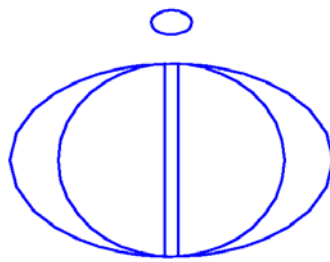


DICTRA



User's Guide

Version 25



News in DICTRA version 25

DICTRA version 25 contains new features and improvements as described below.

- In DICTRA 25 we consider diffusion of elements, instead of species as was the case in earlier versions. This is a large change that has been introduced in order to obtain a better treatment of diffusion in phases that is modelled with the same specie on several sub-lattices, e.g. phases showing chemical ordering, as well as to manage phases modelled with charged species, e.g. Cr^{2+} , Cr^{3+} etc.
- It's now possible to treat diffusion in ionic phases (e.g. oxides) containing charged species (e.g. Cr^{3+} , O^{2-}). This is managed by treating the diffusion of the corresponding elements (e.g. Cr, O).
- In order to treat diffusion in phases where the same specie is present on more than on one single sub-lattice, then a new database diffusion model, invoked by the keyword "GENERAL" inside the TDB file, has been introduced. Using this model the mobilities for specie present on several sub-lattices are specified separately for each sub-lattice. See the new DICTRA Example i3. Note that for phases modelled with a contribution from chemical ordering the database diffusion model keyword should still be "ORDERED"
- A boundary condition "GAS" has been introduced in order to manage a mobile outer boundary condition, e.g. for simulating the growth of an external oxide layer. See the new DICTRA Example i3.
- Better generation of automatic start values for activities/potentials at a moving phase interface. This has resulted in improved simulation stability for so-called moving phase-boundary problems.
- A so-called "labyrinth factor" can now be specified in each region. This simply allows a user the possibility to increase or reduce all the diffusion coefficients in a particular region by a function or a constant factor.
- The diffusion model used for stoichiometric phases has been rewritten, and due to a generalized treatment, then fluxes for all elements for which mobility data is available are now calculated, and also used in the simulation, e.g. considering a binary Fe-C system and BCC region surrounded by an FCC region (both phases are modelled with only Fe species on the first sub-lattice), now also the flux of Fe and not as previously only the flux of C is calculated.

- The maximum time-step allowed by the automatic time-step control in DICTRA is now dependent upon the high time limit for each function interval.
- Extensions in the homogenisation model, e.g. new options available for selecting homogenization function, see section 4.2.9.
- New version is based on TCC version S, which contains improvements that may be useful in DICTRA.
- New version is backward compatible with earlier version of DICTRA.

NEWS IN DICTRA VERSION 25	2
1. INTRODUCTION	8
2. HOW TO READ THIS MANUAL	9
3. BASIC CONCEPTS	9
3.1 GENERAL	9
3.2 CELLS, REGIONS AND INTERFACES	9
3.3 REGIONS AND GRID	10
3.4 GEOMETRIES	10
3.5 PHASES	11
3.6 COMPOSITIONS.....	11
4. COMMANDS IN THE DICTRA MODULE	12
4.1 INTRODUCTION	12
4.2 COMMANDS FOR SETTING UP THE PROBLEM.....	13
<i>SET_CONDITION GLOBAL</i>	14
<i>ENTER_REGION</i>	14
<i>ENTER_GRID_COORDINATES</i>	14
<i>ENTER_PHASE_IN_REGION</i>	15
<i>ENTER_COMPOSITIONS</i>	15
<i>SET_CONDITION BOUNDARY</i>	15
<i>ENTER_GEOMETRICAL_EXPONENT</i>	15
<i>COARSENING_MODEL</i>	16
<i>PARA_EQUILIBRIUM_MODEL</i>	16
<i>HOMOGENIZATION_MODEL</i>	16
<i>SET_SIMULATION_TIME</i>	16
<i>SET-ACCURACY</i>	16
<i>SET_ALL_START_VALUES</i>	16
<i>SAVE_WORKSPACES</i>	17
<i>SIMULATE_REACTION</i>	17
4.3 COMMAND GROUPS IN THE DICTRA MODULE.....	17
4.3.1 <i>General module commands</i>	18
<i>BACK</i>	18
<i>EXIT</i>	18
<i>GOTO_MODULE</i>	18
<i>HELP</i>	18
<i>MACRO_FILE_OPEN</i>	19
<i>PATCH</i>	19
<i>POST_PROCESSOR</i>	19
<i>READ_WORKSPACES</i>	19
<i>SAVE_WORKSPACES</i>	19
<i>SET_INTERACTIVE_MODE</i>	20
4.3.2 <i>Basic commands for setting up problems</i>	20
<i>ENTER_COMPOSITIONS</i>	20
<i>ENTER_GEOMETRICAL_EXPONENT</i>	22
<i>ENTER_GRID_COORDINATES</i>	22
<i>ENTER_PHASE_IN_REGION</i>	23
<i>ENTER_REGION</i>	28

<i>SET_CONDITION</i>	28
<i>SET_SIMULATION_TIME</i>	31
<i>SIMULATE_REACTION</i>	31
4.3.3 <i>Listing commands</i>	31
<i>LIST_REGION</i>	32
<i>LIST_PROFILES</i>	32
<i>LIST_CONDITIONS</i>	32
<i>LIST_MOBILITY_DATA</i>	32
<i>LIST_TIMESTEPS</i>	33
<i>CHECK_DIFFUSION_MATRIX</i>	33
<i>TABULATE_MOBILITY_DATA</i>	33
4.3.4 <i>Simulation condition commands</i>	34
<i>SET_ACCURACY</i>	34
<i>SET_NUMERICAL_LIMITS</i>	34
<i>SET_SIMULATION_CONDITION</i>	35
<i>SET_REFERENCE_STATE</i>	37
4.3.5 <i>Auxiliary commands</i>	38
<i>SELECT_TIMESTEP</i>	38
<i>ENTER_LABYRINTH_FUNCTION</i>	38
<i>ENTER_MOBILITY_DATA</i>	39
<i>AMEND_MOBILITY_DATA</i>	39
<i>SET_FIRST_INTERFACE</i>	39
<i>DEBUGGING</i>	39
<i>POLY_COMMAND</i>	39
<i>SET_ALL_START_VALUES</i>	39
4.3.6 <i>Cell commands</i>	40
<i>SELECT_CELL</i>	40
<i>CREATE_NEW_CELL</i>	40
<i>AMEND_CELL_DISTRIBUTION</i>	41
4.3.7 <i>Coarsening and limited interfacial mobility commands</i>	41
<i>COARSENING_MODEL</i>	41
<i>SET_SURFACE_TENSION</i>	41
4.3.8 <i>Para-equilibrium model command</i>	42
<i>PARA_EQUILIBRIUM_MODEL</i>	42
4.3.9 <i>HOMOGENIZATION model command</i>	42
<i>HOMOGENIZATION_MODEL</i>	43
<i>ENTER_HOMOGENIZATION_FUN</i>	44
<i>UTILITIES_HOMOGENIZATION</i>	46
5. POST PROCESSOR	47
5.1 <i>INTRODUCTION</i>	47
5.2 <i>BASIC COMMANDS</i>	47
<i>BACK</i>	47
<i>EXIT</i>	48
<i>HELP</i>	48
<i>INFORMATION</i>	48
<i>LIST_PLOT_SETTINGS</i>	48
<i>MAKE_EXPERIMENTAL_DATAFILE</i>	48
<i>PLOT_DIAGRAM</i>	48
<i>DUMP_DIAGRAM (PC/WINDOWS ONLY)</i>	49

<i>SET_DIAGRAM_AXIS</i>	49
<i>SET_INDEPENDENT_VARIABLE</i>	54
<i>SET_PLOT_CONDITION</i>	54
<i>SET_PLOT_FORMAT</i>	56
5.3 ADVANCED COMMANDS	56
5.3.1 <i>Specific commands</i>	56
<i>DIFFERENTIATE_VALUES</i>	56
<i>ENTER_SYMBOL</i>	56
<i>INTEGRATE_VALUES</i>	57
<i>LIST_SYMBOLS</i>	58
<i>LIST_REGION_NAMES</i>	58
<i>LIST_TIME_STEPS</i>	58
<i>SELECT_CELL</i>	58
5.3.2 <i>General commands</i>	59
<i>APPEND_EXPERIMENTAL_DATA</i>	59
<i>LABEL_CURVES</i>	62
<i>PATCH_WORKSPACE</i>	62
<i>PRINT_DIAGRAM (PC/WINDOWS Only)</i>	63
<i>QUICK_EXPERIMENTAL_PLOT</i>	63
<i>REINITIATE_PLOT_SETTINGS</i>	63
<i>SET_AXIS_LENGTH</i>	63
<i>SET_AXIS_PLOT_STATUS</i>	63
<i>SET_AXIS_TEXT_STATUS</i>	63
<i>SET_AXIS_TYPE</i>	64
<i>SET_COLOR</i>	64
<i>SET_DIAGRAM_TYPE</i>	64
<i>SET_FONT</i>	65
<i>SET_INTERACTIVE_MODE</i>	65
<i>SET_PLOT_OPTIONS</i>	65
<i>SET_PLOT_SIZE</i>	66
<i>SET_PREFIX_SCALING</i>	66
<i>SET_RASTER_STATUS</i>	66
<i>SET_SCALING_STATUS</i>	66
<i>SET_TITLE</i>	67
<i>SET_TRUE_MANUAL_SCALING</i>	67
<i>SET_TIC_TYPE</i>	67
6. HINTS	67
6.1 GENERAL	68
6.2 MOVING BOUNDARY PROBLEMS.....	68
6.3 CELL CALCULATIONS	69
6.4 DIFFUSION IN DISPERSED SYSTEMS.....	69
6.5 COOPERATIVE GROWTH	69
7. DICTRA & DIFFUSIVITIES	69
7.1. INTRODUCTION	70
7.2. MODELING OF THE ATOMIC MOBILITY.....	70
7.3. RELATIONS BETWEEN DIFFUSION COEFFICIENTS AND ATOMIC MOBILITIES.....	72
7.3.1 <i>Phenomenological coefficients</i>	72
7.3.2 <i>Interdiffusion coefficients</i>	73

7.3.3 Intrinsic diffusion coefficients.....	74
7.3.4 Self-diffusion coefficient	75
7.3.5 Impurity diffusion coefficient.....	75
7.4. How to create a kinetic database.....	76
7.4.1 Simple Ni-Al database for dilute face-centered cubic Ni-alloys	76
7.4.2 Optimized Ni-Al database for the face-centered cubic phase	77
REFERENCES	78
APPENDIX A, DICTRA EXTENSIONS TO THE DATABASE DEFINITION FILE	
SYNTAX.....	79
APPENDIX B, A SIMPLE NI-AL DATABASE FOR DILUTE NI-ALLOYS.....	82
APPENDIX C, ASSESSED NI-AL DATABASE.....	83

1. INTRODUCTION

DICTRA is a general software package for simulation of Diffusion Controlled TRANSformations in multicomponent systems. Any number of components may be treated (provided that necessary thermodynamic and kinetic data are available). DICTRA is particularly suitable for treating problems involving a moving boundary, e.g. Stefan problems. The boundary conditions may be given in a rather flexible way, which enables the user to treat problems of practical interest. Examples of problems that may be treated by DICTRA are:

One-phase problems:

- * Homogenisation of alloys
- * Carburizing and decarburizing of e.g. steel in austenitic state

Moving boundary problems:

- * Growth or dissolution of precipitates
- * Coarsening of precipitates
- * Microsegregation during solidification
- * Austenite to ferrite transformations
- * Growth of intermediate phases in compounds
- * Nitriding and nitrocarburization

Long-range diffusion in multi-phase systems:

- * Carburizing of high-temperature alloys
- * Interdiffusion in compounds, e.g. coating systems

Cooperative growth:

- * Growth of pearlite in alloyed steels

Deviation from local equilibrium:

- * Calculations under paraequilibrium conditions

The program is based on a numerical solution of the multicomponent diffusion equations in the various regions of a material assuming that thermodynamic equilibrium holds locally at all phase interfaces. DICTRA is interfaced with THERMO-CALC which handles all thermodynamic calculations needed by DICTRA.

DICTRA is essentially divided into 4 modules, namely

- Solution of diffusion equations
- Calculation of thermodynamic equilibrium
- Solution of flux-balance equations
- Displacement of phase interface positions and adjustment of grid points etc.

In addition there is a post processor that enables the user to plot and list data from a simulation, e.g. concentration profiles, particle size as a function of time etc., and also a database module to handle thermodynamic and kinetic data.

The user interface is built up around a number of concepts which will be defined in chapter 3.

2. HOW TO READ THIS MANUAL

The basic concepts used in this manual and in the DICTRA program are defined and discussed in CHAPTER 3. It is recommended to start reading this chapter. A brief description of each command is given in CHAPTER 4, which is intended mainly as a reference. Glance through chapter 4. The post processor and its commands are described in CHAPTER 5. If something goes wrong you may find some help in CHAPTER 6. In a separate volume a number of running examples are collected. This is probably the most instructive chapter. Read the examples and try them out yourself. When you want to try your own problems find an example that is similar and modify it in accordance with your own problem.

3. BASIC CONCEPTS

3.1 General

Before a simulation is started a number of conditions must be fixed. The initial state of the system and its boundary conditions must all be defined. Some parameters involving the numerical calculations must be given. Some of those may be given by the program as default values but others have to be supported by the user. The basic concepts used when defining problems in DICTRA are presented in this chapter.

3.2 Cells, regions and interfaces

DICTRA regards a system as divided into cells. The simplest system consists of at least one cell. If there are several cells these are interconnected under the assumption of diffusional equilibrium and there are thus no differences in diffusion potentials between cells. Cells may exchange matter, however, a system of cells form a closed system. A cell contains one or several regions in which the diffusion problem is to be solved. The size of a cell is fixed during the whole simulation whereas the size of a region may grow or shrink. Two

neighbouring regions are separated by an interface which is usually mobile although its migration rate may be very low. Such an interface is called inner interface and the condition at such an interface comes out as a result of the simulation. The boundary of a cell is called outer interface and the condition of this type of interface may be affected by the user's choice of boundary conditions.

3.3 Regions and grid

The diffusion equation is solved on a region which must contain at least one phase but may contain several phases. A region must also contain a number of gridpoints situated at given positions which may be adjusted as a result of the simulation. The composition is only known at the gridpoints and is assumed to vary linearly between the gridpoints. In a case where a region contains several phases one of those must be chosen as a matrix in which the diffusion problem is solved. The amount and composition of the other phases are those given by thermodynamic equilibrium keeping the over-all composition at the gridpoint fixed.

Regions can be given arbitrary names, though regions created automatically by the program during a simulation will take the name of the created phase with R_ added in front. This is used when inactive phases are entered into a region.

The grid points in a region may be distributed linearly, geometrically or entered point by point. When the grid points are distributed linearly the points are equally spaced in the region, when distributed geometrically the spacing is defined by a geometrical series, which is controlled by a user defined factor where a value less than one and larger than zero will yield a closer spacing at the right side of the region and a value larger than one will instead yield a closer spacing at the left side. The inverses of the geometrical factors give corresponding spacing at either side of the region.

3.4 Geometries

The geometry of the problem is defined by a geometrical exponent. The program handles problems that can be reduced to 1-dimensional geometries. The geometrical exponent can take the values 0, 1 or 2.

Giving the geometries:

0. Planar geometry.

This corresponds to an infinitely wide plate of a certain thickness.

1. Cylindrical geometry.

This corresponds to an infinitely long cylinder of a certain radius.

2. Spherical geometry.
Sphere of a certain radius.

The size of the system is defined by the sum of sizes of the regions.

In the global coordinate system the position where the coordinate is zero is at the left outer boundary in the planar case and in the cylindrical and the spherical cases it is the centre. Accordingly the coordinate with the highest value is in the planar case the right outer boundary and for the cylindrical and spherical geometries the only outer boundary. In the case where several cells are used they are always connected at this outer boundary.

3.5 Phases

A region may contain one or several phases. A phase can be introduced with the status ACTIVE or INACTIVE where active is default. The inactive status means that the driving force for precipitation (denoted DGM in POLY-3) of the phase is monitored continuously. If it exceeds a predefined positive value the phase will take part in the simulation and the phase status is automatically changed into the active status. A new region is then created and given the name of the phase preceded by R_. If a phase is given an inactive status it will upon entering the calculations be of matrix type, see below.

A phase may be of three different types, matrix, spheroid or lamellar type. If there is only one phase in a region that phase is automatically of the matrix type. The spheroid type is used to treat one or several dispersed phases in a matrix. It should be noticed that unless the homogenization model is invoked, then diffusion is only treated in the matrix phase and the spheroid phases are assumed to be homogeneous and in equilibrium with the matrix at each point. The lamellar type is used to simulate the growth of a eutectic or eutectoid region. So far the program can only treat the growth, but not the dissolution, of such a region.

3.6 Compositions

The DICTRA program works internally with two types of composition variables, i.e. site-fractions and u-fractions, although the user may use also wt%, weight fraction or mole fraction for convenience.

The site-fractions are used in setting up the problem and interfacing with POLY-3 whereas the u-fractions are used in the diffusion equations. The different concentration variables are explained below.

Site-fractions y_k :

The site fraction of a species k , y_k , is the fraction of equivalent lattice sites occupied by species k . It is the only concentration variable that uniquely defines the composition and the constitution of a phase and it is thus necessary to use the site fraction in the storage of the data during a simulation.

U-fractions u_k :

The u-fraction of a component k is defined as

$$u_k = \frac{x_k}{\sum x_k}$$

where the summation is taken over the substitutional elements only. The choice of the volume fixed frame of reference in the calculations make it necessary to use a composition variable which is related to the volume. The definition of the u-fraction is based upon the assumption that a species may or may not contribute to the volume of a phase. An interstitial species is assumed to not contribute to the volume.

This definition makes it necessary in the mobility database to define which species do not contribute to the volume. This is done with the keyword ZERO-VOLUME-SPECIES, followed by a list of those species.

4. COMMANDS IN THE DICTRA MODULE

4.1 Introduction

All commands in the DICTRA monitor are listed in Table 1, see below. In the following section the most important commands will be discussed.

AMEND_CELL_DISTRIBUTION
AMEND_MOBILITY_DATA
BACK
CHECK_DIFFUSION_MATRIX
COARSENING_MODEL
CREATE_NEW_CELL
DEBUGGING
DELETE_REGION
ENTER_COMPOSITIONS
ENTER_EFFECTIVE_FUNCTION
ENTER_GEOMETRICAL_EXPONENT

ENTER_GRID_COORDINATES
ENTER_HOMOGENIZATION_FUN
ENTER_LABYRINTH_FUNCTION
ENTER_MOBILITY_DATA
ENTER_PHASE_IN_REGION
ENTER_REGION
EXIT
GOTO_MODULE
HELP
HOMOGENIZATION_MODEL
LIST_CONDITIONS
LIST_MOBILITY_DATA
LIST_PROFILES
LIST_REGION
LIST_TIMESTEPS
MACRO_FILE_OPEN
PARA_EQUILIBRIUM_MODEL
PATCH
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_STOICH_FACTOR
SET_SURFACE_TENSION
SIMULATE_REACTION
TABULATE_MOBILITY_DATA
UTILITIES_HOMOGENIZATION

4.2 Commands for setting up the problem

Before the Dictra monitor is entered the user has to enter thermodynamic and kinetic data from the database module:

- Switch to the appropriate thermodynamic database, define the phases and the components in the system, and then retrieve the data (for more information, see TDB User's Guide available in the Thermo-Calc User's Guide).

- Switch to the appropriate mobility database, define the phases and the components in the system, and then retrieve the data.

Thereafter the Dictra monitor is entered and the initial conditions and the various simulation conditions are defined.

SET_CONDITION GLOBAL

Define the conditions that reduce the degrees of freedom at the phase interface.

A global condition is either pressure (P), temperature (T) or the heat content removal (Q), these may be specified as functions of time, the syntax for this is approximately the same as used in the GES (Gibbs Energy System) in Thermo-Calc to specify temperature ranges for thermodynamic parameters.

ENTER_REGION

Enter a region into the system. The name of the region can be arbitrarily chosen. The new region is by default attached to the right side of the last region in the cell.

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 may be of the type LINEAR, READ_POINT_BY_POINT, GEOMETRIC or DOUBLE_GEOMETRIC.

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

ENTER_PHASE_IN_REGION

Enter a phase into an earlier defined region. At this time it is determined whether the phase is active or inactive, the type of phase is also entered and may be of MATRIX, LAMELLAR or SPHEROID type.

ENTER_COMPOSITIONS

Enter the composition into the phases in a named region. The composition of the phase may be given in, site-fraction, mole-fraction, mole-percent, weight-fraction, weight-percent or u-fraction. The composition profile may be entered by the user or be read from a file.

SET_CONDITION_BOUNDARY

Define the boundary conditions for the system. Boundary conditions may be set for both the upper and the lower side of the system. The conditions may be of types:

FIX_FLUX_VALUE
STATE_VARIABLE_VALUE
POTENTIAL_FLUX_FUNCTION
ITERATIVE_ACTIVITY_FLUX_FUNCTION
ACTIVITY_FLUX_FUNCTION
CLOSED_SYSTEM
MIXED_ZERO_FLUX_AND_ACTIVITY
GAS

The different alternatives may in most cases be functions of both TIME, T (temperature) and P (pressure).

The default is CLOSED_SYSTEM which is equivalent to setting the fluxes of all components to zero at the boundary. This is also the default if no boundary conditions were to be entered.

ENTER_GEOMETRICAL_EXPONENT

Enter the geometrical exponent which defines the geometry of the system. The geometrical exponent ranges from 0 to 2 corresponding to planar, cylindrical and spherical geometry, respectively. If no geometrical exponent is entered then planar geometry is assumed by default.

COARSENING_MODEL

This command invokes a simplified model present in DICTRA for treating coarsening, see 4.3.7.

PARA_EQUILIBRIUM_MODEL

This command invokes a model for simulation of a moving boundary problem assuming that para-equilibrium conditions apply at the moving interface, see 4.3.8.

HOMOGENIZATION_MODEL

This command invokes the homogenization model that may be applied to simulate long-range diffusion through a multiphase mixture, under the assumption that local equilibrium holds at each node point, see 4.2.9.

SET_SIMULATION_TIME

Set the simulation time. The automatic time step control is recommended. The smallest time step and the initial time step must be chosen with some care reflecting the time scale of the problem in the initial stage.

SET-ACCURACY

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

SET_ALL_START_VALUES

This command enables the user to enter start values for various unknown quantities, such as velocities and potentials.

SAVE_WORKSPACES

Save the setup on a store-file before starting the simulation.

SIMULATE_REACTION

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

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

SIMULATE_REACTION YES

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

For more details on the commands used to setup the simulation, please refer to the next sections, the examples and the on-line help.

4.3 Command groups in the DICTRA module

The commands in the DICTRA-module can be divided into the following groups:

- general module commands
- basic commands for setting up problems
- listing commands
- simulation condition commands
- auxiliary commands
- cell commands

A complete description of all commands divided into subject groups follows in the next sections. The text in these sections are extracted from the online help and can therefore also at any time be accessed from within the program. In the following sections the use of all commands is described. All sections start with a plain listing of the commands presented therein, and then follow in alphabetic order a detailed description of the commands. In order to increase the readability, each command is preceded with a " " and each sub-prompt with a " ". A sub-prompt appears whenever a command expects more input from the user.

4.3.1 General module commands

BACK **MACRO_FILE_OPEN** **SAVE_WORKSPACES**
EXIT **PATCH** **SET_INTERACTIVE_MODE**
GOTO_MODULE **POST_PROCESSOR** **HELP**
READ_WORKSPACES

These commands are common in all modules in the DICTRA and THERMO-CALC package. They are used in transferring the control to the different modules, getting help and handling the workspaces.

BACK

This command gives the control back to the most recent module. From the post-processor one goes 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 by user are lost.

GOTO_MODULE

The user may select another module by this command.

MODULE NAME

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

HELP

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

COMMAND

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

MACRO_FILE_OPEN

Macro is a convenient way of predefining sequences of commands on a file and then executing them by the MACRO command. This is useful when the same calculation is made often with just small changes. One good case for applying this is when calculating diagrams from an assessment. With a macro file all commands can be stored on a file and you just type MACRO <filename>. The macro file can contain any legal DICTRA commands. The macro must be terminated with EXIT or in the SYS, DICTRA, POLY-3 or POST module with the command SET_INTERACTIVE.

Macro filename:

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

PATCH

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

POST_PROCESSOR

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

READ_WORKSPACES

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

File name

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

SAVE_WORKSPACES

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

File name

Name of the file where the workspaces shall be saved on.
The default file extension is DIC.

Overwrite current file content

Proceed with SAVE

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

SET_INTERACTIVE_MODE

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

4.3.2 Basic commands for setting up problems

ENTER_COMPOSITION	ENTER_PHASE_IN_REGION
SET_SIMULATION_TIME	ENTER_GEOMETRICAL_EXPO
ENTER_REGION	SIMULATE_REACTION
ENTER_GRID_COORDINATE	SET_CONDITION

These are the necessary commands to setup and simulate a problem with the DICTRA module. The commands have superficially been described in the previous chapter.

ENTER_COMPOSITIONS

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

REGION NAME

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

PHASE NAME

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

USE EQUILIBRIUM VALUE

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

DEPENDENT SUBSTITUTIONAL SPECIES

A dependent substitutional species is required in order to be able to determine which species are independent. The program will then only

query for the compositions of the independent species. NOTE: Sometimes the dependent species is chosen by the program and thus this question is never given. This maybe due to stoichiometric constraints or to the fact that it has been set already in the kinetics database due to the model selected for the diffusion.

DEPENDENT INTERSTITIAL SPECIES

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

COMPOSITION TYPE

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

SITE_FRACTION
MOLE_FRACTION
MOLE_PERCENT
WEIGHT_FRACTION
WEIGHT_PERCENT
U_FRACTION

TYPE

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

LINEAR
READ_POINT_BY_POINT
FUNCTION
GEOMETRIC

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

For example the function:

$$3+2\text{hs}(x-1e-4)$$

Provide a concentration of 3 at the left side and 5 at the right side with a sharp step in the concentration profile at $1e-4\text{m}=100\mu\text{m}$.

VALUE OF FIRST POINT

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

VALUE OF LAST POINT

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

INPUT FILE

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

VALUE OF POINT

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

VALUE OF R IN THE GEOMETRICAL SERIE

Use the same geometrical factor as for the geometrical grid.

VOLUME FRACTION OF

Initial volume fraction of a spheroid phase.

ENTER_GEOMETRICAL_EXPONENT

This command enters the geometrical exponent which defines the geometry of system. The program handles 1-dimensional geometries defined by the geometrical exponent. These geometries are:

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

GEOMETRICAL EXPONENT

An integer value between 0 and 2 is required.

ENTER_GRID_COORDINATES

Command specifies the size of a region, as well as the distribution of grid points in the region.

REGION NAME

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

WIDTH OF REGION

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

TYPE

Type of grid to entered, possible alternatives are

LINEAR
READ_POINT_BY_POINT
GEOMETRIC
DOUBLE_GEOMETRIC

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

NUMBER OF POINTS

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

INPUT FILE

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

VALUE OF POINT

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

VALUE OF R IN THE GEOMETRICAL SERIES

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

VALUE OF R IN THE GEOMETRICAL SERIES FOR LOWER PART OF REGION

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

VALUE OF R IN THE GEOMETRICAL SERIES FOR UPPER PART OF REGION

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

ENTER_PHASE_IN_REGION

This command enters a phase into an earlier defined region.

ACTIVE OR INACTIVE PHASE

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

REGION NAME

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

PHASE TYPE

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

MATRIX
LAMELLAR
SPHEROID

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

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

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

PHASE NAME

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

COMPOSITION SET

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

ATTACH TO REGION NAMED

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

ATTACHED TO THE RIGHT OF

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

REQUIRED DRIVING FORCE FOR PRECIPITATION

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

CONDITION TYPE

Boundary condition used if the inactive phase becomes stable.

Specific sub-prompts for the phase type LAMELLAR.

Enter name of "ALPHA" phase

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

Enter name of "BETA" phase

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

Enter name of "GAMMA" phase

Enter the GES phase name for the GAMMA matrix phase.

Enter "ALPHA"/"BETA" surface tension:

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

Enter "ALPHA"/"GAMMA" surface tension:

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

Enter "BETA"/"GAMMA" surface tension:

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

Optimum growth condition factor /2/:

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

Name of dependent element

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

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

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

Volume diffusion model.

Boundary diffusion model.

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

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

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

AUTOMATIC

MIXED

TDB

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

DQ(X)=

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

k' =

k'' =

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

DF_boundary(X) =

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

DQ_boundary(X) =

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

DF_volume(X) =

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

DQ_volume(X) =

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

Automatic start values for the S0 determination /Y/:

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

Critical thickness of "ALPHA" lamella:

If you answered N on the previous question this prompt will appear. The critical thickness of ALPHA is about 0.9 of 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

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

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

Critical thickness of "BETA" lamella:

The critical thickness of BETA is about 0.1 of S_0 , see above.

Automatic start values on potentials /Y/:

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

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

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

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

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

Growth rate V:

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

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

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

Automatic start values on other variables /Y/:

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

Fraction of "ALPHA" phase:

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

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

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

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

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

ENTER_REGION

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

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.

SET_CONDITION

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

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

GLOBAL OR BOUNDARY CONDITION

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

VARIABLE

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

BOUNDARY

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

CONDITION TYPE

Defines the type of boundary condition to be specified. The different alternatives may in most cases be functions of both TIME, T (temperature) and P (pressure).

Legal alternatives are:

FIX_FLUX_VALUE
STATE_VARIABLE_VALUE
POTENTIAL_FLUX_FUNCTION
ACTIVITY_FLUX_FUNCTION
ITERATIVE_ACTIVITY_FLUX_FUNCTION
CLOSED_SYSTEM
MIXED_ZERO_FLUX_AND_ACTIVITY
GAS

The default is CLOSED_SYSTEM which is equivalent to setting the fluxes of all components to zero at the boundary. This is also the default boundary condition.

Fix flux value

The flux for the independent components given as a function of time, temperature and pressure.

State variable expression

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

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. Note that the activities are those with user defined reference states.

Iterative activity flux function

Same as activity flux function above. However, an iterative scheme is used to determine the flux. This method may be used instead of activity flux function when the latter has problems.

Closed system

Corresponds to a fix flux value, which is set to zero at all times.

Mixed zero flux and activity

The flux of selected components will be set to zero and the activity of others may be set to a prescribed value.

State variable expression

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.

GAS

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

LOW TIME LIMIT

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

HIGH TIME LIMIT

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

ANY MORE RANGES

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

TYPE OF CONDITION FOR COMPONENT

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

SET_SIMULATION_TIME

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

END TIME FOR INTEGRATION

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

AUTOMATIC TIMESTEP CONTROL

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

MAX TIMESTEP DURING INTEGRATION

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

TIMESTEP DURING INTEGRATION

Fixed timestep used when the automatic timestep procedure is disabled.

INITIAL TIMESTEP

Timestep used as the initial timestep.

SMALLEST ACCEPTABLE TIMESTEP

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

SIMULATE_REACTION

Start the simulation with this command.

4.3.3 Listing commands

LIST_REGION

TABULATE_MOBILITY_DATA

LIST_TIMESTEPS

CHECK_DIFFUSION_MATRIX

LIST_MOBILITY_DATA

LIST_PROFILES

LIST_CONDITIONS

The listing commands lists entered and simulated data. The commands may be used to check the entered data before a simulation and to obtain numerical values of a simulation result.

LIST_REGION

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

OUTPUT FILE

File where the information is to be written.

LIST_PROFILES

Lists profiles in the cell.

NAME OF REGION

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

OUTPUT FILE

File where the information is to be written.

COMPOSITION TYPE

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

SITE_FRACTION
MOLE_FRACTION
WEIGHT_FRACTION
U_FRACTION

COMPONENTS

The output information may be limited to the specified components.

CONSTITUENTS

The output information may be limited to the specified constituents.

LIST_CONDITIONS

Lists the conditions set with the SET_CONDITION command.

OUTPUT FILE

File where the information is to be written.

LIST_MOBILITY_DATA

List the previously entered mobility data.

OUTPUT FILE

File where the information is to be written.

LIST_TIMESTEPS

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

CHECK_DIFFUSION_MATRIX

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

PHASE NAME

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

CONCENTRATION OF

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

Pressure

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

Temperature

Temperature at which diffusion coefficient matrix is to be displayed.

OPTIONS

Use one or several of DLPBMXOE

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

TABULATE_MOBILITY_DATA

Tabulate the previously entered mobility data for a phase.

Phase

Phase for which the mobility data is to be tabulated.

Diffusing species

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

Pressure

Pressure at which the mobility data is to be tabulated.

Low temperature limit

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

High temperature limit

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

Step in temperature

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

4.3.4 Simulation condition commands

SET_ACCURACY**SET_NUMERICAL_LIMITS****SET_SIMULATION_CONDITION****SET_REFERENCE_STATE**

These commands are used to change the conditions of a simulation. In many cases the default settings of these parameters will suffice but it is however common that it is necessary to change these values in order to obtain a successful simulation.

SET_ACCURACY

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

MAX RELATIVE ERROR

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

MAX ABSOLUTE ERROR

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

SET_NUMERICAL_LIMITS

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

REQUIRED SUM OF SQUARES IN NS01A

Required accuracy during the solution of the fluxbalance equations.

MAX NUMBER OF CALLS TO CALFUN OF NS01A

The maximum number of iterations when solving the fluxbalance equations. This number acts as a "safety valve", a moderate choice is

$10 * (\text{number_of_interfaces} * (\text{number_of_components} - 1))$

but use a larger value if necessary.

STEP USED BY NS01A

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

MAX STEP USED BY NS01A

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

MAX NUMBER OF EQUIDISTANT POINTS IN A REGION

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

FRACTION OF REGION ASSIGNED TO THE INTERFACE

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

SMALLEST NUMBER USED IN SCALING FLUX EQUATIONS

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

DEFAULT DRIVING FORCE FOR INACTIVE PHASES

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

SET_SIMULATION_CONDITION

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

NS01A PRINT CONTROL

Determines whether data should be printed about the iterative procedure to solve fluxbalance equations. This parameter is normally set

to 0 but can be set to 1 when difficulties with convergence occur. NS01A will then print out the values used in the iterations and the residuals.

FLUX CORRECTION FACTOR

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

NUMBER OF DELTA TIMESTEPS IN CALLING MULDIFF

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

CHECK INTERFACE POSITION

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

VARY POTENTIALS OR ACTIVITIES

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

ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT

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

SAVE WORKSPACE ON FILE

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

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

DEGREE OF IMPLICITY WHEN INTEGRATING PDEs

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

0.0	Euler forwards
0.5	Trapezoidal rule
1.0	Euler backwards

MAX TIMESTEP CHANGE PER TIMESTEP

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

USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION

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

ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF

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

SET_REFERENCE_STATE

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

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

Component

The name of the component must be given.

Reference state

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

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

Temperature

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

Pressure

One may select the pressure for the reference state.

4.3.5 Auxiliary commands

SELECT_TIMESTEP	AMEND_MOBILITY_DATA
POLY_COMMAND	ENTER_LABYRINTH_FUNCTION
SET_FIRST_INTERFACE	SET_ALL_START_VALUES
ENTER_MOBILITY_DATA	DEBUGGING

The auxiliary commands do not fall under any other category. However, they are very useful in many cases.

SELECT_TIMESTEP

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

TIMESTEP

The timestep to be selected, legal syntax is:

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

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

DELETE ALL OTHER TIMESTEPS

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

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.

ENTER_MOBILITY_DATA

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

AMEND_MOBILITY_DATA

Mobility data may be changed interactively by this command.

SET_FIRST_INTERFACE

This command sets the coordinate of the first interface in the cell.
Default value is zero

COORDINATE FOR FIRST INTERFACE

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

DEBUGGING

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

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

The level of debugging information to be displayed.

POLY_COMMAND

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

To Poly

Command line sent to the POLY-3 module.

SET_ALL_START_VALUES

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

START VALUE FOR VELOCITY OF INTERFACE

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

START VALUE FOR POTENTIAL

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

VARYING SPECIES IN INTERFACE

The species which potential is treated as unknown.

AUTOMATIC STARTING VALUES FOR PHASE COMPOSITIONS

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

4.3.6 Cell commands

SELECT_CELL CREATE_NEW_CELL AMEND_CELL_DISTRIBUTION

These commands are used to setup and manipulate cells in the DICTRA module. Cells can be used to model immobile phase interfaces and precipitates with size distributions. The coupling between the cells is achieved by enforcing the same diffusion potentials ($\mu_k - \mu_n$) at the outer boundary of the cells for the independent components. Here μ_n is the chemical potential of a reference component. In order to maintain the overall massbalance the net flux between the cells is assumed to be zero. The individual fluxes in each cell is multiplied by a factor (CELL DISTRIBUTION FACTOR) which by default is unity, another value may however be used in order to describe a precipitate size distribution.

SELECT_CELL

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

Number

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

CREATE_NEW_CELL

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

CELL DISTRIBUTION FACTOR

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

AMEND_CELL_DISTRIBUTION

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

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.

4.3.7 Coarsening and limited interfacial mobility commands

COARSENING_MODEL

SET_SURFACE_TENSION

These commands are used to enable the simplified model for calculating coarsening in multicomponent systems in the DICTRA module. The calculations are performed in one cell on a maximum size particle which is assumed to 1.5 times the size of the average particle size. The SET_SURFACE_TENSION command is also utilized for simulating a case with a limited interfacial mobility.

COARSENING_MODEL

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

ENABLE COARSENING MODEL

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

SET_SURFACE_TENSION

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

FUNCTION

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

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

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

The molar volume should be given relative to the molar volume used by default in DICTRA, $1 \cdot 10^{-5}$ (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 $0.71 \cdot 10^{-5}$ (m³/mole), the entered function should be

$$2 \cdot 0.5 \cdot 0.71 \cdot (7/6) / X;$$

4.3.8 Para-equilibrium model command

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 several ways (AUTO, value%, -value and value), see below.

PARA_EQUILIBRIUM_MODEL

This command enables or disables the use of the para-equilibrium model.

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.

4.3.9 HOMOGENIZATION model command

HOMOGENIZATION_MODEL UTILITIES_HOMOGENIZATION

ENTER_HOMOGENIZATION_FUN

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 the region one of them is entered as MATRIX phase and all other phases as SPHEROID, but it does not matter which one is entered as matrix phase and it will not affect simulations. Homogenization model simulations differs from all other DICTRA simulations in that it is implemented using an implicit finite volume method in order to increase numerical stability (degree of implicitness can be chosen using the SET_SIMULATION_CONDITIONS command). Because of this, and other factors, homogenization model simulations will generally run slower than other comparable DICTRA simulations. The homogenization model should only be used for single region, single cell simulations.

HOMOGENIZATION_MODEL

This command enables or disables the use of the homogenization model and its default settings.

ENABLE_HOMOGENIZATION

Enter yes to enable the homogenization model.

USE_DEFAULT_SETTINGS

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

ADD_IDEAL_FLUX_CONTRIBUTION

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

USE_INTERPOLATION_SCHEME

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

-Enter what is essentially the number of steps in composition space between the minimum and maximum mole fraction. 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.

-Enter whether interpolation data should be recalculated when the composition range changes. If yes is entered there is still some elasticity

in the scheme so that data will not be recalculated if the changes are reasonably small.

-Enter whether the scheme should be validated and calibrated. The computational cost for validation and calibration is not insignificant and it is recommended that this setting only be used initially (in a trial run lasting a few time-steps) to get an idea of the necessary number of steps. Sub-prompts for this setting are calibration interval, minimum and maximum number of steps and the lower and upper error bound.

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

USE GLOBAL MINIMIZATION

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

USE INDIVIDUAL EQUILIBRIA FOR EACH NODE

Enter yes or no whether an individual equilibria should be defined for each spatial node. Depending on simulation conditions, using individual equilibria may reduce the risk for non-converged equilibrium calculations and may also speed up simulations. Enabling this setting is superfluous if global minimization is used.

EVALUATE JACOBIAN EVERY TIME-STEP

Entering yes will force the jacobian to be evaluated at the beginning of every time-step

ENTER_HOMOGENIZATION_FUN

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

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

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

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

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

The varieties with "excluded phases" are useful in several respects. First, if a phase is modelled as having zero solubility for a component, the mobility of that component in that phase is undefined, which causes a (non-terminal) error. Setting a phase as "excluded" causes the mobility of all components in that phase to be set to zero. Second, often there are some "major" matrix

solid solution phases and some "minor" precipitate phases. If the mobilities in the minor precipitate phases are zero the lower Hashin-Shtrikman bound is useless as it will produce a kinetic coefficient that is zero. However, using homogenization function #9 the excluded phases will not be considered when evaluating which phase has the most sluggish kinetics.

UTILITIES_HOMOGENIZATION

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

USE AVERAGED VOLUME-FIXED FLUX FOR MIXED BC

Enabling this setting causes the in-/outward flux to/from the system due to a boundary condition of type "mixed" to be evaluated using an average composition instead of balancing the fluxes using only the dependent component.

SET TEMPERATURE ACCORDING TO SOLIDUS TEMPERATURE

Enabling this setting causes the global temperature to be set such that it strives towards a certain value $T_{\text{target}} = T_{\text{sol}} - X$, where X is a value supplied by the user. The rate by which the temperature approaches T_{target} is also supplied by the user. The solidus temperature is determined with a ± 1 K accuracy. This setting can be useful for optimizing homogenisation heat treatments. Note that the liquid phase must be entered into the system in order for this utility to be used. The global temperature as a function of time will be saved to disk on a file "TEMP.TXT". The corresponding time will be saved to "TIME.TXT". The minimum solidus temperature will be saved to "TSOL.TXT". The node point with the minimum solidus temperature will be saved to "NODETSOL.TXT".

QUASI-NON-ISOTHERMAL SIMULATION

As the name implies this setting is used to perform simulations where temperature varies across the domain. However, the heat of transport is disregarded, thus "Quasi". The temperature at each node point (starting with the first node and ending with the last) at specific moments in time should be supplied by the user in a file "TEMP.TXT" and the corresponding temporal vector in a file "TIME.TXT". Thus, if the number of rows in file TIME.TXT is M and the number of node points is N , the number of rows in TEMP.TXT should be $M \cdot N$. Linear interpolation is used at intermediate points in time. Both files should contain column vectors with entries in format D28.16. Temperatures at node points are evaluated at the beginning of each time-step, which means that the maximum time-step should be chosen with some care.

5. POST PROCESSOR

5.1 Introduction

In order to be able to perform any plotting or printing, you have to specify what variables should be plotted on the diagram axis or printed in the table columns. For this purpose we have the commands SET_DIAGRAM_AXIS and ENTER TABLE. After having set both X- and Y-axis variables (and possibly a Z-axis which will appear as tick marks on the XY-curve), or table columns, you also have to specify the so-called plot condition and independent variable. It is important to realize that it is not sufficient just to define the axis variables before plotting/printing. As the simulation has both a time and a space coordinate, and we can only have one independent variable (time or space) in our plots or tabulations, the other variable must be set fixed during the plot/tabulation. This is specified with the SET_INDEPENDENT_VARIABLE and SET_PLOT_CONDITION commands, respectively. If you are heading for a table, use the command TABULATE. If you prefer a graphical plot, you additionally have to specify what type of graphical device you are using with the command SET_PLOT_FORMAT.

The command repertoire of the POST PROCESSOR has been divided into two categories. In principle, the 'Basic Commands' are sufficient for an easy and straight forward production of most types of plots and tables. The purpose of the 'Advanced Commands' is to supply the user with some additional utility commands that allows him to manipulate the default appearance of a plot.

In the two following sections the use of all commands is described. Both sections start with a plain listing of the commands presented therein, then follow in alphabetic order a detailed description of the commands.

5.2 Basic Commands

BACK	PLOT_DIAGRAM	EXIT
SET_DIAGRAM_AXIS	HELP	
DUMP_DIAGRAM	SET_INDEPENDENT_VARIABLE	
INFORMATION	SET_PLOT_CONDITION	
LIST_PLOT_SETTINGS	SET_PLOT_FORMAT	
MAKE_EXPERIMENTAL_DATAFILE		

BACK

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

EXIT

Terminates the program and returns to the operating system.

HELP

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

Command

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

INFORMATION

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

WHICH SUBJECT

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

PURPOSE

STATE VARIABLES

INTEGRAL VARIABLES

AUXILIARY VARIABLES

PLOT CONDITION AND INDEPENDENT VARIABLE

BASIC METHODOLOGY

LIST_PLOT_SETTINGS

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

MAKE_EXPERIMENTAL_DATAFILE

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

Output file

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

PLOT_DIAGRAM

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

PLOT FILE

The name of the file or graphical device

DUMP_DIAGRAM (PC/WINDOWS ONLY)

This command is an alternative command for producing plots in the PC/Windows environment. Supported graphical formats are PNG,BMP,PDF,JPEG,TIFF. The plot is saved to a file.

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

Specifies which graphical format should be used.

RESOLUTION (LOW,MEDIUM,HIGH)

Specifies the resolution of the plot.

SET_DIAGRAM_AXIS

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

AXIS (X,Y OR Z)

Specifies for which axis to set a variable.

VARIABLE

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

NONE	INTEGRAL VARIABLES
FUNCTIONS	AUXILIARY VARIABLES
STATE VARIABLES	

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

FOR COMPONENT

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

IN REGION

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

FOR PHASE

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

INTERFACE

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

TYPE

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

REGION NAME

Name of the region wherein the local distance is measured.

Below follows a more complete description of all valid axis variables

NONE

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

FUNCTIONS

Functions are identified by their names which have been entered with the command ENTER FUNCTION. Use the LIST_SYMBOLS command to get a list of valid function names.

STATE VARIABLES

State variables in the POST PROCESSOR has a similar meaning as those defined in POLY-3. Examples of state variables are temperature, mole fraction, enthalpy etc. In POLY-3 a general notation method based on character mnemonics has been designed for a predefined set of state variables. These are presented in the table below.

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

<u>MNEMONIC</u>	<u>MEANING</u>
Intensive properties	
T	temperature
P	pressure
AC(component)	activity

MU(component) chemical potential

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

Extensive property \bar{Z} at each grid point:

Z	ext. prop. \bar{Z} at each grid point.
ZM	ext. prop. \bar{Z} per moles of atoms.
ZW	ext. prop. \bar{Z} per mass (gram).
ZV	ext. prop. \bar{Z} per volume (m ³).

Extensive property \bar{Z} for a phase at each grid point:

Z	ext. prop. \bar{Z} for the current amount of the phase.
ZM	ext. prop. \bar{Z} per mole of atoms of the phase.
ZW	ext. prop. \bar{Z} per mass (gram) of the phase.
ZV	ext. prop. \bar{Z} per volume (m ³) of the phase.
ZF	ext. prop. \bar{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.

Remark: instead of the mnemonics NM and BW, X and W can be used to designate mole fraction and mass fraction.

Total amount (note: suffixes M, W and V can be applied)

N	Number of moles.
B	Mass.

Note, the legal combination BW is not very interesting as it will always be unity! BV is the density.

Amount of a phase (note: suffixes M, W and V can be applied)

NP(phase) Number of moles of a phase.

BP(phase) Mass of a phase.

VP(phase) Volume of a phase.

Remark: the normalizing properties are calculated at each grid point.

Constitution

Y(phase,species#sublattice) site fraction

Note: This quantity is dependent upon the model chosen for the phase.

INTEGRAL VARIABLES

An integral variable is a quantity that has been obtained by integration in space over the whole system or over a specific region. In a planar geometry values are given per unit area, in a cylindrical geometry they are given per unit length, and in a spherical geometry they are absolute values.

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	READING
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,

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

Example:

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.

AUXILIARY VARIABLES

As a complement to state variables and integral variables the following auxiliary variables have been defined. The variables may also be called by their mnemonic names, which are shown in the rightmost column. These are convenient to use in user defined functions.

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

*) 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 region.

Additional auxiliary variables only present as mnemonics

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)	¹⁰ log 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)	¹⁰ log 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)	$Q=R(\ln(DC\{T_1\}) - \ln(DC\{T_1+e\}))/((1/(T_1+e)) - 1/T_1)$
QT(phase,J)	$Q=R(\ln(DT\{T_1\}) - \ln(DT\{T_1+e\}))/((1/(T_1+e)) - 1/T_1)$
QI(phase,J,K,N)	$Q=R(\ln(DI\{T_1\}) - \ln(DI\{T_1+e\}))/((1/(T_1+e)) - 1/T_1)$
FC(phase,J,K,N)	$D_0=\exp(\ln(DC\{T_1\})+Q/R/T_1)$
FT(phase,J)	$D_0=\exp(\ln(DT\{T_1\})+Q/R/T_1)$
FI(phase,J,K,N)	$D_0=\exp(\ln(DI\{T_1\})+Q/R/T_1)$

SET_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. When plotting a diagram you must choose either one to vary along the curve, i.e. the independent variable, the other one is then the plot condition. N.B. When plotting integral quantities TIME should be independent variable.

VARIABLE

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

TYPE

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

NAME OF REGION

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

SET_PLOT_CONDITION

There are two "free" variables after a simulation done by DICTRA. One is the simulation TIME, the other one is a DISTANCE in the system. In general, when plotting a diagram you must choose either type as fixed (i.e. the plot condition), the other one is then the independent variable. However, when

plotting integral quantities, plot condition is automatically set to INTEGRAL and TIME is chosen as independent variable. N.B. You cannot mix different kinds of plot conditions. However, for TIME and DISTANCE you may supply up to 15 different condition values, see sub-prompt VALUE(S) below. The plot condition chosen is printed on a separate line above the diagram.

CONDITION

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

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

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

INTERFACE

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

TYPE

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

NAME OF REGION

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

AT UPPER INTERFACE OF REGION

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

UPPER OR LOWER INTERFACE OF REGION

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

VALUE(S)

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

SET_PLOT_FORMAT

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

Graphic Device number

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

5.3 Advanced Commands

The advanced commands are split into two different sub-groups. In the first group, we have some utility commands that are related to DICTRA simulations. In the second group, we present general POST PROCESSOR commands for the manipulation of diagrams.

5.3.1 Specific commands

ENTER_SYMBOL

LIST_REGION_NAMES

LIST_SYMBOLS

INTEGRATE_VALUES

LIST_TIME_STEPS

SELECT_CELL

TABULATE

DIFFERENTIATE_VALUES

DIFFERENTIATE_VALUES

Differentiate the plotted curve.

ENTER_SYMBOL

This command defines a symbolic name that represents either a table or an 'arbitrary' function. Legal variables in functions and columns in tables are

state variables, auxiliary variables, integral variables or previously defined functions. Functions are a useful feature of the POST PROCESSOR for defining quantities that are convenient for the user.

Function or table /FUNCTION/:

Select what kind of symbol to enter.

NAME:

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

Function:

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

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

&

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

Variable(s):

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

INTEGRATE_VALUES

Integrate the plotted curve.

LIST_SYMBOLS

Lists a specific or all symbols defined.

NAME:

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

LIST_REGION_NAMES

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

LIST_TIME_STEPS

Lists all integration time steps.

SELECT_CELL

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

Number

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

TABULATE

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

Name:

Give the symbolic name of the table.

Output file /SCREEN/:

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

5.3.2 General commands

APPEND_EXPERIMENTAL_DATA	SET_FONT
LABEL_CURVES	SET_INTERACTIVE_MODE
PATCH_WORKSPACE	SET_PLOT_OPTIONS
QUICK_EXPERIMENTAL_PLOT	SET_PLOT_SIZE
REINITIATE_PLOT_SETTINGS	SET_PREFIX_SCALING
SET_AXIS_LENGTH	SET_RASTER_STATUS
SET_AXIS_PLOT_STATUS	SET_SCALING_STATUS
SET_AXIS_TEXT_STATUS	SET_TIC_TYPE
SET_AXIS_TYPE	SET_TITLE
SET_COLOR	SET_TRUE_MANUAL_SCALING
SET_DIAGRAM_TYPE	

APPEND_EXPERIMENTAL_DATA

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

USE EXPERIMENTAL (Y OR N)

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

EXPERIMENTAL DATAFILE:

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

PROLOGUE NUMBER:

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

DATASET NUMBER(S):

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

A brief introduction to DATAPLOT.

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

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

The below presented syntax must be used for the DATAPLOT file. For a more complete reference see *User's Guide to Dataplot Graphical Language*.

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:

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:

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

Select one X and one Y variable
BLOCK GOC=C3,DWR; X1=C1+273.15; X2=C1; Y=C1+C2*4.184;
or multiple X and one Y variable
BLOCK GOC=C4,MWAS; X=C1+273.15; Y1=C2*4.184; Y2=C3;
or one X and multiple Y variables
BLOCK GOC=C5,DWA; X1=C1; X2=C4; Y1=C2*4.184; Y2=C3;
or multiple XY pairs

BLOCKEND

DRAWLINE x,y x,y ...

TEXT text or ~name (of a string, see below)
If output to a PostScript device and the postscript hardcopy fonts are used, most LTEXT codes will work in text string. Consult your LTEXT or DATAPLOT manual about such codes.

ATTRIBUTE TOP, CENTER or BOTTOM

STRING name text
The text string may contain text formatting codes namely: ^S# to set font size, ^G for greek font, ^F# to set font type, ^U# for positioning the text upwards, ^D# for positioning the text downwards, ^R# for positioning the text to the right, ^L# for positioning the text to the left, and finally ^N for printing without updating current position to the end of the character. These text formatting codes only work for soft fonts not hardcopy postscript fonts.

INCLUDE filename

CLIP ON or OFF

SYMBOLSIZE rnumb

FUNCTION Y=203(X); or X=203(Y); <start end steps GOC>
The < > denotes an optional parameter.

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

PCFUNCTION Y=203(X); or X=203(Y); <start end steps GOC>
The < > denotes an optional parameter. May be used to add a function to the current path.

Legal GOC are:

W = World coordinates (* DEFAULT)

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

Examples:

```

700      2.54
50       1.91      WRDS
1.1      0.9       NS3
100      20'This is a text

```

or

```

BLOCK GOC=C3,MWAS; X=C1+273.15; Y=C2*4.184;
600   -1400   S1'text
700   -1500
BLOCKEND

```

LABEL_CURVES

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

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

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

LABEL CURVES

Toggle the option by giving YES or NO.

PATCH_WORKSPACE

This command is only for those who think they know what they are doing. *The use of this command is definitely not encouraged.* You easily corrupt the whole internal data structure of the POST PROCESSOR! If you use it by mistake(?!), type an @ at the ADDRESS: prompt in order to return to the POST PROCESSOR.

PRINT_DIAGRAM (PC/WINDOWS Only)

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

QUICK_EXPERIMENTAL_PLOT

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

REINITIATE_PLOT_SETTINGS

All parameters describing the diagram will be given default values.

SET_AXIS_LENGTH

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

AXIS

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

AXIS LENGTH

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

SET_AXIS_PLOT_STATUS

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

AXIS PLOT (Y OR N)

The user can specify to plot axis or not.

SET_AXIS_TEXT_STATUS

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

AXIS (X, Y OR Z)

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

AUTOMATIC AXIS TEXT (Y OR N)

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

AXIS TEXT

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

SET_AXIS_TYPE

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

AXIS (X, Y or Z)

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

AXIS TYPE

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

SET_COLOR

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

- Text and axis Color
- Diagram Color
- DATAPLOT Color

SET_DIAGRAM_TYPE

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

TRIANGULAR DIAGRAM (Y OR N)

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

PLOT 3:RD AXIS

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

CLIP ALONG THE 3:RD AXIS

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

SET_FONT

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

SELECT FONTNUMBER

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

FONT SIZE

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

SET_INTERACTIVE_MODE

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

SET_PLOT_OPTIONS

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

PLOT HEADER

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

PLOT LOGO

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

PLOT FOOTER

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

WHITE COUNTOURED PS CHARS

Toggle the option of having a thin white contour around postscript characters (only on postscript devices).

PLOT REMOTE EXPONENTS

Toggle the plot of the remote exponents on the axis.

PLOT CELL#

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

PLOT-CONDITION STATUS

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

SET_PLOT_SIZE

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

RELATIVE PLOT SIZE

Enter the relative scaling factor.

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, ...

AXIS (X OR Y)

The user must specify X or Y axis.

USE PREFIX SCALING

Enables or disables prefix scaling by giving YES or NO.
Give an integer value to select a prefix power of your own.

SET_RASTER_STATUS

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

RASTER PLOT

Enables or disables the raster plot.

SET_SCALING_STATUS

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

AXIS (X, Y OR Z)

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

AUTOMATIC SCALING (Y OR N)

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

MIN VALUE

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

MAX VALUE

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

SET_TITLE

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

TITLE

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

SET_TRUE_MANUAL_SCALING

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

AXIS (X or Y)

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

SET_TIC_TYPE

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

TIC TYPE

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

TIC TYPE > 0 → tic marks on the outside of the axis

TIC TYPE < 0 → tic marks on the inside of the axis

6. HINTS

6.1 General

When you run your setup file make sure to check that all commands have been correctly entered and accepted by the program.

Always try to simplify your problem as much as possible at least in the beginning. If, for instance, you have an alloy with five or six components try to sort out the main components and make a first simulation with those components only. Then in a second run you can add further components if necessary.

Start using low accuracy and refine it in a second run. Check the profiles and the overall mass balance. If the accuracy is insufficient improve the accuracy values. Do not start out with too rigid constraints because it will only result in unreasonable computational times (and probably numerous other problems).

If large fluctuations occur in the profiles one can try to modify the grid or the timestep somewhat. Usually the timestep should be increased and this is accomplished by lowering the accuracy. Often the profiles can be improved if the pde's (partial differential equations) are integrated implicitly. This is accomplished by setting the parameter DEGREE OF IMPLICITITY WHEN INTEGRATING PDEs in the command SET_SIMULATION_CONDITION to 1.

To see what happens (and also see some of the commands that are sent to POLY-3) switch on the debug flag with the command DEBUG YES. This may give valuable information when the simulations do not converge or when the program crashes.

6.2 Moving boundary problems

Try using the automatic starting values as a first try. If the first time step does not converge amend the starting values for the velocities, usually to smaller values.

If the simulation fails during the first timestep check how the starting values affect the residuals. This is done by setting the parameter NS01A PRINT CONTROL in the command SET-SIMULATION-CONDITION to 1. The program will then print out the tried unknown value and the residual for each flux balance equation in each iteration. The equations are organized in the order that the first unknown is always the migration rate of the phase interfaces followed by the unknown potentials. All unknowns are scaled by the starting value or the calculated value in the previous timestep if such exists.

Check the grid distribution at the interfaces. If the grid is too coarse then the fluxes may be less well defined.

Use activities instead of potentials when the content of one ore more of the components becomes very low. In that case the activity approaches 0, which is more easy to handle than a potential that approaches infinity. This is done by setting the parameter VARY POTENTIALS OR ACTIVITIES in the command SET_SIMULATION_CONDITION to ACTIVITIES.

6.3 Cell calculations

In cell calculations, determine start values for each cell separately and thereafter connect together the individual cells. It might even be necessary to start out by simulating in planar and/or cylindrical geometry in order to determine sufficient starting values for a spherical case.

6.4 Diffusion in dispersed systems

It is important to realize that the maximum timestep allowed or the highest timestep actually taken in the calculation will affect the final result. Particularly this will be the case when one or more of the diffusing species have low solubility in the matrix phase. This is because a supersaturation is created in the matrix phase during a diffusion step and if too large timesteps are allowed too high supersaturations are created. Therefore, always check your result by performing a second simulation with a maximum timestep that is ten times lower than in the first run. If the results differ much between the first and the second run decrease the timestep again with a factor of ten and perform a third run and so on until the results can be trusted.

If a simulation fails because the program is not able to calculate the initial equilibrium or the equilibrium at some point at a later stage of the simulation, try to calculate the initial equilibrium yourself using Thermo-Calc and enter the composition and the fraction of each phase separately instead of having the program calculating it. Also enter starting values for each phase with the command SET-ALL-START-VALUES.

6.5 Cooperative growth

Try to calculate the A1e temperature with Thermo-Calc and start your simulation at a temperature slightly below that one. Use the equations given in the interactive help in order to estimate S0 and the growth rate.

7. DICTRA & Diffusivities

How to construct a kinetic database - a short guide

7.1. Introduction

In order to perform simulations using DICTRA, both thermodynamic and kinetic descriptions are needed. Moreover, the results and the accuracy of the simulations critically depend on the quality of these descriptions. The thermodynamic descriptions are available from the Thermo-Calc^[1] system. Consult the Thermo-Calc User's guide^[2] for more information about the Thermo-Calc database system. Kinetic descriptions are available within the DICTRA system, e.g. the MOB^[3] solution database, which is one source which contains kinetic data for several binary, some ternary, and even a few higher order systems. However, so far there is much less kinetic data which has been systematically assessed in the same way as thermodynamic data and there is thus a need to remedy this situation.

In the theoretical treatment of diffusive reactions one usually works with diffusion coefficients which are evaluated from experimental measurements. In a multicomponent system a large number of diffusion coefficients have to be evaluated, and moreover, they are generally functions of alloy composition and are interrelated. A database would thus be very complex. A superior alternative is to store atomic mobilities in the database, rather than diffusion coefficients. The number of parameters which need to be stored in a multicomponent system will then be substantially reduced and the parameters are independent. The diffusion coefficients, which are used in the simulations, can then be obtained as a product of a thermodynamic and a kinetic factor. The thermodynamic factor is essentially the second derivatives of the molar Gibbs energy with respect to the concentrations, and is known if the system has been assessed thermodynamically. The kinetic factor contains the atomic mobilities, which are stored in the kinetic database. The purpose of this text is to describe how concentration, temperature and pressure dependence of the atomic mobility can be modeled, as well as to describe relations between the different diffusion coefficients and the atomic mobility. In addition, the purpose of this text is to demonstrate how a mobility database can be created.

7.2. Modeling of the atomic mobility

From absolute-reaction rate theory arguments the mobility coefficient for an element B, M_B , may be divided into a frequency factor M_B^0 and an activation enthalpy Q_B i.e.

$$M_B = M_B^0 \exp\left(-\frac{Q_B}{RT}\right) \frac{1}{RT} {}^{mg} \Gamma \quad (1)$$

${}^{mg} \Gamma$ is a factor taking into account the effect of the ferromagnetic transition^[4]. ${}^{mg} \Gamma$ is a function of the alloy composition. It has been suggested^[5] that one should expand the logarithm of the frequency factor, $\ln M_B$ rather than the value itself, thus the mobility, M_B is expressed as:

$$M_B = \exp\left(\frac{RT \ln M_B^0}{RT}\right) \exp\left(-\frac{Q_B}{RT}\right) \frac{1}{RT} {}^{mg} \Gamma \quad (2)$$

Both $RT \ln M_B^0$ and Q_B will in general depend upon the composition, the temperature, and the pressure. In the spirit of the Calphad approach^[6], the composition dependency of these two factors, is represented with a linear combination of the values at each endpoint of the composition space, and a Redlich-Kister expansion, viz.

$$\Phi_B = \sum_i x_i \Phi_B^i + \sum_i \sum_{j>i} x_i x_j \left[\sum_{r=0}^m {}^r \Phi_B^{i,j} (x_i - x_j)^r \right] \quad (3)$$

where Φ_B represents $RT \ln M_B$ or $-Q_B$. Φ_B^i is the value of Φ_B for pure i and thus represents one of the endpoint values in the composition space. ${}^r \Phi_B^i$ are binary interaction parameters. The commas separate different species interacting with each other. x_i and x_j are mole fractions of elements i and j respectively. Each individual Φ parameter, i.e. Φ_B^i and ${}^r \Phi_B^i$ is stored in the database and may be expressed as a polynomial in temperature and pressure, if necessary. The Φ_B^i and ${}^r \Phi_B^i$ are referred to in the database as MF and MQ parameters, e.g.

$$\text{MF}(\text{BCC_A2\&CR,Ni:VA;0}) = R^*T^* \text{LN}(+8.50\text{E-}05)$$

is used to represent the frequency factor to the mobility of Cr in pure Ni, i.e. $RT \ln M_{Cr}^{Ni0}$, whereas:

$$\text{MQ}(\text{BCC_A2\&CR,Ni:VA;0}) = -2.18\text{E}+05$$

represents $-Q_{Cr}^{Ni}$. The magnetic effect is represented by Jönsson's model^[4].

$${}^{mg} \Gamma = \exp(6\alpha\xi) \exp\left(\frac{-\alpha\xi Q_B}{RT}\right) \quad (4)$$

where ξ represents the state of the magnetic order ($0 < \xi < 1$) at the temperature under consideration and α is treated as a constant, approximately equal to 0.3 in bcc alloys. For fcc alloys the ferromagnetic effect on diffusion is

usually neglectable, i.e. $\alpha=0$. When there is magnetic ordering it is thus necessary to make the division into MF and MQ because ${}^{mg}\Gamma$ depends on Q_B , i.e. MQ. The full expression then becomes:

$$RT \ln[RTM_B] = RT \ln M_B^0 - Q_B + RT \ln {}^{mg}\Gamma = \sum MF + \sum MQ + RT \ln {}^{mg}\Gamma$$

Both MF and MQ may be arbitrary polynomials in temperature and if there is no magnetic effect, i.e. $RT \ln \text{upmg}\$grG\$ = 0$, it is sufficient to enter either one of them. For example, the mobility of Cr in pure Ni may as well be stored as:

$$MF(\text{FCC_A1\&CR,Ni:VA;0}) = 0$$

and

$$MQ(\text{FCC_A1\&CR,Ni:VA;0}) = -Q_{Cr}^{Ni} + RT \ln M_{Cr}^{Ni0}$$

In order to build a database it is necessary to find values on MF and MQ (or when no magnetic effect is considered MQ alone). In many cases such data can be found in the literature. The tracer diffusivity D_B^* is directly related to the mobility M_B by means of the Einstein relation

$$D_B^* = RTM_B \tag{5}$$

and when there is no magnetic effect on the mobility, e.g. ${}^{mg}\Gamma = 1$, then from Eq's (2) and (5) it is found that:

$$MQ = RT \ln M_B^0 - Q_B = RT \ln D_B^* \tag{6}$$

vp18In a more complex database the model parameters are determined from an optimization procedure, where all experimental information is taken into account, see e.g. Refs. 7 and 8.

7.3. Relations between diffusion coefficients and atomic mobilities

7.3.1 Phenomenological coefficients

For crystalline phases the vacancy-exchange mechanism of diffusion is predominant, i.e. diffusion occurs by atoms jumping into neighboring vacant lattice sites. From the absolute reaction rate theory, and by assuming that the vacancy concentration is governed by thermodynamic equilibrium, the diffusional flux of a component k in the lattice fixed frame of reference can be expressed as^[9]:

$$\tilde{J}_k = -c_k y_{Va} \Omega_{kVa} \frac{\partial \mu_k}{\partial z} \quad (7)$$

Here c_k is the amount of k per unit volume, y_{Va} is the fraction of vacant lattice sites on the sublattice where k is dissolved, Ω_{kVa} is a kinetic parameter which gives the rate of exchange if there is a vacancy adjacent to a k -atom, and μ_k is the chemical potential of component k . The mobility M_k is here defined as:

$$M_k = y_{Va} \Omega_{kVa} \quad \text{when } k \text{ is substitutional,} \quad (8a)$$

$$M_k = \Omega_{kVa} \quad \text{when } k \text{ is interstitial.} \quad (8b)$$

From Eqs. (7), 8(a) and 8(b) it is possible to identify the so called phenomenological parameters that relate the flux of k to all the driving forces, i.e. $L_{kk} = c_k M_k$ when k is substitutional, $L_{kk} = c_k y_{Va} M_k$ when k is interstitial, and $L_{ki} = 0$ when $k \neq i$. The fluxes in the lattice-fixed frame of reference may now be expressed as:

$$\tilde{J}_k = -\sum_{i=1}^n L_{ki} \frac{\partial \mu_i}{\partial z} = -L_{kk} \frac{\partial \mu_k}{\partial z} \quad (9)$$

Transformation to the volume-fixed frame of reference, or the number-fixed frame of reference with respect to the substitutional elements, which may be regarded as the same, if as assumed in DICTRA, the partial molar volumes are independent of concentration, and the partial molar volumes of the interstitials are neglected, yields

$$J_k = -\sum_{i=1}^n L'_{ki} \frac{\partial \mu_i}{\partial z} \quad (10)$$

where

$$L'_{ki} = \sum_{j=1}^n (\delta_{jk} - c_k V_j) L_{ji} \quad (11)$$

where δ_{jk} is the Kronecker delta, i.e., = 1 when $j=k$ and 0 otherwise. V_j is the partial molar volume of element j .

7.3.2 Interdiffusion coefficients

Generally, it is much more convenient to express the fluxes as functions of concentration gradients, rather than gradients in chemical potential. This is accomplished by rewriting Eq. (10) using the chain rule of derivation, i.e.

$$J_k = -\sum_{i=1}^n L'_{ki} \sum_{j=1}^n \frac{\partial \mu_i}{\partial c_j} \frac{\partial c_j}{\partial z} \quad (12)$$

or equally if the unreduced diffusivities, D_{kj} are introduced,

$$J_k = -\sum_{j=1}^n D_{kj} \frac{\partial c_j}{\partial z} \quad (13)$$

The D_{kj} matrix introduced in Eq. (13) may be identified by comparing with Eq. (12),

$$D_{kj} = \sum_{i=1}^n L'_{ki} \frac{\partial \mu_i}{\partial c_j} \quad (14)$$

The $\partial \mu_i / \partial c_j$ are purely thermodynamic quantities, sometimes they are referred to as thermodynamic factors. It is now evident that the diffusivities may be looked upon as consisting of two separate parts, one purely thermodynamic and one kinetic.

There is a relation between the n concentration gradients in Eq. (13) and for practical calculations one usually chooses to eliminate one of them. The reduced diffusivities in a volume-fixed frame of reference, where it is assumed that all the substitutional species have the same partial molar volumes, and furthermore, only the substitutional species contribute to the volume, i.e. the DICTRA frame of reference, is expressed as,

$$D_{kj}^n = D_{kj} - D_{kn} \quad (\text{when } j \text{ is substitutional}), \quad (15a)$$

$$D_{kj}^n = D_{kj} \quad (\text{when } j \text{ is interstitial}), \quad (15b)$$

where n is taken as the dependent species. Using these diffusivities Eq. (13) now becomes,

$$J_k = -\sum_{j=1}^{n-1} D_{kj}^n \frac{\partial c_j}{\partial z} \quad (16)$$

Eq. (16) contains the so-called interdiffusion coefficients, sometimes referred to as chemical diffusivities. These diffusivities may be evaluated experimentally from e.g. diffusion couple experiments.

7.3.3 Intrinsic diffusion coefficients

The individual or intrinsic diffusion coefficients, that are defined in the lattice-fixed frame of reference by:

$$\tilde{J}_k = -\sum_{j=1}^{n-1} {}^i D_{kj}^n \frac{\partial c_j}{\partial z} \quad (17)$$

can also be evaluated from diffusion couple experiments, if in addition to concentration profiles the Kirkendall velocity can be estimated from the movement of inert markers. As the interdiffusion coefficients, the intrinsic diffusion coefficients can also be calculated from the mobilities. However, this time by applying the chain rule of derivation on Eq. 9 and remembering that $L_{ki} = 0$ when $k \neq i$

$$\tilde{J}_k = -\sum_{i=1}^n L_{kk} \frac{\partial \mu_k}{\partial c_j} \frac{\partial c_j}{\partial z} \quad (18)$$

The intrinsic diffusion coefficients may be identified in Eq. 18 as:

$${}^i D_{kj} = L_{kk} \frac{\partial \mu_k}{\partial c_j} \quad (19)$$

Also here there is a relation between the n concentration gradients. If one of the concentrations are chosen as dependent, and if the same approximation as previously used for the partial molar volumes of the different elements is applied, then the intrinsic diffusion coefficients defined in Eq. 17 are finally found.

$${}^i D_{kj}^n = {}^i D_{kj} - {}^i D_{kn} \quad (\text{when } j \text{ is substitutional}), \quad (20a)$$

$${}^i D_{kj}^n = {}^i D_{kj} \quad (\text{when } j \text{ is interstitial}), \quad (20b)$$

7.3.4 Self-diffusion coefficient

The self-diffusion coefficient of A is the diffusivity of A in the limit of pure A. Studies of self-diffusion usually utilize radioactive tracer atoms A^* of the same element.

7.3.5 Impurity diffusion coefficient

When the diffusion of a solute B in a solvent A is studied at an extremely small concentration of B, which e.g. radio tracers permit, then the impurity diffusion coefficient of B in A is observed.

7.4. How to create a kinetic database

Naturally, the handling and storage of kinetic data will benefit from the use of some kind of database management. Thus, the TDB database definition file syntax described in Manager's guide to Database Module TDB, found in the Thermo-Calc User's guide^[2] has been extended to incorporate a few new keywords needed when storing kinetic data. The DICTRA extensions to the database definition file syntax are described in Appendix A.

A kinetic database may be established with different levels of ambition. If experimental data are available a complete assessment of the atomic mobilities can be performed from which the diffusion coefficient matrix can be calculated. To make a complete assessment however, is a rather time consuming task and hence a simpler approach may sometimes be useful. Also, since experimental data are lacking for many systems the simpler approach may be applied in order to have at least a qualitative result.

It will now be demonstrated in principle how a simple and an optimized Ni-Al database for the face-centered cubic phase can be created.

7.4.1 Simple Ni-Al database for dilute face-centered cubic Ni-alloys

The first step to be taken when creating either a simple or a more advanced kinetic database is to define element, phase, and constituent data for the considered system. This is simply accomplished by copying this information from the appropriate thermodynamic database (i.e. the thermodynamic database which are later going to be used for the simulation). For the simple Ni-Al database, which can be found in Appendix B, the data was taken from the SSOL database^[10].

In addition to this, it is necessary to provide some data on the molar volume of the various phases, and to define zero-volume species. The former is provided by the parameter VS, and so far no ambitious attempts have been made in order to enter any quantitative data. Thus, at the moment it is assumed in the database that all phases have the same molar volumes. The elements which do not contribute to the volume are defined by the command ZEROVOLUME_SPECIES. In the Ni-Al case Va will be the only zero-volume specie. Now it is time to define the diffusion model to be used. As can be seen in Appendix A, this is accomplished by the keyword DIFFUSION. In the simple Ni-Al database, Appendix B, the default model was chosen and thus there is no need to specify a diffusion model.

Finally, it is time to provide the mobility parameters, the MF's ($RT \ln M_B^0$) and MQ's ($-Q_B$). Since in the simple Ni-Al database the default diffusion model is used and not the magnetic, there is no need to separate the MF's and the

MQ's. Thus, as previously shown it is possible to merge these two parameters into one single parameter, e.g. $MQ = -Q_B + RT \ln M_B^0$. If for the simple Ni-Al database it's assumed that the mobilities are independent of concentration, then only two parameters are needed, i.e. the mobilities of Al in Ni, and Ni in Ni. This data can be extracted from data on the impurity diffusion coefficient of Al in pure Ni and from data on the self-diffusion coefficient of Ni. The parameters in Appendix B were extracted from the following data:

$$D_{Al}^{Ni} = 7.5 \cdot 10^{-4} \exp\left(\frac{-284000}{RT}\right) \quad (m^2 / s)$$

$$D_{Ni}^{Ni} = 2.26 \cdot 10^{-4} \exp\left(\frac{-287000}{RT}\right) \quad (m^2 / s)$$

Figure B1 shows the interdiffusion coefficient ($D_{AlAl}^{Ni} = D_{NiNi}^{Al}$) in the Ni-Al system at 1200°C as a function of Al-concentration. The solid line was calculated from the data in Appendix B. The symbols are experimental data from Yamamoto et al.^[11]. Evidently, in this case it was possible to predict the concentration dependency of the interdiffusion coefficient rather well assuming concentration independent mobilities.

7.4.2 Optimized Ni-Al database for the face-centered cubic phase

If experimental data is available, it is possible to use this information in order to optimize the mobility parameters and creating a more complete database. The data from Yamamoto et al.^[11] was used in example f2 in DICTRA's example volume in order to optimize the interaction parameters, $MQ(\text{FCC_A1\&AL,AL,NI:VA})$ and $MQ(\text{FCC_A1\&NI,AL,NI:VA})$. In addition, in this example proper end points on the Al-side were used. These new end points were extracted from the impurity diffusion coefficient of Ni in Al, and from the self-diffusion coefficient of Al. These end points can of course also be assessed in an optimization procedure if multiple experimental data exist. Appendix C is a database which has been created from the optimization result in example f2. Figure C1 shows a comparison between the calculated interdiffusion coefficient and the experimentally measured one.

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Appendix A, DICTRA extensions to the database definition file syntax

PARAMETER [special GES parameter name] [low temp. limit]
[FTP-function] [upper temp limit] {Ref. Index} !

The keyword PARAMETER allows for, in addition to the GES parameter names for thermodynamic data, five extensions suitable for kinetic data. Valid extensions to GES parameter names are:

MQ	←	Activation enthalpy for mobility equation.
MF	←	Pre-exponential factor for mobility equation.
DQ	←	Activation enthalpy for diffusivity equation.
DF	←	Pre-exponential factor for diffusivity equation.
VS	←	Volume counted per mole of volume carrying species.

Examples:

```
PARAMETER MQ(BCC_A2&CO,FE:VA) 298.15 -232000; 6000 N 8!
PARAMETER MF(BCC_A2&CO,FE:VA) 298.15 +R*T*LN(13.0E-5); 6000 N 8!
PARAMETER DQ(FCC_A1&AL,*) 298.15 -284000+R*T*LN(7.5E-4); 6000 N 10!
PARAMETER DF(FCC_A1&AL,*) 298.15 0; 6000 N 10!
PARAMETER VS(FCC_A1) 298.15 1.0E-5; 6000 N !
```

DIFFUSION [keyword] [phase name] [additional parameter(s)] !

The keyword DIFFUSION specifies what type of diffusion model to use for a phase if the default model is not wanted. In the default model the full diffusion matrix is calculated. A diffusivity is calculated from the different mobilities and the thermodynamic factors.

The former ones are calculated as

$$M = \exp\left(\sum MF / RT\right) \exp\left(\sum MQ / RT\right) / RT$$

where Σ stands for a weighted summation of the different MF's and MQ's plus possibly a Redlich-Kister term.

Valid model keyword are:

NONE	Remark: no diffusion in this phase
DILUTE	constitution list of dependent species in each sublattice must be given as additional parameter. Only the diagonal terms

in the diffusion matrix are calculated.

$$M = \exp\left(\sum DF / RT\right) \exp\left(\sum DQ / RT\right)$$

MAGNETIC the so-called ALPHA and ALPHA2 parameters must be given as additional parameters. ALPHA is for the substitutional magnetic model and ALPHA2 for the interstitial one. By appending an "&" (and) and a specie name after the alpha keyword one can supply individual values for the different species. The full diffusion matrix is calculated.

USE_POLY3 for phases which are modeled with the same species on several sublattices, e.g. Sigma and $M_{23}C_6$. For such phases it's necessary to perform equilibrium calculations using POLY-3 in order to calculate the diffusivities. The full diffusion matrix is calculated. From DICTRA ver. 25 a better option is to use the diffusion model GENERAL described below.

ORDERED Used for phases with chemical ordering. A contribution to the activation enthalpy of the mobility depending on the degree of long-range order is added. The model has been tested on the B2-BCC phase of the Al-Fe, Al-Ni, and Al-Fe-Ni systems, see Helander and Ågren, *Acta mater.*, **47** (1999), pp.1141-1152 and Helander and Ågren, *Acta mater.*, **47** (1999), pp.3291-3300. The contribution from ordering is added to the mobility of the disordered state. The disordered state is found in a separate phase which must be given when using this keyword.

GENERAL Used for phases that is modelled with the same specie on several sub-lattices, as well as to manage phases modelled with charged species e.g. Cr^{3+} etc. Mobilities are specified separately for each sub-lattice. Note that for phases modelled with a contribution from chemical ordering the database diffusion model keyword should still be "ORDERED"

Examples:

```
DIFFUSION NONE SIGMA !
DIFFUSION DILUTE CEMENTITE : FE : C : !
DIFFUSION MAGNETIC BCC_A2 ALPHA=0.3 ALPHA2&C=1.8 ALPHA2&N=0.6 !
DIFFUSION USE_POLY3 M23C6 !
DIFFUSION ORDERED B2_BCC DISORDER_PHASE BCC_A2 !
DIFFUSION GENERAL SPINEL !
```

ZEROVOLUME_SPECIES [list of species] !

In DICTRA one has applied the assumption that the volume is carried by the

substitutional elements only. The interstitial elements are assumed to have zero molar volumes. The keyword ZERO_VOLUME_SPECIES takes as argument a list of which species are to be considered as zero volume ones.

Examples:

```
ZERO_VOLUME_SPECIES VA C N !
```


Figure B1

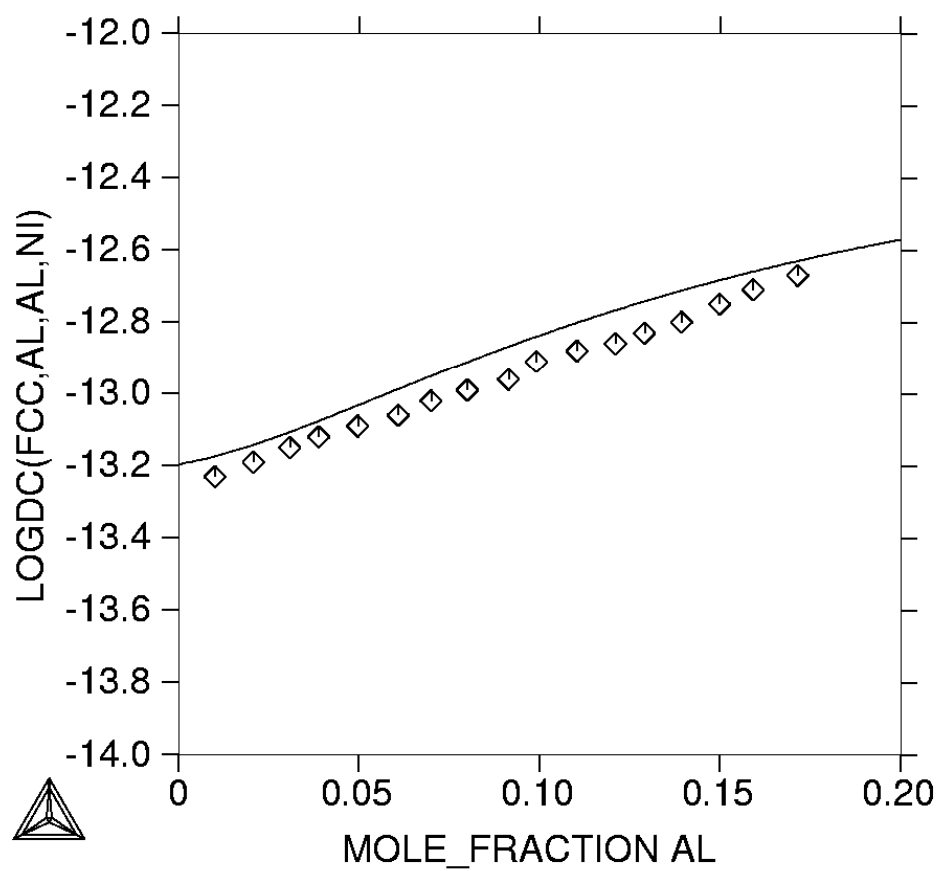


Figure C1

