DICTRA Module User Guide

Thermo-Calc 4.1

DICTRA Module User Guide

Contents

1   Introduction

DICTRA is a module in the Thermo-Calc software package for simulation of diffusion controlled transformations in multicomponent systems. The simulation calculations in DICTRA are both time- and space-dependent.

DICTRA is particularly suitable for solving diffusion problems that includes a moving boundary (so-called Stefan problems). The multicomponent diffusion equations in the various regions of a material are solved under the assumption that thermodynamic equilibrium holds locally at all phase interfaces. Simulations are one-dimensional and three different geometries can be performed: planar, cylindrical and spherical.

You can set the boundary conditions in many different ways. This allows you to solve many types of problems:

- 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 para-equilibrium conditions

1.1   Documentation for DICTRA

Apart from this document, you can use the following documentation to learn more about how to use DICTRA:

DICTRA Command Reference
> contains information about all the commands that are available in the DICTRA module. For each command there is a brief description of what the command does, what the command's parameters are (if any), and what kind of values you can give the parameters

Online help in DICTRA
> contains information about modules, commands, and conditions

DICTRA Examples Collection

> contains example macro files that demonstrate different ways in which you can use DICTRA. See .

Thermo-Calc Console Mode User Guide

> describes how to get started using Thermo-Calc in the Console mode.

1.1.1 This User Guide

Target group

This user guide is intended for new users of the DICTRA module in the Thermo-Calc program. It is expected that such a user has some familiarity with the Thermo-Calc console mode and its command-line interface. Furthermore, it is expected that such a user understands the basics of thermodynamics.

Purpose

This DICTRA User Guide is intended to get you started using the DICTRA module. It gives you a brief overview of the program and its various components, and describes in generic terms how you can define your system of components, set up and perform simulations, as well as visualize the results.

Content

Chapter 2 briefly describes some general features of the DICTRA module. This chapter also includes a description of the typical workflow when using DICTRA. Chapter 3 describes important basic concepts of the DICTRA software.

Chapters 4, 5 and 6 then follows your typical workflow for using DICTRA. Chapter 4 describes how you define which elements your system contains and retrieve necessary thermodynamic and kinetic data about the elements. Chapter 5 describes how you configure and run simulations, and chapter 6 how you plot the simulation results. Finally, chapter 7 contains some recommendations and guidelines for configuring and troubleshooting different kinds of simulations.

Note that this User Guide is only a guide to get you started using DICTRA. Once you have learned the basics from this User Guide, you can turn to other learning resources.

The following conventions will be used throughout this User Guide:

- Console command name are written in small upper case letters. For example, the command for calculating an equilibrium is COMPUTE_EQUILIBRIUM.

- Examples of how you can use a command are written like this:

      SET_CONDITION GLOBAL

- Menu items are referred to by the menu name and the name of the item, separated by a vertical line ("|"). For example, "select Menu | Print PS" means, select the menu item "Print PS" from the "Menu" menu.

1.1.2 Using online help

At the command line prompt in the Console, you can access online help information in several ways:

- To get a list of all the available commands in the current module, simply type a question mark ("?") and press the enter key.
- To get a description of a specific command, use HELP followed by the name of the command. Note that you can only get online help information about a command that is available in the module that you are currently in.
- To get more general information about the system, use INFORMATION. You will be requested to specify about which subject want information. Answer "?" in response and you will get a list of all the subjects on which you can get more information. Note that this subject list is specific to the module you are currently in.

1.1.3 Contents of the DICTRA Examples Collection

To learn more about how to use DICTRA, you can run and study the examples in the *DICTRA Examples Collection*. This is a collection of macro files that you can run in DICTRA. Each example consists of three macro files: a "setup" macro, a "run" macro and a "plot" macro. You must run these three macros in order.

The pdf document *DICTRA Examples* contains the contents of the macro files and the output with which DICTRA responds. The macros are also extensively commented.

The table in Appendix 1: DICTRA Examples Collection provides a brief description of each example in the collection.

1.2 Program overview

DICTRA consists of two Thermo-Calc modules: the DICTRA_MONITOR module and the DIC_PARROT module. In this user guide, the abbreviated name "the DICTRA module" will be used to refer to the DICTRA_MONITOR module.

The DIC_PARROT module is used for assessing experimental data and using such data to optimise calculations. This user guide does not cover how to use the DIC_PARROT module.

For more information about the various modules that are available in Thermo-Calc, see the *Thermo-Calc Console Mode User Guide*.

1.3 Licenses for using DICTRA

The DICTRA module in Thermo-Calc requires a separate DICTRA license. Without such a license, you cannot enter the DICTRA module.

If you are using a network client installation of Thermo-Calc, then you may not be able to enter the DICTRA module even if you have access to a license server with a valid network license file. This is because other clients that are part of your network installation may have "checked out" all instances of the DICTRA license that the network license allows you to run simultaneously. A DICTRA license is checked out when you enter the DICTRA module and it is checked back in when you leave the module.

To display information about who has checked out licenses from your license server, use the SYS command DISPLAY_LICENSE_INFO, or select "Show License Info" from the "Help" main menu.

Note that if you have entered and used the PARROT module, then you will not be able to enter the DIC_PARROT module during the same session. You must close down Thermo-Calc and launch the program again to enter DIC_PARROT. If you try to enter DIC_PARROT after having been in the PARROT module earlier in the session, you will get the following message:

```
DICTRA PARROT disabled after using PARROT
```

2 Using the DICTRA module

The enter the DICTRA module, enter GOTO_MODULE DICTRA in the Thermo-Calc console.

2.1 Using log, macro, and workspace files

DICTRA makes use of a few different kinds of files: log files (*.LOG), macro files (*.DCM) and workspace files (*.DIC).

2.1.1 Using Log files

Log files are plain text files used to save a sequence of commands. Log files can be edited in a text editor.

To start saving your input into such a file, use SET_LOG_FILE in the SYS module, followed by the name of the file that you want to save your command sequence to.

If you want to save DICTRA's output in the log file as well, use SET_ECHO before the SET_LOG_FILE command. Doing this is often useful if you want to use the log file later as a macro file.

2.1.2 Using Macro files

Macro files are plain text files used to save a sequence of commands that can be loaded and executed. Macro files can be edited in a text editor. You add comments to the file by starting a line with "@@".

To run a macro file, use MACRO_FILE_OPEN in the SYS or DICTRA module, followed by the name of the macro file. DICTRA will then immediately execute the command sequence that the file contains.

The macro must end with EXIT or, if you want to remain in the console and continue to use the program, in the SYS, DICTRA, POLY, or POST module with the command SET_INTERACTIVE.

2.1.3 Using workspace files

You can save all the data in your current workspace by first using SAVE_WORKSPACES which is available in the DICTRA module. The workspace will contains all the settings you have specified and the result of any calculations you have performed after using SAVE_WORKSPACES. Consequently, the command opens a workspace in which all data is saved which is generated after the SAVE_WORKSPACE command has been executed. The saved data will include original and modified thermodynamic data, your last set of conditions and options, and the results of any simulation.

To load the data and calculation results of a workspace file, use the READ_WORKSPACES command that is available in the DICTRA module.

2.2 Writing functions

You will sometimes have to specify functions when you set up your system in DICTRA. For example, you may want to make global and boundary conditions vary as a function of time. All of the following operators can be used in writing functions. Use a semi-colon (";") to mark the end of a function.

Operator	Description
+, -, *, /	addition, subtraction, multiplication, division
**	exponentiation
SQRT(X)	square root
EXP(X)	Exponential
LOG(X)	natural logarithm
LOG10(X)	base 10 logarithm
SIN(X), COS(X), ATAN(X)	sinus, cosinus and arctangent
SIGN(X)	sign function SIGN(X) is -1 when X<0, is 0 when X=0 and is 1 when X>0.
ERF(X)	error function

2.3 Specifying time-dependent profiles

In using DICTRA you will often be prompted to specify a time-dependent profile for some condition.

To define such profiles or intervals, you will be prompted to enter the following information:

"LOW TIME LIMIT"   This determines the time at which the function will start to apply.

 "HIGH TIME LIMIT"   This determines the time at which the function will stop to apply. To set the high limit to the time when the simulation ends, enter an asterisk ("*").

"ANY MORE RANGES"   Enter "Y" to specify an additional range with a time-dependent function, which will start to apply at the time step after the high time limit of the previous range have been reached. Enter "N" if you do not want to specify any more ranges.

2.4 Typical workflow

The following figure represent the typical workflow when you set up a problem and run a simulation in DICTRA. The solid arrows represent your typical movements between the modules. The dashed arrows represent movement of data within DICTRA.
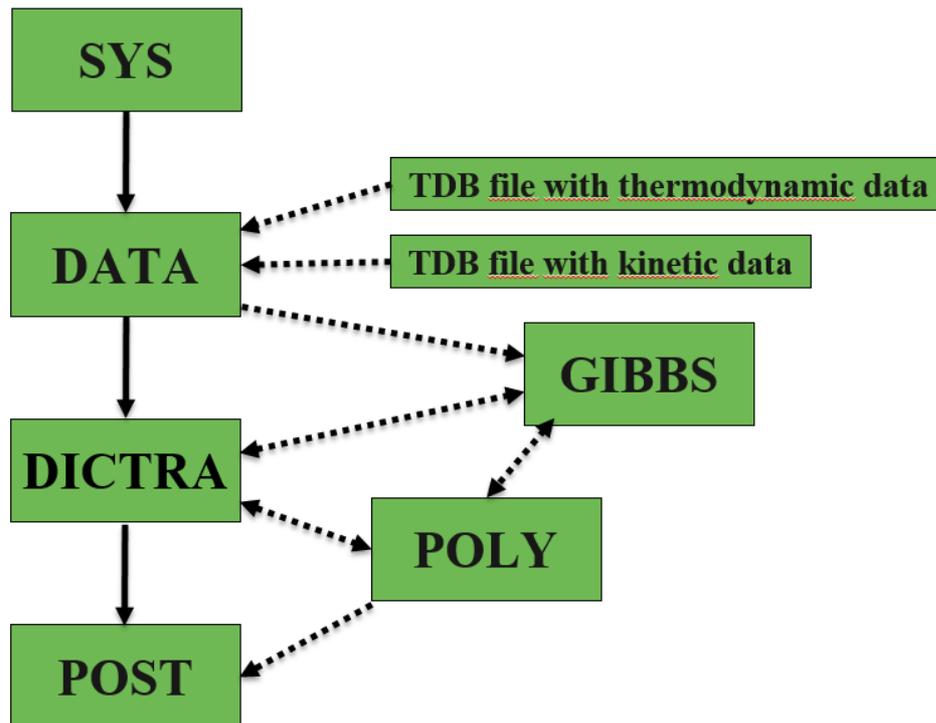
The basic workflow is the following:

1. When you start Thermo-Calc, you find yourself in the SYS module.

2. Define your system in the DATA module: Before performing your calculation, you must define your system and retrieve thermodynamic data as well as kinetic data. The data is retrieved from database files, and the data needed for describing your system is sent to the GIBBS module. See chapter 0 for more information.

3. When you have done this, DICTRA will be able to access the retrieved data. The retrieved data will also be accessible to the POLY module, which will be involved in simulations that require that equilibrium calculations are performed.

4. Set the initial state of the system, define its geometry and boundary conditions in the DICTRA module. The simplest system has one cell that contains one region, but you may put additional regions in a cell and put additional cells in your system. You must also define which phases each region contains. In the DICTRA module, you can set various parameters for the numerical calculations as well, such as at which grid points in the system where you want to perform calculations.

5. Run the simulation from within the DICTRA module.

6. Plot and visualize your data in the POST module. You can choose which data to plot and change the appearance of the diagram in a host of ways. You can save the diagram as an image file (in many different formats). See chapter 6 for more information.

3 Basic concepts

The basic concepts used when defining problems in DICTRA are presented in the following.

3.1 System, cells and regions

In DICTRA, your system will normally consist of one cell. This cell contains one or several regions in which the diffusion problem is to be solved. A system of diffusion equations will be solved for each region. The size of the system is simply the sum of sizes of all the regions in all the system's cells.

The interface between two regions will typically move as the result of a simulation, that is, the regions will grow or shrink. Such an interface is called an "inner interface". The boundary of a cell is called an outer interface and the condition of this type of interface may be affected by the user's choice of boundary conditions.

For some simulations, it will be useful to have several cells in your system. Matter can move between cells. However, it is assumed that there is diffusional equilibrium between all cells (this means that there are no differences in diffusion potentials between cells). In other words, the size of a cell is fixed during the simulation.

The system is by default a closed system, which means that matter cannot move across its boundaries. However, you can change this setting for both the lower boundary (left side/centre) and the upper boundary (right side/surface) of the system. You can also set these boundary conditions to vary as a function of time, temperature and/or pressure.

3.2 Global conditions

There are a number of global parameters that will influence the rate of the diffusion in your simulation: temperature, pressure, and heat content removal. All these parameters are defined as functions of time. It is also possible to let the temperature be a function of the spatial position, and heat content removal as a function of temperature or pressure.

For heat content removal, the amount of extracted heat per time unit is normalized and the size of the system is normalized to 1 mole of atoms.

3.3 Geometry and coordinates

DICTRA can only handle diffusion problems where composition vary along one spatial coordinate. The geometry of your system can be planar, cylindrical or spherical. A planar geometry corresponds to an infinitely wide plate of a certain thickness. A cylindrical geometry corresponds to an infinitely long cylinder of a certain radius. Finally, a spherical geometry corresponds to a sphere with a certain radius.

If your system has a planar geometry, then the lower boundary (the zero coordinate) is at the left side of the system. The upper boundary (the coordinate with the highest value) is at the right side of the system. If your system has a cylindrical or spherical geometry then the lower boundary (the zero coordinate) is by default at the centre of the cylinder/sphere. The upper boundary (the coordinate with the highest value) is at the "surface" of the cylinder/sphere. For cylindrical and spherical geometry it is possible to enter a leftmost coordinate that is larger than zero to allow for "tube" and "hollow sphere" geometries.

3.4 Regions and grid

A region contains one or more phases. If a region contains several phases one of those must be entered as a "matrix" phase whereas the others are entered as type "spheroid".

A region must also contain a number of grid points. The composition is only known at these grid points and DICTRA assumes that the composition varies linearly between them. The amount and composition of all the phases present at a single grid point in a certain region are those given by thermodynamic equilibrium keeping the over-all composition at the grid point fixed.

3.5 Phases

Each region contains one or more phases. A phase may be of three different types, matrix, spheroid or lamellar type.

Matrix	The matrix phase is the region's primary phase. If there is only one phase in a region, then that phase is automatically of the matrix type.
Spheroid	This type is used to treat one or several dispersed phases in a matrix. It should be noticed that unless the homogenization model is invoked, which happen automatically when a spheroid phase is entered, then diffusion is only considered in the matrix phase; the spheroid phases then only act as sources and sinks of the diffusing elements.
Lamellar	This type is used to simulate the growth of a eutectic or eutectoid region. The program can only treat the growth, but not the dissolution, of such a region. The pearlite calculation model will be used for a phase that is Lamellar.

A phase can be introduced with the status "active" or "inactive", where active is default. An inactive phase is a phase which will not participate in the calculations until it has become stable.

If a phase is inactive, then the driving force for precipitation of the phase is continuously monitored. When the driving force exceeds a predefined positive value, the phase will take part in the simulation and the phase automatically becomes active. A new region is then created and the formerly inactive phase is entered as the matrix phase of the new region. The name of the region is set to the name of the phase that just became active but with "R_" added as a prefix.

3.6 Compositions

The DICTRA program uses two types of composition variables internally, namely site-fractions and u-fractions, although you may also use for example weight fraction or mole fraction.

The site-fractions are used in setting up the problem and interfacing with POLY-3. 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.

The u-fractions are used in the diffusion equations. The u-fraction of a component k is defined as

$$u_k = \frac{x_k}{\sum_{j \in S} x_j}$$

The summation is only performed over the substitutional elements. The choice of the volume fixed frame of reference in the calculations make it convenient 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 element is assumed to not contribute to the volume. Substitutional elements are assumed to contribute equally to volume.

3.7 Types of problems

DICTRA is used to simulate diffusion-controlled transformations in multicomponent alloys. The following subsections briefly characterizes some of the types of problems that DICTRA simulations can handle.

For more information on how to use DICTRA to run different kinds of simulations, see the *DICTRA Examples Collection*. See Appendix 1: DICTRA Examples Collection for a list of all the available examples.

3.7.1 Diffusion in a single-phase system

The simplest type of simulation you can perform in DICTRA is a simulation of how certain components in one phase diffuse over time in that single phase. To simulate this kind of problem, you just need to create one region and enter one phase into that region. You can set up the system under various conditions by defining profiles for how temperature and pressure will change over time, or for how the boundary conditions of the region will change over time.

3.7.2 Moving boundary multi-phase system

With two regions in a single cell you can simulate how diffusion causes phase transformations. For example, you can simulate how an individual particle grow or dissolve as a function of time. The result is a simulation of how the boundary between the regions migrate over time. As in the case of a one-phase simulation, you can set up the system under various conditions by defining profiles for how temperature will change overtime, or for how the boundary conditions of the region change overtime.
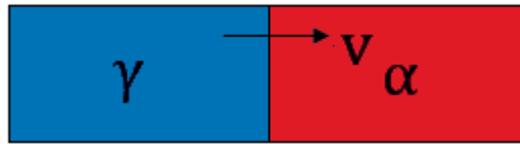
Normally, simulations in DICTRA are performed under the assumption that thermodynamic equilibrium holds locally at all phase interfaces. However, it is also possible to simulate a moving phase boundary problem while assuming that para-equilibrium conditions apply at the phase boundary.
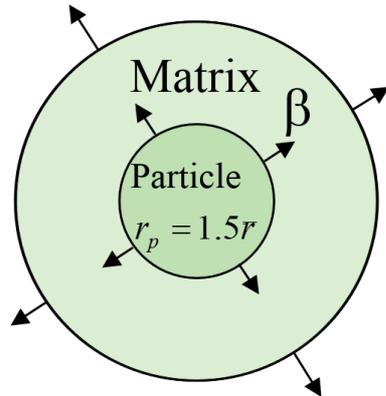
3.7.3 Coarsening processes

You can run a simulation of a coarsening process in DICTRA. In accordance with Lifshitz-Slyozov-Wagner theory, this is done by assuming that the coarsening can be simulated by calculating the growth of a single particle of the maximum size in the particle size distribution.

3.7.4 Diffusion in disperse systems

You can perform simulations where one or more dispersed phases are present in a matrix phase. For example, you can simulate how carburization causes precipitation of carbides in an austenitic matrix phase. The dispersed phases act as point sinks or sources of solute atoms in the simulation and their fraction and composition is calculated from the average composition in each node, assuming that equilibrium holds locally in each volume element.
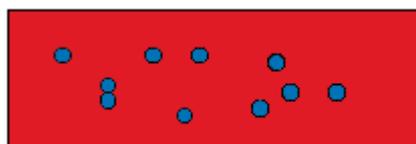
There are two ways in which you can simulate diffusion in a system that contains a dispersed phase, but it is strongly recommended that you use the so-called homogenization model. The homogenization model allows you to take into account diffusion in all phases for which you have kinetic data; the homogenization model treat all phases in the same way regardless of which phase was entered as type matrix and which phases were entered as type spheroid.
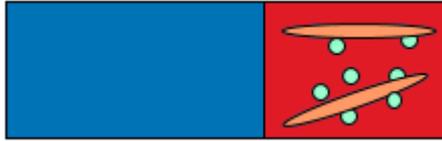
3.7.5 Cooperative growth

You can simulate the growth of pearlite in alloyed steels by calculating the Eutectoid reaction γ→α+β, where α and β grow cooperatively as a lamellar aggregate into the γ matrix.

4   System definition: retrieving data

In order to perform a simulation in DICTRA, both a thermodynamic database and a kinetic database is needed. The thermodynamic database is a normal Thermo-Calc database, whereas the kinetic database contains information about the atomic mobility of individual components in various phases.

To avoid that the diffusion problem will be unsolvable, , it is recommended that you make the problem as simple as possible. Therefore, define your system with as few components and phases as possible.

4.1   How to define your system

To define your system means to select its components and to retrieve thermodynamic and/or kinetic data about those components from an appropriate database. This section describes how you do this in the DATA module.

Pre-requisites

To define your system, you must be in the DATA module. Use GOTO_MODULE DATA to enter it.

Procedure

To define your system, follow these steps:

Step	Action
1	Use SWITCH_DATABASE to select database. Unless you directly specify the name of the database as a parameter to the command, the available databases will be listed, and you will be prompted to specify which you want to use.
2	Use DEFINE_ELEMENTS followed by a list of the elements that you want in your system. (To list the elements that are available in your current database, use LIST_DATABASE ELEMENTS.)
3	To make sure that you do not retrieve phases from the database that you do not need, use REJECT PHASES *.
4	Restore the phases that should be included using RESTORE PHASES.
5	Use GET_DATA to read from the database and send the thermodynamic data about your system to the GIBBS and DICTRA workspace.
6	Use APPEND_DATABASE to select the database from which you want to retrieve kinetic data.
7	Define your elements and specify whether to reject and restore any phases. Do this in exactly the same way as you would for the thermodynamics data (see the preceding step 2, 3 and 4).
8	Use GET_DATA to read from the database and add the kinetic data to the thermodynamic data that already exists in the GIBBS and DICTRA workspace.

Use APPEND_DATABASE again if you want to add thermodynamic or kinetic data from yet another database. When you have retrieved all the data you need, you can proceed to the DICTRA module.

5   Configuring your DICTRA calculation

This section describes in general terms what options you have when setting up your problem in DICTRA.

5.1 Setting global conditions

Use SET_CONDITION GLOBAL to set global conditions. Global conditions include temperature (T), heat content removal (Q) and pressure (P). They reduce the degrees of freedom for equilibrium calculations. Note that if the heat content removal is specified only the initial temperature should be entered with the SET_INITIAL_TEMPERATURE command. In practice, the pressure is rarely specified. By default the pressure is assumed to be constant and equal to 1 bar.

For each condition, you can define a profile over time that consists of several intervals of time, or "ranges", with each such range having its own function that defines the value of the condition.

Temperature can be entered as a function of time (TIME) and/or spatial coordinate (X). The pressure condition can be defined as a function of time (TIME). The heat content removal can be defined as a function of temperature (T), pressure (P) and/or time (TIME).

For example, the following function could specify a cooling rate if it is used to specify how the global condition temperature (T) changes with time (TIME) during a certain range:

```
1900-1*TIME;
```

5.2 Specifying the geometry

A system in DICTRA will by default have a planar geometry. To change the geometry of the system, use ENTER_GEOMETRICAL_EXPONENT followed by a numeral 0, 1 or 2. The numerals correspond to the following geometries:

'0' = Planar geometry.

'1' = Cylindrical geometry.

'2' = Spherical geometry.

With a cylindrical or spherical geometry, the system's zero coordinate (left boundary) is at the centre of the cylinder or sphere. The highest coordinate (right boundary) is defined by the cylinder's or sphere's radius. If you want a geometry corresponding to a tube or a hollow sphere, then use SET_FIRST_INTERFACE to locate the system's left boundary at a coordinate that is greater than zero.

5.3 Entering regions and gridpoints

You enter a new region by specifying its name and, unless it is the first region, how it should be located with respect to one already existing region. The size of a region is determined when you enter a grid into the region.

5.3.1 How to create a region

This section describes how to enter a new region in your system.

Pre-requisites

You must have defined your system before you create a region. See section 0.

Procedure

To enter a new region, follow these steps:

Step	Action
1	Use ENTER_REGION to enter a region into the system.
2	Enter an arbitrary name for the region at the "REGION NAME" prompt. If this is the first region you create in your system, then the procedure stops here. Otherwise, you will continue to the next step.
3	Enter the name of an already existing region to which the new region will be attached.
4	Specify whether the new region should be "ATTACHED TO THE RIGHT OF" the existing region. Enter "Y" to attach to the existing region's right side or "N" to attach it to its left side. If your system has a cylindrical or spherical geometry, then this is a question of whether to put the new region outside the existing region, so that the new region surrounds the existing one, or to put it at the existing region's centre, so that the existing region will surround the new region.

5.3.2 How to put a grid in region

This section describes how you specify the size and grid point distribution to use in a region.

Pre-requisites

You must have created the region that you will enter a grid in.

Procedure

To specify the size and grid point distribution for a region, follow these steps:

Step	Action
1	Use ENTER_GRID_COORDINATES followed by the name of the region.
2	Specify the width of the region in meters. .
3	Enter how many grid points that the region should contain at the "NUMBER OF POINTS" prompt.
4	Specify the type of grid point distribution you want to have in the region. ・ "LINEAR": A linear grid will give an equally spaced grid.

- "READ_POINT_BY_POINT": This allows you to read a number of specific grid points from a data file. The input source from which to read the points when entering values point by point. If you want to enter the grid points at the terminal, then enter "READ_POINT_BY_POINT TERMINAL".

- "GEOMETRIC": A geometrical grid will yield a varying density of grid points in the region.. You will be prompted to enter the "VALUE OF R IN THE GEOMETRICAL SERIES", which determines the distribution. A geometrical factor larger than one will yield a higher density of grid points at the lower end of the region and a factor smaller than one will yield a higher density of grid points at the upper end of the region.

- "DOUBLE_GEOMETRIC": A double geometrical grid makes it possible to have a high number of grid points in the middle or at both ends of a region. You will be prompted to specify two geometrical factors. "VALUE OF R IN THE GEOMETRICAL SERIE FOR LOWER PART OF REGION" determines the distribution in the the lower (left) part of a region, while the "VALUE OF R IN THE GEOMETRICAL SERIE FOR UPPER PART OF REGION" determines the distribution in the upper (right) part of a region.

5.4 Setting boundary conditions

Boundary conditions are conditions that define how matter behaves at the boundaries of your system. By default, matter is not allowed to cross the system boundaries.

The following types of boundary conditions are available:

FIX_FLUX_VALUE   Enter functions that yield the flux times the molar volume for the independent components. May be a function of time, temperature and pressure. Use this boundary condition with caution since it may cause unrealistic compositions.

STATE_VARIABLE_VALUE

A legal equilibrium condition 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. Conditions for temperature and pressure should not be specified here since they are taken from the global conditions.

POTENTIAL_FLUX_FUNCTION

This is used to take into account the finite rate of a surface reaction. The flux for the independent components must be given in the format:

$$J_k = f_k(T, P, TIME) * \left[POTENTIAL_k^N - g_k(T, P, TIME) \right]$$

The functions f and g may have time (TIME), temperature (T), and/or pressure (P) as arguments. N is an integer. The potentials are those with user defined reference states.

ACTIVITY_FLUX_FUNCTION

This is used to take into account the finite rate of a surface reaction. The flux for the independent components must be given in the format:

$$J_k = f_k(T, P, TIME) * \left[ACTIVITY_k^N - g_k(T, P, TIME) \right]$$

The functions f and g may have time (TIME), temperature (T), and/or pressure (P) as arguments. N is an integer. 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. This is the default boundary condition.

MIXED_ZERO_FLUX_AND_ACTIVITY

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

GAS   This is the only boundary condition that may cause a change in system volume. 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.

5.4.1 How to set a boundary condition

This section describes the procedure for setting boundary conditions.

Pre-requisites

You must have defined your system and created a region. See section 0.

Procedure

To set a boundary condition, follow these steps:

Step	Action
1	Use SET_CONDITION BOUNDARY.
2	Specify whether you want to set the LOWER or the UPPER boundary.

3   Specify which condition type you want to set the boundary to.

4   Enter any parameter values that are necessary for the condition type you have chosen.

5   Specify the "LOW TIME LIMIT", when the function you will define will start to apply.

6   If required, enter the function that will be applied during the time interval. For most condition types, the function may have time, temperature and pressure as arguments.

7   Enter the "HIGH TIME LIMIT" for the interval.

8   If you want to define a different function for another time interval, then enter "Y" when prompted with "ANY MORE RANGES". You will then be requested to enter another function for the next range.

        When you have defined functions for all the ranges you want, enter "N" at the "ANY MORE RANGES" prompt.

5.5 Entering phases in regions

When a region has been defined, you must enter one or more phases in the region. How many phases you should enter, and of which types, depend on the kind of simulation you want to run. Note that there is no supersaturation locally within a given region. Here are three examples:

   · If you want to simulate diffusion of components within one phase, then you should enter one matrix into the region.
   · If you want to simulate how an interface between regions move, then enter two regions with at least one phase in each.
   · If you want to simulate growth of one or more dispersed phases in a matrix phase, then enter one matrix phase and one or more spheroid phases.

5.5.1 How to enter a phase in a region

Pre-requisite

You must have created at least one region in which to enter the phase.

Procedure

To enter a phase in a region, follow these steps:

Step	Action
1	Use ENTER_PHASE_IN_REGION to enter a phase in a previously created region.
2	Specify whether the phase is to be "ACTIVE" or "INACTIVE". If you enter an inactive phase, then you will be requested to specify the following: · Enter the name of the region and the side of that region which the phase will be attached to.

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

- Enter the "CONDITION TYPE" that the phase boundary condition should be set to if the inactive phase becomes stable. (Inactive phases will only be considered in the simulation calculations once it has become stable.)

If you enter an active phase, the procedure is as follows.

3   Specify the "REGION NAME" for the region in which the phase is to be entered.

4   Specify the "PHASE TYPE". A phase can be of type "MATRIX", "LAMELLAR" or "SPHEROID" (see section 3.5). You can only enter a "SPHEROID" phase if a "MATRIX" phase has already been created. You can only enter one matrix phase in each region.

5   Enter the "PHASE NAME". You can append a hash sign ("#") and a digit at the end of the phase name to designate the composition set number (e.g. "FCC#2"). If you do not append this and the phase has more than one composition set, then you will immediately be prompted to specify a composition set number.

5.6 Entering compositions in phases

When you specify the composition of a phase, you do this by specifying the distribution of the phase within its region—a composition profile.

5.6.1 How to specify the composition of a phase in a region

This section describes how you specify the initial composition of a specific phase in a region.

Pre-requisites

You must have already entered the phase that you want to specify the composition for.

Procedure

To specify the composition of a phase, follow these steps:

Step	Action
1	Use ENTER_COMPOSITIONS to enter a composition of a phase in a certain region.
2	Enter the "REGION NAME" of the region in which the phase has previously been entered.
3	Enter the "PHASE NAME" of the phase whose composition you want to specify.

4   If the phase is of the spheroid type, then you will be prompted to choose whether to "USE EQUILIBRIUM VALUE". If you enter "Y", then DICTRA will automatically calculate the equilibrium fractions of the phase and its constitution at the start of the simulation. You will also be prompted to specify the initial "VOLUME FRACTION OF" the spheroid phase.

5   Enter which of the components is the "DEPENDENT COMPONENT". Note that sometimes the dependent component is automatically set by DICTRA and you will not be prompted to set it.

6   Enter which "COMPOSITION TYPE" to use for the constitution of the phase. The alternative are the following:

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

7   Enter the "TYPE" of the composition distribution (that is, the type of composition profile). The alternatives are:

- "LINEAR": A linear distribution will give an equally spaced composition distribution. You will be prompted to specify the composition at the first (leftmost) grid point ("VALUE OF FIRST POINT") and at the last (rightmost) grid point ("VALUE OF LAST POINT").

- "READ_POINT_BY_POINT": This allows you to read the composition at each grid point. The specification of these can either be read from a DATA-file that you will be prompted to select or entered directly at the terminal. If you want to enter them at the terminal, then enter "READ_POINT_BY_POINT TERMINAL".

- "GEOMETRIC": A geometrical distribution will yield a higher concentration of the component at the lower end of the region if a geometrical factor larger than one is given and a higher concentration at the upper end of the region if the factor is smaller than one. You will be prompted to specify the "VALUE OF R IN THE GEOMETRICAL SERIES" which determines the distribution.

- "FUNCTION": The composition profile can be given as a function of the global distance denoted 'gd'. Useful functions include the error function ("erf(gd)") and the heavy-side step function ("hs(gd)"). For example, the function "3+2hs(x-1e-4)" will specify a concentration of 3 at the region's left side and 5 at the region's right side, with a sharp step in the concentration profile at 1e-4m=100μm.

5.7 Adding cells

If you add cells to a system, then each new cell is always placed next to the system's right outer boundary. Use CREATE_NEW_CELL to add a cell.

5.8 Setting up and running a simulation

This section describes the order in which you will typically set up your system in DICTRA and run a simulation.

Setting up a problem and running the simulation so that it successfully converges may require some fine-tuning and troubleshooting. Here are some general advice to keep in mind when you start to set up and run a simulation. For more specific recommendations about troubleshooting for different kinds of simulation problems, see section 0.

- Initially, simplify your problem as much as possible. For example, if you have an alloy with five or six components, then run a simulation with only the main components first. When this simulation works, you can then add more components in case that is necessary.

- Start with a low accuracy and refine it on a second run. If you start with a high accuracy setting, then computing the simulation will take much longer, and it is more likely that you will run into problems. Check the profiles and the overall mass balance, and if the accuracy is insufficient then you can improve the accuracy values. To change the accuracy, use SET_ACCURACY and increase or decrease "MAX RELATIVE ERROR" and "MAX ABSOLUTE ERROR".

- If you get large fluctuations in the composition or phase boundary profiles, then you can try modifying the grid or the time step of the simulation. You can increase the time step by lowering the accuracy if automatic time step control is used (this is the default). If you increase the tolerated relative and/or absolute error with SET_ACCURACY, then the automatic time step control will increase the time step.

- The composition or phase boundary profiles can often also be improved if the partial differential equations (PDEs) are integrated fully implicitly. To integrate the PDEs in this way, use SET_SIMULATION_CONDITION to set the parameter "DEGREE OF IMPLICITY WHEN INTEGRATING PDEs" to a value of '1'.

- To receive more detailed information about what is happening during the simulation, you can use DEBUG YES. If your simulations fail to converge, then this may provide you with clues about what the source of the failure is.

5.8.1 How to set up and run a simulation

This procedure describes the typical produce for setting up a problem and running a simulation.

Pre-requisites

Before you can set up a problem and start a simulation, you must have retrieved thermodynamic and kinetic data and defined your system. For information about how to do this, see section 0.

Procedure

To set up a problem and run a simulation, follow these steps:

Step	Action
1	Set conditions that hold globally in the system using SET_CONDITION GLOBAL. Normally, this will be the temperature condition.
2	Enter a region into the current cell using ENTER_REGION. Give the region an arbitrary name. If the region that you create is not the cell's first region, then it will by default be attached to the right side of the last region created in the cell.
3	For each region, use ENTER_GRID_COORDINATES to specify the region's size (width) as well as the type of grid and the number of grid points to be used in the region. The size is specified in meters.
4	Use ENTER_PHASE_IN_REGION to enter a phase into a region. Specify whether the phase is active/inactive, which type of phase it is, and what the name of the phase is.
5	Use ENTER_COMPOSITIONS to specify the initial composition of a phase that you have entered in a region. You can specify the composition in terms of 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.
6	Use SET_CONDITION BOUNDARY to set non-default boundary conditions.
7	Use ENTER_GEOMETRICAL_EXPONENT to enter the geometrical exponen that defines the geometry of the system. If you do not specify the geometrical exponent, then it will be assumed that the system has a planar geometry.
8	Use SET_SIMULATION_TIME to set the simulation time.
9	If you want to use a specific model for the simulation calculations, then set DICTRA to use that model. For more information, see section 5.9.
10	You are now ready to run the simulation. However, it is recommended that you use SAVE_WORKSPACES to save the setup of your problem before running the simulation.
11	Use SIMULATE_REACTION to start the simulation. To ensure that the simulation will be run with default settings, use SIMULATE_REACTION YES, otherwise you may be prompted to specify certain values during the running of the simulations (if phases appear or disappear in the simulation).

5.9 Different simulation models

Depending on how you have configured your DICTRA calculation, DICTRA will use different kinds of models when performing the simulation. In the case of some models, you must explicitly set DICTRA to use them.

The following table lists the different models used in DICTRA:

Model	Description
The coarsening model	You must explicitly set DICTRA to use this model with the COARSENING_MODEL command. The model allows you to perform coarsening simulations. To use this mode, you should configure your calculation in the following way: • Have one cell only, with a single particle that is 1.5 times larger than the average particle size. • The matrix phase should be in contact with the maximum size particle on the left/lower side, and then the model will specify a local equilibrium with an average sized particle on the right/upper side. The surface energy will then result in growth of both the maximum size particle and the matrix phase. Use SET_SURFACE_TENSION to enter the surface energy to enable coarsening.
The para-equilibrium model	You must explicitly set DICTRA to use this model with the PARA_EQUILIBRIUM_MODEL command. The model allows you to calculate a moving phase boundary problem while assuming that para-equilibrium conditions hold at the boundary. You can only simulate a single moving boundary in one cell. Substitutional components will, in effect, be regarded as one composite component. The composition of the substitutional components in the phase that is to be dissolved in several ways. Enter "AUTO" to set it to the value at the region's lower or upper boundary; enter a value followed by a percentage sign ("%") to set it to a certain percentage from the moving boundary inside the region; enter a hyphen ("-") followed by a value to set it to a fixed distance from the moving boundary; or simply enter a value to set the composition to that specific value.
The homogenization model	If you enter a spheroid phase when you configure your calculation, then the homogenization model will automatically be used by DICTRA. This is useful when you want to simulate long-range diffusion through a multiphase mixture, under the assumption that local equilibrium holds at each node point.

	You can also explicitly set DICTRA to use the model with the HOMOGENIZATION_MODEL command. This way, you can use the homogenization model also when calculating a moving boundary problem.
	When the homogenization model is used, simulations are run using an implicit finite volume method to increase numerical stability. Because of this, and other factors, homogenization model simulations will generally run slower than other comparable DICTRA simulations. You can increase or decrease the "DEGREE OF IMPLICITY WHEN INTEGRATING PDEs" with the SET_SIMULATION_CONDITIONS command.
The disperse model	This model can be used to calculate diffusion of a phase that is dispersed in a matrix phase. However, it is recommended that you use the homogenization model for this type of calculation instead. The disperse model has the following limitations: · There must be a continuous matrix phase otherwise the simulation will break down. · There is no implicit integration of the partial differential equations (PDEs), leading to a lower accuracy. · Only diffusion in the matrix phase can be simulated. It will be assumed that no diffusion occurs in the dispersed phase.
The thermomigration model	The thermomigration model allows you to simulate thermally induced diffusion in temperature gradients. To use the model, you must set the temperature to depend on the spatial coordinate (x) in you calculation. In addition, you must also enter the heat of transport quantity (Q^*) using the ENTER_HEAT_TRANSFER_PARAMETER command. You must enter this parameter separately for each component in each phase. The model will automatically be used by DICTRA when you have done this.
The grain-boundary model	You must explicitly set DICTRA to use this model with the GB_MODEL command. This model allows you to simulate grain-boundary and dislocation-assisted diffusion. The grain-boundaries and the dislocations will contribute to the total amount of diffusion according to their weighted fractions. The parameters are entered separately for each region in order to allow for different expression for different phases.
The pearlite model	This model is automatically used by DICTRA if there is lamellar phase in a region.

6 Visualization

You can plot or tabulate the results of your DICTRA simulation in the post-processor module, also called the POST module. The diagram is presented on a plot tab in the Console Results window. Once the simulation results have been plotted, you can then change its appearance in the "Plot Properties" window, which you open by right-clicking on the plot tab and selecting "Properties" from the pop-up menu.

6.1.1 How to plot your simulation results

Plotting a diagram is to graphically represent how a dependent variable varies with an independent variable. The independent variable is either distance or time.

Pre-requisites

To plot a diagram, you must already have run your simulation in the DICTRA module and you must have entered the POST module. Note that you use POST to enter the POST module (using GOTO_MODULE POST will lead to a "NO SUCH MODULE" message). The POST command is only available in the DICTRA module.

Procedure

To plot a diagram, follow these steps:

Step	Action

1	Use SET_DIAGRAM_AXIS to specify which variables that should be plotted on the X- and Y-axes of the diagram. One of these axes must be set to either "TIME" or "DISTANCE". For example, to set the X-axis to plot the distance from the lower boundary of the calculation (rather than from the lower boundary of the current region) and the Y-axis to plot the weight-percent composition of the Si element, you would enter the following at the POST module prompt:
	
	`SET_DIAGRAM_AXIS X DISTANCE GLOBAL`
	
	`SET_DIAGRAM AXIS Y WEIGHT-PERCENT SI`
	
	You may also specify a Z-axis, which will be represented as tick marks on the curve in the XY-plane.
	
	When you set one of the axes to "TIME" or "DISTANCE", then that variable automatically becomes the independent variable. In rare cases, you may not want the independent variable to be plotted along an axis. In that case, you must use SET_INDEPENDENT_VARIABLE to set this variable to either "TIME" or "DISTANCE".

2	Since the calculations in your simulation depend on both time and a spatial coordinate, one of these variables must be fixed during the plotting of a graph. Use SET_PLOT_CONDITION to set which variable that should be kept fixed. You can set any of the following variables as the fixed plot condition: • "TIME": The integration time.

- "DISTANCE": The distance in the system (from the lower boundary).
- "INTERFACE": At the location of a certain interface between two phases.
- "INTEGRAL": The value of the plot condition is integrated over the phase, region or system volume.

If you select "TIME", then you can enter more than one value if you separate them by commas. One graph will be plotted for each value.

3   Use PLOT SCREEN to plot the diagram.

The plot of the simulation results on a tab in the Console Results window. The following screenshot shows the plot from example 2a in the DICTRA Examples Collection, where distance has been set as the independent variable and the weight-percent of Ni is plotted on the Y-axis. The plot condition is "TIME": the plot shows four graphs, each showing the spatial distribution of Ni in the region at the time steps 0, 1e5, 3e5, and 10e5.
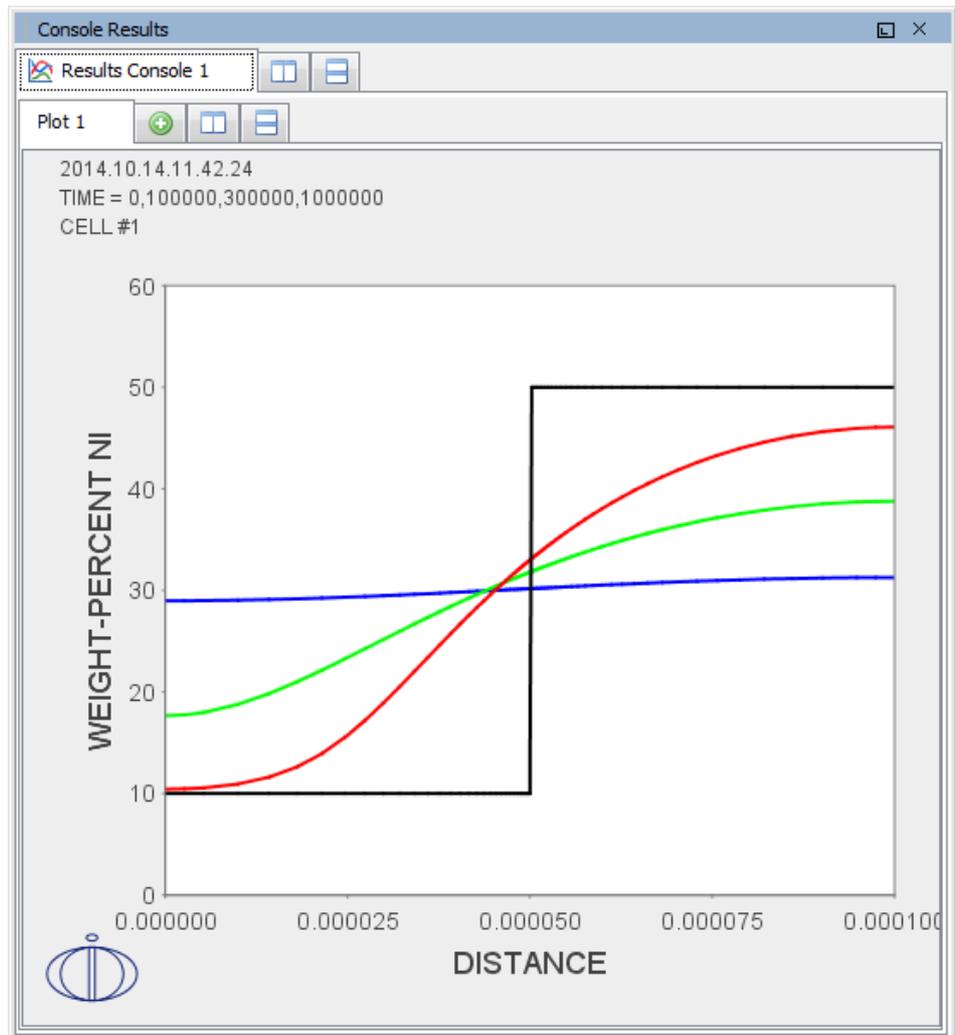
You can also print the plotted graphs direct to a postscript-file by using PLOT followed by a filename.

6.1.2 Modifying the appearance of the diagram

To change the appearance of your diagram, right click on the diagram and select "Properties" from the pop-up menu. This will open up a Plot Properties window. Here you can, for example, change the fonts and colours used, and enter a title for your diagram.

You can also change the colour, stroke (solid/dashed/dotted/dash_dot) and line width of a particular series of lines in the plot by double-clicking one of the lines in the series. In this way, you can also toggle whether data points should be shown or not for a series of lines. The crosshair cursor turns into a cursor resembling a pointing hand when it is placed over a line that can clicked but if you hold down Ctrl, this will not happen (the cursor will continue to be shown as a crosshair).

To configure the default settings for plotting, select "Options" from the "Tools" main menu and open the "Plotting" tab under Console Mode.

6.1.3 Saving your diagram

When a diagram has been plotted, there are several ways in which you can save it:

MAKE_EXPERIMENTAL_DATAFILE

> Use this to save all the data about the plotted diagram in an EXP-file. An EXP-file is a plain text file that describes the diagram in the DATAPLOT graphical language. See the *DATAPLOT User Guide* for more information. Note that information about the underlying calculations that the diagram is based on is not saved in an EXP-file.

DUMP_DIAGRAM

> Use this to save the diagram image to a PS, PDF, SVG, EMF, GIF, or PNG file. You will be asked which format to save it.

Right click on diagram |Save Plot

> Do this to save the diagram image in a variety of image file formats.

PRINT_DIAGRAM

> Use this to print a hard copy of the diagram.

6.2 How to tabulate your simulation results

You can tabulate your simulation results in a table.

Pre-requisites

To tabulate the simulation results, you must already have run your simulation in the DICTRA module and you must have entered the POST module. Note that you use POST to enter the POST module (using GOTO_MODULE POST will lead to a "NO SUCH MODULE" message). The POST command is only available in the DICTRA module.

Procedure

To tabulate your results, follow these steps:

Step	Action

1   Use ENTER_SYMBOL TABLE to specify which variables that should be
        shown in the table columns. Separate the variables by commas
        (",").

2   Use SET_INDEPENDENT_VARIABLE to specify which variable that the
        rows in the table should represent.

3   Use TABULATE to generate the table.

7   Troubleshooting

The following section contains some general advice to consider in order to avoid having your simulation fail to converge when you calculate different kinds of problems in DICTRA.

7.1.1 Moving boundary problems

Use the automatic starting values when you run the simulation the first time. If the first time step does not converge try decreasing the starting values for the velocities. Alternatively, increase the duration of the first time step.

If the simulation fails during the first time step, then check how the starting values affect the residuals. You can do this by setting the parameter "NS01A PRINT CONTROL" with SET_SIMULATION_CONDITION to 1. DICTRA will then print the tried unknown value and the residual for each flux balance equation in each iteration. The equations are organized so that the first unknown value is always the migration rate of the phase interfaces followed by the unknown potentials. All unknown values are scaled by the starting value or the calculated value in the previous time step.

Check the grid distribution at the interfaces. If the grid is too coarse or too fine-grained then the fluxes may not be defined well.

Use activities instead of potentials when the content of one or more of the components becomes very low. If you do this, then the activity will approach zero, which is easier to handle than a potential that approaches infinity. Use SET_SIMULATION_CONDITION to set the parameter "VARY POTENTIALS OR ACTIVITIES" to "ACTIVITIES".

7.1.2 Cell calculations

In cell calculations, determine start values for each cell separately and thereafter connect the individual cells. You can even start out simulating in planar and/or cylindrical geometry in order to determine sufficient starting values if you want to use a spherical geometry.

7.1.3 Diffusion in dispersed systems

If you simulate diffusion in a dispersed system and the homogenization model is turned off, then time integration will be explicit. The maximum time step allowed, or the highest time step actually taken in the calculation, will affect the final result of the simulation. This effect will be most evident if one or more of the diffusing species have low solubility in the matrix phase. When this is the case, a supersaturation is created in the matrix phase during a diffusion step and if too large a time step is allowed, then too much supersaturation is created. Consequently, always check your results by performing a second simulation with a maximum time step that is ten times lower than in the first run. If there is large difference in results between the first and the second run, then decrease the time step again with a factor of ten and perform a third run. Repeat this process until the results can be trusted.

If a simulation fails because the program is not able to calculate an equilibrium, then try to calculate the initial equilibrium yourself using Thermo-Calc and enter the composition and fraction of each phase separately instead of having DICTRA calculate it. Also enter starting values for each phase with the command SET_ALL_START_VALUES. Alternatively, you may force DICTRA to use certain start values using SET_SIMULATION_CONDITIONS.

7.1.4 Cooperative growth

If your simulation fails to converge, try calculating the A1e temperature with Thermo-Calc and start your simulation at a temperature slightly below that temperature. Use the equations given in the interactive help in order to estimate S0 and the growth rate.

8 Appendix 1: DICTRA Examples Collection

The following table lists and briefly describes the examples in the *DICTRA Examples Collection*.

Example	Description
One-Phase problems	
a1	Homogenisation of a binary Fe-Ni alloy (Initially we assume a linear concentration)
a2	Homogenisation of a binary Fe-Ni alloy (Initially we assume a step profile)
a3	Uphill diffusion in an Fe-Si-C alloy
a4a	Carburization of binary Fe-C allow (Comparison with an analytical erf-solution)
a4b	Carburization of binary Fe-C allow (A surface reaction controls the flux of C)
a6	C-diffusion through a tube wall
Moving boundary problems	
b1a	Austenite to ferrite transformation in a binary Fe-C alloy
b1b	Austenite to ferrite transformation in a binary Fe-C alloy (Inactive ferrite)
b1c	Austenite to ferrite transformation in a binary Fe-C alloy (Gradual cooling down)
b2	Cementite dissolution in an Fe-Cr-C alloy
b3	Dissolution of 23-carbide in an austenitic matrix
b4a	Solidfication path of a Fe-18%Cr-8%Ni alloy (Eutectic reaction)
b4b	Solidfication path of a Fe-18%Cr-8%Ni alloy (Peritectic reaction)
b4c	Solidfication path of a Fe-18%Cr-8%Ni alloy (Peritectic reaction, homogenenous liquid)
b4d	Solidfication path of a Fe-18%Cr-8%Ni alloy (Peritectic reaction, heat-flux controls the Temperature)
b5	Diffusion couple of Fe-Ni-Cr alloys
b6	Microsegregation of phosphorus
Cell calculations	
c1	"Carbon cannon" in ferrite/austenite Fe-C system, two-cell calculation
c2	Cementite dissolution in an Fe-Cr-C alloy (Three different particle sizes)
Diffusion in dispersed systems	
d1a	Carburization of Ni-25%Cr alloy

d1b	Carburization of Ni-25%Cr alloy, using homogenization model
d2a	Diffusion couple of Fe-Cr-Ni alloys (Initially we have a step-profile)
d2b	Diffusion couple of Fe-Cr-Ni alloys, using homogenization model (Initially we have a step-profile)
d3	Diffusion couple of Fe-Cr-Ni alloys (Using the new model)
Cooperative growth	
e1	Growth of pearlite in an Fe-Mn-C alloy
Coarsening	
f1	Coarsening of M6C precipitate in an Fe-Mo-C alloy
Kinetic data	
g1	Checking diffusivities in an Fe-Ni alloy
g2	Optimization of mobilities in Ni-Al fcc alloys
Deviation from local equilibrium	
h1	ferrite/austenite diffusion couple with interface mobility
h2	ferrite/austenite para-equilibrium in an Fe-Ni-C alloy
h3	Diffusion in a temperature gradient
Diffusion in complex phases	
i1	Diffusion in a system with B2-ordering
i2	Diffusion of carbon in cementite
i3a	Diffusion in iron oxide
i3b	Diffusion in iron oxide with a GB contribution