



DICTRA User Guide
Version 2015b



1. Contents

1. Contents	2
2. Introduction to DICTRA.....	3
2.1 About DICTRA	3
2.2 Typographical Conventions	4
2.3 Help Resources	4
2.4 DICTRA Examples Collection.....	5
2.5 Opening a Macro File.....	6
2.6 DICTRA Licenses.....	11
2.7 Using this Guide.....	12
3. Working in DICTRA	13
3.1 Terminology.....	13
3.2 Typical DICTRA Module Workflow	13
3.3 DICTRA File Formats	14
3.3.1 Log Files	14
3.3.2 Macro Files	14
3.3.3 Workspace Files.....	15
3.4 Operators and Functions.....	15
3.5 Specifying Time-Dependent Profiles	15
4. Basic Concepts.....	16
4.1 System, Cells and Regions	16
4.2 Global Conditions	16
4.3 Geometry and Coordinates	16
4.4 Regions and Grids.....	17
4.5 Phases.....	17
4.6 Composition Variables.....	18
4.7 DICTRA Simulation Types	18
4.7.1 Diffusion in a Single-Phase System.....	18
4.7.2 Moving Boundary Multi-Phase System	19
4.7.3 Coarsening Processes	19
4.7.4 Diffusion in Disperse Systems	19
4.7.5 Cooperative Growth	20
5. System Definition: Retrieving Data.....	21
5.1 Defining a System	21
6. Configuring a DICTRA Calculation	22
6.1 Setting Global Conditions	22
6.2 Specifying the Geometry	22
6.3 Regions and Gridpoints	23
6.3.1 Creating a Region	23
6.3.2 Adding Gridpoints to a Region	23

6.4	Boundary Conditions	24
6.4.1	Setting Boundary Conditions	25
6.5	Phases in Regions	25
6.5.1	Entering Phases in a Region.....	25
6.6	Compositions in Phases	26
6.6.1	Specifying Phase Compositions in a Region	26
6.7	Adding (Creating) Cells	27
7.	DICTRA Simulations	28
7.1	Tips for a Successful Simulation	28
7.2	Setting Up and Running a Simulation	28
7.3	Simulation Models.....	29
7.4	Importing a Scheil Segregation Profile	31
8.	Plotting Simulations in the POST Module	33
8.1	Plotting Simulation Results.....	33
8.2	Editing the Plot Properties	34
8.3	Saving Diagrams	35
8.4	Tabulating Simulation Results	35
9.	Troubleshooting	36
9.1	Moving Boundary Problems	36
9.2	Cell Calculations.....	36
9.3	Diffusion in Dispersed Systems	37
9.4	Cooperative Growth	37

2. Introduction to DICTRA

This guide is for new users of DICTRA in the Thermo-Calc program. It is expected that you have familiarity with the Thermo-Calc Console Mode.

- [About DICTRA](#)
- [Typographical Conventions](#)
- [Help Resources](#)
- [DICTRA Examples Collection](#)
- [Opening a Macro File](#)
- [DICTRA Licenses](#)
- [Using this Guide](#)

2.1 About DICTRA

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

DICTRA is suitable for solving diffusion problems that include 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 ways, enabling you to solve different types of problems.

Problem type	Examples
One-phase problems	• Homogenization of alloys • Carburising and decarburising 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
Long-range diffusion in multi-phase systems	• Carburizing of high-temperature alloys • Interdiffusion in compounds, e.g. coating systems • Nitriding and nitrocarburization
Cooperative growth	• Growth of pearlite in alloyed steels
Deviation from local equilibrium	• Calculations under para-equilibrium conditions

2.2 Typographical Conventions

The following conventions are used in this guide:

Convention	Definition
Forward arrow →	The forward arrow symbol → instructs you to select a series of menu items in a specific order. For example, Tools→Options is equivalent to: From the Tools menu, select Options .
Boldface font	A boldface font indicates that the given word(s) are shown that way in on a toolbar button or as a menu selection. For example, if you are told to select a menu item in a particular order, such as Tools→Options , or to click Save .
<i>Italic</i> font	An <i>italic</i> font indicates the introduction of important terminology. Expect to find an explanation in the same paragraph or elsewhere in the guide.
COMMAND	This font and all capital letters indicates that this is a COMMAND used in the Console Mode terminal. Examples of how you can use a command are written like this: SET_CONDITION T=1000 P=1E5 X(C)=0.01 N=1
HELP	Text in blue and underline is a link to another section. In this document commands are also sections. Clicking this link will take you to more detail about a particular command.
<Enter>	Text with <angle brackets> indicates a keyboard entry. Usually to press <Enter> (or Return).
code and code bold	A code font shows a programming code or code example. The code bold font highlights the entry.
Important	 Provides important information and indicates that more detail is located in the linked or named topic.
Note	 The information can be of use to you. It is recommended that you read the text or follow the link to more information.
Examples	 Go to the example collection to learn more.

2.3 Help Resources

Before using this guide, review the *Thermo-Calc User Guide* for details about using Console Mode, as well as the *Console Mode Command Reference*. After reviewing this guide, see the *DICTRA Command Reference*.

Online Help

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

- To access some feature help in Graphical Mode, in the lower left corner of the Configuration window, click the help button  for information about the active tab or node.

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

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

PDFs

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

2.4 DICTRA Examples Collection

To learn more about how to use the DICTRA software you can open and run the example files. These macro files (with the extension *.DCM) include comments, which you can either run in Thermo-Calc or open and read in a text editor. If you read the macro file in a text editor, you do not see the output that Thermo-Calc gives in response to the commands stored in the macro file.

Examples on the Website

You can find the Graphical and Console Mode examples on the [website](#) under **Examples**. The example files are also included in the installation.

EXAMPLES ^

Thermo-Calc Graphical Mode

Description of a few selected examples to get started using Graphical Mode in Thermo-Calc

[Thermo-Calc Graphical Mode Examples Guide](#)

[Thermo-Calc Graphical Mode Examples](#)

Thermo-Calc Console Mode

More than 50 examples using Console Mode in Thermo-Calc

[Examples guide](#)

[Example files for Windows](#)

[Example files for Mac and Linux](#)

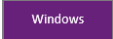
Installed Examples

The default directories where the software and its components are installed, vary by platform and user type. The pdf document *DICTRA Examples* contains the contents of the macro files and the output with which DICTRA responds.

 On a Windows network user login, the Thermo-Calc and DICTRA Examples and Materials folders are located here **C:\Users\Public\Documents\Thermo-Calc\2015b**. The TC_PRISMA Examples folder is located here **C:\Users\<user>\Documents\Thermo-Calc\2015b**. For all products, the manuals are located here **C:\Program Files\Thermo-Calc\2015b\Manuals**.

 On Windows, once Thermo-Calc is installed, you can also locate the Thermo-Calc and DICTRA Examples and Materials folders, plus all the Manuals using the shortcuts located in the Start menu. Go to **Start → All Programs > Thermo-Calc** and click **Examples**, **Manuals**, or **Materials** as required to open the applicable folder. The TC_PRISMA Examples folder is currently available from here **C:\Users\<user>\Documents\Thermo-Calc\2015b**.

In the table, <user> stands for the username and <version> for the version of Thermo-Calc, for example 2015b.

OS	User type	Default directory
	Normal user	- Users\<user>\Thermo-Calc\<version> - Users\<user>\Documents\Thermo-Calc\<version> - My documents
	Administrator	- Program Files\Thermo-Calc\<version> - Users\Public\Documents\Thermo-Calc\<version> - Public documents
	Administrator (user name and password required)	Examples and manuals in /Users/Shared/Thermo-Calc/<version> To go to this folder, in Finder, from the Go main menu select Go to folder. Enter the above file path and click Go.
	Non root user	home/<user>/Thermo-Calc/<version>
	Root user	usr/local/Thermo-Calc/<version>

2.5 Opening a Macro File

Navigate to the file location, where each set of file examples is in its own folder. 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.

Name

 exa1	Name
 exa2a	 plot.DCM
 exa2b	 run.DCM
 exa3	 setup.DCM
 exa4	

To begin, double-click the **setup.DCM** file to open it. It launches a new session of Thermo-Calc and opens in Console Mode. If you have an instance of Thermo-Calc open in Console Mode, you can also drag and drop the file to run the macro.

Descriptions of the DICTRA Example Collection

No.	Description
One-Phase problems	
a1	Homogenization of a binary Fe-Ni alloy (Initially a linear concentration is assumed).
a2a	Homogenization of a binary Fe-Ni alloy (Initially a step profile is assumed).
a2b	Simple homogenization of a binary Fe-Ni alloy. This example is identical to a2a however, it uses implicit time integration instead of the trapetzoidal method for solving the PDEs.
a3	Uphill diffusion in an Fe-Si-C alloy. Setup file for the simulation of uphill diffusion in a ternary single phase austenite matrix due to the classical darken experiment published by I.S. Darken: Trans. Aime, v. 180 (1949), pp. 430-438. In this setup two pieces of austenite (3.80 wt%Si, 0.49 wt%C) and (0.05 wt%Si, 0.45 wt%C) are put together and are subsequently annealed at 1050 C for 13 days. As both pieces are austenite they must be entered into the same region. we can accomplish this by giving the compositions of Si and C in each gridpoint individually. For convenience we store these data on file.
a4	Carburization of binary Fe-C alloy (comparison with an analytical erf-solution). This is a simple binary simulation with just one single phase region. The numerical simulation is compared with an analytical erf-solution. A special database is created, erf.tdb, in which the diffusion coefficient is set to a concentration independent value.
a5	Simulation of carburization of a binary Fe - 0.15 wt% C alloy. A mixture of 40% n2 and 60% cracked methanol was used as carrier gas. The carburizing "carbon potential" in the gas is 0.85 wt%. A surface reaction controls the flux of c at the surface.
a6	C-diffusion through a tube wall. A simple example on diffusion through a tube wall. The tube-material is an Fe-0.6%Mn-0.7%Si-0.05%C alloy. On the inside wall a carbon activity of 0.9 is maintained whereas on the outside the C-activity is very low. This example demonstrates the use of the command SET-FIRST-INTERFACE as well as the use of MIXED boundary conditions.
a7	DICTRA simulation of a homogenization heat treatment. The initial segregation profile is created from a Scheil calculation (see macro create_initial_profile.TCM). The command INPUT_SCHEIL_PROFILE in the DICTRA monitor performs most of the setup. Only time and temperature must be entered after the INPUT_SCHEIL_PROFILE command is executed.

Moving boundary problems

No.	Description
b1a	Austenite to ferrite transformation in a binary Fe-C alloy. Setup file for calculating a ferrite (BCC)/austenite (FCC) transformation in a binary Fe-C alloy. The initial state is an austenite of 2 mm thickness. The composition of the austenite is Fe-0.15wt%C. After austenitisation the specimen is quenched down to 1050K. The system is assumed closed, so we do not set any boundary conditions (closed system is default). Ferrite is expected to grow into the austenite. For this reason we start with a thin region with ferrite adjacent to the austenite.
b1b	Austenite to ferrite transformation in a binary Fe-C alloy (Inactive ferrite). Same problem as in exb1a but now we set up the problem with ferrite as an inactive phase adjacent to the initial austenite.
b1c	Austenite to ferrite transformation in a binary Fe-C alloy (gradual cooling down). Same problem as in exb1a and exb1b but now we start the simulation at a higher temperature and assume a gradual cooling down to 1050 K. When 1050 K is reached, the temperature is kept constant and thus have an isothermal transformation. As in exb1b we have ferrite as an inactive phase adjacent to the initial austenite.
b2	Cementite dissolution in an Fe-Cr-C alloy. Setup file for calculating the dissolution of a spherical cementite particle in an austenite matrix. This case is from Z.-K. Liu, L. Höglund, B. Jönsson and J. Ågren: <i>Metall. Trans. A</i> , v. 22A (1991), pp. 1745-1752. In order to achieve the correct average composition in the calculation it is necessary to take into account the fact that the calculation in DICTRA is setup using the volume fraction of the phases. To calculate the initial state at the heat treatment temperature we need first to determine the state at the normalizing temperature. To calculate the volume fraction of the phases we need to enter a number of functions that calculate these quantities.
b3	Dissolution of 23-carbide in an austenitic matrix. Setup file for calculating the dissolution of a M23C6 particle in an austenite matrix. A film of ferrite is allowed to nucleate around the carbide during the precipitation.
b4a	Solidification path of a Fe-18%Cr-8%Ni alloy (eutectic reaction). This examples demonstrates the solidification path of an Fe-18%Cr-8%Ni alloy. A eutectic reaction is assumed, LIQUID → BCC + FCC. Hence the BCC and FCC regions should be on separate sides of the liquid region. Comparison is made with both a Scheil-Gulliver simulation and equilibrium solidification conditions, both made with Thermo-Calc.
b4b	Solidification path of an Fe-18%Cr-8%Ni alloy (peritectic reaction). Same as exb4a but, now a peritectic reaction is assumed, LIQUID + BCC → FCC. Hence the FCC region should appear in between the LIQUID and the BCC. Comparison is made with both a Scheil-Gulliver simulation and equilibrium solidification conditions, both made with Thermo-Calc.
b4c	Solidification path of an Fe-18%Cr-8%Ni alloy (peritectic reaction, homogeneous liquid). Same as exb4b but, now we will amend the diffusivity data for the LIQUID and use a very high value for the diffusivity in order to simulate a case where it is assumed the composition in the LIQUID is always homogeneous. This case should be considered less realistic.
b4d	Solidification path of an Fe-18%Cr-8%Ni alloy (peritectic reaction, heat-flux controls the temperature). Same as exb4b but, instead of controlling the temperature the amount heat extracted is given. Comparison is made with both a Scheil-Gulliver simulation and equilibrium solidification conditions, both made with Thermo-Calc.

No.	Description
b5	Diffusion couple of Fe-Ni-Cr alloys. This example demonstrates the evaluation of a ternary Fe-Cr-Ni diffusion couple. A thin slice of ALPHA phase (38%Cr,0%Ni) is clamped between two thicker slices of GAMMA phase (27%Cr, 20%Ni). The assembly is subsequently heat treated at 1373K. This setup corresponds to diffusion couple in M. Kajihara, C.-B. Lim and M. Kikuchi: <i>ISIJ International</i> , v. 33 (1993), pp. 498-507. See also M. Kajihara and M. Kikuchi: <i>Acta. Metall. Mater.</i> , v. 41 (1993), pp. 2045-2059.
b6	Microsegregation of phosphorus. This example illustrates the effect of microsegregation of phosphorus during peritectic solidification in steel.
b7	This example shows how to enter dispersed phases on either side of a phase interface. The particular case shows how the kinetics of a ferrite to austenite transformation is affected by simultaneous precipitation of niobium carbide. The transformation is caused by carburization.

Cell calculations

c1	Carbon cannon in ferrite/austenite Fe-C system, two-cell calculation. This example simulates what happens to a FERRITE plate that has inherited the carbon content of its parent AUSTENITE. The FERRITE plate formed is embedded in an AUSTENITE matrix. This setup corresponds to a proposed mechanism for formation of WIDMANNSTÄTTEN FERRITE or for the FERRITE phase of the BAINITE structure. It is assumed that the phase boundary between FERRITE and AUSTENITE is immobile, this is achieved in the simulation by putting the FERRITE and the AUSTENITE in two different cells. See also M. Hillert, L. Höglund and J. Ågren: <i>Acta Metall. Mater.</i> , v.41 (1993), pp. 1951-1957.
c2	Cementite dissolution in an Fe-Cr-C alloy (three different particle sizes). Setup file for calculating the dissolution of CEMENTITE particles in an AUSTENITE matrix. This case is identical to exb2 except that we here have three different particle sizes. Altogether six particles are considered using three different cells. This in order to be able to represent some size distribution among the CEMENTITE particles. See also Z.-K. Liu, L. Höglund, B. Jönsson and J. Ågren: <i>Metall.Trans.A 22A</i> (1991), pp. 1745-1752.

Diffusion in dispersed systems

d1a	Carburization of Ni-25%Cr alloy. Setup file for carburization of a Ni-25Cr alloy. In this case the M3C2 and M7C3 carbides are entered as spheroid phases in a FCC matrix. This case is from A. Engström, L. Höglund and J. Ågren: <i>Metall. Trans. A</i> , v. 25A (1994), pp. 1127-1134. This simulation can be run with either the DISPERSED SYSTEM MODEL or the HOMOGENIZATION MODEL. In this example the DISPERSED SYSTEM MODEL is used, which requires that the default HOMOGENIZATION MODEL is disabled. With the DISPERSED SYSTEM MODEL the command ENTER_LABYRINTH_FUNCTION is used to take into account the impeding effect of dispersed phases on long-range diffusion. For the HOMOGENIZATION MODEL the command ENTER_HOMOGENIZATION_FUNCTION should be used.
d1b	Carburization of Ni-25%Cr alloy, using homogenization model. Setup file for carburization of a Ni-25Cr alloy. In this case the M3C2 and M7C3 carbides are entered as spheroid phases in a FCC matrix. This case is from A. Engström, L. Höglund and J. Ågren: <i>Metall. Trans. A</i> , v. 25A (1994), pp. 1127-1134. This simulation can be run with either the DISPERSED SYSTEM MODEL or the HOMOGENIZATION MODEL. Here the default HOMOGENIZATION MODEL is used and then ENTER_HOMOGENIZATION_FUNCTION should be used instead of ENTER_LABYRINTH_FUNCTION.

No.	Description
d2a	Diffusion couple of Fe-Cr-Ni alloys (initially with a step-profile). Setup file for calculating the interdiffusion in a diffusion couple between a two-phase (FCC+BCC) and a single-phase (FCC) Fe-Ni-Cr ALLOY. This case is from A. Engström: <i>Scand. J. Met.</i> , vol. 24, 1995, pp.12-20. This simulation can be run with either the DISPERSED SYSTEM MODEL or the HOMOGENIZATION MODEL. In this example the DISPERSED SYSTEM MODEL is used, which requires that the default HOMOGENIZATION MODEL is disabled. With the DISPERSED SYSTEM MODEL the command ENTER_LABYRINTH_FUNCTION is used to take into account the impeding effect of dispersed phases on long-range diffusion. For the HOMOGENIZATION MODEL the command ENTER_HOMOGENIZATION_FUNCTION should be used.
d2b	Diffusion couple of Fe-Cr-Ni alloys, using homogenization model (initially with a step-profile). Setup file for calculating the interdiffusion in a diffusion couple between a two-phase (FCC+BCC) and a single-phase (FCC) Fe-Ni-Cr alloy. This case is from A. Engström: <i>Scand. J. Met.</i> , vol. 24, 1995, pp.12-20. This simulation can be run with either the DISPERSED SYSTEM MODEL or the HOMOGENIZATION MODEL. The default HOMOGENIZATION MODEL is used and then ENTER_HOMOGENIZATION_FUNCTION is used instead of ENTER_LABYRINTH_FUNCTION.
d3	Diffusion couple of Fe-Cr-Ni alloys (using the new model). This example shows the use of the homogenization model. It is taken from H. Larsson and A Engström, <i>Acta Mater</i> , v.54 (2006), pp. 2431-2439. Experimental data from A Engström, <i>Scand J Metall</i> , v.243 (1995), p. 12. The homogenization model can be used for multiphase simulations like the dispersed system model, but unlike the dispersed system model there is no need to have a single continuous matrix phase and, furthermore, there is no need to limit the size of time-steps. The set-up is performed in the same manner as for the dispersed system model, which means that a certain phase is entered as the matrix phase and the other phases are entered as spheroidal, but the choice of matrix phase does not affect the simulation.
Cooperative growth	
e1	Growth of pearlite in an Fe-Mn-C alloy. This is an example file for a setup and a calculation of PEARLITE growth in an Fe - 0.50wt%C - 0.91wt%Mn steel.
Coarsening	
f1	Coarsening of M ₆ C precipitate in an Fe-Mo-C alloy. Setup file for calculating the Ostwald-ripening of a spherical M ₆ C carbide in an AUSTENITE matrix.
Kinetic data	
g1	Kinetic data file for checking mobilities and diffusivities in an Fe-Ni alloy.
g2	Optimization of mobilities in Ni-Al fcc alloys. Kinetic data file for reading thermodynamic data and setting up the kinetic parameters which are needed for an optimization of the FCC phase in the binary Ni-Al system. See also A. Engström and J. Ågren: Assessment of Diffusional Mobilities in Face-Centered Cubic Ni-Cr-Al Alloys, in the February issue of <i>Z. Metallkunde</i> , 1996.
Deviation from local equilibrium	
h1	Ferrite/austenite diffusion couple with interface mobility. Setup file for calculating the growth of FERRITE into AUSTENITE with a limited interface mobility. This is achieved by adding a Gibbs-energy contribution to the FERRITE using the SET-SURFACE-ENERGY command.

No.	Description
h2	Ferrite/austenite para-equilibrium in an Fe-Ni-C alloy. Setup file for calculation of the growth of FERRITE into AUSTENITE in an Fe-2.02%Ni-0.0885%C alloy using the para-equilibrium model. The results are compared with experimental information from Hutchinson, C. R., A. Fuchsmann, and Yves Brechet. "The diffusional formation of ferrite from austenite in Fe-C-Ni alloys." <i>Met. Mat. Trans A</i> 35.4 (2004): 1211-1221.
h3	Diffusion in a temperature gradient. This calculation shows how a temperature gradient induces diffusion.
Diffusion in complex phases	
i1	Diffusion in a system with B2-ordering. Diffusion in including effects from chemical ordering. The datafile AlFeNi-data.TDB contains both a thermodynamic and kinetic description for the ordered and disordered bcc.
i2	Diffusion of carbon in cementite. This example demonstrates the use of the model for calculation of diffusion through a stoichiometric phase. The flux of a component in the stoichiometric phase is assumed to be proportional to the difference in chemical potential at each side of the stoichiometric phase multiplied with the mobility for the component in the phase. The mobility is assessed from experimental information and is basically the tracer diffusivity for the component. This calculation is compared with experimental data where a sample of pure iron has been exposed to a gas atmosphere with a certain carbon activity. The weight gain is then measured as a function of time. The experimental data is obtained from Ozturk B., Fearing V. L., Ruth A. Jr. and Simkovich G., <i>Met Trans A</i> , vol 13A (1982), pp 1871-1873.
i3a	Diffusion in iron oxide. Oxidation of iron sample and consequent growth of an oxide layer.
i3b	Diffusion in iron oxide with a GB contribution. Oxidation of iron sample and consequent growth of an oxide layer using the grain boundary diffusion contribution model.

2.6 DICTRA Licenses

You can start (and install) the Thermo-Calc software without a valid license but you cannot do any calculations. To show information about the available and installed licenses, from the main menu select **Help → Show License Info**.

DICTRA in Thermo-Calc requires a separate license. If you are using a network client installation of Thermo-Calc, then you may not be able to use DICTRA 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 DICTRA that the network license allows you to run simultaneously. A DICTRA license is checked out when you enter DICTRA and it is checked back in when you exit.

 Search the online help or see the [Thermo-Calc Installation Guide](#) on the website for more information about license types.

If you try to enter DIC_PARROT after having been in the PARROT module earlier in the session, this message displays `DICTRA PARROT disabled after using PARROT`. To enter DIC_PARROT relaunch Thermo-Calc and enter these commands starting in the SYS module: `GOTO_MODULE DIC_PAR`.

2.7 Using this Guide

Before using this guide, review the *Thermo-Calc User Guide* and the *Console Mode Command Reference* for details about Console Mode. After reviewing this guide, see the *DICTRA Command Reference*.

This guide includes an overview of the program and its 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.

[Working in DICTRA](#) introduces you to the terminology, workflow and file formats in DICTRA.

The next section is an overview of [Basic Concepts](#) of the DICTRA software including descriptions of cells, regions, phase, and phases, for example. The section also gives examples of the different simulation types to prepare you for defining your own system.

The next sections walk you through the concepts and general workflow to set up a DICTRA simulation.

[System Definition: Retrieving Data](#) describes how you define the system and retrieve thermodynamic and kinetic data about the elements.

[Configuring a DICTRA Calculation](#) and [DICTRA Simulations](#) describes how you configure and run simulations, and [Plotting Simulations in the POST Module](#) explains how to plot the simulation results.

The [Troubleshooting](#) section has some recommendations and guidelines to adjust configurations and settings if you have difficulty with any of the steps.

3. Working in DICTRA

```

Console
Console 1

Thermo-Calc / DICTRA
Only for use at Thermo-Calc Software
Local contact pumbaa.thermocalc.se

SYS:GOTO_MODULE DICTRA
NO TIME STEP DEFINED
DIC>

```

Open Thermo-Calc in Console Mode. In the SYS module, type `GOTO_MODULE DICTRA`. Type `?` for a list of available DICTRA commands, which are described in detail in the *Console Mode Command Reference* and the *DICTRA Command Reference*.

- [Terminology](#)
- [Typical DICTRA Module Workflow](#)
- [DICTRA File Formats](#)
- [Operators and Functions](#)
- [Specifying Time-Dependent Profiles](#)

3.1 Terminology

DICTRA consists of two Thermo-Calc modules: the DICTRA_MONITOR module and the DIC_PARROT module. In this guide, *DICTRA* and *DICTRA module* are used interchangeably to refer to the DICTRA_MONITOR module.

The DIC_PARROT module assesses experimental data and uses this data to optimise calculations. See the *Console Mode Command Reference* for more information about using the DIC_PARROT module.

3.2 Typical DICTRA Module Workflow

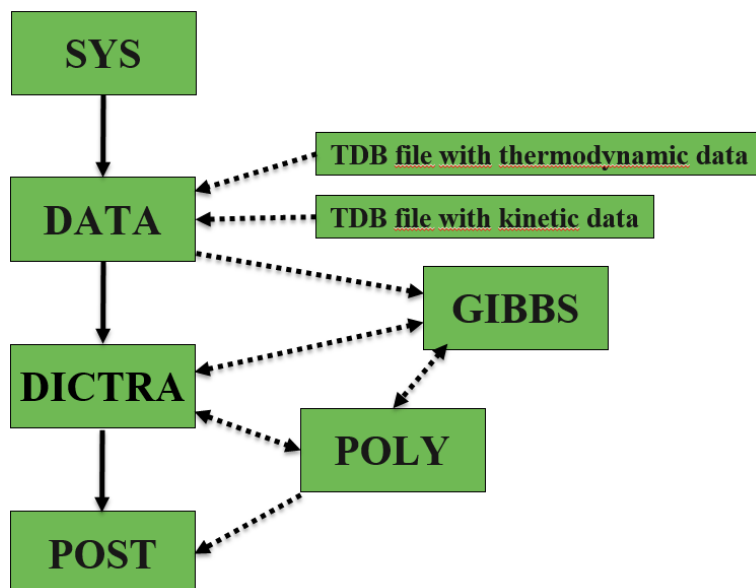


Figure 1: An example of a typical DICTRA module workflow.

Figure 1 represent the typical workflow when you set up a problem and run a simulation in DICTRA. The solid arrows represent the typical movements between the modules. The dashed arrows represent movement of data within DICTRA. The basic workflow is as follow.

1. You are in the **SYS** module when you start Thermo-Calc in Console Mode.
 In the **DATA** module define the system. Before performing a calculation, you must define your system and retrieve thermodynamic and kinetic data. The data is retrieved from database files (*.TDB).
 The data needed to describe a system is sent to the **GIBBS** module. When the data is in GIBBS, DICTRA can access the retrieved data. The retrieved data is accessible to the **POLY** module, which is involved in simulations that require that equilibrium calculations are performed.
2. In the **DICTRA** module:
 - Set the initial state of the system and define its geometry and boundary conditions. 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.
 - Define which phases each region contains.
 - Set various parameters for the numerical calculations.
 - Run the simulation from within the DICTRA module.
3. In the **POST** module plot and visualize your data.
 - Choose the data to plot
 - Change the appearance of the diagram
 - Save the diagram as an image file (in many different formats).

3.3 DICTRA File Formats

DICTRA uses different file formats: *log* files (*.LOG), *macro* files (*.DCM) and *workspace* files (*.DIC).

3.3.1 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 a log file, in the SYS module type `SET_LOG_FILE`, followed by the name of the file that you want to save your command sequence to.
- When creating a command sequence, and if you want to save DICTRA's output in the log file, type `SET_ECHO` before the `SET_LOG_FILE` command. This is useful if you later want to use the log file as a macro file.

3.3.2 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. When creating a command sequence, you add comments to the file by starting a line with @@.

- To run a macro file, in the SYS or DICTRA module type `MACRO_FILE_OPEN`, followed by the name of the macro file. DICTRA runs the command sequence that the file contains.

- To remain in the console and keep working in DICTRA, in the SYS, DICTRA, POLY, or POST module add the command `SET_INTERACTIVE` at the end at the end of the macro file. Alternatively, use `EXIT` as the final command.

3.3.3 Workspace Files

You can save all the data in your current workspace. At the `DIC` prompt, type `SAVE_WORKSPACES`. The command opens the workspace, which contains all the data, specified settings and the result of any calculations performed. The saved data includes original and modified thermodynamic data, the last set of conditions and options, and the results of any simulations.

To load the data and calculation results of a workspace file, at the `DIC` prompt type `READ_WORKSPACES`.

3.4 Operators and Functions

Sometimes you need to specify functions when setting up a system in DICTRA. For example, to make global and boundary conditions vary as a function of time. The following operators can be used in writing functions. Use a semi-colon (;) to mark the end of a function.

Available operators for writing functions

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

3.5 Specifying Time-Dependent Profiles

In DICTRA you are often prompted to specify a time-dependent profile for a condition. To define these profiles or intervals, enter information as follows and refer to the *DICTRA Command Reference* for more information:

Command profile	Description
LOW TIME LIMIT	To determine the time when the function starts to apply.
HIGH TIME LIMIT	To determine the time when the function stops applying. Use an asterisk (*) to set the high limit to the time when the simulation ends.
ANY MORE RANGES	Enter <code>Y</code> to specify an additional range with a time-dependent function, which starts to apply at the time step after the high time limit of the previous range is reached.

4. Basic Concepts

This section introduces you to the basic concepts to solve problems in DICTRA.

- [System, Cells and Regions](#)
- [Global Conditions](#)
- [Geometry and Coordinates](#)
- [Regions and Grids](#)
- [Phases](#)
- [Composition Variables](#)
- [DICTRA Simulation Types](#)

4.1 System, Cells and Regions

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

The interface between two regions typically moves as the result of a simulation, that is, the regions 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 choice of boundary conditions.

For some simulations it is useful to have several cells in a 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.

By default this is 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.

4.2 Global Conditions

There are several global parameters that influence the diffusion rate in simulations: temperature, pressure and heat content removal. These parameters are defined as functions of time. The temperature can also be a function of the spatial position, and heat content removal can be 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 one mole of atoms. Also see [Setting Global Conditions](#).

4.3 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. If the 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.

A *cylindrical* geometry corresponds to an infinitely long cylinder of a certain radius. A *spherical* geometry corresponds to a sphere with a certain radius.

For cylindrical and spherical geometries, 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. You can enter a leftmost coordinate that is larger than zero to allow for tube and hollow sphere geometries. Also see [Specifying the Geometry](#).

4.4 Regions and Grids

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 *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. Also see [Regions and Gridpoints](#).

4.5 Phases

Each region contains one or more *phases*. A phase can be of the *matrix*, *spheroid* or *lamellar* type. A phase can be introduced with the status *active* (the default) or *inactive*.

An inactive phase is a phase which does not participate in the calculations until it is 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 takes 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 $R_{\text{}}$ added as a prefix. Also see [Phases in Regions](#) and [Compositions in Phases](#).

Phase type	Description
Matrix	The region's primary phase. If there is only one phase in a region, then that phase is automatically a matrix.
Spheroid	Used to treat one or several dispersed phases in a matrix. Unless the homogenization model is invoked, which happens 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	Used to simulate the growth of a eutectic or eutectoid region. The software only treats the growth, not the dissolution, of such a region. The <i>pearlite calculation model</i> is used for a phase that is lamellar.

4.6 Composition Variables

DICTRA uses two types of composition variables: site-fractions and u-fractions, although you can also use weight fraction or mole fraction, for example.

The *site-fractions* are used to set up the problem and interface 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 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.

4.7 DICTRA Simulation Types

DICTRA is used to simulate diffusion-controlled transformations in multicomponent alloys. The following are some of the types of simulations DICTRA can handle.



Also see [DICTRA Examples Collection](#).

4.7.1 Diffusion in a Single-Phase System

The simplest DICTRA simulation is one where certain components in one phase diffuse over time in that single phase. To simulate this, you 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 change over time, or for how the boundary conditions of the region change over time.

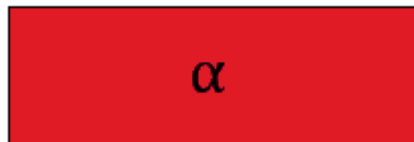


Figure 2: Simulate diffusion in a single-phase system.

4.7.2 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 changes overtime, or for how the boundary conditions of the region change overtime.

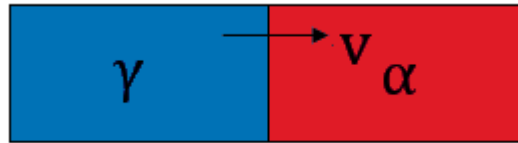


Figure 3: Simulate a moving boundary multi-phase system.

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.

4.7.3 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.

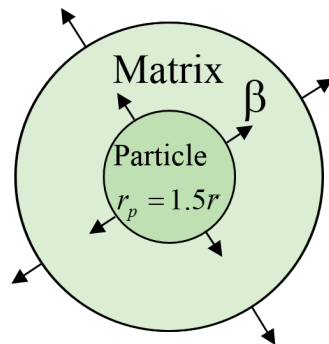


Figure 4: Simulate a coarsening process.

4.7.4 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 the fraction and composition is calculated from the average composition in each node, assuming that equilibrium holds locally in each volume element.

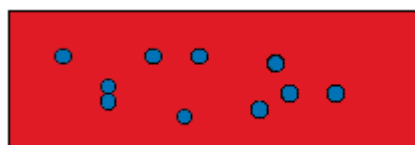


Figure 5: Simulate diffusion in a disperse system.

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 *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.



Figure 6: Simulate diffusion with the homogenization model.

4.7.5 Cooperative Growth

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

5. 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 making the diffusion problem 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.

 Search the online help or refer to the [DICTRA Command Reference](#) on the website for details about the specific commands. The next section, [Defining a System](#) is a short summary.

5.1 Defining a System

1. Open Thermo-Calc in Console Mode. At the SYS prompt, type
`GOTO_MODULE DATA.`
2. Use SWITCH_DATABASE to select database. Unless you directly specify the name of the database as a parameter to the command, the available databases are listed. Specify the one to use.
3. Use DEFINE_ELEMENTS followed by a list of the elements that you want in your system. (To list the elements available in the current database, type
`LIST_DATABASE ELEMENTS.`)
4. Use REJECT with the keyword, `phases` to make sure that unnecessary phases are not retrieved from the database.
5. Use RESTORE with the keyword, `phases` to restore any phases that have been excluded.
6. Use GET_DATA to read from the database and send the thermodynamic data about your system to the GIBBS and DICTRA workspace.
7. Use APPEND_DATABASE to select the database from which you want to retrieve kinetic data.
8. 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).
9. 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.
10. Use APPEND_DATABASE again to add thermodynamic or kinetic data from another database. When all the data needed is retrieved, you can start using the DICTRA module.

6. Configuring a DICTRA Calculation

This section describes in general terms what options you have when setting up your problem in DICTRA. Search the online help or refer to the [DICTRA Command Reference](#) on the website for details about the specific commands.

- [Setting Global Conditions](#)
- [Specifying the Geometry](#)
- [Regions and Gridpoints](#)
- [Boundary Conditions](#)
- [Phases in Regions](#)
- [Compositions in Phases](#)
- [Adding \(Creating\) Cells](#)

6.1 Setting Global Conditions

Use SET_CONDITION GLOBAL to set global conditions. Global conditions include temperature (T), heat content removal (Q) and pressure (P), and these reduce the degrees of freedom for equilibrium calculations. Also see [Global Conditions](#).



If the heat content removal is specified then 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 range having its own function to define 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;`

6.2 Specifying the Geometry

By default a DICTRA system has a planar geometry. To change the geometry of the system, use ENTER_GEOMETRICAL_EXPONENT followed by a number 0 (planar), 1 (cylindrical) or 2 (spherical). See [Geometry and Coordinates](#).

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.

6.3 Regions and Gridpoints

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 a grid is entered into the region. Also see [System, Cells and Regions](#) and [Regions and Grids](#).

6.3.1 Creating a Region

1. Complete the section [Defining a System](#).
2. Use ENTER_REGION to enter a region into the system.
3. Enter an arbitrary name for the region at the REGION NAME prompt.
4. If this is the first region you create in your system, then the procedure stops here. Otherwise, continue to the next step.
5. Enter the name of an already existing region to which the new region is attached.
6. 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.
7. If the 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 surrounds the new region.

6.3.2 Adding Gridpoints to a Region

1. Complete the sections [Defining a System](#) and [Creating a Region](#).
2. Use ENTER_GRID_COORDINATES followed by the name of the region.
3. Specify the width of the region in meters. .
4. At the NUMBER OF POINTS prompt enter the number of grid points for the region.
5. Specify the type of grid point distribution to have in the region.
 - LINEAR, for an equally spaced grid.
 - READ_POINT_BY_POINT 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. To enter the grid points at the terminal, enter READ_POINT_BY_POINT TERMINAL.
 - GEOMETRIC for a grid that yields a varying density of grid points in the region. Enter the VALUE OF R IN THE GEOMETRICAL SERIES, which determines the distribution. A geometrical factor larger than one yields a higher density of grid points at the lower end of the region and a factor smaller than one yields a higher density of grid points at the upper end of the region.
 - DOUBLE_GEOMETRIC to have a high number of grid points in the middle or at both ends of a region. Specify two geometrical factors. VALUE OF R IN THE GEOMETRICAL SERIES FOR LOWER PART OF REGION for the distribution in the lower (left) part of a region, and VALUE OF R IN THE GEOMETRICAL SERIES FOR UPPER PART OF SUBREGION for the distribution in the upper (right) part of a region.

6.4 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. Also refer to the SET_CONDITION command described in the *DICTRA Command Reference*.

Boundary condition	Description
FIX_FLUX_VALUE	Enter functions that yield the flux times the molar volume for the independent components. Can be a function of time, temperature and pressure. Use this boundary condition with caution as 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 should be used with care as no checks are done in advance to determine if it is a legal expression. Do not specify the conditions for temperature and pressure here as these are taken from the global conditions.
POTENTIAL_FLUX_FUNCTION	Use to take into account the finite rate of a surface reaction. The flux for the independent components must be given in the format: $J_k = f_k(T, P, TIME) * [POTENTIAL_k^N - g_k(T, P, TIME)]$ 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	Use to take into account the finite rate of a surface reaction. The flux for the independent components must be given in the format: $J_k = f_k(T, P, TIME) * [ACTIVITY_k^N - g_k(T, P, TIME)]$ 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 but an iterative scheme is used to determine the flux. Use this if the other command encounters 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 is set to zero and the activity of others may be set to a prescribed value.
GAS	This option can cause a change in system volume. The flux of selected components is set to zero and the activity of others can be set to a prescribed value. Use this to treat an expanding system, e.g. the growth of an external oxide scale.

6.4.1 Setting Boundary Conditions

1. Complete the sections [Defining a System](#) and [Creating a Region](#).
2. Use SET_CONDITION BOUNDARY. Then 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 define starts to apply.
6. If required, enter the function that is 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. Then enter another function for the next range.
9. When you have defined functions for all the ranges you want, enter N at the ANY MORE RANGES prompt.

6.5 Phases in Regions

When defining a region you need to enter one or more phases into the region. The number and type of phases depends on the simulation you want to run. Also see [Phases](#).



There is no supersaturation locally within a given region.

- To simulate diffusion of components within one phase, enter one matrix into the region.
- To simulate how an interface between regions moves, enter two regions with at least one phase in each.
- To simulate growth of one or more dispersed phases in a matrix phase, enter one matrix phase and one or more spheroid phases.

6.5.1 Entering Phases in a Region

1. Complete the sections [Defining a System](#) and [Creating a Region](#).
2. Use ENTER_PHASE_IN_REGION. Specify whether the phase is to be ACTIVE or INACTIVE.
3. For an inactive phase, specify the following:
 - Enter the name of the region and the side of that region which the phase is 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 are only considered in the simulation calculations once it is stable.)
4. For an active phase specify the following:

- `REGION NAME` for the region in which the phase is to be entered.
- `PHASE TYPE` -`MATRIX`, `LAMELLAR` or `SPHEROID`. `SPHEROID` is only available if a `MATRIX` phase is created first. You can only enter one matrix phase in each region.
- 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 are prompted to specify a composition set number.

6.6 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. Also see [Phases](#).

6.6.1 Specifying Phase Compositions in a Region

1. Complete the sections [Defining a System](#), [Creating a Region](#) and [Entering Phases in a Region](#).
2. Use `ENTER_COMPOSITIONS` to enter a composition of a phase in a certain region.
3. Enter the `REGION NAME` of the region in which the phase has previously been entered.
4. Enter the `PHASE NAME` of the phase whose composition you want to specify.
5. If the phase is spheroid, then for `USE EQUILIBRIUM VALUE` enter `Y` to automatically calculate the equilibrium fractions of the phase and its constitution at the start of the simulation. Specify the initial `VOLUME FRACTION OF` the spheroid phase.
6. Enter the `DEPENDENT COMPONENT`. Sometimes the dependent component is automatically set by DICTRA and there is no prompt.
7. Enter a `COMPOSITION TYPE` for the constitution of the phase. The options are:
 - `SITE_FRACTION`
 - `MOLE_FRACTION`
 - `MOLE_PERCENT`
 - `WEIGHT_FRACTION`
 - `WEIGHT_PERCENT`
 - `U_FRACTION`
8. Enter the `TYPE` of composition distribution (that is, the type of composition profile). The options are:
 - `LINEAR` to have an equally spaced composition distribution. 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` to read the composition at each grid point. The specification of these can either be read from a `DATA`-file that you are 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` for a distribution that yields 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 are prompted to specify the `VALUE OF R IN THE GEOMETRICAL SERIES` which determines the distribution.
- `FUNCTION` for 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)` specifies 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 $1\text{e-}4\text{m}=100\mu\text{m}$.

6.7 Adding (Creating) 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.

7. DICTRA Simulations

This section describes the typical order in which the system in DICTRA is set up to run a simulation.

Setting up a problem and running the simulation so that it successfully converges may require some fine-tuning and [Troubleshooting](#).

- [Tips for a Successful Simulation](#)
- [Setting Up and Running a Simulation](#)
- [Simulation Models](#)

7.1 Tips for a Successful Simulation

Simplify your problem as much as possible

For example, if you have an alloy with five or six components, first run a simulation with only the main components. When this simulation works, you can then add more components as 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 takes much longer, and problems are more likely. 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.

Modify the grid or time step

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 (the default). If you increase the tolerated relative and/or absolute error with SET_ACCURACY, then the automatic time step control increases the time step.

Integrate the PDEs

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.

Debug

To receive more detailed information about what is happening during the simulation, you can use DEBUG Y. If your simulations fails to converge, then this may give you some clues about the source of the failure.

7.2 Setting Up and Running a Simulation

1. Before you can set up a problem and start a simulation, you must have retrieved thermodynamic and kinetic data and defined your system. See [System Definition: Retrieving Data](#).
2. Set conditions that hold globally in the system using SET_CONDITION GLOBAL. Normally, this is the temperature condition.

3. 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 by default it is attached to the right side of the last region created in the cell.
4. 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.
5. 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.
6. 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 a user or be read from a file.
7. Use `SET_CONDITION BOUNDARY` to set non-default boundary conditions.
8. Use `ENTER_GEOMETRICAL_EXPONENT` to enter the geometrical exponent that defines the geometry of the system. If you do not specify the geometrical exponent, then it is assumed that the system has a planar geometry.
9. Use `SET_SIMULATION_TIME` to set the simulation time.
10. If you want to use a specific model for the simulation calculations, then set DICTRA to use that model. See [Simulation Models](#).
11. 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.
12. Use `SIMULATE_REACTION` to start the simulation. To ensure that the simulation is 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).

7.3 Simulation Models

Based on how the DICTRA calculation is configured, the software uses different kinds of models to perform the simulation. For some models, you must explicitly set DICTRA to use them.



Also refer to the individual commands described in the *DICTRA Command Reference*.

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, configure the calculation as follows:

- 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 specifies a local equilibrium with an average sized particle on the right/upper side.
- The surface energy then results in growth of both the maximum size particle and the matrix phase. Use SET_SURFACE_TENSION to enter the surface energy to enable coarsening.

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 are, in effect, 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.

HOMOGENIZATION_MODEL

If you enter a spheroid phase when you configure your calculation, then the homogenization model is automatically 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 generally run slower than other comparable DICTRA simulations. You can increase or decrease the DEGREE OF IMPLICIT WHEN INTEGRATING PDEs with the SET_SIMULATION_CONDITIONS command.

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 breaks 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 is assumed that no diffusion occurs in the dispersed phase.

There is no specific command to activate this model. It is only available if a phase of type "spheroid" is entered in a region. After a spheroid phase has been entered the homogenization model must explicitly be inactivated in order to run the simulation with the dispersed model. This is done by entering `HOMOGENIZATION_MODEL NO`.

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 your 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 is automatically used by DICTRA once this is done.



See DICTRA example exh3 *Deviation from local equilibrium*.

Grain-boundary model (GB_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 contribute to the total amount of diffusion according to the weighted fractions. The parameters are entered separately for each region in order to allow for different expression for different phases.

Pearlite Model

This model is automatically used by DICTRA if there is lamellar phase in a region.

7.4 Importing a Scheil Segregation Profile

You can import a previously calculated Scheil segregation profile into DICTRA. A Scheil calculation is a conservative estimate of the segregation that occurs during solidification and is therefore useful when estimating the necessary time/temperature for a homogenizing heat treatment.

From a practical point of view it is also a simple and fast calculation compared to a more accurate, but computationally more difficult, DICTRA simulation.

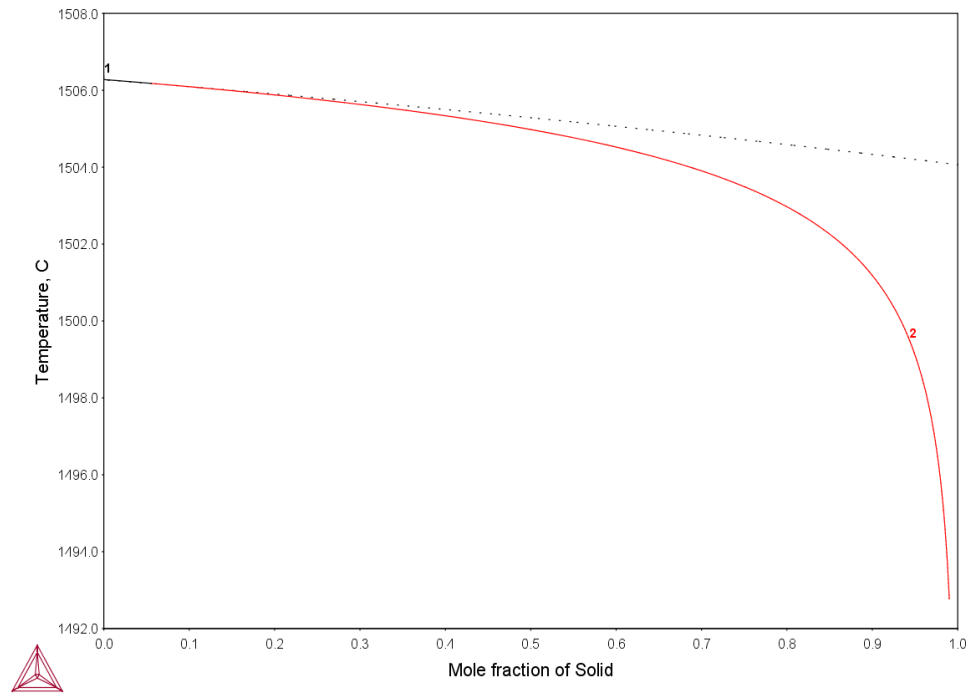


In order to limit the computational effort, this feature cannot be combined with the *fast diffusers* option in the Scheil module. See the *Thermo-Calc Console Mode Command Reference* for information about the Scheil commands. Also search the online help and refer to the *DICTRA Command Reference Guide*,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



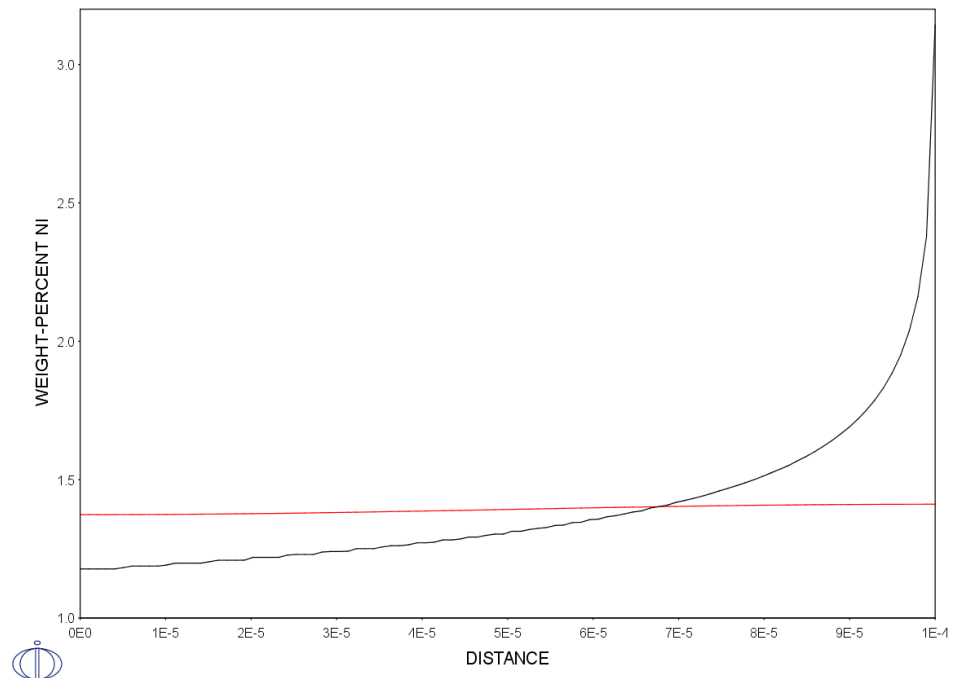
In the following example, taken from [DICTRA Examples Collection](#) number **a7**, the Scheil segregation profile for a ferritic stainless steel (Fe-17Cr-1.4Ni-1Mn) was calculated in the Scheil module in Thermo-Calc.

2015.11.10.11.51.39
FEDEMO: CR, FE, MN, NI
T=1779.52, W(CR)=0.17, W(NI)=1.4E-2, W(MN)=1E-2, P=1E5, N=1



The profile was then imported into DICTRA and a one hour homogenizing heat treatment at 1200 °C was simulated. For the DICTRA simulation a domain size of 100 μ m was assumed, which approximately corresponds to the secondary dendrite arm spacing. The plot below show the initial and final Ni profile.

2015.11.10.11.53.36
TIME = 0.3600
CELL #1



8. Plotting Simulations in the POST Module

You can plot or tabulate the results of your DICTRA simulation in the POST_PROCESSOR module, also called the POST module and accessed within DICTRA. The resulting diagram is on a plot tab in the Console Results window. Once the simulation results are plotted, you can then change its appearance in the Plot Properties window.

- [Plotting Simulation Results](#)
- [Editing the Plot Properties](#)
- [Saving Diagrams](#)
- [Tabulating Simulation Results](#)

8.1 Plotting 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.

1. Complete all the sections to run your DICTRA simulation (see [System Definition: Retrieving Data](#), [Configuring a DICTRA Calculation](#), and [DICTRA Simulations](#)).
2. In DICTRA, at the DIC prompt type POST_PROCESSOR (or just POST).
3. Use SET_DIAGRAM_AXIS to specify the variables to plot on the X- and Y-axes of the diagram. One of the 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, at the POST prompt type:

```
SET_DIAGRAM_AXIS X DISTANCE GLOBAL
SET_DIAGRAM_AXIS Y WEIGHT-PERCENT SI
```

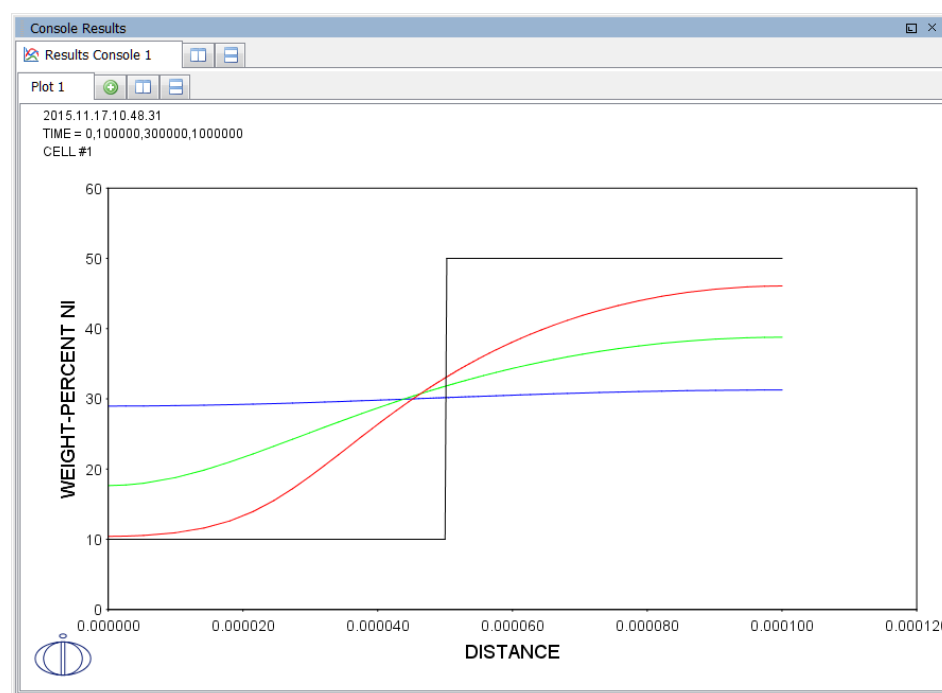
You can specify a Z-axis, which is represented as tick marks on the curve in the XY-plane.

When one of the axes is set to TIME or DISTANCE, the variable automatically becomes the independent variable. If you do not want the independent variable plotted along an axis, use SET_INDEPENDENT_VARIABLE and set it to TIME or DISTANCE.

4. Simulation calculations depend on both time and a spatial coordinate; these variables must be fixed during the plotting process. Use SET_PLOT_CONDITION to set the variable to keep fixed. These variables can be set 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.
5. For TIME, more than one value can be entered using commas to separate the values. One graph is plotted for each value.

6. Use PLOT SCREEN to plot the diagram.
7. The plot is added as a tab to the **Console Results** window. The plot example below is from example 2a in the [DICTRA Examples Collection](#). Distance is set as the independent variable and the weight-percent of Ni is on the Y-axis. The plot condition is TIME: the plot shows four graphs, each with the spatial distribution of Ni in the region at the time steps 0, 1e5, 3e5, and 10e5.
8. To print the plotted graphs direct to a postscript-file, type PLOT and a filename.
9. In the **Plot** window, right click the diagram and choose **Properties** to adjust its appearance and colors.

 See [Editing the Plot Properties](#) and the *Thermo-Calc User Guide* for more information.



8.2 Editing the Plot Properties

To change the appearance of a plotted diagram, right click the diagram and select **Properties**. In the **Plot Properties** window you can change the fonts and colours, and add a title, for example.

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 be clicked but if you hold down Ctrl, this does not happen (the cursor continues to be shown as a crosshair).

 To configure the default settings for plotting, from the main menu, select **Tools→Options**. For Console Mode click the **Plotting** tab. See the *Thermo-Calc User Guide* for more information.

8.3 Saving Diagrams

To save a plotted diagram you can do any of the following:

- Use `MAKE_EXPERIMENTAL_DATAFILE` 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. Note that information about the underlying calculations that the diagram is based on is not saved in an EXP-file.



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

- Use `DUMP_DIAGRAM` to save the diagram image to a PS, PDF, SVG, EMF, GIF, or PNG file. You are asked which format to save it.
- In the **Console Results** window, right click a diagram and select **Save Plot**. From the list, choose the file format to save it in.
- Use `PRINT_DIAGRAM` to print a hard copy of the diagram.

8.4 Tabulating Simulation Results

1. Complete all the sections to run your DICTRA simulation.
2. In DICTRA, at the DIC prompt type `POST_PROCESSOR` (or just `POST`).
3. Use `ENTER_SYMBOL TABLE` to specify which variables that should be shown in the table columns. Separate the variables by commas (,).
4. Use `SET_INDEPENDENT_VARIABLE` to specify which variable that the rows in the table should represent.
5. Use `TABULATE` to generate the table.

9. 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.

- [Moving Boundary Problems](#)
- [Cell Calculations](#)
- [Diffusion in Dispersed Systems](#)

9.1 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 then prints 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 approaches 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`.

9.2 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.

9.3 Diffusion in Dispersed Systems

If you simulate diffusion in a dispersed system and the homogenization model is turned off, then time integration is explicit. The maximum time step allowed, or the highest time step actually taken in the calculation, affects the final result of the simulation. This effect is 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`.

9.4 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 S_0 and the growth rate.