAL THICKNESS OF "ALPHA" LAMELLA:

If you answered N this prompt displays. The critical thickness of ALPHA is about 0.9 of S_0 , 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

	$S = 1.75 \cdot 10^{-5} (A_{1e} - T)^{-1}$ <p>The equation may be used as a start value approx. for alloyed steels. However, use the A_{1e} temperature of the steel.</p> <p>CRITICAL THICKNESS OF "BETA" LAMELLA:</p> <p>The critical thickness of BETA is about 0.1 of S_0, see above.</p> <p>AUTOMATIC START VALUES ON POTENTIALS /Y/:</p> <p>Enter Y if you want automatic start values for the unknown potentials.</p> <p>GIVE POTENTIALS FOR "ALPHA"/"GAMMA" EQUIL.</p> <p>If you answered N this prompt displays. Enter start values for the unknown potentials, MU, at the ALPHA/GAMMA phase boundary.</p> <p>GIVE POTENTIALS FOR "BETA"/"GAMMA" EQUIL.</p> <p>Enter start values for the unknown potentials, MU, at the BETA/GAMMA phase boundary.</p> <p>GROWTH RATE V:</p> <p>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:</p> $S = 8 \cdot 10^{-9} (A_{1e} - T)^2$ <p>The equation may be used as a start value approx. for alloyed steels. However, use the A_{1e} of the steel.</p> <p>AUTOMATIC START VALUES ON OTHER VARIABLES /Y/:</p> <p>Enter Y if you want automatic start values for the unknowns in the determination of the growth rate.</p> <p>FRACTION OF "ALPHA" PHASE:</p> <p>Enter a guess on the fraction of the ALPHA phase. For pearlite it is about 0.9.</p> <p>GIVE POTENTIALS FOR "ALPHA"/"GAMMA" EQUIL.</p> <p>Enter start values for the unknown potentials, MU, at the ALPHA/GAMMA phase boundary.</p> <p>GIVE POTENTIALS FOR "BETA"/"GAMMA" EQUIL.</p> <p>Enter start values for the unknown potentials, MU, at the BETA/GAMMA phase boundary.</p>
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3.19 ENTER_REGION

Enter a region into the system. Enter this before entering a grid or any phases.

Syntax	ENTER_REGION
Prompt	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.
--	---

3.20 GB_MODEL

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 contribute to the total amount of diffusion according to the weighted fractions.

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:

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

where

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

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

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

where

- δ : the grainboundary thickness (typical value $0.5 \cdot 10^{10}$)
- d : the grainsize as a function of time and temperature (typical value $25 \cdot 10^{-6}$)
- ρ : the dislocation density as a function of time and temperature
- b : burgersvector (typical value $1 \cdot 10^{-10}$)
- M^{bulk} : the mobility in the bulk (δ/d being the fraction of grain boundaries in the bulk and $\rho \cdot b^2$ being the fraction of dislocations in the bulk)

Syntax	GB_MODEL
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3.21 HOMOGENIZATION_MODEL

Enable or disable 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 does 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 implicitity can be chosen using the [SET SIMULATION CONDITION](#) command). Because of this, and other factors, homogenization model simulations generally run slower than other comparable DICTRA simulations.

Syntax	HOMOGENIZATION_MODEL
Prompt	<p>ENABLE HOMOGENIZATION</p> <p>Y to enable the homogenization model.</p> <p>USE DEFAULT SETTINGS</p> <p>Y to use default settings for the homogenization model. If N is entered these sub-prompts appear.</p> <p>ADD IDEAL FLUX CONTRIBUTION</p> <p>Enter Y or N. If yes is entered a 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.</p> <p>USE INTERPOLATION SCHEME</p> <p>Enter Y or N. The interpolation scheme may speed up simulations significantly. If yes is entered several sub-prompts appear:</p> <ul style="list-style-type: none"> • 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 is not 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. <p>USE GLOBAL MINIMIZATION</p>

	<p>Enter Y or N whether global minimization should be used in equilibrium calculations. In general, using global minimization significantly increases the CPU time for a given simulation, but there is also a significantly reduced risk for non-converged equilibrium calculations.</p> <p>REFRESH JACOBIAN EVERY ITERATION</p> <p>Entering Y increases computational demand for each iteration, but may in some cases improve convergence rate.</p> <p>DEFAULT GRID PARAMETER VALUES</p> <p>These settings only affect moving phase boundary simulations where the grid changes during the simulation. Entering 'no' causes the following sub-prompts to appear</p> <ul style="list-style-type: none"> • 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.
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3.22 INPUT_SCHEIL_PROFILE

 As per normal procedure, and before entering the DICTRA monitor, you need to read thermodynamic and kinetic data to use this command.

This command takes a previously calculated Scheil segregation profile and performs most of the setup needed to use that profile in a DICTRA simulation, for example a homogenizing heat treatment.

The command creates a region called SCHEIL_REGION. You then create a linear grid and enter the composition read from the file containing the segregation profile.

After issuing this command, you specify simulation time ([SET SIMULATION TIME](#)) and simulation temperature ([SET CONDITION](#), enter GLOBAL and variable T) to finalize setup.

 In order to limit the computational effort, this feature cannot be combined with the *fast diffusers* option in the Scheil module. Also search the online help and refer to the *DICTRA User Guide*, *Thermo-Calc User Guide* and *Thermo-Calc Console Mode Command Reference* for detailed information about Scheil simulations.

Syntax	INPUT_SCHEIL_PROFILE
Prompt	<p>ENTER FILE LOCATION OF SCHEIL SEGREGATION PROFILE</p> <p>In interactive mode (the command line), a file dialogue window opens. Navigate to the file containing the Scheil profile. Alternately, if you are working from a macro file, the line should contain the name of the file.</p> <p>ENTER WIDTH OF REGION</p> <p>Enter the width of the region [m] that contains the Scheil profile. This typically corresponds to the secondary dendrite arm spacing.</p> <p>ENTER MAIN SOLID SOLUTION PHASE</p> <p>Enter the name of one of the main solid solution phases. In the next prompt you can enter other phases that enter the simulation.</p> <p>SHOULD MORE PHASES BE ENTERED IN THE REGION</p> <p>Enter Y to enter more phases then enter the phase name as prompted next.</p> <p>ENTER PHASE NAME</p> <p>Enter the name of another phase that should be entered into the region.</p>

3.23 LIST_CONDITIONS

Lists the conditions set with the [SET_CONDITION](#) command.

Syntax	LIST_CONDITIONS
Prompt	<p>OUTPUT FILE</p> <p>File where the information is to be written.</p>

3.24 LIST_MOBILITY_DATA

Lists the mobility data from the database or entered interactively by the [ENTER_MOBILITY_DATA](#) command. This command does not work for encrypted databases.

Syntax	LIST_MOBILITY_DATA
Prompt	<p>OUTPUT FILE</p> <p>File where the information is to be written.</p>

3.25 LIST_MOBILITY_ESTIMATES

Lists the mobility estimate entered interactively by the [ENTER_MOBILITY_ESTIMATE](#) command.

Syntax	LIST_MOBILITY_ESTIMATES
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3.26 LIST_PROFILES

Lists the concentration profiles and grid coordinates in the cell.

Syntax	LIST_PROFILES
Prompt	<p>NAME OF REGION Name of region(s) in which the profiles are to be listed.</p> <p>OUTPUT FILE File where the information is to be written.</p> <p>COMPOSITION TYPE Composition type in which the profiles are to be written. Legal composition types are:</p> <ul style="list-style-type: none"> • SITE_FRACTION • MOLE_FRACTION • WEIGHT_FRACTION • U_FRACTION <p>COMPONENTS The output information may be limited to the specified components.</p> <p>CONSTITUENTS The output information may be limited to the specified constituents.</p>

3.27 LIST_REGION

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

Syntax	LIST_REGION
Prompt	<p>OUTPUT FILE File where the information is to be written.</p>

3.28 LIST_TIMESTEPS

List time steps in the workspace and those stored on file during a simulation. This for the DICTRA module.

Syntax	LIST_TIMESTEPS
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3.29 MACRO_FILE_OPEN

Use this to predefine sequences of commands on a file and then execute them with 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.

3.30 PARA_EQUILIBRIUM_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 these ways: AUTO, value%, -value and value.

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.

3.31 POLY_COMMAND

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.

3.32 POST_PROCESSOR

Gives control to the post processor which has its own command repertoire. See [POST PROCESSOR Commands](#).

Syntax	POST_PROCESSOR
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3.33 READ_WORKSPACES

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

Syntax	READ_WORKSPACES
Prompt	<p>FILE NAME</p> <p>Name of the file where the workspaces shall be read from. The default file extension is dic.</p>

3.34 SAVE_WORKSPACES

The workspaces in DICTRA, POLY-3 and GES5 are saved on a file. Return to the state before the SAVE command by entering a READ command. The SAVE command should normally be given before starting a simulation with [SIMULATE REACTION](#).

Syntax	SAVE_WORKSPACES
Prompt	<p>FILE NAME</p> <p>Name of the file where the workspaces shall be saved on.</p> <p>The default file extension is DIC.</p> <p>OVERWRITE CURRENT FILE CONTENT</p> <p>PROCEED WITH SAVE</p> <p>There is already a file with this name and if you answer Y the previous content is overwritten. If you have results from SIMULATE_REACTION these are lost when SAVE is used. You may append several results by the SIMULATE_REACTION command without destroying the previous results but SAVE erases them all.</p>

3.35 SELECT_CELL

Selects the current cell from the list of existing cells and enables you to enter and display data into that cell. This is a DICTRA command. Also see the POST PROCESSOR command of the same name, [SELECT_CELL](#).

Syntax	SELECT_CELL
Prompt	<p>NUMBER</p> <p>Specify the cell number by giving an integer or one of the key words NEXT or PREVIOUS.</p>

3.36 SELECT_TIMESTEP

Select a time step from those stored on file during a simulation. The profiles can be listed and simulation can be continued from this time step.

Syntax	SELECT_TIMESTEP
Prompt 33,	<p>TIMESTEP</p> <p>The time step to be selected, legal syntax is:</p> <ul style="list-style-type: none"> • FIRST • LAST • time • #nnn • #? <p>When selecting a time no interpolation is performed but the time step closest to the time entered is selected. #nnn can be obtained from the number given by LIST_TIMESTEPS or by typing #?.</p> <p>DELETE ALL OTHER TIMESTEPS</p> <p>Clears the current workspace from all other time steps except the one selected. This is necessary if the simulation is to be continued from this time step.</p>

3.37 SET_ACCURACY

Enter the accuracy requirements to use in the determination of the time step when using the automatic time step procedure. 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
Prompt	<p>MAX RELATIVE ERROR</p> <p>The maximum allowed relative error of the profile during one time step integration.</p> <p>MAX ABSOLUTE ERROR</p> <p>Maximum allowed absolute error of the profile during one time step integration. This parameter must be chosen with some relation to the smallest concentration in the profiles.</p>

3.38 SET_ALL_START_VALUES

Enter starting values for various quantities, such as velocities and potentials.

Syntax	SET_ALL_START_VALUES
Prompt	<p>START VALUE FOR VELOCITY OF INTERFACE</p> <p>A starting value for velocity at the named interface is required.</p> <p>START VALUE FOR POTENTIAL</p> <p>A starting value for a potential at the named interface is required. If an AUTOMATIC value is specified the program attempts to determine a starting value and also selects a suitable component for which the potential is varied.</p> <p>VARYING SPECIES IN INTERFACE</p> <p>The species which potential is treated as unknown.</p> <p>AUTOMATIC STARTING VALUES FOR PHASE COMPOSITIONS</p> <p>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.</p>

3.39 SET_CONDITION

Define conditions to reduce the degrees of freedom at equilibrium or defines the boundary conditions at the outer rims of the system. Use it 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.

DICTRA uses a constant molar volume, which is included in the flux, i.e. the unit of flux as entered in boundary conditions is:

$$\text{flux} * \text{molar volume} = \text{mol} * \text{m}^{-2} * \text{s}^{-1} * \text{m}^3 * \text{mol}^{-1} = \text{m} * \text{s}^{-1}$$

Syntax:	SET_CONDITION
Prompt:	<p>GLOBAL OR BOUNDARY CONDITION</p> <p>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.</p> <p>VARIABLE</p> <p>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.</p> <p>BOUNDARY</p>

Defines on which side of the system the boundary conditions are to be specified. Options 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 options 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.

Options 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:

$$J_k = f_k(T, P, TIME) * [ACTIVITY_k^N - g_k(T, P, TIME)]_{or}$$

$$J_k = f_k(T, P, TIME) * [POTENTIAL_k^N - g_k(T, P, TIME)]_{where f}$$

and g may be functions of time (TIME), temperature (T), and pressure (P), and N is an integer.



The activities are those with user defined reference states. The function f_k is the mass transfer coefficient, g_k is the activity of the corresponding species in the gas and N is a stoichiometric coefficient. For more details see L. Sproge and J. Ågren, "Experimental and theoretical studies of gas consumption in the gas carburizing process" *J. Heat Treat.* 6, 9–19 (1988).

- **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 is set to zero and the activity of others may be set to a prescribed value.
- **GAS:** The flux of selected components is 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

	<p>The lower time limit to be used when entering a time dependent function.</p> <p>HIGH TIME LIMIT</p> <p>The upper time limit to be used when entering a time dependent function. An asterisk * indicates the high limit as infinity.</p> <p>ANY MORE RANGES</p> <p>To specify whether any additional time dependent functions exists or not.</p> <p>TYPE OF CONDITION FOR COMPONENT</p> <p>The type of condition when setting a boundary condition of the type MIXED. Options are ZERO_FLUX and ACTIVITY.</p>
--	---

3.40 SET_FIRST_INTERFACE

Set the coordinate of the first interface in the cell, when a value other than zero is required, for instance when simulating diffusion through a tube wall or a hollow sphere. The default value is zero.

Syntax	SET_FIRST_INTERFACE
Prompt	<p>COORDINATE FOR FIRST INTERFACE</p> <p>The coordinate to which the first interface is to be set.</p>


3.41 SET_INITIAL_TEMPERATURE

Use this 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
Prompt	INITIAL TEMPERATURE /2000/

3.42 SET_INTERACTIVE

Useful in demonstration or macro files in order to stop the execution of the command file and pass over input focus to the keyboard.

 In the DICTRA POST_PROCESSOR this is called SET_INTERACTIVE_MODE but it is the same command.

Syntax	<p>SET_INTERACTIVE</p> <p>SET_INTERACTIVE_MODE</p>
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3.43 SET_NUMERICAL_LIMITS

Set parameters 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	<p>REQUIRED SUM OF SQUARES IN NS01A Required accuracy during the solution of the flux-balance equations.</p> <p>MAX NUMBER OF CALLS TO CALFUN OF NS01A The maximum number of iterations when solving the flux-balance equations. This number acts as a <i>safety valve</i>, a moderate choice is $10 * (\text{number_of_interfaces} * (\text{number_of_components} - 1))$ but use a larger value if necessary.</p> <p>STEP USED BY NS01A A user supplied parameter which is used to calculate the estimates of the partial derivatives numerically when solving the flux-balance equations.</p> <p>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 flux-balance equations.</p> <p>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.</p> <p>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.</p> <p>SMALLEST NUMBER USED IN SCALING FLUX EQUATIONS The flux-balance equations are scaled by the velocities calculated in the previous time step. 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.</p> <p>DEFAULT DRIVING FORCE FOR INACTIVE PHASES Sets the necessary driving force needed before an inactive phase is allowed to start to precipitate.</p>

3.44 SET_REFERENCE_STATE

The reference state for a component is important when using activities, chemical potentials and enthalpies and it 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. You can select the reference state of a component if the reference state in the database is not suitable.

Syntax	SET_REFERENCE_STATE
Prompt	<p>COMPONENT</p> <p>The name of the component must be given.</p> <p>REFERENCE STATE</p> <p>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.</p> <p>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 calculates the Gibbs energy of all possible states with the phase with the pure component at the current temperature and selects the most stable one.</p> <p>TEMPERATURE</p> <p>Select the temperature for the reference state. The value * means the temperature used for the calculation.</p> <p>PRESSURE</p> <p>Select the pressure for the reference state.</p>

3.45 SET_SIMULATION_CONDITION

Set parameters used to control output and certain parameters during the simulation.

Syntax	SET_SIMULATION_CONDITION
Prompt	<p>NS01A PRINT CONTROL</p> <p>Determines whether data should be printed about the iterative procedure to solve flux-balance equations. This parameter is normally set to 0 but can be set to 1 when difficulties with convergence occur. NS01A prints out the values used in the iterations and the residuals.</p> <p>FLUX CORRECTION FACTOR</p>

<p>This parameter controls if the flux correction scheme should be used in the calculations. The value should normally always be 1.</p> <p>NUMBER OF DELTA TIMESTEPS IN CALLING MULDIFF</p> <p>This parameter specifies the number of equally large time steps that one time step should be subdivided into.</p> <p>CHECK INTERFACE POSITION</p> <p>This parameter determines whether the time step is to be controlled by the phase interface displacement during the simulation.</p> <p>VARY POTENTIALS OR ACTIVITIES</p> <p>Determines whether the program should use the potential or the activity of a component in order to find the correct tie line 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.</p> <p>ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT</p> <p>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 time step.</p> <p>SAVE WORKSPACE ON FILE</p> <p>This parameter determines whether the workspaces are to be saved on file during the course of the simulation. Options are Y to always save on file, N to never save on file, or ## to save every n:th time on file (## is a integer value ranging from 0 to 99).</p> <p>DEGREE OF IMPLICITITY WHEN INTEGRATING PDES</p> <p>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).</p> <ul style="list-style-type: none"> • 0.0 Euler forwards • 0.5 Trapezoidal rule • 1.0 Euler backwards <p>MAX TIMESTEP CHANGE PER TIMESTEP</p> <p>Factor specifying the maximum increase in the time step taken from one time step to another. If 2 is given the maximum time step is twice as long as the previous time step taken.</p> <p>USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION</p> <p>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 Y, then these equilibrium calculations are performed using forced starting values in POLY_3.</p> <p>ALWAYS CALCULATE STIFFNES MATRIX IN MULDIFF</p>
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	<p>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 N, it is only calculated at the first iteration and a constant stiffness matrix is used to obtain the solution to the PDEs. This then leads to an implicit solution and therefore the degree of implicitly is automatically set to 1.</p>
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3.46 SET_SIMULATION_TIME

Enter the time specific conditions for a simulation.

Syntax	SET_SIMULATION_TIME
Prompt	<p>END TIME FOR INTEGRATION</p> <p>The time up to which the simulation is to be carried out.</p> <p>AUTOMATIC TIMESTEP CONTROL</p> <p>Determines whether the time step should be controlled by an automatic procedure or not. If you answer N you are prompted for the fixed time step to use during the simulation. The time step determined by the automatic time step control procedure is controlled by the parameters set by the command SET_ACCURACY.</p> <p>MAX TIMESTEP DURING INTEGRATION</p> <p>The maximum time step allowed during the simulation. This is required when using the automatic procedure to determine the time step.</p> <p>TIMESTEP DURING INTEGRATION</p> <p>Fixed time step used when the automatic time step procedure is disabled.</p> <p>INITIAL TIMESTEP</p> <p>Time step used as the initial time step.</p> <p>SMALLEST ACCEPTABLE TIMESTEP</p> <p>The smallest time step allowed during the simulation. This is required when using the automatic procedure to determine the time step.</p>

3.47 SET_SURFACE_TENSION

This command enters a distance- and velocity-dependent function which is added to the Gibbs energy of the phase at left side of each phase interface. This can then be used to emulate the effect of surface tension on the equilibrium between at the phase interface or limited phase mobility.

Enter a surface energy function which adds 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 substitutional atoms. This command is also used to simulate a limited interfacial mobility control where the energy function is a function of the interface velocity.

It is used to enter the surface energy to enable coarsening. However, it can also be used to simulate a case with a limited interfacial mobility.

This function should only be used in spherical geometries if the function is solely dependent of the interface position.

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, 1×10^{-5} (m³/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 M₆C as an example with surface tension 0.5 (J/m²) and molar volume of 0.71×10^{-5} (m³/mole), the entered function should be $2*0.5*0.71*(7/6)/X$;

Commonly the surface tension function is defined as:

$$\text{delta-G} = 2 * \text{SIGMA} * V_m / R$$

The function to be entered will then be:

$$2*\text{SIGMA}/X;$$

A limited interface mobility can be expressed as:

$$\text{delta-G} = v * V_m / \text{const}$$

The function to be entered is then:

$$v/"\text{const}";$$



The expression is multiplied by the partial molar volume of the substitutional components.

Syntax	SET_SURFACE_TENSION
Prompt	FUNCTION

3.48 SIMULATE_REACTION

Start the simulation. If given without any argument, you are prompted for certain values during simulations where phases appear or disappear.

Syntax	SIMULATE_REACTION
Prompt	<p>The command can also be given with the argument YES typed on the same line:</p> <p>SIMULATE_REACTION YES</p> <p>With the YES argument, default values are used during simulation and no user input can be given. This is especially useful when using DICTRA in batch mode.</p>

3.49 STORE_HOMOGENIZATION_DATA

Read/write the interpolation scheme data to file. The interpolation scheme is an option of the homogenization model that is used to speed up simulations. Use if this option can speed up simulations further.

Syntax	STORE_HOMOGENIZATION_DATA
Prompt	<p>STORE/READ HOMOGENIZATION MODEL INTERPOLATION DATA <Y/N></p> <p>Answering Y or N enables/disables read/write of interpolation scheme data to file.</p>

3.50 SWITCH_MODEL

Select the solver to be tried first and if only one solver should be used.

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

Syntax	SWITCH_MODEL
Prompt	<p>ENABLE AUTOMATIC SWITCH OF MODEL (Y/N)</p> <p>Determines if one or two solvers should be used.</p> <p>TRY CLASSIC FIRST (Y/N)</p> <p>Determines which of the two solvers should be tried first.</p> <p>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.</p> <ul style="list-style-type: none"> • HOMOGENIZATION_MODEL • ENTER_HOMOGENIZATION_FUNCTION • UTILITIES_HOMOGENIZATION <p>For some selections and set-ups only one of the two solvers is allowed.</p>


3.51 UTILITIES_HOMOGENIZATION

Use this with the homogenization model for the available utilities.

Syntax	UTILITIES_HOMOGENIZATION
Prompt	SET TEMPERATURE ACCORDING TO SOLIDUS TEMPERATURE

Set the global temperature such that it goes to a certain value $T_{\text{target}}=T_{\text{sol}}-X$, where X is an entered value. Also enter the rate by which the temperature approaches T_{target} . The solidus temperature is determined with a ± 1 K accuracy.

Input guesses of the minimum and maximum temperature to occur during the simulation. This utility can be useful to optimise homogenisation heat treatments.

 The liquid phase must be entered into the system.

DUMP RESULTS TO TEXT FILES

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

READ INITIAL COMPOSITION FROM TEXT FILE

Select Y 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 Y 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 is 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.

ENTER INACTIVE PHASES INTO ONE REGION

Select Y 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 Y 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

Save the average finite volume composition instead of a converted piece-wise linear composition.

SET CONSTANT PHASE ADDITION

Add constant Gibbs energy contributions to phases (in J/mol formula unit).

USE ELEMENT MOBILITY PREFACTOR

Enter constant factors which the mobilities of elements are multiplied with in all phases.

ENTER ELEMENT MOBILITY ESTIMATE

	<p>Interactively enter a constant mobility estimate for specific elements in specific phases. This can be used to enter mobility estimates in phases for which there is no assessed data. Estimates entered here override database values.</p> <p>ENTER MINIMUM SAVE INTERVAL</p> <p>Enter a minimum time interval (in seconds) that must pass between subsequent saved time-steps. This is useful in cases where a large number of small time-steps may occur in order to keep down the size of the result file.</p> <p>SIMPLIFIED EVALUATION OF ACTIVITY BOUNDARY CONDITION</p> <p>With this setting enabled the fluxes on boundaries are evaluated directly from the activity gradient, i.e. without taking into account the change of state on the boundary caused by the prescribed boundary activities.</p> <p>ENTER EXPLICIT LIMITS ON COMPOSITION</p> <p>Use this setting with caution to explicitly enter upper and lower limits on composition for all components (in mole fraction).</p> <p>ENTER CHEMICAL POTENTIAL CONTRIBUTION</p> <p>Enter a function (in valid poly-3 syntax) that is evaluated separately at all grid points and added to the chemical potential of all elements. The contribution affects the flux between grid points.</p> <p>DO NOT BALANCE EXTERNAL BOUNDARY FLUXES</p> <p>For all boundary conditions except type GAS, the flux of substitutional elements into the domain is balanced with the flux of the dependent substitutional elements such that the size of the domain is preserved. Enabling this setting disables the balancing of the substitutional fluxes.</p> <p>FIX EXTERNAL BOUNDARY FLUX OF DEPENDENT COMPONENT</p> <p>Enter a constant flux on the boundary of the dependent substitutional component. For all boundary conditions except type GAS, this flux is otherwise set to a value such that the net substitutional flux is zero.</p> <p>MODIFIED KINETICS ON BOUNDARY</p> <p>Use this to modify the kinetics on the boundary and enter a factor. If the factor is greater/smaller than one, the mobilities of all elements on the boundary is set equal to the maximum/minimum mobility of all elements times the factor. This can be useful in order to quickly saturate an outermost finite volume.</p>
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4 POST PROCESSOR Commands

- [Purpose and Methodology](#)
- [Plot Condition and Independent Variable](#)
- [APPEND EXPERIMENTAL DATA](#)
- [DETERMINE KIRK PLANE](#)
- [DIFFERENTIATE VALUES](#)
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- [SET RASTER STATUS](#)
- [SET SCALING STATUS](#)
- [SET TIC TYPE](#)
- [SET TITLE](#)
- [SET TRUE MANUAL SCALING](#)

4.1 Purpose and Methodology

The purpose of the POST PROCESSOR is to read and process data from the internal data structure of DICTRA in order to present the result of a simulation in either* GRAPHICAL (command [PLOT DIAGRAM](#)) or* TABULAR FORM (command [MAKE EXPERIMENTAL DATAFILE](#)).

Before plotting/printing, you have to specify what variables should be plotted on the diagram axis or printed in the table columns. For this purpose there is a command [SET DIAGRAM AXIS](#). After having SET both X- and Y-axis variables, you have to SET also plot condition and independent variable. It is also possible to specify a Z-axis. Its values appear as tick marks on the XY-curve.

4.2 Plot Condition and Independent Variable

There are two free variables after a simulation done by DICTRA. One is the simulation TIME, the other is a DISTANCE in the system.

In general, when plotting a diagram you MUST set either type as fixed, i.e. the *plot condition*, use command [SET PLOT CONDITION](#). The plot condition chosen is printed on a separate line above the diagram.

The other variable is then the independent variable, use command [SET INDEPENDENT VARIABLE](#). The independent variable is used as stepping variable. It varies along the calculated curve.

Legal plot conditions

- **TIME:** Integration time
- **DISTANCE:** Distance in system. It may be a GLOBAL distance counted from the rightmost interface of the system. Alternatively, it may be LOCAL. The distance is then counted from the LOWER interface of the specific region prompted for.
- **INTERFACE:** At a certain interface. An interface is identified by the NAME of the adjacent region, with the addition that you will be prompted to specify if the interface is at the upper or lower end of the region.
- **INTEGRAL:** Is automatically SET when using an INTEGRAL VARIABLE as axis variable.
- **TIE_LINE:** At a certain interface. Allows you to plot a certain quantity from both sides of an interface. The typical application is for plotting tie-lines.

Legal independent variables

- **TIME:** Integration time. Is automatically SET when using an INTEGRAL VARIABLE' or TIME as axis variable.
- **DISTANCE:** Space coordinate. It may be GLOBAL. It is then counted from the rightmost interface of the system. Alternatively, it may be LOCAL. The distance is then counted from the LOWER interface of the specific region prompted for.

4.3 APPEND_EXPERIMENTAL_DATA

Add experimental data and text on a calculated diagram. The experimental data and text are added to a file prepared according to the syntax of the DATAPLOT graphical language. The picture generated from the data is superimposed on the ordinary graphical output from the POST PROCESSOR. The experimental data file can be created with 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 dumps a calculated diagram on a file according to the DATAPLOT syntax. With the aid of a basic 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	<p>USE EXPERIMENTAL (Y OR N)</p> <p>Specify whether the data from an experimental data file should be included in the next plot. If N, no experimental data is plotted.</p> <p>EXPERIMENTAL DATAFILE</p> <p>Specify the name of the file with the experimental data. Default file extension is exp.</p>

	<p>PROLOGUE NUMBER</p> <p>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.</p> <p>DATASET NUMBER(S)</p> <p>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.</p> <p>For more information about DATAPLOT, see About DATAPLOT.</p>
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4.4 DETERMINE_KIRK_PLANE

To use this command a certain time must be set as plot condition. You are prompted for the position of a plane at time zero. The position of the plane at the plot condition time is then calculated. The difference in position is equal to the Kirkendall shift, i.e. how much an inert marker would drift in the material due to a net flux of vacancies.

Syntax	DETERMINE_KIRK_PLANE
Prompt	INITIAL ZERO PLANE /-1/

4.5 DIFFERENTIATE_VALUES

Differentiate the plotted curve.

Syntax	DIFFERENTIATE_VALUES
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4.6 DUMP_DIAGRAM


An alternative way to create plots. Supported graphical formats are PNG, BMP, PDF, JPEG and TIFF. The plot is saved to a file.

Syntax	DUMP_DIAGRAM
Prompt	<p>OUTPUT FORMAT (PNG, BMP, PDF, JPEG, TIFF)</p> <p>Specifies which graphical format to use.</p> <p>RESOLUTION (LOW, MEDIUM, HIGH)</p> <p>Specifies the resolution of the plot.</p>

4.7 ENTER_SYMBOL

Define a symbolic name to represent 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 to define quantities.

Syntax	ENTER_SYMBOL
Prompt	FUNCTION OR TABLE /FUNCTION/

	<p>Select what kind of symbol to enter.</p> <p>NAME</p> <p>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 =.</p> <p>FUNCTION</p> <p>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:</p> <ul style="list-style-type: none"> • <code>POI (CEM, U) -POI (CEM, L) ;</code> The thickness of the region named CEMENTITE • <code>AC (CR) /X (FCC, CR) ;</code> The activity coefficient for Cr in phase FCC • <code>SQRT (TIME) ;</code> The square root of the simulation time <p>&</p> <p>The ampersand & sub-prompt displays if the function was not terminated by a semicolon. It allows a 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.</p> <p>VARIABLE (S)</p> <p>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.</p> <p> The independent variable is always printed in the first column.</p>
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4.8 INFORMATION

Some general information about the POST PROCESSOR module is given.

Syntax	INFORMATION <SUBJECT>
Prompt	<p>WHICH SUBJECT</p> <p>Select which subject you want additional information about. Type ? to get a list of topics.</p> <ul style="list-style-type: none"> • PURPOSE • STATE VARIABLES • INTEGRAL VARIABLES

	<ul style="list-style-type: none"> • AUXILIARY VARIABLES • PLOT CONDITION AND INDEPENDENT VARIABLE • BASIC METHODOLOGY
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4.9 INTEGRATE_VALUES

Integrate the plotted curve.

Syntax	INTEGRATE_VALUES
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4.10 LABEL_CURVES

Create labels. Each label is explained with to the right of the diagram.

For example: 1. X: X(CR); Y: TIME; PC:3 is read as 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
Prompt	LABEL CURVES Select Y or N.


4.11 LIST_PLOT_SETTINGS

Lists the present values of most parameters specifying the type of diagram to be plotted.

Syntax	LIST_PLOT_SETTINGS
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4.12 LIST_REGION_NAMES

Lists all region names defined.

 All region names have a #-sign and the cell number appended.

Syntax	LIST_REGION_NAMES
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4.13 LIST_SYMBOLS

Lists a specific or all symbols defined.

Syntax	LIST_SYMBOLS
Prompt	NAME Give the name of a symbol or an asterisk * to list all defined symbols.

4.14 LIST_TIME_STEPS

Lists all integration time steps. This for the POST PROCESSOR module.

Syntax	LIST_TIME_STEPS
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4.15 MAKE_EXPERIMENTAL_DATAFILE

Save graphical information in a file with the DATAPLOT format (also see [APPEND_EXPERIMENTAL_DATA](#) and [About DATAPLOT Files](#)). To merge two or more diagrams from separate calculations, use this command to export it and add them together with a normal text editor.

Syntax	MAKE_EXPERIMENTAL_DATAFILE
Prompt	<p>OUTPUT FILE</p> <p>File where the graphical information is written. Default file extension is <code>exp</code>.</p>

4.16 PLOT_DIAGRAM

Plot graphical information on the specified device using the plot format set by [SET_PLOT_FORMAT](#).

Syntax	PLOT_DIAGRAM
Prompt	<p>PLOT FILE</p> <p>The name of the file or graphical device.</p>

4.17 PRINT_DIAGRAM

Print the diagram using the printers defined in Windows. It is only available for a Windows operating system.

Syntax	PRINT_DIAGRAM
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4.18 QUICK_EXPERIMENTAL_PLOT

Defines a pair of axes, 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 data file.

It 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. See [APPEND_EXPERIMENTAL_DATA](#) for information about the format of the data file.

Syntax	QUICK_EXPERIMENTAL_PLOT
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4.19 REINITIATE_PLOT_SETTINGS


All parameters describing the diagram are given as default values.

Syntax	REINITIATE_PLOT_SETTINGS
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4.20 SELECT_CELL

Select the cell data to be processed. You can only plot data from one cell at a time. Type ? to get a list of valid cell numbers. This is a POST PROCESSOR command. Also see the DICTRA command of the same name, [SELECT_CELL](#).

 The current cell number is displayed as a part of the POST PROCESSOR prompt.

Syntax	SELECT_CELL
Prompt	<p>NUMBER</p> <p>Number of the cell to be selected. Specify cell number by giving an integer or one of the key words NEXT or PREVIOUS.</p> <p>TABULATE</p> <p>Tabulate a named table.</p> <p> The independent variable is always printed in the first column.</p> <p>NAME</p> <p>Give the symbolic name of the table.</p> <p>OUTPUT FILE /SCREEN/</p> <p>Select output device/file. Press Enter to get output on the screen.</p>

4.21 SET_AXIS_LENGTH

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. 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	<p>AXIS</p> <p>Specify the axis to set the axis length.</p> <p>AXIS LENGTH</p> <p>Specify the relative axis length. The relative length 1 corresponds to 10 tic-marks on the axis.</p>

4.22 SET_AXIS_PLOT_STATUS

Specify to plot a diagram axis. Use it to merge different diagrams on a pen-plotter or to obtain the diagram faster. The default to plot the axes.

Syntax	SET_AXIS_PLOT_STATUS
Prompt	<p>AXIS PLOT</p> <p>Y or N to plot axis.</p>

4.23 SET_AXIS_TEXT_STATUS

Change the axis text from the automatic text given by the axis specification to another text.

Syntax	SET_AXIS_TEXT_STATUS
Prompt	<p>AXIS (X, Y OR Z)</p> <p>Specify which axis text status to change (if the axis type is INVERSE, X2 or Y2 may be used to set the corresponding opposite linear axis text).</p> <p>AUTOMATIC AXIS TEXT (Y OR N)</p> <p>Specify if automatic axis text is to be used or not.</p> <p>AXIS TEXT</p> <p>Enter axis text.</p>

4.24 SET_AXIS_TYPE

Select a linear, logarithmic or inverse axis.

Syntax	SET_AXIS_TYPE
Prompt	<p>AXIS (X, Y OR Z)</p> <p>Specify which axis to change the axis type.</p> <p>AXIS TYPE</p> <p>Specify which axis type to set. Select LINEAR (default), LOGARITHMIC or INVERSE. Only the three first characters are needed.</p>

4.25 SET_COLOR

On devices that support colors/(line types), select different colors/(line types) for:

- Text and axis Color
- Diagram Color
- DATAPLOT Color

Syntax	SET_COLOR
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4.26 SET_DIAGRAM_AXIS

Specify the axis variables of a plot. At least two axis variables (x and y) must be specified.

Syntax	SET_DIAGRAM_AXIS
Prompt	<p>AXIS (X, Y OR Z)</p> <p>Specifies the axis to set a variable.</p> <p>VARIABLE</p>

	<p>Specifies the variable to plot along this axis. A variable is specified by its mnemonic or name. The valid variable mnemonics and names are explained below. The variable types are:</p> <ul style="list-style-type: none"> • NONE: To clear an axis setting. • INTEGRAL VARIABLES: A quantity 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: Identified by a name which is entered with <code>ENTER FUNCTION</code>. Use the <code>LIST_SYMBOLS</code> command to get a list of valid function names. • AUXILIARY VARIABLES: As a complement to state variables and integral variables the auxiliary variables are defined. The variables can be called by their mnemonic names, which are shown in the rightmost column. These are useful in user-defined functions. • STATE VARIABLES: State variables in the POST module are similar to 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 is designed for a predefined set of state variables. <p>For more information about state variables, integral variables and auxiliary variables, see State, Integral and Auxiliary Variables.</p> <p>Depending on the axis variable some sub-prompts may be available.</p> <p><code>FOR COMPONENT</code></p> <p>When an activity, flux, mole-, weight- or U-fraction or percent is plotted the name of the component must be supplied.</p> <p><code>IN REGION</code></p> <p>When the lamellar spacing, e.g. for pearlite, is plotted the name of the region must be supplied.</p> <p><code>FOR PHASE</code></p> <p>When the lamellar thickness, e.g. for ferrite in pearlite, is plotted the name of the phase must be supplied.</p> <p><code>INTERFACE</code></p> <p>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.</p> <p><code>TYPE</code></p>
--	--

	<p>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 are prompted for.</p> <p>REGION NAME</p> <p>Name of the region wherein the local distance is measured.</p>
--	--

4.27 SET_DIAGRAM_TYPE

Set the diagram to a square (the default) or triangular plot (Gibbs triangle).

Syntax	SET_DIAGRAM_TYPE
Prompt	<p>TRIANGULAR DIAGRAM</p> <p>Select Y for a triangular plot.</p> <p>PLOT 3:RD AXIS</p> <p>For triangular plots is selected specify if a 3:rd axis, connecting the end points of the x- and y-axis is plotted.</p> <p>CLIP ALONG THE 3:RD AXIS</p> <p>Remove all lines outside the region limited by a line joining the end points of the X- and Y-axis.</p>

4.28 SET_FONT

Select the font to use 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	<p>SELECT FONTNUMBER</p> <p>Give the number for the font to select. Type ? to get an online list of the available fonts.</p> <p>FONT SIZE</p> <p>A value of 0.3 is recommended.</p>

4.29 SET_INDEPENDENT_VARIABLE

There are two free variables after a simulation is done in 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.



When plotting integral quantities TIME should be the independent variable.

Syntax	SET_INDEPENDENT_VARIABLE
Prompt	VARIABLE

	<p>Select which variable TIME (integration time) or DISTANCE (space coordinate) to treat as the independent variable</p> <p>TYPE</p> <p>When choosing distance as independent variable 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 are prompted for.</p> <p>NAME OF REGION</p> <p>For a LOCAL distance supply the name of the region within which the distance is measured. Type a ?, to get a list of valid region names.</p>
--	---

4.30 SET_PLOT_CONDITION

There are two free variables after a simulation is done in 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	<p>CONDITION</p> <p>Specify the type of condition to set. Valid conditions are:</p> <ul style="list-style-type: none"> • 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. <p>Depending on the condition some or none of these sub-prompts may display.</p> <p>INTERFACE</p> <p>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 ? to get a full list of relevant region names.</p> <p>TYPE</p>

	<p>When distance is chosen as plot condition 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 are prompted for.</p> <p>NAME OF REGION</p> <p>Give the name of the region within which the distance is measured.</p> <p>AT UPPER INTERFACE OF REGION</p> <p>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.</p> <p>UPPER OR LOWER INTERFACE OF REGION</p> <p>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.</p> <p>VALUE (S)</p> <p>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.</p>
--	---

4.31 SET_PLOT_FORMAT

Adjust the format of the graphical output to another graphical device. Usually the default device is a Tektronix-4010 terminal. This default can be changed with the SET_PLOT_ENVIRONMENT command in the SYSTEM MONITOR or by your TC.INI file, see separate documentation.

Syntax	SET_PLOT_FORMAT
Prompt	<p>GRAPHIC DEVICE NUMBER</p> <p>Depending on the available hardware different plot formats may be available. These are listed with a ?. With some formats there can be additional sub-prompts asking for e.g. font type and size.</p>

4.32 SET_PLOT_OPTIONS

Toggle on/off the plotting options on the diagram.

Syntax	SET_PLOT_OPTIONS
Prompt	<p>PLOT HEADER</p> <p>Toggle the plot of the DICTRA-header text above the diagram.</p> <p>PLOT LOGO</p> <p>Toggle the plot of the DICTRA logotype at lower-left corner of the diagram.</p> <p>PLOT FOOTER</p>

	<p>Toggle the plot of the footer identifier text (only on postscript devices).</p> <p>WHITE COUNTOURED PS CHARS</p> <p>Toggle the option of having a thin white contour around postscript characters (only on postscript devices).</p> <p>PLOT REMOTE EXPONENTS</p> <p>Toggle the plot of the remote exponents on the axis.</p> <p>PLOT CELL#</p> <p>Toggle the plot of the cell number text at the upper-right corner of the diagram.</p> <p>PLOT-CONDITION STATUS</p> <p>Toggle the plot of the plot-condition status line above the diagram.</p>
--	---

4.33 SET_PLOT_SIZE

Specify a relative scale factor to change the size of the diagram. The default value of the scaling factor depends on what output device is chosen by the [SET_PLOT_FORMAT](#) command. The default plot size is adjusted to the chosen device.

Syntax	SET_PLOT_SIZE
Prompt	<p>RELATIVE PLOT SIZE</p> <p>Enter the relative scaling factor.</p>

4.34 SET_PREFIX_SCALING

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	<p>AXIS (X OR Y)</p> <p>Specify X- or Y- axis.</p> <p>USE PREFIX SCALING</p> <p>Enables or disables prefix scaling, Y or N. Give an integer value to select a prefix power of your own.</p>

4.35 SET_RASTER_STATUS

Set to have a raster plotted in the diagram. Default is no raster plotted.

Syntax	SET_RASTER_STATUS
Prompt	<p>RASTER PLOT (Y OR N) /Y/</p> <p>Enables (Y) or disables (N) the raster plot.</p>

4.36 SET_SCALING_STATUS

Choose between manual or automatic scaling on a specified axis. If manual scaling is chosen 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	<p>AXIS (X, Y OR Z) Specify what axis to set the scaling status.</p> <p>AUTOMATIC SCALING (Y OR N) Automatic (Y) and manual (N) scaling.</p> <p>MIN VALUE For manual scaling specify the value of the starting point of the specified axis.</p> <p>MAX VALUE For manual scaling specify the value of the end point of the specified axis.</p>

4.37 SET_TIC_TYPE

Change the size of the tic marks and the placement either inside or outside of the axis.

Syntax	SET_TIC_TYPE
Prompt	<p>TIC TYPE Place on either the inside or the outside of the diagram axis. The absolute value of TIC TYPE determines the length.</p> <ul style="list-style-type: none"> • TIC TYPE > 0 (outside the axis) • TIC TYPE < 0 (inside the axis)

4.38 SET_TITLE

Specify a title that displays on all listings and diagrams from the POST PROCESSOR.

Syntax	SET_TITLE
Prompt	<p>TITLE Enter the title to include on all output. There is a maximum length of about 60 characters.</p>

4.39 SET_TRUE_MANUAL_SCALING

Set to manual scaling instead of the default where the tic marks on the axis are placed in even intervals using the whole axis length. The scaling routine adjusts the given minimum and maximum values slightly to accomplish this. 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 the axis you want to toggle between automatic adjustment or avoiding the adjustment of the given maximum and minimum values.

5 About DATAPLOT Files

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



For more information about DATAPLOT search the online help or refer to the *DATAPLOT User Guide*.

All prologues must be placed before the first DATASET statement.

The syntax must be used for the DATAPLOT file.

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

Keyword	Parameters
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)
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.

Keyword	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><code>=0</code> , <code><video>=NORMAL</code> and <code><mode>=TRANSPARENT</code> . To set a new current pattern supply any or all of the optional parameters. <code><code></code> is a single letter 0-9, A-Z or a-t (if <code><code>=t</code> supply also a number in the range 0.00 - 1.00, e.g. PAINT t 0.25.) <code><video></code> is a string reading NORMAL or INVERSE. <code><mode></code> is a string reading TRANSPARENT or OPAQUE.
PCFUNCTION Y=203(X); or X=203(Y);	<code><start end steps GOC></code> The <code><></code> 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 plot box 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
    
```

6 State, Integral and Auxiliary Variables

- [State Variables](#)
- [Intensive Properties](#)
- [Extensive Properties](#)
- [Integral Variables](#)
- [Auxiliary Variables](#)

6.1 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 a 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.

6.2 Intensive Properties

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

6.3 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.

Mnemonic	Description
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 is always 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.
Y(phase,species#sublattice)	site fraction (this quantity is dependent upon the model chosen for the phase)

6.4 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.
- IVV(Austenite) is the volume fraction of Austenite in a single cell calculation.
- IVV(2, Austenite) is the volume fraction of Austenite in Cell 2 for a multi cell calculation.

6.5 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

Name	Mnemonic	Argument
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)	$D0=\exp(\ln(DI\{T1\})+Q/R/T1)$