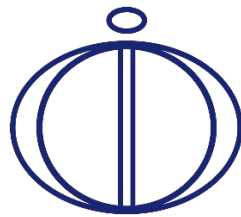


# Diffusion Module (DICTRA) Example Macros

Thermo-Calc Version 2026a



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### [exa1](#)

One-phase problem. Homogenization of a binary Fe-Ni alloy. In this example it is assumed there is initially a linear Ni-concentration profile. -----

### [exa2a](#)

One-phase problem. Homogenization of a binary Fe-Ni alloy. A Ni rich and a Ni lean alloy are put together and initially there is a step profile. -----

### [exa2b](#)

One-phase problem. Homogenization of a binary Fe-Ni alloy. This example is identical to a2a but instead it uses implicit time integration instead of the trapezoidal method for solving the PDEs. -----

### [exa3](#)

One-phase problem. Uphill diffusion in an Fe-Si-C alloy This is an example to simulate uphill diffusion in a ternary single phase austenite matrix due to the classical Darken experiment published by L.S. Darken: Trans. Aime, v.180 (1949), pp. 430-438.

### [exa4](#)

One-phase problem. Carburization of binary Fe-C alloy: Comparison to an analytical erf solution This is a simple binary simulation with a single phase region. The numerical simulation is compared with an analytical erf solution. For this reason a special database erf.tdb is created where the diffusion coefficient is set to a concentration independent value. -----

### [exa5](#)

One-phase problem. Carburization of a binary Fe-0.15 wt% C alloy. A mixture of 40% N2 and 60% cracked methanol is 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. -----

### [exa6](#)

One-phase problem. Diffusion through a tube wall. A simple example about 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 MIXED boundary conditions. -----

### [exa7](#)

One phase example. 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 set up. Only time and temperature must be entered after the INPUT\_SCHEIL\_PROFILE command is executed. -----

### [exb1a](#)

Moving boundary problem. Austenite to ferrite transformation in a binary Fe-C alloy This example calculates a ferrite(BCC)/austenite(FCC) transformation in a binary Fe-C alloy. The initial state is an austenite of 2mm thickness. The composition of the austenite is Fe-0.15wt%C.

### [exb1b](#)

Moving boundary problem. Austenite to ferrite transformation in a binary Fe-C alloy This is the same example as in exb1a but now the problem is with ferrite as an inactive phase adjacent to the initial austenite. -----

### [exb1c](#)

Moving boundary problem. Austenite to ferrite transformation in a binary Fe-C alloy This is the same example as in exb1a and exb1b but now the simulation starts at a higher temperature and assumes a gradual cooling down to 1050 K.

### [exb2](#)

Description could not be found

### [exb3](#)

Moving boundary example. Dissolution of 23-carbide in an austenitic matrix This example calculates the dissolution of an M23C6 particle in an austenite matrix. A film of ferrite is allowed to nucleate around the carbide during the precipitation. -----

### [exb4a](#)

Moving boundary problem. Solidification path of an Fe-18%Cr-8%Ni alloy: Eutectic reaction This example 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 done in Thermo-Calc. -----

### [exb4b](#)

Moving boundary problem. Solidification path of an Fe-18%Cr-8%Ni alloy: Peritectic reaction This example is the 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 done in Thermo-Calc. -----

### [exb4c](#)

Moving boundary problem. Solidification path of an Fe-18%Cr-8%Ni alloy This example is the same as exb4b but now the diffusivity data is amended for the LIQUID and a high value for the diffusivity is used to simulate a case where it is assumed that the composition in the LIQUID is always homogeneous. This example is less realistic than exb4b. Comparison is made with both a Scheil-Gulliver simulation and equilibrium solidification conditions, both done in Thermo-Calc. -----

### [exb4d](#)

Moving boundary problem. Solidification path of an Fe-18%Cr-8%Ni alloy This example is the same as exb4b but instead of controlling the temperature the amount of heat extracted is given. Comparison is made with both a Scheil-Gulliver simulation and equilibrium solidification conditions, both done in Thermo-Calc. -----

### [exb5](#)

Moving boundary problem. Ternary 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 1373 K. This example corresponds to diffusion couple A in M. Kajihara, C.-B. Lim and M. Kikuchi: ISIJ International 33 (1993), pp. 498-507. See also M. Kajihara and M. Kikuchi: Acta Metall.Mater. 41 (1993), pp.2045-2059. -----

### [exb6](#)

Moving boundary problem. Microsegregation of phosphorus This example illustrates the effect of microsegregation of phosphorus during peritectic solidification in steel. -----

[exb7](#)

This example modifies the database interactively, which is not yet supported by GES6. Therefore, we enforce the use of GES5.

[exc1](#)

Cell calculation. Carbon in ferrite/austenite: Fe-C system, 2-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. Hägglund and J. Ågren: Acta Metall. Mater. 41 (1993), pp.1951-1957. -----

[exc2](#)

Cell calculation. Cementite dissolution in an Fe-Cr-C alloy: Three particle sizes and three different cells This example calculates the dissolution of cementite particles in an austenite matrix. This example is the same as exc1 but instead there are three particle sizes. A total of six particles are considered using three different cells. This is to represent some size distribution among the cementite particles. See also Z.-K. Liu, L. Hägglund, B. Jansson and J. Ågren: Metall.Trans.A, v. 22A (1991), pp. 1745-1752. -----

[exd1a](#)

Diffusion in dispersed systems. Carburization of Ni-25%Cr alloy: Dispersed system model This example is about carburization of a Ni-25Cr alloy. In this case the M3C2 and M7C3 carbides are entered as spheroid phases in a FCC matrix. 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. This case is from A. Engström, L. Hägglund and J. Ågren: Metall.Trans.A v. 25A (1994), pp. 1127-1134. -----

[exd1b](#)

Diffusion in dispersed systems. Carburization of Ni-25%Cr alloy: Homogenization model This example is about 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. Hägglund and J. Ågren: Metall.Trans. A, v.25A (1994), pp. 1127-1134. This simulation can be run with the DISPERSED SYSTEM MODEL or HOMOGENIZATION MODEL. The default HOMOGENIZATION MODEL is used and then ENTER\_HOMOGENIZATION\_FUNCTION should be used instead of ENTER\_LABYRINTH\_FUNCTION. -----

[exd2a](#)

Diffusion in dispersed systems. Diffusion couple of Fe-Cr-Ni alloys: Dispersed system model This example calculates 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: Scand. J. Met., v. 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. -----

[exd2b](#)

Diffusion in dispersed systems. Diffusion couple of Fe-Cr-Ni alloys: Homogenization model This example calculates 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: Scand. J. Met., v. 24, 1995, pp.12-20. 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. -----

[exd3](#)

Diffusion in dispersed systems. Diffusion couple of Fe-Cr-Ni alloys: Homogenization model This example uses the homogenization model. It is taken from H. Larsson and A. Engström, Acta. Mater. v.54 (2006), pp. 2431-2439. Experimental data from A. Engström, Scand J Metall, 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 will not affect the simulation. -----

[exe1](#)

Cooperative growth. Growth of pearlite in an Fe-Mn-C alloy An example of pearlite growth in an Fe-0.50wt%C-0.91wt%Mn steel. -----

[exf1](#)

Coarsening problem. Coarsening of M6C precipitate in an Fe-Mo-C alloy This example calculates the Ostwald-ripening of a spherical M6C carbide in an austenite matrix. -----

[exg1](#)

Kinetic data example. Checking mobilities and diffusivities in an Fe-Ni alloy This is an example file to check the mobilities and diffusivities in an Fe-Ni alloy. -----

[exg2](#)

Kinetic data example. Optimization of mobilities in Ni-Al fcc alloys A file for reading thermodynamic data and setting up the kinetic parameters that 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 Z. Metallkunde, Feb. 1996). -----

[exh1](#)

Deviation from local equilibrium. Ferrite/austenite diffusion couple with interface mobility This example calculates the growth of ferrite into austenite with a limited interface mobility. this is done by adding a Gibbs-energy contribution to the ferrite using the SET-SURFACE-ENERGY command. -----

[exh2](#)

Deviation from local equilibrium. Ferrite/austenite para-equilibrium in an Fe-Ni-C alloy This example calculates 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." Metall. Mat. Trans. A 35.4 (2004): 1211-1221. -----

[exh3](#)

Deviation from local equilibrium. Diffusion induced by a temperature gradient (thermomigration) This calculation shows how a temperature gradient induces diffusion. -----

[exi1](#)

Diffusion in complex phases. Diffusion in a system with B2 ordering This example shows diffusion in a system with B2 ordering. The datafile AlFeNi-data.TDB contains both a thermodynamic and kinetic description for the ordered and disordered BCC. -----

[exi2](#)

Diffusion in complex phases. 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.

[exi3a](#)

Diffusion in complex phases. Diffusion in iron oxide (FeO) This example shows the oxidation of an iron sample and the consequent growth of an oxide layer. -----

[exi3b](#)

Diffusion in complex phases. Diffusion in iron oxide (FeO) with a grain boundary contribution This example shows the oxidation of an iron sample and consequent growth of an oxide layer using the grain boundary diffusion contribution model. -----



## **One-Phase Problems**

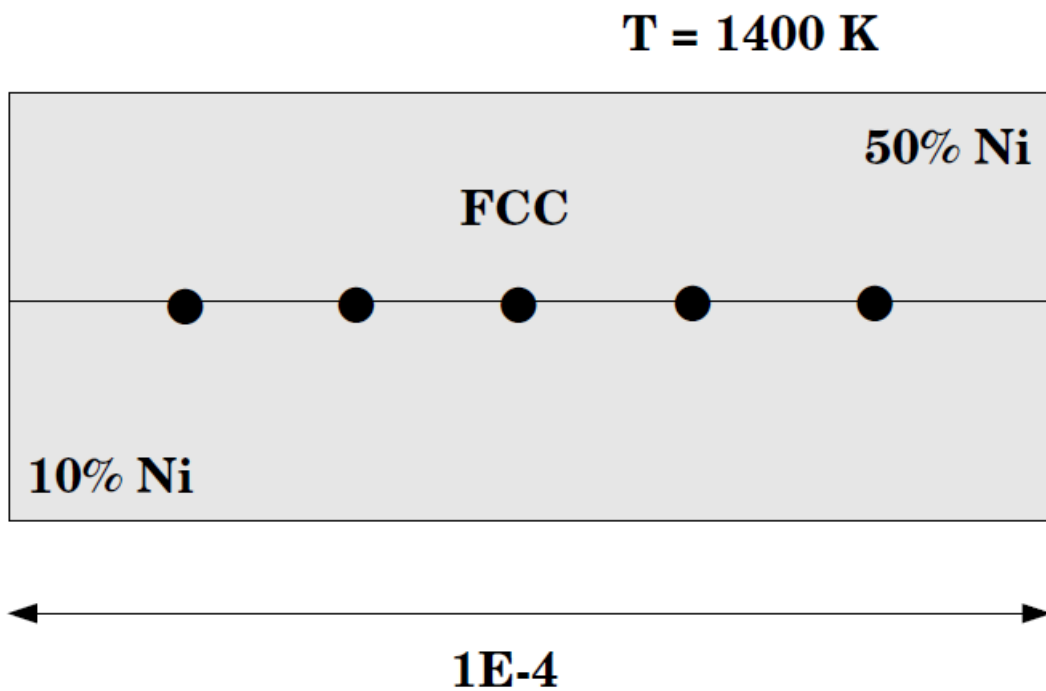




## Example exa1

### Homogenization of a binary Fe-Ni alloy: Linear Concentration Profile

Simple homogenization of a binary Fe-Ni alloy. It is assumed there is initially a linear Ni-concentration profile.



## Results

### exal-setup

#### SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

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Software running on Windows 64-bit wordlength  
Compiler: Intel Fortran Compiler 2025.0.0  
License library version: 9.7.0.0036  
Linked: Nov 19 2025 at 14:44:36

```
SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exal\setup.DCM.test"
```

```
SYS: @@
```

```
SYS: @@ One-phase problem.
```

```
SYS: @@ Homogenization of a binary Fe-Ni alloy.
```

```
SYS: @@ In this example it is assumed there is initially a linear
```

```
SYS: @@ Ni-concentration profile.
```

```
SYS: @@-----
```

```
SYS:
```

```
SYS: @@
```

```
SYS: @@ START BY GOING TO THE DATABASE MODULE
```

```
SYS: @@
```

```
SYS: goto module
```

```
MODULE NAME: data
```

```
THERMODYNAMIC DATABASE module
```

```
Database folder:
```

```
C:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\databases\da
```

```
ta
```

```
Current database: Steels/Fe-Alloys v12.0
```

```
VA /- DEFINED
```

```
DICTRA_FCC_A1 REJECTED
```

```
TDB_TCFE12:
```

```
TDB_TCFE12: @@
```

```
TDB_TCFE12: @@ USE THERMODYNAMIC DATABASE TO RETRIEVE DATA
```

```
TDB_TCFE12: @@
```

```
TDB_TCFE12: switch_database
```

```
Use one of these databases
```

```
TCFE12 = Steels/Fe-Alloys v12.0
```

```
TCFE9 = Steels/Fe-Alloys v9.3
```

```
SSUB6 = SGTE Substances v6.0
```

```
FEDEMO = Iron Demo Database v6.0
```

```
MOB2 = Alloys Mobility v2.7
```

```
MOBFE7 = Steels/Fe-Alloys Mobility v7.1
```

```
MOBFE4 = Steels/Fe-Alloys Mobility v4.0
```

```
MOBFE2 = Steels/Fe-Alloys Mobility v2.0
```

```
MFEDEMO = Fe-Alloys Mobility demo database v5.0
```

```
USER = User defined Database
```

```
DATABASE NAME /TCFE12/: fedemo
```

```
Current database: Iron Demo Database v6.0
```

```
VA /- DEFINED
```

```
TDB_FEDEMO:
```

```
TDB_FEDEMO: @@
```

```
TDB_FEDEMO: @@ DEFINE THE SYSTEM TO WORK WITH
```

```
TDB_FEDEMO: @@
```

```
TDB_FEDEMO: define_system
```

```
ELEMENTS: fe ni
```

```
FE NI DEFINED
```

```
TDB_FEDEMO:
```

```
TDB_FEDEMO: @@
```

```
TDB_FEDEMO: @@ EXCLUDE THE THERMODYNAMIC DATA FOR THE PHASES THAT ARE NOT NEEDED
```

```
TDB_FEDEMO: @@
```

```
TDB_FEDEMO: reject
```

```
ELEMENTS, SPECIES, PHASES, CONSTITUENT OR SYSTEM: /PHASES/: phase
```

```
PHASES: *
```

```
GAS:G LIQUID:L BCC_A2
```

```
C14_LAVES CBCC_A12 CUB_A13
```

```
FCC_A1 HCP_A3 REJECTED
```

```
TDB_FEDEMO:
```

```
TDB_FEDEMO: @@
```

```
TDB_FEDEMO: @@ RESTORE THE THERMODYNAMIC DATA FOR THE FCC PHASE
```

```
TDB_FEDEMO: @@
```

```
TDB_FEDEMO: restore
```

```
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /ELEMENTS/: phase
```

```
PHASES: fcc
```

```
FCC_A1 RESTORED
```

```
TDB_FEDEMO:
```

```
TDB_FEDEMO: @@
```

```
TDB_FEDEMO: @@ RETRIEVE DATA FROM THE DATABASE FILE
TDB_FEDEMO: @@
TDB_FEDEMO: get_data
08:38:49,782 [Thread-0] INFO  JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....
```

Use the command LIST\_REFERENCES to see the list of references for assessed data

-OK-

```
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ MOBILITY/DIFFUSIVITY DATA ARE STORED IN A SEPARATE DATABASE FILE.
TDB_FEDEMO: @@ SWITCH TO THE MOBILITY DATABASE TO RETRIEVE DATA
TDB_FEDEMO: @@
TDB_FEDEMO: append_database
Use one of these databases

TCFE12 = Steels/Fe-Alloys v12.0
TCFE9  = Steels/Fe-Alloys v9.3
SSUB6  = SGTE Substances v6.0
FEDEMO = Iron Demo Database v6.0
MOB2   = Alloys Mobility v2.7
MOBFE7 = Steels/Fe-Alloys Mobility v7.1
MOBFE4 = Steels/Fe-Alloys Mobility v4.0
MOBFE2 = Steels/Fe-Alloys Mobility v2.0
MFEDEMO = Fe-Alloys Mobility demo database v5.0
USER    = User defined Database
```

```
DATABASE NAME /FEDEMO/: mfedemo
Current database: Fe-Alloys Mobility demo database v5.0
```

```
VA DEFINED
APP: define_system
ELEMENTS: fe ni
FE NI DEFINED
APP: reject
ELEMENTS, SPECIES, PHASES, CONSTITUENT OR SYSTEM: /PHASES/: phase
PHASES: *
BCC_A2 FCC_A1 LIQUID:L
REJECTED
APP:
APP: restore
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /ELEMENTS/: phase
PHASES: fcc
FCC_A1 RESTORED
APP:
APP: get_data
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....
```

Use the command LIST\_REFERENCES to see the list of references for assessed data

-OK-

```
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP
APP: @@
APP: goto_module
MODULE NAME: dictra_monitor
NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set_condition
GLOBAL OR BOUNDARY CONDITION /GLOBAL/: global
VARIABLE : T
LOW TIME LIMIT /0/: 0
T(TIME,X)= 1400;
HIGH TIME LIMIT /*/: *
ANY MORE RANGES /N/: N
DIC>
DIC> @@
DIC> @@ START BY ENTERING A REGION
DIC> @@
DIC> enter_region
REGION NAME : austenite
DIC>
DIC> @@
DIC> @@ ENTER A GRID INTO THE REGION
DIC> @@
DIC> @@ FOR SIMPLICITY, AN EQUIDISTANT GRID IS USED
DIC> @@
DIC> enter_grid_coordinates
REGION NAME : /AUSTENITE/: austenite
WIDTH OF REGION /1/: 1e-4
TYPE /AUTO/: AUTO
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE active PHASE INTO THE REGION
DIC> @@
DIC> enter_phase_in_region
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /AUSTENITE/: austenite
PHASE TYPE /MATRIX/: matrix
PHASE NAME : /NONE/: fcc#1
DIC>
DIC> @@
DIC> @@ ENTER AN INITIAL Ni COMPOSITION INTO THE PHASE. A LINEAR
DIC> @@ VARIATION IN THE REGION IS ASSUMED.
DIC> @@
DIC> enter_compositions
REGION NAME : /AUSTENITE/: austenite
```

```
PHASE NAME: /FCC_A1/: fcc#1
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: weight_percent
PROFILE FOR /NI/: ni
TYPE /LINEAR/: linear
VALUE OF FIRST POINT : 10
VALUE OF LAST POINT : /10/: 50
DIC>
DIC> @@
DIC> @@ THE BOUNDARY CONDITION IS A CLOSED SYSTEM AS WE DO NOT SPECIFY
DIC> @@ ANYTHING ELSE
DIC> @@
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set_simulation_time
END TIME FOR INTEGRATION /.1/: 1E6
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /100000/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO FILE AND EXIT
DIC> @@
DIC> save_workspaces exal Y
DIC>
DIC> set_interactive
--OK--
DIC>
```

exal-run

DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exal\run.DCM.test"

DIC>

DIC>

DIC> @@ exal\_run.DCM

DIC>

DIC> @@

DIC> @@ FILE FOR RUNNING EXAMPLE a1

DIC> @@

DIC> goto\_module

MODULE NAME: dictra\_monitor

TIME STEP AT TIME 0.00000E+00

DIC>

DIC> read\_workspaces exal

OK

DIC>

DIC> @@

DIC> @@ Start the simulation

DIC> @@

DIC> simulate\_reaction

INFO: Default responses (if any) will be applied during the simulation. Use "SIMULATE\_REACTION NO" instead for manual input.

Region: AUSTENITE

linear 50 points

DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE

U-FRACTION IN SYSTEM: FE = .709679836161099 NI = .290320163838901

TOTAL SIZE OF SYSTEM: 1E-04 [m]

U-FRACTION IN SYSTEM: FE = .709679836161099 NI = .290320163838901

TOTAL SIZE OF SYSTEM: 1E-04 [m]

TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .709679836161099 NI = .290320163838901

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.10010000E-03 DT = 0.10000000E-03 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .709679836161099 NI = .290320163838901

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.40010010 DT = 0.40000000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .709679836161099 NI = .290320163838901

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 1197.6953 DT = 1197.2952 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .709679836161099 NI = .290320163838901

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 3592.2856 DT = 2394.5903 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .7096798361611 NI = .290320163838901

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 8381.4662 DT = 4789.1806 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .7096798361611 NI = .290320163838901

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 1 seconds

TIME = 17959.827 DT = 9578.3613 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .7096798361611 NI = .290320163838901

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 37116.550 DT = 19156.723 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .7096798361611 NI = .2903201638389

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 75429.995 DT = 38313.445 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .709679836161099 NI = .290320163838901

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 152056.89 DT = 76626.890 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .7096798361611 NI = .2903201638389

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 252056.89 DT = 100000.00 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .7096798361611 NI = .2903201638389

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 352056.89 DT = 100000.00 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .7096798361611 NI = .2903201638389

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 452056.89 DT = 100000.00 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .709679836161099 NI = .290320163838901

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 552056.89 DT = 100000.00 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .7096798361611 NI = .2903201638389

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 652056.89 DT = 100000.00 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .7096798361611 NI = .290320163838899

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 752056.89 DT = 100000.00 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .709679836161101 NI = .290320163838899

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 852056.89 DT = 100000.00 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .709679836161102 NI = .290320163838898

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 952056.89 DT = 100000.00 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .709679836161101 NI = .290320163838899

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 1000000.0 DT = 47943.115 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .709679836161101 NI = .290320163838899

TOTAL SIZE OF SYSTEM: 1E-04 [m]

MUST SAVE WORKSPACE ON FILE

WORKSPACE SAVED ON FILE

RECLAIMING WORKSPACE

DELETING TIME-RECORD FOR TIME 0.0000000

DELETING TIME-RECORD FOR TIME 0.10000000E-06

DELETING TIME-RECORD FOR TIME 0.10010000E-03

DELETING TIME-RECORD FOR TIME 0.40010010

DELETING TIME-RECORD FOR TIME 1197.6953

```
DELETING TIME-RECORD FOR TIME 3592.2856
DELETING TIME-RECORD FOR TIME 8381.4662
DELETING TIME-RECORD FOR TIME 17959.827
DELETING TIME-RECORD FOR TIME 37116.550
DELETING TIME-RECORD FOR TIME 75429.995
DELETING TIME-RECORD FOR TIME 152056.89
DELETING TIME-RECORD FOR TIME 252056.89
DELETING TIME-RECORD FOR TIME 352056.89
DELETING TIME-RECORD FOR TIME 452056.89
DELETING TIME-RECORD FOR TIME 552056.89
DELETING TIME-RECORD FOR TIME 652056.89
DELETING TIME-RECORD FOR TIME 752056.89
DELETING TIME-RECORD FOR TIME 852056.89
```

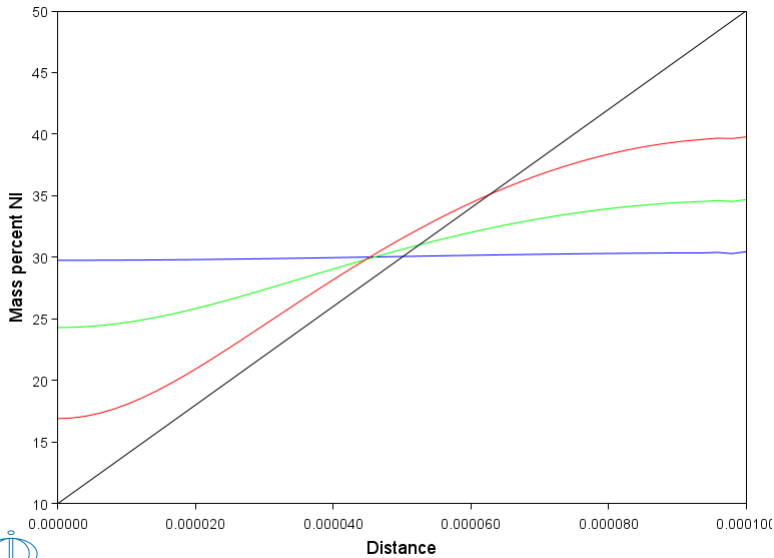
```
KEEPING TIME-RECORD FOR TIME 952056.89
AND FOR TIME 1000000.0
WORKSPACE RECLAIMED
```

```
TIMESTEP AT 1000000.00 SELECTED
```

```
DIC>
DIC> @@
DIC> @@ THE SIMULATION IS FINISHED
DIC> @@
DIC>
DIC> set_interactive
--OK--
DIC>
```

exal-plot

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exal\plot.DCM.test"
DIC>
DIC>
DIC> @@ exal_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE a1
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> goto_module
MODULE NAME: dictra_monitor
TIME STEP AT TIME 1.00000E+06
DIC> read_workspaces exal
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post_processor
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1:
POST-1: @@
POST-1: @@ PLOT SOME CONCENTRATION PROFILES
POST-1: @@
POST-1: set_diagram_axis
AXIS (X, Y OR Z) : x
VARIABLE : distance
INFO: Distance is set as independent variable
DISTANCE : /GLOBAL/: global
POST-1:
POST-1: set_diagram_axis
AXIS (X, Y OR Z) : y
VARIABLE : weight-percent
FOR COMPONENT : ni
POST-1:
POST-1: set_plot_condition
CONDITION /TIME/: time
VALUE(S) /LAST/: 0 1e5 3e5 1e6
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot_diagram
```



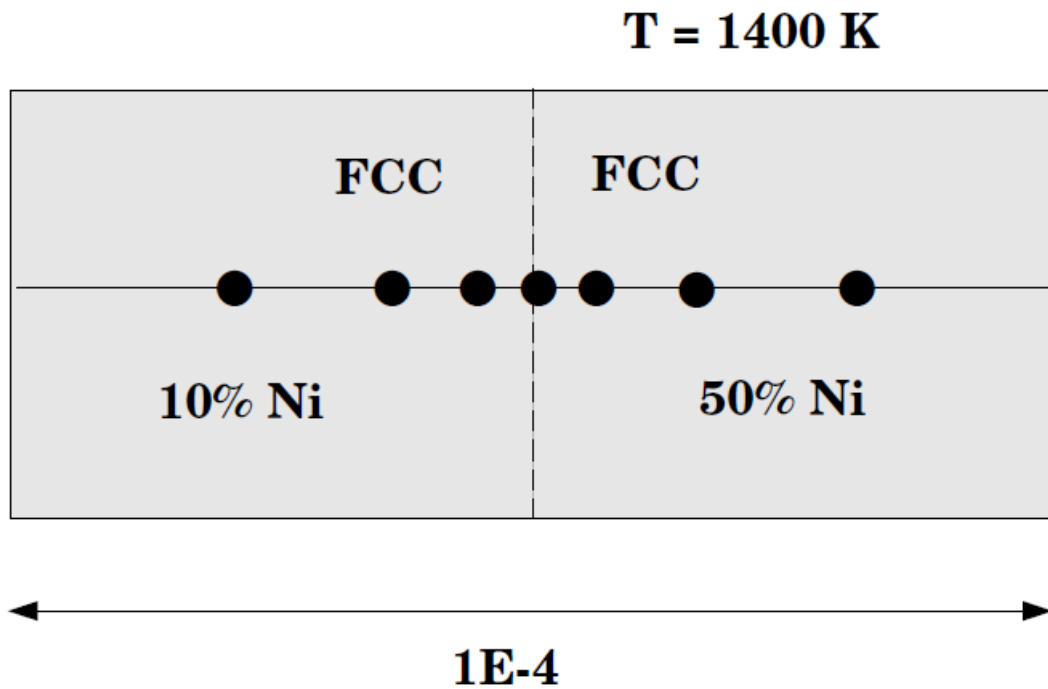
```
POST-1:
POST-1:
POST-1:
POST-1: @?<Hit_return_to_continue>
POST-1:
POST-1: set_interactive
--OK--
POST-1:
```



## Example exa2a

### Homogenization of a binary Fe-Ni alloy: Step-profile

Simple homogenization of a binary Fe-Ni alloy. A Ni rich and a Ni lean alloy are put together and initially there is a step profile.



## exa2a-setup

### SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,  
Stockholm, Sweden

Software running on Windows 64-bit wordlength  
Compiler: Intel Fortran Compiler 2025.0.0  
License library version: 9.7.0.0036  
Linked: Nov 19 2025 at 14:44:36

```
SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exa2a\setup.DCM.test"
```

```
SYS: @@
SYS: @@ One-phase problem.
SYS: @@ Homogenization of a binary Fe-Ni alloy.
SYS: @@ A Ni rich and a Ni lean alloy are put together and initially
SYS: @@ there is a step profile.
SYS: @@-----
SYS:
SYS: @@ exa2a_setup.DCM
SYS:
SYS: @@
SYS: @@ IN exa1 ALL THE COMMANDS WERE WRITTEN IN FULL BUT NOW ABBREVIATED
SYS: @@ COMMANDS ARE USED
SYS: @@
SYS:
SYS: @@
SYS: @@ FIRST DEFINE A LOG-FILE FOR THIS EXAMPLE
SYS: @@
SYS: set_log_file setup
Heading:
SYS: @@
SYS: @@ NOW GO TO THE DATABASE MODULE
SYS: @@
SYS: go da
... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\databases\da
ta
Current database: Steels/Fe-Alloys v12.0

VA                /- DEFINED
DICTRA_FCC_A1    REJECTED
TDB_TCFE12:
TDB_TCFE12: @@
TDB_TCFE12: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA
TDB_TCFE12: @@
TDB_TCFE12: sw FEDEMO
... the command in full is SWITCH_DATABASE
Current database: Iron Demo Database v6.0

VA                /- DEFINED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ DEFINE THE SYSTEM TO WORK WITH
TDB_FEDEMO: @@
TDB_FEDEMO: def-system fe ni
... the command in full is DEFINE_SYSTEM
FE                NI    DEFINED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ EXCLUDE THE THERMODYNAMIC DATA FOR THE PHASES THAT ARE NOT NEEDED
TDB_FEDEMO: @@
TDB_FEDEMO: rej ph * all
... the command in full is REJECT
GAS:G             LIQUID:L             BCC_A2
C14 LAVES        CBCC_A12             CUB_A13
FCC_A1           HCP_A3    REJECTED
TDB_FEDEMO: res ph fcc
... the command in full is RESTORE
FCC_A1    RESTORED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ RETRIEVE DATA FROM THE DATABASE FILE
TDB_FEDEMO: @@
TDB_FEDEMO: get
... the command in full is GET_DATA
08:41:48,180 [Thread-0] INFO  JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ...

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ MOBILITY/DIFFUSIVITY DATA ARE STORED IN A SEPARATE DATABASE FILE.
TDB_FEDEMO: @@ SWITCH TO THE MOBILITY DATABASE TO RETRIEVE DATA
TDB_FEDEMO: @@
TDB_FEDEMO: app
... the command in full is APPEND_DATABASE
Use one of these databases

TCFE12 = Steels/Fe-Alloys v12.0
TCFE9  = Steels/Fe-Alloys v9.3
SSUB6  = SGTE Substances v6.0
FEDEMO = Iron Demo Database v6.0
MOB2   = Alloys Mobility v2.7
MOBFE7 = Steels/Fe-Alloys Mobility v7.1
MOBFE4 = Steels/Fe-Alloys Mobility v4.0
MOBFE2 = Steels/Fe-Alloys Mobility v2.0
```





```
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO FILE AND EXIT
DIC> @@
DIC> save exa2a Y
... the command in full is SAVE_WORKSPACES
DIC>
DIC> set-inter
... the command in full is SET_INTERACTIVE
--OK--
DIC>
```

exa2a-run

DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC:MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exa2a\run.DCM.test"

... the command in full is MACRO\_FILE\_OPEN

DIC>

DIC>

DIC> @@ exa2a\_run.DCM

DIC>

DIC> @@

DIC> @@ FILE FOR RUNNING EXAMPLE a2a

DIC> @@

DIC>

DIC> @@

DIC> @@ ENTER THE DICTRA MONITOR AN READ SETUP FROM FILE

DIC> @@

DIC> go d-m

... the command in full is GOTO\_MODULE

TIME STEP AT TIME 0.00000E+00

DIC>

DIC> read exa2a

... the command in full is READ\_WORKSPACES

... the command in full is DEFINE\_COMPONENTS

... the command in full is SELECT\_EQUILIBRIUM

OK

DIC>

DIC> @@

DIC> @@ START THE SIMULATION

DIC> @@

DIC> simulate

... the command in full is SIMULATE\_REACTION

INFO: Default responses (if any) will be applied during the simulation. Use "SIMULATE\_REACTION NO" instead for manual input.

DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE

... the command in full is SET\_NUMERICAL\_LIMITS

U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383

TOTAL SIZE OF SYSTEM: 1E-04 [m]

U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383

TOTAL SIZE OF SYSTEM: 1E-04 [m]

2 GRIDPOINT(S) ADDED TO CELL #1 REGION: AUSTENITE

TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .29111175459383

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.10010000E-03 DT = 0.10000000E-03 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .29111175459383

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.40010010 DT = 0.40000000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 8.1787785 DT = 7.7786784 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 23.736135 DT = 15.557357 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .29111175459383

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 1 seconds

TIME = 54.850849 DT = 31.114714 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .29111175459383

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 117.08028 DT = 62.229428 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 241.53913 DT = 124.45886 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .29111175459383

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 490.45684 DT = 248.91771 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .29111175459383

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 988.29226 DT = 497.83542 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 1983.9631 DT = 995.67084 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 3975.3048 DT = 1991.3417 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .29111175459383

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 7957.9881 DT = 3982.6834 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 15923.355 DT = 7965.3667 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 31854.088 DT = 15930.733 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 63715.555 DT = 31861.467 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 127438.49 DT = 63722.934 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 227438.49 DT = 100000.00 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 327438.49 DT = 100000.00 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383

```
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep          0 seconds
TIME = 427438.49 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406168 NI = .291111754593832
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep          0 seconds
TIME = 527438.49 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep          0 seconds
TIME = 627438.49 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .291111754593829
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep          1 seconds
TIME = 727438.49 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406171 NI = .291111754593829
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep          0 seconds
TIME = 827438.49 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406171 NI = .291111754593829
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep          0 seconds
TIME = 927438.49 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .291111754593831
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep          0 seconds
TIME = 1000000.0 DT = 72561.511 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406171 NI = .291111754593828
TOTAL SIZE OF SYSTEM: 1E-04 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 0.0000000
DELETING TIME-RECORD FOR TIME 0.100000000E-06
DELETING TIME-RECORD FOR TIME 0.100100000E-03
DELETING TIME-RECORD FOR TIME 0.40010010
DELETING TIME-RECORD FOR TIME 8.1787785
DELETING TIME-RECORD FOR TIME 23.736135
DELETING TIME-RECORD FOR TIME 54.850849
DELETING TIME-RECORD FOR TIME 117.08028
DELETING TIME-RECORD FOR TIME 241.53913
DELETING TIME-RECORD FOR TIME 490.45684
DELETING TIME-RECORD FOR TIME 988.29226
DELETING TIME-RECORD FOR TIME 1983.9631
DELETING TIME-RECORD FOR TIME 3975.3048
DELETING TIME-RECORD FOR TIME 7957.9881
DELETING TIME-RECORD FOR TIME 15923.355
DELETING TIME-RECORD FOR TIME 31854.088
DELETING TIME-RECORD FOR TIME 63715.555
DELETING TIME-RECORD FOR TIME 127438.49
DELETING TIME-RECORD FOR TIME 227438.49
DELETING TIME-RECORD FOR TIME 327438.49
DELETING TIME-RECORD FOR TIME 427438.49
DELETING TIME-RECORD FOR TIME 527438.49
DELETING TIME-RECORD FOR TIME 627438.49
DELETING TIME-RECORD FOR TIME 727438.49
DELETING TIME-RECORD FOR TIME 827438.49

KEEPING TIME-RECORD FOR TIME 927438.49
AND FOR TIME 1000000.0
WORKSPACE RECLAIMED

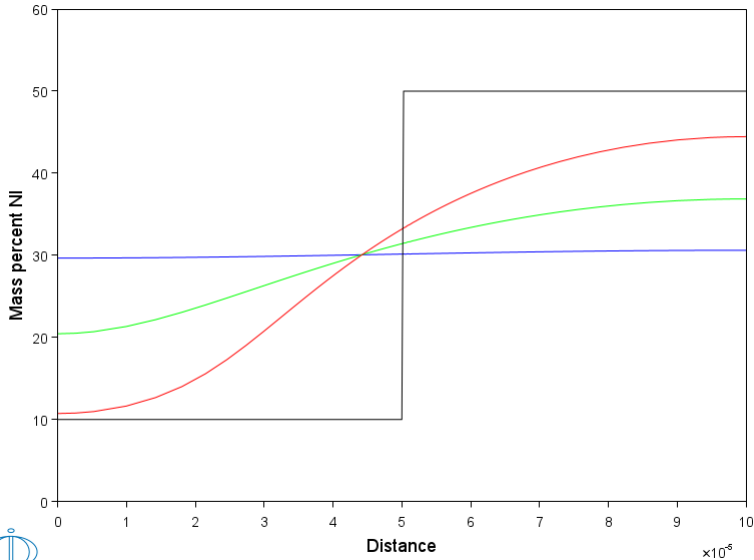
TIMESTEP AT 1000000.00 SELECTED
```

```
DIC>
DIC> @@
DIC> @@ THE SIMULATION IS FINISHED
DIC> @@
DIC>
DIC> set-inter
... the command in full is SET_INTERACTIVE
--OK--
DIC>
```

exa2a-plot

DIC>About

```
NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exa2a\plot.DCM.test"
... the command in full is MACRO_FILE_OPEN
DIC>
DIC>
DIC> @@ exa2a_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE a2a
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
... the command in full is GOTO_MODULE
TIME STEP AT TIME 1.00000E+06
DIC>
DIC> read exa2a
... the command in full is READ_WORKSPACES
... the command in full is DEFINE_COMPONENTS
... the command in full is SELECT_EQUILIBRIUM
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
... the command in full is POST_PROCESSOR
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1:
POST-1: @@
POST-1: @@ PLOT SOME NI-CONCENTRATION PROFILES
POST-1: @@
POST-1: s-d-a
... the command in full is SET_DIAGRAM_AXIS
AXIS (X, Y OR Z) : x
VARIABLE : dist
INFO: Distance is set as independent variable
... the command in full is SET_INDEPENDENT_VARIABLE
DISTANCE : /GLOBAL/: glo
POST-1:
POST-1: s-d-a
... the command in full is SET_DIAGRAM_AXIS
AXIS (X, Y OR Z) : y
VARIABLE : weight-percent
FOR COMPONENT : ni
POST-1:
POST-1: s-p-c
... the command in full is SET_PLOT_CONDITION
CONDITION /TIME/: time
VALUE(S) /LAST/: 0 1e5 3e5 1e6
POST-1:
POST-1: @@
POST-1: @@ SET SCALING ON Y-AXIS BEFORE PLOTTING
POST-1: @@
POST-1: s-s-s
... the command in full is SET_SCALING_STATUS
AXIS (X, Y OR Z) : y
AUTOMATIC SCALING (Y OR N) /N/: n
MIN VALUE : 0
MAX VALUE : 60
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
... the command in full is MAKE_EXPERIMENTAL_DATAFILE
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
... the command in full is PLOT_DIAGRAM
```



POST-1:  
POST-1:

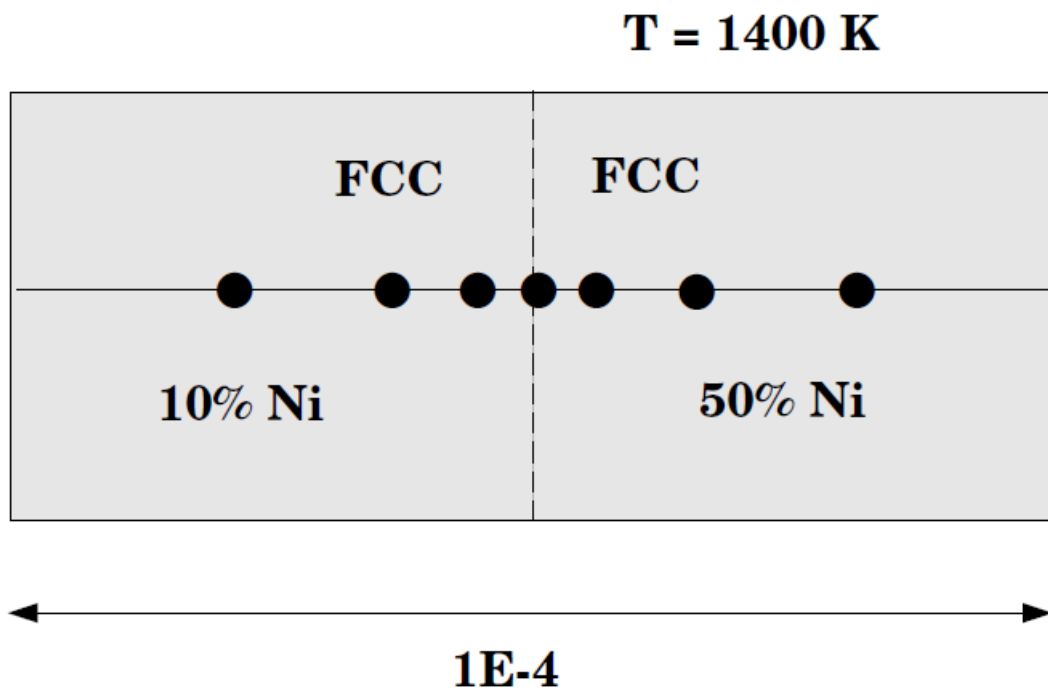
```
POST-1:
POST-1: @?<Hit_return_to_continue>
POST-1:
POST-1: set-inter
... the command in full is SET_INTERACTIVE_MODE
--OK--
POST-1:
```



## Example exa2b

### Homogenization of a binary Fe-Ni alloy

Simple homogenization of a binary Fe-Ni alloy. We have put together a Ni rich and a Ni lean alloy. This example is identical to exa2a. However, in this example implicit time integration is used instead of the trapezoidal method for solving the PDEs.



## exa2b-setup

### SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,  
Stockholm, Sweden

Software running on Windows 64-bit wordlength  
Compiler: Intel Fortran Compiler 2025.0.0  
License library version: 9.7.0.0036  
Linked: Nov 19 2025 at 14:44:36

```
SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exa2b\setup.DCM.test"
```

```
SYS: @@
SYS: @@ One-phase problem.
SYS: @@ Homogenization of a binary Fe-Ni alloy.
SYS: @@ This example is identical to a2a but instead it uses implicit time
SYS: @@ integration instead of the trapezoidal method for solving the PDEs.
SYS: @@-----
SYS:
SYS: @@ exa2b_setup.DCM
SYS:
SYS: @@
SYS: @@ FIRST DEFINE A LOG-FILE FOR THIS EXAMPLE
SYS: @@
SYS: set_log_file setup
Heading:
SYS: @@
SYS: @@ THEN GO TO THE DATABASE MODULE
SYS: @@
SYS: go da
... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\databases\da
ta
Current database: Steels/Fe-Alloys v12.0

VA          /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE12:
TDB_TCFE12: @@
TDB_TCFE12: @@ USE THE TCFE DATABASE FOR THERMODYNAMIC DATA
TDB_TCFE12: @@
TDB_TCFE12: sw fedemo
... the command in full is SWITCH_DATABASE
Current database: Iron Demo Database v6.0

VA          /- DEFINED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ DEFINE THE SYSTEM TO WORK WITH
TDB_FEDEMO: @@
TDB_FEDEMO: def-system fe ni
... the command in full is DEFINE_SYSTEM
FE          NI DEFINED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ EXCLUDE THE THERMODYNAMIC DATA FOR THE PHASES THAT ARE NOT NEEDED
TDB_FEDEMO: @@
TDB_FEDEMO: rej ph * all
... the command in full is REJECT
GAS:G          LIQUID:L          BCC_A2
C14_LAVES          CBCC_A12          CUB_A13
FCC_A1          HCP_A3 REJECTED
TDB_FEDEMO: res ph fcc
... the command in full is RESTORE
FCC_A1 RESTORED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ RETRIEVE DATA FROM THE DATABASE FILE
TDB_FEDEMO: @@
TDB_FEDEMO: get
... the command in full is GET_DATA
08:44:45,594 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ...

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ MOBILITY/DIFFUSIVITY DATA ARE STORED IN A SEPARATE DATABASE FILE.
TDB_FEDEMO: @@ SWITCH TO THE MOBILITY DATABASE TO RETRIEVE DATA.
TDB_FEDEMO: @@
TDB_FEDEMO: app
... the command in full is APPEND_DATABASE
Use one of these databases

TCFE12 = Steels/Fe-Alloys v12.0
TCFE9  = Steels/Fe-Alloys v9.3
SSUB6  = SGTE Substances v6.0
FEDEMO = Iron Demo Database v6.0
MOB2   = Alloys Mobility v2.7
MOBFE7 = Steels/Fe-Alloys Mobility v7.1
MOBFE4 = Steels/Fe-Alloys Mobility v4.0
MOBFE2 = Steels/Fe-Alloys Mobility v2.0
MFEDEMO = Fe-Alloys Mobility demo database v5.0
USER    = User defined Database

DATABASE NAME /FEDEMO/: mfedemo
Current database: Fe-Alloys Mobility demo database v5.0
```





```
INITIAL TIMESTEP : /1E-07/:  
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:  
DIC>  
DIC>  
DIC> @@  
DIC> @@ SAVE THE SET UP TO FILE AND EXIT  
DIC> @@  
DIC> save exa2b Y  
... the command in full is SAVE_WORKSPACES  
DIC>  
DIC> set-inter  
... the command in full is SET_INTERACTIVE  
--OK--  
DIC>
```

exa2b-run

DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exa2b\run.DCM.test"

... the command in full is MACRO\_FILE\_OPEN

DIC>

DIC>

DIC> @@ exa2b\_run.DCM

DIC>

DIC> @@

DIC> @@ FILE FOR RUNNING EXAMPLE a2b

DIC> @@

DIC>

DIC> @@

DIC> @@ ENTER THE DICTRA MONITOR AN READ SETUP FROM FILE

DIC> @@

DIC>

go d-m

... the command in full is GOTO\_MODULE

TIME STEP AT TIME 0.00000E+00

DIC> read exa2b

... the command in full is READ\_WORKSPACES

... the command in full is DEFINE\_COMPONENTS

... the command in full is SELECT\_EQUILIBRIUM

OK

DIC>

DIC> @@

DIC> @@ Start the simulation

DIC> @@

DIC> simulate

... the command in full is SIMULATE\_REACTION

INFO: Default responses (if any) will be applied during the simulation. Use "SIMULATE\_REACTION NO" instead for manual input.

... the command in full is SET\_NUMERICAL\_LIMITS

U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383

TOTAL SIZE OF SYSTEM: 1E-04 [m]

U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383

TOTAL SIZE OF SYSTEM: 1E-04 [m]

2 GRIDPOINT(S) ADDED TO CELL #1 REGION: AUSTENITE

TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .29111175459383

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.10010000E-03 DT = 0.10000000E-03 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .29111175459383

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.40010010 DT = 0.400000000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 8.1725731 DT = 7.7724730 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 23.717519 DT = 15.544946 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .29111175459383

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 54.807411 DT = 31.089892 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 116.98720 DT = 62.179784 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 241.34676 DT = 124.35957 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 490.06590 DT = 248.71914 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 987.50417 DT = 497.43827 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 1982.3807 DT = 994.87654 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .29111175459383

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 3972.1338 DT = 1989.7531 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 7951.6400 DT = 3979.5062 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 15910.652 DT = 7959.0123 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 31828.677 DT = 15918.025 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 63664.726 DT = 31836.049 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .708888245406171 NI = .291111754593829

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 127336.83 DT = 63672.099 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .708888245406166 NI = .291111754593834

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 227336.83 DT = 100000.00 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .708888245406162 NI = .291111754593838

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 327336.83 DT = 100000.00 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: FE = .70888824540616 NI = .29111175459384

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 1 seconds

```
TIME = 427336.83 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406162 NI = .291111754593838
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 527336.83 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406164 NI = .291111754593836
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 627336.83 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406161 NI = .291111754593839
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 727336.83 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406161 NI = .291111754593839
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 827336.83 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406163 NI = .291111754593837
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 927336.83 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406163 NI = .291111754593837
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 1000000.0 DT = 72663.175 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406167 NI = .291111754593833
TOTAL SIZE OF SYSTEM: 1E-04 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 0.0000000
DELETING TIME-RECORD FOR TIME 0.100000000E-06
DELETING TIME-RECORD FOR TIME 0.100100000E-03
DELETING TIME-RECORD FOR TIME 0.40010010
DELETING TIME-RECORD FOR TIME 8.1725731
DELETING TIME-RECORD FOR TIME 23.717519
DELETING TIME-RECORD FOR TIME 54.807411
DELETING TIME-RECORD FOR TIME 116.98720
DELETING TIME-RECORD FOR TIME 241.34676
DELETING TIME-RECORD FOR TIME 490.06590
DELETING TIME-RECORD FOR TIME 987.50417
DELETING TIME-RECORD FOR TIME 1982.3807
DELETING TIME-RECORD FOR TIME 3972.1338
DELETING TIME-RECORD FOR TIME 7951.6400
DELETING TIME-RECORD FOR TIME 15910.652
DELETING TIME-RECORD FOR TIME 31828.677
DELETING TIME-RECORD FOR TIME 63664.726
DELETING TIME-RECORD FOR TIME 127336.83
DELETING TIME-RECORD FOR TIME 227336.83
DELETING TIME-RECORD FOR TIME 327336.83
DELETING TIME-RECORD FOR TIME 427336.83
DELETING TIME-RECORD FOR TIME 527336.83
DELETING TIME-RECORD FOR TIME 627336.83
DELETING TIME-RECORD FOR TIME 727336.83
DELETING TIME-RECORD FOR TIME 827336.83

KEEPING TIME-RECORD FOR TIME 927336.83
AND FOR TIME 1000000.0
WORKSPACE RECLAIMED

TIMESTEP AT 1000000.00 SELECTED
```

```
DIC>
DIC> @@
DIC> @@ THE SIMULATION IS FINISHED
DIC> @@
DIC>
DIC> set-inter
... the command in full is SET_INTERACTIVE
--OK--
DIC>
```

## exa2b-plot

DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exa2b\plot.DCM.test"

... the command in full is MACRO\_FILE\_OPEN

DIC>

DIC>

DIC> @@ exa2b\_plot.DCM

DIC>

DIC> @@

DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE a2b

DIC> @@

DIC> @@

DIC> @@

DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE

DIC> @@

DIC> go d-m

... the command in full is GOTO\_MODULE

TIME STEP AT TIME 1.00000E+06

DIC> read exa2b

... the command in full is READ\_WORKSPACES

... the command in full is DEFINE\_COMPONENTS

... the command in full is SELECT\_EQUILIBRIUM

OK

DIC>

DIC> @@

DIC> @@ GO TO THE POST PROCESSOR

DIC> @@

DIC> post

... the command in full is POST\_PROCESSOR

POST PROCESSOR VERSION 1.7

Implemented by Bjorn Jonsson

POST-1:

POST-1:

POST-1: @@

POST-1: @@ PLOT SOME CONCENTRATION PROFILES

POST-1: @@

POST-1: s-d-a

... the command in full is SET\_DIAGRAM\_AXIS

AXIS (X, Y OR Z) : x

VARIABLE : dist

INFO: Distance is set as independent variable

... the command in full is SET\_INDEPENDENT\_VARIABLE

DISTANCE : /GLOBAL/: glo

POST-1:

POST-1: s-d-a

... the command in full is SET\_DIAGRAM\_AXIS

AXIS (X, Y OR Z) : y

VARIABLE : w-p

FOR COMPONENT : ni

POST-1:

POST-1: s-p-c

... the command in full is SET\_PLOT\_CONDITION

CONDITION /TIME/: time

VALUE(S) /LAST/: 0 1e5 3e5 1e6

POST-1:

POST-1: @@

POST-1: @@ SET SCALING ON Y-AXIS BEFORE PLOTTING

POST-1: @@

POST-1: s-s-s

... the command in full is SET\_SCALING\_STATUS

AXIS (X, Y OR Z) : y

AUTOMATIC SCALING (Y OR N) /N/: n

MIN VALUE : 0

MAX VALUE : 60

POST-1:

POST-1:

POST-1: SET\_EXP\_FILE\_FORMAT 5

POST-1: MAKE c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\unite\distribution\macroResult.exp Y

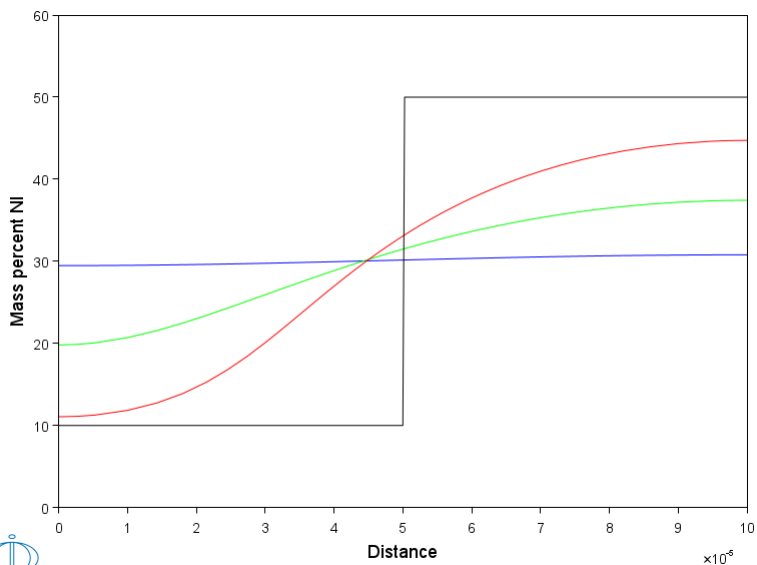
... the command in full is MAKE\_EXPERIMENTAL\_DATAFILE

POST-1: SET\_EXP\_FILE\_FORMAT 10

POST-1:

POST-1: plot

... the command in full is PLOT\_DIAGRAM



POST-1:

POST-1:

POST-1:

```
POST-1: @?<Hit_return_to_continue>
POST-1:
POST-1: set-inter
... the command in full is SET_INTERACTIVE_MODE
--OK--
POST-1:
```

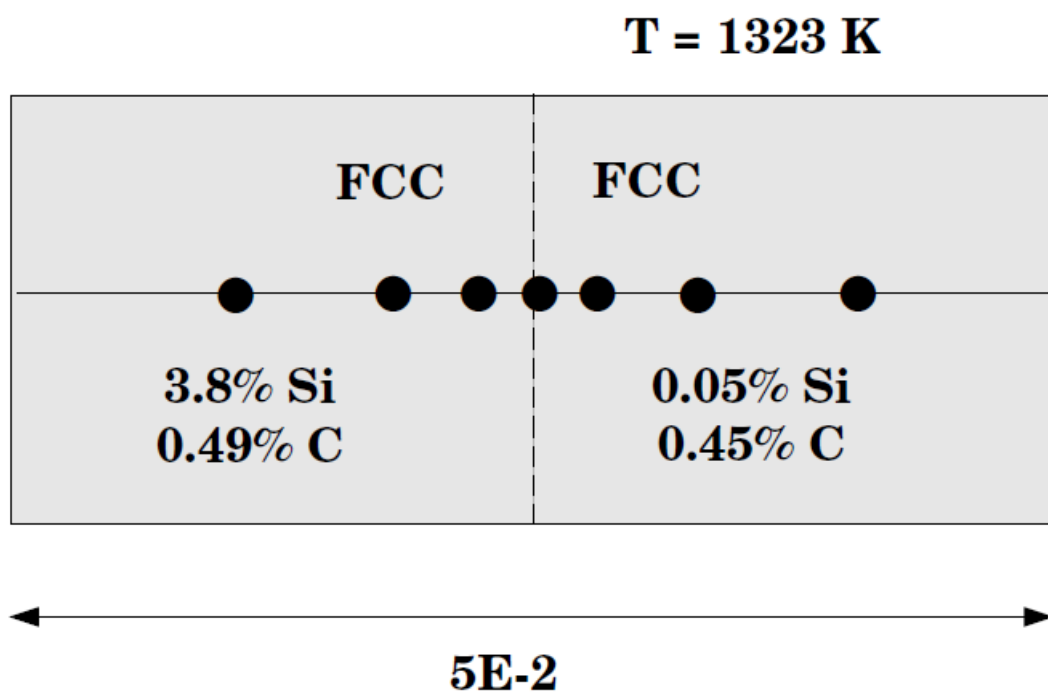


## Example exa3

### Uphill diffusion in an Fe-Si-C alloy

Simulation of uphill diffusion in a ternary single phase austenite matrix due to the classical darken experiment published by L.S. Darken (Trans. Aime, v.180 (1949), pp. 430-438).

In this example, 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. This is done by giving the compositions of Si and C in each gridpoint individually. These data are then stored on file.



## exa3-setup

### SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,  
Stockholm, Sweden

Software running on Windows 64-bit wordlength  
Compiler: Intel Fortran Compiler 2025.0.0  
License library version: 9.7.0.0036  
Linked: Nov 19 2025 at 14:44:36

```
SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exa3\setup.DCM.test"
```

```
SYS: @@
SYS: @@ One-phase problem.
SYS: @@ Uphill diffusion in an Fe-Si-C alloy
SYS: @@ This is an example to simulate uphill diffusion in a ternary single
SYS: @@ phase austenite matrix due to the classical Darken experiment published
SYS: @@ by L.S. Darken: Trans. Aime, v.180 (1949), pp. 430-438.
SYS: @@
SYS: @@ In this example two pieces of austenite (3.80 wt%Si, 0.49 wt%C) and
SYS: @@ (0.05 wt%Si, 0.45 wt%C) are put together and are subsequently annealed
SYS: @@ at 1050C for 13 days. As both pieces are austenite they must be entered
SYS: @@ into the same region. This is done by individually giving the compositions
SYS: @@ of Si and C in each grid point. These data are then stored to file.
SYS: @@-----
SYS:
SYS: @@ darken_setup.DCM
SYS:
SYS: @@
SYS: @@ Note that LOG-FILES used previously in examples a2a and a2b are
SYS: @@ no longer used.
SYS: @@
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASE
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\databases\da
ta
Current database: Steels/Fe-Alloys v12.0

VA          /-  DEFINED
DICTRA_FCC_A1  REJECTED
TDB_TCFE12:
TDB_TCFE12: @@
TDB_TCFE12: @@ USE A TCFE DATABASE FOR THE THERMODYNAMIC DATA
TDB_TCFE12: @@
TDB_TCFE12: sw tcfe9
Current database: Steels/Fe-Alloys v9.3

VA          /-  DEFINED
L12_FCC      B2_BCC          DICTRA_FCC_A1
REJECTED
TDB_TCFE9: def-sys fe si c
FE          SI              C
DEFINED
TDB_TCFE9: rej ph * all
GAS:G      LIQUID:L        BCC_A2
FCC_A1     HCP_A3          CBCC_A12
CUB_A13    DIAMOND_FCC_A4  GRAPHITE
CEMENTITE  M23C6          M7C3
M5C2       KSI_CARBIDE     FE4N_LP1
FECN_CHI   LAVES_PHASE_C14 M3SI
CR3SI      FE2SI           FESI2_H
FESI2_L    MSI             M5SI3
AL4C3      FE8SI2C         SIC
AL5FE4     MP_B31            M2P_C22
REJECTED
TDB_TCFE9: res ph fcc
FCC_A1 RESTORED
TDB_TCFE9: get
08:47:43,630 [Thread-0] INFO  JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ...

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE MOBILITY DATA
TDB_TCFE9: @@
TDB_TCFE9: app mobfe4
Current database: Steels/Fe-Alloys Mobility v4.0

VA  DEFINED
B2_BCC REJECTED
APP: def-sys fe si c
FE          SI              C
DEFINED
APP: rej ph * all
BCC_A2     CEMENTITE       FCC_A1
FE4N_LP1   HCP_A3            LIQUID:L
REJECTED
APP: res ph fcc
FCC_A1 RESTORED
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
```

FUNCTIONS ....

Use the command LIST\_REFERENCES to see the list of references for assessed data

--OK--

```
APP: @@
APP: @@ ENTER THE DICTRA MONITOR
APP: @@
APP: go d-m
NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 1323; * N
DIC>
DIC> @@
DIC> @@ ENTER THE REGION austenite
DIC> @@
DIC> enter-region
REGION NAME : austenite
DIC>
DIC> @@
DIC> @@ ENTER THE GRID
DIC> @@ NOTE THAT GRID POINT DISTANCES ARE SMALLEST AROUND THE MIDDLE
DIC> @@
DIC> enter-grid
REGION NAME : /AUSTENITE/: austenite
WIDTH OF REGION /1/: 50E-3
TYPE /AUTO/: AUTO
DIC>
DIC> @@
DIC> @@ ENTER THE PHASE INTO A REGION (BOTH PIECES ARE AUSTENITIC)
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /AUSTENITE/: austenite
PHASE TYPE /MATRIX/: matrix
PHASE NAME : /NONE/: fcc#1
DIC>
DIC> @@
DIC> @@ ENTER COMPOSITIONS INTO THE PHASE
DIC> @@
DIC> enter-composition
REGION NAME : /AUSTENITE/: austenite
PHASE NAME : /FCC_A1/: fcc#1
DEPENDENT COMPONENT ? /SI/: FE
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: C func 0.49-0.04*hs(x-25e-3);
PROFILE FOR /SI/: SI func 3.80-3.75*hs(x-25e-3);
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME AND OTHER SIMULATION PARAMETERS
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 1e10
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /1E+09/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC> save exa3 Y
DIC>
DIC> set-inter
--OK--
DIC>
```

exa3-run

DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exa3\run.DCM.test"

DIC>

DIC>

DIC> @@ darken\_run.DCM

DIC>

DIC> @@

DIC> @@ ENTER THE DICTRA MONITOR

DIC> @@

DIC> go d-m

TIME STEP AT TIME 0.00000E+00

DIC>

DIC> @@

DIC> @@ READ SETUP FROM FILE AND START SIMULATION

DIC> @@

DIC> read exa3

OK

DIC>

DIC> sim

INFO: Default responses (if any) will be applied during the simulation. Use "SIMULATE\_REACTION NO" instead for manual input.

Region: AUSTENITE

geometric 0.833333 dense at 0.250000E-01 36 points

geometric 1.20000 dense at 0.250000E-01 35 points

DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE

U-FRACTION IN SYSTEM: C = .0215351645464254 FE = .962915638654286

SI = .0370843613457148

TOTAL SIZE OF SYSTEM: .05 [m]

U-FRACTION IN SYSTEM: C = .0215351645464254 FE = .962915638654286

SI = .0370843613457148

TOTAL SIZE OF SYSTEM: .05 [m]

TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .0215351645464254 FE = .962915638654286

SI = .0370843613457148

TOTAL SIZE OF SYSTEM: .05 [m]

CPU time used in timestep 0 seconds

TIME = 0.10010000E-03 DT = 0.10000000E-03 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .0215351645464254 FE = .962915638654286

SI = .0370843613457148

TOTAL SIZE OF SYSTEM: .05 [m]

CPU time used in timestep 0 seconds

TIME = 0.40010010 DT = 0.40000000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .0215351645464253 FE = .962915638654286

SI = .0370843613457148

TOTAL SIZE OF SYSTEM: .05 [m]

CPU time used in timestep 0 seconds

TIME = 39.307408 DT = 38.907308 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .0215351645464254 FE = .962915638654286

SI = .0370843613457148

TOTAL SIZE OF SYSTEM: .05 [m]

CPU time used in timestep 0 seconds

TIME = 117.12202 DT = 77.814615 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .0215351645464254 FE = .962915638654286

SI = .0370843613457148

TOTAL SIZE OF SYSTEM: .05 [m]

CPU time used in timestep 0 seconds

TIME = 272.75125 DT = 155.62923 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .0215351645464254 FE = .962915638654286

SI = .0370843613457148

TOTAL SIZE OF SYSTEM: .05 [m]

CPU time used in timestep 0 seconds

TIME = 584.00971 DT = 311.25846 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .0215351645464257 FE = .962915638654286

SI = .0370843613457148

TOTAL SIZE OF SYSTEM: .05 [m]

CPU time used in timestep 0 seconds

TIME = 1206.5266 DT = 622.51692 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .0215351645464264 FE = .962915638654286

SI = .0370843613457148

TOTAL SIZE OF SYSTEM: .05 [m]

CPU time used in timestep 0 seconds

TIME = 2451.5605 DT = 1245.0338 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .0215351645464265 FE = .962915638654285

SI = .0370843613457148

TOTAL SIZE OF SYSTEM: .05 [m]

CPU time used in timestep 1 seconds

TIME = 4941.6282 DT = 2490.0677 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .0215351645464267 FE = .962915638654286

SI = .0370843613457148

TOTAL SIZE OF SYSTEM: .05 [m]

CPU time used in timestep 0 seconds

TIME = 9921.7635 DT = 4980.1354 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .0215351645464267 FE = .962915638654286

SI = .0370843613457148

TOTAL SIZE OF SYSTEM: .05 [m]

CPU time used in timestep 0 seconds

TIME = 19882.034 DT = 9960.2708 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .0215351645464261 FE = .962915638654286

SI = .0370843613457148

TOTAL SIZE OF SYSTEM: .05 [m]

CPU time used in timestep 0 seconds

TIME = 39802.576 DT = 19920.542 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .0215351645464252 FE = .962915638654286

SI = .0370843613457148

TOTAL SIZE OF SYSTEM: .05 [m]

CPU time used in timestep 0 seconds

TIME = 79643.659 DT = 39841.083 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .0215351645464261 FE = .962915638654286

SI = .0370843613457148

TOTAL SIZE OF SYSTEM: .05 [m]

CPU time used in timestep 1 seconds

TIME = 159325.82 DT = 79682.166 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .0215351645464378 FE = .962915638654285

SI = .0370843613457148

TOTAL SIZE OF SYSTEM: .05 [m]

CPU time used in timestep 0 seconds

TIME = 318690.16 DT = 159364.33 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .021535164546488 FE = .962915638654285

SI = .0370843613457148

TOTAL SIZE OF SYSTEM: .05 [m]

CPU time used in timestep 0 seconds

TIME = 637418.82 DT = 318728.66 SUM OF SQUARES = 0.0000000

```

U-FRACTION IN SYSTEM: C = .0215351645466408 FE = .962915638654285
SI = .0370843613457148
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep 0 seconds
TIME = 1274876.1 DT = 637457.33 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351645470029 FE = .962915638654285
SI = .0370843613457148
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep 0 seconds
TIME = 2549790.8 DT = 1274914.7 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351645470028 FE = .962915638654285
SI = .0370843613457148
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep 0 seconds
TIME = 5099620.1 DT = 2549829.3 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351645468634 FE = .962915638654285
SI = .0370843613457148
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep 1 seconds
TIME = 10199279. DT = 5099658.6 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .021535164546573 FE = .962915638654285
SI = .0370843613457148
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep 0 seconds
TIME = 20398596. DT = 10199317. SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351645463065 FE = .962915638654285
SI = .0370843613457148
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep 0 seconds
TIME = 40797230. DT = 20398634. SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .021535164546185 FE = .962915638654285
SI = .0370843613457148
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep 0 seconds
TIME = 81594499. DT = 40797269. SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351645461055 FE = .962915638654285
SI = .0370843613457148
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep 0 seconds
TIME = 0.16318904E+09 DT = 81594538. SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351645460831 FE = .962915638654285
SI = .0370843613457148
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep 0 seconds
TIME = 0.32637811E+09 DT = 0.16318908E+09 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351645461223 FE = .962915638654285
SI = .0370843613457148
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep 0 seconds
TIME = 0.65275627E+09 DT = 0.32637815E+09 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351645462032 FE = .962915638654285
SI = .0370843613457148
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep 0 seconds
TIME = 0.13055126E+10 DT = 0.65275630E+09 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351645463127 FE = .962915638654285
SI = .0370843613457148
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep 0 seconds
TIME = 0.23055126E+10 DT = 0.10000000E+10 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351645465151 FE = .962915638654285
SI = .0370843613457148
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep 0 seconds
TIME = 0.33055126E+10 DT = 0.10000000E+10 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351645467281 FE = .962915638654285
SI = .0370843613457148
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep 1 seconds
TIME = 0.43055126E+10 DT = 0.10000000E+10 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351645471859 FE = .962915638654285
SI = .0370843613457148
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep 0 seconds
TIME = 0.53055126E+10 DT = 0.10000000E+10 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351645478041 FE = .962915638654285
SI = .0370843613457148
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep 0 seconds
TIME = 0.63055126E+10 DT = 0.10000000E+10 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .021535164548421 FE = .962915638654285
SI = .0370843613457148
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep 0 seconds
TIME = 0.73055126E+10 DT = 0.10000000E+10 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351645487861 FE = .962915638654285
SI = .0370843613457148
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep 0 seconds
TIME = 0.83055126E+10 DT = 0.10000000E+10 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .021535164548902 FE = .962915638654285
SI = .0370843613457149
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep 0 seconds
TIME = 0.93055126E+10 DT = 0.10000000E+10 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351645489791 FE = .962915638654285
SI = .0370843613457148
TOTAL SIZE OF SYSTEM: .05 [m]
CPU time used in timestep 0 seconds
TIME = 0.10000000E+11 DT = 0.69448743E+09 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0215351645490017 FE = .962915638654285
SI = .0370843613457148
TOTAL SIZE OF SYSTEM: .05 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 0.0000000
DELETING TIME-RECORD FOR TIME 0.10000000E-06
DELETING TIME-RECORD FOR TIME 0.10010000E-03
DELETING TIME-RECORD FOR TIME 0.40010010
DELETING TIME-RECORD FOR TIME 39.307408
DELETING TIME-RECORD FOR TIME 117.12202
DELETING TIME-RECORD FOR TIME 272.75125
DELETING TIME-RECORD FOR TIME 584.00971
DELETING TIME-RECORD FOR TIME 1206.5266
DELETING TIME-RECORD FOR TIME 2451.5605

```

DELETING TIME-RECORD FOR TIME 4941.6282  
DELETING TIME-RECORD FOR TIME 9921.7635  
DELETING TIME-RECORD FOR TIME 19882.034  
DELETING TIME-RECORD FOR TIME 39802.576  
DELETING TIME-RECORD FOR TIME 79643.659  
DELETING TIME-RECORD FOR TIME 159325.82  
DELETING TIME-RECORD FOR TIME 318690.16  
DELETING TIME-RECORD FOR TIME 637418.82  
DELETING TIME-RECORD FOR TIME 1274876.1  
DELETING TIME-RECORD FOR TIME 2549790.8  
DELETING TIME-RECORD FOR TIME 5099620.1  
DELETING TIME-RECORD FOR TIME 10199279.  
DELETING TIME-RECORD FOR TIME 20398596.  
DELETING TIME-RECORD FOR TIME 40797230.  
DELETING TIME-RECORD FOR TIME 81594499.  
DELETING TIME-RECORD FOR TIME 0.16318904E+09  
DELETING TIME-RECORD FOR TIME 0.32637811E+09  
DELETING TIME-RECORD FOR TIME 0.65275627E+09  
DELETING TIME-RECORD FOR TIME 0.13055126E+10  
DELETING TIME-RECORD FOR TIME 0.23055126E+10  
DELETING TIME-RECORD FOR TIME 0.33055126E+10  
DELETING TIME-RECORD FOR TIME 0.43055126E+10  
DELETING TIME-RECORD FOR TIME 0.53055126E+10  
DELETING TIME-RECORD FOR TIME 0.63055126E+10  
DELETING TIME-RECORD FOR TIME 0.73055126E+10  
DELETING TIME-RECORD FOR TIME 0.83055126E+10

KEEPING TIME-RECORD FOR TIME 0.93055126E+10  
AND FOR TIME 0.10000000E+11  
WORKSPACE RECLAIMED

TIMESTEP AT 0.10000000E+11 SELECTED

DIC>  
DIC> set-inter  
--OK--  
DIC>

## exa3-plot

### DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exa3\plot.DCM.test"

DIC>

DIC>

DIC> @@ darken\_plot.DCM

DIC>

DIC> @@

DIC> @@ ENTER THE DICTRA MODULE AND SPECIFY THE STORE-RESULT FILE

DIC> @@

DIC> go d-m

TIME STEP AT TIME 1.00000E+10

DIC> read exa3

OK

DIC>

DIC> @@

DIC> @@ ENTER THE DICTRA POST PROCESSOR

DIC> @@

DIC> post

POST PROCESSOR VERSION 1.7

Implemented by Bjorn Jonsson

POST-1:

POST-1: @@

POST-1: @@ PLOT THE CONCENTRATION PROFILE FOR Si AT TIMES 0, 1E5, 1123200, 1E7,

POST-1: @@ 1E8, 1E9 AND 1E10 S

POST-1: @@

POST-1: @@ SET DISTANCE IN SYSTEM AS X-AXIS, WEIGHT-% SI ON Y-AXIS AND SPECIFY

POST-1: @@ FOR WHICH SIMULATION TIMES TO PLOT THE PROFILES.

POST-1: @@

POST-1: set-diagram-axis x distance global

INFO: Distance is set as independent variable

POST-1: set-diagram-axis y weight-percent si

POST-1: set-plot-condition time 0 1E5 1123200 1e7 1E8 1E9 1E10

POST-1:

POST-1: @@

POST-1: @@ PLOT THE DIAGRAM

POST-1: @@

POST-1: set-title

TITLE : Figure a3.1

POST-1:

POST-1: SET\_EXP\_FILE\_FORMAT 5

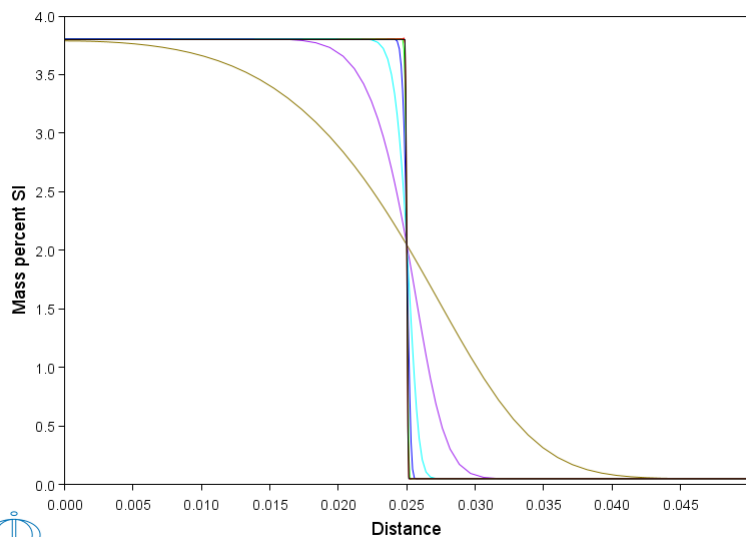
POST-1: MAKE c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\unite\distribution\macroResult.exp Y

POST-1: SET\_EXP\_FILE\_FORMAT 10

POST-1:

POST-1: plot

Figure a3.1



POST-1:

POST-1:

POST-1:

POST-1: Hit RETURN to continue

POST-1: @@

POST-1: @@ PLOT THE CONCENTRATION PROFILES FOR C

POST-1: @@

POST-1: @@ WE ONLY NEED TO CHANGE THE Y-AXIS

POST-1: @@

POST-1: set-diagram-axis y w-p c

POST-1: set-title Figure a3.2

POST-1:

POST-1: SET\_EXP\_FILE\_FORMAT 5

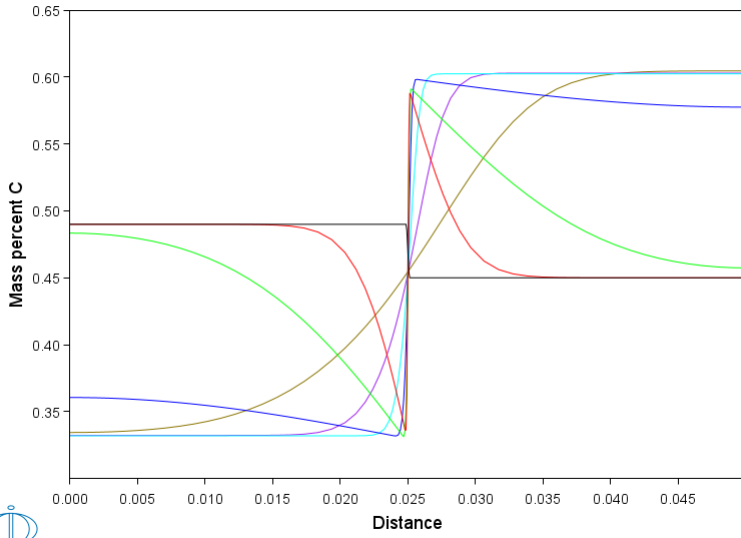
POST-1: MAKE c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\unite\distribution\macroResult.exp Y

POST-1: SET\_EXP\_FILE\_FORMAT 10

POST-1:

POST-1: plot

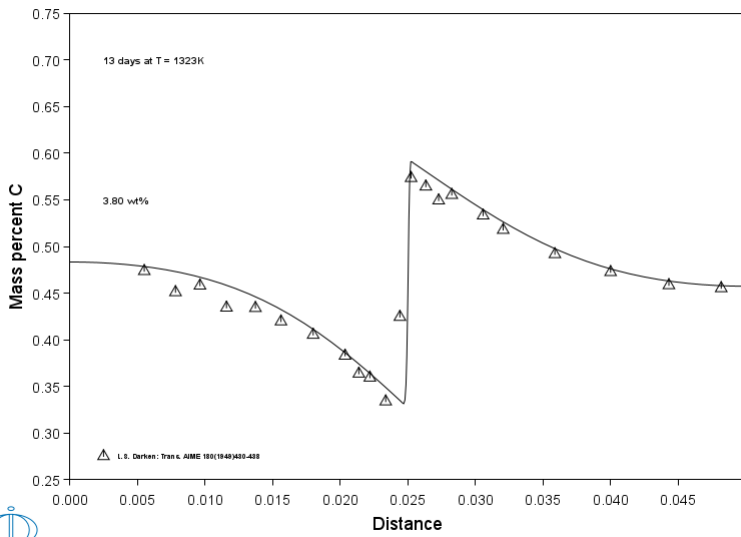
Figure a3.2



```

POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1: @@
POST-1: @@ COMPARE WITH DARKEN'S EXPERIMENTS
POST-1: @@
POST-1: append_experimental_data yes exa3.exp 0; 1
POST-1:
POST-1: set-plot-condition time 1123200
POST-1:
POST-1: s-s-s
AXIS (X, Y OR Z) : y
AUTOMATIC SCALING (Y OR N) /N/: n
MIN VALUE : 0.25
MAX VALUE : 0.75
POST-1:
POST-1: set-title Figure a3.3
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
    
```

Figure a3.3



```

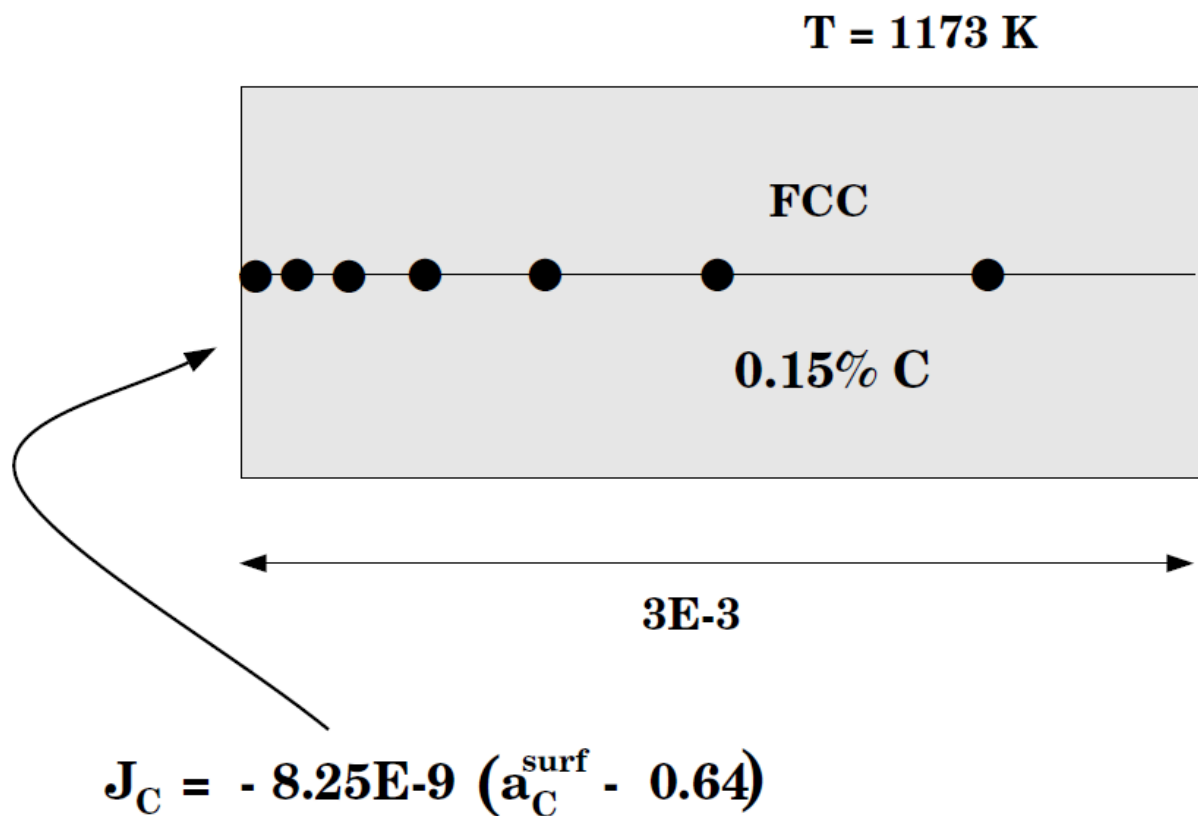
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1: set-inter
--OK--
POST-1:
    
```



## Example exa5

### Carburization of a binary Fe-0.15 wt% C alloy: A surface reaction controls the flux of C at the surface

A mixture of 40% N<sub>2</sub> and 60% cracked methanol is used as carrier gas. The carburizing "carbon potential" in the gas is 0.85 wt%.

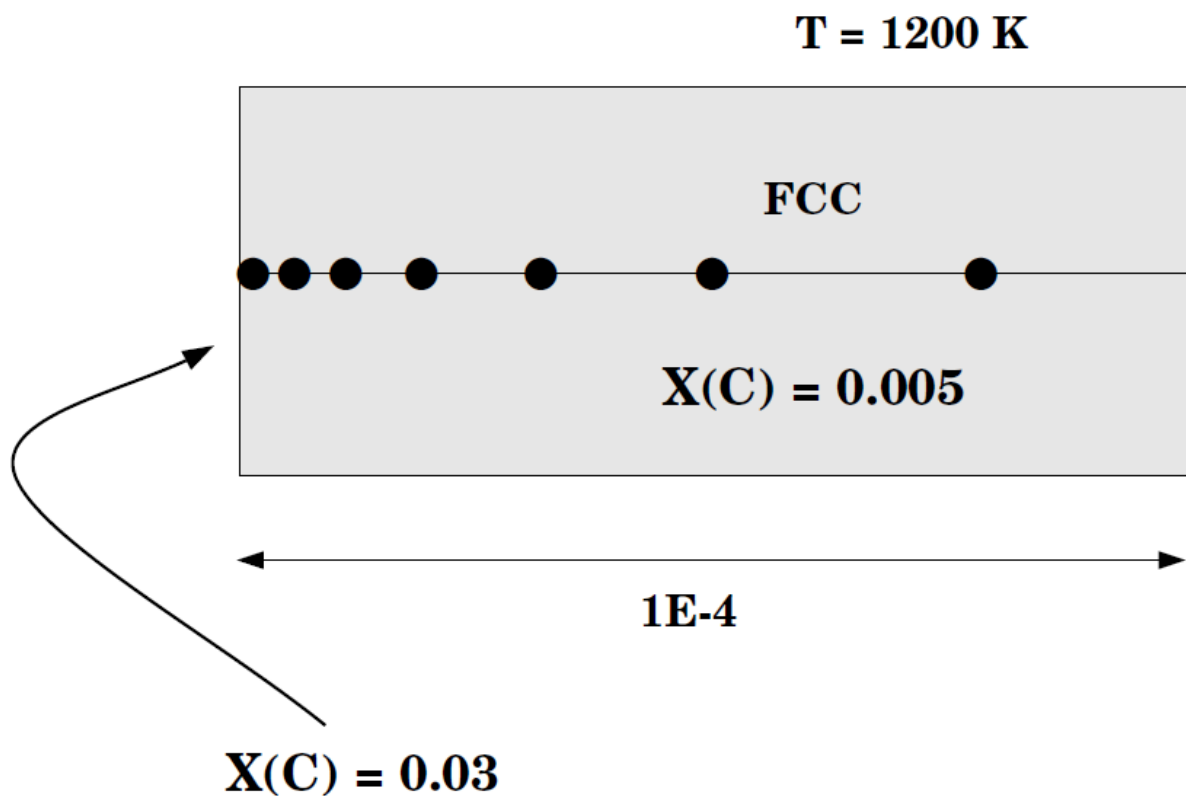




## Example exa4

### Carburization of a binary Fe-C alloy: Comparison to analytical erf solution

This is a simple binary simulation with one single phase region. It compares a numerical simulation with an analytical erf-solution. For this reason a special database is created (*erf.tdb*) where the diffusion coefficient is set to a concentration independent value.



## exa4-setup

### SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,  
Stockholm, Sweden

Software running on Windows 64-bit wordlength  
Compiler: Intel Fortran Compiler 2025.0.0  
License library version: 9.7.0.0036  
Linked: Nov 19 2025 at 14:44:36

```
SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exa4\setup.DCM.test"
```

```
SYS: @@  
SYS: @@ One-phase problem.  
SYS: @@ Carburization of binary Fe-C alloy: Comparison to an analytical erf solution  
SYS: @@ This is a simple binary simulation with a single phase region.  
SYS: @@ The numerical simulation is compared with an analytical erf solution.  
SYS: @@ For this reason a special database erf.tdb is created where the  
SYS: @@ diffusion coefficient is set to a concentration independent value.  
SYS: @@-----
```

```
SYS:  
SYS: @@ exa4_setup.DCM  
SYS:  
SYS:  
SYS: @@  
SYS: @@ READ THE DATA FROM THE DATABASES  
SYS: @@  
SYS: go da  
THERMODYNAMIC DATABASE module  
Database folder:  
C:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\databases\da  
ta  
Current database: Steels/Fe-Alloys v12.0
```

```
VA /- DEFINED  
DICTRA FCC_A1 REJECTED  
TDB_TCFE12: sw FEDEMO  
Current database: Iron Demo Database v6.0
```

```
VA /- DEFINED  
TDB_FEDEMO: def-system fe,c  
FE C DEFINED  
TDB_FEDEMO: rej-ph *  
GAS:G LIQUID:L BCC_A2  
C14 LAVES CBCC_A12 CEMENTITE_D011  
CUB_A13 DIAMOND_A4 FCC_A1  
GRAPHITE_A9 HCP_A3 KSI_CARBIDE  
M23C6_D84 M5C2 M7C3_D101  
REJECTED
```

```
TDB_FEDEMO: rest-ph fcc  
FCC_A1 RESTORED  
TDB_FEDEMO: get  
08:50:51,494 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***  
REINITIATING GES .....  
ELEMENTS .....  
SPECIES .....  
PHASES .....  
PARAMETERS ...  
FUNCTIONS ....
```

Use the command LIST\_REFERENCES to see the list of references for assessed data

```
-OK-  
TDB_FEDEMO:  
TDB_FEDEMO: append user exa4.TDB  
Current database: User defined Database  
This database does not support the DATABASE_INFORMATION command
```

```
VA DEFINED  
08:50:52,366 [Thread-0] INFO TDBFileParser: USER_1068030556_22, number of lines read: 29  
08:50:52,425 [Thread-0] INFO DatabaseUtils: Parsing of USER_1068030556_22 completed in 62 ms
```

```
TDB_APP: def-system fe,c  
FE C DEFINED  
TDB_APP: rej-ph *  
FCC_A1 REJECTED  
TDB_APP: rest-ph fcc  
FCC_A1 RESTORED  
TDB_APP: get  
08:50:53,139 [Thread-0] INFO Database: Preparing system for use: USER_1068030556_22  
ELEMENTS .....  
SPECIES .....  
PHASES .....  
PARAMETERS ...  
FUNCTIONS ....
```

```
-OK-  
TDB_APP:  
TDB_APP: @@  
TDB_APP: @@ GO TO THE DICTRA MODULE AND SET UP THE SYSTEM  
TDB_APP: @@  
TDB_APP: go d-m  
NO TIME STEP DEFINED  
DIC>  
DIC> @@  
DIC> @@ ENTER GLOBAL CONDITION T  
DIC> @@  
DIC> set-cond glob T 0 1200; * N  
DIC>  
DIC> @@  
DIC> @@ ENTER THE REGION steel  
DIC> @@  
DIC> enter-region  
REGION NAME : steel  
DIC>  
DIC> @@  
DIC> @@ ENTER THE GRID  
DIC> @@ CARBON ENTERS THE SYSTEM FROM THE LOWER BOUNDARY AND CONSEQUENTLY  
DIC> @@ MORE POINTS ARE REQUIRED AT THAT BOUNDARY. THIS IS WHY A GEOMETRIC
```

```
DIC> @@ GRID IS USED.
DIC> @@
DIC> enter-grid
REGION NAME : /STEEL/: steel
WIDTH OF REGION /1/: 1E-4
TYPE /AUTO/: AUTO
DIC>
DIC> @@
DIC> @@ ENTER THE PHASE INTO THE REGION
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /STEEL/: steel
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITION IN THE FCC PHASE
DIC> @@
DIC> enter-composition
REGION NAME : /STEEL/: steel
PHASE NAME: /FCC_A1/: fcc#1
COMPOSITION TYPE /MOLE_FRACTION/: mole-fraction
PROFILE FOR /C/: c
TYPE /LINEAR/: linear
VALUE OF FIRST POINT : 0.005
VALUE OF LAST POINT : /5E-3/: 0.005
08:50:54,699 [Thread-0] INFO Phase: Preparing phase for use: FCC_A1
DIC>
DIC>
DIC> @@
DIC> @@ SET A FIXED COMPOSITION AS THE BOUNDARY VALUE
DIC> @@
DIC> set-condition
GLOBAL OR BOUNDARY CONDITION /GLOBAL/: boundary
BOUNDARY /LOWER/: lower
CONDITION TYPE /CLOSED_SYSTEM/: state-variable-value
State variable expression #1 : /N=1/: n=1
State variable expression #2 : x(c)=0.03
DIC>
DIC>
DIC> @@
DIC> @@ SET A SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 100
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /10/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC>
DIC> save exa4 Y
DIC>
DIC> set-inter
--OK--
DIC>
```

exa4-run

DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exa4\run.DCM.test"

DIC>

DIC>

DIC> @@ exa4\_run.DCM

DIC>

DIC> @@

DIC> @@ FILE FOR RUNNING EXAMPLE a4

DIC> @@

DIC>

DIC> @@

DIC> @@ ENTER THE DICTRA MONITOR AND READ THE STORE RESULT FILE

DIC> @@

DIC> go d-m

TIME STEP AT TIME 0.00000E+00

DIC> read exa4

OK

DIC>

DIC> @@

DIC> @@ START THE SIMULATION

DIC> @@

DIC> sim

INFO: Default responses (if any) will be applied during the simulation. Use "SIMULATE\_REACTION NO" instead for manual input.

Region: STEEL  
geometric 1.20000 dense at 0.00000 57 points  
DEGREE OF IMPLICIT SET TO TRAPEZOIDAL RULE  
U-FRACTION IN SYSTEM: C = .00502512562814071 FE = 1  
TOTAL SIZE OF SYSTEM: 1E-04 [m]  
U-FRACTION IN SYSTEM: C = .00502512562814071 FE = 1  
TOTAL SIZE OF SYSTEM: 1E-04 [m]  
TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .00505812483736605 FE = 1  
TOTAL SIZE OF SYSTEM: 1E-04 [m]  
CPU time used in timestep 0 seconds  
TIME = 0.10010000E-03 DT = 0.10000000E-03 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .00505918131292522 FE = 1  
TOTAL SIZE OF SYSTEM: 1E-04 [m]  
CPU time used in timestep 0 seconds  
TIME = 0.39379161E-02 DT = 0.38378161E-02 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .005088438297452 FE = 1  
TOTAL SIZE OF SYSTEM: 1E-04 [m]  
CPU time used in timestep 0 seconds  
TIME = 0.11613548E-01 DT = 0.76756322E-02 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .00512323510928179 FE = 1  
TOTAL SIZE OF SYSTEM: 1E-04 [m]  
CPU time used in timestep 0 seconds  
TIME = 0.26964813E-01 DT = 0.15351264E-01 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .00516937716229967 FE = 1  
TOTAL SIZE OF SYSTEM: 1E-04 [m]  
CPU time used in timestep 0 seconds  
TIME = 0.57667341E-01 DT = 0.30702529E-01 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .00523281439554546 FE = 1  
TOTAL SIZE OF SYSTEM: 1E-04 [m]  
CPU time used in timestep 0 seconds  
TIME = 0.11907240 DT = 0.61405057E-01 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .00532134417798201 FE = 1  
TOTAL SIZE OF SYSTEM: 1E-04 [m]  
CPU time used in timestep 0 seconds  
TIME = 0.24188251 DT = 0.12281011 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .00544573917126831 FE = 1  
TOTAL SIZE OF SYSTEM: 1E-04 [m]  
CPU time used in timestep 0 seconds  
TIME = 0.48750274 DT = 0.24562023 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .00562110184346364 FE = 1  
TOTAL SIZE OF SYSTEM: 1E-04 [m]  
CPU time used in timestep 0 seconds  
TIME = 0.97874320 DT = 0.49124046 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .00586871098233561 FE = 1  
TOTAL SIZE OF SYSTEM: 1E-04 [m]  
CPU time used in timestep 0 seconds  
TIME = 1.9612241 DT = 0.98248092 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .00621860525716751 FE = 1  
TOTAL SIZE OF SYSTEM: 1E-04 [m]  
CPU time used in timestep 0 seconds  
TIME = 3.9261860 DT = 1.9649618 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .00671317488999983 FE = 1  
TOTAL SIZE OF SYSTEM: 1E-04 [m]  
CPU time used in timestep 0 seconds  
TIME = 7.8561096 DT = 3.9299237 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .00741220811437077 FE = 1  
TOTAL SIZE OF SYSTEM: 1E-04 [m]  
CPU time used in timestep 0 seconds  
TIME = 15.715957 DT = 7.8598473 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .00840038142848028 FE = 1  
TOTAL SIZE OF SYSTEM: 1E-04 [m]  
CPU time used in timestep 1 seconds  
TIME = 25.715957 DT = 10.000000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .00934017906507076 FE = 1  
TOTAL SIZE OF SYSTEM: 1E-04 [m]  
CPU time used in timestep 0 seconds  
TIME = 35.715957 DT = 10.000000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .0101085679608066 FE = 1  
TOTAL SIZE OF SYSTEM: 1E-04 [m]  
CPU time used in timestep 0 seconds  
TIME = 45.715957 DT = 10.000000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .0107752067656887 FE = 1  
TOTAL SIZE OF SYSTEM: 1E-04 [m]  
CPU time used in timestep 0 seconds  
TIME = 55.715957 DT = 10.000000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .011372261459059 FE = 1  
TOTAL SIZE OF SYSTEM: 1E-04 [m]  
CPU time used in timestep 0 seconds  
TIME = 65.715957 DT = 10.000000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .011917828517872 FE = 1  
TOTAL SIZE OF SYSTEM: 1E-04 [m]  
CPU time used in timestep 0 seconds  
TIME = 75.715957 DT = 10.000000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .0124232979419724 FE = 1  
TOTAL SIZE OF SYSTEM: 1E-04 [m]  
CPU time used in timestep 0 seconds  
TIME = 85.715957 DT = 10.000000 SUM OF SQUARES = 0.0000000

```
U-FRACTION IN SYSTEM: C = .0128963915090011 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 95.715957 DT = 10.000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .013342629907881 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 100.00000 DT = 4.2840430 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0135266153475069 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 0.0000000
DELETING TIME-RECORD FOR TIME 0.10000000E-06
DELETING TIME-RECORD FOR TIME 0.10010000E-03
DELETING TIME-RECORD FOR TIME 0.39379161E-02
DELETING TIME-RECORD FOR TIME 0.11613548E-01
DELETING TIME-RECORD FOR TIME 0.26964813E-01
DELETING TIME-RECORD FOR TIME 0.57667341E-01
DELETING TIME-RECORD FOR TIME 0.11907240
DELETING TIME-RECORD FOR TIME 0.24188251
DELETING TIME-RECORD FOR TIME 0.48750274
DELETING TIME-RECORD FOR TIME 0.97874320
DELETING TIME-RECORD FOR TIME 1.9612241
DELETING TIME-RECORD FOR TIME 3.9261860
DELETING TIME-RECORD FOR TIME 7.8561096
DELETING TIME-RECORD FOR TIME 15.715957
DELETING TIME-RECORD FOR TIME 25.715957
DELETING TIME-RECORD FOR TIME 35.715957
DELETING TIME-RECORD FOR TIME 45.715957
DELETING TIME-RECORD FOR TIME 55.715957
DELETING TIME-RECORD FOR TIME 65.715957
DELETING TIME-RECORD FOR TIME 75.715957
DELETING TIME-RECORD FOR TIME 85.715957

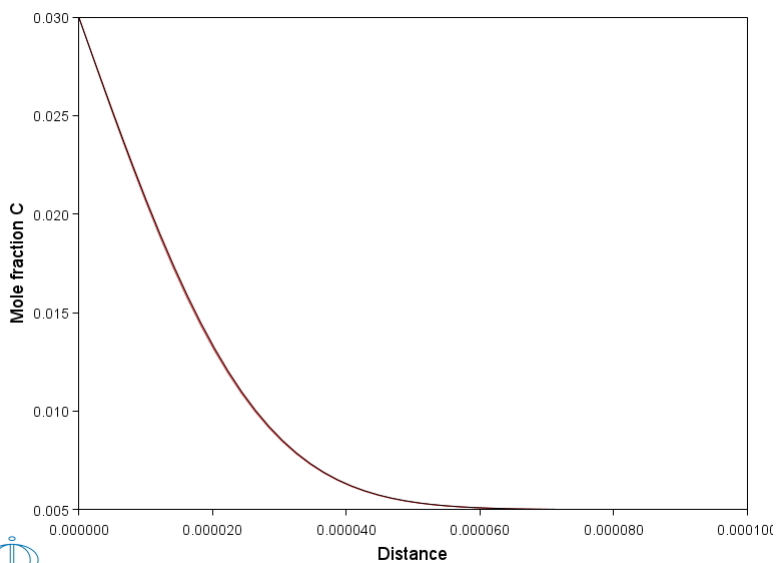
KEEPING TIME-RECORD FOR TIME 95.715957
AND FOR TIME 100.00000
WORKSPACE RECLAIMED

TIMESTEP AT 100.000000 SELECTED
```

```
DIC>
DIC> @@
DIC> @@ THE SIMULATION IS FINISHED
DIC> @@
DIC>
DIC> set-inter
--OK--
DIC>
```

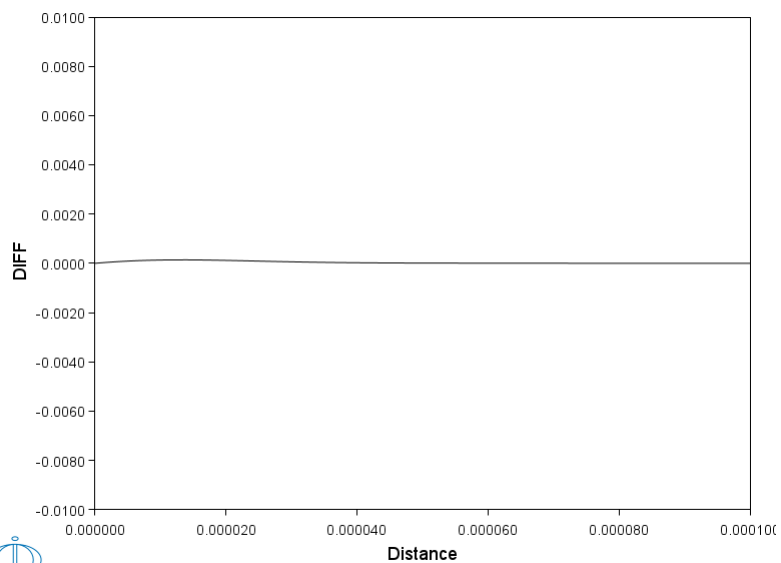
## exa4-plot

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exa4\plot.DCM.test"
DIC>
DIC>
DIC> @@ exa4_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE exa4
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 1.00000E+02
DIC> read exa4
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1: @@
POST-1: @@ PLOT A COMPOSITION PROFILE
POST-1: @@
POST-1: s-d-a x distance global
INFO: Distance is set as independent variable
POST-1: s-d-a y x(c)
POST-1: s-p-c time 25
POST-1:
POST-1: @@
POST-1: @@ ENTER THE ANALYTICAL SOLUTION, CALLED ERF SOL
POST-1: @@
POST-1: enter-symbol
Function or table /FUNCTION/: function
NAME: erfsol
FUNCTION: 0.03-0.025*erf(gd/sqrt(4*dc(fcc,c,c,fe)*25));
POST-1:
POST-1: @@
POST-1: @@ COMPARE THE ANALYTICAL AND NUMERICAL SOLUTIONS
POST-1: @@
POST-1: enter-symbol
Function or table /FUNCTION/: table
NAME: aaa
Variable(s) x(c) erfsol
POST-1:
POST-1: s-d-a y aaa
COLUMN NUMBER /*/: 1 2
POST-1:
POST-1: set-axis-text
AXIS (X, Y OR Z) : y
AUTOMATIC AXIS TEXT (Y OR N) /N/: n
AXIS TEXT : Mole fraction C
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```



```
POST-1:
POST-1:
POST-1:
POST-1: @?<Hit_return_to_continue>
POST-1:
POST-1: @@
POST-1: @@ PLOT THE DIFFERENCE
POST-1: @@
POST-1: enter func diff=x(c)-erfsol;
POST-1: s-d-a y diff
POST-1: s-s-s y n -1e-2 1e-2
POST-1:
```

```
POST-1:  
POST-1: SET_EXP_FILE_FORMAT 5  
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y  
POST-1: SET_EXP_FILE_FORMAT 10  
POST-1:  
POST-1: plot
```



```
POST-1:  
POST-1:  
POST-1:  
POST-1: @?<Hit_return_to_continue>  
POST-1:  
POST-1: set-interactive  
--OK--  
POST-1:
```

## exa5-setup

### SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,  
Stockholm, Sweden

Software running on Windows 64-bit wordlength  
Compiler: Intel Fortran Compiler 2025.0.0  
License library version: 9.7.0.0036  
Linked: Nov 19 2025 at 14:44:36

```
SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exa5\setup.DCM.test"
```

```
SYS: i>?@@
NO SUCH COMMAND, USE HELP
SYS: @@ One-phase problem.
SYS: @@ Carburization of a binary Fe-0.15 wt% C alloy.
SYS: @@ A mixture of 40% N2 and 60% cracked methanol is used as carrier gas.
SYS: @@ The carburizing "carbon potential" in the gas is 0.85 wt%.
SYS: @@ A surface reaction controls the flux of C at the surface.
SYS: @@-----
SYS:
SYS: @@ exa5_setup.DCM
SYS:
SYS: @@
SYS: @@ GO TO THE DATABASES AND READ THE THERMODYNAMIC AND KINETIC DATA
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\databases\da
ta
Current database: Steels/Fe-Alloys v12.0

VA /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE12: sw FEDEMO
Current database: Iron Demo Database v6.0

VA /- DEFINED
TDB_FEDEMO: def-sys fe,c
FE C DEFINED
TDB_FEDEMO: rej-ph *
GAS:G LIQUID:L BCC_A2
C14 LAVES CBCC_A12 CEMENTITE_D011
CUB_A13 DIAMOND_A4 FCC_A1
GRAPHITE_A9 HCP_A3 KSI_CARBIDE
M23C6_D84 MSC2 M7C3_D101
REJECTED
TDB_FEDEMO: rest-ph fcc graphite
FCC_A1 GRAPHITE_A9 RESTORED
TDB_FEDEMO: get
08:53:51,323 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-
TDB_FEDEMO:??
TDB_FEDEMO: append
Use one of these databases

TCFE12 = Steels/Fe-Alloys v12.0
TCFE9 = Steels/Fe-Alloys v9.3
SSUB6 = SGTE Substances v6.0
FEDEMO = Iron Demo Database v6.0
MOB2 = Alloys Mobility v2.7
MOBFE7 = Steels/Fe-Alloys Mobility v7.1
MOBFE4 = Steels/Fe-Alloys Mobility v4.0
MOBFE2 = Steels/Fe-Alloys Mobility v2.0
MFEDEMO = Fe-Alloys Mobility demo database v5.0
USER = User defined Database

DATABASE NAME /FEDEMO/: mfedemo
Current database: Fe-Alloys Mobility demo database v5.0

VA DEFINED
APP: def-sys fe,c
FE C DEFINED
APP: rej-ph *
BCC_A2 FCC_A1 CEMENTITE_D011
LIQUID:L REJECTED
APP: rest-ph fcc
FCC_A1 RESTORED
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-
APP:??
APP: @@
APP: @@ GO TO THE DICTRA MONITOR TO SET UP THE INITIAL STATE OF THE SPECIMEN
APP: @@
APP: go d-m
NO TIME STEP DEFINED
*** ENTERING GRAPHITE_A9 AS A DIFFUSION NONE PHASE
DIC>
DIC> set-cond glob T 0 1173; * N
DIC>
```

```

DIC> @@
DIC> @@ SELECT A REFERENCE STATE FOR THE C ACTIVITY
DIC> @@
DIC> set-ref-state
Component: c
Reference state: graph
Temperature /*/: *
Pressure /100000/: 1e5
DIC>
DIC> @@
DIC> @@ ENTER A REGION, GRID, PHASE AND COMPOSITION
DIC> @@
DIC> enter-region
REGION NAME : steel
DIC>
DIC> enter-grid
REGION NAME : /STEEL/: steel
WIDTH OF REGION /1/: 3E-3
TYPE /AUTO/: AUTO
DIC>
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /STEEL/: steel
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC> enter-composition
REGION NAME : /STEEL/: steel
PHASE NAME: /FCC_A1/: fcc#1
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: c
TYPE /LINEAR/: lin
VALUE OF FIRST POINT : 0.15
VALUE OF LAST POINT : /0.15/: 0.15
DIC>
DIC> @@
DIC> @@ NOW SET THE BOUNDARY CONDITIONS. WE ARE ONLY INTERESTED IN THE
DIC> @@ SURFACE REGION, FOR EXAMPLE IT IS SUFFICIENT TO SET CONDITIONS AT THE
DIC> @@ LOWER BOUNDARY.
DIC> @@
DIC> @@
DIC> @@ Specify the activity flux function which controls the uptake of C.
DIC> @@
DIC> @@ The functions f and g and the parameter N has to be specified.
DIC> @@
DIC> @@
DIC> @@
DIC> @@
DIC> @@ J V = f (variables)*(ACTIVITY -g (variables)) (1)
DIC> @@ k m k k k
DIC> @@
DIC> @@ f and g in equation 1 is the mass-transfer coefficient and
DIC> @@ k k
DIC> @@ the activity of k in the gas, respectively. ACTIVITY in eq. 1 means
DIC> @@ the actual activity of species k at the surface.
DIC> @@
DIC> @@
DIC> @@ The main carburizing reaction for our atmosphere is:
DIC> @@
DIC> @@ CO + H -> C + H O (I)
DIC> @@ 2 <- - 2
DIC> @@
DIC> @@ Following Sproge and Ågren (J. Heat Treating, v6, no 1, 1988 pp. 9-19)
DIC> @@ we calculate the mass-transfer coefficient for carbon, f in
DIC> @@ eq. 1 above by means of eq. 3, 4 and 12 in Sproge and Ågren's paper.
DIC> @@
DIC> @@
DIC> @@
DIC> @@
DIC> @@ A * K * P * sqrt( P )
DIC> @@ I CO H
DIC> @@ 2
DIC> @@ f = ----- / gamma (2)
DIC> @@ a + B * K * P * sqrt( P )
DIC> @@ C I CO H
DIC> @@ 2
DIC> @@
DIC> @@ K is the equilibrium constant for reaction (I)
DIC> @@ I
DIC> @@
DIC> @@ A and B are constants defined in Sproge and Ågren's paper. gamma
DIC> @@ is the activity coefficient for carbon in the steel.
DIC> @@
DIC> @@ Assume a constant value for P * sqrt( P ) = 0.14
DIC> @@ CO H
DIC> @@ 2
DIC> @@ The carbon activity in the gas is controlled by the partial
DIC> @@ pressure of water as can be understood from reaction (I).
DIC> @@
DIC> @@ Assume that the carbon activity, a of the gas is 0.64
DIC> @@ C
DIC> @@ which corresponds to a carburizing "carbon potential" of 0.85 wt%.
DIC> @@
DIC> @@ In this way we may calculate f to 8.25E-9 mol/s.
DIC> @@
DIC>
DIC> set-cond
GLOBAL OR BOUNDARY CONDITION /GLOBAL/: bound
BOUNDARY /LOWER/: lower
CONDITION TYPE /CLOSED_SYSTEM/: activity_flux_function
ENTER THE EXPRESSION AS:
J V = f (variables)*(ACTIVITY -g (variables))
k m k k k
FLUX OF FCC_A1,C
LOW TIME LIMIT /0/: 0
f(T,P,TIME)= -8.25E-9;
HIGH TIME LIMIT /*/: *
ANY MORE RANGES /N/: N
N /1/: 1
LOW TIME LIMIT /0/: 0

```

```
g(T,P,TIME)= 0.64;  
HIGH TIME LIMIT /*/: *  
ANY MORE RANGES /N/: N  
DIC>  
DIC> @@  
DIC> @@ SPECIFY A SIMULATION TIME  
DIC> @@  
DIC> set-simulation-time  
END TIME FOR INTEGRATION /.1/: 18000  
AUTOMATIC TIMESTEP CONTROL /YES/:  
MAX TIMESTEP DURING INTEGRATION /1800/:  
INITIAL TIMESTEP : /1E-07/:  
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:  
DIC>  
DIC> @@  
DIC> @@ SAVE THE SET UP TO FILE  
DIC> @@  
DIC> Save exa5 Y  
DIC>  
DIC> set-inter  
--OK--  
DIC>
```

exa5-run

DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exa5\run.DCM.test"

DIC>

DIC>

DIC> @@ exa5\_run.DCM

DIC>

DIC> @@

DIC> @@ FILE FOR RUNNING EXAMPLE a5

DIC> @@

DIC>

DIC> @@

DIC> @@ ENTER THE DICTRA MONITOR AND READ THE STORE RESULT FILE

DIC> @@

DIC> go d-m

TIME STEP AT TIME 0.00000E+00

\*\*\* ENTERING GRAPHITE\_A9 AS A DIFFUSION NONE PHASE

DIC> read exa5

OK

DIC>

DIC> @@

DIC> @@ Start the simulation

DIC> @@

DIC> sim

INFO: Default responses (if any) will be applied during the simulation. Use "SIMULATE\_REACTION NO" instead for manual input.

Region: STEEL  
geometric 1.20000 dense at 0.00000 57 points  
DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE  
U-FRACTION IN SYSTEM: C = .00698495916383108 FE = 1  
TOTAL SIZE OF SYSTEM: .003 [m]  
U-FRACTION IN SYSTEM: C = .00698495916383108 FE = 1  
TOTAL SIZE OF SYSTEM: .003 [m]  
TIME = 0.1000000E-06 DT = 0.1000000E-06 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .00698495916398348 FE = 1  
TOTAL SIZE OF SYSTEM: .003 [m]  
CPU time used in timestep 0 seconds  
TIME = 0.1001000E-03 DT = 0.1000000E-03 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .00698495931638295 FE = 1  
TOTAL SIZE OF SYSTEM: .003 [m]  
CPU time used in timestep 0 seconds  
TIME = 0.40010010 DT = 0.400000000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .00698556362936311 FE = 1  
TOTAL SIZE OF SYSTEM: .003 [m]  
CPU time used in timestep 1 seconds  
TIME = 4.3766840 DT = 3.9765839 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .00699127311193793 FE = 1  
TOTAL SIZE OF SYSTEM: .003 [m]  
CPU time used in timestep 0 seconds  
TIME = 12.329852 DT = 7.9531678 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .00700200719387827 FE = 1  
TOTAL SIZE OF SYSTEM: .003 [m]  
CPU time used in timestep 1 seconds  
TIME = 28.236188 DT = 15.906336 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .00702208623823577 FE = 1  
TOTAL SIZE OF SYSTEM: .003 [m]  
CPU time used in timestep 0 seconds  
TIME = 60.048859 DT = 31.812671 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .00705900594239566 FE = 1  
TOTAL SIZE OF SYSTEM: .003 [m]  
CPU time used in timestep 1 seconds  
TIME = 123.67420 DT = 63.625343 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .00712525459781422 FE = 1  
TOTAL SIZE OF SYSTEM: .003 [m]  
CPU time used in timestep 0 seconds  
TIME = 250.92489 DT = 127.25069 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .0072405156803945 FE = 1  
TOTAL SIZE OF SYSTEM: .003 [m]  
CPU time used in timestep 1 seconds  
TIME = 505.42626 DT = 254.50137 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .00743394621983935 FE = 1  
TOTAL SIZE OF SYSTEM: .003 [m]  
CPU time used in timestep 0 seconds  
TIME = 1014.4290 DT = 509.00274 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .00774626834606196 FE = 1  
TOTAL SIZE OF SYSTEM: .003 [m]  
CPU time used in timestep 1 seconds  
TIME = 2032.4345 DT = 1018.0055 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .00823209852005916 FE = 1  
TOTAL SIZE OF SYSTEM: .003 [m]  
CPU time used in timestep 0 seconds  
TIME = 3832.4345 DT = 1800.0000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .00888873155588146 FE = 1  
TOTAL SIZE OF SYSTEM: .003 [m]  
CPU time used in timestep 1 seconds  
TIME = 5632.4345 DT = 1800.0000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .00941704184821519 FE = 1  
TOTAL SIZE OF SYSTEM: .003 [m]  
CPU time used in timestep 1 seconds  
TIME = 7432.4345 DT = 1800.0000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .00987244241587805 FE = 1  
TOTAL SIZE OF SYSTEM: .003 [m]  
CPU time used in timestep 1 seconds  
TIME = 9232.4345 DT = 1800.0000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .0102788675108747 FE = 1  
TOTAL SIZE OF SYSTEM: .003 [m]  
CPU time used in timestep 0 seconds  
TIME = 11032.434 DT = 1800.0000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .0106494229829431 FE = 1  
TOTAL SIZE OF SYSTEM: .003 [m]  
CPU time used in timestep 1 seconds  
TIME = 12832.434 DT = 1800.0000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .0109922280612705 FE = 1  
TOTAL SIZE OF SYSTEM: .003 [m]  
CPU time used in timestep 0 seconds  
TIME = 14632.434 DT = 1800.0000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .0113127299083723 FE = 1  
TOTAL SIZE OF SYSTEM: .003 [m]  
CPU time used in timestep 1 seconds  
TIME = 16432.434 DT = 1800.0000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .0116147948085907 FE = 1  
TOTAL SIZE OF SYSTEM: .003 [m]  
CPU time used in timestep 0 seconds

```
TIME = 18000.000    DT = 1567.5655    SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0118650755663949  FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 0.0000000
DELETING TIME-RECORD FOR TIME 0.10000000E-06
DELETING TIME-RECORD FOR TIME 0.10010000E-03
DELETING TIME-RECORD FOR TIME 0.40010010
DELETING TIME-RECORD FOR TIME 4.3766840
DELETING TIME-RECORD FOR TIME 12.329852
DELETING TIME-RECORD FOR TIME 28.236188
DELETING TIME-RECORD FOR TIME 60.048859
DELETING TIME-RECORD FOR TIME 123.67420
DELETING TIME-RECORD FOR TIME 250.92489
DELETING TIME-RECORD FOR TIME 505.42626
DELETING TIME-RECORD FOR TIME 1014.4290
DELETING TIME-RECORD FOR TIME 2032.4345
DELETING TIME-RECORD FOR TIME 3832.4345
DELETING TIME-RECORD FOR TIME 5632.4345
DELETING TIME-RECORD FOR TIME 7432.4345
DELETING TIME-RECORD FOR TIME 9232.4345
DELETING TIME-RECORD FOR TIME 11032.434
DELETING TIME-RECORD FOR TIME 12832.434
DELETING TIME-RECORD FOR TIME 14632.434

KEEPING TIME-RECORD FOR TIME 16432.434
AND FOR TIME 18000.000
WORKSPACE RECLAIMED

TIMESTEP AT 18000.0000 SELECTED
```

```
DIC>
DIC> set-inter
--OK--
DIC>
```

## exa5-plot

### DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exa5\plot.DCM.test"

DIC>

DIC>

DIC> @@ exa5\_plot.DCM

DIC>

DIC> @@

DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE a5

DIC> @@

DIC>

DIC> @@

DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE

DIC> @@

DIC> go d-m

TIME STEP AT TIME 1.80000E+04

\*\*\* ENTERING GRAPHITE\_A9 AS A DIFFUSION NONE PHASE

DIC> read exa5

OK

DIC>

DIC> @@

DIC> @@ ENTER THE POST PROCESSOR

DIC> @@

DIC> post

POST PROCESSOR VERSION 1.7

Implemented by Bjorn Jonsson

POST-1:

POST-1: @@

POST-1: @@ PLOT SOME DIFFERENT CONCENTRATION PROFILES

POST-1: @@

POST-1: s-d-a x dist glo

INFO: Distance is set as independent variable

POST-1: s-d-a y w-p c

POST-1: s-p-c time 100 1000 5000 18000

POST-1:

POST-1:

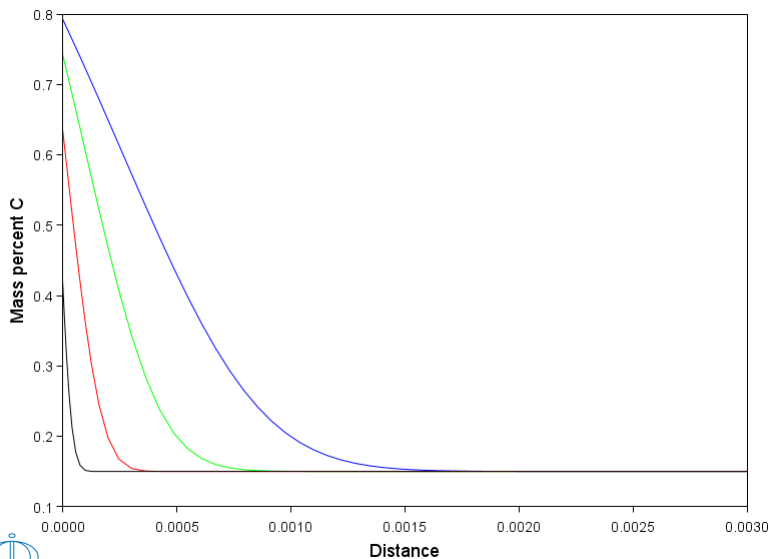
POST-1: SET\_EXP\_FILE\_FORMAT 5

POST-1: MAKE c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\unite\distribution\macroResult.exp Y

POST-1: SET\_EXP\_FILE\_FORMAT 10

POST-1:

POST-1: plot



POST-1:

POST-1:

POST-1:

POST-1: @?<Hit\_return\_to\_continue>

POST-1:

POST-1: @@

POST-1: @@ PLOT THE VARIATION OF THE C ACTIVITY AT THE SURFACE

POST-1: @@

POST-1: s-d-a y acr(c)

POST-1:

POST-1: s-d-a x time

INFO: Time is set as independent variable

POST-1:

POST-1: s-p-c

CONDITION /TIME/: interface

INTERFACE : first

POST-1:

POST-1:

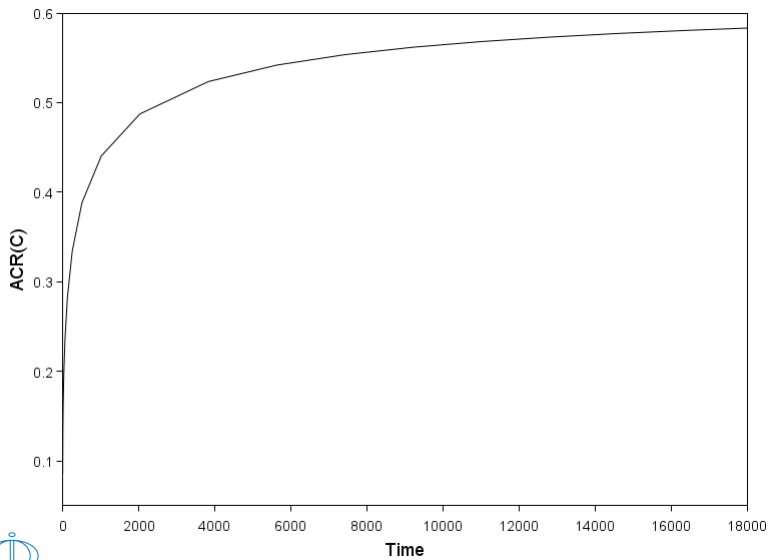
POST-1: SET\_EXP\_FILE\_FORMAT 5

POST-1: MAKE c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\unite\distribution\macroResult.exp Y

OST-1: SET\_EXP\_FILE\_FORMAT 10

POST-1:

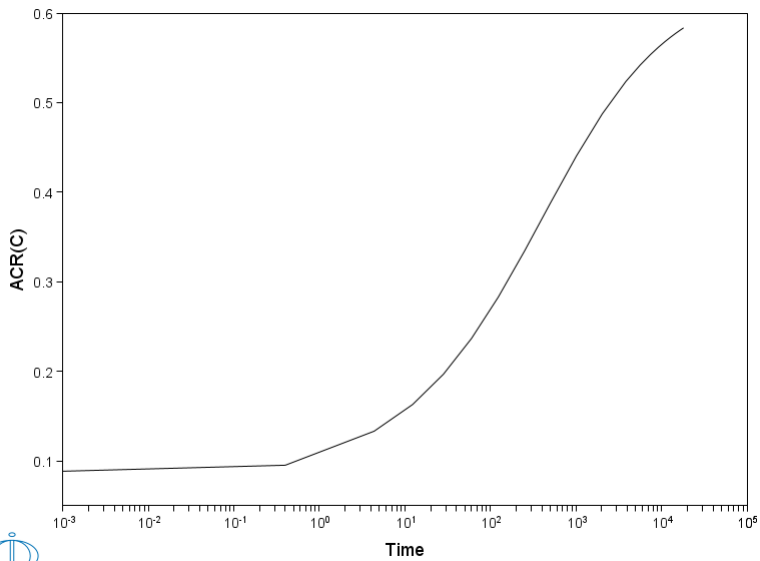
POST-1: plot



```

POST-1:
POST-1:
POST-1:
POST-1: @?<Hit_return_to_continue>
POST-1:
POST-1: @@
POST-1: @@ USE A LOGARITHMIC SCALE ON THE X-AXIS
POST-1: @@
POST-1: set-axis-type
POST-1: AXIS (X, Y OR Z) : x
POST-1: AXIS TYPE /LINEAR/: logarithmic
POST-1:
POST-1: s-s-s x n 0.001 2e4
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

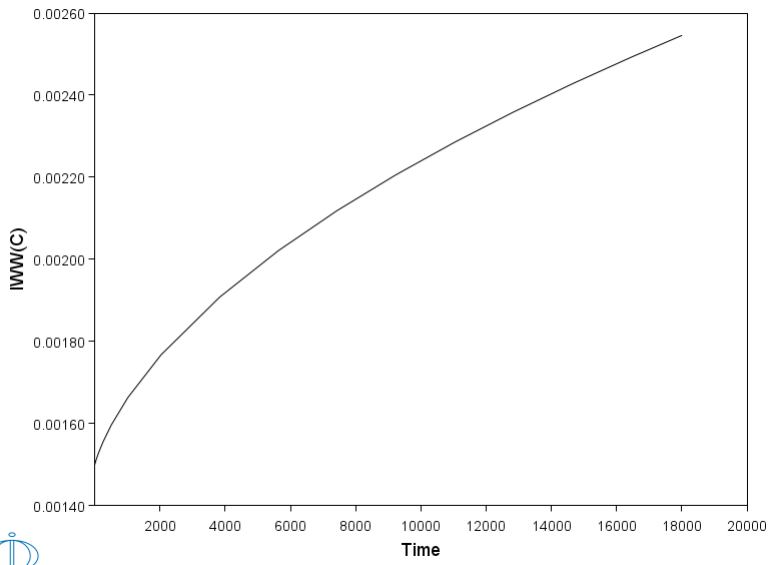
```



```

POST-1:
POST-1:
POST-1:
POST-1: @?<Hit_return_to_continue>
POST-1:
POST-1: @@
POST-1: @@ PLOT THE AVERAGE WEIGHT FRACTION OF C IN THE SPECIMEN
POST-1: @@
POST-1: s-d-a y iww(c)
POST-1:
POST-1: set-ax-ty
POST-1: AXIS (X, Y OR Z) : x
POST-1: AXIS TYPE /LINEAR/: linear
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1:
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

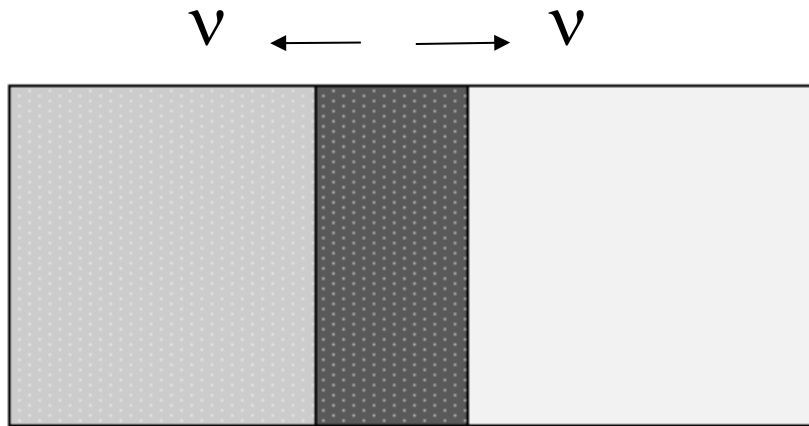
```



```
POST-1:  
POST-1:  
POST-1:  
POST-1: @?<Hit_return_to_continue>  
POST-1:  
POST-1:  
POST-1: set-inter  
--OK--  
POST-1:
```



## Moving Boundary Problems



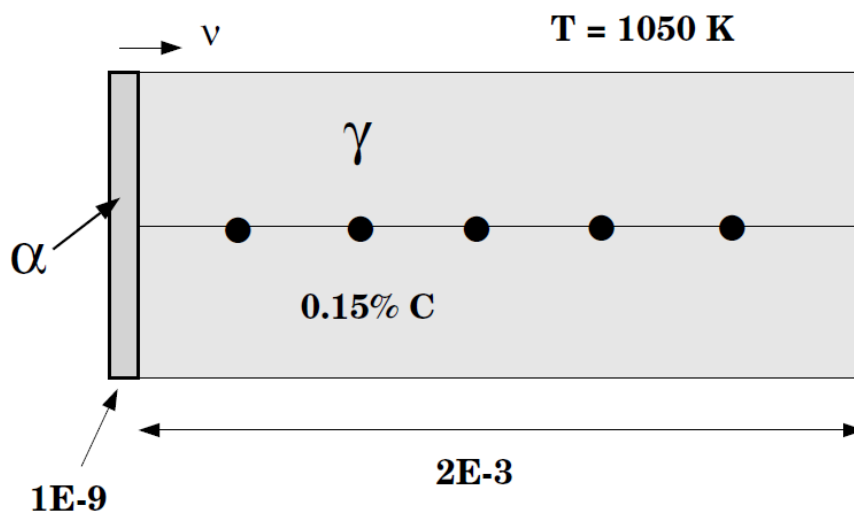
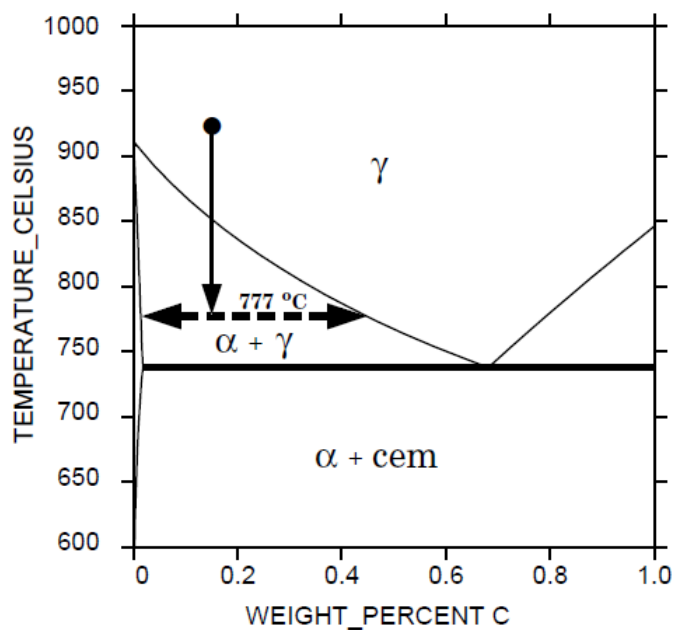


## Example exb1a

### $\gamma$ to $\alpha$ transformation in a binary Fe-C alloy

This example calculates 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 austenitization the specimen has been quenched down to 1050K. The system is assumed closed, no boundary conditions are set (a closed system is the default). Ferrite is expected to grow into the austenite. For this reason you start with a thin region with ferrite adjacent to the austenite.

*Fe - C Phase diagram*



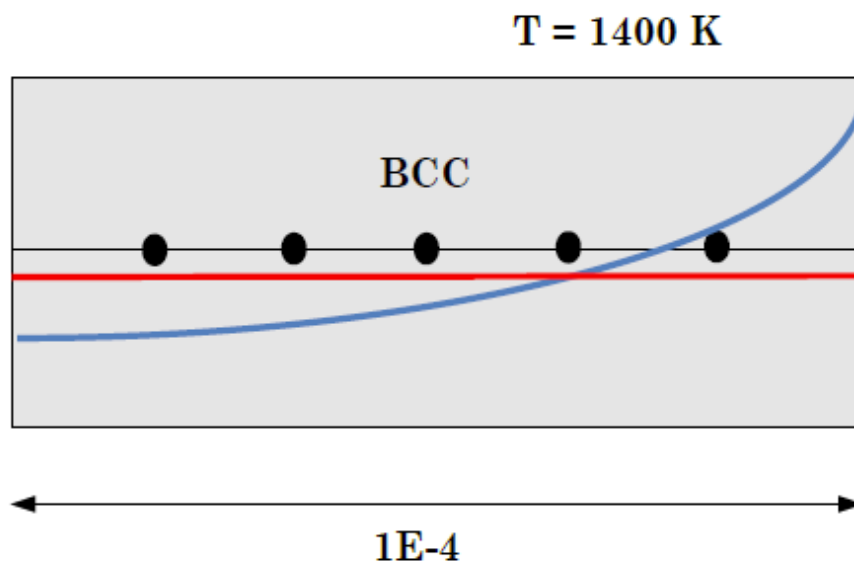


## Example exa7

### Homogenization heat-treatment

(Initial profile imported from Scheil simulation)

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.

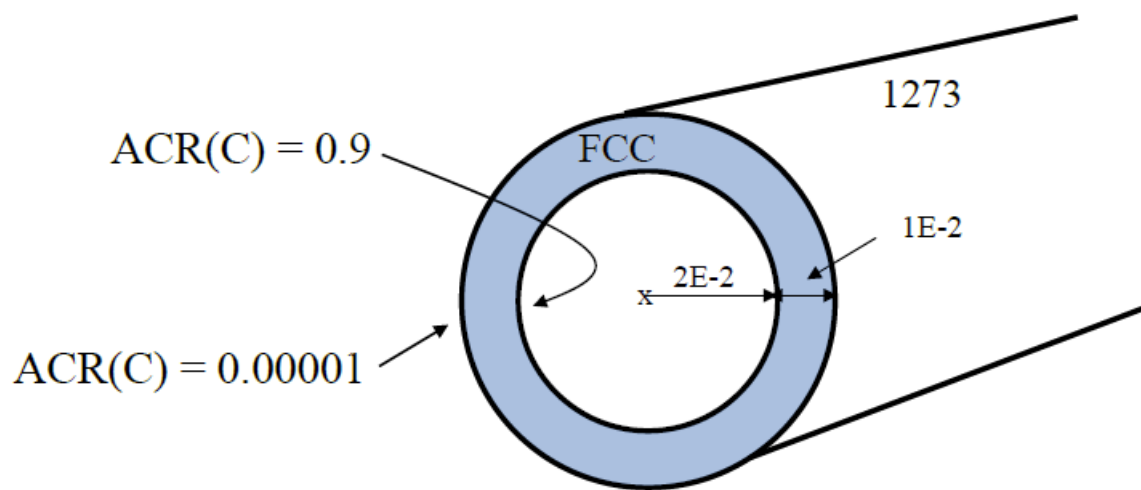




## Example exa6

### Diffusion through a tube wall: Boundary conditions result in a gradient in C-activity

A simple example of 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.



## exa6-setup

### SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,  
Stockholm, Sweden

Software running on Windows 64-bit wordlength  
Compiler: Intel Fortran Compiler 2025.0.0  
License library version: 9.7.0.0036  
Linked: Nov 19 2025 at 14:44:36

```
SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exa6\setup.DCM.test"
```

```
SYS: @@
SYS: @@ One-phase problem.
SYS: @@ Diffusion through a tube wall.
SYS: @@ A simple example about diffusion through a tube wall.
SYS: @@ The tube material is an Fe-0.6%Mn-0.7%Si-0.05%C alloy. On
SYS: @@ the inside wall a carbon activity of 0.9 is maintained whereas on
SYS: @@ the outside the C-activity is very low. This example demonstrates
SYS: @@ the use of the command SET-FIRST-INTERFACE as well as the MIXED
SYS: @@ boundary conditions.
SYS: @@-----
SYS:
SYS: @@ setup.DCM
SYS:
SYS:
SYS: @@
SYS: @@ GO TO THE DATABASE MODULE
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\databases\da
ta
Current database: Steels/Fe-Alloys v12.0

VA          /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE12:
TDB_TCFE12: @@
TDB_TCFE12: @@ USE THE TCFE DATABASE FOR THERMODYNAMIC DATA
TDB_TCFE12: @@
TDB_TCFE12: sw tcfe9
Current database: Steels/Fe-Alloys v9.3

VA          /- DEFINED
LI2_FCC     B2_BCC          DICTRA_FCC_A1
REJECTED
TDB_TCFE9: def-sys fe si mn c
FE          SI          MN
C DEFINED
TDB_TCFE9: rej ph * all
GAS:G      LIQUID:L      BCC_A2
FCC_A1     HCP_A3       CBCC_A12
CUB_A13    DIAMOND_FCC_A4 GRAPHITE
CEMENTITE  M23C6        M7C3
M5C2       KSI_CARBIDE    FE4N_LP1
FECN_CHI   LAVES_PHASE_C14 M3SI
MN9SI2     MN11SI19          MN6SI
G_PHASE    CR3SI          FE2SI
FES12_H    FES12_L          MSI
M5SI3      AL4C3           FE8SI2C
SIC        MN5SIC          CUZN_EPSILON
AL5FE4     MP_B31          M2P_C22
REJECTED
TDB_TCFE9: res ph fcc,grap
FCC_A1     GRAPHITE RESTORED
TDB_TCFE9: get
08:57:00,442 [Thread-0] INFO  JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ...

Use the command LIST_REFERENCES to see the list of references for assessed data
-OK-
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ SWITCH TO A MOBILITY DATABASE TO RETRIIVE KINETIC DATA
TDB_TCFE9: @@
TDB_TCFE9: app
Use one of these databases

TCFE12 = Steels/Fe-Alloys v12.0
TCFE9  = Steels/Fe-Alloys v9.3
SSUB6  = SGTE Substances v6.0
FEDEMO = Iron Demo Database v6.0
MOB2   = Alloys Mobility v2.7
MOBFE7 = Steels/Fe-Alloys Mobility v7.1
MOBFE4 = Steels/Fe-Alloys Mobility v4.0
MOBFE2 = Steels/Fe-Alloys Mobility v2.0
MFEDEMO = Fe-Alloys Mobility demo database v5.0
USER    = User defined Database

DATABASE NAME /TCFE9/: mobfe4
Current database: Steels/Fe-Alloys Mobility v4.0

VA DEFINED
B2_BCC REJECTED
APP: def-sys fe si mn c
FE          SI          MN
C DEFINED
APP: rej ph * all
BCC_A2     CEMENTITE    FCC_A1
FE4N_LP1   HCP_A3           LIQUID:L
```

```
REJECTED
APP: res ph fcc
FCC_A1 RESTORED
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....
```

Use the command LIST\_REFERENCES to see the list of references for assessed data

-OK-

```
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE PROBLEM IS SET UP
APP: @@
APP: go d-m
NO TIME STEP DEFINED
*** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
DIC>
DIC> @@
DIC> @@ ENTER GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 1273; * N
DIC>
DIC> @@
DIC> @@ SET THE REFERENCE STATE FOR CARBON
DIC> @@
DIC> set-ref C grap * 101325
DIC>
DIC> @@
DIC> @@ ENTER A REGION
DIC> @@
DIC> enter-region aus
DIC>
DIC> @@
DIC> @@ ENTER A DOUBLE GEOMETRIC GRID INTO THE REGION
DIC> @@
DIC> enter-grid
REGION NAME : /AUS/: aus
WIDTH OF REGION /1/: 1e-2
TYPE /AUTO/: AUTO
DIC>
DIC> @@
DIC> @@ SET THE GEOMETRY (1 = CYLINDER)
DIC> @@
DIC> enter-geo
GEOMETRICAL EXPONENT /0/: 1
DIC>
DIC> @@
DIC> @@ SET THE FIRST INTERFACE => TUBE
DIC> @@
DIC> set-first-interface
COORDINATE FOR FIRST INTERFACE /0/: 2e-2
DIC>
DIC> @@
DIC> @@ ENTER AN active PHASE IN THE REGION
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /AUS/: aus
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc_al#1
DIC>
DIC> @@
DIC> @@ ENTER INITIAL COMPOSITIONS INTO THE PHASE
DIC> @@
DIC> enter-composition
REGION NAME : /AUS/: aus
PHASE NAME: /FCC_A1/: fcc#1
DEPENDENT COMPONENT ? /SI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: si lin 0.7 0.7
PROFILE FOR /MN/: mn lin 0.6 0.6
PROFILE FOR /SI/: c lin 5e-2 5e-2
DIC>
DIC> @@
DIC> @@ SET THE BOUNDARY CONDITIONS ON BOTH THE LOWER AND UPPER PART OF THE REGION
DIC> @@
DIC> @@ USE MIXED CONDITIONS: AN ACTIVITY CONDITION FOR C AND CLOSED
DIC> @@ SYSTEMS FOR MN AND SI.
DIC> @@
DIC> set-cond
GLOBAL OR BOUNDARY CONDITION /GLOBAL/: boundary
BOUNDARY /LOWER/: lower
CONDITION TYPE /CLOSED_SYSTEM/: mixed
Dependent substitutional element:FE
Dependent interstitial element:VA
TYPE OF CONDITION FOR COMPONENT C /ZERO_FLUX/: activity
LOW TIME LIMIT /0/: 0
ACR(C)(TIME)= 0.9;
HIGH TIME LIMIT /*/: *
ANY MORE RANGES /N/: N
TYPE OF CONDITION FOR COMPONENT MN /ZERO_FLUX/: zero_flux
TYPE OF CONDITION FOR COMPONENT SI /ZERO_FLUX/: zero_flux
DIC>
DIC> set-cond
GLOBAL OR BOUNDARY CONDITION /GLOBAL/: boundary
BOUNDARY /UPPER/: upper
CONDITION TYPE /CLOSED_SYSTEM/: mixed
Dependent substitutional element:FE
Dependent interstitial element:VA
TYPE OF CONDITION FOR COMPONENT C /ZERO_FLUX/: activity
LOW TIME LIMIT /0/: 0
ACR(C)(TIME)= 1e-5;
HIGH TIME LIMIT /*/: *
ANY MORE RANGES /N/: N
TYPE OF CONDITION FOR COMPONENT MN /ZERO_FLUX/: zero_flux
TYPE OF CONDITION FOR COMPONENT SI /ZERO_FLUX/: zero_flux
DIC>
```

```
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 1e9
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /100000000/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC> @@
DIC> @@ SAVE TO FILE
DIC> @@
DIC> save exa6 y
DIC>
DIC> set-inter
--OK--
DIC>
```

exa6-run

DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exa6\run.DCM.test"

DIC>

DIC>

DIC> @@ run.DCM

DIC>

DIC> @@

DIC> @@ FILE FOR RUNNING exa6

DIC> @@

DIC>

DIC> @@

DIC> @@ ENTER THE DICTRA MONITOR AND READ THE STORE RESULT FILE

DIC> @@

DIC> go d-m

TIME STEP AT TIME 0.00000E+00

\*\*\* ENTERING GRAPHITE AS A DIFFUSION NONE PHASE

DIC> read exa6

OK

DIC>

DIC> @@

DIC> @@ Start the simulation

DIC> @@

DIC> simulate

INFO: Default responses (if any) will be applied during the simulation. Use "SIMULATE\_REACTION NO" instead for manual input.

Region: AUS

geometric 1.20000 dense at 0.00000 35 points

geometric 0.833333 dense at 0.100000E-01 36 points

DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE

U-FRACTION IN SYSTEM: C = .00115488575879621 FE = .490055682684517

MN = .00302988813183617 SI = .00691442924890043

TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]

U-FRACTION IN SYSTEM: C = .00115488575879621 FE = .490055682684517

MN = .00302988813183617 SI = .00691442924890043

TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]

TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00116918857196932 FE = .490055682684517

MN = .00302988813183617 SI = .00691442924890043

TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]

CPU time used in timestep 0 seconds

TIME = 0.10010000E-03 DT = 0.10000000E-03 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00116925677511611 FE = .490055682684517

MN = .00302988813183617 SI = .00691442924890043

TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]

CPU time used in timestep 1 seconds

TIME = 3.7171296 DT = 3.7170295 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00119293284978174 FE = .490055682684522

MN = .00302988813183677 SI = .00691442924889472

TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]

CPU time used in timestep 0 seconds

TIME = 11.151189 DT = 7.4340590 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00121675295851969 FE = .490055682684526

MN = .00302988813183727 SI = .00691442924889021

TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]

CPU time used in timestep 0 seconds

TIME = 26.019307 DT = 14.868118 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00124742195297911 FE = .490055682684531

MN = .00302988813183786 SI = .00691442924888482

TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]

CPU time used in timestep 1 seconds

TIME = 55.755543 DT = 29.736236 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00128911390005542 FE = .490055682684537

MN = .0030298881318386 SI = .00691442924887818

TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]

CPU time used in timestep 0 seconds

TIME = 115.22801 DT = 59.472472 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00134703651660225 FE = .490055682684544

MN = .0030298881318395 SI = .00691442924887014

TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]

CPU time used in timestep 1 seconds

TIME = 234.17296 DT = 118.94494 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00142832106681786 FE = .490055682684552

MN = .00302988813184054 SI = .00691442924886107

TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]

CPU time used in timestep 0 seconds

TIME = 472.06285 DT = 237.88989 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00154296869660367 FE = .490055682684559

MN = .00302988813184158 SI = .00691442924885257

TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]

CPU time used in timestep 0 seconds

TIME = 947.84262 DT = 475.77978 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00170514012818242 FE = .490055682684562

MN = .00302988813184217 SI = .00691442924884914

TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]

CPU time used in timestep 0 seconds

TIME = 1899.4022 DT = 951.55955 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00193499994805703 FE = .490055682684551

MN = .00302988813184128 SI = .00691442924886167

TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]

CPU time used in timestep 1 seconds

TIME = 3802.5213 DT = 1903.1191 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00226140370551408 FE = .490055682684509

MN = .00302988813183727 SI = .00691442924890687

TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]

CPU time used in timestep 0 seconds

TIME = 7608.7595 DT = 3806.2382 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00272584528526073 FE = .490055682684477

MN = .00302988813183441 SI = .00691442924894202

TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]

CPU time used in timestep 0 seconds

TIME = 15221.236 DT = 7612.4764 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00338827312489028 FE = .490055682684529

MN = .00302988813184169 SI = .00691442924888304

TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]

CPU time used in timestep 0 seconds

TIME = 30446.189 DT = 15224.953 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00433631630407219 FE = .490055682684635

MN = .00302988813185701 SI = .00691442924876118

TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]

CPU time used in timestep 1 seconds

TIME = 60896.094 DT = 30449.906 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00570002964090365 FE = .490055682684757

MN = .00302988813187498 SI = .0069144292486217  
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]  
CPU time used in timestep 0 seconds  
TIME = 121795.91 DT = 60899.811 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .00767412084728369 FE = .490055682684913  
MN = .00302988813189467 SI = .00691442924844635  
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]  
CPU time used in timestep 0 seconds  
TIME = 243595.53 DT = 121799.62 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .0105195649513181 FE = .490055682685137  
MN = .00302988813192002 SI = .00691442924819631  
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]  
CPU time used in timestep 1 seconds  
TIME = 487194.77 DT = 243599.25 SUM OF SQUARES = 0.0000000

output ignored...

... output resumed

TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]  
CPU time used in timestep 0 seconds  
TIME = 974393.26 DT = 487198.49 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .0161959223170427 FE = .4900556826862  
MN = .0030298881320517 SI = .00691442924700152  
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]  
CPU time used in timestep 0 seconds  
TIME = 1948790.2 DT = 974396.98 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .0165255441524092 FE = .490055682687089  
MN = .00302988813216816 SI = .00691442924599685  
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]  
CPU time used in timestep 1 seconds  
TIME = 3659176.8 DT = 1710386.6 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .0165253603333896 FE = .490055682688707  
MN = .00302988813236503 SI = .00691442924418116  
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]  
CPU time used in timestep 0 seconds  
TIME = 6504445.9 DT = 2845269.0 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .0165252156043225 FE = .4900556826919  
MN = .00302988813272575 SI = .00691442924062761  
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]  
CPU time used in timestep 0 seconds  
TIME = 11499948. DT = 4995502.6 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .0165250199480401 FE = .490055682698835  
MN = .0030298881334676 SI = .00691442923295053  
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]  
CPU time used in timestep 1 seconds  
TIME = 21490954. DT = 9991005.2 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .0165246370574857 FE = .490055682716788  
MN = .00302988813528998 SI = .00691442921317571  
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]  
CPU time used in timestep 0 seconds  
TIME = 41472964. DT = 19982010. SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .0165242743764126 FE = .490055682765089  
MN = .00302988814001775 SI = .00691442916014728  
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]  
CPU time used in timestep 0 seconds  
TIME = 81436985. DT = 39964021. SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .0165240798225428 FE = .490055682897507  
MN = .00302988815269011 SI = .00691442901505678  
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]  
CPU time used in timestep 1 seconds  
TIME = 0.16136503E+09 DT = 79928042. SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .0165243841670119 FE = .490055683239964  
MN = .00302988818594653 SI = .00691442863934314  
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]  
CPU time used in timestep 0 seconds  
TIME = 0.26136503E+09 DT = 0.10000000E+09 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .0165274380561969 FE = .490055683710213  
MN = .00302988823461859 SI = .00691442812042194  
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]  
CPU time used in timestep 0 seconds  
TIME = 0.36136503E+09 DT = 0.10000000E+09 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .0165311427149333 FE = .490055684172888  
MN = .00302988828599814 SI = .00691442760636751  
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]  
CPU time used in timestep 1 seconds  
TIME = 0.46136503E+09 DT = 0.10000000E+09 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .0165343499685237 FE = .49005568461407  
MN = .00302988833774673 SI = .00691442711343715  
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]  
CPU time used in timestep 0 seconds  
TIME = 0.56136503E+09 DT = 0.10000000E+09 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .0165372920835742 FE = .49005568503205  
MN = .00302988838885054 SI = .00691442664435305  
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]  
CPU time used in timestep 0 seconds  
TIME = 0.66136503E+09 DT = 0.10000000E+09 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .0165400639747419 FE = .490055685428352  
MN = .00302988843888551 SI = .00691442619801563  
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]  
CPU time used in timestep 1 seconds  
TIME = 0.76136503E+09 DT = 0.10000000E+09 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .0165427132192147 FE = .49005568580507  
MN = .00302988848767346 SI = .00691442577251001  
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]  
CPU time used in timestep 0 seconds  
TIME = 0.86136503E+09 DT = 0.10000000E+09 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .0165452672694828 FE = .49005568616428  
MN = .00302988853516225 SI = .00691442536581158  
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]  
CPU time used in timestep 0 seconds  
TIME = 0.96136503E+09 DT = 0.10000000E+09 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .0165477435591337 FE = .490055686507851  
MN = .00302988858136234 SI = .00691442497603956  
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]  
CPU time used in timestep 1 seconds  
TIME = 0.10000000E+10 DT = 38634974. SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .016550560658945 FE = .49005568663674  
MN = .00302988859887261 SI = .00691442482964091  
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]  
MUST SAVE WORKSPACE ON FILE  
WORKSPACE SAVED ON FILE  
RECLAIMING WORKSPACE

DELETING TIME-RECORD FOR TIME 0.0000000  
DELETING TIME-RECORD FOR TIME 0.10000000E-06  
DELETING TIME-RECORD FOR TIME 0.10010000E-03  
DELETING TIME-RECORD FOR TIME 3.7171296  
DELETING TIME-RECORD FOR TIME 11.151189  
DELETING TIME-RECORD FOR TIME 26.019307  
DELETING TIME-RECORD FOR TIME 55.755543  
DELETING TIME-RECORD FOR TIME 115.22801  
DELETING TIME-RECORD FOR TIME 234.17296  
DELETING TIME-RECORD FOR TIME 472.06285  
DELETING TIME-RECORD FOR TIME 947.84262  
DELETING TIME-RECORD FOR TIME 1899.4022  
DELETING TIME-RECORD FOR TIME 3802.5213  
DELETING TIME-RECORD FOR TIME 7608.7595  
DELETING TIME-RECORD FOR TIME 15221.236  
DELETING TIME-RECORD FOR TIME 30446.189  
DELETING TIME-RECORD FOR TIME 60896.094  
DELETING TIME-RECORD FOR TIME 121795.91  
DELETING TIME-RECORD FOR TIME 243595.53  
DELETING TIME-RECORD FOR TIME 487194.77  
DELETING TIME-RECORD FOR TIME 974393.26  
DELETING TIME-RECORD FOR TIME 1948790.2  
DELETING TIME-RECORD FOR TIME 3659176.8  
DELETING TIME-RECORD FOR TIME 6504445.9  
DELETING TIME-RECORD FOR TIME 11499948.  
DELETING TIME-RECORD FOR TIME 21490954.  
DELETING TIME-RECORD FOR TIME 41472964.  
DELETING TIME-RECORD FOR TIME 81436985.  
DELETING TIME-RECORD FOR TIME 0.16136503E+09  
DELETING TIME-RECORD FOR TIME 0.26136503E+09  
DELETING TIME-RECORD FOR TIME 0.36136503E+09  
DELETING TIME-RECORD FOR TIME 0.46136503E+09  
DELETING TIME-RECORD FOR TIME 0.56136503E+09  
DELETING TIME-RECORD FOR TIME 0.66136503E+09  
DELETING TIME-RECORD FOR TIME 0.76136503E+09  
DELETING TIME-RECORD FOR TIME 0.86136503E+09

KEEPING TIME-RECORD FOR TIME 0.96136503E+09  
AND FOR TIME 0.10000000E+10  
WORKSPACE RECLAIMED

TIMESTEP AT 0.10000000E+10 SELECTED

DIC>  
DIC> @@  
DIC> @@ THE SIMULATION IS FINISHED  
DIC> @@  
DIC>  
DIC> set-inter  
--OK--  
DIC>

## exa6-plot

DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exa6\plot.DCM.test"

DIC>

DIC>

DIC> @@ exa6\_plot.DCM

DIC>

DIC> @@

DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE exa6

DIC> @@

DIC>

DIC> @@

DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE

DIC> @@

DIC> go d-m

TIME STEP AT TIME 1.00000E+09

\*\*\* ENTERING GRAPHITE AS A DIFFUSION NONE PHASE

DIC> read exa6

OK

DIC>

DIC> @@

DIC> @@ GO TO THE POST PROCESSOR

DIC> @@

DIC> post

POST PROCESSOR VERSION 1.7

Implemented by Bjorn Jonsson

POST-1:

POST-1:

POST-1: @@

POST-1: @@ PLOT THE CONCENTRATION OF C AT DIFFERENT TIMES

POST-1: @@

POST-1: s-d-a x distance global

INFO: Distance is set as independent variable

POST-1: s-d-a y w-p c

POST-1: s-p-c time 0,1e4,2e5,1e7,1e9

POST-1:

POST-1:

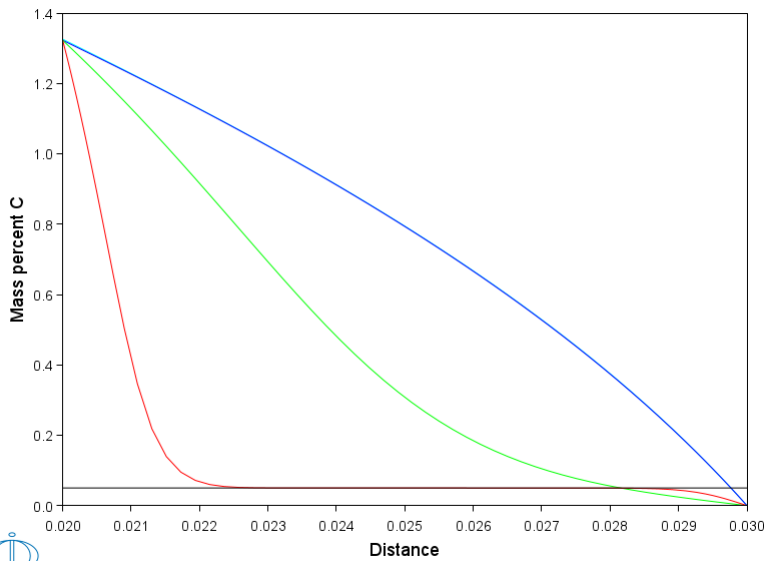
POST-1: SET\_EXP\_FILE\_FORMAT 5

POST-1: MAKE c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\unite\distribution\macroResult.exp Y

POST-1: SET\_EXP\_FILE\_FORMAT 10

POST-1:

POST-1: plot



POST-1:

POST-1:

POST-1:

POST-1:Hit RETURN to continue

POST-1:

POST-1: @@

POST-1: @@ PLOT THE ACTIVITY OF C

POST-1: @@

POST-1: s-d-a y acr(c)

POST-1:

POST-1:

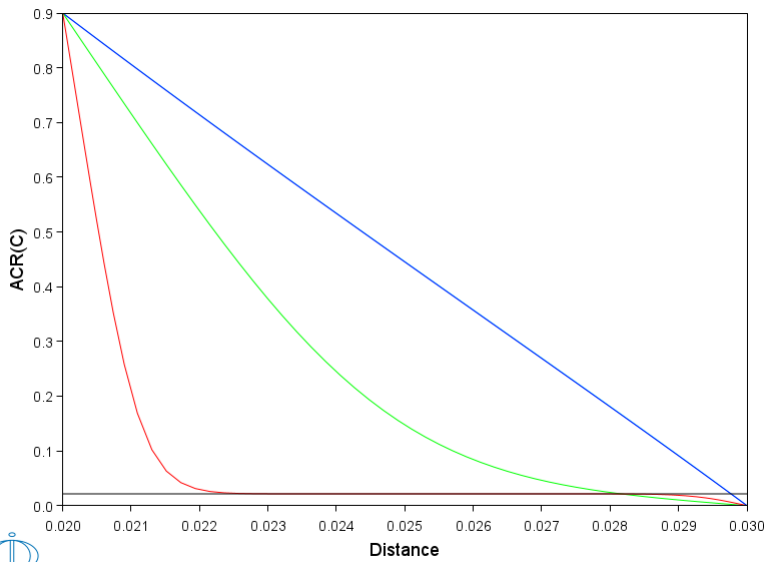
POST-1: SET\_EXP\_FILE\_FORMAT 5

POST-1: MAKE c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\unite\distribution\macroResult.exp Y

POST-1: SET\_EXP\_FILE\_FORMAT 10

POST-1:

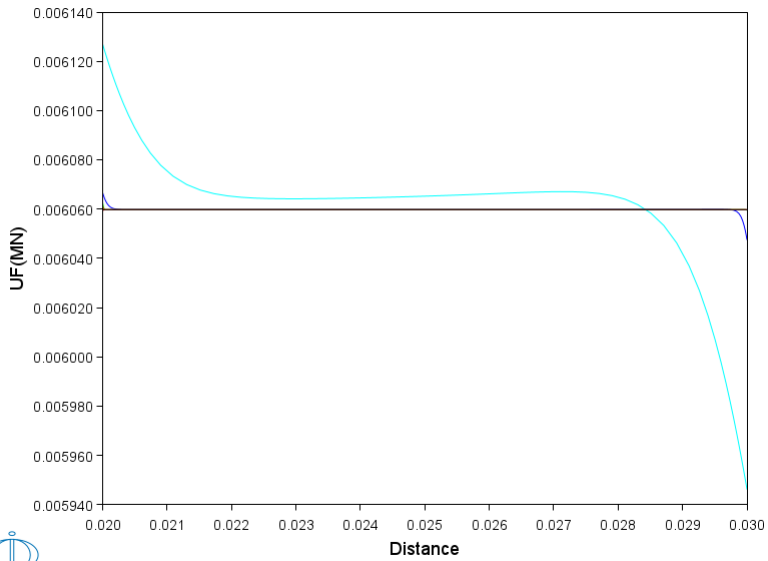
POST-1: plot



```

POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ LET US LOOK AT THE MN AND SI PROFILES
POST-1: @@
POST-1: @@ WE PLOT THE U-FRACTION OF MN AND SI WHICH WILL BE INDEPENDENT
POST-1: @@ OF THE C-CONCENTRATION.
POST-1: @@
POST-1: s-d-a y u-f mn
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

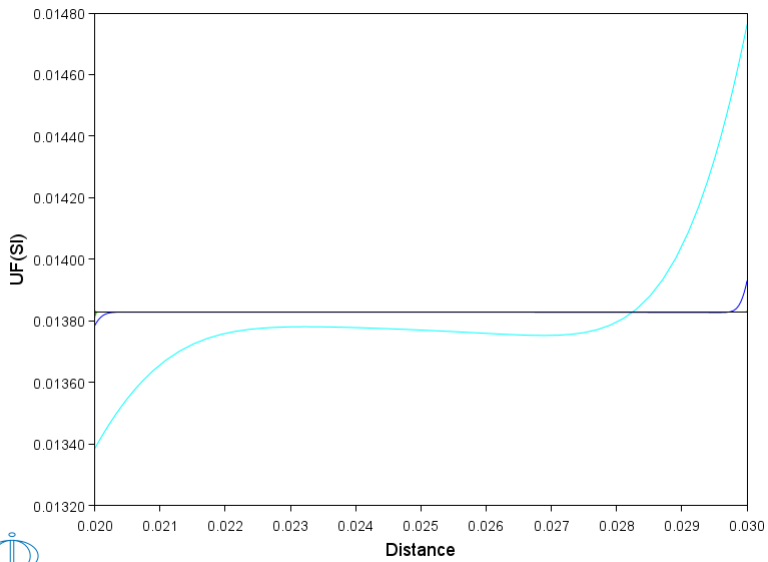
```



```

POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: s-d-a y u-f si
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

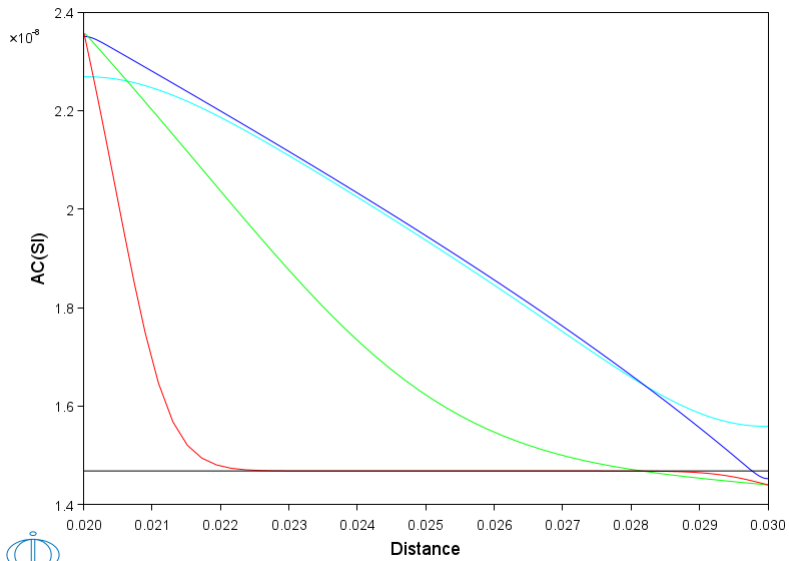
```



```

POST-1:
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ FINALLY, LOOK AT THE ACTIVITY PROFILES OF SI
POST-1: @@
POST-1: s-d-a y ac(si)
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

```



```

POST-1:
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: set-inter
--OK--
POST-1:

```

## exa7-setup

### SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,  
Stockholm, Sweden

Software running on Windows 64-bit wordlength  
Compiler: Intel Fortran Compiler 2025.0.0  
License library version: 9.7.0.0036  
Linked: Nov 19 2025 at 14:44:36

```
SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exa7\setup.DCM.test"
```

```
SYS: @@ One phase example.
```

```
SYS: @@ Homogenization heat treatment
```

```
SYS: @@ The initial segregation profile is created from a Scheil
```

```
SYS: @@ calculation (see macro create_initial_profile.TCM). The command
```

```
SYS: @@ INPUT_SCHEIL_PROFILE in the DICTRA MONITOR performs most of the
```

```
SYS: @@ set up. Only time and temperature must be entered after the
```

```
SYS: @@ INPUT_SCHEIL_PROFILE command is executed.
```

```
SYS: @@-----
```

```
SYS:
```

```
SYS: @@ In this example only a single phase, ferrite, is entered in the simulation
```

```
SYS: go da
```

```
THERMODYNAMIC DATABASE module
```

```
Database folder:
```

```
C:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\databases\da
```

```
ta
```

```
Current database: Steels/Fe-Alloys v12.0
```

```
VA /- DEFINED
```

```
DICTRA FCC_A1 REJECTED
```

```
TDB_TCFE12: sw FEDEMO
```

```
Current database: Iron Demo Database v6.0
```

```
VA /- DEFINED
```

```
TDB_FEDEMO: def-sys fe cr ni mn
```

```
FE CR NI
```

```
MN DEFINED
```

```
TDB_FEDEMO: rej ph *
```

```
GAS:G LIQUID:L BCC_A2
```

```
C14_LAVES CBCC_A12 CHI_A12
```

```
CUB_A13 DIAMOND_A4 FCC_A1
```

```
HCP_A3 SIGMA_D8B REJECTED
```

```
TDB_FEDEMO: rest ph bcc
```

```
BCC_A2 RESTORED
```

```
TDB_FEDEMO: get
```

```
09:00:58,282 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
```

```
REINITIATING GES .....
```

```
ELEMENTS .....
```

```
SPECIES .....
```

```
PHASES .....
```

```
PARAMETERS ...
```

```
FUNCTIONS ....
```

```
Use the command LIST_REFERENCES to see the list of references for assessed data
```

```
-OK-
```

```
TDB_FEDEMO:
```

```
TDB_FEDEMO: app MFEDEMO
```

```
Current database: Fe-Alloys Mobility demo database v5.0
```

```
VA DEFINED
```

```
APP: def-sys fe cr ni mn
```

```
FE CR NI
```

```
MN DEFINED
```

```
APP: rej ph *
```

```
BCC_A2 FCC_A1 LIQUID:L
```

```
REJECTED
```

```
APP: rest ph bcc
```

```
BCC_A2 RESTORED
```

```
APP: get
```

```
ELEMENTS .....
```

```
SPECIES .....
```

```
PHASES .....
```

```
PARAMETERS ...
```

```
FUNCTIONS ....
```

```
Use the command LIST_REFERENCES to see the list of references for assessed data
```

```
-OK-
```

```
APP:
```

```
APP: go dict-mon
```

```
NO TIME STEP DEFINED
```

```
DIC>
```

```
DIC>
```

```
DIC> @@ THE INPUT_SCHEIL_PROFILE COMMAND PERFORMS MOST OF THE SET UP
```

```
DIC> input_scheil_profile
```

```
INFO: SCHEIL_REGION CREATED
```

```
FILE NAME /XF.TXT/: segregation_profile.TXT
```

```
ENTER WIDTH OF REGION /1/: 100e-6
```

```
INFO: LINEAR GRID IN SCHEIL_REGION ENTERED WITH 100 GRID POINTS
```

```
ENTER MAIN SOLID SOLUTION PHASE
```

```
PHASE NAME: bcc#1
```

```
INFO: CHANGING DEPENDENT COMPONENT FROM NI TO FE
```

```
INFO: COMPOSITION PROFILE ENTERED IN REGION
```

```
SHOULD MORE PHASES BE ENTERED IN THE REGION /NO/: n
```

```
INFO: TO COMPLETE SETUP, ENTER TEMPERATURE AND
```

```
SIMULATION TIME
```

```
DIC>
```

```
DIC>
```

```
DIC> @@ ENTER THE HEAT TREATMENT TEMPERATURE
```

```
DIC> s-cond
```

```
GLOBAL OR BOUNDARY CONDITION /GLOBAL/: glob
```

```
VARIABLE : t
```

```
LOW TIME LIMIT /0/: 0 1473; * n
```

```
DIC>
```

```
DIC>
```

```
DIC> @@ ENTER A SIMULATION TIME
DIC> se-si-ti
END TIME FOR INTEGRATION /.1/: 3600
AUTOMATIC TIMESTEP CONTROL /YES/: y
MAX TIMESTEP DURING INTEGRATION /360/: 360
INITIAL TIMESTEP : /1E-07/: 1e-7
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/: 1e-9
DIC>
DIC>
DIC> save exa7 y
DIC>
DIC> set-inter
--OK--
DIC>
```

exa7-run

DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC-MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exa7\run.DCM.test"

DIC> go dict-mon

TIME STEP AT TIME 0.00000E+00

DIC>

DIC> read exa7

OK

DIC>

DIC> sim

INFO: Default responses (if any) will be applied during the simulation. Use "SIMULATE\_REACTION NO" instead for manual input.

DEGREE OF IMPLICIT SET TO TRAPEZOIDAL RULE

U-FRACTION IN SYSTEM: CR = .180420497424242 FE = .796498787878788

MN = .00999016878282828 NI = .0130905459141414

TOTAL SIZE OF SYSTEM: 1E-04 [m]

U-FRACTION IN SYSTEM: CR = .180420497424242 FE = .796498787878788

MN = .00999016878282828 NI = .0130905459141414

TOTAL SIZE OF SYSTEM: 1E-04 [m]

TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .180420497424242 FE = .796498787878788

MN = .00999016878282829 NI = .0130905459141414

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 1 seconds

TIME = 0.10010000E-03 DT = 0.10000000E-03 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .180420497424242 FE = .796498787878788

MN = .00999016878282829 NI = .0130905459141414

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.43088419 DT = 0.43078409 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .180420497424243 FE = .796498787878788

MN = .00999016878282829 NI = .0130905459141414

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 1 seconds

TIME = 1.2924524 DT = 0.86156818 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .180420497424243 FE = .796498787878788

MN = .00999016878282823 NI = .0130905459141414

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 3.0155887 DT = 1.7231364 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .180420497424242 FE = .796498787878787

MN = .00999016878282903 NI = .0130905459141414

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 1 seconds

TIME = 6.4618615 DT = 3.4462727 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .180420497424241 FE = .796498787878781

MN = .00999016878283682 NI = .0130905459141414

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 13.354407 DT = 6.8925455 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .180420497424229 FE = .796498787878749

MN = .00999016878287914 NI = .0130905459141424

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 27.139498 DT = 13.785091 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .180420497424222 FE = .796498787878759

MN = .00999016878287931 NI = .0130905459141401

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 54.709680 DT = 27.570182 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .180420497424197 FE = .79649878787879

MN = .00999016878287965 NI = .0130905459141337

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 1 seconds

TIME = 109.85004 DT = 55.140364 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .180420497424141 FE = .796498787878856

MN = .00999016878288083 NI = .0130905459141224

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 220.13077 DT = 110.28073 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .180420497424055 FE = .79649878787895

MN = .00999016878288576 NI = .0130905459141088

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 440.69223 DT = 220.56145 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .180420497423961 FE = .79649878787904

MN = .00999016878289935 NI = .013090545914099

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 800.69223 DT = 360.00000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .180420497423905 FE = .796498787879083

MN = .00999016878291508 NI = .0130905459140971

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 1160.6922 DT = 360.00000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .180420497423885 FE = .796498787879095

MN = .00999016878292113 NI = .0130905459140983

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 1 seconds

TIME = 1520.6922 DT = 360.00000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .180420497423872 FE = .796498787879106

MN = .00999016878292266 NI = .0130905459140985

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 1880.6922 DT = 360.00000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .180420497423861 FE = .796498787879119

MN = .00999016878292224 NI = .0130905459140979

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 2240.6922 DT = 360.00000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .180420497424024 FE = .79649878787892

MN = .00999016878295051 NI = .0130905459141057

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 2600.6922 DT = 360.00000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .180420497424179 FE = .796498787878731

MN = .00999016878297196 NI = .0130905459141176

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 2960.6922 DT = 360.00000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .180420497424306 FE = .796498787878574

MN = .00999016878299062 NI = .0130905459141293

TOTAL SIZE OF SYSTEM: 1E-04 [m]

```
CPU time used in timestep          0 seconds
TIME = 3320.6922      DT = 360.00000      SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .180420497424408 FE = .796498787878447
MN = .00999016878300579 NI = .0130905459141394
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep          1 seconds
TIME = 3600.0000      DT = 279.30777      SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .180420497424463 FE = .796498787878379
MN = .00999016878301374 NI = .0130905459141449
TOTAL SIZE OF SYSTEM: 1E-04 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME      0.0000000
DELETING TIME-RECORD FOR TIME      0.100000000E-06
DELETING TIME-RECORD FOR TIME      0.100100000E-03
DELETING TIME-RECORD FOR TIME      0.43088419
DELETING TIME-RECORD FOR TIME      1.2924524
DELETING TIME-RECORD FOR TIME      3.0155887
DELETING TIME-RECORD FOR TIME      6.4618615
DELETING TIME-RECORD FOR TIME      13.354407
DELETING TIME-RECORD FOR TIME      27.139498
DELETING TIME-RECORD FOR TIME      54.709680
DELETING TIME-RECORD FOR TIME      109.85004
DELETING TIME-RECORD FOR TIME      220.13077
DELETING TIME-RECORD FOR TIME      440.69223
DELETING TIME-RECORD FOR TIME      800.69223
DELETING TIME-RECORD FOR TIME      1160.6922
DELETING TIME-RECORD FOR TIME      1520.6922
DELETING TIME-RECORD FOR TIME      1880.6922
DELETING TIME-RECORD FOR TIME      2240.6922
DELETING TIME-RECORD FOR TIME      2600.6922
DELETING TIME-RECORD FOR TIME      2960.6922

KEEPING TIME-RECORD FOR TIME      3320.6922
AND FOR TIME                      3600.0000
WORKSPACE RECLAIMED

TIMESTEP AT      3600.0000      SELECTED
```

```
DIC>
DIC> set-inter
--OK--
DIC>
```

exa7-plot

DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exa7\plot.DCM.test"

DIC> go dict-mon

TIME STEP AT TIME 3.60000E+03

DIC>

DIC> read exa7

OK

DIC>

DIC> post

POST PROCESSOR VERSION 1.7

Implemented by Bjorn Jonsson

POST-1:

POST-1: s-p-c time 0,3600

POST-1: s-d-a x d g

INFO: Distance is set as independent variable

POST-1: s-d-a y w-p mn

POST-1:

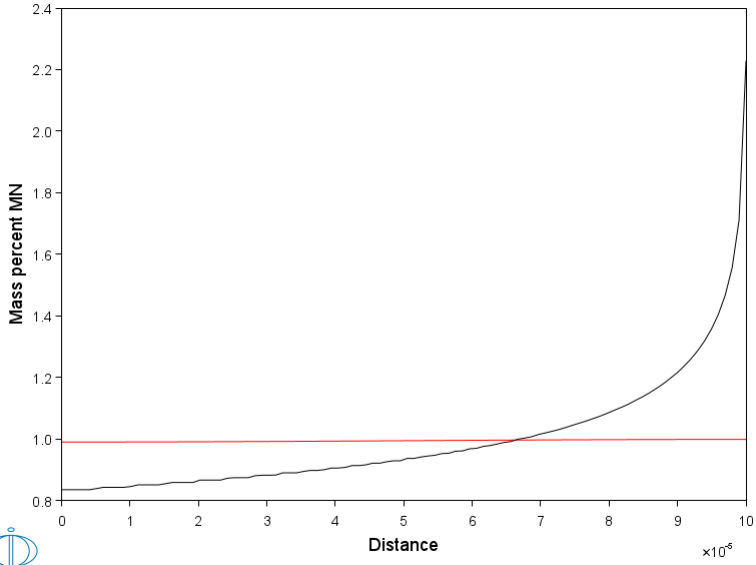
POST-1: SET\_EXP\_FILE\_FORMAT 5

POST-1: MAKE c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\unite\distribution\macroResult.exp Y

POST-1: SET\_EXP\_FILE\_FORMAT 10

POST-1:

POST-1: plot



POST-1:

POST-1: @@ Hit enter for the next plot

POST-1: @?

POST-1:

POST-1: s-d-a y w-p ni

POST-1:

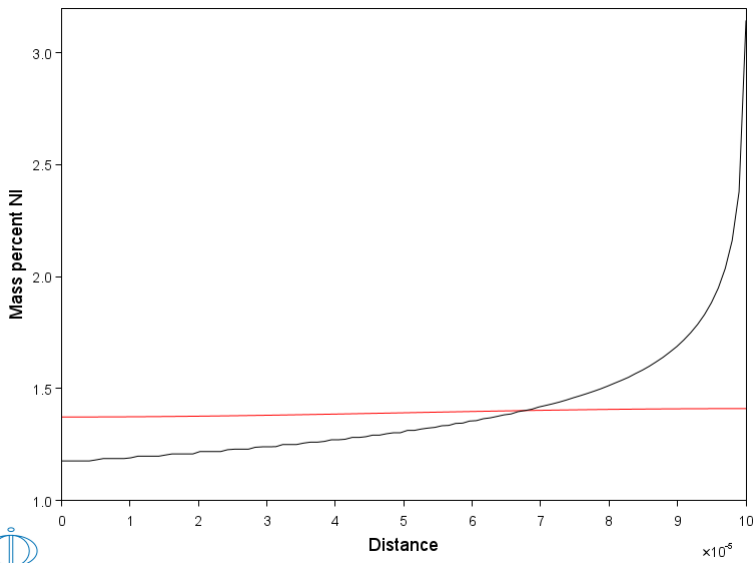
POST-1: SET\_EXP\_FILE\_FORMAT 5

POST-1: MAKE c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\unite\distribution\macroResult.exp Y

POST-1: SET\_EXP\_FILE\_FORMAT 10

POST-1:

POST-1: plot



POST-1:

POST-1: set-inter

--OK---

POST-1:

## exbla-setup

### SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,  
Stockholm, Sweden

Software running on Windows 64-bit wordlength  
Compiler: Intel Fortran Compiler 2025.0.0  
License library version: 9.7.0.0036  
Linked: Nov 19 2025 at 14:44:36

```
SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exbla\setup.DCM.test"
```

```
SYS: @@
SYS: @@ Moving boundary problem.
SYS: @@ Austenite to ferrite transformation in a binary Fe-C alloy
SYS: @@ This example calculates a ferrite(BCC)/austenite(FCC) transformation
SYS: @@ in a binary Fe-C alloy. The initial state is an austenite of 2mm
SYS: @@ thickness. The composition of the austenite is Fe-0.15wt%C.
SYS: @@
SYS: @@ After austenitization the specimen is quenched down to 1050K.
SYS: @@ The system is assumed closed, so no boundary conditions are set
SYS: @@ (a closed system is the default). Ferrite is expected to grow
SYS: @@ into the austenite, which is why we start with a thin
SYS: @@ region with ferrite adjacent to the austenite.
SYS: @@-----
SYS:
SYS: @@ exbla_setup.DCM
SYS:
SYS:
SYS: @@
SYS: @@ START BY GOING TO THE DATABASE MODULE
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\databases\da
ta
Current database: Steels/Fe-Alloys v12.0

VA                /- DEFINED
DICTRA FCC_A1     REJECTED
TDB_TCFE12:
TDB_TCFE12: @@
TDB_TCFE12: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE THE DATA
TDB_TCFE12: @@
TDB_TCFE12: sw FEDEMO
Current database: Iron Demo Database v6.0

VA                /- DEFINED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ DEFINE THE SYSTEM TO WORK WITH
TDB_FEDEMO: @@
TDB_FEDEMO: def-sys fe c
FE                C DEFINED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ EXCLUDE THE THERMODYNAMIC DATA FOR THE PHASES THAT ARE NOT NEEDED
TDB_FEDEMO: @@
TDB_FEDEMO: rej ph * all
GAS:G             LIQUID:L                 BCC_A2
C14_LAVES         CBCC_A12                 CEMENTITE_D011
CUB_A13           DIAMOND_A4                FCC_A1
GRAPHITE_A9       HCP_A3                 KSI_CARBIIDE
M23C6_D84         M5C2                  M7C3_D101
REJECTED
TDB_FEDEMO: res ph fcc bcc
FCC_A1           BCC_A2 RESTORED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ RETRIEVE DATA FROM THE DATABASE FILE
TDB_FEDEMO: @@
TDB_FEDEMO: get
09:03:58,960 [Thread-0] INFO  JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ MOBILITY/DIFFUSIVITY DATA ARE STORED IN A SEPARATE DATABASE FILE.
TDB_FEDEMO: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE DATA
TDB_FEDEMO: @@
TDB_FEDEMO: append
Use one of these databases

TCFE12 = Steels/Fe-Alloys v12.0
TCFE9  = Steels/Fe-Alloys v9.3
SSUB6  = SGTE Substances v6.0
FEDEMO = Iron Demo Database v6.0
MOB2   = Alloys Mobility v2.7
MOBFE7 = Steels/Fe-Alloys Mobility v7.1
MOBFE4 = Steels/Fe-Alloys Mobility v4.0
MOBFE2 = Steels/Fe-Alloys Mobility v2.0
MFEDEMO = Fe-Alloys Mobility demo database v5.0
USER    = User defined Database

DATABASE NAME /FEDEMO/: MFEDEMO
Current database: Fe-Alloys Mobility demo database v5.0

VA DEFINED
```

```

APP: def-sys fe c
FE C DEFINED
APP: rej ph * all
BCC A2 FCC_A1 CEMENTITE_D011
LIQUID:L REJECTED
APP: res ph fcc bcc
FCC A1 BCC_A2 RESTORED
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

```

Use the command LIST\_REFERENCES to see the list of references for assessed data

-OK-

```

APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP
APP: @@
APP: go d-m
NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER GLOBAL CONDITION T
DIC> @@
DIC> set-condition global T 0 1050; * N
DIC>
DIC> @@
DIC> @@ START BY ENTERING THE REGIONS ferrite AND austenite WHERE WE
DIC> @@ PUT THE BCC AND FCC PHASE, RESPECTIVELY. THE FERRITE REGION IS
DIC> @@ ASSUMED INITIALLY TO BE VERY THIN, 1E-9 METERS.
DIC> @@
DIC> enter-region
REGION NAME : ferrite
DIC>
DIC> enter-region
REGION NAME : austenite
ATTACH TO REGION NAMED /FERRITE/:
ATTACHED TO THE RIGHT OF FERRITE /YES/:
DIC>
DIC> @@
DIC> @@ ENTER GRIDS INTO THE REGIONS
DIC> @@
DIC> enter-grid
REGION NAME : /FERRITE/: ferrite
WIDTH OF REGION /1/: 1e-9
TYPE /AUTO/: linear
NUMBER OF POINTS /50/: 10
DIC>
DIC> enter-grid austenite
WIDTH OF REGION /1/: 20e-4
TYPE /AUTO/: geo
NUMBER OF POINTS /50/: 100
VALUE OF R IN THE GEOMETRICAL SERIE : 1.05
DIC>
DIC>
DIC> @@
DIC> @@ ENTER active PHASES INTO THE REGIONS
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /FERRITE/: ferrite
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: bcc
DIC>
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /AUSTENITE/: austenite
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC>
DIC> @@
DIC> @@ ENTER AN INITIAL COMPOSITION INTO BCC
DIC> @@
DIC> enter-composition
REGION NAME : /FERRITE/: ferrite
PHASE NAME: /BCC_A2/: bcc
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: C
TYPE /LINEAR/: linear
VALUE OF FIRST POINT : 0.01
VALUE OF LAST POINT : /1E-2/: 0.01
DIC>
DIC> @@
DIC> @@ ENTER AN INITIAL COMPOSITION INTO FCC
DIC> @@
DIC> enter-composition
REGION NAME : /AUSTENITE/: austenite
PHASE NAME: /FCC_A1/: fcc#1
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: C
TYPE /LINEAR/: linear
VALUE OF FIRST POINT : 0.15
VALUE OF LAST POINT : /0.15/: 0.15
DIC>
DIC>
DIC> @@
DIC> @@ THE BOUNDARY CONDITION IS A CLOSED SYSTEM AS WE DO NOT SPECIFY
DIC> @@ ANYTHING ELSE
DIC> @@
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time

```

```
END TIME FOR INTEGRATION /.1/: 1e9
AUTOMATIC TIMESTEP CONTROL /YES/: YES
MAX TIMESTEP DURING INTEGRATION /100000000/: 1e8
INITIAL TIMESTEP : /1E-07/: 1E-7
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/: 1E-7
DIC>
DIC>
DIC> @@
DIC> @@ IMPLICIT (1) TIME INTEGRATION IS USED INSTEAD OF THE MORE ACCURATE
DIC> @@ (BUT LESS STABLE) TRAPETZOIDAL METHOD WHICH IS THE DEFAULT.
DIC> @@
DIC> set-option DEGREE_OF_IMPLICITY 1.0
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exbla Y
DIC>
DIC> set-inter
--OK--
DIC>
```

exbla-run

DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exbla\run.DCM.test"

DIC>

DIC>

DIC> @@ exbla\_run.DCM

DIC>

DIC> @@

DIC> @@ FILE FOR RUNNING EXAMPLE bia

DIC> @@

DIC>

DIC> @@

DIC> @@ ENTER THE DICTRA MONITOR AND READ THE STORE RESULT FILE

DIC> @@

DIC> go d-m

TIME STEP AT TIME 0.000000E+00

DIC> read exbla

OK

DIC>

DIC> @@

DIC> @@ START THE SIMULATION

DIC> @@

DIC> simulate

INFO: Default responses (if any) will be applied during the simulation. Use "SIMULATE\_REACTION NO" instead for manual input.

Trying old scheme

U-FRACTION IN SYSTEM: C = .00698495590385911 FE = 1

TOTAL SIZE OF SYSTEM: .002000001 [m]

U-FRACTION IN SYSTEM: C = .00698495590385911 FE = 1

TOTAL SIZE OF SYSTEM: .002000001 [m]

4 GRIDPOINT(S) ADDED TO CELL #1 REGION: FERRITE

1 GRIDPOINT(S) ADDED TO CELL #1 REGION: AUSTENITE

0.115717401092532 0.115717856446369 111.048227048957 0.112984276791639 0.104050479021637 9.078830416795058

002 7.040904723184642E-002 3.472489916122559E-002 1.786881247439455E-003 9.193858915072814E-

006 1.857932633733402E-009 6.961181207827499E-020 TIME = 0.10000000E-06 DT = 0.10000000E-

06 SUM OF SQUARES = 0.69611812E-19

CELL # 1 VELOCITY AT INTERFACE # 2 IS 9.7160434 AND 9.7160434

POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.97260434E-06

U-FRACTION IN SYSTEM: C = .0069849386866348 FE = 1

TOTAL SIZE OF SYSTEM: .002000001 [m]

11 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: FERRITE

18 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: AUSTENITE

CPU time used in timestep 0 seconds

3.924867797234691E-003 3.925632782452177E-003 2.584529651866910E-005 1.486336496202991E-005 1.819317395067808E-

006 2.382916455095352E-009 8.205700881550707E-010 1.188241281818198E-010 3.399651142650408E-

021 TIME = 0.30000000E-06 DT = 0.20000000E-06 SUM OF SQUARES = 0.33996511E-20

CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.39752367E-05 AND 0.39752367E-05

POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.97260514E-06

U-FRACTION IN SYSTEM: C = .00698493868666082 FE = 1

TOTAL SIZE OF SYSTEM: .002000001 [m]

CPU time used in timestep 0 seconds

3.401999976038911E-009 3.365290685772431E-009 4.093695838798279E-014 1.545477732805252E-018 TIME = 0.70000000E-

06 DT = 0.40000000E-06 SUM OF SQUARES = 0.15454777E-17

CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.39679940E-05 AND 0.39679940E-05

POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.97260672E-06

U-FRACTION IN SYSTEM: C = .00698493868665902 FE = 1

TOTAL SIZE OF SYSTEM: .002000001 [m]

CPU time used in timestep 0 seconds

4.098253737021600E-009 4.058109820116081E-009 8.006954446087587E-015 1.502870138493581E-018 TIME = 0.15000000E-

05 DT = 0.80000000E-06 SUM OF SQUARES = 0.15028701E-17

CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.39679475E-05 AND 0.39679475E-05

POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.97260990E-06

U-FRACTION IN SYSTEM: C = .00698493868665542 FE = 1

TOTAL SIZE OF SYSTEM: .002000001 [m]

1 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: FERRITE

CPU time used in timestep 0 seconds

4.093819624242715E-009 4.053733166299584E-009 1.044582208539704E-015 4.719935580229088E-019 TIME = 0.31000000E-

05 DT = 0.16000000E-05 SUM OF SQUARES = 0.47199356E-18

CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.39678579E-05 AND 0.39678579E-05

POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.97261625E-06

U-FRACTION IN SYSTEM: C = .00698493868664821 FE = 1

TOTAL SIZE OF SYSTEM: .002000001 [m]

1 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: FERRITE

CPU time used in timestep 0 seconds

4.084485200528954E-009 4.044439967759275E-009 1.480555155016377E-015 4.155720032801227E-023 TIME = 0.63000000E-

05 DT = 0.32000000E-05 SUM OF SQUARES = 0.41557200E-22

CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.39676764E-05 AND 0.39676764E-05

POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.97262894E-06

U-FRACTION IN SYSTEM: C = .00698493868663385 FE = 1

TOTAL SIZE OF SYSTEM: .002000001 [m]

1 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: FERRITE

CPU time used in timestep 0 seconds

output ignored...

... output resumed

32 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: FERRITE

CPU time used in timestep 0 seconds

2.611831128559994E-005 2.612247732488457E-005 1.163693146018181E-

018 TIME = 0.61258999E+09 DT = 0.10000000E+09 SUM OF SQUARES = 0.11636931E-17

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.50743205E-16 AND -0.50743205E-16

POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.13801335E-02

U-FRACTION IN SYSTEM: C = .00697896446883887 FE = 1

TOTAL SIZE OF SYSTEM: .002000001 [m]

1 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: AUSTENITE

CPU time used in timestep 0 seconds

5.667696996320780E-006 5.667214108148784E-006 4.934237366947947E-

021 TIME = 0.71258999E+09 DT = 0.10000000E+09 SUM OF SQUARES = 0.49342374E-20

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.16645896E-15 AND -0.16645896E-15

POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.13801169E-02

U-FRACTION IN SYSTEM: C = .00697913421325872 FE = 1

TOTAL SIZE OF SYSTEM: .002000001 [m]

1 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: AUSTENITE

CPU time used in timestep 0 seconds  
1.759335210588360E-004 1.759423470102133E-004 8.020718929993898E-  
021 TIME = 0.81258999E+09 DT = 0.10000000E+09 SUM OF SQUARES = 0.80207189E-20  
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.48723311E-15 AND 0.48723311E-15  
POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.13801656E-02  
U-FRACTION IN SYSTEM: C = .006978637363447 FE = 1  
TOTAL SIZE OF SYSTEM: .002000001 [m]  
32 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: FERRITE

CPU time used in timestep 0 seconds  
1.489740793056276E-004 1.489978523102500E-004 2.905911973058217E-  
019 TIME = 0.91258999E+09 DT = 0.10000000E+09 SUM OF SQUARES = 0.29059120E-18  
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.12097389E-15 AND -0.12097389E-15  
POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.13801535E-02  
U-FRACTION IN SYSTEM: C = .00697876072504328 FE = 1  
TOTAL SIZE OF SYSTEM: .002000001 [m]  
1 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: AUSTENITE

CPU time used in timestep 0 seconds  
1.028394579648291E-005 1.028549662054664E-005 5.156398795723296E-  
022 TIME = 0.10000000E+10 DT = 87410009. SUM OF SQUARES = 0.51563988E-21  
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.38684973E-16 AND 0.38684973E-16  
POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.13801569E-02  
U-FRACTION IN SYSTEM: C = .0069787262430949 FE = 1  
TOTAL SIZE OF SYSTEM: .002000001 [m]

MUST SAVE WORKSPACE ON FILE  
WORKSPACE SAVED ON FILE  
RECLAIMING WORKSPACE  
DELETING TIME-RECORD FOR TIME 0.0000000  
DELETING TIME-RECORD FOR TIME 0.10000000E-06  
DELETING TIME-RECORD FOR TIME 0.30000000E-06  
DELETING TIME-RECORD FOR TIME 0.70000000E-06  
DELETING TIME-RECORD FOR TIME 0.15000000E-05  
DELETING TIME-RECORD FOR TIME 0.31000000E-05  
DELETING TIME-RECORD FOR TIME 0.63000000E-05  
DELETING TIME-RECORD FOR TIME 0.12700000E-04  
DELETING TIME-RECORD FOR TIME 0.25500000E-04  
DELETING TIME-RECORD FOR TIME 0.51100000E-04  
DELETING TIME-RECORD FOR TIME 0.10230000E-03  
DELETING TIME-RECORD FOR TIME 0.20470000E-03  
DELETING TIME-RECORD FOR TIME 0.40950000E-03  
DELETING TIME-RECORD FOR TIME 0.81910000E-03  
DELETING TIME-RECORD FOR TIME 0.16383000E-02  
DELETING TIME-RECORD FOR TIME 0.32767000E-02  
DELETING TIME-RECORD FOR TIME 0.65535000E-02  
DELETING TIME-RECORD FOR TIME 0.13107100E-01  
DELETING TIME-RECORD FOR TIME 0.26214300E-01  
DELETING TIME-RECORD FOR TIME 0.52428700E-01  
DELETING TIME-RECORD FOR TIME 0.10485750  
DELETING TIME-RECORD FOR TIME 0.20971510  
DELETING TIME-RECORD FOR TIME 0.41943030  
DELETING TIME-RECORD FOR TIME 0.83886070  
DELETING TIME-RECORD FOR TIME 1.6777215  
DELETING TIME-RECORD FOR TIME 3.3554431  
DELETING TIME-RECORD FOR TIME 6.7108863  
DELETING TIME-RECORD FOR TIME 13.421773  
DELETING TIME-RECORD FOR TIME 26.843545  
DELETING TIME-RECORD FOR TIME 53.687091  
DELETING TIME-RECORD FOR TIME 107.37418  
DELETING TIME-RECORD FOR TIME 214.74836  
DELETING TIME-RECORD FOR TIME 429.49673  
DELETING TIME-RECORD FOR TIME 858.99346  
DELETING TIME-RECORD FOR TIME 1717.9869  
DELETING TIME-RECORD FOR TIME 3435.9738  
DELETING TIME-RECORD FOR TIME 6871.9477  
DELETING TIME-RECORD FOR TIME 13743.895  
DELETING TIME-RECORD FOR TIME 27487.791  
DELETING TIME-RECORD FOR TIME 54975.581  
DELETING TIME-RECORD FOR TIME 109951.16  
DELETING TIME-RECORD FOR TIME 219902.33  
DELETING TIME-RECORD FOR TIME 439804.65  
DELETING TIME-RECORD FOR TIME 879609.30  
DELETING TIME-RECORD FOR TIME 1759218.6  
DELETING TIME-RECORD FOR TIME 3518437.2  
DELETING TIME-RECORD FOR TIME 7036874.4  
DELETING TIME-RECORD FOR TIME 14073749.  
DELETING TIME-RECORD FOR TIME 28147498.  
DELETING TIME-RECORD FOR TIME 56294995.  
DELETING TIME-RECORD FOR TIME 0.11258999E+09  
DELETING TIME-RECORD FOR TIME 0.21258999E+09  
DELETING TIME-RECORD FOR TIME 0.31258999E+09  
DELETING TIME-RECORD FOR TIME 0.41258999E+09  
DELETING TIME-RECORD FOR TIME 0.51258999E+09  
DELETING TIME-RECORD FOR TIME 0.61258999E+09  
DELETING TIME-RECORD FOR TIME 0.71258999E+09  
DELETING TIME-RECORD FOR TIME 0.81258999E+09

KEEPING TIME-RECORD FOR TIME 0.91258999E+09  
AND FOR TIME 0.10000000E+10  
WORKSPACE RECLAIMED

TIMESTEP AT 0.10000000E+10 SELECTED

DIC>  
DIC>  
DIC>  
DIC> @@  
DIC> @@ THE SIMULATION IS FINISHED  
DIC> @@  
DIC>  
DIC> set-inter  
--OK--  
DIC>

# exbla-plot

DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exbla\plot.DCM.test"

DIC>

DIC>

DIC> @@ exbla\_plot.DCM

DIC>

DIC> @@

DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE bla

DIC> @@

DIC>

DIC> @@

DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE

DIC> @@

DIC> go d-m

TIME STEP AT TIME 1.00000E+09

DIC> read exbla

OK

DIC>

DIC> @@

DIC> @@ GO TO THE POST PROCESSOR

DIC> @@

DIC> post

POST PROCESSOR VERSION 1.7

Implemented by Bjorn Jonsson

POST-1:

POST-1:

POST-1: @@

POST-1: @@ PLOT THE CARBON CONCENTRATIONS AT DIFFERENT TIMES

POST-1: @@

POST-1: s-d-a x distance global

INFO: Distance is set as independent variable

POST-1: s-d-a y w-p c

POST-1: s-p-c time 1e3,1e5,1e9

POST-1:

POST-1:

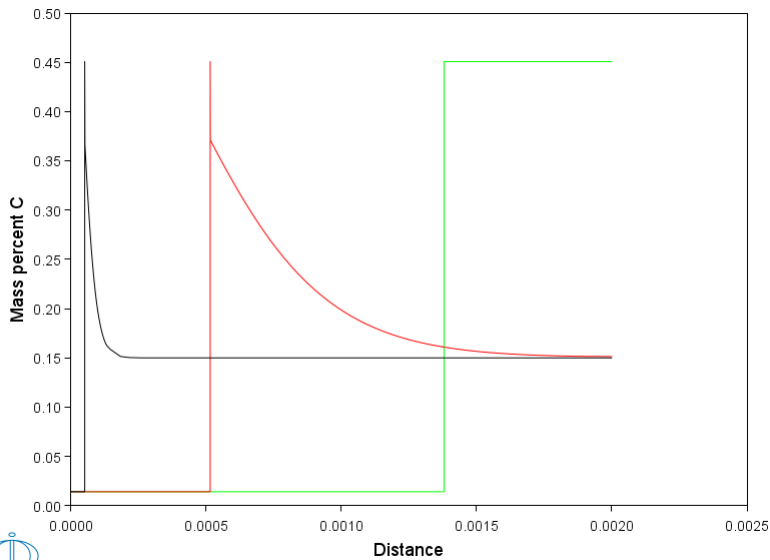
POST-1: SET\_EXP\_FILE\_FORMAT 5

POST-1: MAKE c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\unite\distribution\macroResult.exp Y

POST-1: SET\_EXP\_FILE\_FORMAT 10

POST-1:

POST-1: plot



POST-1:

POST-1:

POST-1: @?

POST-1:

POST-1: sel-plot new

POST-1:

POST-1: @@

POST-1: @@ PLOT THE POSITION OF THE BCC/FCC INTERPHASE

POST-1: @@

POST-1: s-d-a x time

INFO: Time is set as independent variable

POST-1: s-d-a y

VARIABLE : pos

INTERFACE : aus

UPPER OR LOWER INTERFACE OF REGION AUSTENITE#1 /LOWER/: lower

POST-1:

POST-1: set\_axis\_type

AXIS (X, Y OR Z) : x

AXIS TYPE /LINEAR/: log

POST-1:

POST-1: s-s-s

AXIS (X, Y OR Z) : x

AUTOMATIC SCALING (Y OR N) /N/: n

MIN VALUE : 10

MAX VALUE : 1e9

POST-1:

POST-1:

POST-1: SET\_EXP\_FILE\_FORMAT 5

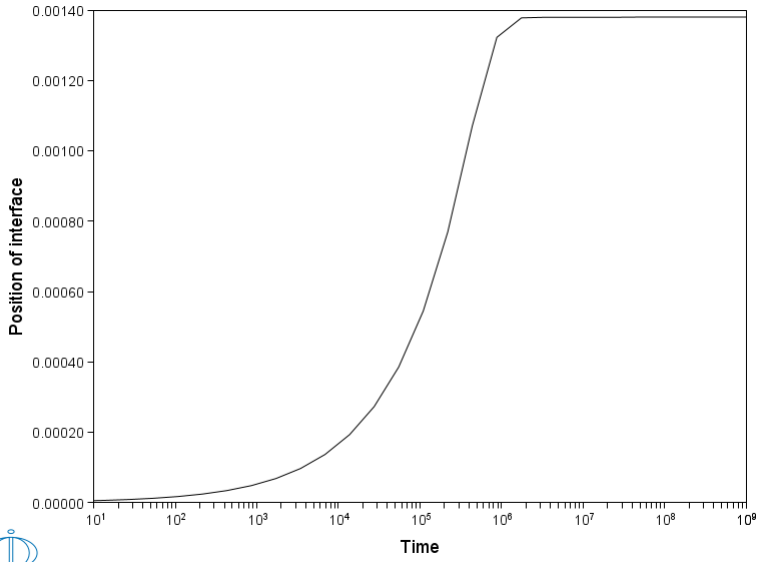
POST-1: MAKE c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\unite\distribution\macroResult.exp Y

POST-1:

OST-1: SET\_EXP\_FILE\_FORMAT 10

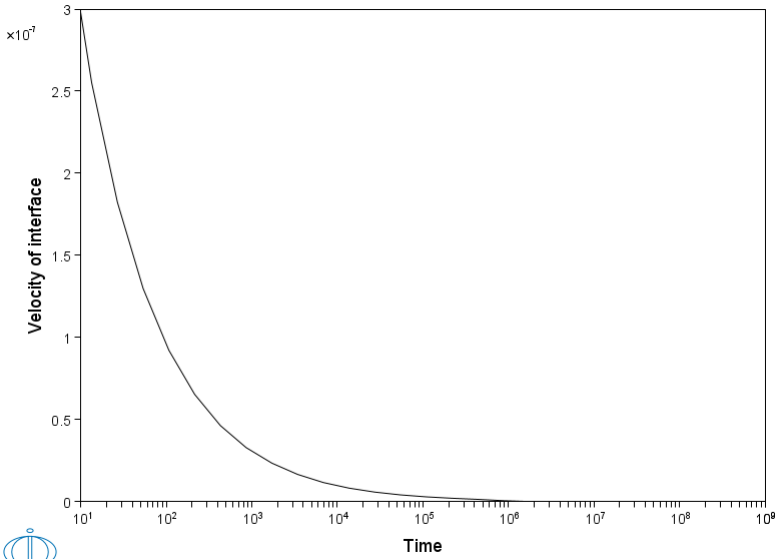
POST-1:

POST-1: plot



```

POST-1:
POST-1:@?
POST-1:
POST-1: sel-plot new
POST-1:
POST-1:
POST-1: @@
POST-1: @@ PLOT THE VELOCITY OF THE BCC/FCC INTERPHASE
POST-1: @@
POST-1: s-d-a
AXIS (X, Y OR Z) : y
VARIABLE : velocity
INTERFACE : aus
UPPER OR LOWER INTERFACE OF REGION AUSTENITE#1 /LOWER/: lower
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
  
```



```

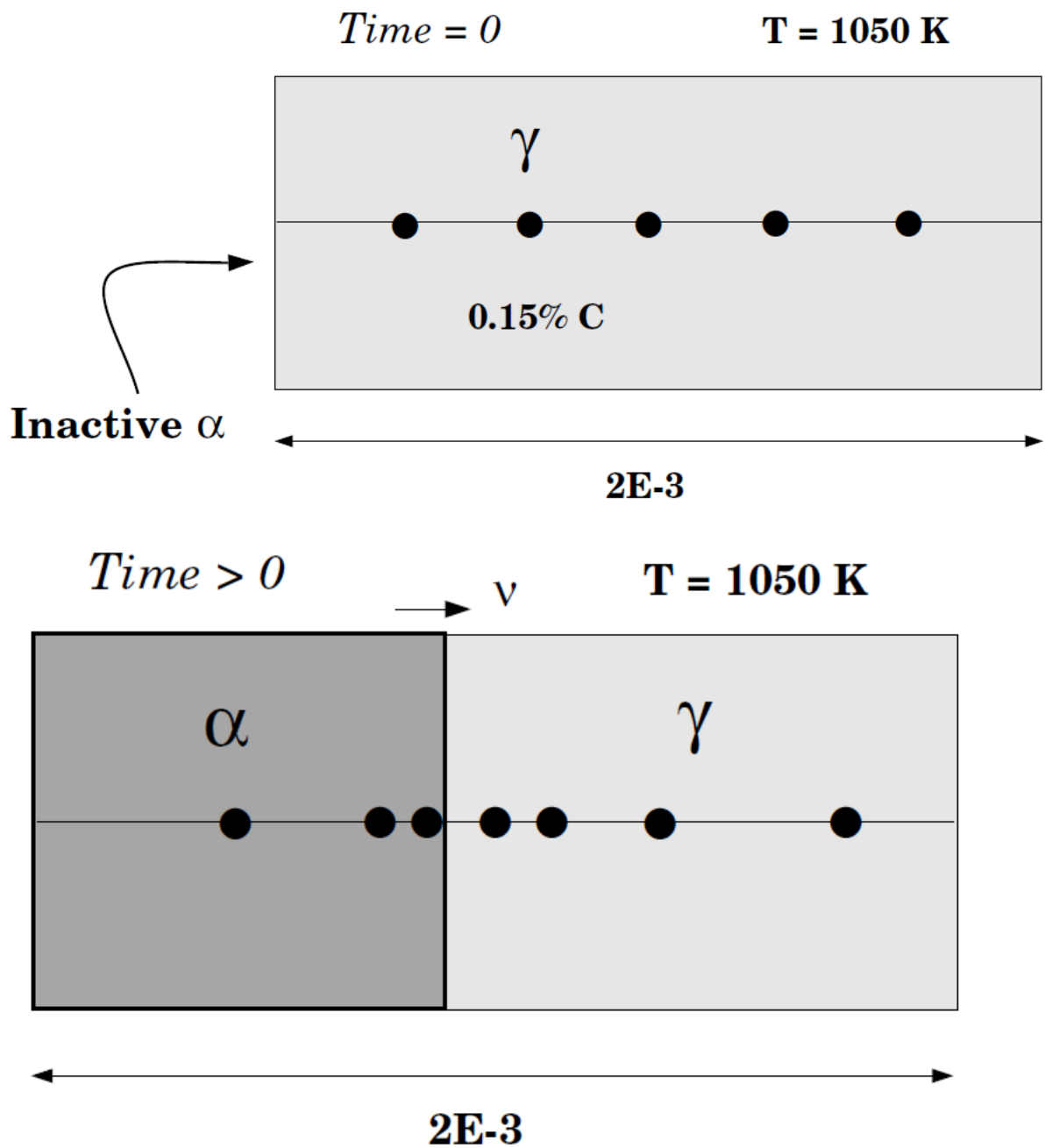
POST-1:
POST-1:
POST-1:
POST-1:
POST-1: set-inter
--OK--
POST-1:
  
```



## Example exb1b

### $\gamma$ to $\alpha$ transformation in a binary Fe-C alloy: Inactive $\alpha$

This is the same example as in exb1a but now the problem is with ferrite as an inactive phase adjacent to the initial austenite.



## exblb-setup

### SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,  
Stockholm, Sweden

Software running on Windows 64-bit wordlength  
Compiler: Intel Fortran Compiler 2025.0.0  
License library version: 9.7.0.0036  
Linked: Nov 19 2025 at 14:44:36

```
SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exblb\setup.DCM.test"
```

```
SYS: @@
SYS: @@ Moving boundary problem.
SYS: @@ Austenite to ferrite transformation in a binary Fe-C alloy
SYS: @@ This is the same example as in exbla but now the problem is with
SYS: @@ ferrite as an inactive phase adjacent to the initial austenite.
SYS: @@-----
SYS:
SYS: @@ exblb_setup.DCM
SYS:
SYS: @@
SYS: @@ START BY GOING TO THE DATABASE MODULE
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\databases\da
ta
Current database: Steels/Fe-Alloys v12.0

VA                /-  DEFINED
DICTRA_FCC_A1    REJECTED
TDB_TCFE12:
TDB_TCFE12: @@
TDB_TCFE12: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA
TDB_TCFE12: @@
TDB_TCFE12: sw FEDEMO
Current database: Iron Demo Database v6.0

VA                /-  DEFINED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ DEFINE THE SYSTEM TO WORK WITH
TDB_FEDEMO: @@
TDB_FEDEMO: def-sys fe c
FE                C  DEFINED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ EXCLUDE THE THERMODYNAMIC DATA FOR THE PHASES THAT ARE NOT NEEDED
TDB_FEDEMO: @@
TDB_FEDEMO: rej ph * all
GAS:G            LIQUID:L            BCC_A2
C14_LAVES        CBCC_A12           CEMENTITE_D011
CUB_A13          DIAMOND_A4         FCC_A1
GRAPHITE_A9      HCP_A3             KSI_CARBIDE
M23C6_D84        MSC2              M7C3_D101
REJECTED
TDB_FEDEMO: res ph fcc bcc
FCC_A1           BCC_A2  RESTORED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ RETRIEVE DATA FROM THE DATABASE FILE
TDB_FEDEMO: @@
TDB_FEDEMO: get
09:06:59,984 [Thread-0] INFO  JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS .....

Use the command LIST_REFERENCES to see the list of references for assessed data
-OK-
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ MOBILITY/DIFFUSIVITY DATA ARE STORED IN A SEPARATE DATABASE FILE.
TDB_FEDEMO: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE THE DATA.
TDB_FEDEMO: @@
TDB_FEDEMO: app
Use one of these databases

TCFE12 = Steels/Fe-Alloys v12.0
TCFE9  = Steels/Fe-Alloys v9.3
SSUB6  = SGTE Substances v6.0
FEDEMO = Iron Demo Database v6.0
MOB2   = Alloys Mobility v2.7
MOBFE7 = Steels/Fe-Alloys Mobility v7.1
MOBFE4 = Steels/Fe-Alloys Mobility v4.0
MOBFE2 = Steels/Fe-Alloys Mobility v2.0
MFEDEMO = Fe-Alloys Mobility demo database v5.0
USER    = User defined Database

DATABASE NAME /FEDEMO/: MFEDEMO
Current database: Fe-Alloys Mobility demo database v5.0

VA  DEFINED
APP: def-sys fe c
FE                C  DEFINED
APP: rej ph * all
BCC_A2            CEMENTITE_D011
LIQUID:L REJECTED
APP: res ph fcc bcc
FCC_A1           BCC_A2  RESTORED
APP: get
```

ELEMENTS .....  
SPECIES .....  
PHASES .....  
PARAMETERS ...  
FUNCTIONS .....

Use the command LIST\_REFERENCES to see the list of references for assessed data

-OK-

```
APP: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP
APP: @@
APP: go d-m
      NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 1050; * N
DIC>
DIC> @@
DIC> @@ START BY ENTERING THE REGION austenite WHERE WE PUT THE fcc PHASE
DIC> @@
DIC> enter-region
REGION NAME : austenite
DIC>
DIC> @@
DIC> @@ ENTER THE GRID INTO THE REGION
DIC> @@
DIC> enter-grid
REGION NAME : /AUSTENITE/: austenite
WIDTH OF REGION /1/: 20e-4
TYPE /AUTO/: GEO
NUMBER OF POINTS /50/: 100
VALUE OF R IN THE GEOMETRICAL SERIE : 1.05
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE active PHASES INTO THE REGIONS
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /AUSTENITE/: austenite
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC> @@
DIC> @@ ENTER THE inactive PHASES INTO THE REGIONS
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inactive
ATTACH TO REGION NAMED /AUSTENITE/: austenite
ATTACHED TO THE RIGHT OF AUSTENITE /YES/: no
PHASE NAME: /NONE/: bcc
REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-5
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITION FOR FCC
DIC> @@
DIC> enter-composition
REGION NAME : /AUSTENITE/: austenite
PHASE NAME: /FCC_A1/: fcc#1
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: C
TYPE /LINEAR/: lin
VALUE OF FIRST POINT : 0.15
VALUE OF LAST POINT : /0.15/: 0.15
DIC>
DIC> @@
DIC> @@ THE BOUNDARY CONDITION IS A CLOSED SYSTEM AS WE DO NOT SPECIFY
DIC> @@ ANYTHING ELSE
DIC> @@
DIC>
DIC> list-prof,,,,,,,,
INTERFACE AT GLOBAL COORDINATE X = 0.00000E+00
REGION AUSTENITE
COORDINATE NP(FCC_A1) X(FCC_A1,C) X(FCC_A1,FE)
0 1 .00693651 .993063
8.04898E-07 1 .00693651 .993063
1.65004E-06 1 .00693651 .993063
2.53744E-06 1 .00693651 .993063
3.46921E-06 1 .00693651 .993063
4.44757E-06 1 .00693651 .993063
5.47485E-06 1 .00693651 .993063
6.55349E-06 1 .00693651 .993063
7.68606E-06 1 .00693651 .993063
8.87526E-06 1 .00693651 .993063
1.01239E-05 1 .00693651 .993063
1.1435E-05 1 .00693651 .993063
1.28117E-05 1 .00693651 .993063
1.42572E-05 1 .00693651 .993063
1.57749E-05 1 .00693651 .993063
1.73685E-05 1 .00693651 .993063
1.90419E-05 1 .00693651 .993063
2.07989E-05 1 .00693651 .993063
2.26437E-05 1 .00693651 .993063
2.45808E-05 1 .00693651 .993063
2.66147E-05 1 .00693651 .993063
2.87504E-05 1 .00693651 .993063
3.09928E-05 1 .00693651 .993063
3.33473E-05 1 .00693651 .993063
3.58196E-05 1 .00693651 .993063
3.84155E-05 1 .00693651 .993063
4.11411E-05 1 .00693651 .993063
4.40031E-05 1 .00693651 .993063
4.70081E-05 1 .00693651 .993063
5.01634E-05 1 .00693651 .993063
5.34765E-05 1 .00693651 .993063
5.69552E-05 1 .00693651 .993063
6.06079E-05 1 .00693651 .993063
```

6.44432E-05	1	.00693651	.993063
6.84703E-05	1	.00693651	.993063
7.26987E-05	1	.00693651	.993063
7.71385E-05	1	.00693651	.993063
8.18003E-05	1	.00693651	.993063
8.66952E-05	1	.00693651	.993063
9.18349E-05	1	.00693651	.993063
9.72315E-05	1	.00693651	.993063
1.02898E-04	1	.00693651	.993063
1.08848E-04	1	.00693651	.993063
1.15095E-04	1	.00693651	.993063
1.21655E-04	1	.00693651	.993063
1.28542E-04	1	.00693651	.993063
1.35774E-04	1	.00693651	.993063
1.43368E-04	1	.00693651	.993063
1.51341E-04	1	.00693651	.993063
1.59713E-04	1	.00693651	.993063
1.68504E-04	1	.00693651	.993063
1.77734E-04	1	.00693651	.993063
1.87426E-04	1	.00693651	.993063
1.97602E-04	1	.00693651	.993063
2.08287E-04	1	.00693651	.993063
2.19506E-04	1	.00693651	.993063
2.31286E-04	1	.00693651	.993063
2.43655E-04	1	.00693651	.993063
2.56643E-04	1	.00693651	.993063
2.7028E-04	1	.00693651	.993063
2.84599E-04	1	.00693651	.993063
2.99634E-04	1	.00693651	.993063
3.1542E-04	1	.00693651	.993063
3.31996E-04	1	.00693651	.993063
3.49401E-04	1	.00693651	.993063
3.67676E-04	1	.00693651	.993063
3.86865E-04	1	.00693651	.993063
4.07013E-04	1	.00693651	.993063
4.28168E-04	1	.00693651	.993063
4.50382E-04	1	.00693651	.993063
4.73706E-04	1	.00693651	.993063
4.98196E-04	1	.00693651	.993063
5.2391E-04	1	.00693651	.993063
5.50911E-04	1	.00693651	.993063
5.79261E-04	1	.00693651	.993063
6.09029E-04	1	.00693651	.993063
6.40286E-04	1	.00693651	.993063
6.73105E-04	1	.00693651	.993063
7.07565E-04	1	.00693651	.993063
7.43748E-04	1	.00693651	.993063
7.8174E-04	1	.00693651	.993063
8.21632E-04	1	.00693651	.993063
8.63519E-04	1	.00693651	.993063
9.075E-04	1	.00693651	.993063
9.5368E-04	1	.00693651	.993063
.00100217	1	.00693651	.993063
.00105308	1	.00693651	.993063
.00110654	1	.00693651	.993063
.00116267	1	.00693651	.993063
.00122161	1	.00693651	.993063
.0012835	1	.00693651	.993063
.00134848	1	.00693651	.993063
.00141671	1	.00693651	.993063
.00148835	1	.00693651	.993063
.00156357	1	.00693651	.993063
.00164255	1	.00693651	.993063
.00172548	1	.00693651	.993063
.00181256	1	.00693651	.993063
.001904	1	.00693651	.993063
.002	1	.00693651	.993063

INTERFACE AT GLOBAL COORDINATE X = 2.00000E-03

```

DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 1e9
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /10000000/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ IMPLICIT (1) TIME INTEGRATION IS USED INSTEAD OF THE MORE ACCURATE
DIC> @@ (BUT LESS STABLE) TRAPETZOIDAL METHOD WHICH IS THE DEFAULT.
DIC> @@
DIC> set-option DEGREE_OF_IMPLICIT 1.0
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exblb Y
DIC>
DIC> set-inter
--OK--
DIC>

```

exbib-run

DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exbib\run.DCM.test"

DIC>

DIC>

DIC> @@ exbib\_run.DCM

DIC>

DIC> @@

DIC> @@ FILE FOR RUNNING EXAMPLE bib

DIC> @@

DIC>

DIC> @@

DIC> @@ ENTER THE DICTRA MONITOR AND READ THE STORE RESULT FILE

DIC> @@

DIC> go d-m

TIME STEP AT TIME 0.000000E+00

DIC> read exbib

OK

DIC>

DIC> @@

DIC> @@ START THE SIMULATION

DIC> @@

DIC> sim y

INFO: Default responses (if any) will be applied during the simulation. Use "SIMULATE\_REACTION NO" instead for manual input.

U-FRACTION IN SYSTEM: C = .00698495916383108 FE = 1

TOTAL SIZE OF SYSTEM: .002 [m]

U-FRACTION IN SYSTEM: C = .00698495916383108 FE = 1

TOTAL SIZE OF SYSTEM: .002 [m]

1 GRIDPOINT(S) ADDED TO CELL #1 REGION: AUSTENITE

INFO: PHASE BCC\_A2 IS SCHEDULED TO APPEAR

1 GRIDPOINT(S) ADDED TO CELL #1 REGION: AUSTENITE

REGION STATUS CHANGE, ITERATING: TIME= 0.50000000E-07

1 GRIDPOINT(S) ADDED TO CELL #1 REGION: AUSTENITE

REGION STATUS CHANGE, ITERATING: TIME= 0.25000000E-07

TIME = 0.25000000E-07 DT = 0.25000000E-07

U-FRACTION IN SYSTEM: C = .00698495916383108 FE = 1

TOTAL SIZE OF SYSTEM: .002 [m]

MUST SAVE WORKSPACE ON FILE

WORKSPACE SAVED ON FILE

RECLAIMING WORKSPACE

KEEPING TIME-RECORD FOR TIME 0.0000000

AND FOR TIME 0.25000000E-07

WORKSPACE RECLAIMED

Trying old scheme 3

START VALUE(S) FOR INTERFACE #2 R\_BCC\_A2/AUSTENITE, CELL #1

-----  
20 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: AUSTENITE

Trying old scheme 3

U-FRACTION IN SYSTEM: C = .00698156310125388 FE = 1

TOTAL SIZE OF SYSTEM: .002 [m]

U-FRACTION IN SYSTEM: C = .00698156310125388 FE = 1

TOTAL SIZE OF SYSTEM: .002 [m]

1 GRIDPOINT(S) ADDED TO CELL #1 REGION: R\_BCC\_A2

4.848065353536785E-003 4.848091905343611E-003 0.640161288181735 3.043446661679094E-003 4.863748717832611E-

003 5.207814605731493E-003 2.964933799699408E-003 4.124118149768927E-003 2.854849216965825E-

003 2.900580522124421E-003 2.874656387338556E-003 2.860055810344646E-003 2.855270672160098E-

003 2.855476546657522E-003 2.854734016801175E-003 2.854760790301994E-003 2.854774332530540E-

003 2.854727109430693E-003 2.854729190774520E-003 2.854729446829519E-003 2.854726782500090E-

003 2.854727019195424E-003 2.854726875628526E-003 2.854726788763905E-003 2.854726808796026E-003

ERROR RETURN FROM NS01A BECAUSE THERE HAVE BEEN 25 CALLS OF CALFUN

RESCALING

4 GRIDPOINT(S) ADDED TO CELL #1 REGION: R\_BCC\_A2

2.866274113410890E-003 2.866165756161273E-003 7.120621596271988E-003 9.77088982496736E-004 2.455448035442813E-

003 7.629037466095791E-005 7.738742468887819E-005 9.537961602733466E-006 5.350404292657428E-

007 7.494705349070975E-011 8.665068991379627E-016 4.475882884430830E-025 TIME = 0.12500000E-06 DT = 0.10000000E-

06 SUM OF SQUARES = 0.44758829E-24

CELL # 1 VELOCITY AT INTERFACE # 2 IS 20.508379 AND 20.508379

POSITION OF INTERFACE R\_BCC\_A2 / AUSTENITE IS 0.30508379E-05

U-FRACTION IN SYSTEM: C = .00698116131758942 FE = 1

TOTAL SIZE OF SYSTEM: .002 [m]

CPU time used in timestep 1 seconds

8 GRIDPOINT(S) ADDED TO CELL #1 REGION: R\_BCC\_A2

1.622043683846508E-004 1.622367887784417E-004 7.833396504907085E-010 5.412785760911286E-010 6.572998732089805E-

011 4.472325000686400E-013 1.465950470830037E-013 9.643738601951300E-012 4.360979563915932E-

014 1.264297758897139E-011 1.460133055602959E-014 1.431308683654039E-011 5.145413903971377E-

015 1.528994825611976E-011 1.861836721905488E-015 1.587334855613868E-011 6.837235644616751E-016

output ignored...

... output resumed

TOTAL SIZE OF SYSTEM: .002 [m]

7 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: R\_BCC\_A2

CPU time used in timestep 0 seconds

2.605771336599939E-005 2.605874004060590E-005 1.908742751358646E-

017 TIME = 0.66706428E+09 DT = 0.10000000E+09 SUM OF SQUARES = 0.19087428E-16

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.20098632E-15 AND -0.20098632E-15

POSITION OF INTERFACE R\_BCC\_A2 / AUSTENITE IS 0.13798088E-02

U-FRACTION IN SYSTEM: C = .00698226857547703 FE = 1

TOTAL SIZE OF SYSTEM: .002 [m]

1 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: AUSTENITE

CPU time used in timestep 0 seconds

7.133791546665525E-005 7.134470143220694E-005 2.480895576768879E-

022 TIME = 0.76706428E+09 DT = 0.10000000E+09 SUM OF SQUARES = 0.24808956E-21

CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.21716814E-15 AND 0.21716814E-15

POSITION OF INTERFACE R\_BCC\_A2 / AUSTENITE IS 0.13798305E-02

U-FRACTION IN SYSTEM: C = .0069820471208938 FE = 1

TOTAL SIZE OF SYSTEM: .002 [m]

29 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: R\_BCC\_A2

CPU time used in timestep 0 seconds

8.338690001653589E-005 8.339482740199053E-005 1.770087011002676E-

028 TIME = 0.86706428E+09 DT = 0.10000000E+09 SUM OF SQUARES = 0.17700870E-27

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.23491983E-15 AND -0.23491983E-15

POSITION OF INTERFACE R\_BCC\_A2 / AUSTENITE IS 0.13798070E-02  
U-FRACTION IN SYSTEM: C = .00698228667754199 FE = 1  
TOTAL SIZE OF SYSTEM: .002 [m]  
1 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: AUSTENITE

CPU time used in timestep 0 seconds  
5.418843480567073E-005 5.419534772435475E-005 1.129096246098665E-  
027 TIME = 0.96706428E+09 DT = 0.10000000E+09 SUM OF SQUARES = 0.11290962E-26  
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.13071835E-15 AND 0.13071835E-15  
POSITION OF INTERFACE R\_BCC\_A2 / AUSTENITE IS 0.13798201E-02  
U-FRACTION IN SYSTEM: C = .00698215337908559 FE = 1  
TOTAL SIZE OF SYSTEM: .002 [m]  
17 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: R\_BCC\_A2

CPU time used in timestep 0 seconds  
2.073373790420605E-005 2.073611727676384E-005 2.587623169920472E-  
028 TIME = 0.10000000E+10 DT = 32935717. SUM OF SQUARES = 0.25876232E-27  
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.95160811E-16 AND -0.95160811E-16  
POSITION OF INTERFACE R\_BCC\_A2 / AUSTENITE IS 0.13798170E-02  
U-FRACTION IN SYSTEM: C = .00698218533960413 FE = 1  
TOTAL SIZE OF SYSTEM: .002 [m]

MUST SAVE WORKSPACE ON FILE

WORKSPACE SAVED ON FILE

RECLAIMING WORKSPACE

DELETING TIME-RECORD FOR TIME 0.0000000  
DELETING TIME-RECORD FOR TIME 0.25000000E-07  
DELETING TIME-RECORD FOR TIME 0.12500000E-06  
DELETING TIME-RECORD FOR TIME 0.19118010E-04  
DELETING TIME-RECORD FOR TIME 0.57104030E-04  
DELETING TIME-RECORD FOR TIME 0.13307607E-03  
DELETING TIME-RECORD FOR TIME 0.28502015E-03  
DELETING TIME-RECORD FOR TIME 0.58890831E-03  
DELETING TIME-RECORD FOR TIME 0.11966846E-02  
DELETING TIME-RECORD FOR TIME 0.24122373E-02  
DELETING TIME-RECORD FOR TIME 0.48433425E-02  
DELETING TIME-RECORD FOR TIME 0.97055531E-02  
DELETING TIME-RECORD FOR TIME 0.19429974E-01  
DELETING TIME-RECORD FOR TIME 0.38878816E-01  
DELETING TIME-RECORD FOR TIME 0.77776501E-01  
DELETING TIME-RECORD FOR TIME 0.15557187  
DELETING TIME-RECORD FOR TIME 0.31116261  
DELETING TIME-RECORD FOR TIME 0.62234408  
DELETING TIME-RECORD FOR TIME 1.2447070  
DELETING TIME-RECORD FOR TIME 2.4894329  
DELETING TIME-RECORD FOR TIME 4.9788847  
DELETING TIME-RECORD FOR TIME 9.9577884  
DELETING TIME-RECORD FOR TIME 19.915596  
DELETING TIME-RECORD FOR TIME 39.831210  
DELETING TIME-RECORD FOR TIME 79.662439  
DELETING TIME-RECORD FOR TIME 159.32490  
DELETING TIME-RECORD FOR TIME 318.64981  
DELETING TIME-RECORD FOR TIME 637.29964  
DELETING TIME-RECORD FOR TIME 1274.5993  
DELETING TIME-RECORD FOR TIME 2549.1986  
DELETING TIME-RECORD FOR TIME 5098.3973  
DELETING TIME-RECORD FOR TIME 10196.795  
DELETING TIME-RECORD FOR TIME 20393.589  
DELETING TIME-RECORD FOR TIME 40787.178  
DELETING TIME-RECORD FOR TIME 81574.357  
DELETING TIME-RECORD FOR TIME 163148.71  
DELETING TIME-RECORD FOR TIME 326297.43  
DELETING TIME-RECORD FOR TIME 652594.85  
DELETING TIME-RECORD FOR TIME 1305189.7  
DELETING TIME-RECORD FOR TIME 2610379.4  
DELETING TIME-RECORD FOR TIME 5220758.8  
DELETING TIME-RECORD FOR TIME 10441518.  
DELETING TIME-RECORD FOR TIME 20883035.  
DELETING TIME-RECORD FOR TIME 41766071.  
DELETING TIME-RECORD FOR TIME 83532141.  
DELETING TIME-RECORD FOR TIME 0.16706428E+09  
DELETING TIME-RECORD FOR TIME 0.26706428E+09  
DELETING TIME-RECORD FOR TIME 0.36706428E+09  
DELETING TIME-RECORD FOR TIME 0.46706428E+09  
DELETING TIME-RECORD FOR TIME 0.56706428E+09  
DELETING TIME-RECORD FOR TIME 0.66706428E+09  
DELETING TIME-RECORD FOR TIME 0.76706428E+09  
DELETING TIME-RECORD FOR TIME 0.86706428E+09

KEEPING TIME-RECORD FOR TIME 0.96706428E+09  
AND FOR TIME 0.10000000E+10  
WORKSPACE RECLAIMED

TIMESTEP AT 0.10000000E+10 SELECTED

DIC>

DIC>

DIC>

DIC>

DIC>

DIC> @@

DIC> @@ THE SIMULATION IS FINISHED

DIC> @@

DIC>

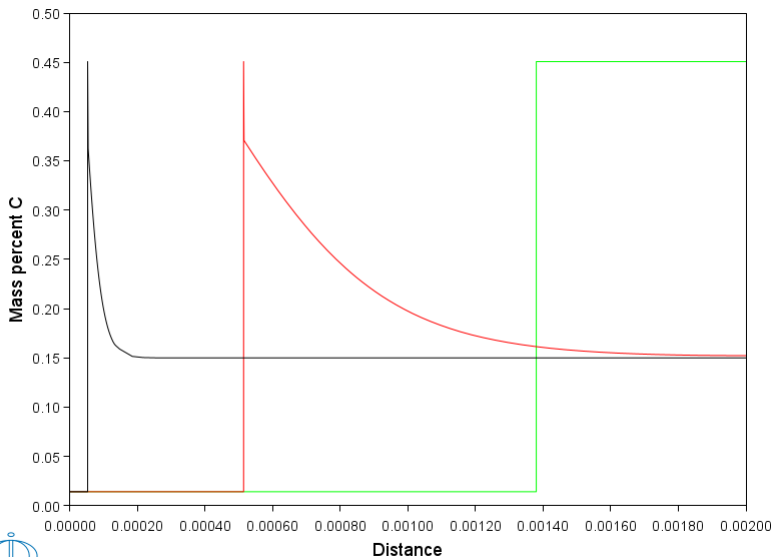
DIC> set-inter

--OK--

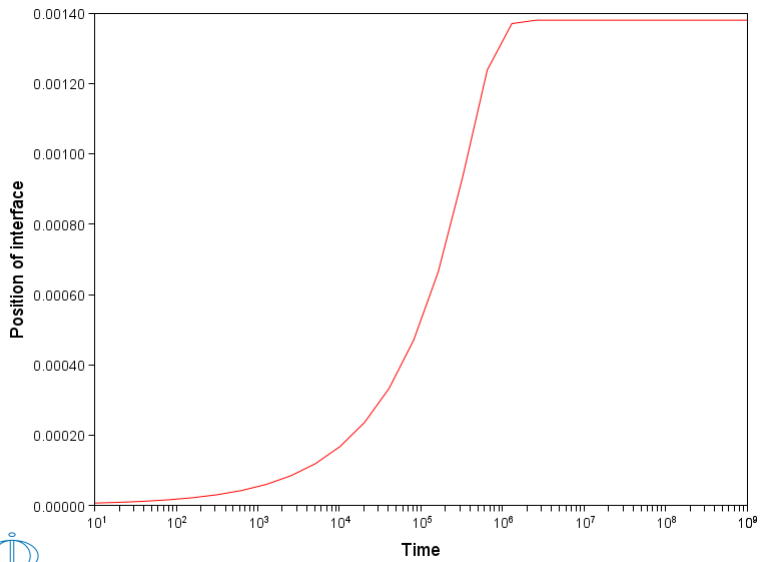
DIC>

## exbib-plot

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exbib\plot.DCM.test"
DIC>
DIC>
DIC> @@ exbib_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE blb
DIC> @@
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 1.00000E+09
DIC> read exbib
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1:
POST-1: @@
POST-1: @@ PLOT THE CARBON CONCENTRATIONS AT DIFFERENT TIMES
POST-1: @@
POST-1: s-d-a y w-p c
POST-1: s-d-a x dist glob
INFO: Distance is set as independent variable
POST-1: s-p-c time 1e3,1e5,1e9
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

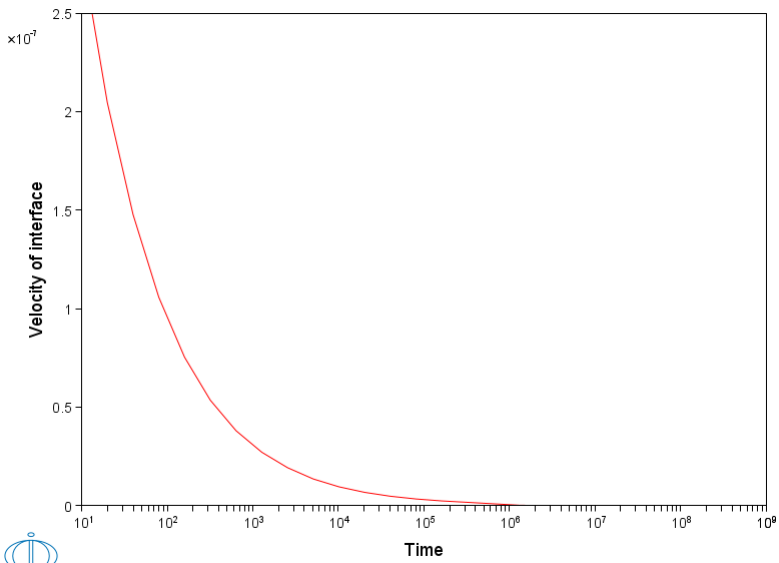


```
POST-1:
POST-1:
POST-1: Hit RETURN to continue
POST-1:
POST-1: sel-plot new
POST-1:
POST-1: @@
POST-1: @@ PLOT THE POSITION OF THE BCC/FCC INTERPHASE
POST-1: @@
POST-1: s-d-a x time
INFO: Time is set as independent variable
POST-1: s-d-a y
VARIABLE : pos
INTERFACE : aus
UPPER OR LOWER INTERFACE OF REGION AUSTENITE#1 /LOWER/: lower
POST-1:
POST-1: set_axis_type
AXIS (X, Y OR Z) : x
AXIS TYPE /LINEAR/: log
POST-1:
POST-1: s-s-s
AXIS (X, Y OR Z) : x
AUTOMATIC SCALING (Y OR N) /N/: n
MIN VALUE : 10
MAX VALUE : 1e9
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
WORKING ...
WORKING ... OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```



```

POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: sel-plot new
POST-1:
POST-1: @@
POST-1: @@ PLOT THE VELOCITY OF THE BCC/FCC INTERPHASE
POST-1: @@
POST-1: s-d-a
AXIS (X, Y OR Z) : y
VARIABLE : velocity
INTERFACE : aus
UPPER OR LOWER INTERFACE OF REGION AUSTENITE#1 /LOWER/: lower
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
WORKING ...
WORKING ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
  
```



```

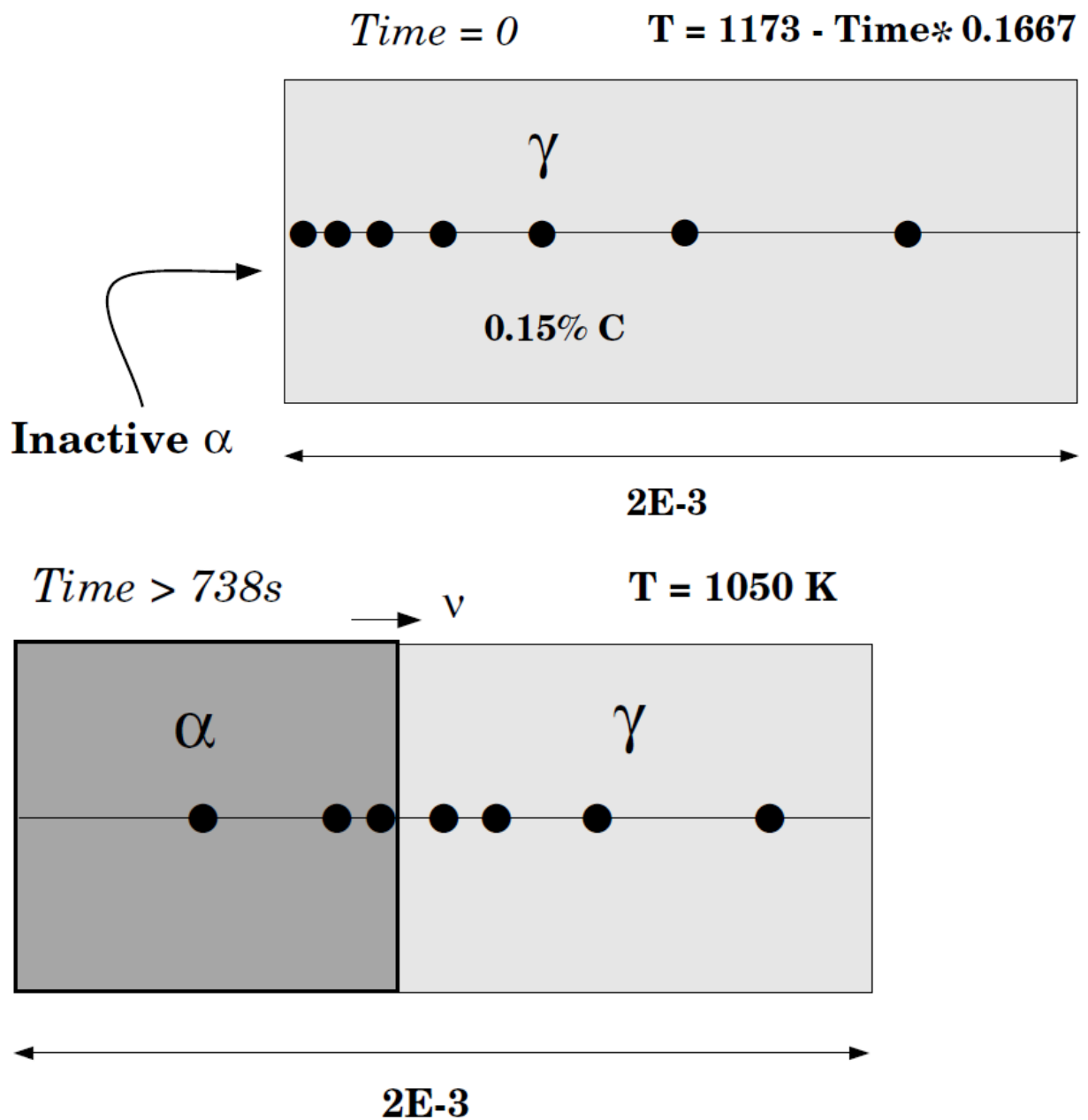
POST-1:
POST-1:
POST-1:
POST-1:
POST-1: set-inter
--OK--
POST-1:
  
```



## Example exb1c

### $\gamma$ to $\alpha$ transformation in a binary Fe-C alloy: Gradual cool down to 1050 K

This is the same example as in exb1a and exb1b but now the simulation starts at a higher temperature and assumes a gradual cooling down to 1050 K. When 1050 K is reached, the temperature is kept constant and thus has an isothermal transformation. As in exb1b, ferrite is in an inactive phase adjacent to the initial austenite.



## exblc-setup

### SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,  
Stockholm, Sweden

Software running on Windows 64-bit wordlength  
Compiler: Intel Fortran Compiler 2025.0.0  
License library version: 9.7.0.0036  
Linked: Nov 19 2025 at 14:44:36

```
SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exblc\setup.DCM.test"
```

```
SYS: @@
SYS: @@ Moving boundary problem.
SYS: @@ Austenite to ferrite transformation in a binary Fe-C alloy
SYS: @@ This is the same example as in exbla and exblb but now the
SYS: @@ simulation starts at a higher temperature and assumes a gradual cooling
SYS: @@ down to 1050 K.
SYS: @@
SYS: @@ When 1050 K is reached, the temperature is kept constant and thus has an
SYS: @@ isothermal transformation. As in exblb ferrite is an inactive
SYS: @@ phase adjacent to the initial austenite.
SYS: @@-----
SYS:
SYS: @@ exblc_setup.DCM
SYS:
SYS: @@
SYS: @@ START BY GOING TO THE DATABASE MODULE
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\databases\da
ta
Current database: Steels/Fe-Alloys v12.0

VA          /-  DEFINED
DICTRA FCC_A1 REJECTED
TDB_TCFE12:
TDB_TCFE12: @@
TDB_TCFE12: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA
TDB_TCFE12: @@
TDB_TCFE12: sw FEDEMO
Current database: Iron Demo Database v6.0

VA          /-  DEFINED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ DEFINE THE SYSTEM TO WORK WITH
TDB_FEDEMO: @@
TDB_FEDEMO: def-sys fe c
FE          C  DEFINED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ EXCLUDE THE THERMODYNAMIC DATA FOR THE PHASES THAT ARE NOT NEEDED
TDB_FEDEMO: @@
TDB_FEDEMO: rej ph * all
GAS:G      LIQUID:L          BCC_A2
C14_LAVES  CBCC_A12         CEMENTITE_D011
CUB_A13    DIAMOND_A4       FCC_A1
GRAPHITE_A9 HCP_A3            KSI_CARBIIDE
M23C6_D84  M5C2            M7C3_D101
REJECTED
TDB_FEDEMO: res ph fcc bcc
FCC_A1     BCC_A2  RESTORED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ RETRIEVE DATA FROM THE DATABASE FILE
TDB_FEDEMO: @@
TDB_FEDEMO: get
09:10:00,934 [Thread-0] INFO  JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

Use the command LIST_REFERENCES to see the list of references for assessed data
-OK-
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ MOBILITY/DIFFUSIVITY DATA ARE STORED IN A SEPARATE DATABASE FILE.
TDB_FEDEMO: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE DATA
TDB_FEDEMO: @@
TDB_FEDEMO: app
Use one of these databases

TCFE12 = Steels/Fe-Alloys v12.0
TCFE9  = Steels/Fe-Alloys v9.3
SSUB6  = SGTE Substances v6.0
FEDEMO = Iron Demo Database v6.0
MOB2   = Alloys Mobility v2.7
MOBFE7 = Steels/Fe-Alloys Mobility v7.1
MOBFE4 = Steels/Fe-Alloys Mobility v4.0
MOBFE2 = Steels/Fe-Alloys Mobility v2.0
MFEDEMO = Fe-Alloys Mobility demo database v5.0
USER    = User defined Database

DATABASE NAME /FEDEMO/: MFEDEMO
Current database: Fe-Alloys Mobility demo database v5.0

VA  DEFINED
APP: def-sys fe c
FE          C  DEFINED
APP: rej ph * all
```

```
BCC_A2          FCC_A1          CEMENTITE_D011
LIQUID:L REJECTED
APP: res ph fcc bcc
FCC_A1          BCC_A2  RESTORED
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS .....
```

Use the command LIST\_REFERENCES to see the list of references for assessed data

-OK-

```
APP: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP
APP: @@
APP: go d-m
NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER GLOBAL CONDITION T
DIC> @@
DIC> @@ ASSUME THAT THE COOLING RATE IS 10K/MINUTE DOWN TO 1050K
DIC> @@
DIC> set-cond
GLOBAL OR BOUNDARY CONDITION /GLOBAL/: glob
VARIABLE : T
LOW TIME LIMIT /0/: 0
T(TIME,X)= 1173-time*0.1667;
HIGH TIME LIMIT /*/: 738
ANY MORE RANGES /N/: y
T(TIME,X)= 1050;
HIGH TIME LIMIT /*/: *
ANY MORE RANGES /N/: N
DIC>
DIC> @@
DIC> @@ START BY ENTERING THE REGION austenite WHERE WE PUT THE fcc PHASE
DIC> @@
DIC> enter-region
REGION NAME : austenite
DIC>
DIC> @@
DIC> @@ ENTER THE GRID INTO THE REGION
DIC> @@
DIC> enter-grid
REGION NAME : /AUSTENITE/: austenite
WIDTH OF REGION /1/: 20e-4
TYPE /AUTO/: AUTO
DIC>
DIC> @@
DIC> @@ ENTER THE active PHASES INTO THE REGIONS
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /AUSTENITE/: austenite
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC> @@
DIC> @@ ENTER THE inactive PHASES INTO THE REGIONS
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inact
ATTACH TO REGION NAMED /AUSTENITE/: austenite
ATTACHED TO THE RIGHT OF AUSTENITE /YES/: no
PHASE NAME: /NONE/: bcc
REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-5
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITION FOR FCC
DIC> @@
DIC> enter-composition
REGION NAME : /AUSTENITE/: austenite
PHASE NAME: /FCC_A1/: fcc#1
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: C
TYPE /LINEAR/: lin
VALUE OF FIRST POINT : 0.15
VALUE OF LAST POINT : /0.15/: 0.15
DIC>
DIC> @@
DIC> @@ THE BOUNDARY CONDITION IS A CLOSED SYSTEM AS WE DO NOT SPECIFY
DIC> @@ ANYTHING ELSE.
DIC> @@
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 738
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /73.8/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC> @@
DIC> @@ IMPLICIT (1) TIME INTEGRATION IS USED INSTEAD OF THE MORE ACCURATE
DIC> @@ (BUT LESS STABLE) TRAPETZOIDAL METHOD WHICH IS THE DEFAULT.
DIC> @@
DIC> set-option DEGREE_OF_IMPLICITY 1.0
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exblc Y
DIC>
```

```
DIC> set-inter  
--OK--  
DIC>
```

exb1c-run

DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exb1c\run.DCM.test"

DIC>

DIC>

DIC> @@ exb1c\_run.DCM

DIC>

DIC> @@

DIC> @@ FILE FOR RUNNING EXAMPLE exb1c

DIC> @@

DIC> go d-m

TIME STEP AT TIME 0.00000E+00

DIC> read exb1c

OK

DIC>

DIC> @@

DIC> @@ START THE SIMULATION

DIC> @@

DIC> sim

INFO: Default responses (if any) will be applied during the simulation. Use "SIMULATE\_REACTION NO" instead for manual input.

Region: AUSTENITE

geometric 1.20000 dense at 0.00000 57 points

U-FRACTION IN SYSTEM: C = .00698495916383109 FE = 1

TOTAL SIZE OF SYSTEM: .002 [m]

U-FRACTION IN SYSTEM: C = .00698495916383109 FE = 1

TOTAL SIZE OF SYSTEM: .002 [m]

TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00698495916383109 FE = 1

TOTAL SIZE OF SYSTEM: .002 [m]

CPU time used in timestep 0 seconds

TIME = 0.10010000E-03 DT = 0.10000000E-03 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00698495916383108 FE = 1

TOTAL SIZE OF SYSTEM: .002 [m]

CPU time used in timestep 0 seconds

TIME = 1.7794466 DT = 1.7793465 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00698495916383108 FE = 1

TOTAL SIZE OF SYSTEM: .002 [m]

CPU time used in timestep 0 seconds

TIME = 5.3381396 DT = 3.5586930 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00698495916383108 FE = 1

TOTAL SIZE OF SYSTEM: .002 [m]

CPU time used in timestep 0 seconds

TIME = 12.455526 DT = 7.1173861 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00698495916383109 FE = 1

TOTAL SIZE OF SYSTEM: .002 [m]

CPU time used in timestep 0 seconds

TIME = 26.690298 DT = 14.234772 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00698495916383109 FE = 1

TOTAL SIZE OF SYSTEM: .002 [m]

CPU time used in timestep 0 seconds

TIME = 55.159842 DT = 28.469544 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00698495916383109 FE = 1

TOTAL SIZE OF SYSTEM: .002 [m]

CPU time used in timestep 0 seconds

TIME = 92.059842 DT = 36.900000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00698495916383108 FE = 1

TOTAL SIZE OF SYSTEM: .002 [m]

CPU time used in timestep 0 seconds

TIME = 128.95984 DT = 36.900000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00698495916383109 FE = 1

TOTAL SIZE OF SYSTEM: .002 [m]

CPU time used in timestep 0 seconds

TIME = 165.85984 DT = 36.900000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00698495916383109 FE = 1

TOTAL SIZE OF SYSTEM: .002 [m]

CPU time used in timestep 0 seconds

TIME = 202.75984 DT = 36.900000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00698495916383109 FE = 1

TOTAL SIZE OF SYSTEM: .002 [m]

CPU time used in timestep 0 seconds

TIME = 239.65984 DT = 36.900000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00698495916383109 FE = 1

TOTAL SIZE OF SYSTEM: .002 [m]

CPU time used in timestep 0 seconds

TIME = 276.55984 DT = 36.900000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00698495916383109 FE = 1

TOTAL SIZE OF SYSTEM: .002 [m]

CPU time used in timestep 0 seconds

INFO: PHASE BCC\_A2 IS SCHEDULED TO APPEAR

INFO: BACKTRACING WITH SMALLER TIMESTEP 9.2250

TIME = 285.78484 DT = 9.2250000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00698495916383109 FE = 1

TOTAL SIZE OF SYSTEM: .002 [m]

CPU time used in timestep 0 seconds

INFO: PHASE BCC\_A2 IS SCHEDULED TO APPEAR

REGION STATUS CHANGE, ITERATING: TIME= 295.00984

REGION STATUS CHANGE, ITERATING: TIME= 290.39734

REGION STATUS CHANGE, ITERATING: TIME= 288.09109

REGION STATUS CHANGE, ITERATING: TIME= 289.24422

REGION STATUS CHANGE, ITERATING: TIME= 288.66765

REGION STATUS CHANGE, ITERATING: TIME= 288.95594

REGION STATUS CHANGE, ITERATING: TIME= 288.81180

REGION STATUS CHANGE, ITERATING: TIME= 288.73972

REGION STATUS CHANGE, ITERATING: TIME= 288.77576

REGION STATUS CHANGE, ITERATING: TIME= 288.75774

REGION STATUS CHANGE, ITERATING: TIME= 288.74873

REGION STATUS CHANGE, ITERATING: TIME= 288.75324

TIME = 288.75324 DT = 2.9683960

U-FRACTION IN SYSTEM: C = .00698495916383109 FE = 1

TOTAL SIZE OF SYSTEM: .002 [m]

MUST SAVE WORKSPACE ON FILE

WORKSPACE SAVED ON FILE

RECLAIMING WORKSPACE

DELETING TIME-RECORD FOR TIME 0.0000000

DELETING TIME-RECORD FOR TIME 0.10000000E-06

DELETING TIME-RECORD FOR TIME 0.10010000E-03

DELETING TIME-RECORD FOR TIME 1.7794466

DELETING TIME-RECORD FOR TIME 5.3381396

DELETING TIME-RECORD FOR TIME 12.455526

DELETING TIME-RECORD FOR TIME 26.690298

DELETING TIME-RECORD FOR TIME 55.159842

DELETING TIME-RECORD FOR TIME 92.059842

```
DELETING TIME-RECORD FOR TIME 128.95984
DELETING TIME-RECORD FOR TIME 165.85984
DELETING TIME-RECORD FOR TIME 202.75984
DELETING TIME-RECORD FOR TIME 239.65984
DELETING TIME-RECORD FOR TIME 276.55984

KEEPING TIME-RECORD FOR TIME 285.78484
AND FOR TIME 288.75324
WORKSPACE RECLAIMED
Trying old scheme 3
START VALUE(S) FOR INTERFACE #2 R_BCC_A2/AUSTENITE, CELL #1
-----
Trying old scheme 3
U-FRACTION IN SYSTEM: C = .0069816240380179 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
U-FRACTION IN SYSTEM: C = .0069816240380179 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
1 GRIDPOINT(S) ADDED TO CELL #1 REGION: R_BCC_A2
```

output ignored...

... output resumed

```
TIME = 0.44276225E+09 DT = 0.10000000E+09 SUM OF SQUARES = 0.54017547E-21
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.38762941E-16 AND 0.38762941E-16
POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS 0.13786592E-02
U-FRACTION IN SYSTEM: C = .00699399188702824 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
1 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: R_BCC_A2

CPU time used in timestep 0 seconds
1.403407489400562E-004 1.403591057696059E-004 4.346038603478281E-
017 TIME = 0.54276225E+09 DT = 0.10000000E+09 SUM OF SQUARES = 0.43460386E-16
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.20098536E-16 AND -0.20098536E-16
POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS 0.13786572E-02
U-FRACTION IN SYSTEM: C = .00699401238226739 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
1 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: AUSTENITE

CPU time used in timestep 0 seconds
9.017858690391845E-006 9.020271482103977E-006 1.248071023428739E-
020 TIME = 0.64276225E+09 DT = 0.10000000E+09 SUM OF SQUARES = 0.12480710E-19
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.49723170E-17 AND -0.49723170E-17
POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS 0.13786567E-02
U-FRACTION IN SYSTEM: C = .00699401745272732 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
1 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: AUSTENITE

CPU time used in timestep 0 seconds
4.341532094479382E-005 4.341663060354274E-005 9.820511580670602E-
019 TIME = 0.74276225E+09 DT = 0.10000000E+09 SUM OF SQUARES = 0.98205116E-18
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.27434605E-16 AND 0.27434605E-16
POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS 0.13786594E-02
U-FRACTION IN SYSTEM: C = .00699399894766214 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
1 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: R_BCC_A2

CPU time used in timestep 0 seconds
5.229084408867828E-005 5.229877462615132E-005 2.006819806129132E-
025 TIME = 0.84276225E+09 DT = 0.10000000E+09 SUM OF SQUARES = 0.20068198E-24
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.85704577E-17 AND -0.85704577E-17
POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS 0.13786585E-02
U-FRACTION IN SYSTEM: C = .00699399821624293 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
1 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: AUSTENITE

CPU time used in timestep 0 seconds
1.959794758807766E-005 1.959643097242937E-005 6.675784762387637E-
029 TIME = 0.94276225E+09 DT = 0.10000000E+09 SUM OF SQUARES = 0.66757848E-28
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.30105396E-16 AND -0.30105396E-16
POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS 0.13786555E-02
U-FRACTION IN SYSTEM: C = .00699402891585532 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
1 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: AUSTENITE

CPU time used in timestep 0 seconds
2.362913132365089E-004 2.363098123700666E-004 2.781799323798323E-
018 TIME = 0.10000000E+10 DT = 57237752. SUM OF SQUARES = 0.27817993E-17
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.45867886E-16 AND 0.45867886E-16
POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS 0.13786582E-02
U-FRACTION IN SYSTEM: C = .00699400214391535 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 738.00000
DELETING TIME-RECORD FOR TIME 755.01850
DELETING TIME-RECORD FOR TIME 789.05550
DELETING TIME-RECORD FOR TIME 857.12950
DELETING TIME-RECORD FOR TIME 993.27750
DELETING TIME-RECORD FOR TIME 1265.5735
DELETING TIME-RECORD FOR TIME 1810.1655
DELETING TIME-RECORD FOR TIME 2899.3495
DELETING TIME-RECORD FOR TIME 5077.7175
DELETING TIME-RECORD FOR TIME 9434.4536
DELETING TIME-RECORD FOR TIME 18147.926
DELETING TIME-RECORD FOR TIME 35574.870
DELETING TIME-RECORD FOR TIME 70428.758
DELETING TIME-RECORD FOR TIME 140136.53
DELETING TIME-RECORD FOR TIME 279552.09
DELETING TIME-RECORD FOR TIME 558383.19
DELETING TIME-RECORD FOR TIME 1116045.4
DELETING TIME-RECORD FOR TIME 2231369.8
DELETING TIME-RECORD FOR TIME 4462018.7
DELETING TIME-RECORD FOR TIME 8923316.4
DELETING TIME-RECORD FOR TIME 17845912.
DELETING TIME-RECORD FOR TIME 35691103.
DELETING TIME-RECORD FOR TIME 71381484.
DELETING TIME-RECORD FOR TIME 0.14276225E+09
DELETING TIME-RECORD FOR TIME 0.24276225E+09
DELETING TIME-RECORD FOR TIME 0.34276225E+09
DELETING TIME-RECORD FOR TIME 0.44276225E+09
DELETING TIME-RECORD FOR TIME 0.54276225E+09
```

DELETING TIME-RECORD FOR TIME 0.64276225E+09  
DELETING TIME-RECORD FOR TIME 0.74276225E+09  
DELETING TIME-RECORD FOR TIME 0.84276225E+09

KEEPING TIME-RECORD FOR TIME 0.94276225E+09  
AND FOR TIME 0.10000000E+10  
WORKSPACE RECLAIMED

TIMESTEP AT 0.10000000E+10 SELECTED

DIC>

DIC>

DIC>

DIC>

DIC>

DIC>

DIC> @@

DIC> @@ THE SIMULATION IS FINISHED

DIC> @@

DIC>

DIC> set-inter

--OK--

DIC>

## exb1c-plot

DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exb1c\plot.DCM.test"

DIC>

DIC>

DIC> @@ exb1c\_plot.DCM

DIC>

DIC> @@

DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE b1c

DIC> @@

DIC>

DIC> @@

DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE

DIC> @@

DIC> go d-m

TIME STEP AT TIME 1.00000E+09

DIC> read exb1c

OK

DIC>

DIC> @@

DIC> @@ GO TO THE POST PROCESSOR

DIC> @@

DIC> post

POST PROCESSOR VERSION 1.7

Implemented by Bjorn Jonsson

POST-1:

POST-1:

POST-1: @@

POST-1: @@ PLOT TEMPERATURE VS. TIME

POST-1: @@

POST-1: s-d-a y t

POST-1: s-d-a x time

INFO: Time is set as independent variable

POST-1: s-p-c

CONDITION /TIME/: interface

INTERFACE : austenite

UPPER OR LOWER INTERFACE OF REGION AUSTENITE#1 /LOWER/: lower

POST-1: s-s-s x n 0 1000

POST-1:

POST-1:

POST-1: SET\_EXP\_FILE\_FORMAT 5

POST-1: MAKE c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\unite\distribution\macroResult.exp Y

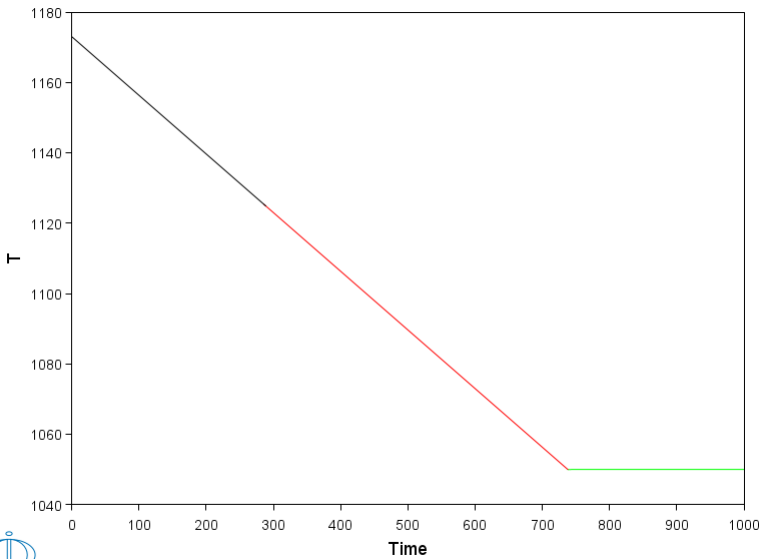
WORKING ...

WORKING ...

OST-1: SET\_EXP\_FILE\_FORMAT 10

POST-1:

POST-1: plot



POST-1:

POST-1:

POST-1:

POST-1:

POST-1: @?<Hit\_return\_to\_continue>

POST-1:

POST-1: @@

POST-1: @@ PLOT VS. LOG TIME

POST-1: @@

POST-1: set-axis-type x log

POST-1: s-s-s x n 10 1e9

POST-1:

POST-1:

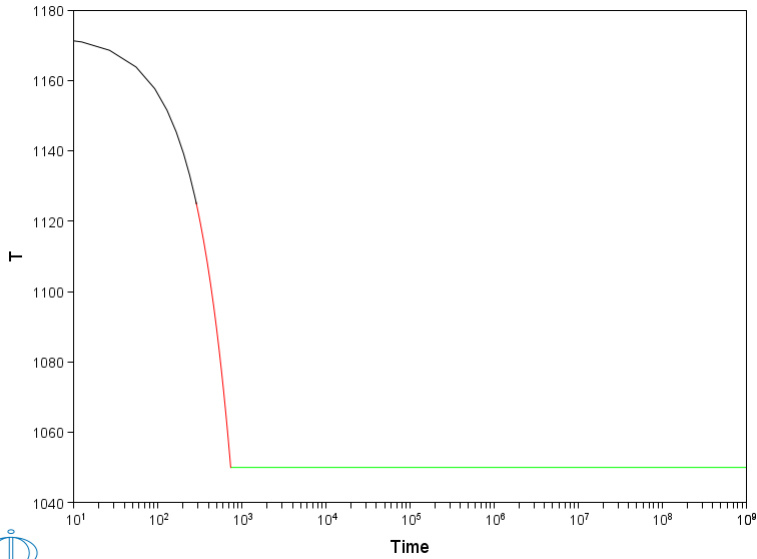
POST-1: SET\_EXP\_FILE\_FORMAT 5

POST-1: MAKE c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\unite\distribution\macroResult.exp Y

POST-1: SET\_EXP\_FILE\_FORMAT 10

POST-1:

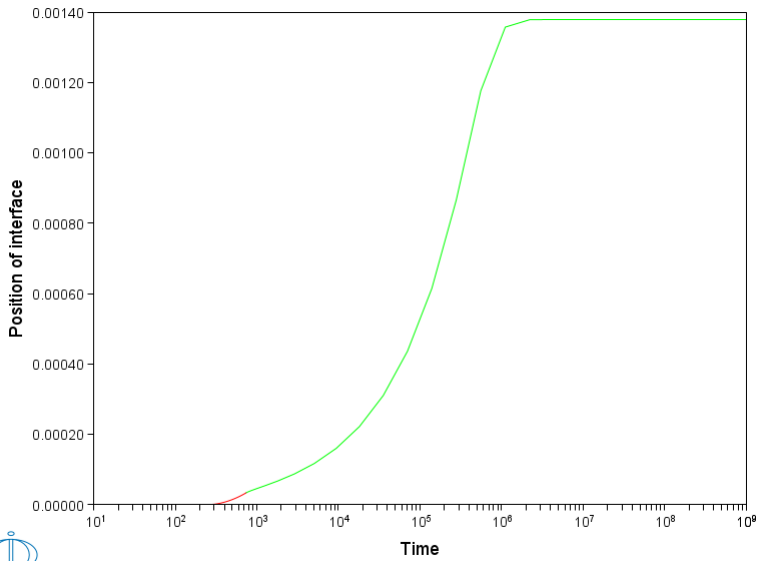
POST-1: plot



```

POST-1:
POST-1:
POST-1:
POST-1: @?<Hit_return_to_continue>
POST-1:
POST-1: @@
POST-1: @@ PLOT THE POSITION OF THE BCC/FCC INTERPHASE
POST-1: @@
POST-1: s-d-a
AXIS (X, Y OR Z) : y
VARIABLE : position
INTERFACE : austenite
UPPER OR LOWER INTERFACE OF REGION AUSTENITE#1 /LOWER/: lower
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
WORKING ...
WORKING ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

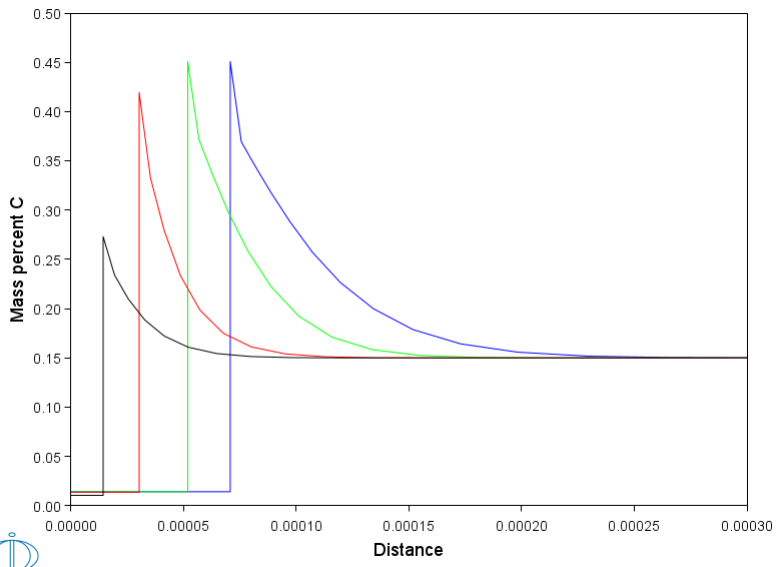
```



```

POST-1:
POST-1:
POST-1:
POST-1: @?<Hit_return_to_continue>
POST-1:
POST-1: @@
POST-1: @@ PLOT THE CARBON CONCENTRATION VS. DISTANCE
POST-1: @@
POST-1: s-d-a y w-p c
POST-1: s-d-a x dis glob
INFO: Distance is set as independent variable
POST-1: s-p-c time 500,700,1200,2000
POST-1: set-axis-type x lin
POST-1: s-s-s x n 0 3e-4
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
WORKING ...OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

```



```

POST-1:
POST-1:
POST-1:
POST-1:
POST-1:??<Hit_return_to_continue>
POST-1: set-inter
--OK--
POST-1:

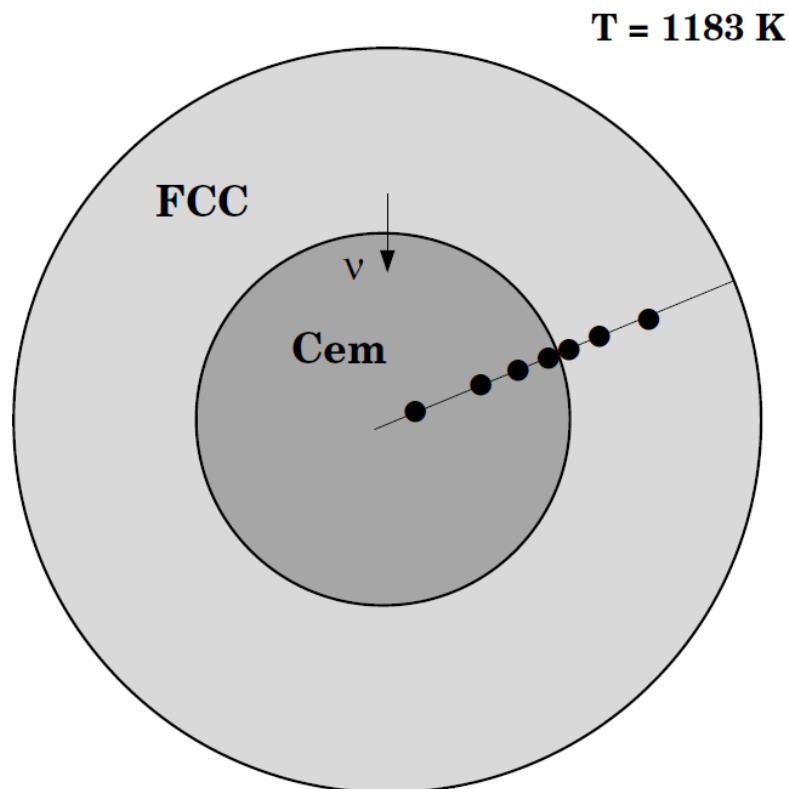
```



## Example exb2

### Cementite dissolution in an Fe-Cr-C alloy

This example calculates 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 (Metall. Trans.A, 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 is set up 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.



## exb2-setup

### SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,  
Stockholm, Sweden

Software running on Windows 64-bit wordlength  
Compiler: Intel Fortran Compiler 2025.0.0  
License library version: 9.7.0.0036  
Linked: Nov 19 2025 at 14:44:36

```
SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exb2\setup.DCM.test"
```

```
SYS: @@
SYS: @@ Moving boundary problem.
SYS: @@ Cementite dissolution in an Fe-Cr-C alloy
SYS: @@ This example calculates the dissolution of a spherical cementite
SYS: @@ particle in an austenite matrix.
SYS: @@ This case is from Z.-K. Liu, L. Högglund, B. Jönsson and J. Ågren:
SYS: @@ Metall. Trans.A, v.22A (1991), pp. 1745-1752.
SYS: @-----
SYS: @@
SYS: @@ In order to achieve the correct average composition in the calculation
SYS: @@ it is necessary to take into account that the calculation is set up
SYS: @@ using the volume fraction of the phases. To calculate the initial
SYS: @@ state at the heat treatment temperature we first need to determine
SYS: @@ the state at the normalizing temperature. To calculate the volume
SYS: @@ fraction of the phases we need to enter a number of functions
SYS: @@ that calculate these quantities. NOTE: The volume fractions are
SYS: @@ determined by assuming that only the substitutional components
SYS: @@ contribute to the volume of a system, whereas the interstitial
SYS: @@ components do not.
SYS: @@
SYS: @@ The total radius of the system can be calculated from the relation:
SYS: @@
SYS: @@      3
SYS: @@      R      V
SYS: @@      cem      cem      f
SYS: @@      ---- = ---- = V
SYS: @@      3      cem
SYS: @@      R      V
SYS: @@      tot      tot
SYS: @@
SYS: @@
SYS: @@
SYS: SET_GES_VERSION
USE GES VERSION 5 OR 6 /6/: 5
SYS: @@ RETRIEVE DATA FROM THE DATABASES
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\databases\da
ta
Current database: Steels/Fe-Alloys v12.0

VA      /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE12:
TDB_TCFE12: @@
TDB_TCFE12: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE THE DATA
TDB_TCFE12: @@
TDB_TCFE12: sw FEDEMO
Current database: Iron Demo Database v6.0

VA      /- DEFINED
TDB_FEDEMO: def-sys fe cr c
FE      CR      C
DEFINED
TDB_FEDEMO: rej ph * all
GAS:G      LIQUID:L      BCC_A2
C14 LAVES      CBCC_A12      CEMENTITE_D011
CHI_A12      CUB_A13      DIAMOND_A4
FCC_A1      GRAPHITE_A9      HCP_A3
KSI CARBIDE      M23C6_D84      M3C2_D510
M5C2      M7C3_D101      SIGMA_D8B
REJECTED
TDB_FEDEMO: res ph fcc bcc cem
FCC_A1      BCC_A2      CEMENTITE_D011
RESTORED
TDB_FEDEMO: get
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
Creating a new composition set FCC_A1#2
PARAMETERS ...
FUNCTIONS ....

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE THE MOBILITY DATA
TDB_FEDEMO: @@
TDB_FEDEMO: app mfedemo
Current database: Fe-Alloys Mobility demo database v5.0

VA DEFINED
APP: def-sys fe cr c
FE      CR      C
DEFINED
APP: rej ph * all
BCC_A2      FCC_A1      CEMENTITE_D011
LIQUID:L REJECTED
APP: res ph fcc cementite
FCC_A1      CEMENTITE_D011 RESTORED
```

```

APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
Creating a new composition set FCC_A1#3
PARAMETERS ...
FUNCTIONS .....

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-
APP:
APP: @@
APP: @@ ENTER THE POLY-3 MONITOR
APP: @@
APP: go p-3

POLY version 3.32
POLY:
POLY: @@
POLY: @@ SET THE CONDITIONS AT THE NORMALIZING TEMPERATURE
POLY: @@
POLY: set-cond T=1008,P=101325,N=1
POLY: set-cond X(CR)=0.0206,X(C)=0.0391
POLY:
POLY: @@
POLY: @@ ENTER FUNCTIONS TO DETERMINE THE VOLUME-FRACTIONS
POLY: @@
POLY: @@ Radius of the cementite particle
POLY: ent-symb var rcem=0.5255e-6;
POLY:
POLY: @@ total number of moles of substitutional components
POLY: ent-symb func nstot=n(fe)+n(cr);
POLY:
POLY: @@ number of moles of substitutional components in cementite
POLY: ent-symb func nscem=n(cem,fe)+n(cem,cr);
POLY:
POLY: @@ volume fraction (U-fraction) of cementite
POLY: ent-symb func vfcem=nscem/nstot;
POLY:
POLY: @@ total radius of the system
POLY: ent-symb func rtot=rcem/vfcem**(1/3);
POLY:
POLY: @@ radius of the surrounding austenite matrix
POLY: ent-symb func rmat=rtot-rcem;
POLY:
POLY:
POLY: @@
POLY: @@ COMPUTE THE EQUILIBRIUM
POLY: @@
POLY: compute-eq
Using global minimization procedure
Calculated 4113 grid points in 0.019 s
Found the set of lowest grid points in 0.001 s
Calculated solution in 0.012 s using 2 iterations. Total time 0.032 s
POLY:
POLY:
POLY: @@
POLY: @@ SHOW THE COMPUTED VALUES TO BE USED IN THE DICTRA CALCULATION
POLY: @@
POLY: show rmat
RMT=5.3924863E-7
POLY: show w(cem,cr),w(bcc,cr),w(bcc,c)
W(CEMENTITE_D011,CR)=0.12581645
W(BCC_A2,CR)=4.4332285E-3
W(BCC_A2,C)=1.5102149E-4
POLY:
POLY: ent var wmatcr=w(bcc,cr);
POLY: ent var wmatc=w(bcc,c);
POLY: ent var wcemcr=w(cem,cr);
POLY:
POLY:
POLY: @@
POLY: @@ ENTER THE DICTRA MONITOR
POLY: @@
POLY: go d-m
NO TIME STEP DEFINED
*** ENTERING BCC_A2 AS A DIFFUSION NONE PHASE
DIC>
DIC> @@
DIC> @@ ENTER GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob t 0 1183; * n
DIC>
DIC> @@
DIC> @@ ENTER THE REGIONS carb AND aus
DIC> @@
DIC> enter-region
REGION NAME : carb
DIC>
DIC> enter-region
REGION NAME : aus
ATTACH TO REGION NAMED /CARB/:
ATTACHED TO THE RIGHT OF CARB /YES/:
DIC> @@
DIC> @@ ENTER GEOMETRICAL GRIDS INTO THE REGIONS
DIC> @@
DIC>
DIC> @@
DIC> @@ THE INITIAL SIZE OF THE CEMENTITE PARTICLE IS ASSUMED TO BE KNOWN
DIC> @@ (IN THIS CASE THE VALUE IS TAKEN FROM LIU ET AL. WHO ESTIMATED THE
DIC> @@ AVERAGE INITIAL DIAMETER OF THE PARTICLES TO 1.051E-6 METERS).
DIC> @@
DIC> enter-grid
REGION NAME : /CARB/: carb
WIDTH OF REGION /1/: rcem
TYPE /AUTO/: AUTO
DIC>
DIC> @@

```

```
DIC> @@ THE SIZE OF THE FCC REGION CAN BE CALCULATED FROM A MASS BALANCE
DIC> @@ AFTER ESTIMATING THE INITIAL COMPOSITIONS IN THE TWO PHASES
DIC> @@
DIC> enter-grid
REGION NAME : /AUS/: aus
WIDTH OF REGION /1/: rmat
TYPE /AUTO/: AUTO
DIC>
DIC> @@
DIC> @@ ENTER PHASES INTO REGIONS
DIC> @@
DIC> enter-phase act carb matrix cementite
DIC> enter-phase act aus matrix fcc#1
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITIONS IN THE PHASES
DIC> @@
DIC> enter-composition
REGION NAME : /CARB/: carb
PHASE NAME: /CEMENTITE D011/: cementite
DEPENDENT COMPONENT ? /FE/: fe
COMPOSITION TYPE /MOLE_FRACTION/: weig-fraction
PROFILE FOR /CR/: cr lin wcemcr wcemcr
DIC>
DIC> enter-composition
REGION NAME : /AUS/: aus
PHASE NAME: /FCC_A1#1/: fcc#1
DEPENDENT COMPONENT ? /FE/: fe
COMPOSITION TYPE /MOLE_FRACTION/: weig-fraction
PROFILE FOR /C/: CR lin wmatcr wmatcr
PROFILE FOR /CR/: C lin wmatc wmatc
DIC>
DIC> @@
DIC> @@ SET TO A SPHERICAL GEOMETRY
DIC> @@
DIC> enter-geo
GEOMETRICAL EXPONENT /0/: 2
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME AND OTHER SIMULATION PARAMETERS
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 10000
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /1000/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exb2 Y
DIC>
DIC> set-inter
--OK--
DIC>
```

exb2-run

DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exb2\run.DCM.test"

DIC>

DIC>

DIC> @@ exb2\_run.DCM

DIC>

DIC> @@

DIC> @@ READ THE SET UP FROM FILE AND START THE SIMULATION

DIC> @@

DIC>

DIC> go d-m

TIME STEP AT TIME 0.00000E+00

\*\*\* ENTERING BCC\_A2 AS A DIFFUSION NONE PHASE

DIC> read exb2

OK

DIC> sim

INFO: Default responses (if any) will be applied during the simulation. Use "SIMULATE\_REACTION NO" instead for manual input.

Region: CARB

geometric 0.833333 dense at 0.525500E-06 58 points

Region: AUS

geometric 1.08382 dense at 0.00000 51 points

DEGREE OF IMPLICIT SET TO TRAPEZOIDAL RULE

Trying old scheme

GENERATING STARTING VALUES FOR CELL # 1 INTERFACE # 2

DETERMINING INITIAL EQUILIBRIUM VALUES

CALCULATING STARTING VALUES: 9 EQUILIBRIUM CALCULATIONS DONE 6 OUT OF 9

04

U-FRACTION IN SYSTEM: C = .0406910188418179 CR = .0214382349908299

FE = .978561765139678

TOTAL SIZE OF SYSTEM: 5.05626559582E-18 [m^3]

U-FRACTION IN SYSTEM: C = .0406910188418179 CR = .0214382349908299

FE = .978561765139678

TOTAL SIZE OF SYSTEM: 5.05626559582E-18 [m^3]

0.175660348248328 0.175701612808876 0.175660403504846 2.957123333729781E-003 7.707887793871315E-

005 1.690889548904206E-005 5.562776867778342E-006 1.479066404490064E-006 1.412228092434950E-

006 3.874041245636360E-007 3.004856193118965E-007 2.976052984421406E-007 2.974033302220243E-

007 2.932922507067780E-007 2.893522382061154E-007 2.815348251005817E-007 2.824718772169510E-

007 2.661546935677175E-007 2.364445524473569E-007 1.814586159121373E-007 1.822641482962206E-

007 9.101299503087152E-008 1.596613000445222E-009 2.088067599073854E-012 7.527983802043017E-

018 TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.71346162E-17

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.42832941E-02 AND -0.42832941E-02

POSITION OF INTERFACE CARB / AUS IS 0.52507167E-06

U-FRACTION IN SYSTEM: C = .040732123121372 CR = .021438336581268

FE = .978561663549239

TOTAL SIZE OF SYSTEM: 5.05626559582E-18 [m^3]

CPU time used in timestep 0 seconds

2.77271904199977E-005 2.773273773310285E-005 2.772713596612424E-005 2.002835653853146E-009 7.555407620527206E-

010 9.239010091274666E-013 5.787187528338812E-019 TIME = 0.30000000E-06 DT = 0.20000000E-

06 SUM OF SQUARES = 0.45694435E-18

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.12394281E-03 AND -0.12394281E-03

POSITION OF INTERFACE CARB / AUS IS 0.52504688E-06

U-FRACTION IN SYSTEM: C = .0407324904420209 CR = .0214383423017019

FE = .978561657828806

TOTAL SIZE OF SYSTEM: 5.05626559582E-18 [m^3]

CPU time used in timestep 1 seconds

4.914773225972526E-006 4.913613218541297E-006 4.914583824931072E-006 2.481536531061057E-006 1.95690770231878E-

006 1.041999135846117E-006 6.930107957357825E-008 9.686519095787612E-013 1.763487087268090E-

017 TIME = 0.68198078E-06 DT = 0.38198078E-06 SUM OF SQUARES = 0.69353217E-17

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.15427964E-03 AND -0.15427964E-03

POSITION OF INTERFACE CARB / AUS IS 0.52498795E-06

U-FRACTION IN SYSTEM: C = .040735146065225 CR = .0214383556812409

FE = .978561644449267

TOTAL SIZE OF SYSTEM: 5.05626559582E-18 [m^3]

1 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: AUS

CPU time used in timestep 0 seconds

8.844088853911705E-007 8.850205938081172E-007 8.843869459699780E-007 4.649899403666994E-007 4.178128550510212E-

007 3.284325666088787E-007 1.817857970660160E-007 1.817633046140124E-007 1.771708811270311E-

008 1.624691978715939E-013 1.000482022309011E-018 TIME = 0.14459423E-05 DT = 0.76396156E-

06 SUM OF SQUARES = 0.26200937E-18

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.12135631E-03 AND -0.12135631E-03

POSITION OF INTERFACE CARB / AUS IS 0.52489524E-06

U-FRACTION IN SYSTEM: C = .0407352705138452 CR = .0214383762063272

FE = .97856162392418

TOTAL SIZE OF SYSTEM: 5.05626559582E-18 [m^3]

CPU time used in timestep 0 seconds

1.038513232878385E-006 1.039247075245704E-006 1.038521895728708E-006 7.20002176175777E-008

output ignored...

... output resumed

U-FRACTION IN SYSTEM: C = .0407662510909206 CR = .0214380716795954

FE = .978561928450912

TOTAL SIZE OF SYSTEM: 5.05626559582E-18 [m^3]

1 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: AUS

CPU time used in timestep 2 seconds

2.140724783563910E-007 2.145004979841646E-007 2.141362471402357E-007 5.160654594656812E-008 1.952775185457182E-

008 2.297648576737977E-012 1.737628569940828E-

016 TIME = 6314.3771 DT = 1000.0000 SUM OF SQUARES = 0.83207635E-16

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.14130507E-10 AND -0.14130507E-10

POSITION OF INTERFACE CARB / AUS IS 0.26623673E-06

U-FRACTION IN SYSTEM: C = .0407664334357307 CR = .0214380677874753

FE = .978561932343032

TOTAL SIZE OF SYSTEM: 5.05626559582E-18 [m^3]

CPU time used in timestep 1 seconds

9.720327142415701E-008 9.744152658146634E-008 9.724120674353808E-008 3.202204430035339E-008 1.303890367511254E-

008 8.772657536632490E-013 2.792532419767100E-

017 TIME = 7314.3771 DT = 1000.0000 SUM OF SQUARES = 0.11293558E-16

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.12493482E-10 AND -0.12493482E-10

POSITION OF INTERFACE CARB / AUS IS 0.25374325E-06

U-FRACTION IN SYSTEM: C = .0407665123632013 CR = .0214380650409061

FE = .978561935089601

TOTAL SIZE OF SYSTEM: 5.05626559582E-18 [m^3]

1 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: AUS

CPU time used in timestep 2 seconds

4.21646499410878E-008 4.229656530269648E-008 4.218541984998433E-008 1.751750361842919E-008 7.921588315648908E-

```

009      3.042072901503781E-013      8.030876548688946E-
018      TIME =      8314.3771      DT =      1000.0000      SUM OF SQUARES =      0.55486176E-17
CELL # 1 VELOCITY AT INTERFACE # 2 IS      -0.11324512E-10 AND      -0.11324512E-10
POSITION OF INTERFACE CARB / AUS IS      0.24241874E-06
U-FRACTION IN SYSTEM:      C = .0407665586064451      CR = .021438063320265
FE = .978561936810242
TOTAL SIZE OF SYSTEM:      5.05626559582E-18 [m^3]
CPU time used in timestep      1 seconds
1.602357697242259E-008      1.609145505745476E-008      1.603158632453903E-008      8.177362736288252E-009      4.212484456971385E-
009      8.134238185912224E-014      2.459483607910364E-
017      TIME =      9314.3771      DT =      1000.0000      SUM OF SQUARES =      0.24344799E-16
CELL # 1 VELOCITY AT INTERFACE # 2 IS      -0.10514429E-10 AND      -0.10514429E-10
POSITION OF INTERFACE CARB / AUS IS      0.23190431E-06
U-FRACTION IN SYSTEM:      C = .0407665686082386      CR = .0214380618411325
FE = .978561938289375
TOTAL SIZE OF SYSTEM:      5.05626559582E-18 [m^3]
CPU time used in timestep      1 seconds
1.007404255701584E-006      1.006919404263611E-006      1.006516338193728E-006      9.435239092746207E-008      1.073534425436613E-
011      6.060170636922464E-017      TIME =      10000.000      DT =      685.62294      SUM OF SQUARES =      0.42361985E-16
CELL # 1 VELOCITY AT INTERFACE # 2 IS      -0.97992402E-11 AND      -0.97992402E-11
POSITION OF INTERFACE CARB / AUS IS      0.22518573E-06
U-FRACTION IN SYSTEM:      C = .0407665610869387      CR = .0214380609255118
FE = .978561939204995
TOTAL SIZE OF SYSTEM:      5.05626559582E-18 [m^3]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME      0.0000000
DELETING TIME-RECORD FOR TIME      0.10000000E-06
DELETING TIME-RECORD FOR TIME      0.30000000E-06
DELETING TIME-RECORD FOR TIME      0.68198078E-06
DELETING TIME-RECORD FOR TIME      0.14459423E-05
DELETING TIME-RECORD FOR TIME      0.29738654E-05
DELETING TIME-RECORD FOR TIME      0.60297117E-05
DELETING TIME-RECORD FOR TIME      0.12141404E-04
DELETING TIME-RECORD FOR TIME      0.24364789E-04
DELETING TIME-RECORD FOR TIME      0.48811559E-04
DELETING TIME-RECORD FOR TIME      0.97705098E-04
DELETING TIME-RECORD FOR TIME      0.19549218E-03
DELETING TIME-RECORD FOR TIME      0.39040662E-03
DELETING TIME-RECORD FOR TIME      0.75073691E-03
DELETING TIME-RECORD FOR TIME      0.13877144E-02
DELETING TIME-RECORD FOR TIME      0.24412376E-02
DELETING TIME-RECORD FOR TIME      0.40939956E-02
DELETING TIME-RECORD FOR TIME      0.65605117E-02
DELETING TIME-RECORD FOR TIME      0.10064324E-01
DELETING TIME-RECORD FOR TIME      0.14884746E-01
DELETING TIME-RECORD FOR TIME      0.21452460E-01
DELETING TIME-RECORD FOR TIME      0.30485537E-01
DELETING TIME-RECORD FOR TIME      0.43317801E-01
DELETING TIME-RECORD FOR TIME      0.62747907E-01
DELETING TIME-RECORD FOR TIME      0.95738120E-01
DELETING TIME-RECORD FOR TIME      0.16171855
DELETING TIME-RECORD FOR TIME      0.29227689
DELETING TIME-RECORD FOR TIME      0.53214421
DELETING TIME-RECORD FOR TIME      1.0118789
DELETING TIME-RECORD FOR TIME      1.9034061
DELETING TIME-RECORD FOR TIME      3.6864605
DELETING TIME-RECORD FOR TIME      7.1077626
DELETING TIME-RECORD FOR TIME      13.306809
DELETING TIME-RECORD FOR TIME      24.555689
DELETING TIME-RECORD FOR TIME      45.854796
DELETING TIME-RECORD FOR TIME      86.774869
DELETING TIME-RECORD FOR TIME      168.61502
DELETING TIME-RECORD FOR TIME      332.29531
DELETING TIME-RECORD FOR TIME      659.65589
DELETING TIME-RECORD FOR TIME      1314.3771
DELETING TIME-RECORD FOR TIME      2314.3771
DELETING TIME-RECORD FOR TIME      3314.3771
DELETING TIME-RECORD FOR TIME      4314.3771
DELETING TIME-RECORD FOR TIME      5314.3771
DELETING TIME-RECORD FOR TIME      6314.3771
DELETING TIME-RECORD FOR TIME      7314.3771
DELETING TIME-RECORD FOR TIME      8314.3771

KEEPING TIME-RECORD FOR TIME      9314.3771
AND FOR TIME      10000.000
WORKSPACE RECLAIMED

TIMESTEP AT      10000.000      SELECTED

```

```

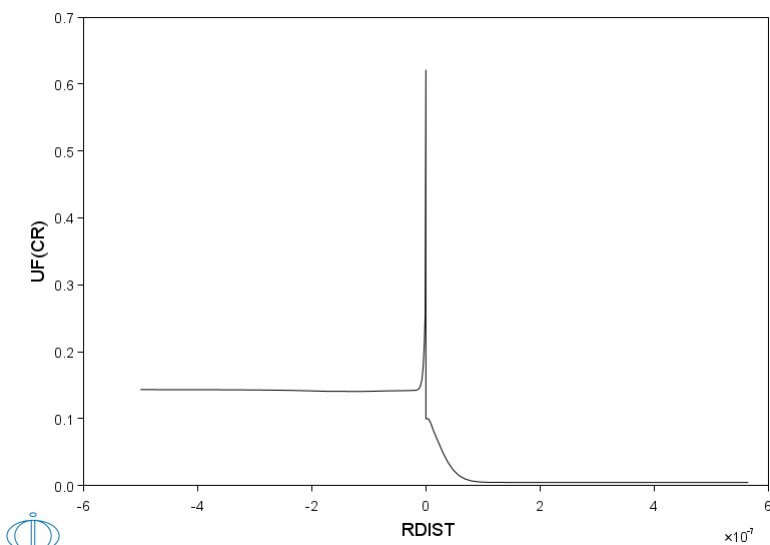
DIC>
DIC>
DIC> set-inter
--OK--
DIC>

```

## exb2-plot

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exb2\plot.DCM.test"
DIC>
DIC>
DIC> @@ exb2_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE b2
DIC> @@
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 1.00000E+04
*** ENTERING BCC_A2 AS A DIFFUSION NONE PHASE
DIC> read exb2
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1: @@
POST-1: @@ LET US PLOT CHROMIUM CONCENTRATION PROFILES
POST-1: @@ WE THEN SET THE DISTANCE AS X-AXIS (NOTE THAT DISTANCE IS AUTOMATICALLY
POST-1: @@ SET AS THE INDEPENDENT VARIABLE) AND U-FRACTION CARBON AS Y-AXIS
POST-1: @@ REMEMBER THAT THE PLOT CONDITION ALSO MUST BE SET.
POST-1: @@
POST-1: @@ NOTICE THAT ALL DISTANCES IN THE DATA FILE ARE GIVEN RELATIVE TO THE
POST-1: @@ CEM/FCC INTERFACE. FOR THIS REASON AN OFFSET MUST BE GIVEN TO THE
POST-1: @@ DATA ACCORDING TO THE ACTUAL PARTICLE RADIUS AT THE SPECIFIED TIME.
POST-1: @@
POST-1: enter-symb
Function or table /FUNCTION/: func
NAME: rdist
FUNCTION: gd-poi(carb,u);
POST-1:
POST-1: s-d-a x rdist
POST-1:
POST-1: s-i-v
VARIABLE /TIME/: dist
DISTANCE : /GLOBAL/: glo
POST-1:
POST-1: s-d-a y uf(cr)
POST-1:
POST-1: s-p-c time 10
POST-1:
POST-1: @@
POST-1: @@ SET THE TITLE ON THE PLOT
POST-1: @@
POST-1: set-title Figure b2.1
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

Figure b2.1



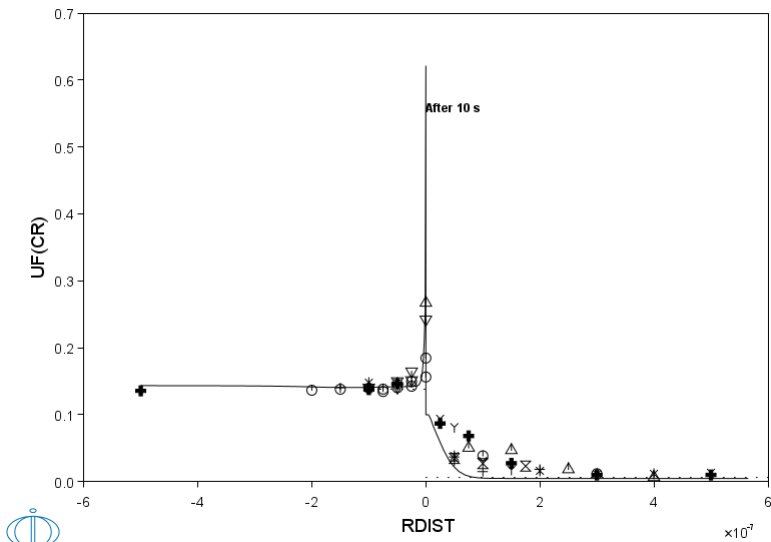
```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1: @?<_hit_return_to_continue_>
POST-1:
POST-1: @@
POST-1: @@ INCLUDE EXPERIMENTAL DATA POINTS ON THE PLOT FOR COMPARISION
POST-1: @@
POST-1: @@ FIRST LIST DATASETS
POST-1: @@
POST-1: app y exb2.exp
PROLOGUE NUMBER: /0/: 0
```

```

DATASET NUMBER(s) : /-1/: -1
  DATASET 1 CONCENTRATION PROFILE T=10S
  DATASET 2 CONCENTRATION PROFILE T=100S
  DATASET 3 CONCENTRATION PROFILE T=1000S
  DATASET 4 CONCENTRATION PROFILE T=10000S
  DATASET 5 VOLUME FRACTION CEMENTITE VS. TIME
  DATASET 6 MEAN PARTICLE DIAMETER VS. TIME
POST-1:
POST-1: @@
POST-1: @@ SELECT THE PROPER DATASET
POST-1: @@
POST-1: app y exb2.exp
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s) : /-1/: 1
POST-1:
POST-1: set-title Figure b2.2
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

```

Figure b2.2

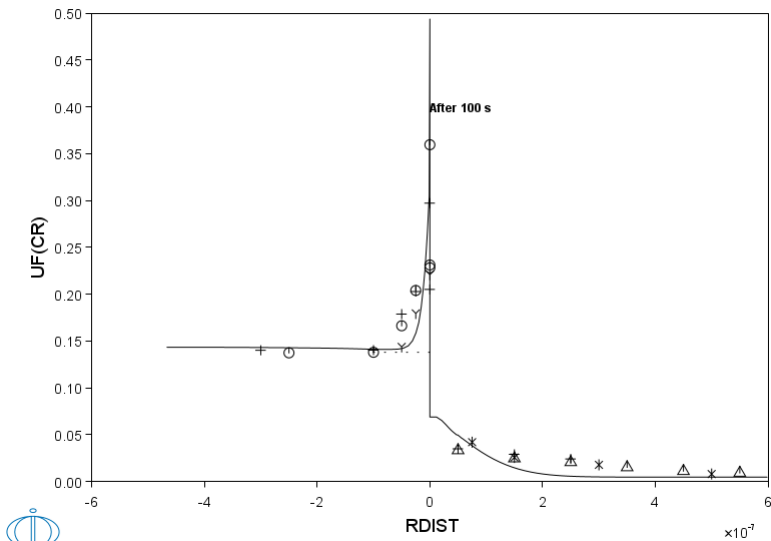


```

POST-1:
POST-1:
POST-1:
POST-1:
POST-1: @?<_hit_return_to_continue_>
POST-1:
POST-1: @@
POST-1: @@ PLOT ALSO FOR 100, 1000 AND 10000 seconds
POST-1: @@
POST-1:
POST-1: s-p-c time 100
POST-1:
POST-1: app y exb2.exp
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s) : /-1/: 2
POST-1:
POST-1: set-title Figure b2.3
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

```

Figure b2.3



```

POST-1:
POST-1:

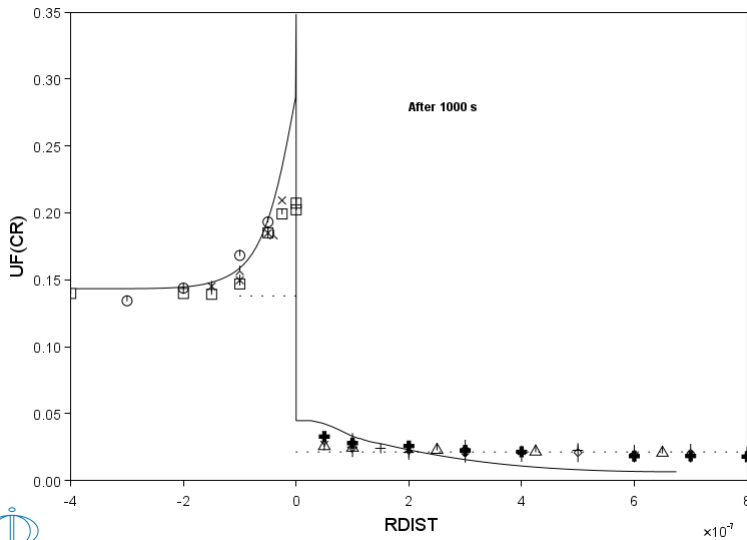
```

```

POST-1:
POST-1:
POST-1:??<_hit_return_to_continue_>
POST-1:
POST-1: s-p-c time 1000
POST-1:
POST-1: app y exb2.exp
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 3
POST-1:
POST-1: set-title Figure b2.4
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

```

Figure b2.4

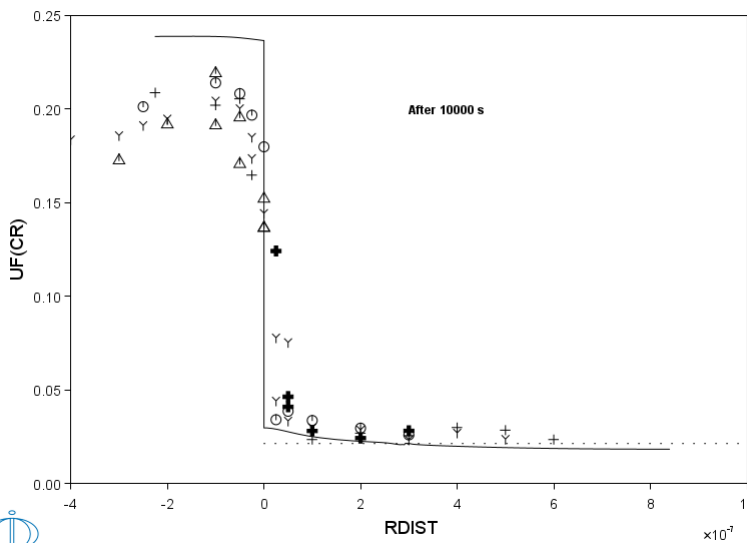


```

POST-1:
POST-1:
POST-1:
POST-1:
POST-1:??<_hit_return_to_continue_>
POST-1:
POST-1: s-p-c time 10000
POST-1:
POST-1: app y exb2.exp
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 4
POST-1:
POST-1: set-title Figure b2.5
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

```

Figure b2.5



```

POST-1:
POST-1:
POST-1:
POST-1:
POST-1:??<_hit_return_to_continue_>
POST-1:
POST-1: @@
POST-1: @@ ALSO PLOT HOW THE VOLUME FRACTION OF CEMENTITE VARIES
POST-1: @@ WITH TIME
POST-1: @@

```

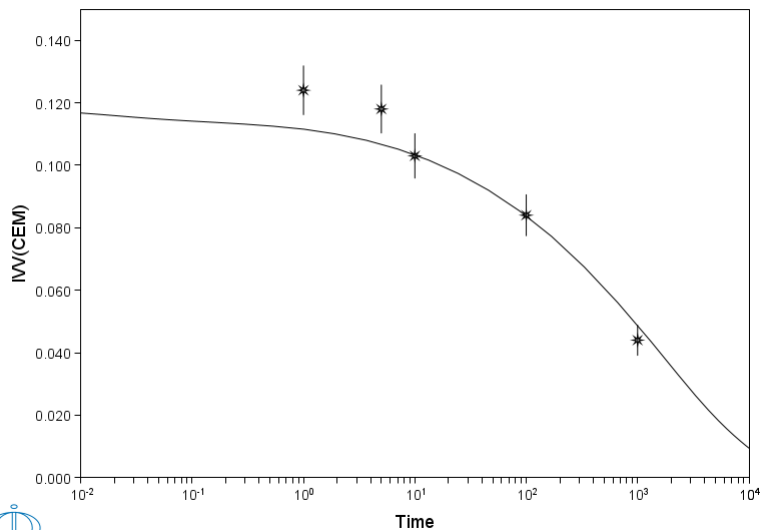
```

POST-1: s-d-a y ivv(cem)
POST-1: s-s-s y n 0 .15
POST-1:
POST-1: s-d-a x time
INFO: Time is set as independent variable
POST-1: set-axis-type x log
POST-1: s-s-s x n .01 10000
POST-1:
POST-1: s-p-c integral
POST-1:
POST-1: app y exb2.exp
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 5
POST-1:
POST-1: set-title Figure b2.6
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y

OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

```

Figure b2.6



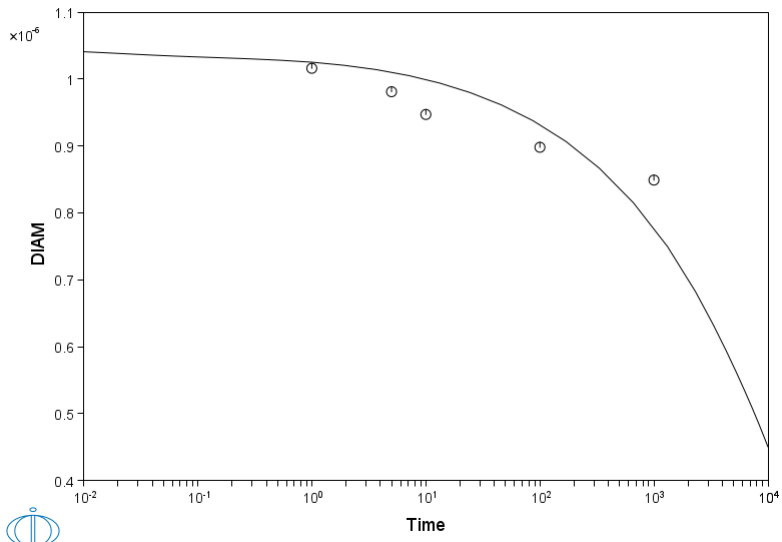
```

POST-1:
POST-1:
POST-1:
POST-1:
POST-1: @?<_hit_return_to_continue_>
POST-1:
POST-1: @@
POST-1: @@ ALSO PLOT HOW THE DIAMETER OF CEMENTITE VARIES WITH TIME
POST-1: @@
POST-1: enter func diam=2*poi(carb,u);
POST-1: s-d-a y diam
POST-1:
POST-1: s-p-c interface carb upper
POST-1:
POST-1: app y exb2.exp
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 6
POST-1:
POST-1: set-title Figure b2.7
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y

OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

```

Figure b2.7



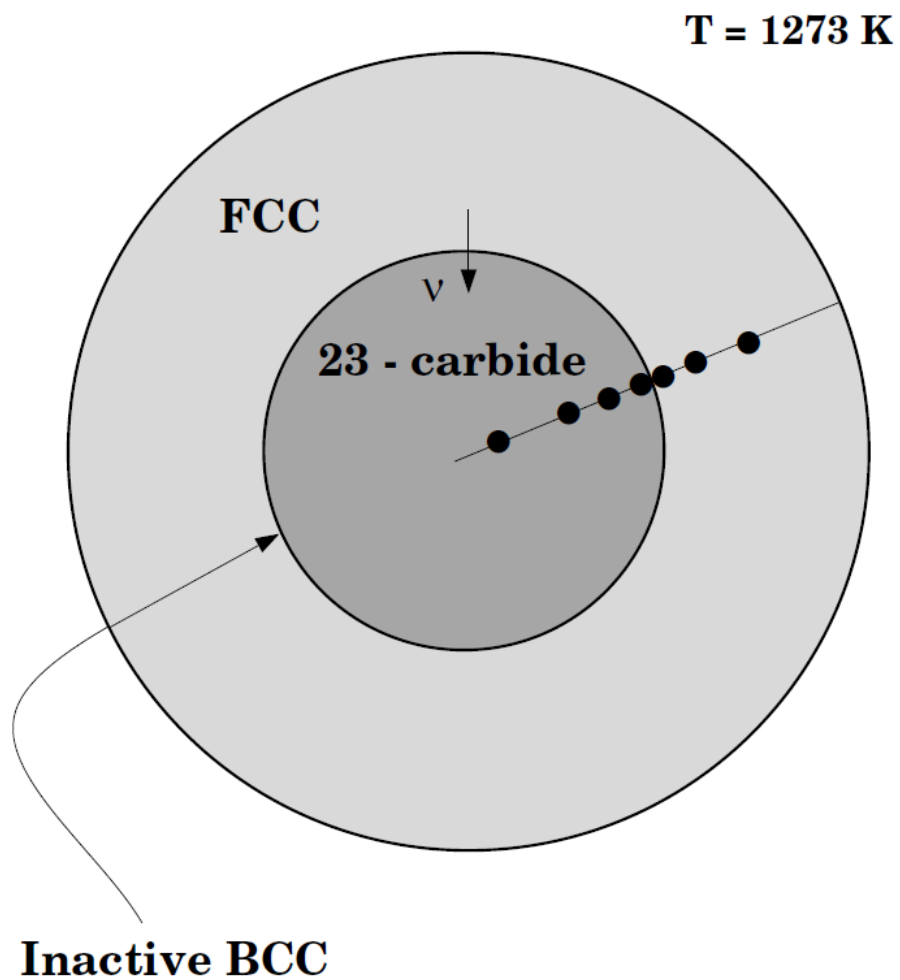
```
POST-1:  
POST-1:  
POST-1:  
POST-1:  
POST-1: @?<_hit_return_to_continue_>  
POST-1:  
POST-1: set-inter  
--OK--  
POST-1:
```



## Example exb3

### Dissolution of 23-carbide in an austenitic matrix

This example calculates the dissolution of an M<sub>23</sub>C<sub>6</sub> particle in an austenite matrix. A film of ferrite is allowed to nucleate around the carbide during the precipitation.



## exb3-setup

### SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,  
Stockholm, Sweden

Software running on Windows 64-bit wordlength  
Compiler: Intel Fortran Compiler 2025.0.0  
License library version: 9.7.0.0036  
Linked: Nov 19 2025 at 14:44:36

```
SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exb3\setup.DCM.test"
```

```
SYS:
```

```
SYS: @@ Moving boundary example.
```

```
SYS: @@ Dissolution of 23-carbide in an austenitic matrix
```

```
SYS: @@ This example calculates the dissolution of an M23C6 particle in an
```

```
SYS: @@ austenite matrix. A film of ferrite is allowed to nucleate around the
```

```
SYS: @@ carbide during the precipitation.
```

```
SYS: @@-----
```

```
SYS:
```

```
SYS: @@
```

```
SYS: @@ RETRIEVE DATA FROM THE DATABASES
```

```
SYS: @@
```

```
SYS: go da
```

```
THERMODYNAMIC DATABASE module
```

```
Database folder:
```

```
C:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\databases\da
```

```
ta
```

```
Current database: Steels/Fe-Alloys v12.0
```

```
VA /- DEFINED
```

```
DICTRA_FCC_A1 REJECTED
```

```
TDB_TCFE12:
```

```
TDB_TCFE12: @@
```

```
TDB_TCFE12: @@ USE A DATABASE FOR THERMODYNAMIC DATA
```

```
TDB_TCFE12: @@
```

```
TDB_TCFE12: sw fedemo
```

```
Current database: Iron Demo Database v6.0
```

```
VA /- DEFINED
```

```
TDB_FEDEMO: def-sys fe c cr
```

```
FE C CR
```

```
DEFINED
```

```
TDB_FEDEMO: rej ph *
```

```
GAS:G LIQUID:L BCC_A2
```

```
C14_LAVES CBCC_A12 CEMENTITE_D011
```

```
CHI_A12 CUB_A13 DIAMOND_A4
```

```
FCC_A1 GRAPHITE_A9 HCP_A3
```

```
KSI_CARBIDE M23C6_D84 M3C2_D510
```

```
M5C2 M7C3_D101 SIGMA_D8B
```

```
REJECTED
```

```
TDB_FEDEMO: res ph fcc bcc m23
```

```
FCC_A1 BCC_A2 M23C6_D84
```

```
RESTORED
```

```
TDB_FEDEMO: get
```

```
09:17:22,976 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
```

```
REINITIATING GES .....
```

```
ELEMENTS .....
```

```
SPECIES .....
```

```
PHASES .....
```

```
Creating a new composition set FCC_A1#2
```

```
PARAMETERS ...
```

```
FUNCTIONS .....
```

```
Use the command LIST_REFERENCES to see the list of references for assessed data
```

```
-OK-
```

```
TDB_FEDEMO:
```

```
TDB_FEDEMO: @@
```

```
TDB_FEDEMO: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE THE MOBILITY DATA
```

```
TDB_FEDEMO: @@
```

```
TDB_FEDEMO: app mfedemo
```

```
Current database: Fe-Alloys Mobility demo database v5.0
```

```
VA DEFINED
```

```
APP: def-sys c cr fe
```

```
C CR FE
```

```
DEFINED
```

```
APP: rej ph *
```

```
BCC_A2 FCC_A1 CEMENTITE_D011
```

```
LIQUID:L REJECTED
```

```
APP: res ph fcc bcc
```

```
FCC_A1 BCC_A2 RESTORED
```

```
APP: get
```

```
ELEMENTS .....
```

```
SPECIES .....
```

```
PHASES .....
```

```
Creating a new composition set FCC_A1#3
```

```
PARAMETERS ...
```

```
FUNCTIONS .....
```

```
Use the command LIST_REFERENCES to see the list of references for assessed data
```

```
-OK-
```

```
APP:
```

```
APP: @@
```

```
APP: @@ ENTER THE DICTRA MONITOR
```

```
APP: @@
```

```
APP: go d-m
```

```
NO TIME STEP DEFINED
```

```
*** ENTERING M23C6_D84 AS A DIFFUSION NONE PHASE
```

```
DIC>
```

```
DIC>
```

```
DIC> @@ THE MOBILITY DATABASE LACKS KINETIC DATA FOR THE M23-CARBIDE
```

```
DIC> @@ SO AN ESTIMATE FOR THE MOBILITIES IN THIS PHASE ARE ENTERED.
```

```
DIC> ent-mob-est M23 c
```

```
M[M23,C](T) = 0;
```

```

NOTE: 1 of 3 parameters entered
DIC>
DIC> ent-mob-est M23 cr
M[M23,CR](T)= 3e-11*exp(-278000/8.3145/T);
NOTE: 2 of 3 parameters entered
DIC>
DIC> ent-mob-est M23 fe
M[M23,FE](T)= 1e-11*exp(-275000/8.3145/T);
NOTE: All necessary parameters entered
DIC>
DIC> @@
DIC> @@ ENTER GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 1273; * N
DIC>
DIC> @@
DIC> @@ ENTER THE REGIONS carbide AND matrix
DIC> @@
DIC> enter-region carbide
DIC> enter-region matrix
ATTACH TO REGION NAMED /CARBIDE/:
ATTACHED TO THE RIGHT OF CARBIDE /YES/:
DIC> @@
DIC> @@ ASSUME SOME REASONABLE SIZE OF THE CARBIDE PARTICLE
DIC> @@
DIC> enter-grid carbide 5.00000000E-7 AUTO
DIC> @@
DIC> @@ THE SIZE OF THE FCC REGION WE CAN CALCULATE FROM A MASS BALANCE
DIC> @@ AFTER ESTIMATING THE INITIAL COMPOSITIONS IN THE TWO PHASES.
DIC> @@
DIC> enter-grid matrix 5.55859755E-7 AUTO
DIC> @@
DIC> @@ ENTER PHASES INTO THE REGION MATRIX. BOUNDARY CONDITIONS ARE GIVEN
DIC> @@ IF THE INACTIVE PHASE bcc IS NUCLEATED
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /CARBIDE/: matrix
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inact
ATTACH TO REGION NAMED /MATRIX/: matrix
ATTACHED TO THE RIGHT OF MATRIX /YES/: no
PHASE NAME: /NONE/: bcc#1
DEPENDENT COMPONENT ? /FE/: fe
REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/:
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> @@
DIC> @@ ENTER THE PHASE INTO THE REGION carbide
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /CARBIDE/: carbide
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: m23c6
DIC>
DIC> @@
DIC> @@ ENTER COMPOSITIONS INTO THE PHASES
DIC> @@
DIC> enter-composition
REGION NAME : /CARBIDE/: carbide
PHASE NAME: /M23C6_D84/: m23c6
DEPENDENT COMPONENT ? /FE/: fe
COMPOSITION TYPE /MOLE_FRACTION/: mole-fraction
PROFILE FOR /CR/: cr lin 0.55079807 0.55079807
DIC>
DIC>
DIC> enter-composition
REGION NAME : /MATRIX/: matrix
PHASE NAME: /FCC_A1#1/: fcc#1
DEPENDENT COMPONENT ? /FE/: fe
COMPOSITION TYPE /MOLE_FRACTION/: mole-fraction
PROFILE FOR /C/: cr lin 8.5203899E-2 8.5203899E-2
PROFILE FOR /CR/: c lin 1.8072433E-4 1.8072433E-4
DIC>
DIC> @@
DIC> @@ SET TO A SPHERICAL GEOMETRY
DIC> @@
DIC> enter-geo
GEOMETRICAL EXPONENT /0/: 2
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME AND OTHER SIMULATION PARAMETERS
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 8000
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /800/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exb3 Y
DIC>
DIC>
DIC>
DIC> set-inter
--OK--
DIC>

```

exb3-run

```

DIC>About
NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exb3\run.DCM.test"
DIC>
DIC>
DIC> @@ exb3_run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING EXAMPLE b3
DIC> @@
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA MONITOR AND READ THE SET UP FROM FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 0.00000E+00
DIC> read exb3
OK
DIC>
DIC> @@
DIC> @@ WHEN THE FERRITE NUCLEATES WE USE DEFAULT VALUES
DIC> @@ AS STARTING VALUES FOR THE WIDTH OF THE NEW REGION
DIC> @@ AND THE VELOCITY OF THE INTERFACES
DIC> @@
DIC>
DIC> @@ START THE SIMULATION
DIC> @@
DIC> sim yes
INFO: Default responses (if any) will be applied during the simulation. Use "SIMULATE_REACTION NO" instead for manual input.
Region: CARBIDE
geometric 0.956620 dense at 0.500000E-06 51 points
Region: MATRIX
geometric 1.05195 dense at 0.00000 50 points
DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
Trying old scheme 4
GENERATING STARTING VALUES FOR CELL # 1 INTERFACE # 2
DETERMINING INITIAL EQUILIBRIUM VALUES
CALCULATING STARTING VALUES: 9 EQUILIBRIUM CALCULATIONS DONE 6 OUT OF 9
U-FRACTION IN SYSTEM: C = .0278637912207471 CR = .149918318671311
FE = .850081681459196
TOTAL SIZE OF SYSTEM: 4.93068569406E-18 [m^3]
U-FRACTION IN SYSTEM: C = .0278637912207471 CR = .149918318671311
FE = .850081681459196
TOTAL SIZE OF SYSTEM: 4.93068569406E-18 [m^3]
0.564525001046130 0.564658892752918 0.564525829496762 1.010918370997740E-002 2.719677100264318E-
004 6.785040686883620E-005 1.215315579807402E-005 4.866561139048117E-006 4.600898530266347E-
006 1.065354242442190E-007 8.588439242735395E-008 5.106291897372686E-008 5.522545709592756E-
008 2.440343683814056E-008 2.876055304151570E-010 1.192136903749214E-015 5.3993350026632977E-
020 TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.73236392E-21
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.18307019E-02 AND -0.18307019E-02
POSITION OF INTERFACE CARBIDE / MATRIX IS 0.49981693E-06
U-FRACTION IN SYSTEM: C = .027878406862065 CR = .149918515634161
FE = .850081484496346
TOTAL SIZE OF SYSTEM: 4.93068569406E-18 [m^3]
CPU time used in timestep 6 seconds
1.169573305641419E-004 1.169808091698651E-004 1.169556456870664E-004 6.196379839283318E-009 3.575390208997375E-
010 5.633278916665288E-016 1.123078553233749E-022 TIME = 0.30000000E-06 DT = 0.20000000E-
06 SUM OF SQUARES = 0.10429154E-21
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.37512517E-04 AND -0.37512517E-04
POSITION OF INTERFACE CARBIDE / MATRIX IS 0.49980943E-06
U-FRACTION IN SYSTEM: C = .0278783962800807 CR = .14991852270919
FE = .850081477421317
TOTAL SIZE OF SYSTEM: 4.93068569406E-18 [m^3]
1 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: MATRIX
CPU time used in timestep 1 seconds
1.635955480785716E-006 1.636388953882924E-006 1.634950881787669E-006 1.008577264185604E-007 2.605673330761522E-
009 3.122189829853064E-014 3.380706863199773E-021 TIME = 0.70000000E-06 DT = 0.40000000E-
06 SUM OF SQUARES = 0.50294281E-21
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.42504001E-04 AND -0.42504001E-04
POSITION OF INTERFACE CARBIDE / MATRIX IS 0.49979243E-06
U-FRACTION IN SYSTEM: C = .0278783834690609 CR = .149918538694267
FE = .85008146143624
TOTAL SIZE OF SYSTEM: 4.93068569406E-18 [m^3]
CPU time used in timestep 1 seconds
1.554949973990134E-004 1.555520585604812E-004 1.554464678200233E-004 4.605861270131429E-008 3.402806768460703E-
010 4.132556837568250E-015 6.323779032804117E-024 TIME = 0.15000000E-05 DT = 0.80000000E-
06 SUM OF SQUARES = 0.97597228E-26
output ignored...

... output resumed

3.460859970899211E-008 3.853190469634759E-012 2.001231773467918E-
017 TIME = 5415.3212 DT = 800.00000 SUM OF SQUARES = 0.31370702E-18
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.73043932E-12 AND -0.73043932E-12
POSITION OF INTERFACE CARBIDE / MATRIX IS 0.39393387E-06
U-FRACTION IN SYSTEM: C = .0278045747992993 CR = .149761222842389
FE = .850238777288118
TOTAL SIZE OF SYSTEM: 4.93068569406E-18 [m^3]
1 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: MATRIX
CPU time used in timestep 2 seconds
6.858629046833883E-008 6.860675426478936E-008 6.851615902357036E-008 4.292891739626284E-008 3.383169652306525E-
008 1.672092142420378E-008 4.330932377463012E-010 3.163126106530902E-016 1.788682455549798E-
019 TIME = 6215.3212 DT = 800.00000 SUM OF SQUARES = 0.17885846E-18
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.31270352E-12 AND -0.31270352E-12
POSITION OF INTERFACE CARBIDE / MATRIX IS 0.39368370E-06
U-FRACTION IN SYSTEM: C = .0278045741427574 CR = .149761222649802
FE = .850238777480705
TOTAL SIZE OF SYSTEM: 4.93068569406E-18 [m^3]
CPU time used in timestep 1 seconds
2.27379115955303E-008 2.274294268683420E-008 2.269665075037888E-008 1.473090656995474E-008 1.327507618347487E-
008 1.072170431932875E-008 6.052324004763496E-009 6.050923875924521E-009 7.828035657731571E-
010 1.529672638853664E-016 TIME = 7015.3212 DT = 800.00000 SUM OF SQUARES = 0.32166961E-16
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.77221693E-13 AND -0.77221693E-13
POSITION OF INTERFACE CARBIDE / MATRIX IS 0.39362193E-06

```

U-FRACTION IN SYSTEM: C = .0278045711605603 CR = .14976122253633

FE = .850238777594177

TOTAL SIZE OF SYSTEM: 4.93068569406E-18 [m^3]

2 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: MATRIX

CPU time used in timestep 1 seconds

7.498872074462225E-009 7.499583350637715E-009 7.474637936974678E-009 4.798597276766772E-009 4.699672603772302E-

009 4.435257557809628E-009 3.992242270087134E-009 3.994347546230775E-009 3.121899460163433E-

009 1.735516641033211E-009 1.783617779399991E-010 4.266439313867035E-014 4.942555297317298E-

020 TIME = 7815.3212 DT = 800.00000 SUM OF SQUARES = 0.49128237E-19

CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.55609981E-13 AND 0.55609981E-13

POSITION OF INTERFACE CARBIDE / MATRIX IS 0.39366641E-06

U-FRACTION IN SYSTEM: C = .0278045718693421 CR = .149761222536683

FE = .850238777593824

TOTAL SIZE OF SYSTEM: 4.93068569406E-18 [m^3]

30 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: CARBIDE

CPU time used in timestep 1 seconds

4.540520188412860E-008 4.540422609731397E-008 4.565368229203065E-008 2.167037238033167E-008 2.150611328750977E-

008 2.116885212786793E-008 2.051269756755002E-008 2.051039107235970E-008 1.922150641194746E-

008 1.677392563020693E-008 1.237154982216541E-008 1.237235227866483E-008 5.577643993147913E-

009 2.423841833983940E-012 6.004102742837816E-

019 TIME = 8000.0000 DT = 184.67878 SUM OF SQUARES = 0.59047825E-18

CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.32313253E-12 AND 0.32313253E-12

POSITION OF INTERFACE CARBIDE / MATRIX IS 0.39372609E-06

U-FRACTION IN SYSTEM: C = .0278045713957348 CR = .149761222535494

FE = .850238777595013

TOTAL SIZE OF SYSTEM: 4.93068569406E-18 [m^3]

MUST SAVE WORKSPACE ON FILE

WORKSPACE SAVED ON FILE

RECLAIMING WORKSPACE

DELETING TIME-RECORD FOR TIME 59.256552

DELETING TIME-RECORD FOR TIME 73.143953

DELETING TIME-RECORD FOR TIME 73.143963

DELETING TIME-RECORD FOR TIME 73.143983

DELETING TIME-RECORD FOR TIME 73.144023

DELETING TIME-RECORD FOR TIME 73.144103

DELETING TIME-RECORD FOR TIME 73.144263

DELETING TIME-RECORD FOR TIME 73.144583

DELETING TIME-RECORD FOR TIME 73.145223

DELETING TIME-RECORD FOR TIME 73.146503

DELETING TIME-RECORD FOR TIME 73.149063

DELETING TIME-RECORD FOR TIME 73.154183

DELETING TIME-RECORD FOR TIME 73.164423

DELETING TIME-RECORD FOR TIME 73.184903

DELETING TIME-RECORD FOR TIME 73.225863

DELETING TIME-RECORD FOR TIME 73.307783

DELETING TIME-RECORD FOR TIME 73.471623

DELETING TIME-RECORD FOR TIME 73.799303

DELETING TIME-RECORD FOR TIME 74.454663

DELETING TIME-RECORD FOR TIME 75.765383

DELETING TIME-RECORD FOR TIME 78.386823

DELETING TIME-RECORD FOR TIME 83.629703

DELETING TIME-RECORD FOR TIME 94.115463

DELETING TIME-RECORD FOR TIME 115.08698

DELETING TIME-RECORD FOR TIME 157.03002

DELETING TIME-RECORD FOR TIME 240.91610

DELETING TIME-RECORD FOR TIME 408.68826

DELETING TIME-RECORD FOR TIME 744.23258

DELETING TIME-RECORD FOR TIME 1415.3212

DELETING TIME-RECORD FOR TIME 2215.3212

DELETING TIME-RECORD FOR TIME 3015.3212

DELETING TIME-RECORD FOR TIME 3815.3212

DELETING TIME-RECORD FOR TIME 4615.3212

DELETING TIME-RECORD FOR TIME 5415.3212

DELETING TIME-RECORD FOR TIME 6215.3212

DELETING TIME-RECORD FOR TIME 7015.3212

KEEPING TIME-RECORD FOR TIME 7815.3212

AND FOR TIME 8000.0000

WORKSPACE RECLAIMED

TIMESTEP AT 8000.00000 SELECTED

DIC>

DIC> set-inter

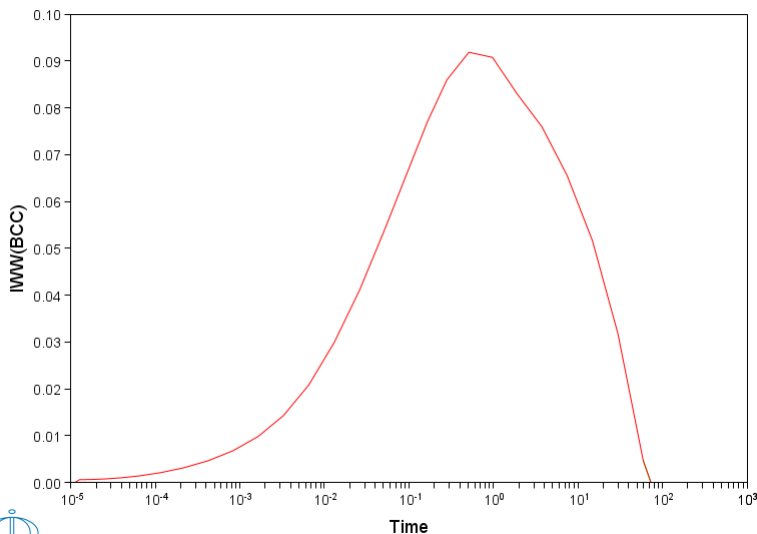
--OK--

DIC>

## exb3-plot

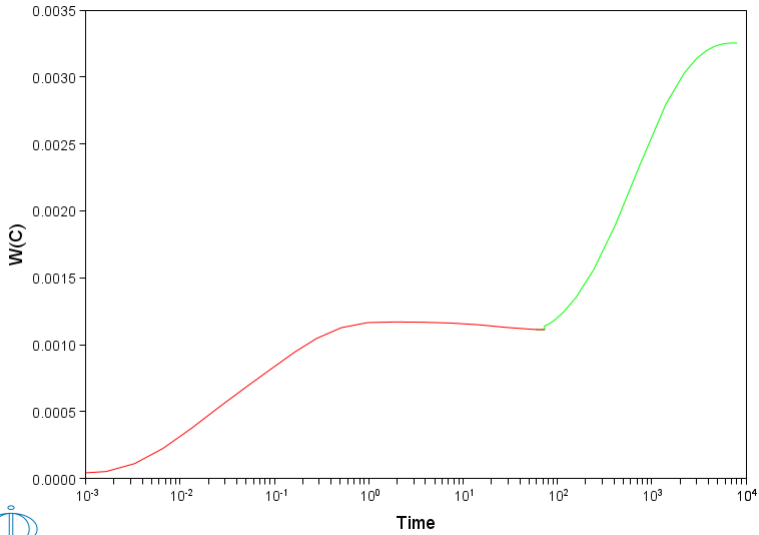
```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exb3\plot.DCM.test"
DIC>
DIC>
DIC> @@ exb3_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE b3
DIC> @@
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA MODULE AND SPECIFY THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 8.00000E+03
DIC> read exb3
OK
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA POST PROCESSOR
DIC> @@
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1: @@
POST-1: @@ LET US SEE HOW THE AMOUNT OF FERRITE VARIED DURING THE
POST-1: @@ SIMULATION
POST-1: @@
POST-1: s-d-a y iwv(bcc)
POST-1: s-d-a x time
INFO: Time is set as independent variable
POST-1: s-ax-tyt x log
POST-1: s-s-s x n 1E-5 1E3
POST-1: s-s-s y n 0 0.1
POST-1:
POST-1: set-tit Figure b3.1
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
WORKING ...
WORKING ... OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

Figure b3.1



```
POST-1:
POST-1:
POST-1: @?<_hit_return_to_continue_>
POST-1:
POST-1: @@
POST-1: @@ NOW LOOK AT THE ALLOYING ELEMENTS AT THE UPPER BOUND OF THE SYSTEM
POST-1: @@
POST-1: s-d-a y w(c)
POST-1: s-s-s x n 1E-3 1E4
POST-1: s-p-c interface last
POST-1:
POST-1: set-tit Figure b3.2
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
WORKING ...
WORKING ... OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

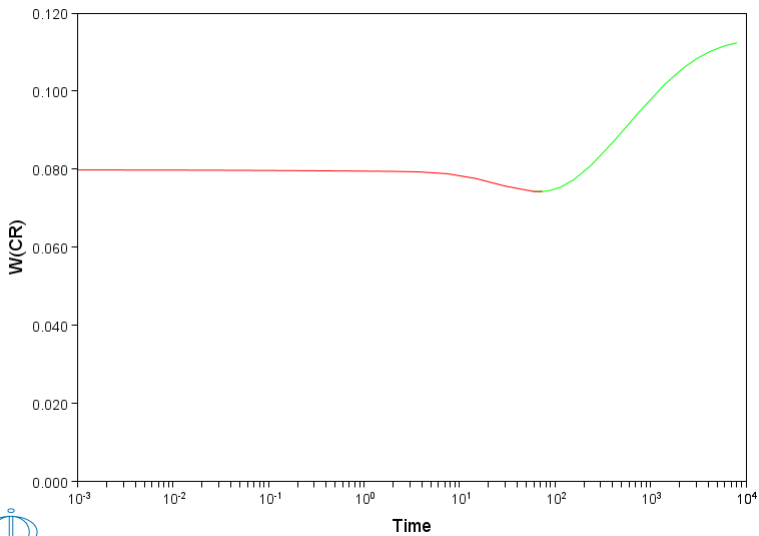
Figure b3.2



```

POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: s-d-a y w(cr)
POST-1: s-s-s y n 0 0.12
POST-1:
POST-1: set-tit Figure b3.3
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
WORKING ...
WORKING ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
    
```

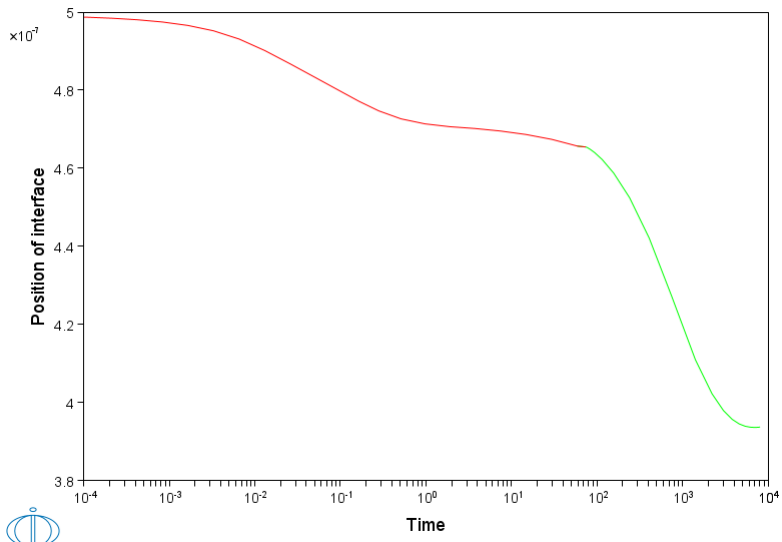
Figure b3.3



```

POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: @@
POST-1: @@ AND FINALLY LOOK AT THE CHANGE OF RADIUS OF THE M23-CARBIDE
POST-1: @@
POST-1: s-d-a y position carbide upper
POST-1: s-s-s x n 1E-4 1E4
POST-1:
POST-1: set-tit Figure b3.4
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
WORKING ...
WORKING ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
    
```

Figure b3.4



```
POST-1:  
POST-1:  
POST-1: @?<_hit_return_to_continue_>  
POST-1:  
POST-1: set-inter  
--OK--  
POST-1:
```



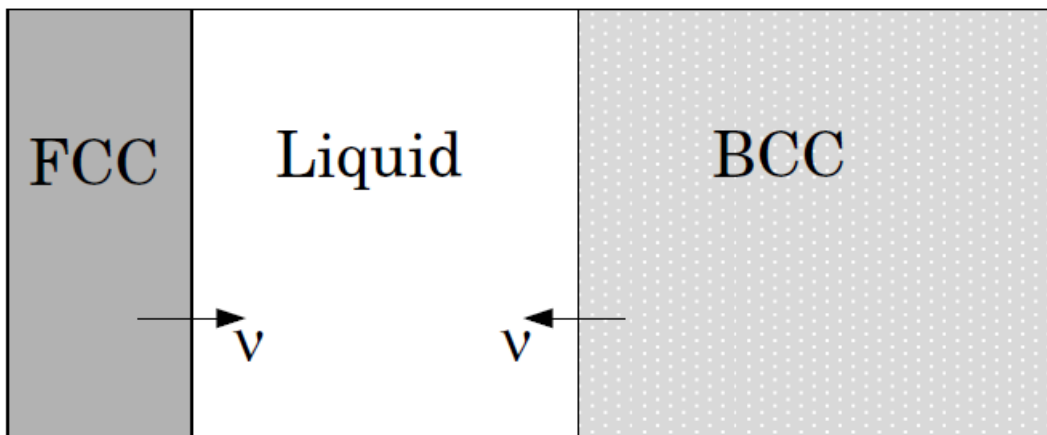
## Example exb4a

### Solidification path of a Fe-18%Cr-8%Ni alloy: Eutectic reaction

This example demonstrates the solidification path of an Fe-18%Cr-8%Ni alloy. A eutectic reaction is assumed, LIQUID  $\rightarrow$  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.

*Time* > 0

**T = 1900 - 1 \* Time K**



**1E-4**

## exb4a-setup

### SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,  
Stockholm, Sweden

Software running on Windows 64-bit wordlength  
Compiler: Intel Fortran Compiler 2025.0.0  
License library version: 9.7.0.0036  
Linked: Nov 19 2025 at 14:44:36

```
SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exb4a\setup.DCM.test"
```

```
SYS: @@  
SYS: @@ Moving boundary problem.  
SYS: @@ Solidification path of an Fe-18%Cr-8%Ni alloy: Eutectic reaction  
SYS: @@ This example demonstrates the solidification path of an Fe-18%Cr-8%Ni  
SYS: @@ alloy. A eutectic reaction is assumed, LIQUID -> BCC + FCC. Hence the  
SYS: @@ BCC and FCC regions should be on separate sides of the liquid region.  
SYS: @@ Comparison is made with both a Scheil-Gulliver simulation and equilibrium  
SYS: @@ solidification conditions, both done in Thermo-Calc.  
SYS: @@-----
```

```
SYS:  
SYS: @@ exb4a_setup.DCM  
SYS:  
SYS:  
SYS: @@  
SYS: @@ START BY GOING TO THE DATABASE MODULE  
SYS: @@  
SYS: go da  
THERMODYNAMIC DATABASE module  
Database folder:  
C:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\databases\da  
ta  
Current database: Steels/Fe-Alloys v12.0
```

```
VA /- DEFINED  
DICTRA_FCC_A1 REJECTED  
TDB_TCFE12:  
TDB_TCFE12: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA  
TDB_TCFE12: sw tcfe9  
Current database: Steels/Fe-Alloys v9.3
```

```
VA /- DEFINED  
L12_FCC B2_BCC DICTRA_FCC_A1  
REJECTED
```

```
TDB_TCFE9:  
TDB_TCFE9: @@ DEFINE THE SYSTEM TO WORK WITH  
TDB_TCFE9: def-sys fe ni cr  
FE NI CR  
DEFINED
```

```
TDB_TCFE9:  
TDB_TCFE9: @@ EXCLUDE THE THERMODYNAMIC DATA FOR THE PHASES THAT ARE NOT NEEDED  
TDB_TCFE9: rej ph /all  
LIQUID:L BCC_A2 FCC_A1  
HCP_A3 CBCC_A12 CUB_A13  
SIGMA CHI_A12 LAVES_PHASE_C14  
CR3SI NBNI3 NI3TI  
CRZN17 BETA1 GAMMA  
AL5FE4 CENI2 CENI5  
REJECTED
```

```
TDB_TCFE9: res ph fcc liq bcc  
FCC_A1 LIQUID:L BCC_A2  
RESTORED
```

```
TDB_TCFE9:  
TDB_TCFE9: @@ RETRIEVE DATA FROM THE DATABASE FILE  
TDB_TCFE9: get  
09:25:59,252 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***  
REINITIATING GES .....  
ELEMENTS .....  
SPECIES .....  
PHASES .....  
PARAMETERS ...  
FUNCTIONS ....
```

Use the command LIST\_REFERENCES to see the list of references for assessed data

```
-OK-  
TDB_TCFE9:  
TDB_TCFE9: @@  
TDB_TCFE9: @@ MOBILITY/DIFFUSIVITY DATA ARE STORED IN A SEPARATE DATABASE FILE.  
TDB_TCFE9: @@ SWITCH TO A MOBILITY DATABASE AND APPEND THE DATA  
TDB_TCFE9: @@  
TDB_TCFE9: app  
Use one of these databases
```

```
TCFE12 = Steels/Fe-Alloys v12.0  
TCFE9 = Steels/Fe-Alloys v9.3  
SSUB6 = SGTE Substances v6.0  
FEDEMO = Iron Demo Database v6.0  
MOB2 = Alloys Mobility v2.7  
MOBFE7 = Steels/Fe-Alloys Mobility v7.1  
MOBFE4 = Steels/Fe-Alloys Mobility v4.0  
MOBFE2 = Steels/Fe-Alloys Mobility v2.0  
MFEDEMO = Fe-Alloys Mobility demo database v5.0  
USER = User defined Database
```

```
DATABASE NAME /TCFE9/: mobfe4  
Current database: Steels/Fe-Alloys Mobility v4.0
```

```
VA DEFINED  
B2_BCC REJECTED  
APP: def-sys fe ni cr  
FE NI CR  
DEFINED  
APP: rej ph /all  
BCC_A2 FCC_A1 HCP_A3  
LIQUID:L REJECTED
```

```

APP: res ph fcc liq bcc
FCC_A1          LIQUID:L          BCC_A2
RESTORED
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP
APP: @@
APP: go d-m
NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER GLOBAL CONDITION T
DIC> @@
DIC> @@ LOWER THE TEMPERATURE TO A RATE OF 1 K/s
DIC> @@
DIC> set-cond glob T 0 1900-1*TIME; * N
DIC>
DIC> @@
DIC> @@ ENTER A REGION CALLED smalta
DIC> @@
DIC> enter-region smalta
DIC>
DIC> @@
DIC> @@ ENTER A DOUBLE GEOMETRIC GRID INTO THE REGION
DIC> @@
DIC> enter-grid
REGION NAME : /SMALTA/: smalta
WIDTH OF REGION /1/: 1e-4
TYPE /AUTO/: AUTO
DIC>
DIC>
DIC> @@
DIC> @@ ENTER active PHASES INTO THE REGION
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /SMALTA/: smalta
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: liq
DIC>
DIC> @@
DIC> @@ ENTER inactive PHASES INTO THE REGION: ONE PHASE ON EACH SIDE OF THE LIQUID
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inact
ATTACH TO REGION NAMED /SMALTA/: smalta
ATTACHED TO THE RIGHT OF SMALTA /YES/: no
PHASE NAME: /NONE/: fcc#1
DEPENDENT COMPONENT ? /NI/: fe
REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-5
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inact
ATTACH TO REGION NAMED /SMALTA/: smalta
ATTACHED TO THE RIGHT OF SMALTA /YES/: yes
PHASE NAME: /NONE/: bcc#1
DEPENDENT COMPONENT ? /NI/: fe
REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-5
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> @@
DIC> @@ ENTER A START COMPOSITION FOR THE LIQUID
DIC> @@
DIC> enter-composition
REGION NAME : /SMALTA/: smalta
PHASE NAME: /LIQUID/: liq
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /CR/: cr lin 18 18
PROFILE FOR /NI/: ni lin 8 8
DIC>
DIC> @@
DIC> @@ THE BOUNDARY CONDITION IS A CLOSED SYSTEM (THE DEFAULT) AS WE DO NOT SPECIFY
DIC> @@ ANYTHING ELSE.
DIC> @@
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 200
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /20/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC> @@
DIC> @@ CHECK THE INTERFACE POSITION. THIS IS TO MAKE SURE THAT THE
DIC> @@ LIQUID REGION DOES NOT SHRINK TOO MUCH DURING A TIMESTEP.
DIC> @@ IN ADDITION THE TIMESTEP IS CONTROLLED BY THE PHASE INTERFACE
DIC> @@ DISPLACEMENT DURING THE SIMULATION.
DIC> @@
DIC> set-option CHECK_INTERFACE_POSITION AUTO
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exb4a Y

```

```
DIC>  
DIC> set-inter  
--OK--  
DIC>
```

exb4a-run

DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exb4a\run.DCM.test"

DIC>

DIC>

DIC> @@ exb4a\_run.DCM

DIC>

DIC> @@

DIC> @@ FILE FOR RUNNING EXAMPLE b4a

DIC> @@

DIC>

DIC> @@

DIC> @@ ENTER THE DICTRA MONITOR AND READ THE SET UP FROM FILE

DIC> @@

DIC> go d-m

TIME STEP AT TIME 0.00000E+00

DIC> read exb4a

OK

DIC>

DIC> @@

DIC> @@ START THE SIMULATION

DIC> @@

DIC> sim yes

INFO: Default responses (if any) will be applied during the simulation. Use "SIMULATE\_REACTION NO" instead for manual input.

Region: SMALTA

geometric 1.18976 dense at 0.00000 35 points

geometric 0.840507 dense at 0.10000E-03 36 points

DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE

INFO: TIMESTEP IS CONTROLLED BY INTERFACE POSITION

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882255

TOTAL SIZE OF SYSTEM: 1E-04 [m]

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882255

TOTAL SIZE OF SYSTEM: 1E-04 [m]

TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882255

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 1 seconds

TIME = 0.24203913E-05 DT = 0.23203913E-05 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882255

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.70611740E-05 DT = 0.46407827E-05 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882255

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.16342739E-04 DT = 0.92815654E-05 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291

NI = .0754116207882255

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.34905870E-04 DT = 0.18563131E-04 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882255

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.72032132E-04 DT = 0.37126261E-04 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882255

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.14628465E-03 DT = 0.74252523E-04 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882255

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.29478970E-03 DT = 0.14850505E-03 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882255

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.59179979E-03 DT = 0.29701009E-03 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882255

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.11858200E-02 DT = 0.59402018E-03 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291

NI = .0754116207882255

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 1 seconds

TIME = 0.23738603E-02 DT = 0.11880404E-02 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291

NI = .0754116207882255

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.47499411E-02 DT = 0.23760807E-02 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291

NI = .0754116207882255

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.95021025E-02 DT = 0.47521615E-02 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291

NI = .0754116207882255

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.19006425E-01 DT = 0.95043229E-02 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291

NI = .0754116207882256

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.38015071E-01 DT = 0.19008646E-01 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291

NI = .0754116207882257

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.76032363E-01 DT = 0.38017292E-01 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291

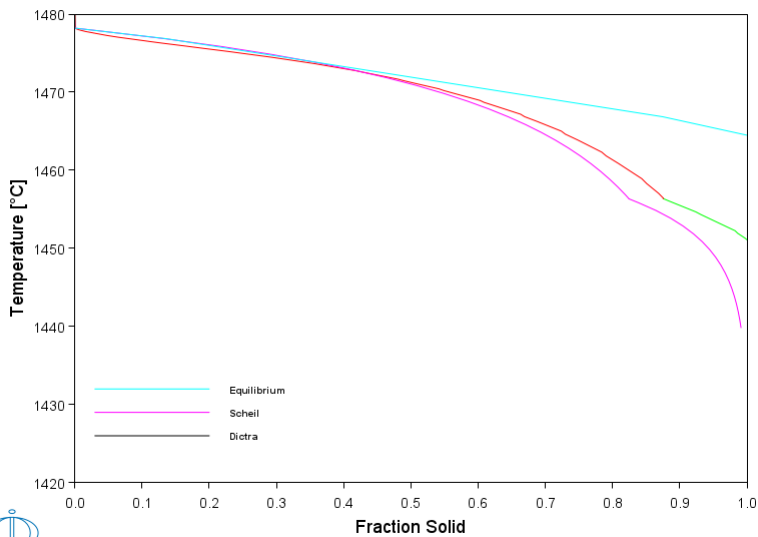


```
DIC> @@  
DIC>  
DIC> set-inter  
--OK--  
DIC>
```

## exb4a-plot

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exb4a\plot.DCM.test"
DIC>
DIC>
DIC> @@ exb4a_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE b4a
DIC> @@
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 2.00000E+02
DIC> read exb4a
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1: set-title Fe-18%Cr-8%Ni
POST-1:
POST-1: @@
POST-1: @@ PLOT THE FRACTION OF SOLID AND COMPARE WITH A SCHEIL-GULLIVER SIMULATION
POST-1: @@ AND EQUILIBRIUM SOLIDIFICATION (DATA ON FILE exb4a.exp)
POST-1: @@
POST-1: enter function fs=1-ivv(liquid);
POST-1: s-d-a x fs
POST-1: s-s-s x n 0 1
POST-1: set-axis-text
AXIS (X, Y OR Z) : x
AUTOMATIC AXIS TEXT (Y OR N) /N/: n
AXIS TEXT : Fraction Solid
POST-1:
POST-1: s-d-a y t-c
POST-1: s-s-s y n 1420 1480
POST-1:
POST-1: s-p-c interface smalta lower
POST-1:
POST-1: app y exb4a.exp 0; 1
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
WORKING ...working ...
WORKING ...working ... OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

Fe-18%Cr-8%Ni



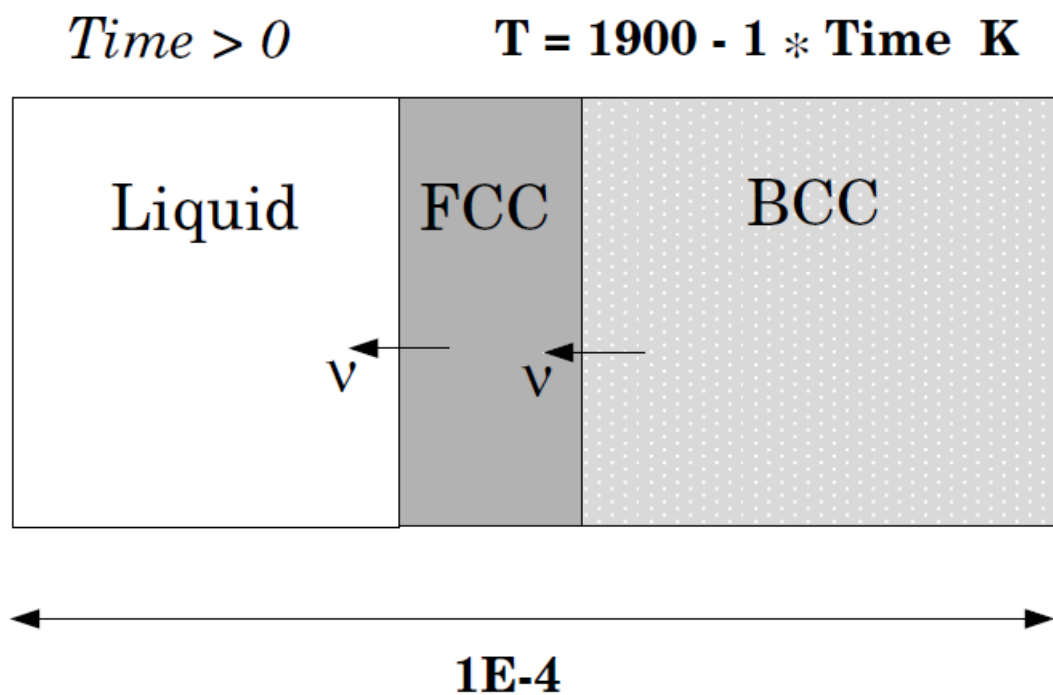
```
POST-1:
POST-1:
POST-1: set-inter
--OK--
POST-1:
```



## Example exb4b

### Solidification path of an Fe-18%Cr-8%Ni alloy: Peritectic reaction

This example is the same as exb4a but now a peritectic reaction is assumed, LIQUID + BCC  $\rightarrow$  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 ThermoCalc.



## exb4b-setup

### SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,  
Stockholm, Sweden

Software running on Windows 64-bit wordlength  
Compiler: Intel Fortran Compiler 2025.0.0  
License library version: 9.7.0.0036  
Linked: Nov 19 2025 at 14:44:36

```
SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exb4b\setup.DCM.test"
```

```
SYS: @@  
SYS: @@ Moving boundary problem.  
SYS: @@ Solidification path of an Fe-18%Cr-8%Ni alloy: Peritectic reaction  
SYS: @@ This example is the same as exb4a but now a peritectic reaction is assumed:  
SYS: @@ LIQUID + BCC -> FCC. Hence the FCC region should appear in between the LIQUID  
SYS: @@ and the BCC. Comparison is made with both a Scheil-Gulliver simulation and  
SYS: @@ equilibrium solidification conditions, both done in Thermo-Calc.  
SYS: @@-----
```

```
SYS: @@  
SYS: @@ exb4b_setup.DCM  
SYS: @@  
SYS: @@  
SYS: @@  
SYS: @@ START BY GOING TO THE DATABASE MODULE  
SYS: @@  
SYS: go da  
THERMODYNAMIC DATABASE module  
Database folder:  
C:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\databases\da  
ta  
Current database: Steels/Fe-Alloys v12.0
```

```
VA /- DEFINED  
DICTRA FCC_A1 REJECTED
```

```
TDB_TCFE12:  
TDB_TCFE12: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA  
TDB_TCFE12: sw fedemo  
Current database: Iron Demo Database v6.0
```

```
VA /- DEFINED
```

```
TDB_FEDEMO:  
TDB_FEDEMO: @@ DEFINE THE SYSTEM TO WORK WITH  
TDB_FEDEMO: def-sys fe ni cr  
FE NI CR  
DEFINED
```

```
TDB_FEDEMO:  
TDB_FEDEMO: @@ EXCLUDE THE THERMODYNAMIC DATA FOR THE PHASES THAT ARE NOT NEEDED  
TDB_FEDEMO: rej ph /all
```

```
GAS:G LIQUID:L BCC_A2  
C14_LAVES CBCC_A12 CHI_A12  
CUB_A13 FCC_A1 HCP_A3  
SIGMA_D8B REJECTED  
TDB_FEDEMO: res ph fcc liq bcc  
FCC_A1 LIQUID:L BCC_A2  
RESTORED
```

```
TDB_FEDEMO:  
TDB_FEDEMO: @@ RETRIEVE DATA FROM THE DATABASE FILE
```

```
TDB_FEDEMO: get  
09:31:42,041 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***  
REINITIATING GES .....  
ELEMENTS .....  
SPECIES .....  
PHASES .....  
PARAMETERS ...  
FUNCTIONS ....
```

Use the command LIST\_REFERENCES to see the list of references for assessed data

```
-OK-
```

```
TDB_FEDEMO:  
TDB_FEDEMO: @@  
TDB_FEDEMO: @@ MOBILITY/DIFFUSIVITY DATA ARE STORED IN A SEPARATE DATABASE FILE.  
TDB_FEDEMO: @@ SWITCH TO A MOBILITY DATABASE AND APPEND THE DATA.  
TDB_FEDEMO: @@  
TDB_FEDEMO: app  
Use one of these databases
```

```
TCFE12 = Steels/Fe-Alloys v12.0  
TCFE9 = Steels/Fe-Alloys v9.3  
SSUB6 = SGTE Substances v6.0  
FEDEMO = Iron Demo Database v6.0  
MOB2 = Alloys Mobility v2.7  
MOBFE7 = Steels/Fe-Alloys Mobility v7.1  
MOBFE4 = Steels/Fe-Alloys Mobility v4.0  
MOBFE2 = Steels/Fe-Alloys Mobility v2.0  
MFEDEMO = Fe-Alloys Mobility demo database v5.0  
USER = User defined Database
```

```
DATABASE NAME /FEDEMO/: mobfe4  
Current database: Steels/Fe-Alloys Mobility v4.0
```

```
VA DEFINED  
B2_BCC REJECTED
```

```
APP: def-sys fe ni cr  
FE NI CR  
DEFINED  
APP: rej ph /all  
BCC_A2 FCC_A1 HCP_A3  
LIQUID:L REJECTED  
APP: res ph fcc liq bcc  
FCC_A1 LIQUID:L BCC_A2  
RESTORED  
APP: get  
ELEMENTS .....  
SPECIES .....
```

PHASES .....  
PARAMETERS ...  
FUNCTIONS ....

Use the command LIST\_REFERENCES to see the list of references for assessed data

-OK-

```
APP: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP
APP: @@
APP: go d-m
NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER GLOBAL CONDITION T
DIC> @@
DIC> @@ LOWER THE TEMPERATURE TO A RATE OF 1 K/s
DIC> @@
DIC> set-cond glob T 0 1900-1*TIME; * N
DIC>
DIC> @@
DIC> @@ ENTER A REGION CALLED smalta
DIC> @@
DIC> enter-region smalta
DIC>
DIC> @@
DIC> @@ ENTER A GEOMETRIC GRID INTO THE REGION
DIC> @@
DIC> enter-grid
REGION NAME : /SMALTA/: smalta
WIDTH OF REGION /1/: 1e-4
TYPE /AUTO/: AUTO
DIC>
DIC> @@
DIC> @@ ENTER active PHASES INTO THE REGION
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /SMALTA/: smalta
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: liq
DIC>
DIC> @@
DIC> @@ ENTER inactive PHASES INTO THE REGION, WITH BOTH PHASES ON THE SAME
DIC> @@ SIDE OF THE LIQUID REGION IN ORDER TO GET A PERITECTIC REACTION.
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inact
ATTACH TO REGION NAMED /SMALTA/: smalta
ATTACHED TO THE RIGHT OF SMALTA /YES/: yes
PHASE NAME: /NONE/: fcc#1
DEPENDENT COMPONENT ? /NI/: fe
REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-5
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inact
ATTACH TO REGION NAMED /SMALTA/: smalta
ATTACHED TO THE RIGHT OF SMALTA /YES/: yes
PHASE NAME: /NONE/: bcc#1
DEPENDENT COMPONENT ? /NI/: fe
REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-5
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> @@
DIC> @@ ENTER THE START COMPOSITION FOR THE LIQUID
DIC> @@
DIC> enter-composition
REGION NAME : /SMALTA/: smalta
PHASE NAME: /LIQUID/: liq
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /CR/: cr lin 18 18
PROFILE FOR /NI/: ni lin 8 8
DIC>
DIC> @@
DIC> @@ THE BOUNDARY CONDITION IS A CLOSED SYSTEM (DEFAULT) AS WE DO NOT SPECIFY
DIC> @@ ANYTHING ELSE.
DIC> @@
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 200
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /20/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ CHECK THE INTERFACE POSITION. THIS IS TO MAKE SURE THAT THE LIQUID REGION
DIC> @@ DOES NOT SHRINK TOO MUCH DURING A TIMESTEP. IN ADDITION, THE TIMESTEP IS
DIC> @@ CONTROLLED BY THE PHASE INTERFACE DISPLACEMENT DURING THE SIMULATION.
DIC> @@
DIC> set-option CHECK_INTERFACE_POSITION yes
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exb4b Y
DIC>
DIC> set-inter
--OK--
DIC>
```

exb4b-run

DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exb4b\run.DCM.test"

DIC>

DIC> @@ exb4b\_run.DCM

DIC>

DIC> @@

DIC> @@ FILE FOR RUNNING EXAMPLE b4b

DIC> @@

DIC>

DIC> @@

DIC> @@ ENTER THE DICTRA MONITOR AND READ THE SET UP FROM FILE

DIC> @@

DIC> go d-m

TIME STEP AT TIME 0.00000E+00

DIC> read exb4b

OK

DIC>

DIC> @@

DIC> @@ START THE SIMULATION

DIC> @@

DIC> sim yes

INFO: Default responses (if any) will be applied during the simulation. Use "SIMULATE\_REACTION NO" instead for manual input.

Region: SMALTA

geometric 0.833333 dense at 0.100000E-03 58 points

DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882254

TOTAL SIZE OF SYSTEM: 1E-04 [m]

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882254

TOTAL SIZE OF SYSTEM: 1E-04 [m]

TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882254

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.71732617E-05 DT = 0.70732617E-05 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882254

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 1 seconds

TIME = 0.21319785E-04 DT = 0.14146523E-04 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882254

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.49612832E-04 DT = 0.28293047E-04 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882254

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.10619893E-03 DT = 0.56586093E-04 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882255

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.21937111E-03 DT = 0.11317219E-03 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882255

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.44571549E-03 DT = 0.22634437E-03 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882255

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.89840423E-03 DT = 0.45268875E-03 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882254

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.18037817E-02 DT = 0.90537750E-03 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882255

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.36145367E-02 DT = 0.18107550E-02 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882255

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 1 seconds

TIME = 0.72360467E-02 DT = 0.36215100E-02 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882255

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.14479067E-01 DT = 0.72430200E-02 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882254

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.28965107E-01 DT = 0.14486040E-01 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882255

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.57937186E-01 DT = 0.28972080E-01 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882256

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.11588135 DT = 0.57944160E-01 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992482 FE = .733068011219292

NI = .0754116207882259

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.23176967 DT = 0.11588832 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291

NI = .0754116207882257

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.46354630 DT = 0.23177664 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: CR = .191520367992484 FE = .73306801121929  
NI = .0754116207882257  
TOTAL SIZE OF SYSTEM: 1E-04 [m]  
CPU time used in timestep 0 seconds  
TIME = 0.92709958 DT = 0.46355328 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: CR = .191520367992481 FE = .733068011219295  
NI = .0754116207882247  
TOTAL SIZE OF SYSTEM: 1E-04 [m]  
CPU time used in timestep 0 seconds  
TIME = 1.8542061 DT = 0.92710656 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: CR = .191520367992471 FE = .733068011219307  
NI = .0754116207882217  
TOTAL SIZE OF SYSTEM: 1E-04 [m]  
CPU time used in timestep 0 seconds

output ignored...

... output resumed

CPU time used in timestep 2 seconds  
5.177595140126708E-008 5.178834804410414E-008 5.138191894024953E-008 2.886814239295225E-009 2.723412029259016E-009  
009 2.348636655291367E-009 1.726157634176269E-009 1.721615066146570E-009 7.501988812431983E-010  
010 5.059921396570343E-014 1.835468130467389E-019  
019 TIME = 198.45743 DT = 0.65536000 SUM OF SQUARES = 0.18289841E-18  
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.25727400E-08 AND -0.25727400E-08  
POSITION OF INTERFACE R\_FCC\_A1 / R\_BCC\_A2 IS 0.10565288E-04  
U-FRACTION IN SYSTEM: CR = .191110607673538 FE = .733546389277693  
NI = .0753430030487688  
TOTAL SIZE OF SYSTEM: 1E-04 [m]  
1 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: R\_BCC\_A2

CPU time used in timestep 2 seconds  
1.314391124064929E-007 1.314463804600718E-007 1.316313914019020E-007 1.238637405936573E-007 1.233278546609284E-007  
007 1.223775491450601E-007 1.201347330734257E-007 1.201382985045189E-007 1.160248294687954E-008  
007 1.077637198778476E-007 9.238001353883692E-008 9.236277415201030E-008 6.495511499158848E-008  
008 2.482668259423956E-008 3.240751602488060E-015 3.722489168076573E-022  
022 TIME = 199.76815 DT = 1.3107200 SUM OF SQUARES = 0.18105038E-21  
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.66845913E-08 AND 0.66845913E-08  
POSITION OF INTERFACE R\_FCC\_A1 / R\_BCC\_A2 IS 0.10574049E-04  
U-FRACTION IN SYSTEM: CR = .191110607676421 FE = .733546389277113  
NI = .075343003046466  
TOTAL SIZE OF SYSTEM: 1E-04 [m]  
30 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: R\_FCC\_A1

CPU time used in timestep 3 seconds  
1.659584620629872E-009 1.659742090425886E-009 1.669036589853826E-009 1.334869919961047E-009 1.322386576707223E-009  
009 1.297312615315943E-009 1.247934639504467E-009 1.247817011528530E-009 1.151997989892740E-009  
009 9.716792536821956E-010 6.570334161547245E-010 6.572262121131271E-010 2.118608423137509E-010  
010 2.518642199310578E-016 3.8499412995576635E-022  
022 TIME = 200.00000 DT = 2.03184798 SUM OF SQUARES = 0.37986776E-21  
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.30153282E-08 AND -0.30153282E-08  
POSITION OF INTERFACE R\_FCC\_A1 / R\_BCC\_A2 IS 0.10573350E-04  
U-FRACTION IN SYSTEM: CR = .191110607675968 FE = .733546389278522  
NI = .0753430030455097  
TOTAL SIZE OF SYSTEM: 1E-04 [m]  
MUST SAVE WORKSPACE ON FILE  
WORKSPACE SAVED ON FILE  
RECLAIMING WORKSPACE

DELETING TIME-RECORD FOR TIME 193.98893  
DELETING TIME-RECORD FOR TIME 197.14672  
DELETING TIME-RECORD FOR TIME 197.14673  
DELETING TIME-RECORD FOR TIME 197.14675  
DELETING TIME-RECORD FOR TIME 197.14679  
DELETING TIME-RECORD FOR TIME 197.14687  
DELETING TIME-RECORD FOR TIME 197.14703  
DELETING TIME-RECORD FOR TIME 197.14735  
DELETING TIME-RECORD FOR TIME 197.14799  
DELETING TIME-RECORD FOR TIME 197.14927  
DELETING TIME-RECORD FOR TIME 197.15183  
DELETING TIME-RECORD FOR TIME 197.15695  
DELETING TIME-RECORD FOR TIME 197.16719  
DELETING TIME-RECORD FOR TIME 197.18767  
DELETING TIME-RECORD FOR TIME 197.22863  
DELETING TIME-RECORD FOR TIME 197.31055  
DELETING TIME-RECORD FOR TIME 197.47439  
DELETING TIME-RECORD FOR TIME 197.80207  
DELETING TIME-RECORD FOR TIME 198.45743

KEEPING TIME-RECORD FOR TIME 199.76815  
AND FOR TIME 200.00000  
WORKSPACE RECLAIMED

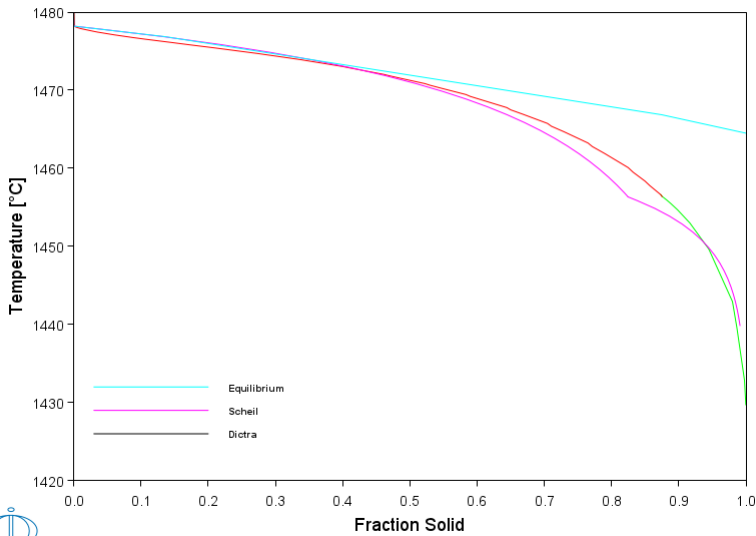
TIMESTEP AT 200.00000 SELECTED

DIC>  
DIC>  
DIC>  
DIC>  
DIC>  
DIC>  
DIC>  
DIC>  
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DIC>  
DIC>  
DIC>  
DIC>  
DIC>  
DIC>  
DIC>  
DIC>  
DIC> @@  
DIC> @@ THE SIMULATION IS FINISHED  
DIC> @@  
DIC>  
DIC> set-inter  
--OK--  
DIC>

exb4b-plot

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exb4b\plot.DCM.test"
DIC>
DIC>
DIC> @@ exb4b_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE b4b
DIC> @@
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 2.00000E+02
DIC> read exb4b
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1: set-title Fe-18%Cr-8%Ni
POST-1:
POST-1: @@
POST-1: @@ PLOT THE FRACTION OF SOLID AND COMPARE WITH A SCHEIL-GULLIVER
POST-1: @@ SIMULATION AND EQUILIBRIUM SOLIDIFICATION (DATA ON FILE exb4.exp)
POST-1: @@
POST-1: enter func fs=1-ivv(liquid);
POST-1: s-d-a x fs
POST-1: s-s-s x n 0 1
POST-1: s-ax-te x n Fraction Solid
POST-1:
POST-1: s-d-a y t-c
POST-1: s-s-s y n 1420 1480
POST-1:
POST-1: s-p-c interf smalta lower
POST-1:
POST-1: app y exb4b.exp 0; 1
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
WORKING ...working ...
WORKING ...working ... OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

Fe-18%Cr-8%Ni



```
POST-1:
POST-1:
POST-1:
POST-1: set-inter
--OK--
POST-1:
```



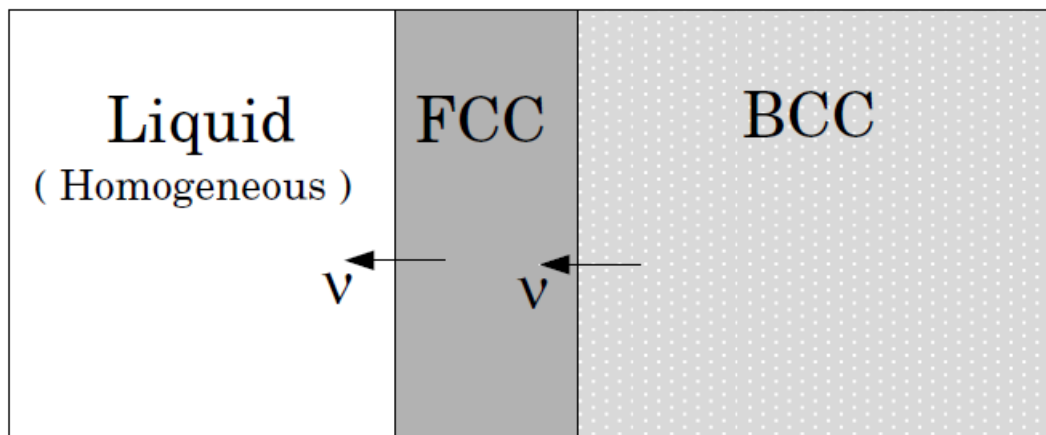
## Example exb4c

### Solidification path of an Fe-18%Cr-8%Ni alloy: Peritectic reaction, homogeneous liquid

This example is the same as exb4b but now the diffusivity data is amended for the LIQUID and a very high value for the diffusivity is used in order to simulate a case where we assume that the composition in the LIQUID is always homogeneous. This case should be considered less realistic than exb4b. Comparison is made with both a Scheil-Gulliver simulation and equilibrium solidification conditions, both made with Thermo-Calc.

*Time > 0*

$$T = 1900 - 1 * \text{Time } K$$



←-----→  
**1E-4**

## exb4c-setup

### SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,  
Stockholm, Sweden

Software running on Windows 64-bit wordlength  
Compiler: Intel Fortran Compiler 2025.0.0  
License library version: 9.7.0.0036  
Linked: Nov 19 2025 at 14:44:36

```
SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exb4c\setup.DCM.test"
```

```
SYS: @@  
SYS: @@ Moving boundary problem.  
SYS: @@ Solidification path of an Fe-18%Cr-8%Ni alloy  
SYS: @@ This example is the same as exb4b but now the diffusivity data is amended  
SYS: @@ for the LIQUID and a high value for the diffusivity is used to simulate a  
SYS: @@ case where it is assumed that the composition in the LIQUID is always  
SYS: @@ homogeneous. This example is less realistic than exb4b.  
SYS: @@ Comparison is made with both a Scheil-Gulliver simulation and equilibrium  
SYS: @@ solidification conditions, both done in Thermo-Calc.
```

```
SYS: @@-----  
SYS:  
SYS: @@ exb4c_setup.DCM  
SYS:  
SYS: @@  
SYS: @@ START BY GOING TO THE DATABASE MODULE  
SYS: @@  
SYS: go da  
THERMODYNAMIC DATABASE module  
Database folder:  
C:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\databases\da  
ta  
Current database: Steels/Fe-Alloys v12.0
```

```
VA /- DEFINED  
DICTRA_FCC_A1 REJECTED  
TDB_TCFE12: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA  
TDB_TCFE12: sw tcfe9  
Current database: Steels/Fe-Alloys v9.3
```

```
VA /- DEFINED  
L12_FCC B2_BCC DICTRA_FCC_A1  
REJECTED
```

```
TDB_TCFE9:  
TDB_TCFE9: @@ DEFINE THE SYSTEM TO WORK WITH  
TDB_TCFE9: def-sys fe ni cr  
FE NI CR  
DEFINED
```

```
TDB_TCFE9:  
TDB_TCFE9: @@ EXCLUDE THE THERMODYNAMIC DATA FOR THE PHASES THAT ARE NOT NEEDED  
TDB_TCFE9: rej ph /all  
LIQUID:L BCC_A2 FCC_A1  
HCP_A3 CBCC_A12 CUB_A13  
SIGMA CHI_A12 LAVES_PHASE_C14  
CR3SI NBNI3 NI3TI  
CRZN17 BETA1 GAMMA  
AL5FE4 CENI2 CENI5  
REJECTED
```

```
TDB_TCFE9: res ph fcc liq bcc  
FCC_A1 LIQUID:L BCC_A2  
RESTORED
```

```
TDB_TCFE9: @@ RETRIEVE DATA FROM THE DATABASE FILE  
TDB_TCFE9: get  
09:38:09,142 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***  
REINITIATING GES .....  
ELEMENTS .....  
SPECIES .....  
PHASES .....  
PARAMETERS ...  
FUNCTIONS .....
```

Use the command LIST\_REFERENCES to see the list of references for assessed data

```
-OK-  
TDB_TCFE9:  
TDB_TCFE9: @@  
TDB_TCFE9: @@ MOBILITY/DIFFUSIVITY DATA ARE STORED IN A SEPARATE DATABASE FILE.  
TDB_TCFE9: @@ SWITCH TO A MOBILITY DATABASE AND APPEND THE DATA.  
TDB_TCFE9: @@  
TDB_TCFE9: app
```

Use one of these databases

```
TCFE12 = Steels/Fe-Alloys v12.0  
TCFE9 = Steels/Fe-Alloys v9.3  
SSUB6 = SGTE Substances v6.0  
FEDEMO = Iron Demo Database v6.0  
MOB2 = Alloys Mobility v2.7  
MOBFE7 = Steels/Fe-Alloys Mobility v7.1  
MOBFE4 = Steels/Fe-Alloys Mobility v4.0  
MOBFE2 = Steels/Fe-Alloys Mobility v2.0  
MFEDEMO = Fe-Alloys Mobility demo database v5.0  
USER = User defined Database
```

```
DATABASE NAME /TCFE9/: mobfe4  
Current database: Steels/Fe-Alloys Mobility v4.0
```

```
VA DEFINED  
B2_BCC REJECTED  
APP: def-sys fe ni cr  
FE NI CR  
DEFINED  
APP: rej ph /all  
BCC_A2 FCC_A1 HCP_A3  
LIQUID:L REJECTED
```

```
APP: res ph fcc liq bcc
FCC_A1          LIQUID:L          BCC_A2
  RESTORED
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....
```

Use the command LIST\_REFERENCES to see the list of references for assessed data

-OK-

```
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP
APP: @@
APP: go d-m
  NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ LIST THE MOBILITIES IN THE LIQUID
DIC> @@
DIC> list-mobility-data ,,liquid
  Sorry, LIST-DATA disabled for this database
DIC>
DIC>
DIC> @@
DIC> @@ AMEND THE DIFFUSIVITY DATA IN THE LIQUID
DIC> @@
DIC> @@ CHANGE TO A DIFFUSIVITY THAT IS 1000 TIMES HIGHER THAN THE
DIC> @@ VALUE IN THE MOBILITY DATABASE. THIS SHOULD BE ENOUGH IN ORDER TO
DIC> @@ ASSUME THAT THE COMPOSITION IN THE LIQUID IS AT ALL TIMES HOMOGENEOUS.
DIC> @@
DIC> amend_mobility_data
PARAMETER:
*** ERROR, PLEASE RE-ENTER EACH PART SEPARATELY
IDENTIFIER: dq
PHASE NAME: liquid&cr
CONSTITUENT: cr
INTERACTING CONSTITUENT:
  DQ(LIQUID&CR#1,CR;0) = Sorry, database encrypted
Do you want to change the number of ranges /NO/: yes
  Reenter ranges
  DQ(LIQUID&CR#1,CR;0) =
LOW TEMPERATURE LIMIT /298.15/: 298.15
FUNCTION: +R*T*LN(1E-06);
HIGH TEMPERATURE LIMIT /6000/: 6000
ANY MORE RANGES /N/: no

*** WARNING, NO MAGNETIC CONTRIBUTION DEFINED

09:38:13,059 [Thread=0] INFO Database: Preparing system for use: MOBFE4_MODIFIED_176363149262716
DIC>
DIC> amend_mobility_data
PARAMETER: dq(liquid&cr,fe;0)
  DQ(LIQUID&CR#1,FE;0) = Sorry, database encrypted
Do you want to change the number of ranges /NO/: y
  Reenter ranges
  DQ(LIQUID&CR#1,FE;0) =
LOW TEMPERATURE LIMIT /298.15/: 298.15 +R*T*LN(1E-06); 6000 n

*** WARNING, NO MAGNETIC CONTRIBUTION DEFINED

DIC>
DIC> am-mob dq(liquid&cr,ni;0)
  DQ(LIQUID&CR#1,NI;0) = Sorry, database encrypted
Do you want to change the number of ranges /NO/: y
  Reenter ranges
  DQ(LIQUID&CR#1,NI;0) =
LOW TEMPERATURE LIMIT /298.15/: 298.15 +R*T*LN(1E-06); 6000 n

*** WARNING, NO MAGNETIC CONTRIBUTION DEFINED

DIC>
DIC> am-mob dq(liquid&ni,cr;0)
  DQ(LIQUID&NI#1,CR;0) = Sorry, database encrypted
Do you want to change the number of ranges /NO/: y
  Reenter ranges
  DQ(LIQUID&NI#1,CR;0) =
LOW TEMPERATURE LIMIT /298.15/: 298.15 +R*T*LN(1E-06); 6000 n

*** WARNING, NO MAGNETIC CONTRIBUTION DEFINED

DIC>
DIC> am-mob dq(liquid&ni,fe;0)
  DQ(LIQUID&NI#1,FE;0) = Sorry, database encrypted
Do you want to change the number of ranges /NO/: y
  Reenter ranges
  DQ(LIQUID&NI#1,FE;0) =
LOW TEMPERATURE LIMIT /298.15/: 298.15 +R*T*LN(1E-06); 6000 n

*** WARNING, NO MAGNETIC CONTRIBUTION DEFINED

DIC>
DIC> am-mob dq(liquid&ni,ni;0)
  DQ(LIQUID&NI#1,NI;0) = Sorry, database encrypted
Do you want to change the number of ranges /NO/: y
  Reenter ranges
  DQ(LIQUID&NI#1,NI;0) =
LOW TEMPERATURE LIMIT /298.15/: 298.15 +R*T*LN(1E-06); 6000 n

*** WARNING, NO MAGNETIC CONTRIBUTION DEFINED

DIC>
DIC> am-mob dq(liquid&fe,cr;0)
  DQ(LIQUID&FE#1,CR;0) = Sorry, database encrypted
```

```

Do you want to change the number of ranges /NO/: y
Reenter ranges
DQ(LIQUID&FE#1,CR;0) =
LOW TEMPERATURE LIMIT /298.15/: 298.15 +R*T*LN(1E-06); 6000 n

*** WARNING, NO MAGNETIC CONTRIBUTION DEFINED

DIC>
DIC> am-mob dq(liquid&fe,fe;0)
DQ(LIQUID&FE#1,FE;0) = Sorry, database encrypted
Do you want to change the number of ranges /NO/: y
Reenter ranges
DQ(LIQUID&FE#1,FE;0) =
LOW TEMPERATURE LIMIT /298.15/: 298.15 +R*T*LN(1E-06); 6000 n

*** WARNING, NO MAGNETIC CONTRIBUTION DEFINED

DIC>
DIC> am-mob dq(liquid&fe,ni;0)
DQ(LIQUID&FE#1,NI;0) = Sorry, database encrypted
Do you want to change the number of ranges /NO/: y
Reenter ranges
DQ(LIQUID&FE#1,NI;0) =
LOW TEMPERATURE LIMIT /298.15/: 298.15 +R*T*LN(1E-06); 6000 n

*** WARNING, NO MAGNETIC CONTRIBUTION DEFINED

DIC>
DIC> list-mobility-data ,,liquid
Sorry, LIST-DATA disabled for this database
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> @@ LOWER THE TEMPERATURE TO A RATE OF 1 K/s
DIC> set-cond glob T 0 1900-1*TIME; * N
DIC>
DIC> @@
DIC> @@ ENTER A REGION CALLED smalta
DIC> @@
DIC> enter-region smalta
DIC>
DIC> @@
DIC> @@ ENTER A GEOMETRIC GRID INTO THE REGION
DIC> @@
DIC> enter-grid
REGION NAME : /SMALTA/: smalta
WIDTH OF REGION /1/: 1e-4
TYPE /AUTO/: AUTO
DIC>
DIC> @@
DIC> @@ ENTER active PHASES INTO THE REGION
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /SMALTA/: smalta
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: liq
DIC>
DIC> @@
DIC> @@ ENTER inactive PHASES INTO THE REGION, BOTH PHASES ON THE SAME SIDE
DIC> @@ OF THE LIQUID REGION IN ORDER TO GET A PERITECTIC REACTION.
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inact
ATTACH TO REGION NAMED /SMALTA/: smalta
ATTACHED TO THE RIGHT OF SMALTA /YES/: yes
PHASE NAME: /NONE/: fcc#1
DEPENDENT COMPONENT ? /NI/: fe
REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-5
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inact
ATTACH TO REGION NAMED /SMALTA/: smalta
ATTACHED TO THE RIGHT OF SMALTA /YES/: yes
PHASE NAME: /NONE/: bcc#1
DEPENDENT COMPONENT ? /NI/: fe
REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-5
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> @@
DIC> @@ ENTER THE START COMPOSITION FOR THE LIQUID
DIC> @@
DIC> enter-composition
REGION NAME : /SMALTA/: smalta
PHASE NAME: /LIQUID/: liq
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /CR/: cr lin 18 18
PROFILE FOR /NI/: ni lin 8 8
09:38:14,800 [Thread-0] INFO Phase: Preparing phase for use: LIQUID
DIC>
DIC> @@
DIC> @@ THE BOUNDARY CONDITION IS A CLOSED SYSTEM (DEFAULT) AS WE DO NOT SPECIFY
DIC> @@ ANYTHING ELSE
DIC> @@
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 200
AUTOMATIC TIMESTEP CONTROL /YES/: yes
MAX TIMESTEP DURING INTEGRATION /20/: 1
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>

```

```
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ CHECK THE INTERFACE POSITION. THIS IS TO MAKE SURE THAT THE LIQUID
DIC> @@ REGION DOES NOT SHRINK TOO MUCH DURING A TIMESTEP. IN ADDITION THE TIMESTEP
DIC> @@ IS CONTROLLED BY THE PHASE INTERFACE DISPLACEMENT DURING THE SIMULATION.
DIC> @@
DIC> set-option CHECK_INTERFACE_POSITION yes
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exb4c Y
DIC>
DIC> set-inter
--OK--
DIC>
```

exb4c-run

DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC-MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exb4c\run.DCM.test"

DIC>

DIC> @@ exb4c\_run.DCM

DIC>

DIC> @@

DIC> @@ FILE FOR RUNNING EXAMPLE b4b

DIC> @@

DIC>

DIC> @@

DIC> @@ ENTER THE DICTRA MONITOR AND READ THE SET UP FROM FILE

DIC> @@

DIC> go d-m

TIME STEP AT TIME 0.00000E+00

DIC> read exb4c

OK

DIC>

DIC> @@

DIC> @@ START THE SIMULATION

DIC> @@

DIC> sim yes

INFO: Default responses (if any) will be applied during the simulation. Use "SIMULATE\_REACTION NO" instead for manual input.

Region: SMALTA

geometric 0.833333 dense at 0.100000E-03 58 points

DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882254

TOTAL SIZE OF SYSTEM: 1E-04 [m]

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882254

TOTAL SIZE OF SYSTEM: 1E-04 [m]

09:39:10,765 [Thread-0] INFO Phase: Preparing phase for use: BCC\_A2

09:39:11,347 [Thread-0] INFO Phase: Preparing phase for use: FCC\_A1

TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882255

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 4 seconds

TIME = 0.30000000E-06 DT = 0.20000000E-06 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882254

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.70000000E-06 DT = 0.40000000E-06 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882255

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.15000000E-05 DT = 0.80000000E-06 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882255

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 1 seconds

TIME = 0.31000000E-05 DT = 0.16000000E-05 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882255

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.63000000E-05 DT = 0.32000000E-05 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882255

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.12700000E-04 DT = 0.64000000E-05 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882255

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.25500000E-04 DT = 0.12800000E-04 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882255

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.51100000E-04 DT = 0.25600000E-04 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882255

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.10230000E-03 DT = 0.51200000E-04 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291

NI = .0754116207882255

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 1 seconds

TIME = 0.20470000E-03 DT = 0.10240000E-03 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882254

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.40950000E-03 DT = 0.20480000E-03 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992484 FE = .73306801121929

NI = .0754116207882254

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.81910000E-03 DT = 0.40960000E-03 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992484 FE = .733068011219291

NI = .0754116207882253

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.16383000E-02 DT = 0.81920000E-03 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992482 FE = .733068011219292

NI = .0754116207882253

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.32767000E-02 DT = 0.16384000E-02 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992479 FE = .733068011219296

NI = .0754116207882255

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.65535000E-02 DT = 0.32768000E-02 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992493 FE = .733068011219281

NI = .0754116207882252



```
DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ THE SIMULATION IS FINISHED
DIC> @@
DIC>
DIC> set-inter
--OK--
DIC>
```

## exb4c-plot

DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exb4c\plot.DCM.test"

DIC>

DIC>

DIC> @@ exb4c\_plot.DCM

DIC>

DIC> @@

DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE b4c

DIC> @@

DIC>

DIC> @@

DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE

DIC> @@

DIC> go d-m

TIME STEP AT TIME 2.00000E+02

DIC> read exb4c

OK

DIC>

DIC> @@

DIC> @@ GO TO THE POST PROCESSOR

DIC> @@

DIC> post

POST-1: POST PROCESSOR VERSION 1.7

Implemented by Bjorn Jonsson

POST-1:

POST-1: set-title Fe-18%Cr-8%Ni

POST-1:

POST-1: @@

POST-1: @@ PLOT THE FRACTION OF SOLID AND COMPARE WITH A SCHEIL-GULLIVER

POST-1: @@ SIMULATION AND EQUILIBRIUM SOLIDIFICATION (DATA ON FILE exb4.exp).

POST-1: @@ IN THIS CASE WE CAN SEE THAT ALL THREE LINES INITIALLY FALL

POST-1: @@ ON THE SAME LINE.

POST-1: @@

POST-1: enter func fs=1-ivv(liquid);

POST-1: s-d-a x fs

POST-1: s-s-s x n 0 1

POST-1: s-ax-te x n Fraction solid

POST-1:

POST-1: s-d-a y t-c

POST-1: s-s-s y n 1420 1480

POST-1:

POST-1: s-p-c interf smalta lower

POST-1:

POST-1: app y exb4c.exp 0; 1

POST-1:

POST-1: SET\_EXP\_FILE\_FORMAT 5

POST-1: MAKE c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\unite\distribution\macroResult.exp Y

WORKING ...

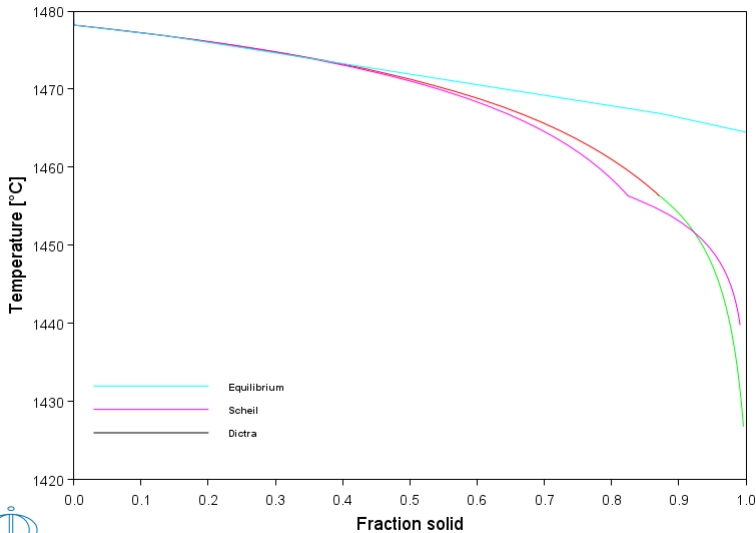
WORKING ...

OST-1: SET\_EXP\_FILE\_FORMAT 10

POST-1:

POST-1: plot

Fe-18%Cr-8%Ni



POST-1:

POST-1:

POST-1: set-inter

--OK--

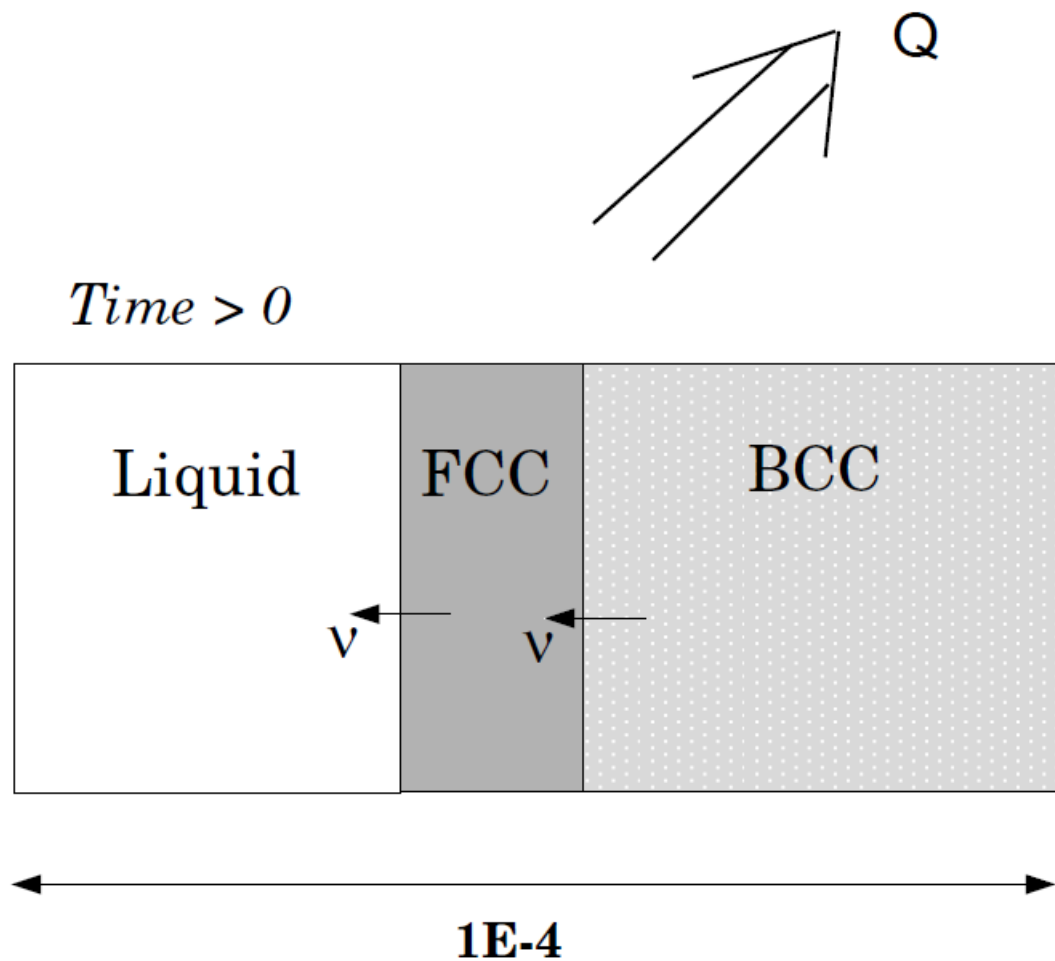
POST-1:



## Example exb4d

### Solidification path of an Fe-18%Cr-8%Ni alloy: Peritectic reaction, heat-flux controls the temperature

This example is the 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.



## exb4d-setup

### SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,  
Stockholm, Sweden

Software running on Windows 64-bit wordlength  
Compiler: Intel Fortran Compiler 2025.0.0  
License library version: 9.7.0.0036  
Linked: Nov 19 2025 at 14:44:36

```
SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exb4d\setup.DCM.test"
```

```
SYS: @@  
SYS: @@ Moving boundary problem.  
SYS: @@ Solidification path of an Fe-18%Cr-8%Ni alloy  
SYS: @@ This example is the same as exb4b but instead of controlling the temperature  
SYS: @@ the amount of heat extracted is given. Comparison is made with both a  
SYS: @@ Scheil-Gulliver simulation and equilibrium solidification conditions,  
SYS: @@ both done in Thermo-Calc.  
SYS: @@-----
```

```
SYS:  
SYS: @@ exb4d_setup.DCM  
SYS:  
SYS: @@  
SYS: @@ START BY GOING TO THE DATABASE MODULE  
SYS: @@  
SYS: go da  
THERMODYNAMIC DATABASE module  
Database folder:  
C:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\databases\da  
ta  
Current database: Steels/Fe-Alloys v12.0
```

```
VA /- DEFINED  
DICTRA_FCC_A1 REJECTED
```

```
TDB_TCFE12:  
TDB_TCFE12: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA
```

```
TDB_TCFE12: sw fedemo  
Current database: Iron Demo Database v6.0
```

```
VA /- DEFINED
```

```
TDB_FEDEMO:  
TDB_FEDEMO: @@ DEFINE THE SYSTEM TO WORK WITH
```

```
TDB_FEDEMO: def-sys fe ni cr  
FE NI CR  
DEFINED
```

```
TDB_FEDEMO:  
TDB_FEDEMO: @@ EXCLUDE THE THERMODYNAMIC DATA FOR THE PHASES THAT ARE NOT NEEDED
```

```
TDB_FEDEMO: rej ph /all  
GAS:G LIQUID:L BCC_A2  
C14_LAVES CBCC_A12 CHI_A12  
CUB_A13 FCC_A1 HCP_A3  
SIGMA_D8B REJECTED
```

```
TDB_FEDEMO: res ph fcc liq bcc  
FCC_A1 LIQUID:L BCC_A2  
RESTORED
```

```
TDB_FEDEMO:  
TDB_FEDEMO: @@ RETRIEVE DATA FROM THE DATABASE FILE
```

```
TDB_FEDEMO: get  
09:45:32,778 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***  
REINITIATING GES .....  
ELEMENTS .....  
SPECIES .....  
PHASES .....  
PARAMETERS ...  
FUNCTIONS ....
```

Use the command LIST\_REFERENCES to see the list of references for assessed data

```
-OK-  
TDB_FEDEMO:  
TDB_FEDEMO: @@  
TDB_FEDEMO: @@ MOBILITY/DIFFUSIVITY DATA ARE STORED IN A SEPARATE DATABASE FILE.  
TDB_FEDEMO: @@ SWITCH TO THE MOBILITY DATABASE AND APPEND THE DATA  
TDB_FEDEMO: @@  
TDB_FEDEMO: app  
Use one of these databases
```

```
TCFE12 = Steels/Fe-Alloys v12.0  
TCFE9 = Steels/Fe-Alloys v9.3  
SSUB6 = SGTE Substances v6.0  
FEDEMO = Iron Demo Database v6.0  
MOB2 = Alloys Mobility v2.7  
MOBFE7 = Steels/Fe-Alloys Mobility v7.1  
MOBFE4 = Steels/Fe-Alloys Mobility v4.0  
MOBFE2 = Steels/Fe-Alloys Mobility v2.0  
MFEDEMO = Fe-Alloys Mobility demo database v5.0  
USER = User defined Database
```

```
DATABASE NAME /FEDEMO/: mobfe2  
Current database: Steels/Fe-Alloys Mobility v2.0  
TCS Steel Mobility Database Version 2.0 from 2011-12-09.
```

```
VA DEFINED
```

```
*** WARNING: This database cannot be used with GES6, temporarily reverting to G  
ES5
```

```
APP: def-sys fe ni cr  
FE NI CR  
DEFINED  
APP: rej ph /all  
BCC_A2 FCC_A1 HCP_A3  
LIQUID:L REJECTED  
APP: res ph fcc liq bcc  
FCC_A1 LIQUID:L BCC_A2  
RESTORED
```

APP: get  
ELEMENTS .....  
SPECIES .....  
PHASES .....  
PARAMETERS ...  
FUNCTIONS .....

Use the command LIST\_REFERENCES to see the list of references for assessed data

-OK-

APP:  
APP: @@  
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP  
APP: @@  
APP: go d-m  
NO TIME STEP DEFINED  
DIC>  
DIC> @@  
DIC> @@ EXTRACT HEAT 91.19 J/mole/s  
DIC> @@  
DIC> set-cond glob Q 0 91.19; \* N  
DIC>  
DIC> @@  
DIC> @@ ENTER AN INITIAL TEMPERATURE  
DIC> @@  
DIC> set-initial-temp 1900  
DIC>  
DIC> @@  
DIC> @@ ENTER A REGION CALLED smalta  
DIC> @@  
DIC> enter-region smalta  
DIC>  
DIC> @@  
DIC> @@ ENTER A GEOMETRIC GRID INTO THE REGION  
DIC> @@  
DIC> enter-grid  
REGION NAME : /SMALTA/: smalta  
WIDTH OF REGION /1/: 1e-4  
TYPE /AUTO/: AUTO  
DIC>  
DIC>  
DIC> @@  
DIC> @@ ENTER active PHASES INTO THE REGION  
DIC> @@  
DIC> enter-phase  
ACTIVE OR INACTIVE PHASE /ACTIVE/: act  
REGION NAME : /SMALTA/: smalta  
PHASE TYPE /MATRIX/: matrix  
PHASE NAME: /NONE/: liq  
DIC>  
DIC> @@  
DIC> @@ ENTER inactive PHASES INTO THE REGION, BOTH PHASES ON THE  
DIC> @@ SAME SIDE OF THE LIQUID REGION TO GET A PERITECTIC REACTION.  
DIC> @@  
DIC> enter-phase  
ACTIVE OR INACTIVE PHASE /ACTIVE/: inact  
ATTACH TO REGION NAMED /SMALTA/: smalta  
ATTACHED TO THE RIGHT OF SMALTA /YES/: yes  
PHASE NAME: /NONE/: fcc#1  
DEPENDENT COMPONENT ? /NI/: fe  
REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-3  
CONDITION TYPE /CLOSED\_SYSTEM/: closed  
DIC>  
DIC> enter-phase  
ACTIVE OR INACTIVE PHASE /ACTIVE/: inact  
ATTACH TO REGION NAMED /SMALTA/: smalta  
ATTACHED TO THE RIGHT OF SMALTA /YES/: yes  
PHASE NAME: /NONE/: bcc#1  
DEPENDENT COMPONENT ? /NI/: fe  
REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-3  
CONDITION TYPE /CLOSED\_SYSTEM/: closed  
DIC>  
DIC> @@  
DIC> @@ ENTER A START COMPOSITION FOR THE LIQUID  
DIC> @@  
DIC> enter-composition  
REGION NAME : /SMALTA/: smalta  
PHASE NAME: /LIQUID/: liq  
DEPENDENT COMPONENT ? /NI/: fe  
COMPOSITION TYPE /MOLE\_FRACTION/: w-p  
PROFILE FOR /CR/: cr lin 18 18  
PROFILE FOR /NI/: ni lin 8 8  
DIC>  
DIC> @@  
DIC> @@ THE BOUNDARY CONDITION IS A CLOSED SYSTEM (DEFAULT) AS WE DO NOT SPECIFY  
DIC> @@ ANYTHING ELSE  
DIC> @@  
DIC> @@  
DIC> @@  
DIC> @@ SET THE SIMULATION TIME  
DIC> @@  
DIC> set-simulation-time  
END TIME FOR INTEGRATION /.1/: 200  
AUTOMATIC TIMESTEP CONTROL /YES/:  
MAX TIMESTEP DURING INTEGRATION /20/:  
INITIAL TIMESTEP : /1E-07/:  
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:  
DIC>  
DIC>  
DIC> @@  
DIC> @@ CHECK THE INTERFACE POSITION. THIS IS TO MAKE SURE THAT THE LIQUID REGION  
DIC> @@ DOES NOT SHRINK TOO MUCH DURING A TIMESTEP. IN ADDITION THE TIMESTEP IS  
DIC> @@ CONTROLLED BY THE PHASE INTERFACE DISPLACEMENT DURING THE SIMULATION.  
DIC> @@  
DIC> set-option CHECK\_INTERFACE\_POSITION yes  
DIC> set-option ALLOW\_AUTOMATIC\_SWITCHING\_OF\_VARYING\_ELE no  
DIC>  
DIC> @@  
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT

```
DIC> @@  
DIC> save exb4d Y  
DIC>  
DIC> set-inter  
--OK--  
DIC>
```

exb4d-run

DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC-MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exb4d\run.DCM.test"

DIC>

DIC> @@ exb4d\_run.DCM

DIC>

DIC> @@

DIC> @@ FILE FOR RUNNING EXAMPLE b4b

DIC> @@

DIC>

DIC> @@

DIC> @@ ENTER THE DICTRA MONITOR AND READ THE SET UP FROM FILE

DIC> @@

DIC> go d-m

TIME STEP AT TIME 0.00000E+00

DIC> read exb4d

OK

DIC>

DIC> @@

DIC> @@ START THE SIMULATION

DIC> @@

DIC> sim

INFO: Default responses (if any) will be applied during the simulation. Use "SIMULATE\_REACTION NO" instead for manual input.

Region: SMALTA

geometric 0.833333 dense at 0.100000E-03 58 points

DEGREE OF IMPLICITITY SET TO TRAPEZOIDAL RULE

TEMPERATURE: 1900.0000 ENTHALPY: 73940.238

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882254

TOTAL SIZE OF SYSTEM: 1E-04 [m]

TEMPERATURE: 1900.0000 ENTHALPY: 73940.238

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882254

TOTAL SIZE OF SYSTEM: 1E-04 [m]

3.863918610063472E-003 3.864691456625800E-003 3.836438015512440E-012 3.779855469070435E-021 TIME = 0.10000000E-

06 DT = 0.10000000E-06 SUM OF SQUARES = 0.37798555E-20

TEMPERATURE: 1900.0000 ENTHALPY: 73940.238

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882254

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

3.862931742460856E-003 3.863704392801343E-003 3.852485041161569E-012 3.839899033642034E-021 TIME = 0.32558285E-

04 DT = 0.32458285E-04 SUM OF SQUARES = 0.38398990E-20

TEMPERATURE: 1899.9999 ENTHALPY: 73940.235

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882254

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

1.543459994304474E-004 1.543768898716917E-004 6.272825248046769E-015 6.272825248046769E-015 1.748662816395658E-

012 2.033049489852038E-026 TIME = 0.97474855E-04 DT = 0.64916570E-04 SUM OF SQUARES = 0.20330495E-25

TEMPERATURE: 1899.9998 ENTHALPY: 73940.229

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882254

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

1.541471559964326E-004 1.541780265386606E-004 6.117175752838604E-015 6.117175752838604E-015 1.746048955043138E-

012 7.808133759302838E-027 TIME = 0.22730799E-03 DT = 0.12983314E-03 SUM OF SQUARES = 0.78081338E-26

TEMPERATURE: 1899.9995 ENTHALPY: 73940.217

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882254

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

1.537498535323091E-004 1.537806842725726E-004 6.054228890287506E-015 6.054228890287506E-015 1.744983991813252E-

012 4.031734655644627E-028 TIME = 0.48697427E-03 DT = 0.25966628E-03 SUM OF SQUARES = 0.40317347E-27

TEMPERATURE: 1899.9990 ENTHALPY: 73940.194

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882254

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

1.529567862365470E-004 1.529875373698845E-004 6.112027788702609E-015 6.112027788702609E-015 1.745963698251880E-

012 6.323380288970213E-027 TIME = 0.10063068E-02 DT = 0.51933256E-03 SUM OF SQUARES = 0.63233803E-26

TEMPERATURE: 1899.9980 ENTHALPY: 73940.146

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882254

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

1.513768021657984E-004 1.514073940879291E-004 6.043942282925615E-015 6.043942282925615E-015 1.744811919408466E-

012 3.194088859274850E-026 TIME = 0.20449719E-02 DT = 0.10386651E-02 SUM OF SQUARES = 0.31940889E-25

TEMPERATURE: 1899.9959 ENTHALPY: 73940.051

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882254

TOTAL SIZE OF SYSTEM: 1E-04 [m]

output ignored...

... output resumed

6.526947291966718E-016 2.176914347918803E-012 6.758339541147391E-016 4.862972565338431E-014 6.758299021566657E-016  
016 1.331491327197846E-014 6.758278754576276E-016 2.176914347918803E-012 6.770119896407681E-016  
016 4.863686018216541E-014 6.770119896256407E-016 1.331295203507202E-014 6.770119896406882E-016

ERROR RETURN FROM NS01A BECAUSE 7 CALLS OF CALFUN FAILED TO IMPROVE THE RESIDUALS

\*\*\* ERROR 1890 IN DCNS01: ERROR RETURN FROM NS01A

ACCEPTING RESIDUAL 6.474221809112478E-016

TIME = 196.62822 DT = 0.50039062 SUM OF SQUARES = 0.64742218E-15

CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.10693836E-06 AND 0.10693836E-06

POSITION OF INTERFACE R\_FCC\_A1 / R\_BCC\_A2 IS 0.56177110E-05

TEMPERATURE: 1704.3501 ENTHALPY: 55952.004

U-FRACTION IN SYSTEM: CR = .191404547713131 FE = .733207675247709

NI = .0753877770391602

TOTAL SIZE OF SYSTEM: 1E-04 [m]

2 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: R\_FCC\_A1

CPU time used in timestep 4 seconds

2.08561990648250E-002 2.085607222032711E-002 2.085621533545253E-002 2.085576666994037E-002 1.838624076190998E-

004 2.777448029025951E-008 1.172154718885017E-012 1.176872420307869E-

016 TIME = 197.62900 DT = 1.0007812 SUM OF SQUARES = 0.64492777E-18

CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.96915158E-07 AND 0.96915158E-07

POSITION OF INTERFACE R\_FCC\_A1 / R\_BCC\_A2 IS 0.57147018E-05  
TEMPERATURE: 1702.1838 ENTHALPY: 55860.743  
U-FRACTION IN SYSTEM: CR = .191404547710647 FE = .733207675250861  
NI = .0753877770384929  
TOTAL SIZE OF SYSTEM: 1E-04 [m]  
4 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: R\_FCC\_A1

CPU time used in timestep 1 seconds  
9.289180495426896E-002 9.289134677966003E-002 9.289187984954131E-002 9.289090699396182E-002 1.311355950720215E-  
003 1.942478159053459E-006 1.783512836526358E-009 1.458971972315604E-014 7.521312597589378E-  
016 7.733559749119407E-013 7.306922173050556E-016 2.633684296895411E-012 3.156993077491077E-  
015 1.765608124367762E-013 3.114127328623319E-015 7.790822239448126E-013 3.114127328633347E-  
015 2.633684296895411E-012 3.124233446951364E-015 1.765608124367762E-013 3.124233446951364E-  
015 7.791020958241830E-013 3.124233446599819E-015 2.633684296895411E-012 3.124250942602367E-015

ERROR RETURN FROM NS01A BECAUSE 7 CALLS OF CALFUN FAILED TO IMPROVE THE RESIDUALS  
RESCALING  
0.390500590918939 0.390499539696817 0.390500744405486 0.390498743964520 6.889379771077427E-  
003 3.533957984476008E-005 1.544573087161034E-007 1.668987402221781E-010 4.957783160626112E-  
013 3.682620229834167E-017 TIME = 199.63056 DT = 2.0015625 SUM OF SQUARES = 0.41039585E-18  
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.17551620E-06 AND 0.17551620E-06  
POSITION OF INTERFACE R\_FCC\_A1 / R\_BCC\_A2 IS 0.60660085E-05  
TEMPERATURE: 1693.5904 ENTHALPY: 55500.051  
U-FRACTION IN SYSTEM: CR = .191404547700898 FE = .73320767526384  
NI = .0753877770352613  
TOTAL SIZE OF SYSTEM: 1E-04 [m]  
27 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: R\_FCC\_A1

CPU time used in timestep 5 seconds  
1.905099861687314E-003 1.905077963207769E-003 1.905104398436018E-003 1.904970649637467E-003 2.711057408494554E-  
007 2.043643386336800E-011 4.573896082428711E-016 1.642536649722262E-015 4.026736315958231E-  
014 8.936143695945022E-015 2.288228284524920E-012 8.432486421868068E-  
025 TIME = 200.00000 DT = 0.36944098 SUM OF SQUARES = 0.54955452E-24  
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.13283678E-06 AND 0.13283678E-06  
POSITION OF INTERFACE R\_FCC\_A1 / R\_BCC\_A2 IS 0.61150838E-05  
TEMPERATURE: 1692.7947 ENTHALPY: 55466.361  
U-FRACTION IN SYSTEM: CR = .191404547696881 FE = .733207675261175  
NI = .0753877770419439  
TOTAL SIZE OF SYSTEM: 1E-04 [m]

MUST SAVE WORKSPACE ON FILE  
WORKSPACE SAVED ON FILE  
RECLAIMING WORKSPACE  
DELETING TIME-RECORD FOR TIME 195.06449  
DELETING TIME-RECORD FOR TIME 195.68998  
DELETING TIME-RECORD FOR TIME 195.75253  
DELETING TIME-RECORD FOR TIME 195.87763  
DELETING TIME-RECORD FOR TIME 196.12782  
DELETING TIME-RECORD FOR TIME 196.62822  
DELETING TIME-RECORD FOR TIME 197.62900

KEEPING TIME-RECORD FOR TIME 199.63056  
AND FOR TIME 200.00000  
WORKSPACE RECLAIMED

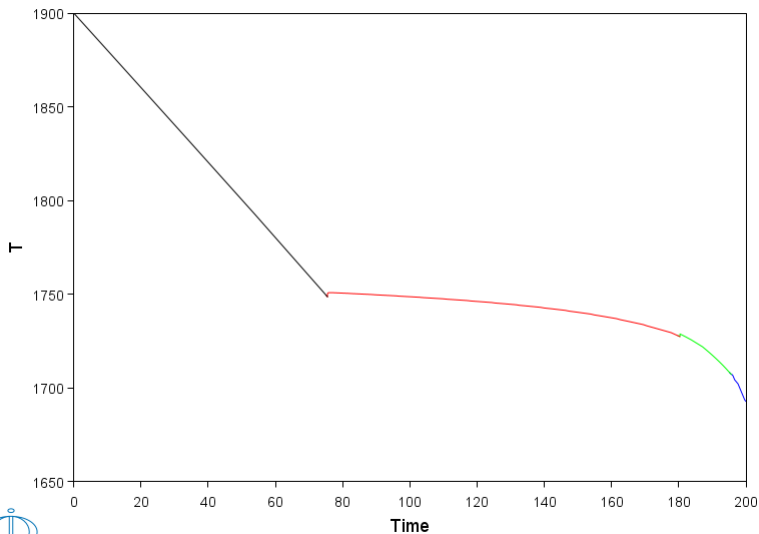
TIMESTEP AT 200.000000 SELECTED

DIC>  
DIC>  
DIC> -1E-6  
NO SUCH COMMAND, USE HELP  
\*\*\* ERROR 666 IN DICMON: NO SUCH COMMAND  
ERROR 666 RESET  
MACRO WAS TERMINATED DUE TO ERROR  
DIC>

## exb4d-plot

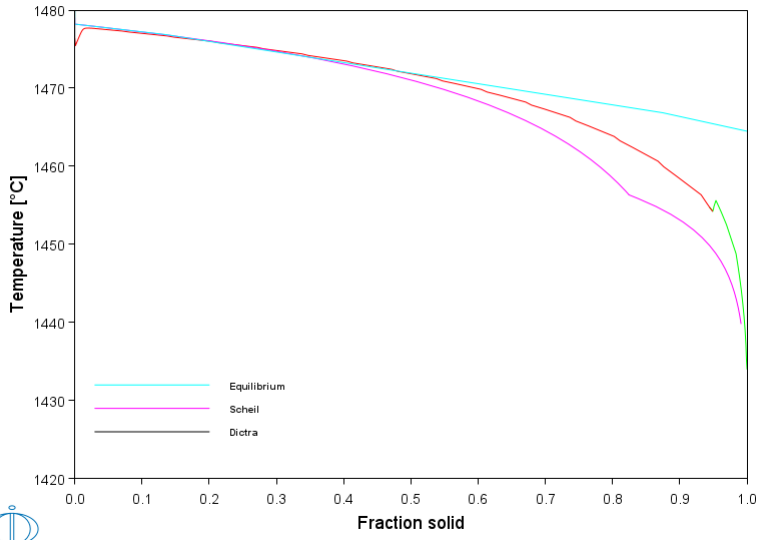
```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exb4d\plot.DCM.test"
DIC>
DIC>
DIC> @@ exb4d_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE b4b
DIC> @@
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 2.00000E+02
DIC> read exb4d
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1: set-title Fe-18%Cr-8%Ni
POST-1:
POST-1: @@
POST-1: @@ PLOT THE FRACTION OF SOLID AND COMPARE WITH SCHEIL-GULLIVER
POST-1: @@ SIMULATION AND EQUILIBRIUM SOLIDIFICATION (DATA ON FILE exb4.exp)
POST-1: @@
POST-1: s-d-a x time
INFO: Time is set as independent variable
POST-1: s-d-a y T
POST-1: s-p-c inter first
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
WORKING ...working ...
WORKING ...working ... OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

Fe-18%Cr-8%Ni



```
POST-1:
POST-1: Hit RETURN to continue
POST-1: enter func fs=1-ivv(liquid);
POST-1: s-d-a x fs
POST-1: s-s-s x n 0 1
POST-1: s-ax-te x n Fraction solid
POST-1:
POST-1: s-d-a y t-c
POST-1: s-s-s y n 1420 1480
POST-1:
POST-1: s-p-c interf smalta lower
POST-1:
POST-1: app y exb4d.exp 0; 1
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
WORKING ...working ...
WORKING ...working ... OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

Fe-18%Cr-8%Ni



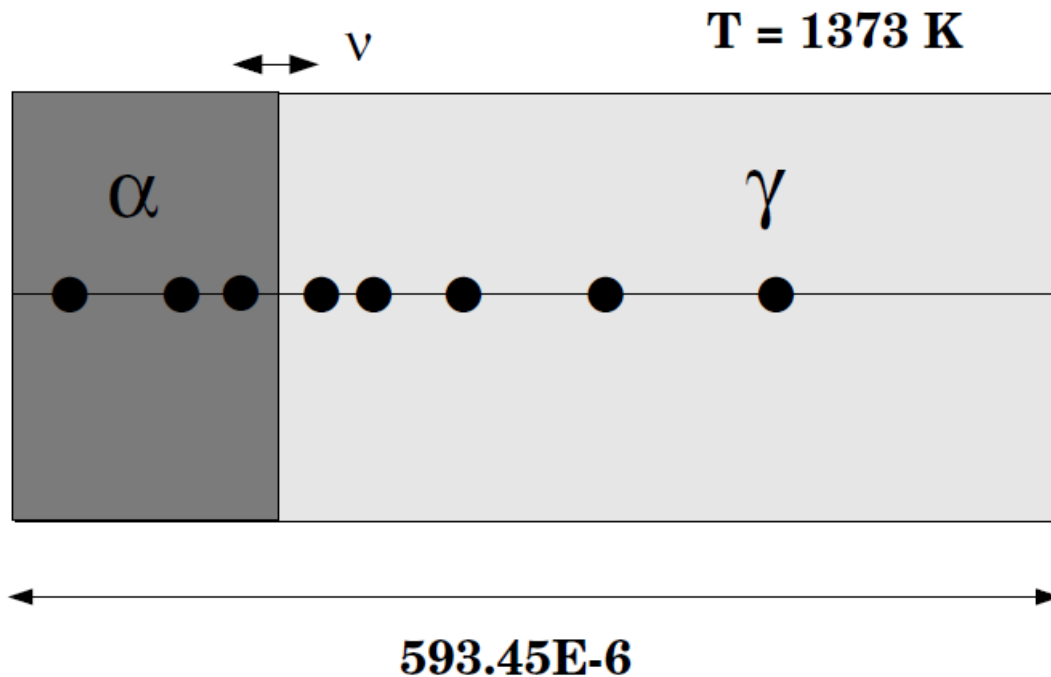
POST-1:  
POST-1:  
POST-1:  
POST-1: set-inter  
--OK--  
POST-1:



## Example exb5

### $\gamma/\alpha/\gamma$ 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 A in M. Kajihara, C.-B. Lim and M. Kikuchi: ISIJ International 33 (1993), pp. 498-507. See also M. Kajihara and M. Kikuchi: Acta Metall.Mater. 41 (1993), pp.2045-2059.



## exb5-setup

### SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,  
Stockholm, Sweden

Software running on Windows 64-bit wordlength  
Compiler: Intel Fortran Compiler 2025.0.0  
License library version: 9.7.0.0036  
Linked: Nov 19 2025 at 14:44:36

```
SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exb5\setup.DCM.test"
```

```
SYS: @@
```

```
SYS: @@ Moving boundary problem.
```

```
SYS: @@ Ternary diffusion couple of Fe-Ni-Cr alloys
```

```
SYS: @@ This example demonstrates the evaluation of a ternary Fe-Cr-Ni diffusion
```

```
SYS: @@ couple. A thin slice of alpha phase (38%Cr, 0%Ni) is clamped between
```

```
SYS: @@ two thicker slices of gamma phase (27%Cr, 20%Ni). The assembly is
```

```
SYS: @@ subsequently heat treated at 1373 K. This example corresponds to diffusion
```

```
SYS: @@ couple A in M. Kajihara, C.-B. Lim and M. Kikuchi: ISIJ International
```

```
SYS: @@ 33 (1993), pp. 498-507. See also M. Kajihara and M. Kikuchi: Acta Metall.Mater.
```

```
SYS: @@ 41 (1993), pp.2045-2059.
```

```
SYS: @@-----
```

```
SYS:
```

```
SYS: @@ exb5_setup.DCM
```

```
SYS:
```

```
SYS: @@
```

```
SYS: @@ GO TO A DATABASE AND READ THE THERMODYNAMIC AND KINETIC DATA
```

```
SYS: @@
```

```
SYS: go da
```

```
THERMODYNAMIC DATABASE module
```

```
Database folder:
```

```
C:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\databases\da
```

```
ta
```

```
Current database: Steels/Fe-Alloys v12.0
```

```
VA /- DEFINED
```

```
DICTRA_FCC_A1 REJECTED
```

```
TDB_TCFE12: sw fedemo
```

```
Current database: Iron Demo Database v6.0
```

```
VA /- DEFINED
```

```
TDB_FEDEMO: def-sys cr fe ni
```

```
CR FE NI
```

```
DEFINED
```

```
TDB_FEDEMO: rej-ph /all
```

```
GAS:G LIQUID:L BCC_A2
```

```
C14_LAVES CBCC_A12 CHI_A12
```

```
CUB_A13 FCC_A1 HCP_A3
```

```
SIGMA_D8B REJECTED
```

```
TDB_FEDEMO: res-ph bcc,fcc
```

```
BCC_A2 FCC_A1 RESTORED
```

```
TDB_FEDEMO: get
```

```
09:51:29,398 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
```

```
REINITIATING GES .....
```

```
ELEMENTS .....
```

```
SPECIES .....
```

```
PHASES .....
```

```
PARAMETERS ...
```

```
FUNCTIONS .....
```

```
Use the command LIST_REFERENCES to see the list of references for assessed data
```

```
-OK-
```

```
TDB_FEDEMO:
```

```
TDB_FEDEMO: app
```

```
Use one of these databases
```

```
TCFE12 = Steels/Fe-Alloys v12.0
```

```
TCFE9 = Steels/Fe-Alloys v9.3
```

```
SSUB6 = SGTE Substances v6.0
```

```
FEDEMO = Iron Demo Database v6.0
```

```
MOB2 = Alloys Mobility v2.7
```

```
MOBFE7 = Steels/Fe-Alloys Mobility v7.1
```

```
MOBFE4 = Steels/Fe-Alloys Mobility v4.0
```

```
MOBFE2 = Steels/Fe-Alloys Mobility v2.0
```

```
MFEDEMO = Fe-Alloys Mobility demo database v5.0
```

```
USER = User defined Database
```

```
DATABASE NAME /FEDEMO/: mfedemo
```

```
Current database: Fe-Alloys Mobility demo database v5.0
```

```
VA DEFINED
```

```
APP: def-sys cr fe ni
```

```
CR FE NI
```

```
DEFINED
```

```
APP: rej-ph /all
```

```
BCC_A2 FCC_A1 LIQUID:L
```

```
REJECTED
```

```
APP: res-ph bcc,fcc
```

```
BCC_A2 FCC_A1 RESTORED
```

```
APP: get
```

```
ELEMENTS .....
```

```
SPECIES .....
```

```
PHASES .....
```

```
PARAMETERS ...
```

```
FUNCTIONS .....
```

```
Use the command LIST_REFERENCES to see the list of references for assessed data
```

```
-OK-
```

```
APP:
```

```
APP: @@
```

```
APP: @@ GO TO THE DICTRA MODULE TO SET UP THE SIMULATION
```

```
APP: @@
```

```
APP: go d-m
```

```
NO TIME STEP DEFINED
```

```
DIC>
```

```
DIC> @@
DIC> @@ SET THE GLOBAL CONDITIONS
DIC> @@
DIC> set-cond glob T 0 1373; * N
DIC>
DIC> @@
DIC> @@ ENTER TWO REGIONS, ONE FOR EACH PHASE
DIC> @@
DIC> enter-region alpha
DIC> enter-region gamma
ATTACH TO REGION NAMED /ALPHA/:
ATTACHED TO THE RIGHT OF ALPHA /YES/:
DIC> @@
DIC> @@ ENTER THE GRID SIZE AND SPACINGS
DIC> @@
DIC> enter-grid alpha 93.45E-6 AUTO
DIC> enter-grid gamma 500.0E-6 AUTO
DIC>
DIC> @@
DIC> @@ SPECIFY WHICH PHASE GOES INTO WHICH REGION
DIC> @@
DIC> enter-phase act alpha matrix bcc
DIC> enter-phase act gamma matrix fcc
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITIONS IN THE PHASES
DIC> @@ IT IS IMPORTANT NOT TO PUT 0%NI IN PHASE BCC,
DIC> @@ ENTER SOME SMALL VALUE INSTEAD
DIC> @@
DIC> enter-composition
REGION NAME : /ALPHA/: alpha
PHASE NAME: /BCC_A2/: bcc
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE FRACTION/: w-f
PROFILE FOR /CR/: cr lin .38 .38
PROFILE FOR /NI/: ni lin 1e-5 1e-5
DIC>
DIC> enter-composition
REGION NAME : /GAMMA/: gamma
PHASE NAME: /FCC_A1/: fcc
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE FRACTION/: w-f
PROFILE FOR /CR/: cr lin .27 .27
PROFILE FOR /NI/: ni lin .28 .28
DIC>
DIC> @@
DIC> @@ SPECIFY THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 36E5
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /360000/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC> SAVE exb5 Y
DIC>
DIC> set-inter
--OK--
DIC>
```

exb5-run

DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exb5\run.DCM.test"

DIC>

DIC>

DIC> @@ exb5\_run.DCM

DIC>

DIC> @@

DIC> @@ FILE FOR RUNNING EXAMPLE b5

DIC> @@

DIC>

DIC> @@

DIC> @@ ENTER THE DICTRA MONITOR AND READ THE SET UP FROM FILE

DIC> @@

DIC> go d-m

TIME STEP AT TIME 0.000000E+00

DIC> read exb5

OK

DIC>

DIC> @@

DIC> @@ START THE SIMULATION

DIC> @@

DIC> simulate

INFO: Default responses (if any) will be applied during the simulation. Use "SIMULATE\_REACTION NO" instead for manual input.

Region: ALPHA

geometric 0.833333 dense at 0.934500E-04 58 points

Region: GAMMA

geometric 1.20000 dense at 0.00000 57 points

DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE

Trying old scheme 4

GENERATING STARTING VALUES FOR CELL # 1 INTERFACE # 2

DETERMINING INITIAL EQUILIBRIUM VALUES

CALCULATING STARTING VALUES: 9 EQUILIBRIUM CALCULATIONS \*\*\* ERROR 1611 IN QTHISS: TOO MANY ITERATIONS

Give the command INFO TROUBLE for help

DONE 6 OUT OF 9 \*\*\* ERROR 1611 IN QTHISS: TOO MANY ITERATIONS

Give the command INFO TROUBLE for help

DONE 9 OUT OF 9 try 1 failed

try 2 failed

try 3 failed

DETERMINED ACTIVITIES ACR(NI) 2.00457405352E-04

UNABLE TO OBTAIN GOOD STARTING VALUE USING THE OLD SCHEME

Trying new scheme

GENERATING STARTING VALUES FOR CELL # 1 INTERFACE # 2

DETERMINING INITIAL EQUILIBRIUM VALUES

CALCULATING STARTING VALUES: 18 EQUILIBRIUM CALCULATIONS DONE 1 OUT OF 18

04

U-FRACTION IN SYSTEM: CR = .305280432605602 FE = .471672082221692

NI = .223047485172706

TOTAL SIZE OF SYSTEM: 5.9345E-04 [m]

U-FRACTION IN SYSTEM: CR = .305280432605602 FE = .471672082221692

NI = .223047485172706

TOTAL SIZE OF SYSTEM: 5.9345E-04 [m]

0.188105170261261 0.188121771941940 0.188103832481157 2.779256912641678E-002 1.57587327625931E-

02 4.124896339306979E-004 5.143494508822299E-006 1.261017697429432E-007 1.146914635563084E-

03 4.569468148236086E-018 TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.36275554E-17

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.60953435 AND -0.60953435

POSITION OF INTERFACE ALPHA / GAMMA IS 0.93389047E-04

U-FRACTION IN SYSTEM: CR = .305280432987362 FE = .471672082631556

NI = .223047484381082

TOTAL SIZE OF SYSTEM: 5.9345E-04 [m]

CPU time used in timestep 0 seconds

1.779115261825630E-002 1.779392776600443E-002 1.779119834418420E-002 1.171890049662968E-004 2.748372297173524E-

006 2.566237882147770E-009 4.187390465705088E-011 2.391880057472405E-011 1.751722898145469E-

010 2.214253811978612E-011 2.214705984352612E-011 2.221152750725942E-011 1.378934454006804E-

010 2.207016118385424E-011 2.205772303523283E-011 2.203286514228735E-011 1.431307667841569E-

010 2.199433512505058E-011 2.191738542649979E-011 2.176389334332356E-011 1.428585240875449E-

010 2.145856875370743E-011 2.085455566267156E-011 1.967299285885644E-011 1.409172320328755E-

010 1.741542504685778E-011 1.332101882153871E-011 6.798640299110062E-012 1.294183760643604E-

010 2.916715438702114E-013 2.029106667799615E-017 TIME = 0.10010000E-03 DT = 0.10000000E-

03 SUM OF SQUARES = 0.21761994E-17

CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.12330140E-06 AND 0.12330140E-06

POSITION OF INTERFACE ALPHA / GAMMA IS 0.93389059E-04

U-FRACTION IN SYSTEM: CR = .305280432986384 FE = .471672082632922

output ignored...

... output resumed

TOTAL SIZE OF SYSTEM: 5.9345E-04 [m]

3 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: GAMMA

CPU time used in timestep 1 seconds

3.539125802032234E-006 3.543659658201383E-006 3.532577278999217E-006 9.534683939078569E-009 7.957515052919483E-

012 2.728196745347149E-017 TIME = 2171568.0 DT = 360000.00 SUM OF SQUARES = 0.28871801E-18

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.77000552E-11 AND -0.77000552E-11

POSITION OF INTERFACE ALPHA / GAMMA IS 0.94156438E-04

U-FRACTION IN SYSTEM: CR = .305280433881236 FE = .471672081895649

NI = .223047484223115

TOTAL SIZE OF SYSTEM: 5.9345E-04 [m]

5 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: GAMMA

CPU time used in timestep 2 seconds

1.910913055911638E-006 1.913835739725634E-006 1.906176349958440E-006 9.785587177056605E-009 1.003840702286194E-

009 5.909964798564086E-014 4.174120598153043E-

021 TIME = 2531568.0 DT = 360000.00 SUM OF SQUARES = 0.65968456E-22

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.66472069E-11 AND -0.66472069E-11

POSITION OF INTERFACE ALPHA / GAMMA IS 0.91763444E-04

U-FRACTION IN SYSTEM: CR = .305280433878176 FE = .471672081912897

NI = .223047484208926

TOTAL SIZE OF SYSTEM: 5.9345E-04 [m]

4 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: GAMMA

CPU time used in timestep 1 seconds

7.763352915100632E-007 7.779573673555813E-007 7.733565297287081E-007 4.526933721971292E-009 8.782730891506061E-

010 1.309666700496760E-014 5.775057878519565E-

022 TIME = 2891568.0 DT = 360000.00 SUM OF SQUARES = 0.44562247E-23

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.59518229E-11 AND -0.59518229E-11

POSITION OF INTERFACE ALPHA / GAMMA IS 0.89620787E-04

U-FRACTION IN SYSTEM: CR = .305280433882621 FE = .47167208190679

```

          NI = .223047484210588
TOTAL SIZE OF SYSTEM: 5.9345E-04 [m]
  5 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: GAMMA

CPU time used in timestep 1 seconds
3.935309888418612E-007 3.945717906831514E-007 3.914381531552864E-007 2.539202899605864E-009 7.956616734816313E-
010 1.322489446442925E-014 3.602395902059583E-
022 TIME = 3251568.0 DT = 360000.00 SUM OF SQUARES = 0.67210309E-23
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.54346504E-11 AND -0.54346504E-11
POSITION OF INTERFACE ALPHA / GAMMA IS 0.87664313E-04
U-FRACTION IN SYSTEM: CR = .305280433881722 FE = .471672081907878
          NI = .223047484210401
TOTAL SIZE OF SYSTEM: 5.9345E-04 [m]
  3 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: GAMMA

CPU time used in timestep 2 seconds
9.202763943316840E-008 9.248958667797537E-008 9.100785475982176E-008 2.192811281867058E-009 1.186326034958367E-
009 7.520254053842260E-011 1.716230829578630E-
016 TIME = 3600000.0 DT = 348432.01 SUM OF SQUARES = 0.12708047E-16
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.50038068E-11 AND -0.50038068E-11
POSITION OF INTERFACE ALPHA / GAMMA IS 0.85920827E-04
U-FRACTION IN SYSTEM: CR = .305280433889326 FE = .471672081890306
          NI = .223047484220368
TOTAL SIZE OF SYSTEM: 5.9345E-04 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 0.0000000
DELETING TIME-RECORD FOR TIME 0.10000000E-06
DELETING TIME-RECORD FOR TIME 0.10010000E-03
DELETING TIME-RECORD FOR TIME 0.30010000E-03
DELETING TIME-RECORD FOR TIME 0.70010000E-03
DELETING TIME-RECORD FOR TIME 0.15001000E-02
DELETING TIME-RECORD FOR TIME 0.31001000E-02
DELETING TIME-RECORD FOR TIME 0.63001000E-02
DELETING TIME-RECORD FOR TIME 0.12700100E-01
DELETING TIME-RECORD FOR TIME 0.25500100E-01
DELETING TIME-RECORD FOR TIME 0.51100100E-01
DELETING TIME-RECORD FOR TIME 0.10230010
DELETING TIME-RECORD FOR TIME 0.20470010
DELETING TIME-RECORD FOR TIME 0.37017658
DELETING TIME-RECORD FOR TIME 0.70112954
DELETING TIME-RECORD FOR TIME 1.3630355
DELETING TIME-RECORD FOR TIME 2.6372138
DELETING TIME-RECORD FOR TIME 5.1855704
DELETING TIME-RECORD FOR TIME 10.282284
DELETING TIME-RECORD FOR TIME 15.055814
DELETING TIME-RECORD FOR TIME 24.602875
DELETING TIME-RECORD FOR TIME 31.094831
DELETING TIME-RECORD FOR TIME 44.078744
DELETING TIME-RECORD FOR TIME 60.484882
DELETING TIME-RECORD FOR TIME 84.239087
DELETING TIME-RECORD FOR TIME 131.74750
DELETING TIME-RECORD FOR TIME 226.76431
DELETING TIME-RECORD FOR TIME 416.79795
DELETING TIME-RECORD FOR TIME 796.86523
DELETING TIME-RECORD FOR TIME 1556.9998
DELETING TIME-RECORD FOR TIME 3008.0232
DELETING TIME-RECORD FOR TIME 5910.0702
DELETING TIME-RECORD FOR TIME 11714.164
DELETING TIME-RECORD FOR TIME 23322.352
DELETING TIME-RECORD FOR TIME 46538.728
DELETING TIME-RECORD FOR TIME 92971.479
DELETING TIME-RECORD FOR TIME 185836.98
DELETING TIME-RECORD FOR TIME 371567.99
DELETING TIME-RECORD FOR TIME 731567.99
DELETING TIME-RECORD FOR TIME 1091568.0
DELETING TIME-RECORD FOR TIME 1451568.0
DELETING TIME-RECORD FOR TIME 1811568.0
DELETING TIME-RECORD FOR TIME 2171568.0
DELETING TIME-RECORD FOR TIME 2531568.0
DELETING TIME-RECORD FOR TIME 2891568.0

KEEPING TIME-RECORD FOR TIME 3251568.0
AND FOR TIME 3600000.0
WORKSPACE RECLAIMED

TIMESTEP AT 3600000.00 SELECTED

```

```

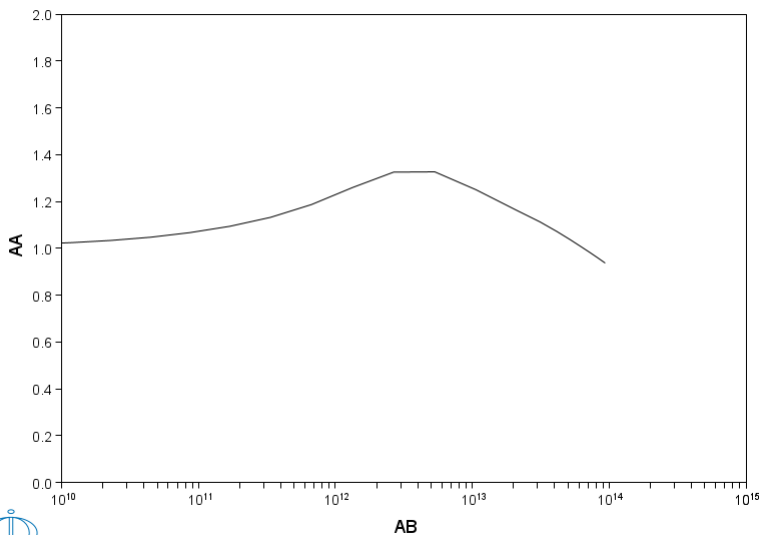
DIC>
DIC> set-inter
--OK--
DIC>

```

## exb5-plot

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exb5\plot.DCM.test"
DIC>
DIC>
DIC> @@ exb5_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE b5
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 3.60000E+06
DIC> read exb5
OK
DIC>
DIC> @@
DIC> @@ ENTER THE POST PROCESSOR, PLOT SOME QUANTITIES AND COMPARE WITH EXPERIMENTS
DIC> @@
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1: set-title Diffusion Couple A
POST-1:
POST-1: @@
POST-1: @@ WE ARE INTERESTED IN THE POSITION OF THE UPPER INTERFACE OF REGION ALPHA
POST-1: @@
POST-1: s-p-c interf alpha upper
POST-1:
POST-1: @@
POST-1: @@ 10 IS THE INITIAL THICKNESS USED FOR NORMALIZATION
POST-1: @@
POST-1: enter func l0=186.9e-6;
POST-1: enter func aa=2*poi(alpha,u)/10;
POST-1: enter func ab=time/10**2;
POST-1: s-i-v time
POST-1:
POST-1: s-d-a x ab
POST-1: s-s-s x n 1e10 1e15
POST-1: s-ax-ty x log
POST-1:
POST-1: s-d-a y aa
POST-1: s-s-s y n 0 2
POST-1:
POST-1: app y exb5.exp
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 7
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

Diffusion Couple A



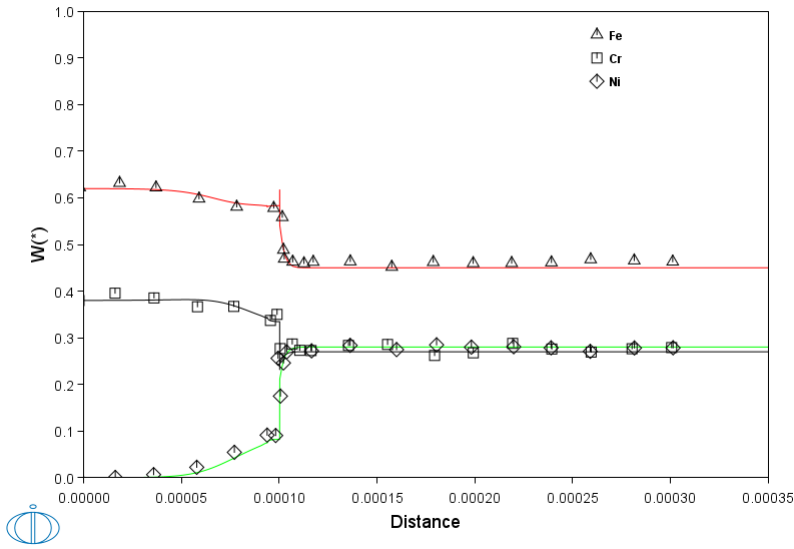
```
POST-1:
POST-1:
POST-1:
POST-1: Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ PLOT THE CONCENTRATION PROFILES FOR DIFFERENT ANNEALING TIMES
POST-1: @@
POST-1: s-d-a x dist glo
INFO: Distance is set as independent variable
POST-1: s-ax-ty x lin
POST-1: s-s-s x n 0 350e-6
POST-1:
POST-1: s-d-a y w(*)
POST-1: s-s-s y n 0 1
POST-1:
POST-1: s-p-c time 3600
```

```

POST-1:
POST-1: app y exb5.exp 0; 1
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

```

Diffusion Couple A

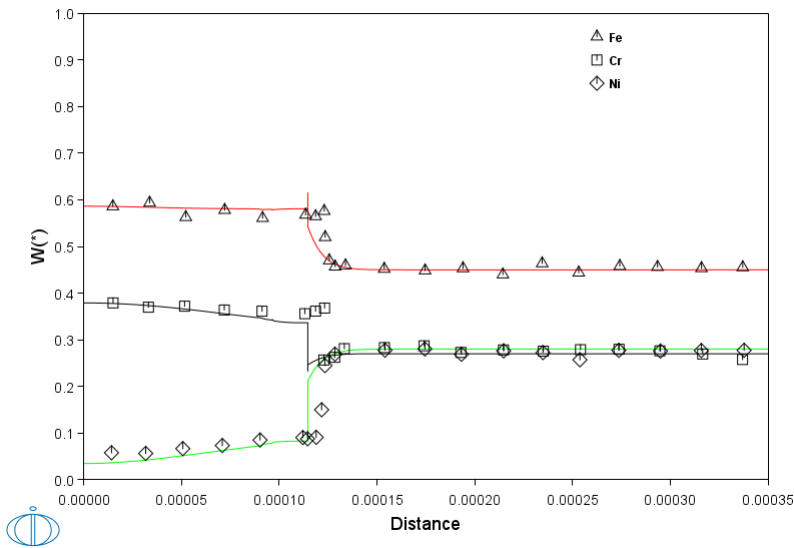


```

POST-1:
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: s-p-c time 36000
POST-1: app y exb5.exp 0; 2
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

```

Diffusion Couple A

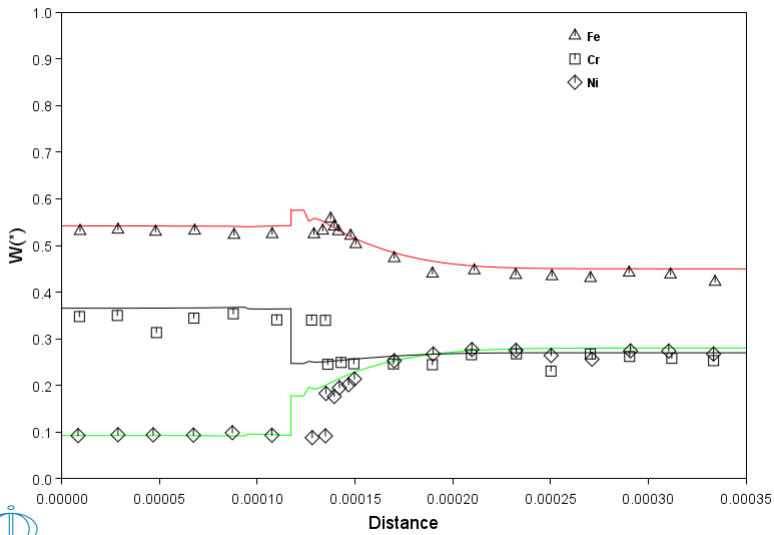


```

POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: s-p-c time 360000
POST-1: app y exb5.exp 0; 3
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

```

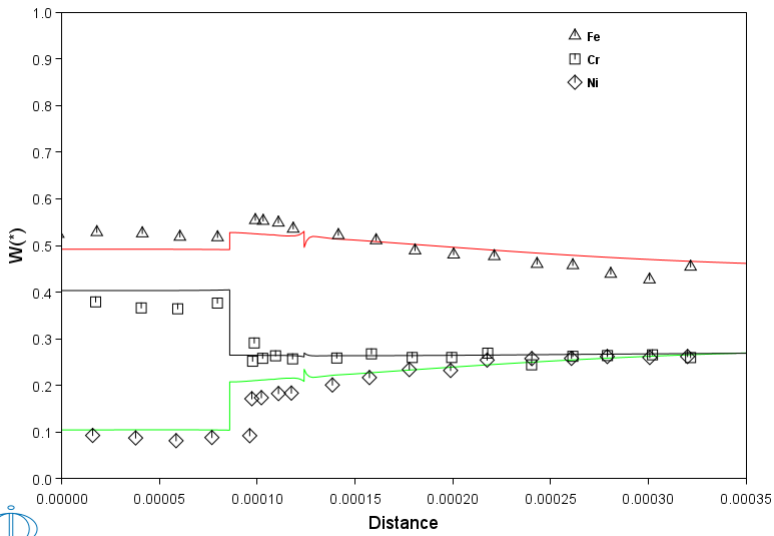
### Diffusion Couple A



```

POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: s-p-c time 3600000
POST-1: app y exb5.exp 0; 4
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
    
```

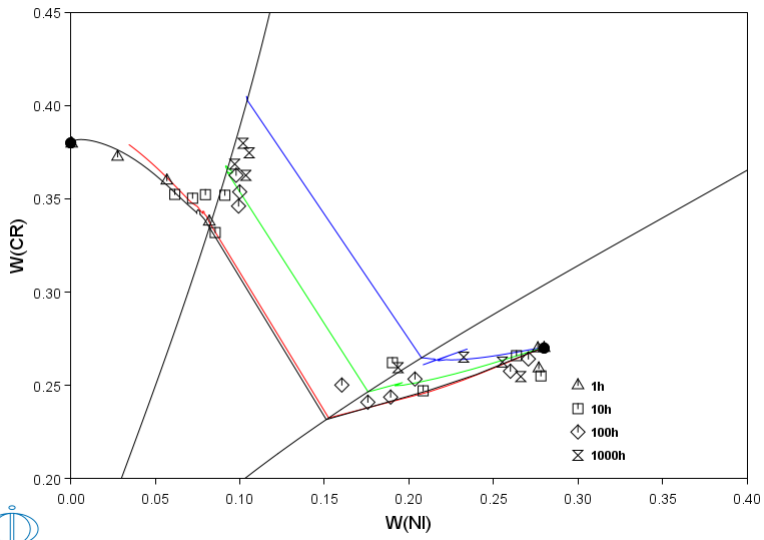
### Diffusion Couple A



```

POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ FINALLY PLOT DIFFERENT DIFFUSION PATHS.
POST-1: @@
POST-1: s-d-a x w(ni)
POST-1: s-s-s x n .00 .40
POST-1:
POST-1: s-d-a y w(cr)
POST-1: s-s-s y n .20 .45
POST-1:
POST-1: s-i-v dist glob
POST-1:
POST-1: s-p-c time 3600,36000,360000,3600000
POST-1:
POST-1: app y exb5.exp 0; 5 6
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
    
```

### Diffusion Couple A



POST-1:  
POST-1:  
POST-1:  
POST-1: set-inter  
--OK--  
POST-1:

## exb6-setup

### SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,  
Stockholm, Sweden

Software running on Windows 64-bit wordlength  
Compiler: Intel Fortran Compiler 2025.0.0  
License library version: 9.7.0.0036  
Linked: Nov 19 2025 at 14:44:36

```
SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exb6\setup.DCM.test"
```

```
SYS: @@
SYS: @@ Moving boundary problem.
SYS: @@ Microsegregation of phosphorus
SYS: @@ This example illustrates the effect of microsegregation
SYS: @@ of phosphorus during peritectic solidification in steel.
SYS: @@-----
SYS:
SYS: @@
SYS: @@ START BY GOING TO THE DATABASE MODULE
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\databases\da
ta
Current database: Steels/Fe-Alloys v12.0

VA          /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE12:
TDB_TCFE12: @@ USE A TCFE DATABASE FOR THERMODYNAMIC DATA
TDB_TCFE12: sw tcfe9
Current database: Steels/Fe-Alloys v9.3

VA          /- DEFINED
L12_FCC     B2_BCC          DICTRA_FCC_A1
REJECTED
TDB_TCFE9:
TDB_TCFE9: @@ DEFINE THE SYSTEM TO WORK WITH
TDB_TCFE9: def-sys fe c si mn p
FE          C          SI
MN          P DEFINED
TDB_TCFE9:
TDB_TCFE9: @@ EXCLUDE THE THERMODYNAMIC DATA FOR THE PHASES THAT ARE NOT NEEDED
TDB_TCFE9: rej ph /all
GAS:G      LIQUID:L      BCC_A2
FCC_A1     HCP_A3       CBCC_A12
CUB_A13    DIAMOND FCC_A4 RED_P
WHITE_P    GRAPHITE     CEMENTITE
M23C6     M7C3         M5C2
KSI_CARBIDE FE4N_LP1    FECN_CHI
LAVES_PHASE_C14 M3SI      MN9SI2
MN11SI19   MN6SI     G_PHASE
CR3SI      FE2SI     FESI2_H
FESI2_L    MSI      M5SI3
AL4C3      FE8SI2C   SIC
MN5SIC     CUZN_EPSILON AL5FE4
MP_B31     CU3P_D021  M2P_C22
M3P_D0E    MN3P_D0E   FENBP
FESI4P4    SIP      SIP2
REJECTED
TDB_TCFE9: res ph fcc liq bcc
FCC_A1     LIQUID:L     BCC_A2
RESTORED
TDB_TCFE9:
TDB_TCFE9: @@ RETRIEVE DATA FROM THE DATABASE FILE
TDB_TCFE9: get
09:55:26,574 [Thread-0] INFO  JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

Use the command LIST_REFERENCES to see the list of references for assessed data
-OK-
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ MOBILITY/DIFFUSIVITY DATA ARE STORED IN A SEPARATE DATABASE FILE.
TDB_TCFE9: @@ SWITCH TO A MOBILITY DATABASE AND APPEND THE DATA.
TDB_TCFE9: @@
TDB_TCFE9: app
Use one of these databases

TCFE12 = Steels/Fe-Alloys v12.0
TCFE9  = Steels/Fe-Alloys v9.3
SSUB6  = SGTE Substances v6.0
FEDEMO = Iron Demo Database v6.0
MOB2   = Alloys Mobility v2.7
MOBFE7 = Steels/Fe-Alloys Mobility v7.1
MOBFE4 = Steels/Fe-Alloys Mobility v4.0
MOBFE2 = Steels/Fe-Alloys Mobility v2.0
MFEDEMO = Fe-Alloys Mobility demo database v5.0
USER    = User defined Database

DATABASE NAME /TCFE9/: mobfe4
Current database: Steels/Fe-Alloys Mobility v4.0

VA DEFINED
B2_BCC REJECTED
APP: def-sys fe c si mn p
FE          C          SI
MN          P DEFINED
APP: rej ph /all
```

```

BCC_A2          CEMENTITE          FCC_A1
FE4N_LP1       HCP_A3              LIQUID:L
  REJECTED
APP: res ph fcc liq bcc
FCC_A1         LIQUID:L            BCC_A2
  RESTORED
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

```

Use the command LIST\_REFERENCES to see the list of references for assessed data

-OK-

```

APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP
APP: @@
APP: go d-m
  NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> @@ LOWER THE TEMPERATURE TO A RATE OF 0.2 K/s
DIC> @@
DIC> set-cond glob T 0 1780-0.2*TIME; * N
DIC>
DIC> @@
DIC> @@ ENTER A REGION CALLED smalta
DIC> @@
DIC> enter-region smalta
DIC>
DIC> @@
DIC> @@ ENTER A DOUBLE GEOMETRIC GRID INTO THE REGION
DIC> @@
DIC> enter-grid
REGION NAME : /SMALTA/: smalta
WIDTH OF REGION /l/: 1e-4
TYPE /AUTO/: AUTO
DIC>
DIC> @@
DIC> @@ ENTER active PHASES INTO THE REGION
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /SMALTA/: smalta
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: liq
DIC>
DIC> @@
DIC> @@ ENTER inactive PHASES INTO THE REGION, BOTH PHASES ON THE SAME SIDE
DIC> @@ OF THE LIQUID REGION TO GET A PERITECTIC REACTION.
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inact
ATTACH TO REGION NAMED /SMALTA/: smalta
ATTACHED TO THE RIGHT OF SMALTA /YES/: no
PHASE NAME: /NONE/: fcc#1
DEPENDENT COMPONENT ? /SI/: fe
  REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-5
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inact
ATTACH TO REGION NAMED /SMALTA/: smalta
ATTACHED TO THE RIGHT OF SMALTA /YES/: no
PHASE NAME: /NONE/: bcc#1
DEPENDENT COMPONENT ? /SI/: fe
  REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-5
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> @@
DIC> @@ ENTER A START COMPOSITION FOR THE LIQUID
DIC> @@
DIC> enter-composition
REGION NAME : /SMALTA/: smalta
PHASE NAME: /LIQUID/: liq
DEPENDENT COMPONENT ? /SI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: c lin 0.4 0.4
PROFILE FOR /MN/: si lin 0.7 0.7
PROFILE FOR /P/: mn lin 0.8 0.8
PROFILE FOR /SI/: p lin 0.03 0.03
DIC>
DIC> @@
DIC> @@ THE BOUNDARY CONDITION IS A CLOSED SYSTEM (DEFAULT) AS WE DO NOT SPECIFY
DIC> @@ ANYTHING ELSE
DIC> @@
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 3000
AUTOMATIC TIMESTEP CONTROL /YES/: yes
MAX TIMESTEP DURING INTEGRATION /300/: 15
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC>
DIC>
DIC> @@ CHECK THE INTERFACE POSITION. THIS IS TO MAKE SURE THAT THE LIQUID REGION
DIC> @@ DOES NOT SHRINK TOO MUCH DURING A TIMESTEP. IN ADDITION THE TIMESTEP IS
DIC> @@ CONTROLLED BY THE PHASE INTERFACE DISPLACEMENT DURING THE SIMULATION.
DIC> @@
DIC> set-option CHECK_INTERFACE_POSITION yes
DIC>

```

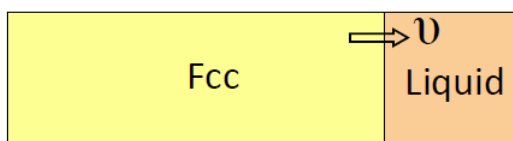
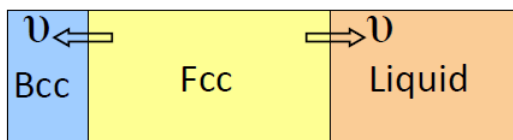
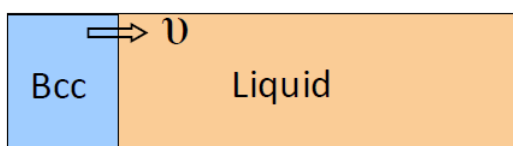
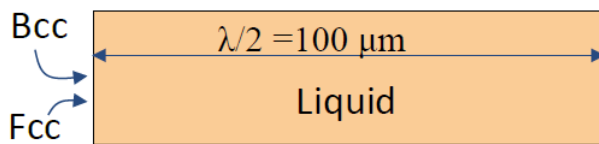
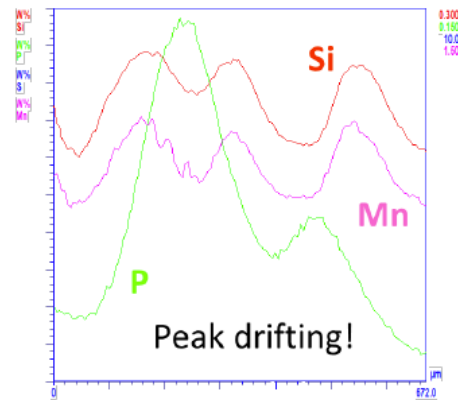
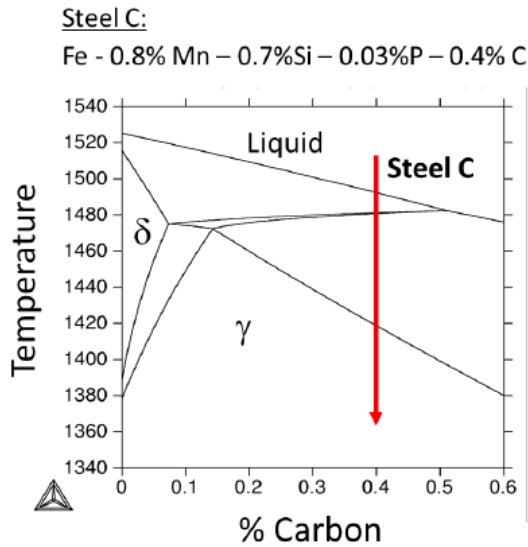
```
DIC> @@  
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT  
DIC> @@  
DIC> save exb6 Y  
DIC> set-inter  
--OK--  
DIC>
```



## Example exb6

### Micro-segregation of phosphorus

This example illustrates the effect of microsegregation of phosphorus during peritectic solidification in steel.



exb6-run

DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exb6\run.DCM.test"

DIC>

DIC>

DIC> @@ exb6\_run.DCM

DIC>

DIC> @@

DIC> @@ READ THE SET UP FROM FILE AND START THE SIMULATION

DIC> @@

DIC>

DIC> go d-m

TIME STEP AT TIME 0.00000E+00

DIC> read exb6

OK

DIC> sim

INFO: Default responses (if any) will be applied during the simulation. Use "SIMULATE\_REACTION NO" instead for manual input.

Region: SMALTA

geometric 1.20000 dense at 0.00000 57 points

DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE

U-FRACTION IN SYSTEM: C = .0185375871047351 FE = .97748186120908

MN = .00810568126669965 P = 5.39133528237327E-04

SI = .0138733239959838

TOTAL SIZE OF SYSTEM: 1E-04 [m]

U-FRACTION IN SYSTEM: C = .0185375871047351 FE = .97748186120908

MN = .00810568126669965 P = 5.39133528237327E-04

SI = .0138733239959838

TOTAL SIZE OF SYSTEM: 1E-04 [m]

TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .0185375871047351 FE = .97748186120908

MN = .00810568126669965 P = 5.39133528237327E-04

SI = .0138733239959838

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 1 seconds

TIME = 0.54150245E-05 DT = 0.53150245E-05 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .0185375871047351 FE = .97748186120908

MN = .00810568126669965 P = 5.39133528237327E-04

SI = .0138733239959838

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.16045073E-04 DT = 0.10630049E-04 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .0185375871047351 FE = .97748186120908

MN = .00810568126669966 P = 5.39133528237327E-04

SI = .0138733239959838

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 1 seconds

TIME = 0.37305171E-04 DT = 0.21260098E-04 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .0185375871047351 FE = .97748186120908

MN = .00810568126669966 P = 5.39133528237327E-04

SI = .0138733239959838

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.79825367E-04 DT = 0.42520196E-04 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .0185375871047351 FE = .97748186120908

MN = .00810568126669966 P = 5.39133528237327E-04

SI = .0138733239959838

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 1 seconds

TIME = 0.16486576E-03 DT = 0.85040391E-04 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .0185375871047351 FE = .97748186120908

MN = .00810568126669966 P = 5.39133528237327E-04

SI = .0138733239959838

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.33494654E-03 DT = 0.17008078E-03 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .0185375871047351 FE = .97748186120908

MN = .00810568126669965 P = 5.39133528237327E-04

SI = .0138733239959838

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.67510811E-03 DT = 0.34016157E-03 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .0185375871047351 FE = .97748186120908

MN = .00810568126669966 P = 5.39133528237327E-04

SI = .0138733239959838

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 1 seconds

TIME = 0.13554312E-02 DT = 0.68032313E-03 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .0185375871047351 FE = .97748186120908

MN = .00810568126669966 P = 5.39133528237327E-04

SI = .0138733239959838

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.27160775E-02 DT = 0.13606463E-02 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .0185375871047351 FE = .97748186120908

MN = .00810568126669966 P = 5.39133528237327E-04

SI = .0138733239959838

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 1 seconds

TIME = 0.54373700E-02 DT = 0.27212925E-02 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .0185375871047351 FE = .97748186120908

MN = .00810568126669965 P = 5.39133528237327E-04

SI = .0138733239959838

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.10879955E-01 DT = 0.54425850E-02 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .0185375871047351 FE = .97748186120908

MN = .00810568126669965 P = 5.39133528237327E-04

SI = .0138733239959838

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.21765125E-01 DT = 0.10885170E-01 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .0185375871047351 FE = .97748186120908

MN = .00810568126669966 P = 5.39133528237326E-04

SI = .0138733239959838

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

TIME = 0.43535465E-01 DT = 0.21770340E-01 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .0185375871047351 FE = .97748186120908

MN = .00810568126669965 P = 5.39133528237326E-04

SI = .0138733239959838

TOTAL SIZE OF SYSTEM: 1E-04 [m]

CPU time used in timestep 0 seconds

```
TIME = 0.87076146E-01 DT = 0.43540680E-01 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .018537587104735 FE = .97748186120908
MN = .00810568126669966 P = 5.39133528237325E-04
SI = .0138733239959838
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 1 seconds
TIME = 0.17415751 DT = 0.87081361E-01 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0185375871047349 FE = .97748186120908
MN = .00810568126669969 P = 5.39133528237323E-04
SI = .0138733239959839
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.34832023 DT = 0.17416272 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0185375871047348 FE = .97748186120908
MN = .00810568126669952 P = 5.39133528237323E-04
SI = .0138733239959838
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.69664567 DT = 0.34832544 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0185375871047347 FE = .97748186120908
MN = .00810568126669964 P = 5.3913352823732E-04
```

output ignored...

... output resumed

```
DELETING TIME-RECORD FOR TIME 1700.1489
DELETING TIME-RECORD FOR TIME 1715.1489
DELETING TIME-RECORD FOR TIME 1730.1489
DELETING TIME-RECORD FOR TIME 1745.1489
DELETING TIME-RECORD FOR TIME 1760.1489
DELETING TIME-RECORD FOR TIME 1775.1489
DELETING TIME-RECORD FOR TIME 1790.1489
DELETING TIME-RECORD FOR TIME 1805.1489
DELETING TIME-RECORD FOR TIME 1820.1489
DELETING TIME-RECORD FOR TIME 1835.1489
DELETING TIME-RECORD FOR TIME 1850.1489
DELETING TIME-RECORD FOR TIME 1865.1489
DELETING TIME-RECORD FOR TIME 1880.1489
DELETING TIME-RECORD FOR TIME 1895.1489
DELETING TIME-RECORD FOR TIME 1910.1489
DELETING TIME-RECORD FOR TIME 1925.1489
DELETING TIME-RECORD FOR TIME 1940.1489
DELETING TIME-RECORD FOR TIME 1955.1489
DELETING TIME-RECORD FOR TIME 1970.1489
DELETING TIME-RECORD FOR TIME 1985.1489
DELETING TIME-RECORD FOR TIME 2000.1489
DELETING TIME-RECORD FOR TIME 2015.1489
DELETING TIME-RECORD FOR TIME 2030.1489
DELETING TIME-RECORD FOR TIME 2045.1489
DELETING TIME-RECORD FOR TIME 2060.1489
DELETING TIME-RECORD FOR TIME 2075.1489
DELETING TIME-RECORD FOR TIME 2090.1489
DELETING TIME-RECORD FOR TIME 2105.1489
DELETING TIME-RECORD FOR TIME 2120.1489
DELETING TIME-RECORD FOR TIME 2135.1489
DELETING TIME-RECORD FOR TIME 2150.1489
DELETING TIME-RECORD FOR TIME 2165.1489
DELETING TIME-RECORD FOR TIME 2180.1489
DELETING TIME-RECORD FOR TIME 2195.1489
DELETING TIME-RECORD FOR TIME 2210.1489
DELETING TIME-RECORD FOR TIME 2225.1489
DELETING TIME-RECORD FOR TIME 2240.1489
DELETING TIME-RECORD FOR TIME 2255.1489
DELETING TIME-RECORD FOR TIME 2270.1489
DELETING TIME-RECORD FOR TIME 2285.1489
DELETING TIME-RECORD FOR TIME 2300.1489
DELETING TIME-RECORD FOR TIME 2315.1489
DELETING TIME-RECORD FOR TIME 2330.1489
DELETING TIME-RECORD FOR TIME 2345.1489
DELETING TIME-RECORD FOR TIME 2360.1489
DELETING TIME-RECORD FOR TIME 2375.1489
DELETING TIME-RECORD FOR TIME 2390.1489
DELETING TIME-RECORD FOR TIME 2405.1489
DELETING TIME-RECORD FOR TIME 2420.1489
DELETING TIME-RECORD FOR TIME 2435.1489
DELETING TIME-RECORD FOR TIME 2450.1489
DELETING TIME-RECORD FOR TIME 2465.1489
DELETING TIME-RECORD FOR TIME 2480.1489
DELETING TIME-RECORD FOR TIME 2495.1489
DELETING TIME-RECORD FOR TIME 2510.1489
DELETING TIME-RECORD FOR TIME 2525.1489
DELETING TIME-RECORD FOR TIME 2540.1489
DELETING TIME-RECORD FOR TIME 2555.1489
DELETING TIME-RECORD FOR TIME 2570.1489
DELETING TIME-RECORD FOR TIME 2585.1489
DELETING TIME-RECORD FOR TIME 2600.1489
DELETING TIME-RECORD FOR TIME 2615.1489
DELETING TIME-RECORD FOR TIME 2630.1489
DELETING TIME-RECORD FOR TIME 2645.1489
DELETING TIME-RECORD FOR TIME 2660.1489
DELETING TIME-RECORD FOR TIME 2675.1489
DELETING TIME-RECORD FOR TIME 2690.1489
DELETING TIME-RECORD FOR TIME 2705.1489
DELETING TIME-RECORD FOR TIME 2720.1489
DELETING TIME-RECORD FOR TIME 2735.1489
DELETING TIME-RECORD FOR TIME 2750.1489
DELETING TIME-RECORD FOR TIME 2765.1489
DELETING TIME-RECORD FOR TIME 2780.1489
DELETING TIME-RECORD FOR TIME 2795.1489
DELETING TIME-RECORD FOR TIME 2810.1489
DELETING TIME-RECORD FOR TIME 2825.1489
DELETING TIME-RECORD FOR TIME 2840.1489
DELETING TIME-RECORD FOR TIME 2855.1489
DELETING TIME-RECORD FOR TIME 2870.1489
DELETING TIME-RECORD FOR TIME 2885.1489
DELETING TIME-RECORD FOR TIME 2900.1489
DELETING TIME-RECORD FOR TIME 2915.1489
DELETING TIME-RECORD FOR TIME 2930.1489
DELETING TIME-RECORD FOR TIME 2945.1489
DELETING TIME-RECORD FOR TIME 2960.1489
DELETING TIME-RECORD FOR TIME 2975.1489
```



## exb6-plot

DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exb6\plot.DCM.test"

DIC>

DIC>

DIC>

DIC> @@

DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE

DIC> @@

DIC> go d-m

TIME STEP AT TIME 3.00000E+03

DIC> read exb6

OK

DIC>

DIC> @@

DIC> @@ GO TO THE POST PROCESSOR

DIC> @@

DIC> post

POST PROCESSOR VERSION 1.7

Implemented by Bjorn Jonsson

POST-1:

POST-1: set-title Fe-0.4%C-0.7%Si-0.8%Mn-0.03%P

POST-1:

POST-1: s-d-a y t-c

POST-1: s-d-a x time

INFO: Time is set as independent variable

POST-1: s-p-c interf first

POST-1:

POST-1: SET\_EXP\_FILE\_FORMAT 5

POST-1: MAKE c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\unite\distribution\macroResult.exp Y

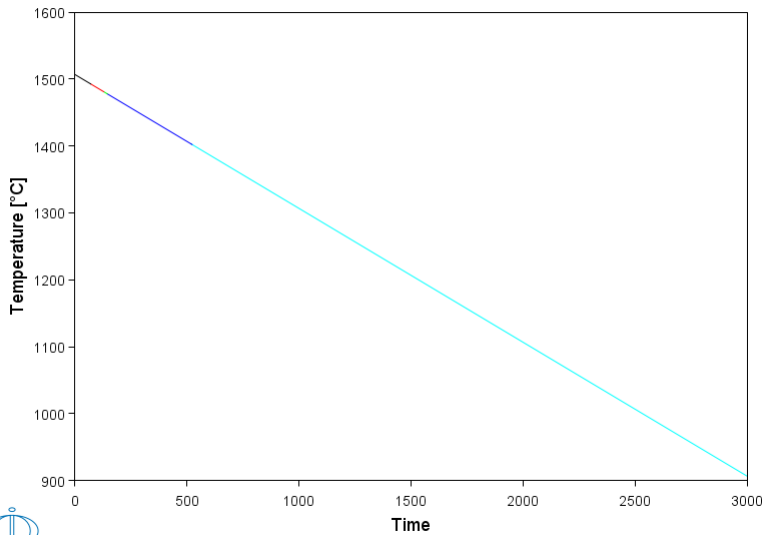
WORKING ...working ...

WORKING ...working ... OST-1: SET\_EXP\_FILE\_FORMAT 10

POST-1:

POST-1: plot

Fe-0.4%C-0.7%Si-0.8%Mn-0.03%P



POST-1:

POST-1: Hit RETURN to continue

POST-1:

POST-1: @@

POST-1: @@ PLOT THE FRACTION OF SOLID

POST-1: @@

POST-1: enter func fs=1-ivv(liq);

POST-1: s-d-a x fs

POST-1: s-s-s x n 0 1

POST-1: s-ax-te x n Fraction solid

POST-1:

POST-1: s-d-a y t-c

POST-1:

POST-1: s-p-c interf smalta lower

POST-1:

POST-1:

POST-1:

POST-1: SET\_EXP\_FILE\_FORMAT 5

POST-1: MAKE c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\unite\distribution\macroResult.exp Y

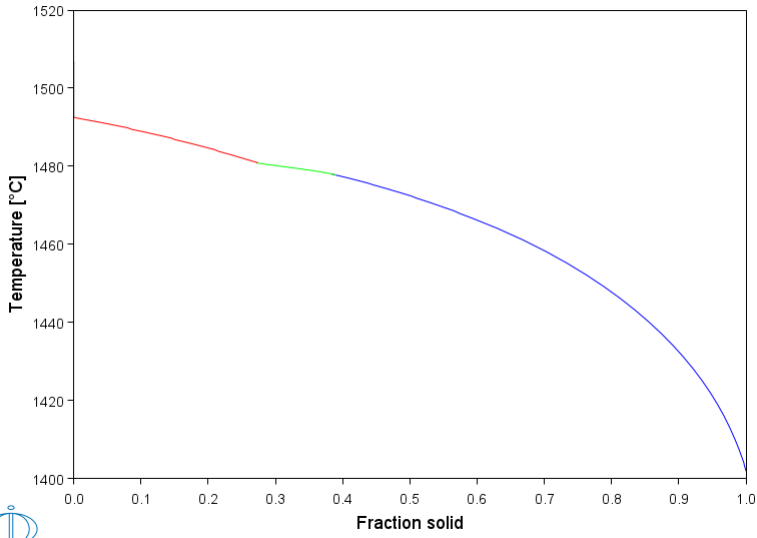
WORKING ...working ...

WORKING ...working ... OST-1: SET\_EXP\_FILE\_FORMAT 10

POST-1:

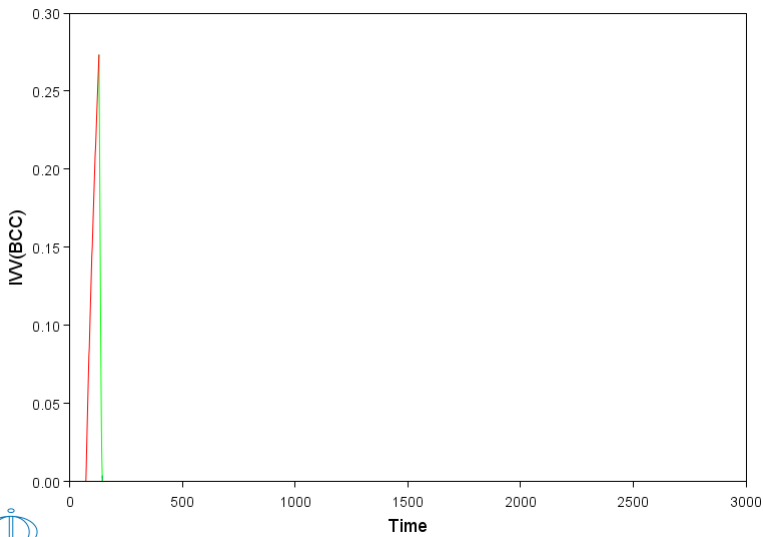
POST-1: plot

Fe-0.4%C-0.7%Si-0.8%Mn-0.03%P



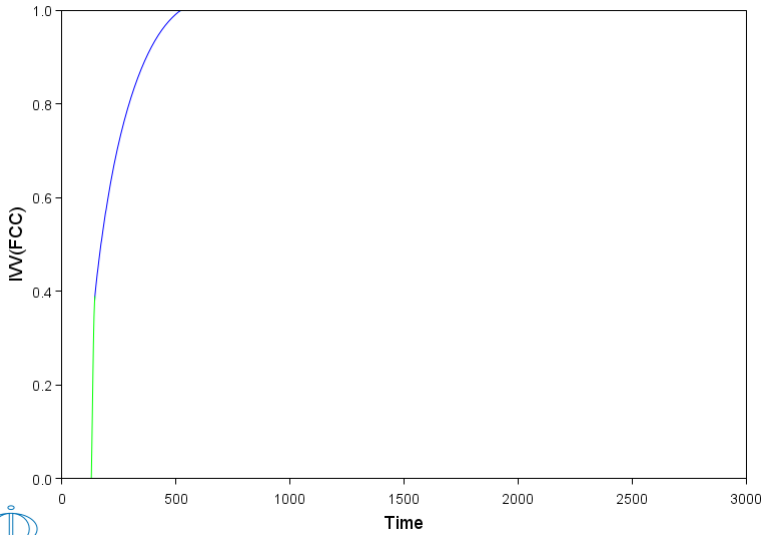
```
POST-1:
POST-1:Hit RETURN to continue
POST-1: s-d-a y ivv(bcc)
POST-1: s-d-a x time
INFO: Time is set as independent variable
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
WORKING ...working ...
WORKING ...working ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

Fe-0.4%C-0.7%Si-0.8%Mn-0.03%P



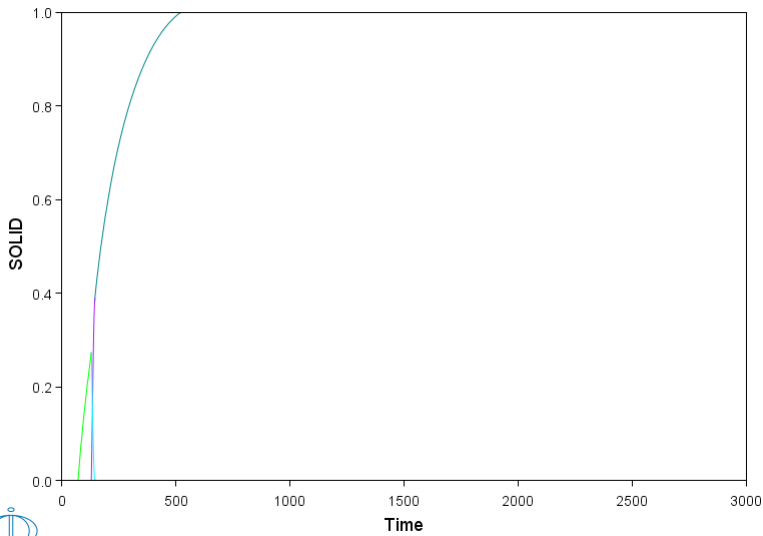
```
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: s-d-a y ivv(fcc)
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
WORKING ...working ...
WORKING ...working ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

Fe-0.4%C-0.7%Si-0.8%Mn-0.03%P



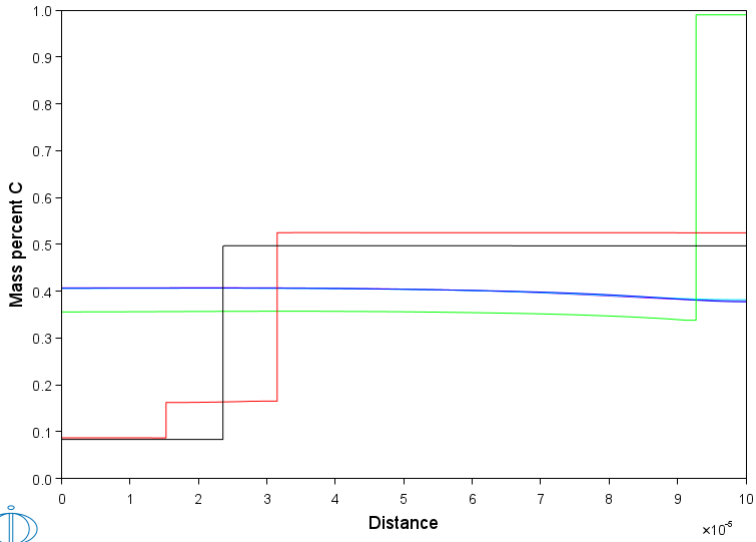
```
POST-1:
POST-1:Hit RETURN to continue
POST-1: ent table solid
Variable(s) ivv(bcc) ivv(fcc)
POST-1:
POST-1: s-d-a y solid
COLUMN NUMBER /*/:
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
WORKING ...working ...
WORKING ...working ... OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

Fe-0.4%C-0.7%Si-0.8%Mn-0.03%P



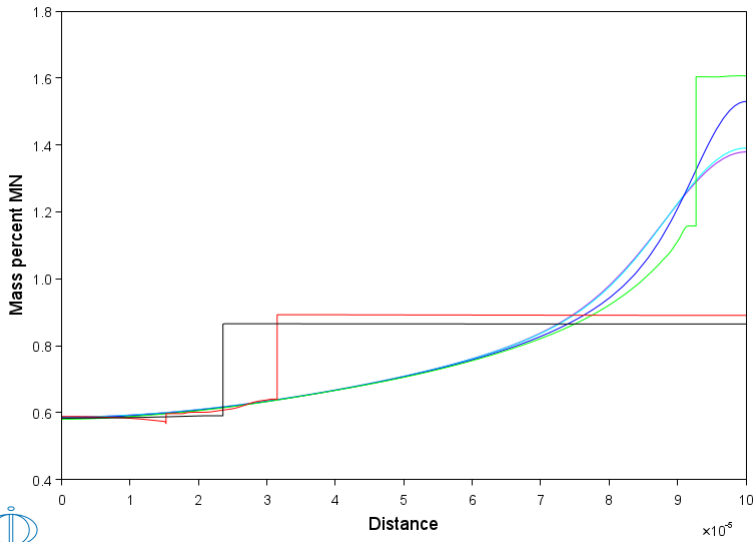
```
POST-1:
POST-1:Hit RETURN to continue
POST-1: s-d-a y w-p c
POST-1: s-d-a x dis gl
INFO: Distance is set as independent variable
POST-1: s-p-c time 120,135,400,700,1500,3000
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
WORKING ...working ...OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

Fe-0.4%C-0.7%Si-0.8%Mn-0.03%P



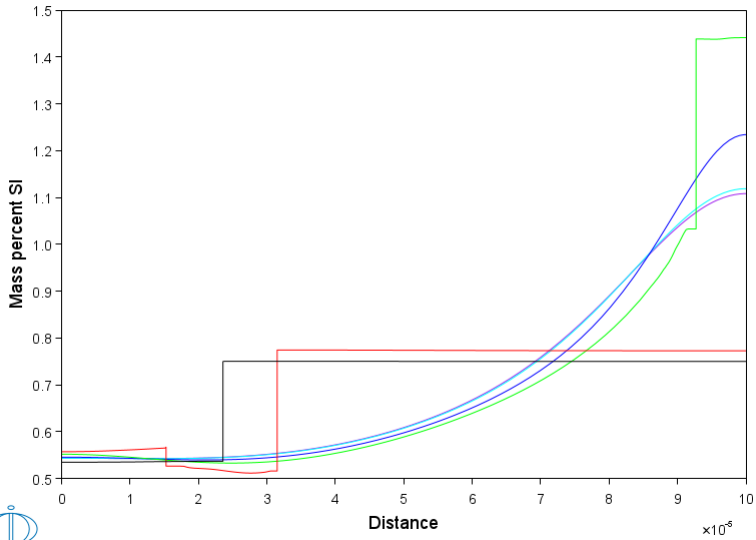
```
POST-1:
POST-1:Hit RETURN to continue
POST-1: s-d-a y w-p mn
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
WORKING ...working ...OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

Fe-0.4%C-0.7%Si-0.8%Mn-0.03%P



```
POST-1:
POST-1:Hit RETURN to continue
POST-1: s-d-a y w-p si
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
WORKING ...working ...OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

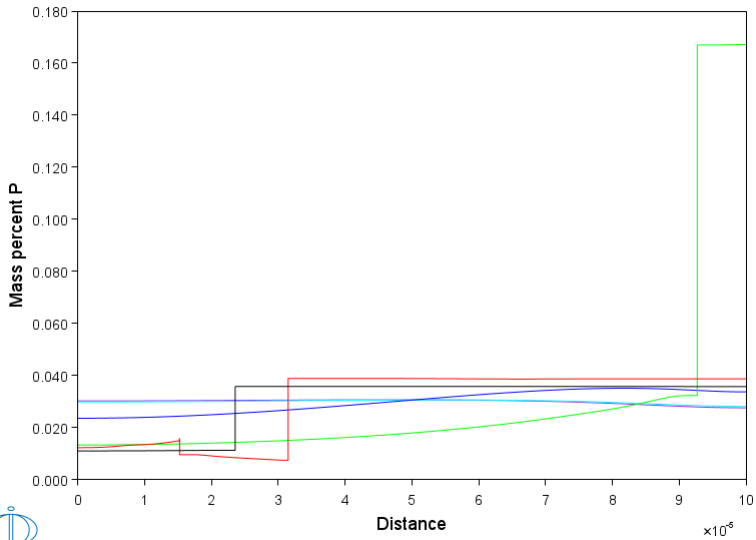
Fe-0.4%C-0.7%Si-0.8%Mn-0.03%P



```

POST-1:
POST-1:Hit RETURN to continue
POST-1: s-d-a y w-p p
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
WORKING ...working ...OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
    
```

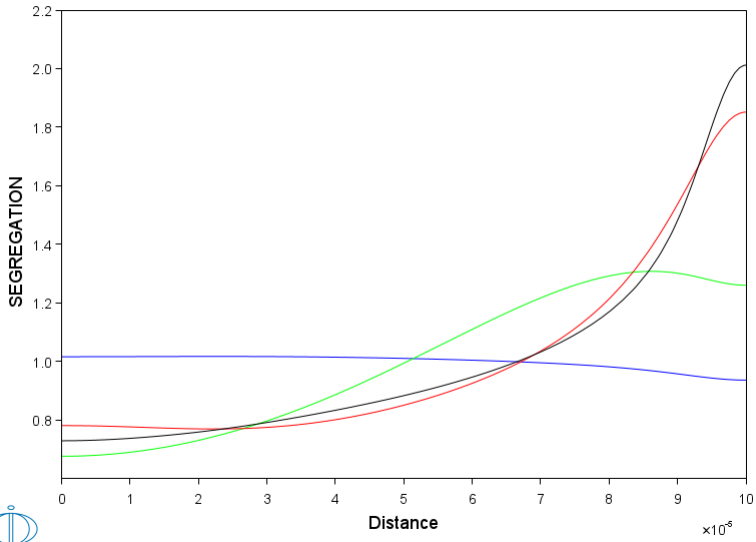
Fe-0.4%C-0.7%Si-0.8%Mn-0.03%P



```

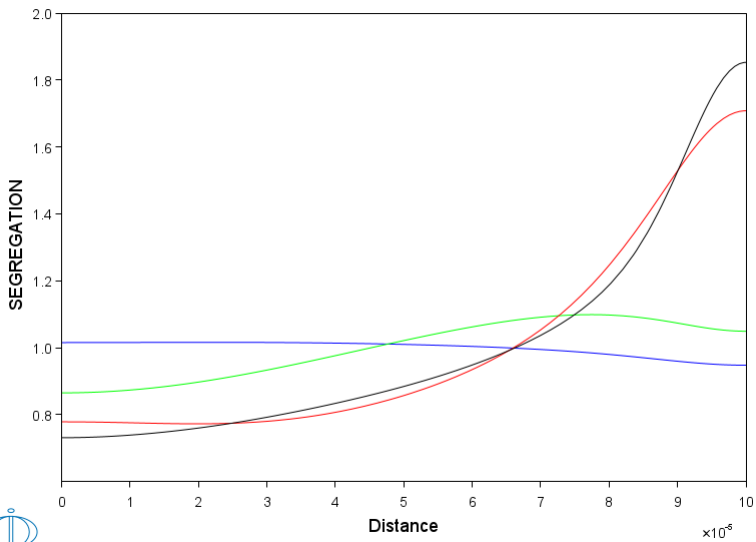
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: ent function mnn
FUNCTION: w(mn)/0.008
&
POST-1: ent function sin
FUNCTION: w(si)/0.007
&
POST-1: ent function pn
FUNCTION: w(p)/0.0003
&
POST-1: ent function cn
FUNCTION: w(c)/0.004
&
POST-1: ent tabel segregation
Variable(s) mnn sin pn cn
POST-1:
POST-1: s-d-a y segregation
COLUMN NUMBER /*/:
POST-1:
POST-1: s-p-c time 610
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
    
```

Fe-0.4%C-0.7%Si-0.8%Mn-0.03%P



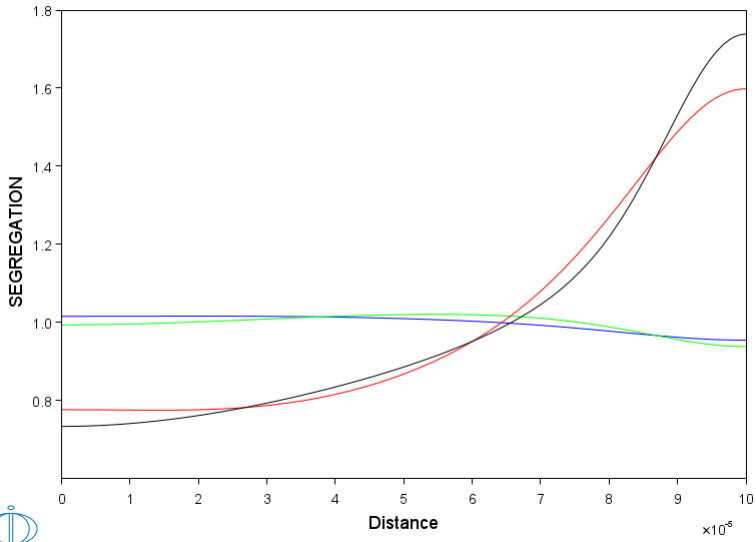
```
POST-1:  
POST-1:Hit RETURN to continue  
POST-1:  
POST-1: s-p-c time 800  
POST-1:  
POST-1: SET_EXP_FILE_FORMAT 5  
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y  
POST-1: SET_EXP_FILE_FORMAT 10  
POST-1:  
POST-1: plot
```

Fe-0.4%C-0.7%Si-0.8%Mn-0.03%P



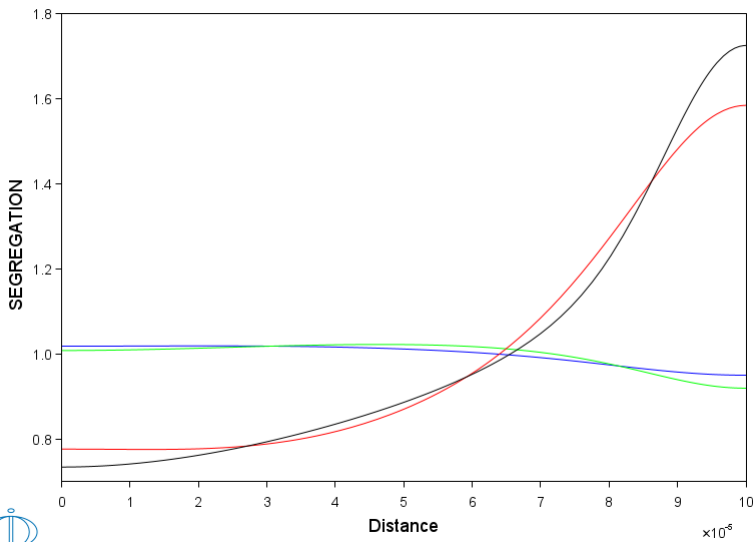
```
POST-1:  
POST-1:Hit RETURN to continue  
POST-1:  
POST-1: s-p-c time 1500  
POST-1:  
POST-1: SET_EXP_FILE_FORMAT 5  
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y  
POST-1: SET_EXP_FILE_FORMAT 10  
POST-1:  
POST-1: plot
```

Fe-0.4%C-0.7%Si-0.8%Mn-0.03%P



```
POST-1:  
POST-1:Hit RETURN to continue  
POST-1:  
POST-1: s-p-c time 3000  
POST-1:  
POST-1: SET_EXP_FILE_FORMAT 5  
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y  
POST-1: SET_EXP_FILE_FORMAT 10  
POST-1:  
POST-1: plot
```

Fe-0.4%C-0.7%Si-0.8%Mn-0.03%P



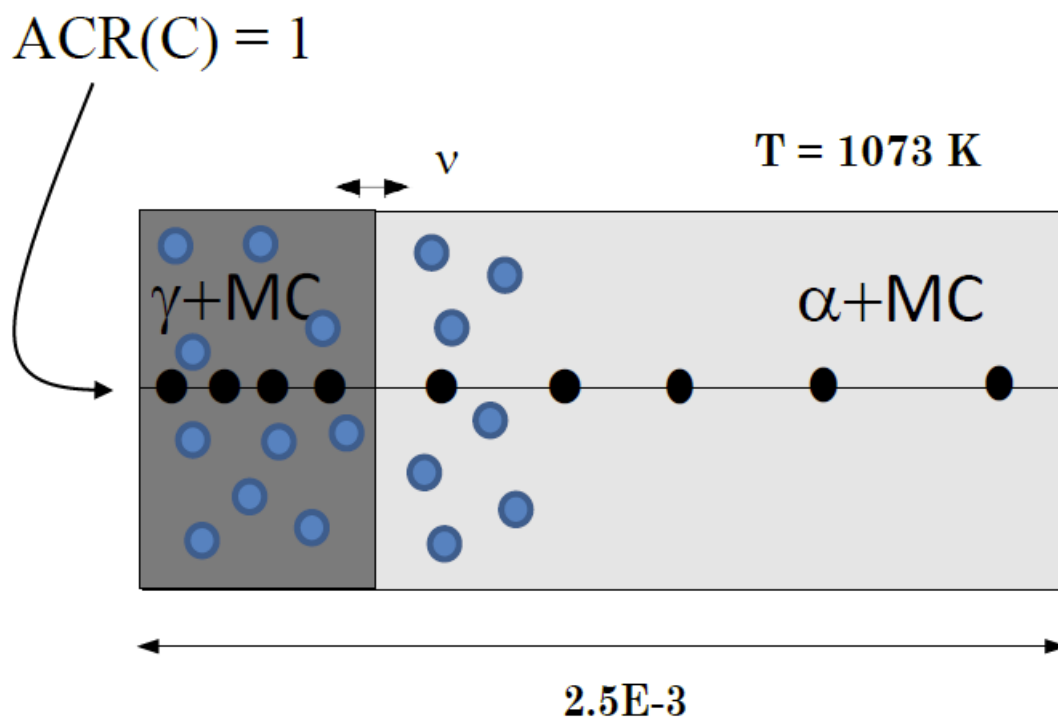
```
POST-1:  
POST-1:Hit RETURN to continue  
POST-1: set-inter  
--OK--  
POST-1:
```



## Example exb7

### Moving boundary problem with multiple phases on each side of the boundary

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.



## exb7-setup

### SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,  
Stockholm, Sweden

Software running on Windows 64-bit wordlength  
Compiler: Intel Fortran Compiler 2025.0.0  
License library version: 9.7.0.0036  
Linked: Nov 19 2025 at 14:44:36

SYS:SYS:MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exb7\setup.DCM"

```
SYS: @@ This example modifies the database interactively, which is not
SYS: @@ yet supported by GES6. Therefore, we enforce the use of GES5.
SYS: set-ges-version 5
SYS:
SYS: @@
SYS: @@ Moving boundary problem.
SYS: @@ Moving boundary problem with multiple phases on each side
SYS: @@ This example shows how to enter dispersed phases on either side
SYS: @@ of a phase interface. The particular case shows how
SYS: @@ the kinetics of a ferrite to austenite transformation is
SYS: @@ affected by simultaneous precipitation of niobium carbide.
SYS: @@ The transformation is caused by carburization.
SYS: @@-----
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASE
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\databases\da
ta
Current database: Steels/Fe-Alloys v12.0

VA          /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE12:
TDB_TCFE12: @@
TDB_TCFE12: @@ USE A TCFE DATABASE FOR THERMODYNAMIC DATA
TDB_TCFE12: @@
TDB_TCFE12: sw tcfe9
Current database: Steels/Fe-Alloys v9.3

VA          /- DEFINED
LI2_FCC     B2_BCC          DICTRA_FCC_A1
REJECTED
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ DEFINE THE SYSTEM TO WORK WITH
TDB_TCFE9: @@
TDB_TCFE9: def-species fe c nb
FE          C              NB
DEFINED
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ EXCLUDE THE THERMODYNAMIC DATA FOR THE PHASES THAT ARE NOT NEEDED
TDB_TCFE9: @@
TDB_TCFE9: rej ph * all
GAS:G       LIQUID:L       BCC_A2
FCC_A1      HCP_A3        CBCC_A12
CUB_A13     DIAMOND_FCC_A4 GRAPHITE
CEMENTITE   M23C6         M7C3
M6C         M5C2             KSI_CARBIDE
Z_PHASE     FE4N_LP1      FECN_CHI
SIGMA       MU_PHASE     LAVES_PHASE_C14
G_PHASE     CR3SI        NBNI3
AL5FE4 REJECTED
TDB_TCFE9: res ph fcc bcc grap
FCC_A1      BCC_A2          GRAPHITE
RESTORED
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ RETRIEVE DATA FROM THE DATABASE FILE
TDB_TCFE9: @@
TDB_TCFE9: get
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
Creating a new composition set FCC_A1#2
PARAMETERS ...
FUNCTIONS ....

Use the command LIST_REFERENCES to see the list of references for assessed data
-OK-
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ NOW APPEND A SSUB DATABASE FROM WHICH WE READ THE THERMODYNAMIC
TDB_TCFE9: @@ DESCRIPTION OF NIOBIUM CARBIDE
TDB_TCFE9: @@
TDB_TCFE9:
TDB_TCFE9: app SSUB6
Current database: SGTE Substances v6.0

VA DEFINED
APP: def-sys fe c nb
FE          C              NB
DEFINED
APP: rej ph *
GAS:G       C0_749NB1_S    C0_877NB1_S
C0_98NB1_S  C_S                     C_L
DIAMOND     CIFE3_S         C1NB1_S
C1NB2_S     C60_S              FE_S
FE_S2       FE_S3              FE_L
```

```
FE2NB1_S          NB_S          NB_L
REJECTED
APP: rest ph c1nb1_s
C1NB1_S RESTORED
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS .....
```

Use the command LIST\_REFERENCES to see the list of references for assessed data

-OK-

```
APP:
APP: @@
APP: @@ MOBILITY/DIFFUSIVITY DATA ARE STORED IN A SEPARATE DATABASE FILE.
APP: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE THE DATA
APP: @@
APP: app mobfe4
Current database: Steels/Fe-Alloys Mobility v4.0
```

```
VA DEFINED
B2_BCC REJECTED
APP: def-sys fe c nb
FE          C          NB
DEFINED
APP: rej ph * all
BCC_A2          CEMENTITE          FCC_A1
FE4N_LP1          HCP_A3          LIQUID:L
REJECTED
APP: res ph fcc bcc
FCC_A1          BCC_A2 RESTORED
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS .....
```

Use the command LIST\_REFERENCES to see the list of references for assessed data

-OK-

```
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP
APP: @@
APP: go d-m
NO TIME STEP DEFINED
*** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
*** ENTERING C1NB1_S AS A DIFFUSION NONE PHASE
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 1073.15; * N
DIC>
DIC> @@
DIC> @@ ENTER REGIONS ferr AND aus
DIC> @@
DIC> enter-region
REGION NAME : ferr
DIC>
DIC> ent-reg
REGION NAME : aus
ATTACH TO REGION NAMED /FERR/: ferr
ATTACHED TO THE RIGHT OF FERR /YES/: n
DIC>
DIC> @@
DIC> @@ ENTER GRIDS INTO REGIONS
DIC> @@
DIC> enter-grid
REGION NAME : /AUS/: ferr
WIDTH OF REGION /1/: 2.499999e-3
TYPE /AUTO/: AUTO
DIC>
DIC>
DIC> enter-grid
REGION NAME : /AUS/: aus
WIDTH OF REGION /1/: 1e-9
TYPE /AUTO/: AUTO
DIC>
DIC>
DIC> @@
DIC> @@ ENTER active PHASES INTO REGIONS
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /AUS/: ferr
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: bcc
DIC>
DIC>
DIC> en-ph
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /AUS/: ferr
PHASE TYPE /MATRIX/: sph
PHASE NAME: /NONE/: c1nb1_s
INFO: EQUILIBRIUM COMPOSITION AND FRACTION OF SPHEROID PHASES USED AS DEFAULT
DIC>
DIC>
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /AUS/: aus
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC>
DIC> en-ph
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /AUS/: aus
```

```

PHASE TYPE /MATRIX/: sph
PHASE NAME: /NONE/: c1nb1_s
INFO: EQUILIBRIUM COMPOSITION AND FRACTION OF SPHEROID PHASES USED AS DEFAULT
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITIONS OF THE PHASES
DIC> @@
DIC> enter-composition
REGION NAME : /AUS/: ferr
PHASE NAME: /BCC_A2/: bcc
DEPENDENT COMPONENT ? /NB/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: c
TYPE /LINEAR/: lin
VALUE OF FIRST POINT : 1e-3
VALUE OF LAST POINT : /1E-3/: 1e-3
PROFILE FOR /NB/: nb
TYPE /LINEAR/: lin
VALUE OF FIRST POINT : 0.28
VALUE OF LAST POINT : /0.28/: 0.28
DIC>
DIC> en-co
REGION NAME : /AUS/: ferr
PHASE NAME: /BCC_A2/: c1nb1_s
USE EQUILIBRIUM VALUE /Y/: y
DIC>
DIC> enter-composition
REGION NAME : /AUS/: aus
PHASE NAME: /FCC_A1#1/: fcc#1
DEPENDENT COMPONENT ? /NB/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: c
TYPE /LINEAR/: lin
VALUE OF FIRST POINT : 0.89
VALUE OF LAST POINT : /0.89/: 0.89
PROFILE FOR /NB/: nb
TYPE /LINEAR/: lin
VALUE OF FIRST POINT : 0.28
VALUE OF LAST POINT : /0.28/: 0.28
DIC>
DIC> en-co
REGION NAME : /AUS/: aus
PHASE NAME: /FCC_A1#1/: c1nb1_s
USE EQUILIBRIUM VALUE /Y/: y
DIC>
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 32400
AUTOMATIC TIMESTEP CONTROL /YES/: y
MAX TIMESTEP DURING INTEGRATION /3240/: 3240
INITIAL TIMESTEP : /1E-07/: 1e-8
SMALLEST ACCEPTABLE TIMESTEP : /1E-08/: 1e-15
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ SET THE REFERENCE PHASE OF CARBON AS GRAPHITE
DIC> @@
DIC> s-ref
Component: c
Reference state: grap
Temperature /*/: *
Pressure /100000/: 1e5
DIC>
DIC> @@
DIC> @@ SET THE BOUNDARY CONDITION.
DIC> @@ THE CARBON ACTIVITY IS THE ONE ON THE BOUNDARY
DIC> @@
DIC> s-cond
GLOBAL OR BOUNDARY CONDITION /GLOBAL/: bound
BOUNDARY /LOWER/: low
CONDITION TYPE /CLOSED_SYSTEM/: mix
Dependent substitutional element:FE
Dependent interstitial element:VA
TYPE OF CONDITION FOR COMPONENT C /ZERO_FLUX/: act
LOW TIME LIMIT /0/: 0
ACR(C)(TIME)= 1.0;
HIGH TIME LIMIT /*/: *
ANY MORE RANGES /N/: N
TYPE OF CONDITION FOR COMPONENT NB /ZERO_FLUX/: zero
DIC>
DIC> @@
DIC> @@ ENABLE THE HOMOGENIZATION MODEL
DIC> @@
DIC> ho y y
INFO: HOMOGENIZATION MODEL ENABLED
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exb7 Y
DIC>
DIC>
DIC> set-inter
--OK--
DIC>

```

exb7-run

DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exb7\run.DCM"

DIC> @@

DIC> @@ READ THE SET UP FROM FILE AND START THE SIMULATION

DIC> @@

DIC>

DIC> go d-m

TIME STEP AT TIME 0.00000E+00

\*\*\* ENTERING GRAPHITE AS A DIFFUSION NONE PHASE

\*\*\* ENTERING C1NB1\_S AS A DIFFUSION NONE PHASE

DIC> read exb7

OK

DIC> sim yes

INFO: Default responses (if any) will be applied during the simulation. Use "SIMULATE\_REACTION NO" instead for manual input.

Region: AUS

geometric 1.00414 dense at 0.00000 25 points

geometric 0.995873 dense at 0.100000E-08 26 points

Region: FERR

geometric 1.02000 dense at 0.00000 50 points

DEGREE OF IMPLICITY SET TO EULER BACKWARD

INFO: not solving in latticefixed frame of reference

STARTING SIMULATION USING HOMOGENIZATION MODEL

-----  
 WARNING: ELEMENT C  
 IS BOTH INTERSTITIAL AND SUBSTITUTIONAL  
 AND RESULTS MUST BE INTERPRETED WITH CARE  
 INFO: PHASE WITH LIMITED SOLUBILITY OF ELEMENT(S) EXIST  
 A FALLBACK PHASE ZZDICTRA\_GHOST WILL BE DEFINED  
 ALONG WITH THE FOLLOWING PARAMETERS:  
 G(ZZDICTRA\_GHOST,C;0)-H298 (GRAPHITE,C;0)  
 G (ZZDICTRA\_GHOST,FE;0)-H298 (BCC\_A2,FE;0)  
 G (ZZDICTRA\_GHOST,NB;0)-H298 (BCC\_A2,NB;0)  
 L(ZZDICTRA\_GHOST,C,FE;0)  
 L(ZZDICTRA\_GHOST,C,NB;0)  
 L(ZZDICTRA\_GHOST,FE,NB;0)  
 INFO: FCC Al#2 is stable but not entered in the simulation

WARNING:C1NB1\_S HAS NO VOLUME FRACTION, CREATING ONE  
 WARNING:C1NB1\_S HAS NO VOLUME FRACTION, CREATING ONE

Starting time-step	t0=	0.0000000	dt=	0.10000000E-07
Error		408		
Starting time-step	t0=	0.97656250E-11	dt=	0.97656250E-11
Starting time-step	t0=	0.19531250E-10	dt=	0.19531250E-10
Starting time-step	t0=	0.39062500E-10	dt=	0.39062500E-10
Starting time-step	t0=	0.78125000E-10	dt=	0.78125000E-10
Starting time-step	t0=	0.15625000E-09	dt=	0.15625000E-09
Starting time-step	t0=	0.31250000E-09	dt=	0.31250000E-09
Starting time-step	t0=	0.62500000E-09	dt=	0.62500000E-09
Starting time-step	t0=	0.93750000E-09	dt=	0.93750000E-09
Starting time-step	t0=	0.12500000E-08	dt=	0.12500000E-08
Starting time-step	t0=	0.15625000E-08	dt=	0.15625000E-08
Starting time-step	t0=	0.21875000E-08	dt=	0.21875000E-08
Starting time-step	t0=	0.28125000E-08	dt=	0.28125000E-08
Starting time-step	t0=	0.34375000E-08	dt=	0.34375000E-08
Starting time-step	t0=	0.40625000E-08	dt=	0.40625000E-08
Starting time-step	t0=	0.46875000E-08	dt=	0.46875000E-08
Starting time-step	t0=	0.53125000E-08	dt=	0.53125000E-08
Starting time-step	t0=	0.59375000E-08	dt=	0.59375000E-08
Starting time-step	t0=	0.65625000E-08	dt=	0.65625000E-08
Starting time-step	t0=	0.71875000E-08	dt=	0.71875000E-08
Starting time-step	t0=	0.78125000E-08	dt=	0.78125000E-08
Starting time-step	t0=	0.84375000E-08	dt=	0.84375000E-08
Starting time-step	t0=	0.90625000E-08	dt=	0.90625000E-08
Starting time-step	t0=	0.96875000E-08	dt=	0.96875000E-08
Starting time-step	t0=	0.10312500E-07	dt=	0.10312500E-07
Starting time-step	t0=	0.10937500E-07	dt=	0.10937500E-07
Starting time-step	t0=	0.11562500E-07	dt=	0.11562500E-07
Starting time-step	t0=	0.12187500E-07	dt=	0.12187500E-07
Starting time-step	t0=	0.12812500E-07	dt=	0.12812500E-07
Starting time-step	t0=	0.13437500E-07	dt=	0.13437500E-07
Starting time-step	t0=	0.14062500E-07	dt=	0.14062500E-07
Starting time-step	t0=	0.14687500E-07	dt=	0.14687500E-07
Starting time-step	t0=	0.15312500E-07	dt=	0.15312500E-07
Starting time-step	t0=	0.15937500E-07	dt=	0.15937500E-07
Starting time-step	t0=	0.16562500E-07	dt=	0.16562500E-07
Starting time-step	t0=	0.17187500E-07	dt=	0.17187500E-07
Starting time-step	t0=	0.17812500E-07	dt=	0.17812500E-07
Starting time-step	t0=	0.18437500E-07	dt=	0.18437500E-07
Starting time-step	t0=	0.19062500E-07	dt=	0.19062500E-07
Starting time-step	t0=	0.19687500E-07	dt=	0.19687500E-07
Starting time-step	t0=	0.20312500E-07	dt=	0.20312500E-07
Starting time-step	t0=	0.20937500E-07	dt=	0.20937500E-07
Starting time-step	t0=	0.21562500E-07	dt=	0.21562500E-07
Starting time-step	t0=	0.22187500E-07	dt=	0.22187500E-07
Starting time-step	t0=	0.22812500E-07	dt=	0.22812500E-07
Starting time-step	t0=	0.23437500E-07	dt=	0.23437500E-07
Starting time-step	t0=	0.24062500E-07	dt=	0.24062500E-07
Starting time-step	t0=	0.24687500E-07	dt=	0.24687500E-07
Starting time-step	t0=	0.25312500E-07	dt=	0.25312500E-07
Starting time-step	t0=	0.25937500E-07	dt=	0.25937500E-07
Starting time-step	t0=	0.26562500E-07	dt=	0.26562500E-07
Starting time-step	t0=	0.27187500E-07	dt=	0.27187500E-07
Starting time-step	t0=	0.27812500E-07	dt=	0.27812500E-07
Starting time-step	t0=	0.28437500E-07	dt=	0.28437500E-07
Starting time-step	t0=	0.29062500E-07	dt=	0.29062500E-07
Starting time-step	t0=	0.29687500E-07	dt=	0.29687500E-07
Starting time-step	t0=	0.30312500E-07	dt=	0.30312500E-07
Starting time-step	t0=	0.30937500E-07	dt=	0.30937500E-07
Starting time-step	t0=	0.31562500E-07	dt=	0.31562500E-07
Starting time-step	t0=	0.32187500E-07	dt=	0.32187500E-07
Starting time-step	t0=	0.32812500E-07	dt=	0.32812500E-07
Starting time-step	t0=	0.33437500E-07	dt=	0.33437500E-07
Starting time-step	t0=	0.34062500E-07	dt=	0.34062500E-07
Starting time-step	t0=	0.34687500E-07	dt=	0.34687500E-07
Starting time-step	t0=	0.35312500E-07	dt=	0.35312500E-07
Starting time-step	t0=	0.35937500E-07	dt=	0.35937500E-07
Starting time-step	t0=	0.36562500E-07	dt=	0.36562500E-07
Starting time-step	t0=	0.37187500E-07	dt=	0.37187500E-07
Starting time-step	t0=	0.37812500E-07	dt=	0.37812500E-07
Starting time-step	t0=	0.38437500E-07	dt=	0.38437500E-07
Starting time-step	t0=	0.39062500E-07	dt=	0.39062500E-07
Starting time-step	t0=	0.39687500E-07	dt=	0.39687500E-07
Starting time-step	t0=	0.40312500E-07	dt=	0.40312500E-07
Starting time-step	t0=	0.40937500E-07	dt=	0.40937500E-07
Starting time-step	t0=	0.41562500E-07	dt=	0.41562500E-07
Starting time-step	t0=	0.42187500E-07	dt=	0.42187500E-07
Starting time-step	t0=	0.42812500E-07	dt=	0.42812500E-07
Starting time-step	t0=	0.43437500E-07	dt=	0.43437500E-07
Starting time-step	t0=	0.44062500E-07	dt=	0.44062500E-07
Starting time-step	t0=	0.44687500E-07	dt=	0.44687500E-07
Starting time-step	t0=	0.45312500E-07	dt=	0.45312500E-07
Starting time-step	t0=	0.45937500E-07	dt=	0.45937500E-07
Starting time-step	t0=	0.46562500E-07	dt=	0.46562500E-07
Starting time-step	t0=	0.47187500E-07	dt=	0.47187500E-07
Starting time-step	t0=	0.47812500E-07	dt=	0.47812500E-07
Starting time-step	t0=	0.48437500E-07	dt=	0.48437500E-07
Starting time-step	t0=	0.49062500E-07	dt=	0.49062500E-07
Starting time-step	t0=	0.49687500E-07	dt=	0.49687500E-07
Starting time-step	t0=	0.50312500E-07	dt=	0.50312500E-07
Starting time-step	t0=	0.50937500E-07	dt=	0.50937500E-07
Starting time-step	t0=	0.51562500E-07	dt=	0.51562500E-07
Starting time-step	t0=	0.52187500E-07	dt=	0.52187500E-07
Starting time-step	t0=	0.52812500E-07	dt=	0.52812500E-07
Starting time-step	t0=	0.53437500E-07	dt=	0.53437500E-07
Starting time-step	t0=	0.54062500E-07	dt=	0.54062500E-07
Starting time-step	t0=	0.54687500E-07	dt=	0.54687500E-07
Starting time-step	t0=	0.55312500E-07	dt=	0.55312500E-07
Starting time-step	t0=	0.55937500E-07	dt=	0.55937500E-07
Starting time-step	t0=	0.56562500E-07	dt=	0.56562500E-07
Starting time-step	t0=	0.57187500E-07	dt=	0.57187500E-07
Starting time-step	t0=	0.57812500E-07	dt=	0.57812500E-07
Starting time-step	t0=	0.58437500E-07	dt=	0.58437500E-07
Starting time-step	t0=	0.59062500E-07	dt=	0.59062500E-07
Starting time-step	t0=	0.59687500E-07	dt=	0.59687500E-07
Starting time-step	t0=	0.60312500E-07	dt=	0.60312500E-07
Starting time-step	t0=	0.60937500E-07	dt=	0.60937500E-07
Starting time-step	t0=	0.61562500E-07	dt=	0.61562500E-07
Starting time-step	t0=	0.62187500E-07	dt=	0.62187500E-07
Starting time-step	t0=	0.62812500E-07	dt=	0.62812500E-07
Starting time-step	t0=	0.63437500E-07	dt=	0.63437500E-07
Starting time-step	t0=	0.64062500E-07	dt=	0.64062500E-07
Starting time-step	t0=	0.64687500E-07	dt=	0.64687500E-07
Starting time-step	t0=	0.65312500E-07	dt=	0.65312500E-07
Starting time-step	t0=	0.65937500E-07	dt=	0.65937500E-07
Starting time-step	t0=	0.66562500E-07	dt=	0.66562500E-07
Starting time-step	t0=	0.67187500E-07	dt=	0.67187500E-07
Starting time-step	t0=	0.67812500E-07	dt=	0.67812500E-07
Starting time-step	t0=	0.68437500E-07	dt=	0.68437500E-07
Starting time-step	t0=	0.69062500E-07	dt=	0.69062500E-07
Starting time-step	t0=	0.69687500E-07	dt=	0.69687500E-07
Starting time-step	t0=	0.70312500E-07	dt=	0.70312500E-07
Starting time-step	t0=	0.70937500E-07	dt=	0.70937500E-07
Starting time-step	t0=	0.71562500E-07	dt=	0.71562500E-07
Starting time-step	t0=	0.72187500E-07	dt=	0.72187500E-07
Starting time-step	t0=	0.72812500E-07	dt=	0.72812500E-07
Starting time-step	t0=	0.73437500E-07	dt=	0.73437500E-07
Starting time-step	t0=	0.74062500E-07	dt=	0.74062500E-07
Starting time-step	t0=	0.74687500E-07	dt=	0.74687500E-07
Starting time-step	t0=	0.75312500E-07	dt=	0.75312500E-07
Starting time-step	t0=	0.75937500E-07	dt=	0.75937500E-07
Starting time-step	t0=	0.76562500E-07	dt=	0.76562500E-07
Starting time-step	t0=	0.77187500E-07	dt=	0.77187500E-07
Starting time-step	t0=	0.77812500E-07	dt=	0.77812500E-07
Starting time-step	t0=	0.78437500E-07	dt=	0.78437500E-07
Starting time-step	t0=	0.79062500E-07	dt=	0.79062500E-07
Starting time-step	t0=	0.79687500E-07	dt=	0.79687500E-07
Starting time-step	t0=	0.80312500E-07	dt=	0.80312500E-07
Starting time-step	t0=	0.80937500E-07	dt=	0.80937500E-07
Starting time-step	t0=	0.81562500E-07	dt=	0.81562500E-07
Starting time-step	t0=	0.82187500E-07	dt=	0.82187500E-07
Starting time-step	t0=	0.82812500E-07	dt=	0.82812500E-07
Starting time-step	t0=	0.83437500E-07	dt=	0.83437500E-07
Starting time-step	t0=	0.84062500E-07	dt=	0.84062500E-07
Starting time-step	t0=	0.84687500E-07	dt=	0.84687500E-07
Starting time-step	t0=	0.85312500E-07	dt=	0.85312500E-07
Starting time-step	t0=	0.85937500E-07	dt=	0.85937500E-07
Starting time-step	t0=	0.86562500E-07	dt=	0.86562500E-07
Starting time-step	t0=	0.87187500E-07	dt=	0.87187500E-07
Starting time-step	t0=	0.87812500E-07	dt=	0.87812500E-07
Starting time-step	t0=	0.88437500E-07	dt=	0.88437500E-07
Starting time-step	t0=	0.89		

```
Starting time-step t0= 0.21823507 dt= 0.52428800E-02
Starting time-step t0= 0.22347795 dt= 0.10485760E-01
Starting time-step t0= 0.23396371 dt= 0.10485760E-01
Starting time-step t0= 0.24444947 dt= 0.10485760E-01
Starting time-step t0= 0.25493523 dt= 0.10485760E-01
Starting time-step t0= 0.26542099 dt= 0.10485760E-01
Starting time-step t0= 0.27590675 dt= 0.20971520E-01
Starting time-step t0= 0.29687827 dt= 0.20971520E-01
Starting time-step t0= 0.31784979 dt= 0.20971520E-01
Starting time-step t0= 0.33882131 dt= 0.20971520E-01
Starting time-step t0= 0.35979283 dt= 0.20971520E-01
Starting time-step t0= 0.38076435 dt= 0.20971520E-01
Starting time-step t0= 0.40173587 dt= 0.20971520E-01
Starting time-step t0= 0.42270739 dt= 0.20971520E-01
Starting time-step t0= 0.44367891 dt= 0.20971520E-01
Starting time-step t0= 0.46465043 dt= 0.20971520E-01
Starting time-step t0= 0.48562195 dt= 0.20971520E-01
Starting time-step t0= 0.50659347 dt= 0.41943040E-01
Starting time-step t0= 0.54853651 dt= 0.41943040E-01
Starting time-step t0= 0.59047955 dt= 0.41943040E-01
Starting time-step t0= 0.63242259 dt= 0.83886080E-01
Starting time-step t0= 0.71630867 dt= 0.83886080E-01
Starting time-step t0= 0.80019475 dt= 0.83886080E-01
Starting time-step t0= 0.88408083 dt= 0.83886080E-01
Starting time-step t0= 0.96796691 dt= 0.83886080E-01
```

output ignored...

... output resumed

```
DELETING TIME-RECORD FOR TIME 25262.422
DELETING TIME-RECORD FOR TIME 25305.372
DELETING TIME-RECORD FOR TIME 25391.271
DELETING TIME-RECORD FOR TIME 25434.221
DELETING TIME-RECORD FOR TIME 25520.120
DELETING TIME-RECORD FOR TIME 25606.019
DELETING TIME-RECORD FOR TIME 25691.919
DELETING TIME-RECORD FOR TIME 25756.343
DELETING TIME-RECORD FOR TIME 25820.768
DELETING TIME-RECORD FOR TIME 25863.718
DELETING TIME-RECORD FOR TIME 25906.667
DELETING TIME-RECORD FOR TIME 25949.617
DELETING TIME-RECORD FOR TIME 25992.567
DELETING TIME-RECORD FOR TIME 26035.516
DELETING TIME-RECORD FOR TIME 26078.466
DELETING TIME-RECORD FOR TIME 26121.416
DELETING TIME-RECORD FOR TIME 26164.365
DELETING TIME-RECORD FOR TIME 26207.315
DELETING TIME-RECORD FOR TIME 26250.265
DELETING TIME-RECORD FOR TIME 26293.214
DELETING TIME-RECORD FOR TIME 26336.164
DELETING TIME-RECORD FOR TIME 26379.114
DELETING TIME-RECORD FOR TIME 26422.063
DELETING TIME-RECORD FOR TIME 26465.013
DELETING TIME-RECORD FOR TIME 26507.963
DELETING TIME-RECORD FOR TIME 26550.912
DELETING TIME-RECORD FOR TIME 26636.812
DELETING TIME-RECORD FOR TIME 26722.711
DELETING TIME-RECORD FOR TIME 26765.661
DELETING TIME-RECORD FOR TIME 26851.560
DELETING TIME-RECORD FOR TIME 26937.459
DELETING TIME-RECORD FOR TIME 26980.409
DELETING TIME-RECORD FOR TIME 27023.359
DELETING TIME-RECORD FOR TIME 27066.308
DELETING TIME-RECORD FOR TIME 27109.258
DELETING TIME-RECORD FOR TIME 27152.208
DELETING TIME-RECORD FOR TIME 27195.157
DELETING TIME-RECORD FOR TIME 27238.107
DELETING TIME-RECORD FOR TIME 27281.057
DELETING TIME-RECORD FOR TIME 27324.006
DELETING TIME-RECORD FOR TIME 27366.956
DELETING TIME-RECORD FOR TIME 27409.906
DELETING TIME-RECORD FOR TIME 27452.855
DELETING TIME-RECORD FOR TIME 27495.805
DELETING TIME-RECORD FOR TIME 27538.755
DELETING TIME-RECORD FOR TIME 27581.704
DELETING TIME-RECORD FOR TIME 27624.654
DELETING TIME-RECORD FOR TIME 27667.604
DELETING TIME-RECORD FOR TIME 27710.553
DELETING TIME-RECORD FOR TIME 27753.503
DELETING TIME-RECORD FOR TIME 27817.928
DELETING TIME-RECORD FOR TIME 27860.877
DELETING TIME-RECORD FOR TIME 27903.827
DELETING TIME-RECORD FOR TIME 27989.726
DELETING TIME-RECORD FOR TIME 28075.626
DELETING TIME-RECORD FOR TIME 28161.525
DELETING TIME-RECORD FOR TIME 28204.475
DELETING TIME-RECORD FOR TIME 28247.424
DELETING TIME-RECORD FOR TIME 28333.324
DELETING TIME-RECORD FOR TIME 28419.223
DELETING TIME-RECORD FOR TIME 28505.122
DELETING TIME-RECORD FOR TIME 28591.022
DELETING TIME-RECORD FOR TIME 28676.921
DELETING TIME-RECORD FOR TIME 28719.871
DELETING TIME-RECORD FOR TIME 28762.820
DELETING TIME-RECORD FOR TIME 28805.770
DELETING TIME-RECORD FOR TIME 28848.720
DELETING TIME-RECORD FOR TIME 28891.669
DELETING TIME-RECORD FOR TIME 28934.619
DELETING TIME-RECORD FOR TIME 28977.569
DELETING TIME-RECORD FOR TIME 29020.518
DELETING TIME-RECORD FOR TIME 29063.468
DELETING TIME-RECORD FOR TIME 29106.418
DELETING TIME-RECORD FOR TIME 29149.368
DELETING TIME-RECORD FOR TIME 29192.317
DELETING TIME-RECORD FOR TIME 29235.267
DELETING TIME-RECORD FOR TIME 29278.217
DELETING TIME-RECORD FOR TIME 29342.641
DELETING TIME-RECORD FOR TIME 29428.540
DELETING TIME-RECORD FOR TIME 29514.440
DELETING TIME-RECORD FOR TIME 29600.339
DELETING TIME-RECORD FOR TIME 29643.289
DELETING TIME-RECORD FOR TIME 29686.238
```

DELETING TIME-RECORD FOR TIME 29750.663  
DELETING TIME-RECORD FOR TIME 29836.562  
DELETING TIME-RECORD FOR TIME 29922.462  
DELETING TIME-RECORD FOR TIME 30008.361  
DELETING TIME-RECORD FOR TIME 30094.260  
DELETING TIME-RECORD FOR TIME 30180.160  
DELETING TIME-RECORD FOR TIME 30266.059  
DELETING TIME-RECORD FOR TIME 30351.958  
DELETING TIME-RECORD FOR TIME 30437.858  
DELETING TIME-RECORD FOR TIME 30523.757  
DELETING TIME-RECORD FOR TIME 30566.707  
DELETING TIME-RECORD FOR TIME 30609.656  
DELETING TIME-RECORD FOR TIME 30652.606  
DELETING TIME-RECORD FOR TIME 30695.556  
DELETING TIME-RECORD FOR TIME 30738.505  
DELETING TIME-RECORD FOR TIME 30781.455  
DELETING TIME-RECORD FOR TIME 30867.354  
DELETING TIME-RECORD FOR TIME 30953.254  
DELETING TIME-RECORD FOR TIME 31039.153  
DELETING TIME-RECORD FOR TIME 31082.103  
DELETING TIME-RECORD FOR TIME 31168.002  
DELETING TIME-RECORD FOR TIME 31253.901  
DELETING TIME-RECORD FOR TIME 31339.801  
DELETING TIME-RECORD FOR TIME 31382.750  
DELETING TIME-RECORD FOR TIME 31425.700  
DELETING TIME-RECORD FOR TIME 31468.650  
DELETING TIME-RECORD FOR TIME 31511.600  
DELETING TIME-RECORD FOR TIME 31554.549  
DELETING TIME-RECORD FOR TIME 31597.499  
DELETING TIME-RECORD FOR TIME 31640.449  
DELETING TIME-RECORD FOR TIME 31683.398  
DELETING TIME-RECORD FOR TIME 31726.348  
DELETING TIME-RECORD FOR TIME 31769.298  
DELETING TIME-RECORD FOR TIME 31812.247  
DELETING TIME-RECORD FOR TIME 31855.197  
DELETING TIME-RECORD FOR TIME 31898.147  
DELETING TIME-RECORD FOR TIME 31941.096  
DELETING TIME-RECORD FOR TIME 31984.046  
DELETING TIME-RECORD FOR TIME 32026.996  
DELETING TIME-RECORD FOR TIME 32069.945  
DELETING TIME-RECORD FOR TIME 32112.895  
DELETING TIME-RECORD FOR TIME 32177.319  
DELETING TIME-RECORD FOR TIME 32220.269  
DELETING TIME-RECORD FOR TIME 32263.219

KEEPING TIME-RECORD FOR TIME 32349.118  
AND FOR TIME 32400.000  
WORKSPACE RECLAIMED

-----  
INTERPOLATION SCHEME USED THIS FRACTION OF  
THE ALLOCATED MEMORY: 0.122439088252744  
EFFICIENCY FACTOR: 29.1910258830722  
MEMORY FRACTION USAGE PER BRANCH:  
0.172677338019014  
8.596093720332654E-002  
9.278505153534618E-002  
-----

DEALLOCATING  
-----

TIMESTEP AT 32400.0000 SELECTED

DIC>  
DIC> set-inter  
--OK--  
DIC>

## exb7-plot

DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exb7\plot.DCM"

DIC>

DIC>

DIC>

DIC> @@

DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE

DIC> @@

DIC> go d-m

TIME STEP AT TIME 3.24000E+04

\*\*\* ENTERING GRAPHITE AS A DIFFUSION NONE PHASE

\*\*\* ENTERING CLNB1\_S AS A DIFFUSION NONE PHASE

DIC> read exb7

OK

DIC>

DIC> @@

DIC> @@ GO TO THE POST PROCESSOR

DIC> @@

DIC> post

POST PROCESSOR VERSION 1.7

Implemented by Bjorn Jonsson

POST-1:

POST-1: @@

POST-1: @@ PLOT THE INTERFACE POSITION AS A FUNCTION OF TIME

POST-1: @@

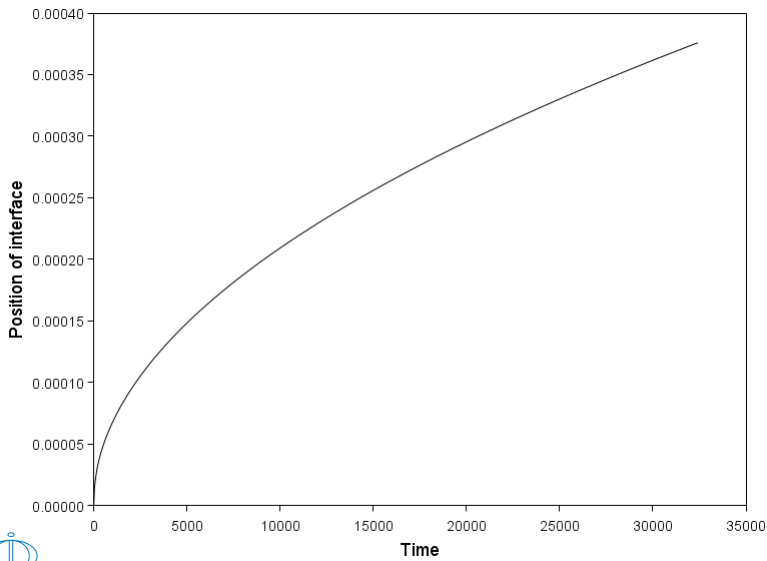
POST-1: s-d-a x time

INFO: Time is set as independent variable

POST-1: s-d-a y po-o-in aus upp

POST-1:

POST-1: plot



POST-1:

POST-1: Hit RETURN to continue

POST-1:

POST-1: @@

POST-1: @@ APPEND DATA FROM A CORRESPONDING SIMULATION

POST-1: @@ WITHOUT NIOBIUM

POST-1: @@

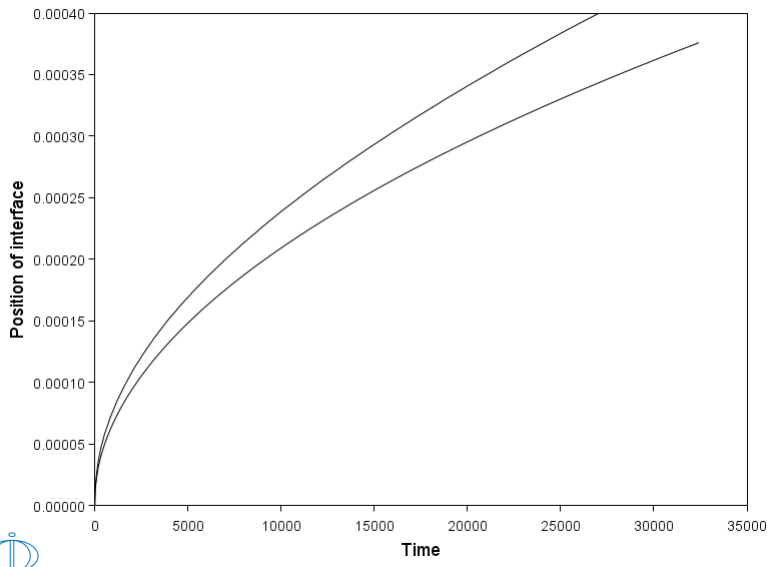
POST-1:

POST-1: app y fec.exp 0

DATASET NUMBER(s): /-1/: 1

POST-1:

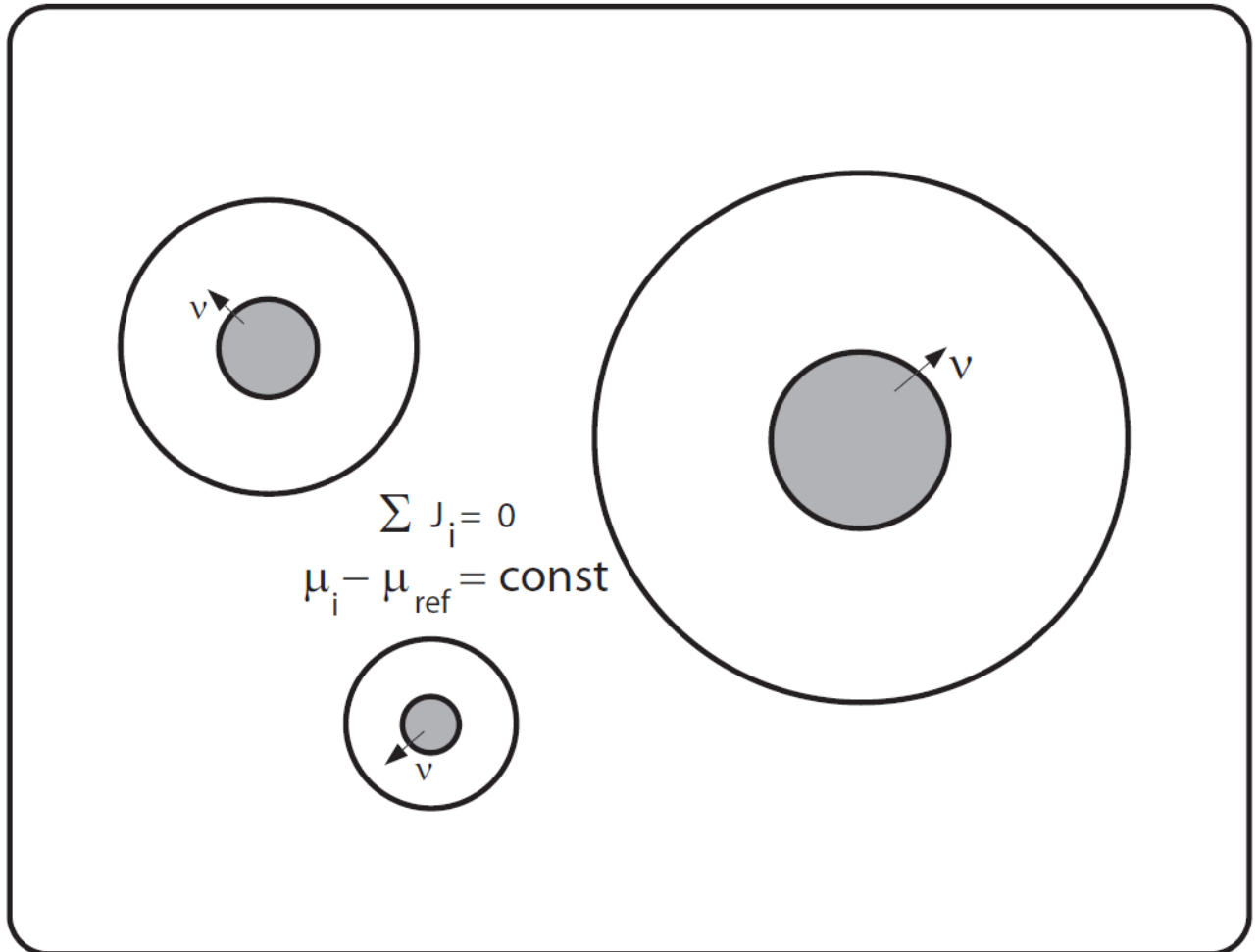
POST-1: plot



POST-1:  
POST-1: set-inter  
--OK--  
POST-1:



## Cell Calculations



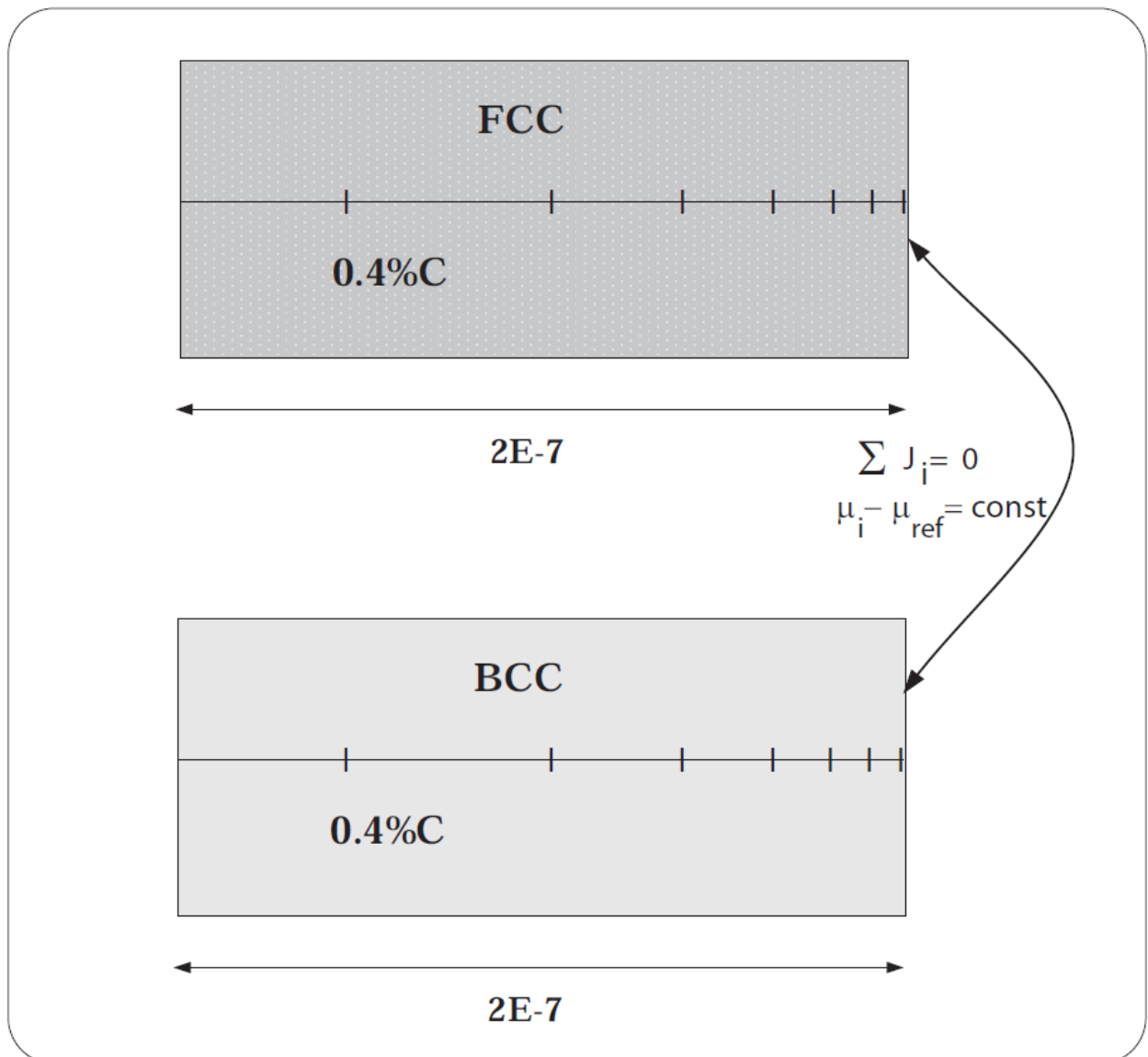


## Example exc1

### 'Carbon cannon' in $\alpha/\gamma$ 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: Acta Metall. Mater. 41 (1993), pp.1951-1957.

$$T = 673\text{K}$$



## excl-setup

### SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,  
Stockholm, Sweden

Software running on Windows 64-bit wordlength  
Compiler: Intel Fortran Compiler 2025.0.0  
License library version: 9.7.0.0036  
Linked: Nov 19 2025 at 14:44:36

```
SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\excl\setup.DCM"
```

```
SYS: i>|@@
NO SUCH COMMAND, USE HELP
SYS: @@ Cell calculation.
SYS: @@ Carbon cannon in ferrite/austenite: Fe-C system, 2-cell calculation
SYS: @@ This example simulates what happens to a ferrite plate that has
SYS: @@ inherited the carbon content of its parent austenite. The ferrite
SYS: @@ plate formed is embedded in an austenite matrix. This setup
SYS: @@ corresponds to a proposed mechanism for formation of WidmannstÄtten
SYS: @@ ferrite or for the ferrite phase of the bainite structure. It is
SYS: @@ assumed that the phase boundary between ferrite and austenite is
SYS: @@ immobile, this is achieved in the simulation by putting the ferrite
SYS: @@ and the austenite in two different cells. See also M. Hillert,
SYS: @@ L. HÄgglund and J. Ågren: Acta Metall. Mater. 41 (1993), pp.1951-1957.
SYS: @@-----
SYS:
SYS: @@ excl_setup.DCM
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASE
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\databases\da
ta
Current database: Steels/Fe-Alloys v12.0

VA                /- DEFINED
DICTRA FCC_A1     REJECTED
TDB_TCFE12:
TDB_TCFE12: @@
TDB_TCFE12: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA
TDB_TCFE12: @@
TDB_TCFE12: sw fedemo
Current database: Iron Demo Database v6.0

VA                /- DEFINED
TDB_FEDEMO: def-sys fe c
FE                C DEFINED
TDB_FEDEMO: rej ph * all
GAS:G             LIQUID:L             BCC_A2
C14_LAVES         CBCC_A12            CEMENTITE_D011
CUB_A13           DIAMOND_A4          FCC_A1
GRAPHITE_A9       HCP_A3              KSI_CARBIDE
M23C6_D84         M5C2                M7C3_D101
REJECTED
TDB_FEDEMO: res ph fcc,bcc
FCC_A1            BCC_A2 RESTORED
TDB_FEDEMO: get
11:04:02,150 [Thread-0] INFO  JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE DATA
TDB_FEDEMO: @@
TDB_FEDEMO: app mfedemo
Current database: Fe-Alloys Mobility demo database v5.0

VA DEFINED
APP: def-sys fe c
FE                C DEFINED
APP: rej ph * all
BCC_A2            FCC_A1              CEMENTITE_D011
LIQUID:L REJECTED
APP: res ph fcc,bcc
FCC_A1            BCC_A2 RESTORED
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR
APP: @@
APP: go d-m
NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
```

```

DIC> set-cond glob T 0 673; * N
DIC>
DIC> @@
DIC> @@ IN THE FIRST CELL
DIC> @@
DIC> @@ ENTER REGION aus CONTAINING AUSTENITE
DIC> @@ ENTER A GEOMETRICAL GRID INTO THAT REGION
DIC> @@ ENTER THE INITIAL COMPOSITION INTO THE AUSTENITE
DIC> @@
DIC> enter-region aus
DIC> enter-grid aus 0.2e-6 AUTO
DIC> enter-phase act aus matrix fcc_a1#1
DIC>
DIC> enter-composition
REGION NAME : /AUS/: aus
PHASE NAME : /FCC_A1/: fcc_a1#1
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: c
TYPE /LINEAR/: lin 0.4 0.4
DIC>
DIC> @@
DIC> @@ IN THE SECOND CELL
DIC> @@
DIC> create-new-cell
CELL DISTRIBUTION FACTOR /1/: 1
CREATING NEW CELL, NUMBER: 2
CELL 2 SELECTED
DIC-2>
DIC-2> @@
DIC-2> @@ ENTER REGION fer CONTAINING FERRITE
DIC-2> @@ ENTER A GEOMETRICAL GRID INTO THAT REGION
DIC-2> @@ ENTER THE INITIAL COMPOSITION INTO THE FERRITE
DIC-2> @@
DIC-2> enter-region fer
DIC-2>
DIC-2>
DIC-2>
DIC-2> enter-grid fer 0.2e-6 AUTO
DIC-2> enter-phase act fer matrix bcc_a2#1
DIC-2>
DIC-2> enter-composition
REGION NAME : /FER/: fer
PHASE NAME : /BCC_A2/: bcc_a2#1
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: c
TYPE /LINEAR/: lin 0.4 0.4
DIC-2>
DIC-2> @@
DIC-2> @@ SET THE SIMULATION TIME AND OTHER SIMULATION PARAMETERS
DIC-2> @@
DIC-2> set-simulation-time
END TIME FOR INTEGRATION /.1/: 0.5
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /.05/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC-2>
DIC-2>
DIC-2>
DIC-2> @@
DIC-2> @@ USE IMPLICIT (1) TIME INTEGRATION
DIC-2> @@
DIC-2> set-option DEGREE_OF_IMPLICITY 1.0
DIC-2>
DIC-2> @@
DIC-2> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC-2> @@
DIC-2> save excl Y
DIC-2>
DIC-2> set-inter
--OK--
DIC-2>

```

excl-run

DIC-2>About

NO SUCH COMMAND, USE HELP

DIC-2>DIC-2>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\excl\run.DCM"

DIC-2>

DIC-2>

DIC-2> @@ excl\_run.DCM

DIC-2>

DIC-2> @@

DIC-2> @@ READ THE WORKSPACE AND START THE SIMULATION

DIC-2> @@

DIC-2> go d-m

TIME STEP AT TIME 0.00000E+00

DIC-2> read excl

OK

DIC> sim

INFO: Default responses (if any) will be applied during the simulation. Use "SIMULATE\_REACTION NO" instead for manual input.

Region: AUS

geometric 0.833333 dense at 0.200000E-06 58 points

Region: FER

geometric 0.866747 dense at 0.200000E-06 56 points

U-FRACTION IN SYSTEM: C = .018673311178274 FE = 1

TOTAL SIZE OF SYSTEM: 4E-07 [m]

U-FRACTION IN SYSTEM: C = .018673311178274 FE = 1

TOTAL SIZE OF SYSTEM: 4E-07 [m]

447946.878608491 447949.425773906 11997.5727803552 509.072302029083 1.64579526427206 2.991014536506762

004 1.873507877807250E-010 2.157620498397347E-020 TIME = 0.10000000E-06 DT = 0.10000000E-

06 SUM OF SQUARES = 0.21576205E-19

U-FRACTION IN SYSTEM: C = .018673311178274 FE = 1

TOTAL SIZE OF SYSTEM: 4E-07 [m]

CPU time used in timestep

6990557.33466302 6990537.78491717 1945697.25852058 208879.794635738 5553.68156963137 18.9610917424286

003 4.905196919524002E-010 TIME = 0.18809712E-05 DT = 0.17809712E-05 SUM OF SQUARES = 0.49051969E-09

U-FRACTION IN SYSTEM: C = .0186752381781978 FE = 1

TOTAL SIZE OF SYSTEM: 4E-07 [m]

CPU time used in timestep

1192344.06100535 1192329.94850616 189579.574181709 12584.7380556981 85.4121357667536 4.689557954150148

002 1.660148003358546E-007 3.211827551363855E-016 TIME = 0.54429136E-05 DT = 0.35619424E-

05 SUM OF SQUARES = 0.32118276E-15

U-FRACTION IN SYSTEM: C = .0186752381781975 FE = 1

TOTAL SIZE OF SYSTEM: 4E-07 [m]

CPU time used in timestep

9352.72460217537 9351.24581868996 8.33131247860036 6.865464737104051E-003 4.679153161748302E-

009 2.627476288683237E-018 TIME = 0.12566798E-04 DT = 0.71238848E-05 SUM OF SQUARES = 0.26274763E-17

U-FRACTION IN SYSTEM: C = .0186752381781976 FE = 1

TOTAL SIZE OF SYSTEM: 4E-07 [m]

CPU time used in timestep

12562.6400754973 12561.6545449903 43.9288662228511 0.130473992862266 1.169682658138010E-

006 3.140511407965565E-014 TIME = 0.26814568E-04 DT = 0.14247770E-04 SUM OF SQUARES = 0.31405114E-13

U-FRACTION IN SYSTEM: C = .0186752381782102 FE = 1

TOTAL SIZE OF SYSTEM: 4E-07 [m]

CPU time used in timestep

1590264.72559312 1590193.66022020 22090.8907443916 225.836918705995 2.529807879096672E-

002 3.445480345719094E-008 4.479609687239584E-018 TIME = 0.55310107E-04 DT = 0.28495539E-

04 SUM OF SQUARES = 0.44796097E-17

U-FRACTION IN SYSTEM: C = .0186752381782102 FE = 1

TOTAL SIZE OF SYSTEM: 4E-07 [m]

CPU time used in timestep

327687.035318517 327661.898987337 1469.72470105990 5.50750601527406 7.888357767448198E-

005 4.277431172052134E-012 TIME = 0.11230118E-03 DT = 0.56991078E-04 SUM OF SQUARES = 0.42774312E-11

U-FRACTION IN SYSTEM: C = .0186752381782691 FE = 1

TOTAL SIZE OF SYSTEM: 4E-07 [m]

CPU time used in timestep

170767.367332731 170754.629137030 847.064841827446 3.49206351563984 6.064520923699286E-

005 4.389923124582143E-012 TIME = 0.22628334E-03 DT = 0.11398216E-03 SUM OF SQUARES = 0.43899231E-11

U-FRACTION IN SYSTEM: C = .0186752381783885 FE = 1

TOTAL SIZE OF SYSTEM: 4E-07 [m]

CPU time used in timestep

71469.1546492401 71463.2474554426 286.706783835063 0.974629802899678 1.147108093787204E-

005 4.630764305921858E-013

output ignored...

... output resumed

8723.73139333764 8714.14888637668 0.142119294131426 2.293429653613097E-006 6.041677043497021E-

016 TIME = 0.19378777 DT = 0.21263337E-01 SUM OF SQUARES = 0.60416770E-15

U-FRACTION IN SYSTEM: C = .0186752381789553 FE = 1

TOTAL SIZE OF SYSTEM: 4E-07 [m]

CPU time used in timestep

3628.51077633945 3623.14317560849 5.106455988690661E-002 2.533716886273999E-007 3.058912087591196E-

017 TIME = 0.21699110 DT = 0.23203332E-01 SUM OF SQUARES = 0.30589121E-16

U-FRACTION IN SYSTEM: C = .0186752381789546 FE = 1

TOTAL SIZE OF SYSTEM: 4E-07 [m]

CPU time used in timestep

343.428217631662 342.020178386370 3.649237162950703E-004 3.883132135689597E-010 1.450665533038300E-

003 1.383662180998518E-020 TIME = 0.24328714 DT = 0.26296039E-01 SUM OF SQUARES = 0.13836622E-19

U-FRACTION IN SYSTEM: C = .0186752381789546 FE = 1

TOTAL SIZE OF SYSTEM: 4E-07 [m]

CPU time used in timestep

154953.127015460 155200.504921007 0.687315762098293 6.734203634684393E-006 2.012407000991206E-

016 TIME = 0.27504833 DT = 0.31761190E-01 SUM OF SQUARES = 0.20124070E-15

U-FRACTION IN SYSTEM: C = .0186752381789549 FE = 1

TOTAL SIZE OF SYSTEM: 4E-07 [m]

CPU time used in timestep

1082965.63954956 1083482.38009993 74.3589963968804 5.678453467944987E-003 2.871632765117707E-

011 TIME = 0.31656380 DT = 0.41515473E-01 SUM OF SQUARES = 0.28716328E-10

U-FRACTION IN SYSTEM: C = .0186752381790661 FE = 1

TOTAL SIZE OF SYSTEM: 4E-07 [m]

CPU time used in timestep

889096.550347434 889476.374328008 71.4735517583633 6.523355538661645E-003 4.517613972818337E-

011 TIME = 0.36656380 DT = 0.50000000E-01 SUM OF SQUARES = 0.45176140E-10

U-FRACTION IN SYSTEM: C = .0186752381792341 FE = 1

TOTAL SIZE OF SYSTEM: 4E-07 [m]

CPU time used in timestep

30667.4576647169 30730.0481919767 2.206536826268009E-002 2.174597970974520E-007 3.148369731517288E-

002 8.800085325441011E-019 TIME = 0.41656380 DT = 0.50000000E-01 SUM OF SQUARES = 0.88000853E-18

U-FRACTION IN SYSTEM: C = .018675238179234 FE = 1

TOTAL SIZE OF SYSTEM: 4E-07 [m]

CPU time used in timestep

96093.7077886222 95993.4121984139 1.36064627479814 1.470015689602965E-005 2.457515992303445E-

```
015      TIME = 0.46656380      DT = 0.50000000E-01 SUM OF SQUARES = 0.24575160E-14
U-FRACTION IN SYSTEM: C = .0186752381792328 FE = 1
TOTAL SIZE OF SYSTEM: 4E-07 [m]
CPU time used in timestep                1 seconds
2902084.90436944      2901466.92691898      786.289143739698      0.212525759670095      1.446423037622219E-
008      9.594350823852117E-020      TIME = 0.50000000      DT = 0.33436199E-01 SUM OF SQUARES = 0.95943508E-19
U-FRACTION IN SYSTEM: C = .0186752381792328 FE = 1
TOTAL SIZE OF SYSTEM: 4E-07 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME      0.00000000
DELETING TIME-RECORD FOR TIME      0.10000000E-06
DELETING TIME-RECORD FOR TIME      0.18809712E-05
DELETING TIME-RECORD FOR TIME      0.54429136E-05
DELETING TIME-RECORD FOR TIME      0.12566798E-04
DELETING TIME-RECORD FOR TIME      0.26814568E-04
DELETING TIME-RECORD FOR TIME      0.55310107E-04
DELETING TIME-RECORD FOR TIME      0.11230118E-03
DELETING TIME-RECORD FOR TIME      0.22628334E-03
DELETING TIME-RECORD FOR TIME      0.45424765E-03
DELETING TIME-RECORD FOR TIME      0.91017628E-03
DELETING TIME-RECORD FOR TIME      0.18220335E-02
DELETING TIME-RECORD FOR TIME      0.36457480E-02
DELETING TIME-RECORD FOR TIME      0.72931770E-02
DELETING TIME-RECORD FOR TIME      0.14588035E-01
DELETING TIME-RECORD FOR TIME      0.29177751E-01
DELETING TIME-RECORD FOR TIME      0.46732906E-01
DELETING TIME-RECORD FOR TIME      0.62920803E-01
DELETING TIME-RECORD FOR TIME      0.80218444E-01
DELETING TIME-RECORD FOR TIME      0.97429297E-01
DELETING TIME-RECORD FOR TIME      0.11527725
DELETING TIME-RECORD FOR TIME      0.13355877
DELETING TIME-RECORD FOR TIME      0.15258192
DELETING TIME-RECORD FOR TIME      0.17252443
DELETING TIME-RECORD FOR TIME      0.19378777
DELETING TIME-RECORD FOR TIME      0.21699110
DELETING TIME-RECORD FOR TIME      0.24328714
DELETING TIME-RECORD FOR TIME      0.27504833
DELETING TIME-RECORD FOR TIME      0.31656380
DELETING TIME-RECORD FOR TIME      0.36656380
DELETING TIME-RECORD FOR TIME      0.41656380

KEEPING TIME-RECORD FOR TIME      0.46656380
AND FOR TIME      0.50000000
WORKSPACE RECLAIMED

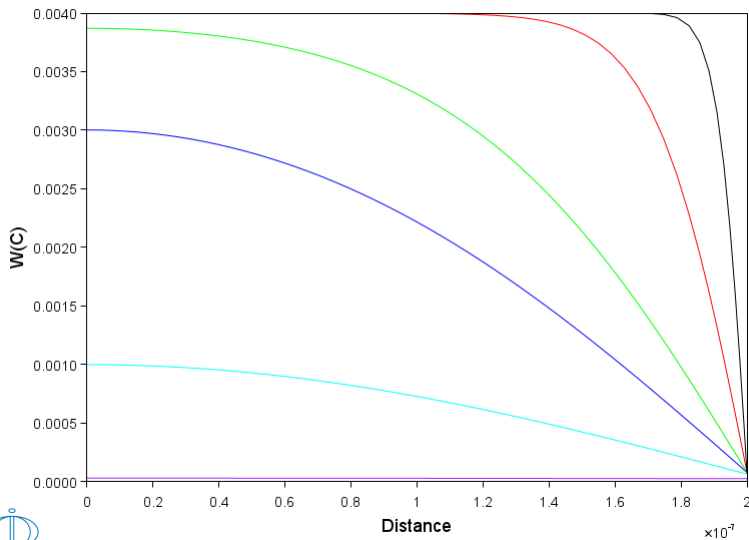
TIMESTEP AT      0.50000000      SELECTED
```

```
DIC>
DIC>
DIC>
DIC> set-inter
--OK--
DIC>
```

## excl-plot

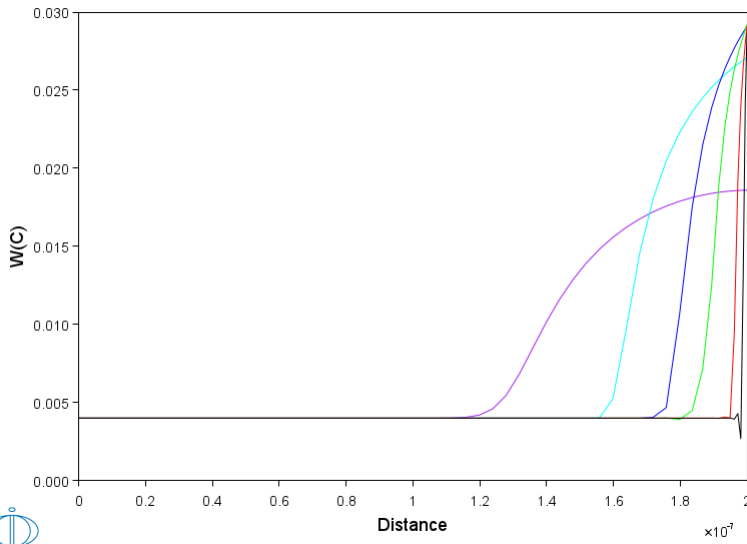
```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\excl\plot.DCM"
DIC>
DIC>
DIC> @@ excl_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE c1
DIC> @@
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 5.00000E-01
DIC> read excl
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1: @@
POST-1: @@ FIRST PLOT CARBON CONCENTRATION PROFILES IN FERRITE (CELL-2)
POST-1: @@ THEN SET THE DISTANCE AS X-AXIS (NOT THAT DISTANCE IS SET INDEPENDENT
POST-1: @@ VARIABLE AUTOMATICALLY) AND W-FRACTION CARBON AS Y-AXIS
POST-1: @@ REMEMBER THAT THE PLOT CONDITION ALSO MUST BE SET.
POST-1: @@
POST-1: select-cell
Number /NEXT/: 2
CELL 2 SELECTED
POST-2:
POST-2: @@
POST-2: @@ NOTICE THAT THE PROMPT INCLUDES THE CURRENT CELL NUMBER
POST-2: @@
POST-2: s-d-a x dist glo
INFO: Distance is set as independent variable
POST-2: s-d-a y w(c)
POST-2: s-p-c time .0001 .001 .01 .03 .1 .5
POST-2:
POST-2: @@
POST-2: @@ SET THE TITLE ON THE PLOTS
POST-2: @@
POST-2: set-title Figure c1.1
POST-2: plot
```

Figure c1.1



```
POST-2:
POST-2:
POST-2:
POST-2: @?<_hit_return_to_continue_>
POST-2:
POST-2: @@
POST-2: @@ DO THE SAME THING FOR THE AUSTENITE (CELL-1)
POST-2: @@
POST-2: select-cell
Number /NEXT/: 1
CELL 1 SELECTED
POST-1: set-title Figure c1.2
POST-1: plot
```

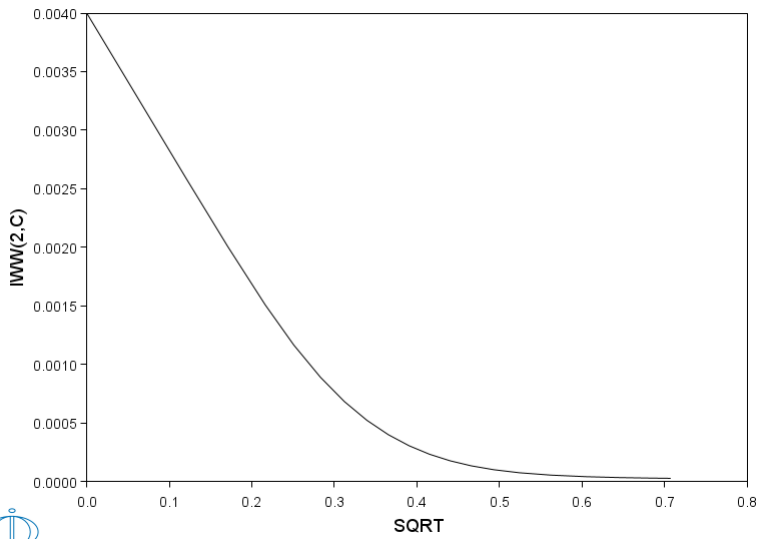
Figure c1.2



```

POST-1:
POST-1:
POST-1:
POST-1: @?<_hit_return_to_continue_>
POST-1: @@
POST-1: @@
POST-1: @@ PLOT THE AVARAGE WEIGHT FRACTION OF CARBON IN FERRITE VS. SQUARE ROOT
POST-1: @@ OF TIME. START BY DEFINING A "SQUARE-ROOT-OF-TIME" FUNCTION.
POST-1: @@
POST-1: sel-cell 2
CELL 2 SELECTED
POST-2: enter func sqrt=sqrt(time);
POST-2: s-d-a x sqrt
POST-2: s-d-a y iw(2,c)
POST-2: s-i-v time
POST-2: set-title Figure c1.3
POST-2: plot
    
```

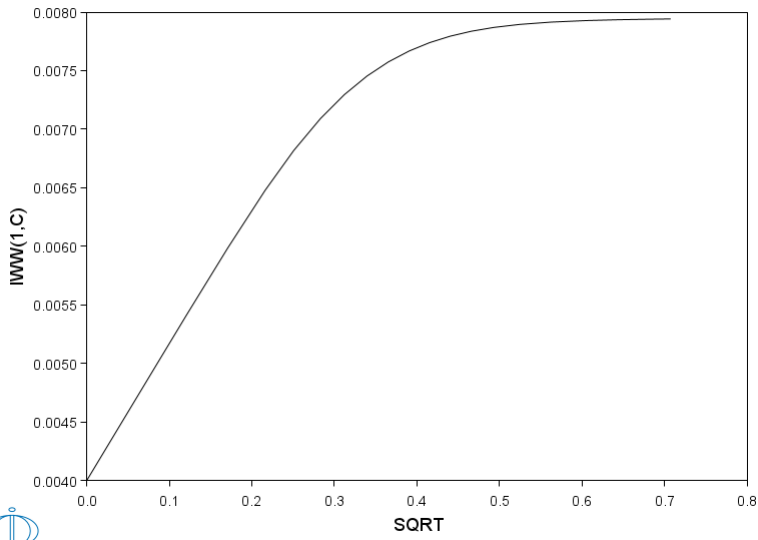
Figure c1.3



```

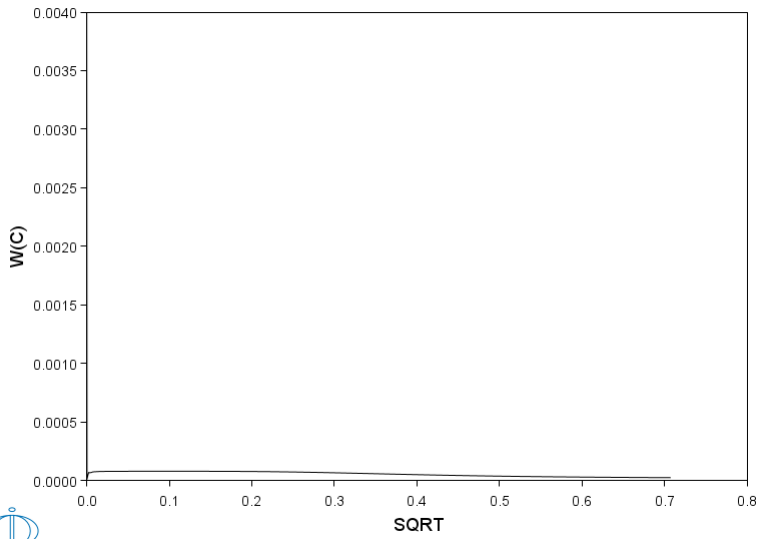
POST-2:
POST-2:
POST-2:
POST-2: @?<_hit_return_to_continue_>
POST-2: @@
POST-2: @@ DO THE SAME THING FOR THE AUSTENITE
POST-2: @@
POST-2: sel-cell 1
CELL 1 SELECTED
POST-1: s-d-a y iw(1,c)
POST-1: set-title Figure c1.4
POST-1: plot
    
```

Figure c1.4



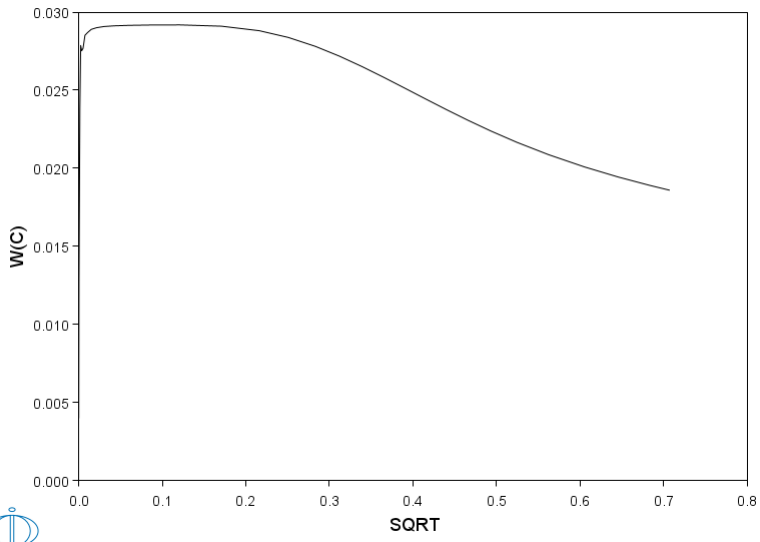
```
POST-1:
POST-1:
POST-1:
POST-1:??<_hit_return_to_continue_>
POST-1:
POST-1: @@
POST-1: @@ PLOT HOW THE CONCENTRATION IN FERRITE AT THE FERRITE/AUSTENITE BOUNDARY
POST-1: @@ V.S SQUARE ROOT OF TIME. THE FERRITE/AUSTENITE BOUNDARY IS REPRESENTED
POST-1: @@ BY THE CELL BOUNDARY I.E. THE "LAST" INTERFACE.
POST-1: @@
POST-1: sel-cell 2
CELL 2 SELECTED
POST-2: s-d-a y w(c)
POST-2: s-p-c interface last
POST-2: set-title Figure c1.5
POST-2: plot
```

Figure c1.5



```
POST-2:
POST-2:
POST-2:
POST-2:??<_hit_return_to_continue_>
POST-2:
POST-2: @@
POST-2: @@ DO THE SAME THING FOR THE AUSTENITE
POST-2: @@
POST-2: sel-cell 1
CELL 1 SELECTED
POST-1: set-title Figure c1.6
POST-1: plot
```

Figure c1.6



```
POST-1:  
POST-1:  
POST-1:  
POST-1: @?<_hit_return_to_continue_>  
POST-1:  
POST-1: set-inter  
--OK--  
POST-1:
```

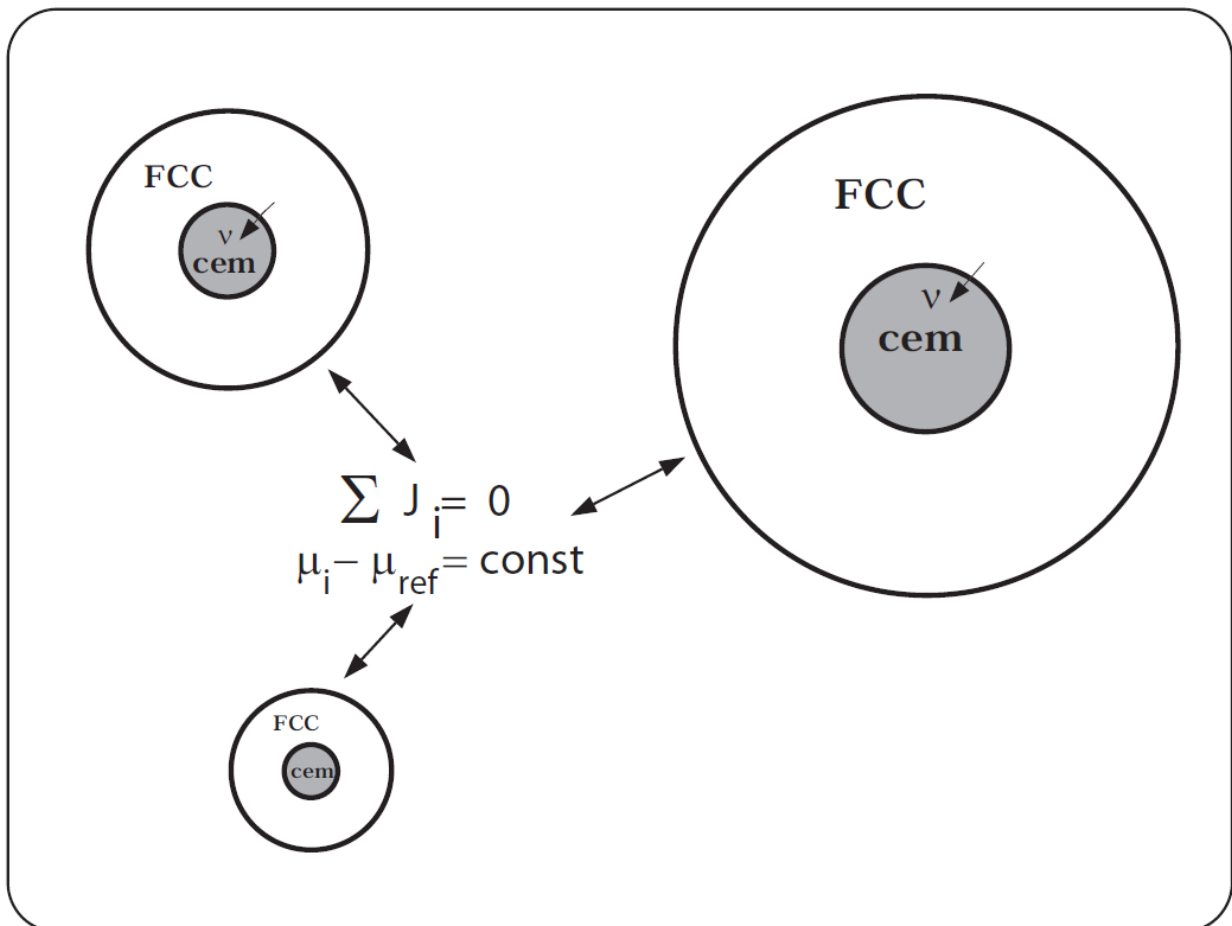


## Example exc2

### Cementite dissolution in an Fe-Cr-C alloy: Three particle sizes and three different cells

This example calculates the dissolution of cementite particles in an austenite matrix. This is the same as exc1 except that there are three particle sizes. Altogether six particles are considered using three different cells. This is to be able to represent some size distribution among the cementite particles. See also Z.-K. Liu, L. Höglund, B. Jönsson and J. Ågren: Metall.Trans.A, v. 22A (1991), pp. 1745-1752.

**T = 1183K**



## exc2-setup

### SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,  
Stockholm, Sweden

Software running on Windows 64-bit wordlength  
Compiler: Intel Fortran Compiler 2025.0.0  
License library version: 9.7.0.0036  
Linked: Nov 19 2025 at 14:44:36

```
SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exc2\setup.DCM"
```

```
SYS: i>?@@
NO SUCH COMMAND, USE HELP
SYS: @@ Cell calculation.
SYS: @@ Cementite dissolution in an Fe-Cr-C alloy: Three particle sizes and
SYS: @@ three different cells
SYS: @@ This example calculates the dissolution of cementite particles
SYS: @@ in an austenite matrix. This example is the same as exc1 but
SYS: @@ instead there are three particle sizes. A total of six
SYS: @@ particles are considered using three different cells. This is to
SYS: @@ represent some size distribution among the cementite particles.
SYS: @@ See also Z.-K. Liu, L. HÅglund, B. JÅnsson and J. Ågren:
SYS: @@ Metall.Trans.A, v. 22A (1991), pp. 1745-1752.
SYS: @@-----
SYS:
SYS: @@ exc2_setup.DCM
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASE
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\databases\da
ta
Current database: Steels/Fe-Alloys v12.0

VA /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE12:
TDB_TCFE12: @@
TDB_TCFE12: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA
TDB_TCFE12: @@
TDB_TCFE12: switch fedemo
Current database: Iron Demo Database v6.0

VA /- DEFINED
TDB_FEDEMO: def-sys fe cr c
FE CR C
DEFINED
TDB_FEDEMO: rej ph * all
GAS:G LIQUID:L BCC_A2
C14_LAVES CBCC_A12 CEMENTITE_D011
CHI_A12 CUB_A13 DIAMOND_A4
FCC_A1 GRAPHITE_A9 HCP_A3
KSI_CARBIDE M23C6_D84 M3C2_D510
M5C2 M7C3_D101 SIGMA_D8B
REJECTED
TDB_FEDEMO: res ph fcc cementite
FCC_A1 CEMENTITE_D011 RESTORED
TDB_FEDEMO: get
11:07:16,403 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
Creating a new composition set FCC_A1#2
PARAMETERS ...
FUNCTIONS ...

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE MOBILITY DATA
TDB_FEDEMO: @@
TDB_FEDEMO: app mfedemo
Current database: Fe-Alloys Mobility demo database v5.0

VA DEFINED
APP: def-sys fe cr c
FE CR C
DEFINED
APP: rej ph * all
BCC_A2 FCC_A1 CEMENTITE_D011
LIQUID:L REJECTED
APP: res ph fcc cementite
FCC_A1 CEMENTITE_D011 RESTORED
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
Creating a new composition set FCC_A1#3
PARAMETERS ...
FUNCTIONS ...

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR
APP: @@
APP: go d-m
NO TIME STEP DEFINED
```

```

DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob t 0 1183; * n
DIC>
DIC> @@-----
DIC> @@ CELL NUMBER ONE - Defining 1 copy of the largest particle
DIC> @@ Since the commands CRE_NEW_CELL or AMEND_CELL are not used for this
DIC> @@ first definition, it is just like any DICTRA setup.
DIC> @@-----
DIC>
DIC> @@
DIC> @@ ENTER REGIONS carb AND aus
DIC> @@
DIC> enter-region carb
DIC> enter-region aus
ATTACH TO REGION NAMED /CARB/:
ATTACHED TO THE RIGHT OF CARB /YES/:
DIC> @@
DIC> @@ ENTER GEOMETRICAL GRIDS INTO THE REGIONS
DIC> @@
DIC>
DIC> @@
DIC> @@ THE SIZE OF THE CEMENTITE PARTICLES ARE KNOWN AS WE ASSUME
DIC> @@ IT HAS BEEN MEASURED.
DIC> @@
DIC> enter-grid
REGION NAME : /CARB/: carb
WIDTH OF REGION /1/: 0.700000e-6
TYPE /AUTO/: GEO
NUMBER OF POINTS /50/: 30
VALUE OF R IN THE GEOMETRICAL SERIE : 0.9
DIC>
DIC> @@
DIC> @@ THE SIZE OF THE FCC REGION CAN BE CALCULATED FROM A MASS BALANCE
DIC> @@ AFTER ESTIMATING THE INITIAL COMPOSITIONS IN THE TWO PHASES.
DIC> @@
DIC> enter-grid
REGION NAME : /AUS/: aus
WIDTH OF REGION /1/: 7.1832993E-7
TYPE /AUTO/: GEO
NUMBER OF POINTS /50/: 30
VALUE OF R IN THE GEOMETRICAL SERIE : 1.1
DIC>
DIC> @@
DIC> @@ ENTER PHASES INTO REGIONS
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /CARB/: carb
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: cementite
DIC>
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /AUS/: aus
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC> @@
DIC> @@ ENTER INITIAL VALUES FOR THE COMPOSITIONS IN THE PHASES
DIC> @@
DIC> enter-composition carb cementite fe w-f
PROFILE FOR /CR/: cr lin 0.12423326 0.12423326
DIC>
DIC> enter-composition aus fcc#1 fe w-f
PROFILE FOR /C/: cr lin 4.6615447E-3 4.6615447E-3
PROFILE FOR /CR/: c lin 1.5135207E-4 1.5135207E-4
DIC>
DIC> @@-----
DIC> @@ CELL NUMBER TWO - Defining 1 copy also of the smallest particle
DIC> @@ This is done by giving the argument 1 at the CRE_NEW_CELL command.
DIC> @@-----
DIC> create-new-cell
CELL DISTRIBUTION FACTOR /1/: 1
CREATING NEW CELL, NUMBER: 2
CELL 2 SELECTED
DIC>
DIC> 2> @@
DIC> 2> @@ ENTER REGIONS carb AND aus
DIC> 2> @@
DIC> 2> enter-region carb
DIC> 2> enter-region aus
ATTACH TO REGION NAMED /CARB/:
ATTACHED TO THE RIGHT OF CARB /YES/:
DIC> 2> @@
DIC> 2> @@ ENTER GEOMETRICAL GRIDS INTO THE REGIONS
DIC> 2> @@
DIC> 2> enter-grid carb 0.300000e-6 GEO 20 0.9
DIC> 2> enter-grid aus 3.0785568E-7 GEO 20 1.1
DIC> 2>
DIC> 2> @@
DIC> 2> @@ ENTER PHASES INTO THE REGIONS
DIC> 2> @@
DIC> 2> enter-phase act carb matrix cementite
DIC> 2> enter-phase act aus matrix fcc#1
DIC> 2>
DIC> 2> @@
DIC> 2> @@ ENTER INITIAL VALUES FOR THE COMPOSITIONS IN THE PHASES
DIC> 2> @@
DIC> 2> enter-composition carb cementite fe w-f
PROFILE FOR /CR/: cr lin 0.12423326 0.12423326
DIC> 2>
DIC> 2> enter-composition aus fcc#1 fe w-f
PROFILE FOR /C/: cr lin 4.6615447E-3 4.6615447E-3
PROFILE FOR /CR/: c lin 1.5135207E-4 1.5135207E-4
DIC> 2>
DIC> 2> @@-----
DIC> 2> @@ CELL NUMBER THREE - Defining 2 copies of the average sized particle

```

```
DIC-2> @@-----
DIC-2> create-new-cell
CELL DISTRIBUTION FACTOR /1/: 2
  CREATING NEW CELL, NUMBER: 3
  CELL 3 SELECTED
DIC-3>
DIC-3> @@
DIC-3> @@ ENTER REGIONS carb AND aus
DIC-3> @@
DIC-3> enter-region carb
DIC-3> enter-region aus
ATTACH TO REGION NAMED /CARB/:
ATTACHED TO THE RIGHT OF CARB /YES/:
DIC-3> @@
DIC-3> @@ ENTER GEOMETRICAL GRIDS INTO THE REGIONS
DIC-3> @@
DIC-3> enter-grid carb 0.525500e-6 GEO 25 0.9
DIC-3> enter-grid aus 5.3926054E-7 GEO 25 1.1
DIC-3>
DIC-3> @@
DIC-3> @@ ENTER PHASES INTO REGIONS
DIC-3> @@
DIC-3> enter-phase act carb matrix cementite
DIC-3> enter-phase act aus matrix fcc#1
DIC-3>
DIC-3> @@
DIC-3> @@ ENTER INITIAL VALUES FOR THE COMPOSITIONS IN THE PHASES
DIC-3> @@
DIC-3> enter-composition carb cementite fe w-f
PROFILE FOR /CR/: cr lin 0.12423326 0.12423326
DIC-3>
DIC-3> enter-composition aus fcc#1 fe w-f
PROFILE FOR /C/: cr lin 4.6615447E-3 4.6615447E-3
PROFILE FOR /CR/: c lin 1.5135207E-4 1.5135207E-4
DIC-3>
DIC-3> @@-----
DIC-3> @@ GLOBAL CONDITIONS - Note: temperature already set.
DIC-3> @@-----
DIC-3>
DIC-3> @@
DIC-3> @@ SET TO A SPHERICAL GEOMETRY
DIC-3> @@
DIC-3> enter-geo 2
DIC-3>
DIC-3>
DIC-3> @@
DIC-3> @@ SET THE SIMULATION TIME
DIC-3> @@
DIC-3> set-simulation-time
END TIME FOR INTEGRATION /.1/: 10000
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /1000/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC-3>
DIC-3> @@
DIC-3> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC-3> @@
DIC-3> save exc2 Y
DIC-3>
DIC-3>
DIC-3> set-inter
--OK--
DIC-3>
```

exc2-run

DIC-3>About

NO SUCH COMMAND, USE HELP

DIC-3>DIC-3>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exc2\run.DCM"

DIC-3>

DIC-3>

DIC-3> @@ exc2\_run.DCM

DIC-3>

DIC-3> @@

DIC-3> @@ READ THE SET UP FROM FILE AND START THE SIMULATION

DIC-3> @@

DIC-3> go d-m

TIME STEP AT TIME 0.00000E+00

DIC-3> read exc2

OK

DIC> sim yes

INFO: Default responses (if any) will be applied during the simulation. Use "SIMULATE\_REACTION NO" instead for manual input.  
DEGREE OF IMPLICITNESS SET TO TRAPEZOIDAL RULE

Trying old scheme 4

GENERATING STARTING VALUES FOR CELL # 1 INTERFACE # 2

DETERMINING INITIAL EQUILIBRIUM VALUES

CALCULATING STARTING VALUES: 9 EQUILIBRIUM CALCULATIONS DONE 6 OUT OF 9

04

Trying old scheme 4

GENERATING STARTING VALUES FOR CELL # 2 INTERFACE # 2

DETERMINING INITIAL EQUILIBRIUM VALUES

CALCULATING STARTING VALUES: 9 EQUILIBRIUM CALCULATIONS DONE 6 OUT OF 9

04

Trying old scheme 4

GENERATING STARTING VALUES FOR CELL # 3 INTERFACE # 2

DETERMINING INITIAL EQUILIBRIUM VALUES

CALCULATING STARTING VALUES: 9 EQUILIBRIUM CALCULATIONS DONE 6 OUT OF 9

04

U-FRACTION IN SYSTEM: C = .0406910187115061 CR = .0214382352209387

FE = .978561764909568

TOTAL SIZE OF SYSTEM: 2.30050996865E-17 [m^3]

U-FRACTION IN SYSTEM: C = .0406910187115061 CR = .0214382352209387

FE = .978561764909568

TOTAL SIZE OF SYSTEM: 2.30050996865E-17 [m^3]

8 GRIDPOINT(S) ADDED TO CELL #1 REGION: CARB

9 GRIDPOINT(S) ADDED TO CELL #1 REGION: AUS

11 GRIDPOINT(S) ADDED TO CELL #2 REGION: CARB

12 GRIDPOINT(S) ADDED TO CELL #2 REGION: AUS

10 GRIDPOINT(S) ADDED TO CELL #3 REGION: CARB

9 GRIDPOINT(S) ADDED TO CELL #3 REGION: AUS

0.562308005161987 0.562344274011782 0.562366853557356 0.562349175215441 0.562308055404654 0.562308076601151

002 3.175413249295662E-002 1.213896739589521E-002 1.062121835683817E-004 1.403438790273176E-

005 3.825371689357113E-006 1.436471950202005E-005 4.649535418442126E-006 3.845602994570142E-

006 3.953076792712090E-006 3.744817358935585E-006 3.788020535983020E-006 3.752696037130689E-

006 3.750979315676525E-006 4.093728631190408E-004 6.107394348874644E-003 3.789577105282956E-

006 3.687373747186901E-006 3.623600664792957E-006 3.626488639510961E-006 3.511997011627082E-

006 3.402323193206890E-006 3.207385177399628E-006 3.013575760568908E-006 3.03483370692124E-

006 2.666125028211296E-006 2.602539804316190E-006 2.328375229342318E-006 1.750312348994674E-

006 1.749273203691536E-006 4.075236951602559E-004 6.106453324145921E-003 1.770380341785491E-

006 1.242047203580392E-006 5.483512043523086E-007 5.480039848778492E-007 1.327538353118446E-

007 2.382133042369882E-008 1.323307162953844E-008 5.542121113340301E-009 1.039962591339205E-

009 2.958801810836022E-010 7.697361894000011E-010 4.032221926558567E-010 2.166092104248856E-

012 6.686618972581373E-017 TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.96243705E-21

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.29712891E-02 AND -0.29712891E-02

POSITION OF INTERFACE CARB / AUS IS 0.69970287E-06

CELL # 2 VELOCITY AT INTERFACE # 2 IS -0.35949743E-02 AND -0.35949743E-02

POSITION OF INTERFACE CARB / AUS IS 0.29964050E-06

CELL # 3 VELOCITY AT INTERFACE # 2 IS -0.36149476E-02 AND -0.36149476E-02

POSITION OF INTERFACE CARB / AUS IS 0.52513851E-06

U-FRACTION IN SYSTEM: C = .040718331897411 CR = .0214509582219592

FE = .978549041908548

TOTAL SIZE OF SYSTEM: 2.30050996865E-17 [m^3]

CPU time used in timestep 5 seconds

2 GRIDPOINT(S) ADDED TO CELL #1 REGION: CARB

1 GRIDPOINT(S) ADDED TO CELL #1 REGION: AUS

2 GRIDPOINT(S) ADDED TO CELL #2 REGION: CARB

1 GRIDPOINT(S) ADDED TO CELL #2 REGION: AUS

2 GRIDPOINT(S) ADDED TO CELL #3 REGION: CARB

1 GRIDPOINT(S) ADDED TO CELL #3 REGION: AUS

0.720078253871675

output ignored...

... output resumed

TOTAL SIZE OF SYSTEM: 2.30050996865E-17 [m^3]

3 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: AUS

04

CPU time used in timestep 6 seconds

2.22966745435616E-002 2.229667475786168E-002 2.229667475323933E-002 2.229817354581277E-002 2.229831021974588E-

002 2.229288884853952E-002 2.229599789674747E-002 1.425119528666322E-003 3.669324639842843E-

006 1.040148781241546E-008 4.192167896667589E-012 1.934402257947536E-

017 TIME = 7165.8351 DT = 1000.0000 SUM OF SQUARES = 0.84728751E-17

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.13177272E-10 AND -0.13177272E-10

POSITION OF INTERFACE CARB / AUS IS 0.42077987E-06

CELL # 3 VELOCITY AT INTERFACE # 2 IS -0.14419647E-10 AND -0.14419647E-10

POSITION OF INTERFACE CARB / AUS IS 0.23638321E-06

U-FRACTION IN SYSTEM: C = .0407440455640011 CR = .0215403703713709

FE = .978459629759136

TOTAL SIZE OF SYSTEM: 2.30050996865E-17 [m^3]

1 GRIDPOINT(S) REMOVED FROM CELL #3 REGION: AUS

04

CPU time used in timestep 5 seconds

3.364345311160721E-002 3.364345324971768E-002 3.364345322365588E-002 3.364519167745175E-002 3.364531099932380E-

002 3.363901560628884E-002 3.364253133539891E-002 2.309312616351048E-003 3.345561560452142E-

006 7.591165941353612E-010 2.319161081122149E-013 7.621818133441375E-

017 TIME = 8165.8351 DT = 1000.0000 SUM OF SQUARES = 0.53143688E-19

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.11743096E-10 AND -0.11743096E-10

POSITION OF INTERFACE CARB / AUS IS 0.40903677E-06

CELL # 3 VELOCITY AT INTERFACE # 2 IS -0.13249555E-10 AND -0.13249555E-10

POSITION OF INTERFACE CARB / AUS IS 0.22313366E-06

U-FRACTION IN SYSTEM: C = .0407440900266383 CR = .0215400101850286

FE = .978459989945479

TOTAL SIZE OF SYSTEM: 2.30050996865E-17 [m^3]

CPU time used in timestep 5 seconds

3.705630166391169E-002 3.705630176337865E-002 3.705630172281395E-002 3.705800171213234E-002 3.705808405673141E-002  
002 3.705189955621500E-002 3.705517870634564E-002 3.158234971095821E-003 4.806272829114568E-006  
006 3.048496197567481E-009 1.034477314758240E-012 2.978972223855546E-016  
016 TIME = 9165.8351 DT = 1000.0000 SUM OF SQUARES = 0.33602577E-18  
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.10620254E-10 AND -0.10620254E-10  
POSITION OF INTERFACE CARB / AUS IS 0.39841652E-06  
CELL # 3 VELOCITY AT INTERFACE # 2 IS -0.12596837E-10 AND -0.12596837E-10  
POSITION OF INTERFACE CARB / AUS IS 0.21053682E-06  
U-FRACTION IN SYSTEM: C = .0407441047083711 CR = .0215397503284518  
FE = .978460249802055  
TOTAL SIZE OF SYSTEM: 2.30050996865E-17 [m^3]  
1 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: AUS  
1 GRIDPOINT(S) REMOVED FROM CELL #3 REGION: AUS

CPU time used in timestep 5 seconds  
4.614833337884686E-002 4.614833346537163E-002 4.614833343952789E-002 4.615003053279432E-002 4.615008115549189E-002  
002 4.614377844854414E-002 4.614661401655567E-002 4.761712383992910E-003 7.908686349474443E-006  
006 7.580574316429073E-009 5.682776786532170E-013 2.653052237587051E-016  
016 TIME = 10000.000 DT = 834.16488 SUM OF SQUARES = 0.10739326E-17  
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.96726218E-11 AND -0.96726218E-11  
POSITION OF INTERFACE CARB / AUS IS 0.39034796E-06  
CELL # 3 VELOCITY AT INTERFACE # 2 IS -0.12034478E-10 AND -0.12034478E-10  
POSITION OF INTERFACE CARB / AUS IS 0.20049808E-06  
U-FRACTION IN SYSTEM: C = .0407440731990143 CR = .0215395772155419  
FE = .978460422914965  
TOTAL SIZE OF SYSTEM: 2.30050996865E-17 [m^3]

MUST SAVE WORKSPACE ON FILE  
WORKSPACE SAVED ON FILE  
RECLAIMING WORKSPACE  
DELETING TIME-RECORD FOR TIME 2676.3768  
DELETING TIME-RECORD FOR TIME 2823.6579  
DELETING TIME-RECORD FOR TIME 2823.6579  
DELETING TIME-RECORD FOR TIME 2823.6579  
DELETING TIME-RECORD FOR TIME 2823.6579  
DELETING TIME-RECORD FOR TIME 2823.6580  
DELETING TIME-RECORD FOR TIME 2823.6582  
DELETING TIME-RECORD FOR TIME 2823.6585  
DELETING TIME-RECORD FOR TIME 2823.6591  
DELETING TIME-RECORD FOR TIME 2823.6604  
DELETING TIME-RECORD FOR TIME 2823.6630  
DELETING TIME-RECORD FOR TIME 2823.6681  
DELETING TIME-RECORD FOR TIME 2823.6783  
DELETING TIME-RECORD FOR TIME 2823.6988  
DELETING TIME-RECORD FOR TIME 2823.7398  
DELETING TIME-RECORD FOR TIME 2823.8217  
DELETING TIME-RECORD FOR TIME 2823.9855  
DELETING TIME-RECORD FOR TIME 2824.3132  
DELETING TIME-RECORD FOR TIME 2824.9686  
DELETING TIME-RECORD FOR TIME 2826.2793  
DELETING TIME-RECORD FOR TIME 2828.9007  
DELETING TIME-RECORD FOR TIME 2834.1436  
DELETING TIME-RECORD FOR TIME 2844.6294  
DELETING TIME-RECORD FOR TIME 2865.6009  
DELETING TIME-RECORD FOR TIME 2907.5439  
DELETING TIME-RECORD FOR TIME 2991.4300  
DELETING TIME-RECORD FOR TIME 3159.2022  
DELETING TIME-RECORD FOR TIME 3494.7465  
DELETING TIME-RECORD FOR TIME 4165.8351  
DELETING TIME-RECORD FOR TIME 5165.8351  
DELETING TIME-RECORD FOR TIME 6165.8351  
DELETING TIME-RECORD FOR TIME 7165.8351  
DELETING TIME-RECORD FOR TIME 8165.8351  
  
KEEPING TIME-RECORD FOR TIME 9165.8351  
AND FOR TIME 10000.000  
WORKSPACE RECLAIMED

TIMESTEP AT 10000.0000 SELECTED

DIC>  
DIC>  
DIC> set-inter  
--OK--  
DIC>

## exc2-plot

DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exc2\plot.DCM"

DIC>

DIC>

DIC> @@ exc2\_plot.DCM

DIC>

DIC> @@

DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE c2

DIC> @@

DIC>

DIC> @@

DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE

DIC> @@

DIC> go d-m

TIME STEP AT TIME 1.00000E+04

DIC> read exc2

OK

DIC>

DIC> @@

DIC> @@ GO TO THE POST PROCESSOR

DIC> @@

DIC> post

POST PROCESSOR VERSION 1.7

Implemented by Bjorn Jonsson

POST-1:

POST-1: @@

POST-1: @@ PLOT THE CHROMIUM CONCENTRATION PROFILES IN THE SAME WAY AS IN exb2

POST-1: @@ BUT NOW FOR EACH PARTICLE. LET US LOOK AT THE PROFILES AFTER 1000s.

POST-1: @@

POST-1: @@

POST-1: @@

POST-1: @@ FIRST CELL

POST-1: @@

POST-1: enter-symb

Function or table /FUNCTION/: func

NAME: rdist

FUNCTION: gd-poi(carb,u);

POST-1:

POST-1: s-d-a x rdist

POST-1:

POST-1: s-d-a y uf(cr)

POST-1:

POST-1: s-i-v

VARIABLE /TIME/: dist

DISTANCE : /GLOBAL/: glo

POST-1:

POST-1: s-p-c time 1000

POST-1:

POST-1: @@

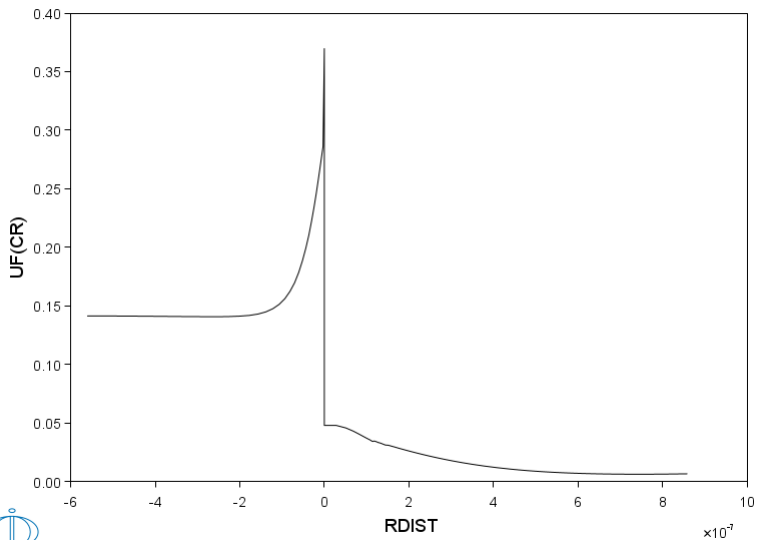
POST-1: @@ SET THE TITLE ON THE PLOT

POST-1: @@

POST-1: set-title Figure C2.1

POST-1: plot

Figure C2.1



POST-1:

POST-1: @@<\_hit\_return\_to\_continue\_>

POST-1:

POST-1: @@

POST-1: @@ SELECT CELL 2

POST-1: @@

POST-1: select-cell

Number /NEXT/: 2

CELL 2 SELECTED

POST-2:

POST-2: enter-symb

Function or table /FUNCTION/: func

NAME: rdist2

FUNCTION: gd-poi(carb,u);

POST-2:

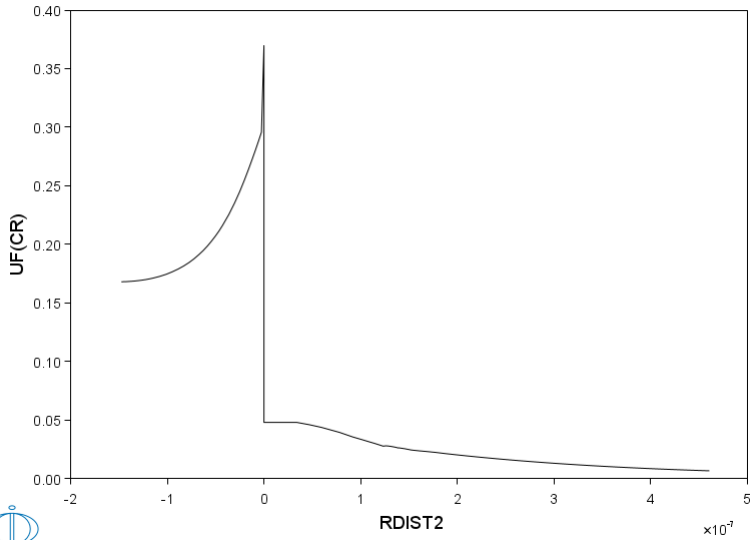
POST-2: s-d-a x rdist2

POST-2:

POST-2: set-title Figure C2.2

POST-2: plot

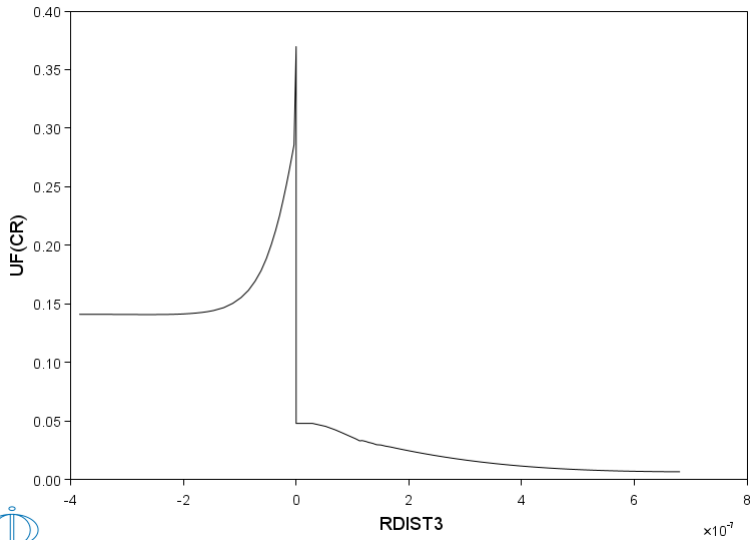
Figure C2.2



```

POST-2:
POST-2:
POST-2:
POST-2: @?<_hit_return_to_continue_>
POST-2:
POST-2: @@
POST-2: @@ SELECT CELL 3
POST-2: @@
POST-2: select-cell 3
      CELL 3 SELECTED
POST-3:
POST-3: enter-symb
Function or table /FUNCTION/: func
NAME: rdist3
FUNCTION: gd-poi(carb,u);
POST-3:
POST-3: s-d-a x rdist3
POST-3:
POST-3: set-title Figure C2.3
POST-3: plot
    
```

Figure C2.3



```

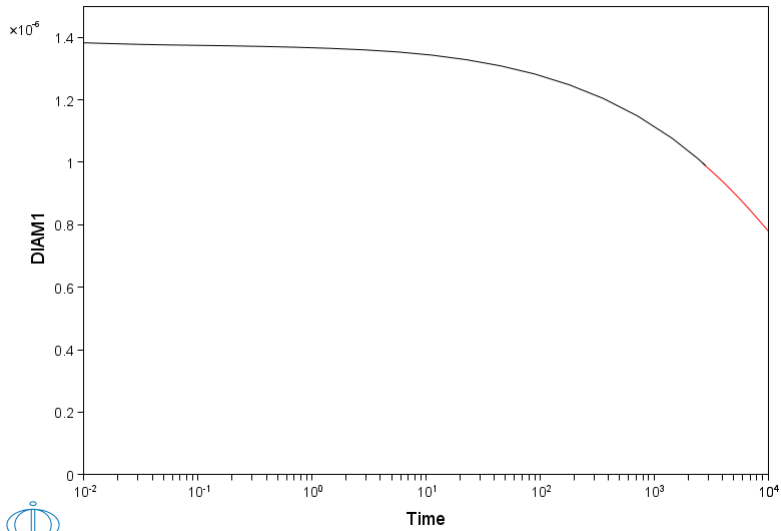
POST-3:
POST-3:
POST-3:
POST-3: @?<_hit_return_to_continue_>
POST-3:
POST-3: @@
POST-3: @@ ALSO PLOT HOW THE DIAMETER OF THE CEMENTITE PARTICLE VARIES
POST-3: @@ WITH TIME IN THE THREE CELLS
POST-3: @@
POST-3: @@
POST-3: @@ SELECT THE FIRST CELL
POST-3: @@
POST-3: sel-cell 1
      CELL 1 SELECTED
POST-1:
POST-1: s-d-a x time
      INFO: Time is set as independent variable
POST-1: s-s-s x n .01 10000
POST-1: set-axis-type x log
POST-1:
POST-1: enter func diam1=2*poi(carb,u);
POST-1: s-d-a y diam1
POST-1: s-s-s y n 0 1.5e-6
POST-1:
    
```

```

POST-1: s-p-c interf carb upp
POST-1:
POST-1: app n
POST-1: set-title Figure C2.4
POST-1: plot
WORKING ...

```

Figure C2.4

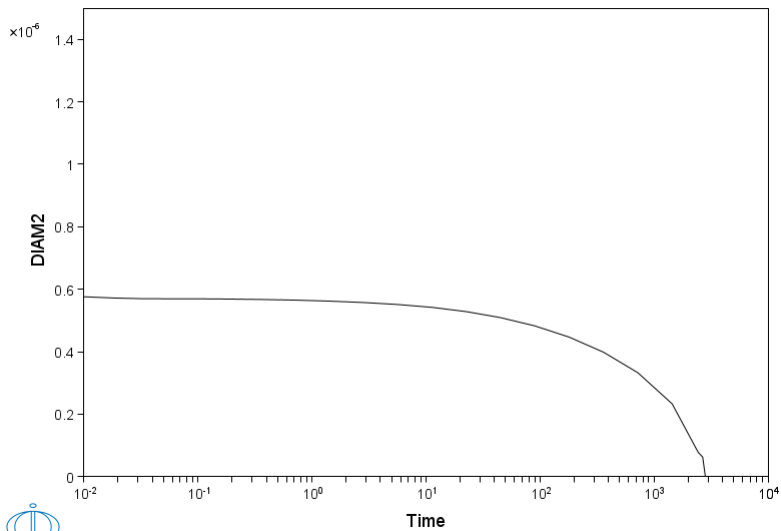


```

POST-1:
POST-1:
POST-1:
POST-1:
POST-1: @?<_hit_return_to_continue_>
POST-1:
POST-1:
POST-1: @@
POST-1: @@ SELECT CELL 2
POST-1: @@
POST-1: sel-cell 2
CELL 2 SELECTED
POST-2:
POST-2: enter func diam2=2*poi(carb,u);
POST-2: s-d-a y diam2
POST-2: s-s-s y n 0 1.5e-6
POST-2:
POST-2: s-p-c interf carb upp
POST-2:
POST-2: set-title Figure C2.5
POST-2: plot
WORKING ...

```

Figure C2.5



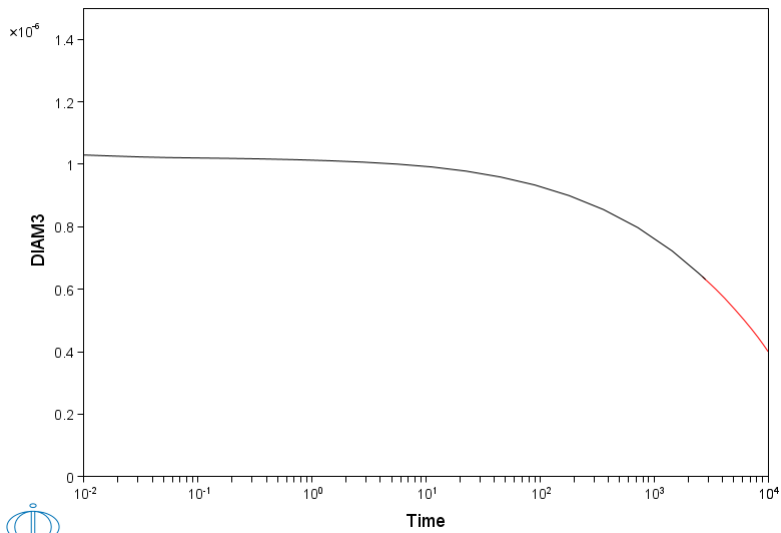
```

POST-2:
POST-2:
POST-2:
POST-2:
POST-2: @?<_hit_return_to_continue_>
POST-2:
POST-2: @@
POST-2: @@ SELECT CELL 3
POST-2: @@
POST-2: sel-cell 3
CELL 3 SELECTED
POST-3:
POST-3: enter func diam3=2*poi(carb,u);
POST-3: s-d-a y diam3
POST-3: s-s-s y n 0 1.5e-6
POST-3:
POST-3: s-p-c interf carb upp
POST-3:
POST-3: set-title Figure C2.6

```

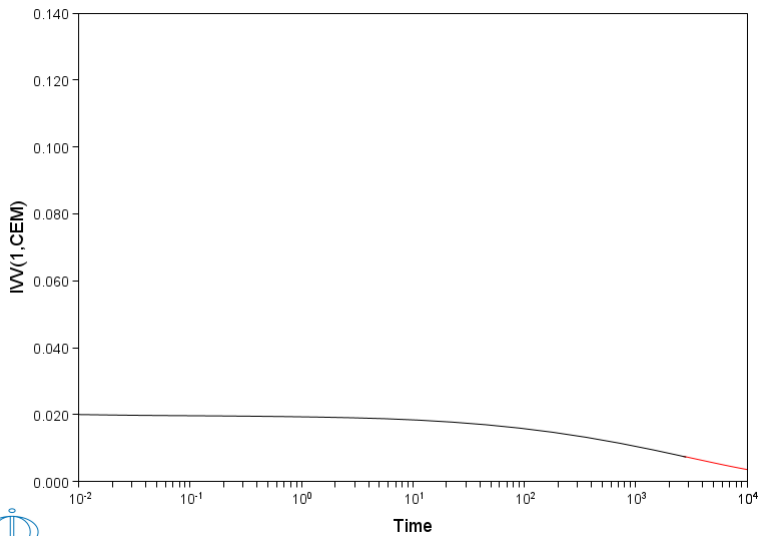
```
POST-3:
POST-3: plot
WORKING ...
```

Figure C2.6



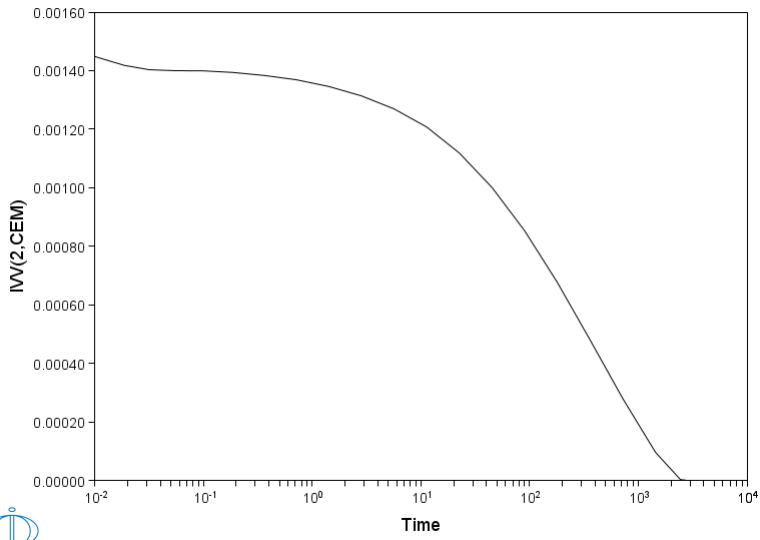
```
POST-3:
POST-3:
POST-3:
POST-3:
POST-3: @?<_hit_return_to_continue_>
POST-3:
POST-3: @@
POST-3: @@ NOW PLOT THE VOLUME FRACTION OF CEMENTITE IN THE THREE CELLS
POST-3: @@
POST-3: s-d-a x time
INFO: Time is set as independent variable
POST-3: s-s-s x n .01 10000
POST-3: set-axis-type x log
POST-3:
POST-3: @@
POST-3: @@ CELL 1
POST-3: @@
POST-3: s-d-a y ivv(1,cem)
POST-3: s-s-s y n 0 0.14
POST-3:
POST-3: s-p-c integral
POST-3:
POST-3: set-title Figure C2.7
POST-3: plot
WORKING ...
```

Figure C2.7



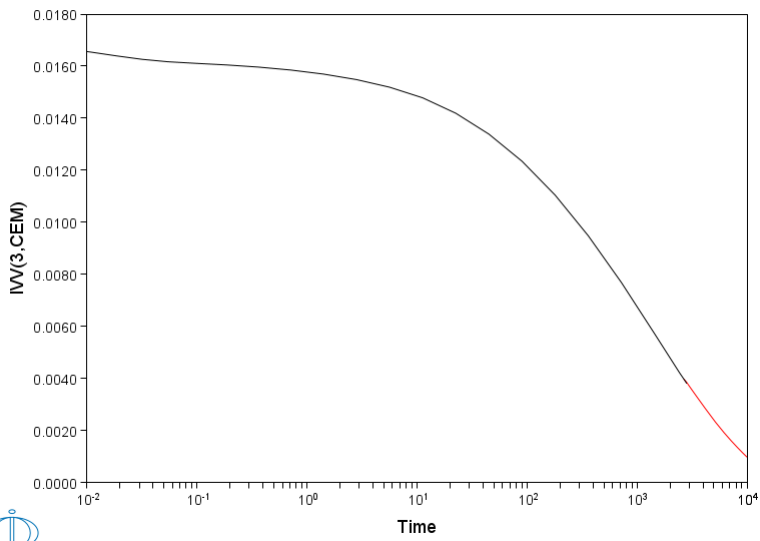
```
POST-3:
POST-3:
POST-3:
POST-3:
POST-3: @?<_hit_return_to_continue_>
POST-3:
POST-3: @@
POST-3: @@ CELL 2
POST-3: @@
POST-3: s-d-a y ivv(2,cem)
POST-3:
POST-3: set-title Figure C2.8
POST-3: plot
WORKING ...
```

Figure C2.8



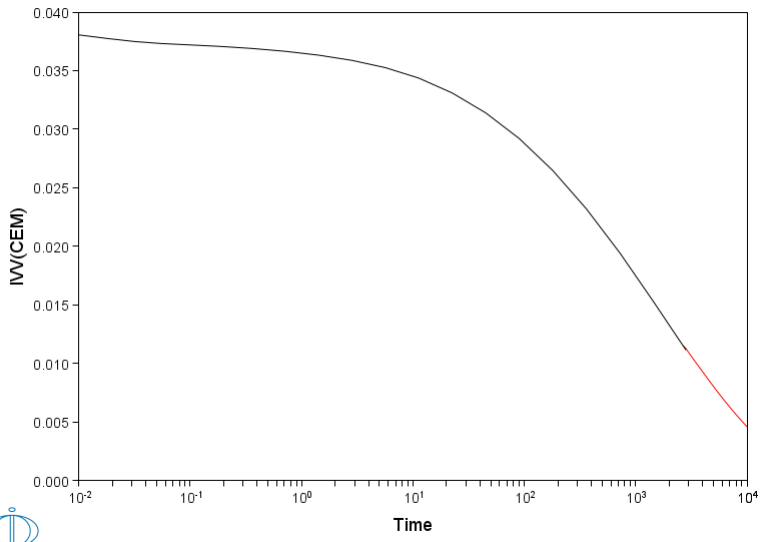
```
POST-3:
POST-3:
POST-3:
POST-3:
POST-3: @?<_hit_return_to_continue_>
POST-3:
POST-3: @@
POST-3: @@ CELL 3
POST-3: @@
POST-3: s-d-a y ivv(3,cem)
POST-3:
POST-3: set-title Figure C2.9
POST-3: plot
WORKING ...
```

Figure C2.9



```
POST-3:
POST-3:
POST-3:
POST-3:
POST-3: @?<_hit_return_to_continue_>
POST-3:
POST-3: @@
POST-3: @@ FINALLY, PLOT HOW THE TOTAL VOLUME FRACTION OF CEMENTITE
POST-3: @@ VARIES WITH TIME.
POST-3: @@
POST-3: s-d-a y ivv(cem)
POST-3:
POST-3: set-title Figure C2.10
POST-3: plot
WORKING ...
```

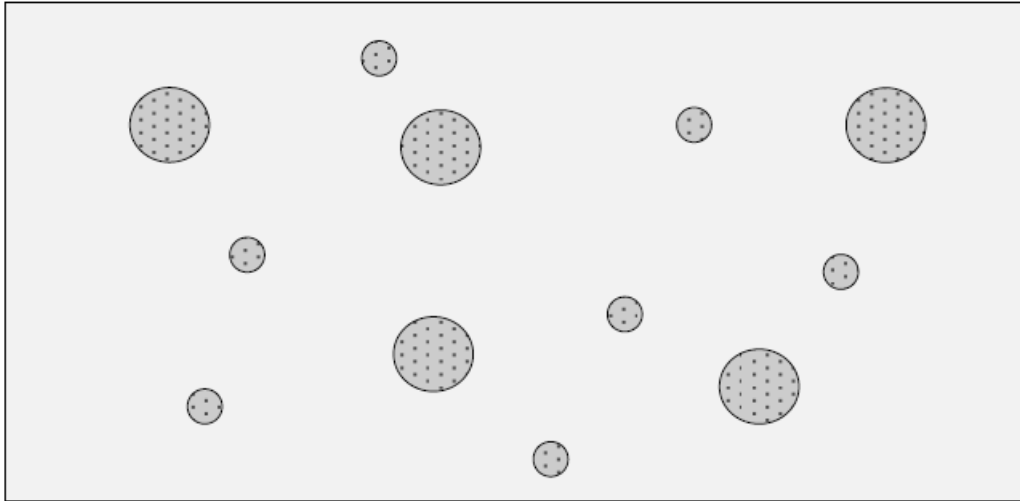
Figure C2.10



```
POST-3:  
POST-3:  
POST-3:  
POST-3:  
POST-3: @?<_hit_return_to_continue_>  
POST-3:  
POST-3: set-inter  
--OK--  
POST-3:
```



## **Diffusion in Dispersed Systems**

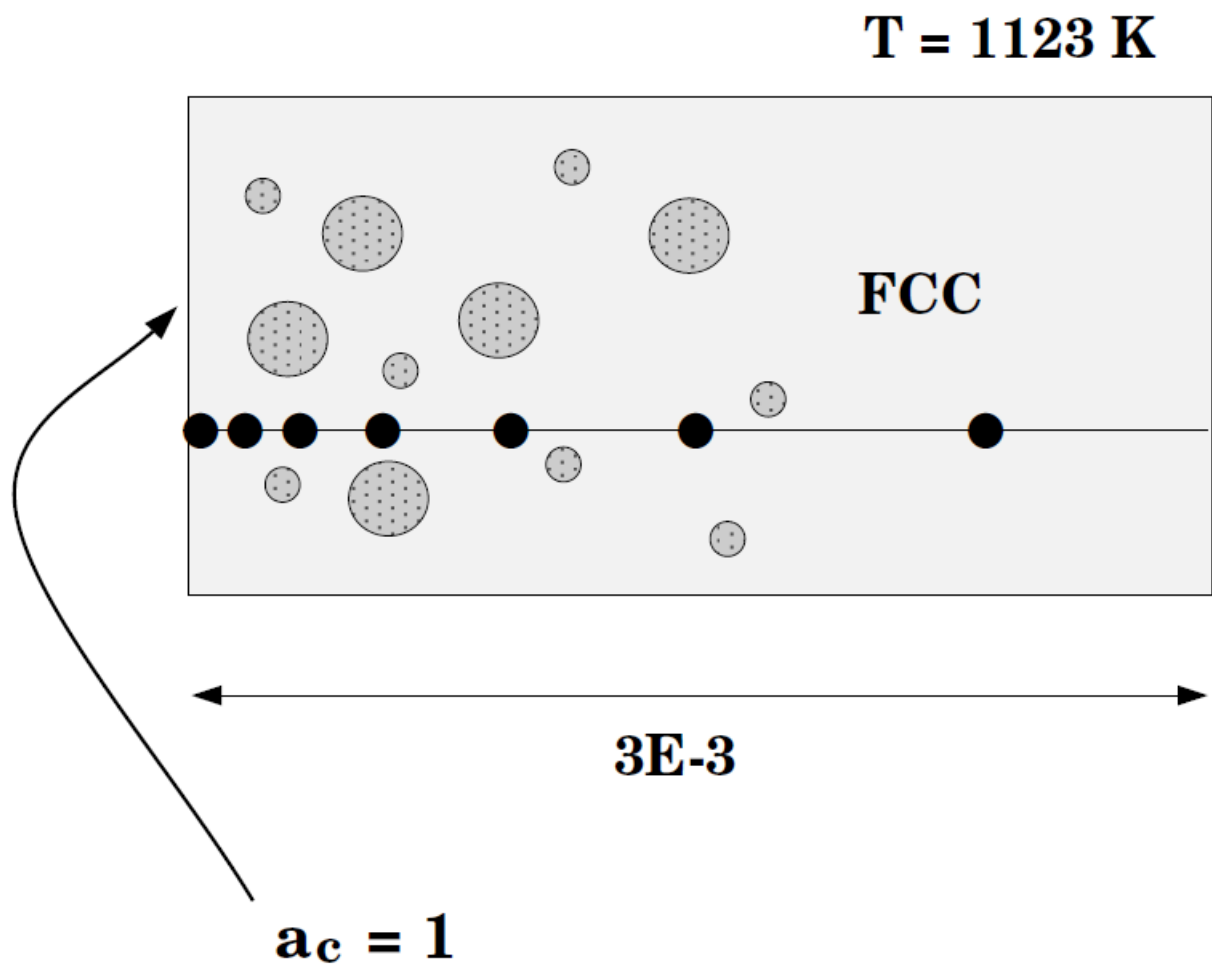




## Example exd1a

### Carburization of a Ni-25% Cr alloy: Dispersed system model

This example is about carburization of a Ni-25Cr alloy. In this case the M<sub>3</sub>C<sub>2</sub> and M<sub>7</sub>C<sub>3</sub> carbides are entered as spheroid phases in a FCC matrix. In this example the DISPERSED SYSTEM MODEL is used. This case is from A. Engström, L. Höglund and J. Ågren: Metall.Trans.A v. 25A (1994), pp. 1127-1134.



## exdia-setup

### SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,  
Stockholm, Sweden

Software running on Windows 64-bit wordlength  
Compiler: Intel Fortran Compiler 2025.0.0  
License library version: 9.7.0.0036  
Linked: Nov 19 2025 at 14:44:36

```
SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exdia\setup.DCM"
```

```
SYS: @@
SYS: @@ Diffusion in dispersed systems.
SYS: @@ Carburization of Ni-25%Cr alloy: Dispersed system model
SYS: @@ This example is about carburization of a Ni-25Cr alloy.
SYS: @@ In this case the M3C2 and M7C3 carbides are entered as
SYS: @@ spheroid phases in a FCC matrix. This simulation can be run
SYS: @@ with either the DISPERSED SYSTEM MODEL or the HOMOGENIZATION MODEL.
SYS: @@ In this example the DISPERSED SYSTEM MODEL is used, which requires
SYS: @@ that the default HOMOGENIZATION MODEL is disabled.
SYS: @@ With the DISPERSED SYSTEM MODEL the command
SYS: @@ ENTER_LABYRINTH_FUNCTION is used to take into account the
SYS: @@ impeding effect of dispersed phases on long-range diffusion.
SYS: @@ For the HOMOGENIZATION MODEL the command
SYS: @@ ENTER_HOMOGENIZATION_FUNCTION should be used.
SYS: @@ This case is from A. Engström, L. Häglund and J. Ågren:
SYS: @@ Metall.Trans.A v. 25A (1994), pp. 1127-1134.
SYS: @@-----
SYS:
SYS: @@ exd1_setup.DCM
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASE
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\databases\da
ta
Current database: Steels/Fe-Alloys v12.0

VA /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE12:
TDB_TCFE12: @@
TDB_TCFE12: @@ USE THE SSOL DATABASE FOR THERMODYNAMIC DATA
TDB_TCFE12: @@
TDB_TCFE12: sw fedemo
Current database: Iron Demo Database v6.0

VA /- DEFINED
TDB_FEDEMO: def-sys ni cr c
NI CR C
DEFINED
TDB_FEDEMO: rej ph * all
GAS:G LIQUID:L BCC_A2
C14_LAVES CBCC_A12 CEMENTITE_D011
CHI_A12 CUB_A13 DIAMOND_A4
FCC_A1 GRAPHITE_A9 HCP_A3
KSI_CARBIDE M23C6_D84 M3C2_D510
M7C3_D101 SIGMA_D8B REJECTED
TDB_FEDEMO: res ph fcc,m7c3,m3c2,grap
FCC_A1 M7C3_D101 M3C2_D510
GRAPHITE_A9 RESTORED
TDB_FEDEMO: get
11:27:29,535 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
Creating a new composition set FCC_A1#2
PARAMETERS ...
FUNCTIONS ...

Use the command LIST_REFERENCES to see the list of references for assessed data
-OK-
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE MOBILITY DATA
TDB_FEDEMO: @@
TDB_FEDEMO: app mfedemo
Current database: Fe-Alloys Mobility demo database v5.0

VA DEFINED
APP: def-sys ni c cr
NI C CR
DEFINED
APP: rej ph * all
BCC_A2 FCC_A1 CEMENTITE_D011
LIQUID:L REJECTED
APP: res ph fcc,m7c3,m3c2,grap
*** ERROR M7C3 INPUT IGNORED
*** ERROR M3C2 INPUT IGNORED
*** ERROR GRAP INPUT IGNORED
FCC_A1 RESTORED
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
Creating a new composition set FCC_A1#3
PARAMETERS ...
FUNCTIONS ...

Use the command LIST_REFERENCES to see the list of references for assessed data
```

```

-OK-
APP: @@
APP: @@ ENTER THE DICTRA MONITOR
APP: @@
APP: go d-m
NO TIME STEP DEFINED
*** ENTERING GRAPHITE_A9 AS A DIFFUSION NONE PHASE
*** ENTERING M3C2_D510 AS A DIFFUSION NONE PHASE
*** ENTERING M7C3_D101 AS A DIFFUSION NONE PHASE
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 1123; * N
DIC> @@
DIC> @@ SET THE REFERENCE STATE FOR CARBON
DIC> @@
DIC> set-reference-state
Component: C
Reference state: grap
Temperature /*/: *
Pressure /100000/: 1E5
DIC> @@
DIC> @@ ENTER THE REGION aus
DIC> @@
DIC> enter-region aus
DIC> @@
DIC> @@ ENTER A GEOMETRICAL GRID INTO THE REGION
DIC> @@
DIC> enter-grid aus 3e-3 geo 100 1.02
DIC> @@
DIC> @@ ENTER A MATRIX PHASE IN THE REGION
DIC> @@
DIC> enter-phase act aus matrix fcc_a1#1
DIC> @@
DIC> @@ ENTER THE START COMPOSITION FOR THE MATRIX PHASE
DIC> @@
DIC> enter-composition
REGION NAME : /AUS/: aus
PHASE NAME : /FCC_A1#1/: fcc#1
DEPENDENT COMPONENT ? /NI/: ni
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: cr
TYPE /LINEAR/: lin 25 25
PROFILE FOR /CR/: c
TYPE /LINEAR/: lin 1e-4 1e-4
DIC> @@
DIC> @@ ENTER SPHEROIDAL PHASES IN THE REGION
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /AUS/: aus
PHASE TYPE /MATRIX/: sph
PHASE NAME : /NONE/: m7c3
INFO: EQUILIBRIUM COMPOSITION AND FRACTION OF SPHEROID PHASES USED AS DEFAULT
DIC> @@
DIC> @@ ENTER A STOICHOMETRIC SPHEROIDAL PHASE IN THE REGION
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /AUS/: aus
PHASE TYPE /MATRIX/: sph
PHASE NAME : /NONE/: m3c2
INFO: EQUILIBRIUM COMPOSITION AND FRACTION OF SPHEROID PHASES USED AS DEFAULT
DIC> @@
DIC> @@ ENTER A START COMPOSITION FOR THE SPHEROIDAL PHASES
DIC> @@
DIC> enter-composition
REGION NAME : /AUS/: aus
PHASE NAME : /FCC_A1#1/: m7c3
USE EQUILIBRIUM VALUE /Y/: Y
DIC> enter-composition
REGION NAME : /AUS/: aus
PHASE NAME : /FCC_A1#1/: m3c2
USE EQUILIBRIUM VALUE /Y/: Y
DIC> @@
DIC> @@ SET THE BOUNDARY CONDITION
DIC> @@
DIC> set-cond
GLOBAL OR BOUNDARY CONDITION /GLOBAL/: boundary
BOUNDARY /LOWER/: lower
CONDITION TYPE /CLOSED_SYSTEM/: mixed
Dependent substitutional element:NI
Dependent interstitial element:VA
TYPE OF CONDITION FOR COMPONENT C /ZERO_FLUX/: activity
LOW TIME LIMIT /0/: 0
ACR(C)(TIME)= 1;
HIGH TIME LIMIT /*/: *
ANY MORE RANGES /N/: N
TYPE OF CONDITION FOR COMPONENT CR /ZERO_FLUX/: zero-flux
DIC> @@
DIC> @@ ENTER THE LABYRINTH FACTOR
DIC> @@
DIC> enter-lab
REGION NAME : aus
f(T,P,VOLFR,X)= volfr**2;
DIC> @@

```

```
DIC> @@ SET THE SIMULATION TIME. REMEMBER TO BE CAREFUL WITH THE
DIC> @@ TIMESTEP WHEN THERE ARE SPHEROIDAL PHASES PRESENT. IN THIS CASE
DIC> @@ THE TIMESTEP IS NOT ALLOWED TO BE LARGER THAN 1800s.
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 3600000
AUTOMATIC TIMESTEP CONTROL /YES/: YES
MAX TIMESTEP DURING INTEGRATION /360000/: 1800
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC> @@
DIC> @@ IN ORDER TO SAVE SOME SPACE ON THE DISK THE RESULT IS STORED
DIC> @@ SELECTIVELY. OTHERWISE THE STORE-RESULT-FILE FROM THIS EXAMPLE
DIC> @@ WOULD BE VERY LARGE.
DIC> @@
DIC> set-option SAVE_WORKSPACE_ON_FILE 99
DIC>
DIC> @@ BY DEFAULT THE "HOMOGENIZATION MODEL" IS USED WHEN MULTIPLE PHASES
DIC> @@ ARE ENTERED IN A SINGLE REGION. FOR THIS EXAMPLE THE HOMOGENIZATION
DIC> @@ MODEL IS DISABLED.
DIC> ho n
HOMOGENIZATION DISABLED
DIC>
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exd1 y
DIC>
DIC> set-inter
--OK--
DIC>
```

exdia-run

DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exdia\run.DCM"

DIC>

DIC>

DIC> @@ exd1\_run.DCM

DIC>

DIC> @@

DIC> @@ READ THE SETUP FILE AND START THE SIMULATION

DIC> @@

DIC> go d-m

TIME STEP AT TIME 0.00000E+00

\*\*\* ENTERING GRAPHITE\_A9 AS A DIFFUSION NONE PHASE

\*\*\* ENTERING M3C2\_D510 AS A DIFFUSION NONE PHASE

\*\*\* ENTERING M7C3\_D101 AS A DIFFUSION NONE PHASE

DIC> read exd1

OK

DIC> sim

INFO: Default responses (if any) will be applied during the simulation. Use "SIMULATE\_REACTION NO" instead for manual input.

DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE

U-FRACTION IN SYSTEM: C = 4.73399450059566E-06 CR = .273386452547573

NI = .726613547452427

TOTAL SIZE OF SYSTEM: .003 [m]

WARNING:M7C3\_D101 HAS NO VOLUME FRACTION, CREATING ONE

WARNING:M3C2\_D510 HAS NO VOLUME FRACTION, CREATING ONE

U-FRACTION IN SYSTEM: C = 4.73399450059567E-06 CR = .273386452547573

NI = .726613547452427

TOTAL SIZE OF SYSTEM: .003 [m]

TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = 8.32233224030127E-05 CR = .273386452547572

NI = .726613547452428

TOTAL SIZE OF SYSTEM: .003 [m]

CPU time used in timestep 0 seconds

TIME = 0.10010000E-03 DT = 0.10000000E-03 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = 1.14491916844134E-04 CR = .273386452547545

NI = .726613547452455

TOTAL SIZE OF SYSTEM: .003 [m]

CPU time used in timestep 0 seconds

TIME = 0.40010010 DT = 0.40000000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = 1.34397473834078E-04 CR = .273386452541228

NI = .726613547458772

TOTAL SIZE OF SYSTEM: .003 [m]

CPU time used in timestep 0 seconds

TIME = 61.226617 DT = 60.826517 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = 1.7323410372616E-04 CR = .273386451404806

NI = .726613548595194

TOTAL SIZE OF SYSTEM: .003 [m]

CPU time used in timestep 1 seconds

TIME = 136.73134 DT = 75.504726 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = 2.15195250520531E-04 CR = .273386450378639

NI = .726613549621361

TOTAL SIZE OF SYSTEM: .003 [m]

CPU time used in timestep 0 seconds

TIME = 246.77995 DT = 110.04860 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = 2.65132643074028E-04 CR = .273386449367933

NI = .726613550632067

TOTAL SIZE OF SYSTEM: .003 [m]

CPU time used in timestep 0 seconds

TIME = 417.73097 DT = 170.95102 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = 3.2670337021943E-04 CR = .273386448427438

NI = .726613551572562

TOTAL SIZE OF SYSTEM: .003 [m]

CPU time used in timestep 0 seconds

TIME = 700.87785 DT = 283.14689 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = 4.03852012958394E-04 CR = .273386447458974

NI = .726613552541026

TOTAL SIZE OF SYSTEM: .003 [m]

CPU time used in timestep 1 seconds

TIME = 1196.7622 DT = 495.88434 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = 5.03958087673235E-04 CR = .273386446322886

NI = .726613553677114

TOTAL SIZE OF SYSTEM: .003 [m]

CPU time used in timestep 0 seconds

TIME = 2136.4657 DT = 939.70351 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = 6.43011746169158E-04 CR = .273386444988439

NI = .726613555011561

TOTAL SIZE OF SYSTEM: .003 [m]

CPU time used in timestep 0 seconds

TIME = 3936.4657 DT = 1800.0000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = 8.3851931757087E-04 CR = .273386443511137

NI = .726613556488862

TOTAL SIZE OF SYSTEM: .003 [m]

CPU time used in timestep 1 seconds

TIME = 5736.4657 DT = 1800.0000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00101736919091153 CR = .273386442681228

NI = .726613557318772

TOTAL SIZE OF SYSTEM: .003 [m]

CPU time used in timestep 0 seconds

TIME = 7536.4657 DT = 1800.0000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00118296843235547 CR = .273386442066148

NI = .726613557933852

TOTAL SIZE OF SYSTEM: .003 [m]

CPU time used in timestep 0 seconds

TIME = 9336.4657 DT = 1800.0000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00133879473943311 CR = .273386441011304

NI = .726613558988696

TOTAL SIZE OF SYSTEM: .003 [m]

CPU time used in timestep 0 seconds

TIME = 11136.466 DT = 1800.0000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00148538356586206 CR = .273386439279047

NI = .726613560720953

TOTAL SIZE OF SYSTEM: .003 [m]

CPU time used in timestep 0 seconds

TIME = 12936.466 DT = 1800.0000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00162329914518437 CR = .273386436825686

NI = .726613563174314

TOTAL SIZE OF SYSTEM: .003 [m]

CPU time used in timestep 1 seconds

TIME = 14736.466 DT = 1800.0000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00175666281801172 CR = .273386434544918

NI = .726613565455081

TOTAL SIZE OF SYSTEM: .003 [m]

```
CPU time used in timestep          0 seconds
TIME = 16509.561 DT = 1773.0953 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00188419609237157 CR = .273386432317836
NI = .726613567682163
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep          0 seconds
TIME = 18202.531 DT = 1692.9700 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00200374276123893 CR = .273386430131738
NI = .726613569868262
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep          0 seconds
TIME = 19871.498 DT = 1668.9675 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00212043303520678 CR = .273386427985713
NI = .726613572014287
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep          1 seconds
TIME = 21585.289 DT = 1713.7906 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00223650931817923 CR = .273386426227093
NI = .726613573772906
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep          0 seconds
TIME = 23385.289 DT = 1800.0000 SUM OF SQUARES = 0.0000000
```

output ignored...

... output resumed

```
CPU time used in timestep          0 seconds
TIME = 3563985.3 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0314537850194298 CR = .2733863252107
NI = .7266136747893
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep          0 seconds
TIME = 3565785.3 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0314617195673842 CR = .273386325190243
NI = .726613674809756
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep          1 seconds
TIME = 3567585.3 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0314696517261714 CR = .27338632516957
NI = .72661367483043
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep          0 seconds
TIME = 3569385.3 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0314775815074803 CR = .273386325148678
NI = .726613674851322
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep          0 seconds
TIME = 3571185.3 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0314855089234026 CR = .27338632512757
NI = .72661367487243
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep          0 seconds
TIME = 3572985.3 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0314934339864118 CR = .273386325106243
NI = .726613674893757
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep          0 seconds
TIME = 3574785.3 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0315013567093432 CR = .273386325084699
NI = .726613674915301
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep          1 seconds
TIME = 3576585.3 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0315092771053743 CR = .273386325062936
NI = .726613674937064
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep          0 seconds
TIME = 3578385.3 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .031517195188006 CR = .273386325040956
NI = .726613674959044
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep          0 seconds
TIME = 3580185.3 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0315251109710436 CR = .273386325018757
NI = .726613674981243
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep          0 seconds
TIME = 3581985.3 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0315330244685791 CR = .27338632499634
NI = .72661367500366
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep          1 seconds
TIME = 3583785.3 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0315409356949736 CR = .273386324973704
NI = .726613675026296
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep          0 seconds
TIME = 3585585.3 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0315488446648401 CR = .273386324950849
NI = .726613675049151
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep          0 seconds
TIME = 3587385.3 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0315567513930271 CR = .273386324927775
NI = .726613675072225
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep          0 seconds
TIME = 3589185.3 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0315646558946027 CR = .273386324904482
NI = .726613675095517
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep          0 seconds
TIME = 3590985.3 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0315725581848389 CR = .27338632488097
NI = .726613675119031
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep          1 seconds
TIME = 3592785.3 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .031580458279197 CR = .273386324857237
NI = .726613675142763
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep          0 seconds
```

```
TIME = 3594585.3 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0315883561933127 CR = .273386324833285
NI = .726613675166715
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 3596385.3 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0315962519429824 CR = .273386324809113
NI = .726613675190887
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 3598185.3 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0316041455441495 CR = .273386324784721
NI = .726613675215279
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 3599985.3 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0316120370128917 CR = .273386324760108
NI = .726613675239892
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 1 seconds
TIME = 3600000.0 DT = 14.711046 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0316121023506871 CR = .273386324759897
NI = .726613675240103
TOTAL SIZE OF SYSTEM: .003 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 0.0000000
DELETING TIME-RECORD FOR TIME 0.10000000E-06
DELETING TIME-RECORD FOR TIME 0.10010000E-03
DELETING TIME-RECORD FOR TIME 163785.29
DELETING TIME-RECORD FOR TIME 341985.29
DELETING TIME-RECORD FOR TIME 520185.29
DELETING TIME-RECORD FOR TIME 698385.29
DELETING TIME-RECORD FOR TIME 876585.29
DELETING TIME-RECORD FOR TIME 1054785.3
DELETING TIME-RECORD FOR TIME 1232985.3
DELETING TIME-RECORD FOR TIME 1411185.3
DELETING TIME-RECORD FOR TIME 1589385.3
DELETING TIME-RECORD FOR TIME 1767585.3
DELETING TIME-RECORD FOR TIME 1945785.3
DELETING TIME-RECORD FOR TIME 2123985.3
DELETING TIME-RECORD FOR TIME 2302185.3
DELETING TIME-RECORD FOR TIME 2480385.3
DELETING TIME-RECORD FOR TIME 2658585.3
DELETING TIME-RECORD FOR TIME 2836785.3
DELETING TIME-RECORD FOR TIME 3014985.3
DELETING TIME-RECORD FOR TIME 3193185.3
DELETING TIME-RECORD FOR TIME 3371385.3
DELETING TIME-RECORD FOR TIME 3549585.3
DELETING TIME-RECORD FOR TIME 3596385.3
DELETING TIME-RECORD FOR TIME 3598185.3

KEEPING TIME-RECORD FOR TIME 3599985.3
AND FOR TIME 3600000.0
WORKSPACE RECLAIMED

TIMESTEP AT 3600000.00 SELECTED
```

```
DIC>
DIC> set-inter
--OK--
DIC>
```

## exdia-plot

### DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exdia\plot.DCM"

DIC>

DIC>

DIC> @@ exd1\_plot.DCM

DIC>

DIC> @@

DIC> @@ FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE exd1

DIC> @@

DIC>

DIC> @@

DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE

DIC> @@

DIC> go d-m

TIME STEP AT TIME 3.60000E+06

\*\*\* ENTERING GRAPHITE\_A9 AS A DIFFUSION NONE PHASE

\*\*\* ENTERING M3C2\_D510 AS A DIFFUSION NONE PHASE

\*\*\* ENTERING M7C3\_D101 AS A DIFFUSION NONE PHASE

DIC> read exd1

OK

DIC>

DIC> @@

DIC> @@ GO TO THE POST PROCESSOR

DIC> @@

DIC> post

POST PROCESSOR VERSION 1.7

Implemented by Bjorn Jonsson

POST-1:

POST-1: @@

POST-1: @@ LOT THE TOTAL CARBON CONCENTRATION PROFILE

POST-1: @@

POST-1: s-d-a y w-p c

POST-1: s-d-a x distance global

INFO: Distance is set as independent variable

POST-1: s-s-s x n 0 2e-3

POST-1: s-p-c time 3600000

POST-1:

POST-1: app y exd1.exp

PROLOGUE NUMBER: /0/: 1

DATASET NUMBER(s): /-1/: 1

POST-1:

POST-1: @@

POST-1: @@ SET THE TITLE ON THE PLOT

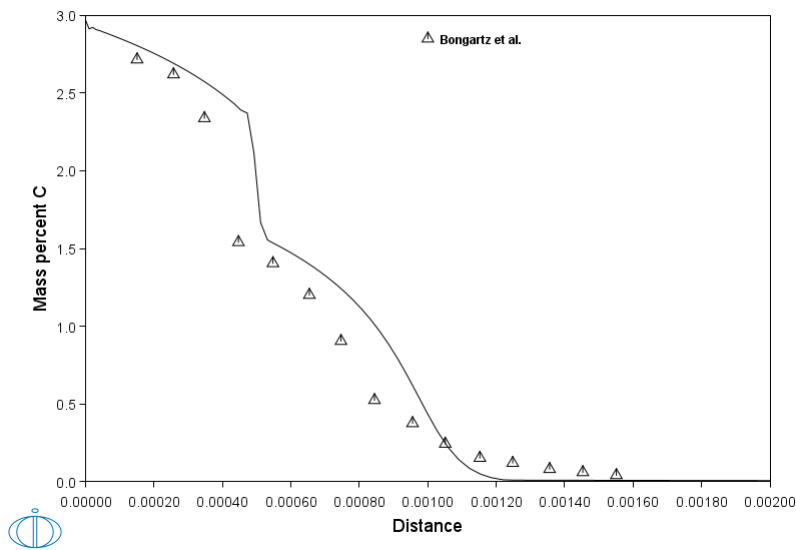
POST-1: @@

POST-1: set-tit d1.1

POST-1:

POST-1: plot

d1.1



POST-1:

POST-1:

POST-1:

POST-1: @?<\_hit\_return\_to\_continue\_>

POST-1:

POST-1: @@

POST-1: @@ NOW PLOT THE AMOUNT OF CARBIDES FORMED

POST-1: @@

POST-1: s-d-a y npm(\*)

POST-1: s-s-s y n 0 0.4

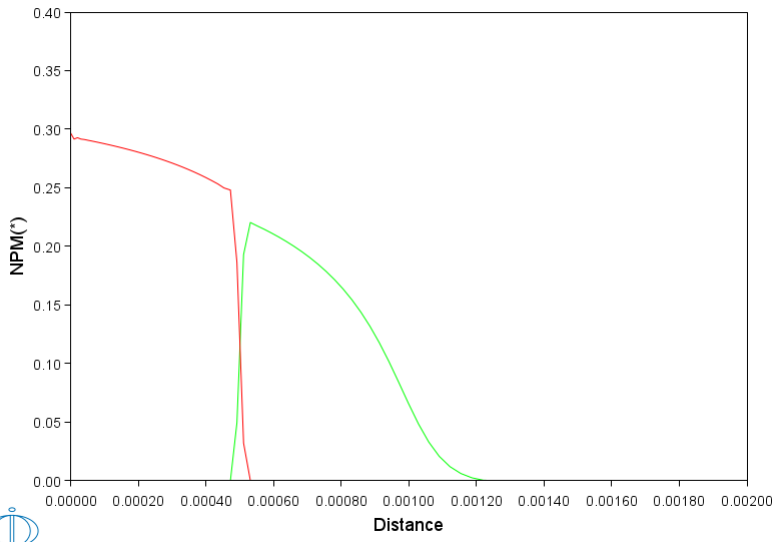
POST-1: app n

POST-1:

POST-1: set-tit d1.2

POST-1: plot

d1.2



```
POST-1:  
POST-1:  
POST-1:  
POST-1: @?<_hit_return_to_continue_>  
POST-1:  
POST-1: set-inter  
--OK--  
POST-1:
```

## exdlib-setup

### SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,  
Stockholm, Sweden

Software running on Windows 64-bit wordlength  
Compiler: Intel Fortran Compiler 2025.0.0  
License library version: 9.7.0.0036  
Linked: Nov 19 2025 at 14:44:36

```
SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exdlib\setup.DCM"
```

```
SYS: i>:@@
NO SUCH COMMAND, USE HELP
SYS: @@ Diffusion in dispersed systems.
SYS: @@ Carburization of Ni-25%Cr alloy: Homogenization model
SYS: @@ This example is about carburization of a Ni-25Cr alloy.
SYS: @@ In this case the M3C2 and M7C3 carbides are entered as
SYS: @@ spheroid phases in a FCC matrix. This case is from
SYS: @@ A. Engström, L. Häglund and J. Ågren: Metall.Trans. A,
SYS: @@ v.25A (1994), pp. 1127-1134.
SYS: @@ This simulation can be run with the DISPERSED SYSTEM MODEL or
SYS: @@ HOMOGENIZATION MODEL. The default HOMOGENIZATION MODEL is used
SYS: @@ and then ENTER_HOMOGENIZATION_FUNCTION should be used instead of
SYS: @@ ENTER_LABYRINTH_FUNCTION.
SYS: @@-----
SYS:
SYS: @@ exdlib_setup.DCM
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASE
SYS: @@
SYS:
SYS: @@ This example modifies the database interactively, which is not
SYS: @@ yet supported by GES6. Therefore, we enforce the use of GES5.
SYS: set-ges-version 5
SYS:
SYS: go da
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\databases\da
ta
Current database: Steels/Fe-Alloys v12.0

VA          /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE12:
TDB_TCFE12: @@
TDB_TCFE12: @@ USE THE SSOL DATABASE FOR THERMODYNAMIC DATA
TDB_TCFE12: @@
TDB_TCFE12: sw fedemo
Current database: Iron Demo Database v6.0

VA          /- DEFINED
TDB_FEDEMO: def-sys ni cr c
NI          CR          C
DEFINED
TDB_FEDEMO: rej ph * all
GAS:G      LIQUID:L      BCC_A2
C14_LAVES  CBCC_A12     CEMENTITE_D011
CHI_A12    CUB_A13      DIAMOND_A4
FCC_A1     GRAPHITE_A9   HCP_A3
KSI_CARBIDE M23C6_D84     M3C2_D510
M7C3_D101  SIGMA_D8B REJECTED
TDB_FEDEMO: res ph fcc,m7c3,m3c2,grap
FCC_A1     M7C3_D101     M3C2_D510
GRAPHITE_A9 RESTORED
TDB_FEDEMO: get
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
Creating a new composition set FCC_A1#2
PARAMETERS ...
FUNCTIONS ...

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE MOBILITY DATA
TDB_FEDEMO: @@
TDB_FEDEMO: app mfedemo
Current database: Fe-Alloys Mobility demo database v5.0

VA DEFINED
APP: def-sys ni c cr
NI          C          CR
DEFINED
APP: rej ph * all
BCC_A2     FCC_A1     CEMENTITE_D011
LIQUID:L REJECTED
APP: res ph fcc,m7c3,m3c2,grap
*** ERROR M7C3 INPUT IGNORED
*** ERROR M3C2 INPUT IGNORED
*** ERROR GRAP INPUT IGNORED
FCC_A1 RESTORED
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
Creating a new composition set FCC_A1#3
PARAMETERS ...
FUNCTIONS ...

Use the command LIST_REFERENCES to see the list of references for assessed data
```

```

-OK-
APP: @@
APP: @@ ENTER THE DICTRA MONITOR
APP: @@
APP: go d-m
NO TIME STEP DEFINED
*** ENTERING GRAPHITE_A9 AS A DIFFUSION NONE PHASE
*** ENTERING M3C2_D510 AS A DIFFUSION NONE PHASE
*** ENTERING M7C3_D101 AS A DIFFUSION NONE PHASE
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 1123; * N
DIC> @@
DIC> @@ SET THE REFERENCE STATE FOR CARBON
DIC> @@
DIC> set-reference-state
Component: C
Reference state: grap
Temperature /*/: *
Pressure /100000/: 1E5
DIC> @@
DIC> @@ ENTER THE REGION aus
DIC> @@
DIC> enter-region aus
DIC> @@
DIC> @@ ENTER A GEOMETRICAL GRID INTO THE REGION
DIC> @@
DIC> enter-grid aus 3e-3 geo 100 1.02
DIC> @@
DIC> @@ ENTER A MATRIX PHASE IN THE REGION
DIC> @@
DIC> enter-phase act aus matrix fcc_a1#1
DIC> @@
DIC> @@ ENTER THE START COMPOSITION FOR THE MATRIX PHASE
DIC> @@
DIC> enter-composition
REGION NAME : /AUS/: aus
PHASE NAME: /FCC_A1#1/: fcc#1
DEPENDENT COMPONENT ? /NI/: ni
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: cr
TYPE /LINEAR/: lin 25 25
PROFILE FOR /CR/: c
TYPE /LINEAR/: lin 1e-4 1e-4
DIC> @@
DIC> @@ ENTER SPHEROIDAL PHASES IN THE REGION
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /AUS/: aus
PHASE TYPE /MATRIX/: sph
PHASE NAME: /NONE/: m7c3
INFO: EQUILIBRIUM COMPOSITION AND FRACTION OF SPHEROID PHASES USED AS DEFAULT
DIC> @@
DIC> @@ ENTER A STOICHOOMETRIC SPHEROIDAL PHASE IN THE REGION
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /AUS/: aus
PHASE TYPE /MATRIX/: sph
PHASE NAME: /NONE/: m3c2
INFO: EQUILIBRIUM COMPOSITION AND FRACTION OF SPHEROID PHASES USED AS DEFAULT
DIC> @@
DIC> @@ ENTER A START COMPOSITION FOR THE SPHEROIDAL PHASES
DIC> @@
DIC> enter-composition
REGION NAME : /AUS/: aus
PHASE NAME: /FCC_A1#1/: m7c3
USE EQUILIBRIUM VALUE /Y/: Y
DIC> enter-composition
REGION NAME : /AUS/: aus
PHASE NAME: /FCC_A1#1/: m3c2
USE EQUILIBRIUM VALUE /Y/: Y
DIC> @@
DIC> @@ SET THE BOUNDARY CONDITION
DIC> @@
DIC> set-cond
GLOBAL OR BOUNDARY CONDITION /GLOBAL/: boundary
BOUNDARY /LOWER/: lower
CONDITION TYPE /CLOSED_SYSTEM/: mixed
Dependent substitutional element:NI
Dependent interstitial element:VA
TYPE OF CONDITION FOR COMPONENT C /ZERO_FLUX/: activity
LOW TIME LIMIT /0/: 0
ACR(C)(TIME)= 1;
HIGH TIME LIMIT /*/: *
ANY MORE RANGES /N/: N
TYPE OF CONDITION FOR COMPONENT CR /ZERO_FLUX/: zero-flux
DIC> @@
DIC> @@ SELECT THE HOMOGENIZATION FUNCTION
DIC> @@
DIC> enter-homo
ENTER HOMOGENIZATION FUNCTION # /5/: 8
SELECTED FUNCTION IS LABYRINTH FACTOR f**2 WITH PRESCRIBED MATRIX PHASE
PHASE NAME: fcc#1

```

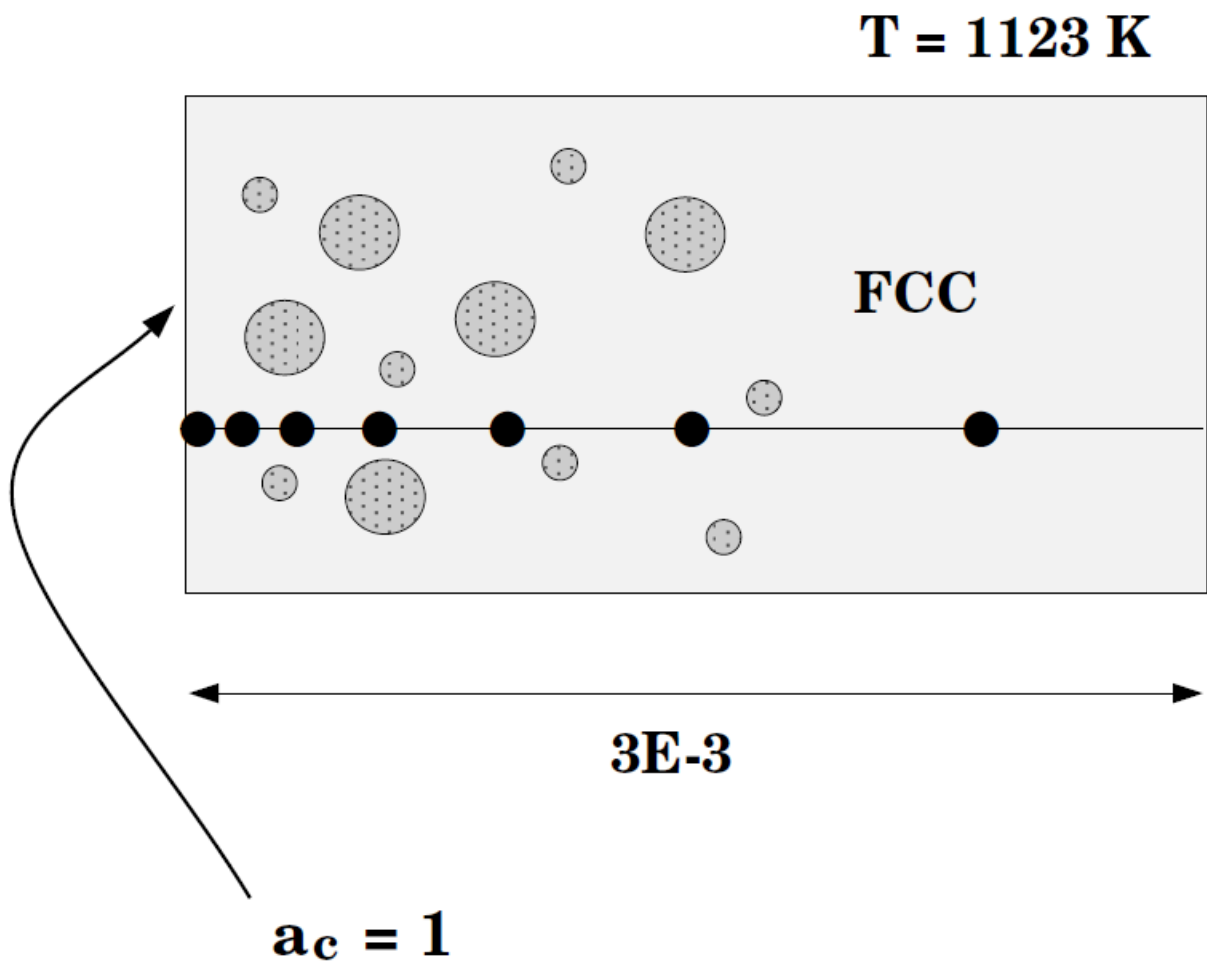
```
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME. REMEMBER TO BE CAREFUL WITH THE
DIC> @@ TIMESTEP WHEN SPHEROIDAL PHASES ARE PRESENT. IN THIS CASE
DIC> @@ THE TIMESTEP IS NOT ALLOWED TO BE LARGER THAN 1800s.
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 3600000
AUTOMATIC TIMESTEP CONTROL /YES/: YES
MAX TIMESTEP DURING INTEGRATION /360000/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC> @@
DIC> @@ TO SAVE SOME SPACE ON THE DISK THE RESULTS ARE STORED SELECTIVELY,
DIC> @@ OTHERWISE THE STORE-RESULT-FILE FROM THIS EXAMPLE WOULD BE
DIC> @@ VERY LARGE.
DIC> @@
DIC> set-option SAVE_WORKSPACE_ON_FILE 99
DIC>
DIC> @@
DIC> @@ SAVE THE SETUP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exdl y
DIC>
DIC> set-inter
--OK--
DIC>
```



## Example exd1b

### Carburization of a Ni-25% Cr alloy: Homogenization model

This example is about carburization of a Ni-25Cr alloy. In this case the M3C2 and M7C3 carbides are entered as spheroid phases in a FCC matrix. It is similar to exd1a except the default HOMOGENIZATION MODEL is used and then ENTER\_HOMOGENIZATION\_FUNCTION should be used instead of ENTER\_LABYRINTH\_FUNCTION. This case is from A. Engström, L. Höglund and J. Ågren: Metall.Trans. A, v.25A (1994), pp. 1127-1134.



exdlb-run

DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exdlb\run.DCM"

DIC>

DIC>

DIC> @@ exdl\_run.DCM

DIC>

DIC> @@

DIC> @@ READ THE SETUP FILE AND START THE SIMULATION

DIC> @@

DIC> go d-m

TIME STEP AT TIME 0.00000E+00

\*\*\* ENTERING GRAPHITE\_A9 AS A DIFFUSION NONE PHASE

\*\*\* ENTERING M3C2\_D510 AS A DIFFUSION NONE PHASE

\*\*\* ENTERING M7C3\_D101 AS A DIFFUSION NONE PHASE

DIC> read exdl

OK

DIC> sim

INFO: Default responses (if any) will be applied during the simulation. Use "SIMULATE\_REACTION NO" instead for manual input.

DEGREE OF IMPLICIT SET TO EULER BACKWARD

INFO: not solving in latticefixed frame of reference

STARTING SIMULATION USING HOMOGENIZATION MODEL

-----

INFO: PHASE WITH LIMITED SOLUBILITY OF ELEMENT(S) EXIST

A FALLBACK PHASE ZZDICTRA\_GHOST WILL BE DEFINED

ALONG WITH THE FOLLOWING PARAMETERS:

G(ZZDICTRA\_GHOST,C;0)-H298 (GRAPHITE,C;0)

G(ZZDICTRA\_GHOST,CR;0)-H298 (BCC\_A2,CR;0)

G(ZZDICTRA\_GHOST,NI;0)-H298 (FCC\_A1,NI;0)

L(ZZDICTRA\_GHOST,C,CR;0)

L(ZZDICTRA\_GHOST,C,NI;0)

L(ZZDICTRA\_GHOST,CR,NI;0)

WARNING:M7C3\_D101 HAS NO VOLUME FRACTION, CREATING ONE

WARNING:M3C2\_D510 HAS NO VOLUME FRACTION, CREATING ONE

Starting time-step t0= 0.0000000 dt= 0.10000000E-06

Starting time-step t0= 0.10000000E-06 dt= 0.20000000E-06

Starting time-step t0= 0.30000000E-06 dt= 0.40000000E-06

Starting time-step t0= 0.70000000E-06 dt= 0.80000000E-06

Starting time-step t0= 0.15000000E-05 dt= 0.16000000E-05

Starting time-step t0= 0.31000000E-05 dt= 0.32000000E-05

Starting time-step t0= 0.63000000E-05 dt= 0.64000000E-05

Starting time-step t0= 0.12700000E-04 dt= 0.12800000E-04

Starting time-step t0= 0.25500000E-04 dt= 0.25600000E-04

Starting time-step t0= 0.51100000E-04 dt= 0.51200000E-04

Starting time-step t0= 0.10230000E-03 dt= 0.10240000E-03

Starting time-step t0= 0.20470000E-03 dt= 0.20480000E-03

Starting time-step t0= 0.40950000E-03 dt= 0.40960000E-03

Starting time-step t0= 0.81910000E-03 dt= 0.81920000E-03

Starting time-step t0= 0.16383000E-02 dt= 0.16384000E-02

Starting time-step t0= 0.32767000E-02 dt= 0.32768000E-02

Starting time-step t0= 0.65535000E-02 dt= 0.65536000E-02

Starting time-step t0= 0.13107100E-01 dt= 0.13107200E-01

Starting time-step t0= 0.26214300E-01 dt= 0.26214400E-01

Starting time-step t0= 0.52428700E-01 dt= 0.52428800E-01

Starting time-step t0= 0.10485750 dt= 0.52428800E-01

Starting time-step t0= 0.15728630 dt= 0.52428800E-01

Starting time-step t0= 0.20971510 dt= 0.52428800E-01

Starting time-step t0= 0.26214390 dt= 0.52428800E-01

Starting time-step t0= 0.31457270 dt= 0.52428800E-01

Starting time-step t0= 0.36700150 dt= 0.10485760

Starting time-step t0= 0.47185910 dt= 0.20971520

Starting time-step t0= 0.68157430 dt= 0.41943040

Starting time-step t0= 1.1010047 dt= 0.41943040

Starting time-step t0= 1.5204351 dt= 0.83886080

Starting time-step t0= 2.3592959 dt= 0.83886080

Starting time-step t0= 3.1981567 dt= 0.83886080

Starting time-step t0= 4.0370175 dt= 0.83886080

Starting time-step t0= 4.8758783 dt= 0.83886080

Starting time-step t0= 5.7147391 dt= 0.83886080

Starting time-step t0= 6.5535999 dt= 0.83886080

Starting time-step t0= 7.3924607 dt= 0.83886080

Starting time-step t0= 8.2313215 dt= 0.83886080

Starting time-step t0= 9.0701823 dt= 0.83886080

Starting time-step t0= 9.9090431 dt= 0.83886080

Starting time-step t0= 10.747904 dt= 0.83886080

Starting time-step t0= 11.586765 dt= 0.83886080

Starting time-step t0= 12.425625 dt= 0.83886080

Starting time-step t0= 13.264486 dt= 0.83886080

Starting time-step t0= 14.103347 dt= 0.83886080

Starting time-step t0= 14.942208 dt= 0.83886080

Starting time-step t0= 15.781069 dt= 0.83886080

Starting time-step t0= 16.619929 dt= 0.83886080

Starting time-step t0= 17.458790 dt= 0.83886080

Starting time-step t0= 18.297651 dt= 0.83886080

Starting time-step t0= 19.136512 dt= 0.83886080

Starting time-step t0= 19.975373 dt= 0.83886080

Starting time-step t0= 20.814233 dt= 0.83886080

Starting time-step t0= 21.653094 dt= 0.83886080

Starting time-step t0= 22.491955 dt= 0.83886080

Starting time-step t0= 23.330816 dt= 0.83886080

Starting time-step t0= 24.169677 dt= 0.83886080

Starting time-step t0= 25.008537 dt= 0.83886080

Starting time-step t0= 25.847398 dt= 0.83886080

Starting time-step t0= 26.686259 dt= 0.83886080

Starting time-step t0= 27.525120 dt= 0.83886080

Starting time-step t0= 28.363981 dt= 0.83886080

Starting time-step t0= 29.202841 dt= 0.83886080

Starting time-step t0= 30.041702 dt= 0.83886080

Starting time-step t0= 30.880563 dt= 0.83886080

Starting time-step t0= 31.719424 dt= 0.83886080

Starting time-step t0= 32.558285 dt= 0.83886080

Starting time-step t0= 33.397145 dt= 0.83886080

Starting time-step t0= 34.236006 dt= 0.83886080

Starting time-step t0= 35.074867 dt= 0.83886080

Starting time-step t0= 35.913728 dt= 0.83886080

Starting time-step t0= 36.752589 dt= 0.83886080

Starting time-step t0= 37.591449 dt= 0.83886080

Starting time-step t0= 38.430310 dt= 1.6777216

Starting time-step t0= 40.108032 dt= 1.6777216

Starting time-step t0= 41.785753 dt= 1.6777216

Starting time-step t0= 43.463475 dt= 1.6777216

Starting time-step t0= 45.141197 dt= 1.6777216

```
Starting time-step t0= 46.818918 dt= 1.6777216
Starting time-step t0= 48.496640 dt= 1.6777216
Starting time-step t0= 50.174361 dt= 1.6777216
Starting time-step t0= 51.852083 dt= 1.6777216
Starting time-step t0= 53.529805 dt= 1.6777216
Starting time-step t0= 55.207526 dt= 1.6777216
Starting time-step t0= 56.885248 dt= 1.6777216
Starting time-step t0= 58.562969 dt= 1.6777216
Starting time-step t0= 60.240691 dt= 1.6777216
Starting time-step t0= 61.918413 dt= 1.6777216
Starting time-step t0= 63.596134 dt= 1.6777216
Starting time-step t0= 65.273856 dt= 1.6777216
Starting time-step t0= 66.951577 dt= 1.6777216
Starting time-step t0= 68.629299 dt= 1.6777216
Starting time-step t0= 70.307021 dt= 1.6777216
Starting time-step t0= 71.984742 dt= 1.6777216
Starting time-step t0= 73.662464 dt= 1.6777216
Starting time-step t0= 75.340185 dt= 1.6777216
Starting time-step t0= 77.017907 dt= 3.3554432
Starting time-step t0= 80.373350 dt= 3.3554432
Starting time-step t0= 83.728793 dt= 3.3554432
Starting time-step t0= 87.084237 dt= 3.3554432
```

output ignored...

... output resumed

```
DELETING TIME-RECORD FOR TIME 2335827.9
DELETING TIME-RECORD FOR TIME 2342699.8
DELETING TIME-RECORD FOR TIME 2349571.8
DELETING TIME-RECORD FOR TIME 2356443.7
DELETING TIME-RECORD FOR TIME 2363315.7
DELETING TIME-RECORD FOR TIME 2370187.6
DELETING TIME-RECORD FOR TIME 2377059.6
DELETING TIME-RECORD FOR TIME 2383931.5
DELETING TIME-RECORD FOR TIME 2390803.5
DELETING TIME-RECORD FOR TIME 2397675.4
DELETING TIME-RECORD FOR TIME 2404547.3
DELETING TIME-RECORD FOR TIME 2411419.3
DELETING TIME-RECORD FOR TIME 2418291.2
DELETING TIME-RECORD FOR TIME 2425163.2
DELETING TIME-RECORD FOR TIME 2432035.1
DELETING TIME-RECORD FOR TIME 2438907.1
DELETING TIME-RECORD FOR TIME 2445779.0
DELETING TIME-RECORD FOR TIME 2452651.0
DELETING TIME-RECORD FOR TIME 2459522.9
DELETING TIME-RECORD FOR TIME 2466394.9
DELETING TIME-RECORD FOR TIME 2473266.8
DELETING TIME-RECORD FOR TIME 2480138.8
DELETING TIME-RECORD FOR TIME 2487010.7
DELETING TIME-RECORD FOR TIME 2493882.7
DELETING TIME-RECORD FOR TIME 2500754.6
DELETING TIME-RECORD FOR TIME 2507626.6
DELETING TIME-RECORD FOR TIME 2514498.5
DELETING TIME-RECORD FOR TIME 2521370.5
DELETING TIME-RECORD FOR TIME 2528242.4
DELETING TIME-RECORD FOR TIME 2535114.4
DELETING TIME-RECORD FOR TIME 2541986.3
DELETING TIME-RECORD FOR TIME 2548858.3
DELETING TIME-RECORD FOR TIME 2555730.2
DELETING TIME-RECORD FOR TIME 2562602.1
DELETING TIME-RECORD FOR TIME 2569474.1
DELETING TIME-RECORD FOR TIME 2576346.0
DELETING TIME-RECORD FOR TIME 2583218.0
DELETING TIME-RECORD FOR TIME 2590090.0
DELETING TIME-RECORD FOR TIME 2596962.0
DELETING TIME-RECORD FOR TIME 2603834.0
DELETING TIME-RECORD FOR TIME 2610706.0
DELETING TIME-RECORD FOR TIME 2617578.0
DELETING TIME-RECORD FOR TIME 2624450.0
DELETING TIME-RECORD FOR TIME 2631322.0
DELETING TIME-RECORD FOR TIME 2638194.0
DELETING TIME-RECORD FOR TIME 2645066.0
DELETING TIME-RECORD FOR TIME 2651938.0
DELETING TIME-RECORD FOR TIME 2658810.0
DELETING TIME-RECORD FOR TIME 2665682.0
DELETING TIME-RECORD FOR TIME 2672554.0
DELETING TIME-RECORD FOR TIME 2679426.0
DELETING TIME-RECORD FOR TIME 2686298.0
DELETING TIME-RECORD FOR TIME 2693170.0
DELETING TIME-RECORD FOR TIME 2700042.0
DELETING TIME-RECORD FOR TIME 2706914.0
DELETING TIME-RECORD FOR TIME 2713786.0
DELETING TIME-RECORD FOR TIME 2720658.0
DELETING TIME-RECORD FOR TIME 2727530.0
DELETING TIME-RECORD FOR TIME 2734402.0
DELETING TIME-RECORD FOR TIME 2741274.0
DELETING TIME-RECORD FOR TIME 2748146.0
DELETING TIME-RECORD FOR TIME 2755018.0
DELETING TIME-RECORD FOR TIME 2761890.0
DELETING TIME-RECORD FOR TIME 2768762.0
DELETING TIME-RECORD FOR TIME 2775634.0
DELETING TIME-RECORD FOR TIME 2782506.0
DELETING TIME-RECORD FOR TIME 2789378.0
DELETING TIME-RECORD FOR TIME 2796250.0
DELETING TIME-RECORD FOR TIME 2803122.0
DELETING TIME-RECORD FOR TIME 2810000.0
DELETING TIME-RECORD FOR TIME 2816872.0
DELETING TIME-RECORD FOR TIME 2823744.0
DELETING TIME-RECORD FOR TIME 2830616.0
DELETING TIME-RECORD FOR TIME 2837488.0
DELETING TIME-RECORD FOR TIME 2844360.0
DELETING TIME-RECORD FOR TIME 2851232.0
DELETING TIME-RECORD FOR TIME 2858104.0
DELETING TIME-RECORD FOR TIME 2864976.0
DELETING TIME-RECORD FOR TIME 2871848.0
DELETING TIME-RECORD FOR TIME 2878720.0
DELETING TIME-RECORD FOR TIME 2885592.0
DELETING TIME-RECORD FOR TIME 2892464.0
DELETING TIME-RECORD FOR TIME 2899336.0
DELETING TIME-RECORD FOR TIME 2906208.0
DELETING TIME-RECORD FOR TIME 2913080.0
DELETING TIME-RECORD FOR TIME 2919952.0
DELETING TIME-RECORD FOR TIME 2926824.0
DELETING TIME-RECORD FOR TIME 2933696.0
DELETING TIME-RECORD FOR TIME 2940568.0
DELETING TIME-RECORD FOR TIME 2947440.0
DELETING TIME-RECORD FOR TIME 2954312.0
DELETING TIME-RECORD FOR TIME 2961184.0
DELETING TIME-RECORD FOR TIME 2968056.0
DELETING TIME-RECORD FOR TIME 2974928.0
DELETING TIME-RECORD FOR TIME 2981800.0
DELETING TIME-RECORD FOR TIME 2988672.0
DELETING TIME-RECORD FOR TIME 2995544.0
DELETING TIME-RECORD FOR TIME 3002416.0
DELETING TIME-RECORD FOR TIME 3009288.0
DELETING TIME-RECORD FOR TIME 3016160.0
DELETING TIME-RECORD FOR TIME 3023032.0
DELETING TIME-RECORD FOR TIME 3029904.0
DELETING TIME-RECORD FOR TIME 3036776.0
DELETING TIME-RECORD FOR TIME 3043648.0
DELETING TIME-RECORD FOR TIME 3050520.0
DELETING TIME-RECORD FOR TIME 3057392.0
DELETING TIME-RECORD FOR TIME 3064264.0
DELETING TIME-RECORD FOR TIME 3071136.0
```

DELETING TIME-RECORD FOR TIME 3088306.1  
DELETING TIME-RECORD FOR TIME 3102050.0  
DELETING TIME-RECORD FOR TIME 3115793.9  
DELETING TIME-RECORD FOR TIME 3129537.8  
DELETING TIME-RECORD FOR TIME 3143281.7  
DELETING TIME-RECORD FOR TIME 3157025.6  
DELETING TIME-RECORD FOR TIME 3170769.5  
DELETING TIME-RECORD FOR TIME 3184513.4  
DELETING TIME-RECORD FOR TIME 3198257.3  
DELETING TIME-RECORD FOR TIME 3212001.2  
DELETING TIME-RECORD FOR TIME 3225745.1  
DELETING TIME-RECORD FOR TIME 3232617.0  
DELETING TIME-RECORD FOR TIME 3239489.0  
DELETING TIME-RECORD FOR TIME 3246360.9  
DELETING TIME-RECORD FOR TIME 3253232.9  
DELETING TIME-RECORD FOR TIME 3260104.8  
DELETING TIME-RECORD FOR TIME 3266976.8  
DELETING TIME-RECORD FOR TIME 3273848.7  
DELETING TIME-RECORD FOR TIME 3280720.7  
DELETING TIME-RECORD FOR TIME 3287592.6  
DELETING TIME-RECORD FOR TIME 3294464.6  
DELETING TIME-RECORD FOR TIME 3301336.5  
DELETING TIME-RECORD FOR TIME 3308208.5  
DELETING TIME-RECORD FOR TIME 3315080.4  
DELETING TIME-RECORD FOR TIME 3321952.4  
DELETING TIME-RECORD FOR TIME 3328824.3  
DELETING TIME-RECORD FOR TIME 3335696.3  
DELETING TIME-RECORD FOR TIME 3349440.2  
DELETING TIME-RECORD FOR TIME 3363184.1  
DELETING TIME-RECORD FOR TIME 3376927.9  
DELETING TIME-RECORD FOR TIME 3390671.8  
DELETING TIME-RECORD FOR TIME 3404415.7  
DELETING TIME-RECORD FOR TIME 3418159.6  
DELETING TIME-RECORD FOR TIME 3431903.5  
DELETING TIME-RECORD FOR TIME 3445647.4  
DELETING TIME-RECORD FOR TIME 3459391.3  
DELETING TIME-RECORD FOR TIME 3473135.2  
DELETING TIME-RECORD FOR TIME 3486879.1  
DELETING TIME-RECORD FOR TIME 3500623.0  
DELETING TIME-RECORD FOR TIME 3514366.9  
DELETING TIME-RECORD FOR TIME 3528110.8  
DELETING TIME-RECORD FOR TIME 3541854.7  
DELETING TIME-RECORD FOR TIME 3555598.6  
DELETING TIME-RECORD FOR TIME 3562470.5  
DELETING TIME-RECORD FOR TIME 3572778.5

KEEPING TIME-RECORD FOR TIME 3586522.3  
AND FOR TIME 3600000.0  
WORKSPACE RECLAIMED

-----  
INTERPOLATION SCHEME USED THIS FRACTION OF  
THE ALLOCATED MEMORY: 5.283679648756118E-002  
EFFICIENCY FACTOR: 65.2378885941645  
-----  
DEALLOCATING  
-----

TIMESTEP AT 3600000.00 SELECTED

DIC>  
DIC> set-inter  
--OK--  
DIC>

# exdib-plot

DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exdib\plot.DCM"

DIC>

DIC>

DIC> @@ exd1\_plot.DCM

DIC>

DIC> @@

DIC> @@ FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE exd1b

DIC> @@

DIC>

DIC> @@

DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE

DIC> @@

DIC> go d-m

TIME STEP AT TIME 3.60000E+06

\*\*\* ENTERING GRAPHITE\_A9 AS A DIFFUSION NONE PHASE

\*\*\* ENTERING M3C2\_D510 AS A DIFFUSION NONE PHASE

\*\*\* ENTERING M7C3\_D101 AS A DIFFUSION NONE PHASE

DIC> read exd1

OK

DIC>

DIC> @@

DIC> @@ GO TO THE POST PROCESSOR

DIC> @@

DIC> post

POST PROCESSOR VERSION 1.7

Implemented by Bjorn Jonsson

POST-1:

POST-1: @@

POST-1: @@ PLOT THE TOTAL CARBON CONCENTRATION PROFILE

POST-1: @@

POST-1: s-d-a y w-p c

POST-1: s-d-a x distance global

INFO: Distance is set as independent variable

POST-1: s-s-s x n 0 2e-3

POST-1: s-p-c time 3600000

POST-1:

POST-1: app y exd1.exp

PROLOGUE NUMBER: /0/: 1

DATASET NUMBER(s): /-1/: 1

POST-1:

POST-1: @@

POST-1: @@ SET A TITLE ON THE PLOT

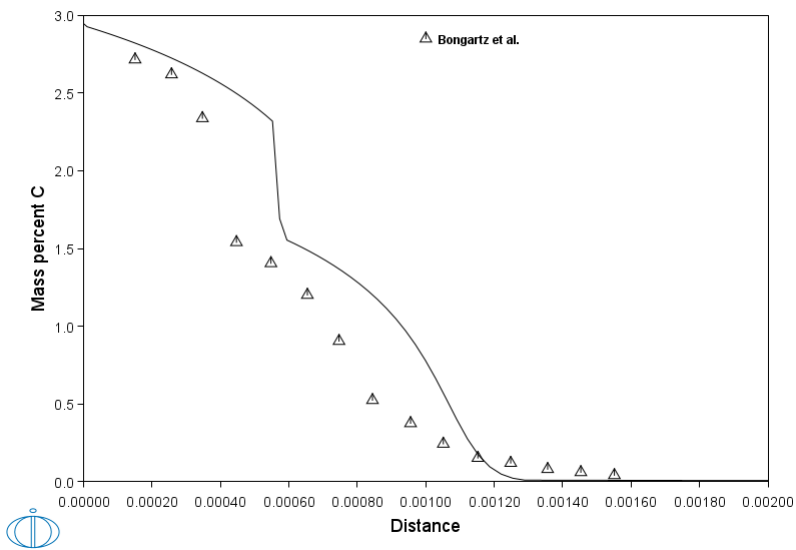
POST-1: @@

POST-1: set-tit d1.1

POST-1:

POST-1: plot

d1.1



POST-1:

POST-1:

POST-1:

POST-1: @?<\_hit\_return\_to\_continue\_>

POST-1:

POST-1: @@

POST-1: @@ PLOT THE AMOUNT OF CARBIDES FORMED

POST-1: @@

POST-1: s-d-a y npm(\*)

POST-1: s-s-s y n 0 0.4

POST-1: app n

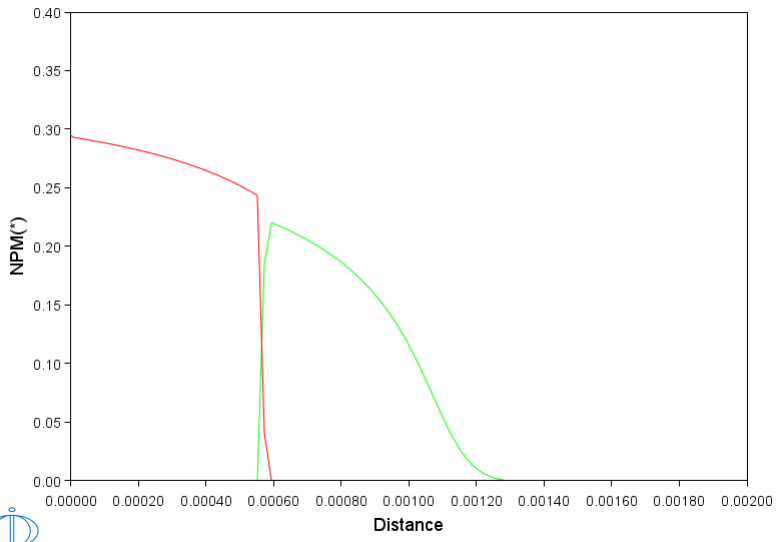
POST-1:

POST-1: set-tit d1.2

POST-1:

POST-1: plot

d1.2



```
POST-1:  
POST-1:  
POST-1:  
POST-1: @?<_hit_return_to_continue_>  
POST-1:  
POST-1: set-inter  
--OK--  
POST-1:
```

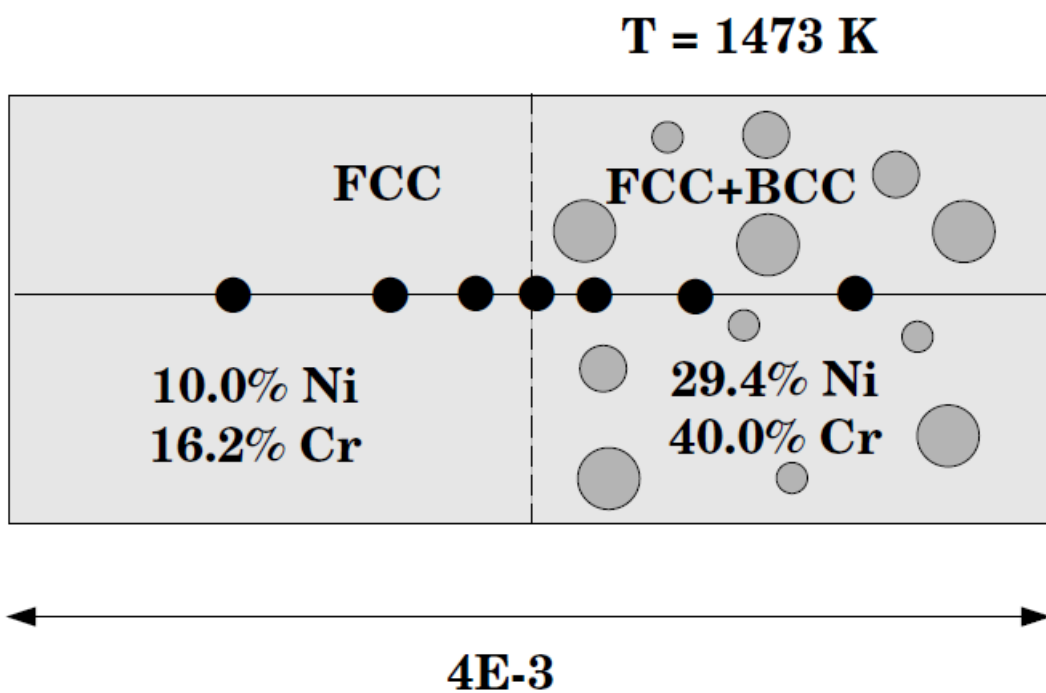


## Example exd2a

### Diffusion couple of Fe-Ni-Cr alloys: Step-profile

This example calculates the interdiffusion in a diffusion couple between a two-phase (FCC+BCC) and a single-phase (FCC) Fe-Ni-Cr alloy. Initially it uses a step profile. This simulation can be run with either the DISPERSED SYSTEM MODEL or the HOMOGENIZATION MODEL. In this example the DISPERSED SYSTEM MODEL is used.

This case is from A. Engström: Scand. J. Met., vol. 24, 1995, pp.12-20.



## exd2a-setup

### SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,  
Stockholm, Sweden

Software running on Windows 64-bit wordlength  
Compiler: Intel Fortran Compiler 2025.0.0  
License library version: 9.7.0.0036  
Linked: Nov 19 2025 at 14:44:36

```
SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exd2a\setup.DCM"
```

```
SYS: @@
SYS: @@ Diffusion in dispersed systems.
SYS: @@ Diffusion couple of Fe-Cr-Ni alloys: Dispersed system model
SYS: @@ This example calculates the interdiffusion in a diffusion
SYS: @@ couple between a two-phase (FCC+BCC) and a single-phase (FCC)
SYS: @@ Fe-Ni-Cr alloy. This case is from A. Engström: Scand. J. Met., v. 24,
SYS: @@ 1995, pp.12-20. This simulation can be run with either the DISPERSED
SYS: @@ SYSTEM MODEL or the HOMOGENIZATION MODEL.
SYS: @@ In this example the DISPERSED SYSTEM MODEL is used, which requires
SYS: @@ that the default HOMOGENIZATION MODEL is disabled.
SYS: @@ With the DISPERSED SYSTEM MODEL the command
SYS: @@ ENTER LABYRINTH_FUNCTION is used to take into account the
SYS: @@ impeding effect of dispersed phases on long-range diffusion.
SYS: @@ For the HOMOGENIZATION MODEL the command
SYS: @@ ENTER_HOMOGENIZATION_FUNCTION should be used.
SYS: @@-----
SYS:
SYS: @@ exd2_setup.DCM
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASE
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\databases\da
ta
Current database: Steels/Fe-Alloys v12.0

VA /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE12: sw fedemo
Current database: Iron Demo Database v6.0

VA /- DEFINED
TDB_FEDEMO: def-sys fe ni cr
FE NI CR
DEFINED
TDB_FEDEMO: rej ph * all
GAS:G LIQUID:L BCC_A2
C14_LAVES CBCC_A12 CHI_A12
CUB_A13 FCC_A1 HCP_A3
SIGMA_D8B REJECTED
TDB_FEDEMO: res ph fcc,bcc
FCC_A1 BCC_A2 RESTORED
TDB_FEDEMO: get
11:43:26,310 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

Use the command LIST_REFERENCES to see the list of references for assessed data
-OK-
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE MOBILITY DATA
TDB_FEDEMO: @@
TDB_FEDEMO: app mfedemo
Current database: Fe-Alloys Mobility demo database v5.0

VA DEFINED
APP: def-sys fe ni cr
FE NI CR
DEFINED
APP: rej ph * all
BCC_A2 FCC_A1 LIQUID:L
REJECTED
APP: res ph fcc,bcc
FCC_A1 BCC_A2 RESTORED
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

Use the command LIST_REFERENCES to see the list of references for assessed data
-OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR
APP: @@
APP: go d-m
NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 1473; * N
DIC>
```

```

DIC> @@
DIC> @@ ENTER THE REGION fer
DIC> @@
DIC> enter-region fer
DIC>
DIC>
DIC> @@
DIC> @@ ENTER GRID INTO THE REGION
DIC> @@
DIC> enter-grid fer 4e-3 auto
DIC>
DIC> @@
DIC> @@ ENTER A MATRIX PHASE IN THE REGION
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act fer matrix fcc
DIC>
DIC> @@
DIC> @@ ENTER THE START COMPOSITION FOR THE MATRIX PHASE
DIC> @@
DIC> enter-composition
REGION NAME : /FER/: fer
PHASE NAME: /FCC_A1/: fcc
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /CR/: cr function 16.2+23.8*HS(x-2e-3);
PROFILE FOR /NI/: ni function 10+19.4*HS(x-2e-3);
DIC>
DIC> @@
DIC> @@ ENTER FERRITE AS THE SPHEROIDAL PHASE IN THE REGION.
DIC> @@ SINCE THE FRACTION OF FERRITE IS SMALL, AND THESE APPEAR
DIC> @@ AS ISOLATED PARTICLES, FERRITE IS ENTERED AS A SPHEROIDAL PHASE
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /FER/: fer
PHASE TYPE /MATRIX/: sph
PHASE NAME: /NONE/: bcc
INFO: EQUILIBRIUM COMPOSITION AND FRACTION OF SPHEROID PHASES USED AS DEFAULT
DIC>
DIC> @@
DIC> @@ ENTER A COMPOSITION FOR THE SPHEROIDAL PHASE
DIC> @@ USE THE EQUILIBRIUM VALUE
DIC> @@
DIC> enter-composition
REGION NAME : /FER/: fer
PHASE NAME: /FCC_A1/: bcc
USE EQUILIBRIUM VALUE /Y/: y
DIC>
DIC>
DIC> @@
DIC> @@ ENTER A LABYRINTH FACTOR
DIC> @@ IN THIS CASE THE LOW DIFFUSIVITY PHASE IS THE MATRIX AND THE
DIC> @@ "EFFECTIVE" DIFFUSIVITY IN THE AUSTENITE+FERRITE TWO-PHASE
DIC> @@ REGION IS EXPECTED TO BE HIGHER THAN THE DIFFUSIVITY IN THE
DIC> @@ AUSTENITE.
DIC> enter-lab
REGION NAME : fer
f(T,P,VOLFR,X)= 1+3*(1-volfr)/volfr;
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME AND OTHER SIMULATION PARAMETERS
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 720000
AUTOMATIC TIMESTEP CONTROL /YES/: YES
MAX TIMESTEP DURING INTEGRATION /72000/: 5000
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC> set-option SAVE_WORKSPACE_ON_FILE 99
DIC>
DIC> @@ BY DEFAULT THE "HOMOGENIZATION MODEL" IS USED WHEN MULTIPLE PHASES
DIC> @@ ARE ENTERED IN A SINGLE REGION. THE HOMOGENIZATION MODEL NEEDS TO BE
DIC> @@ DISABLED FOR THIS EXAMPLE.
DIC> ho n
HOMOGENIZATION DISABLED
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC>
DIC> save exd2 y
DIC>
DIC> set-inter
--OK--
DIC>

```

exd2a-run

DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exd2a\run.DCM"

DIC>

DIC>

DIC> @@ exd2\_run.DCM

DIC>

DIC> @@

DIC> @@ FILE FOR RUNNING THE SIMULATION OF EXAMPLE D2

DIC> @@

DIC>

DIC> @@

DIC> @@ READ THE SETUP FROM FILE AND START THE SIMULATION

DIC> @@

DIC>

DIC> go d-m

TIME STEP AT TIME 0.00000E+00

DIC> read exd2

OK

DIC> sim

INFO: Default responses (if any) will be applied during the simulation. Use "SIMULATE\_REACTION NO" instead for manual input.

Region: FER

geometric 0.833333 dense at 0.200000E-02 36 points

geometric 1.20000 dense at 0.200000E-02 35 points

DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE

U-FRACTION IN SYSTEM: CR = .297939277178739 FE = .517060814291125

NI = .184999908530136

TOTAL SIZE OF SYSTEM: .004 [m]

WARNING:BCC A2 HAS NO VOLUME FRACTION, CREATING ONE

U-FRACTION IN SYSTEM: CR = .297939277178739 FE = .517060814291125

NI = .184999908530136

TOTAL SIZE OF SYSTEM: .004 [m]

TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .297939277178046 FE = .517060814294107

NI = .184999908527847

TOTAL SIZE OF SYSTEM: .004 [m]

CPU time used in timestep 1 seconds

TIME = 0.10010000E-03 DT = 0.10000000E-03 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .29793927648544 FE = .51706081727548

NI = .18499990623908

TOTAL SIZE OF SYSTEM: .004 [m]

CPU time used in timestep 0 seconds

TIME = 0.40010010 DT = 0.40000000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .297939277135146 FE = .517060817343833

NI = .18499990521021

TOTAL SIZE OF SYSTEM: .004 [m]

CPU time used in timestep 0 seconds

TIME = 1101.1611 DT = 1100.7610 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .297941099202627 FE = .517057019687635

NI = .185001881109738

TOTAL SIZE OF SYSTEM: .004 [m]

CPU time used in timestep 0 seconds

TIME = 3302.6831 DT = 2201.5220 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .297942257810931 FE = .517054162996745

NI = .185003579192324

TOTAL SIZE OF SYSTEM: .004 [m]

CPU time used in timestep 0 seconds

TIME = 7705.7271 DT = 4403.0440 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .297942991235041 FE = .517052326688897

NI = .185004682076062

TOTAL SIZE OF SYSTEM: .004 [m]

CPU time used in timestep 1 seconds

TIME = 12705.727 DT = 5000.0000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .297943676929859 FE = .517051286209105

NI = .185005036861036

TOTAL SIZE OF SYSTEM: .004 [m]

CPU time used in timestep 0 seconds

TIME = 17705.727 DT = 5000.0000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .297944185786995 FE = .517050701992937

NI = .185005112220069

TOTAL SIZE OF SYSTEM: .004 [m]

CPU time used in timestep 0 seconds

TIME = 22705.727 DT = 5000.0000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .297944546826876 FE = .517050331194696

NI = .185005121978428

TOTAL SIZE OF SYSTEM: .004 [m]

CPU time used in timestep 0 seconds

TIME = 27705.727 DT = 5000.0000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .297944794978927 FE = .51705007591364

NI = .185005129107433

TOTAL SIZE OF SYSTEM: .004 [m]

CPU time used in timestep 1 seconds

TIME = 32705.727 DT = 5000.0000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .297944953959204 FE = .517049882754367

NI = .185005163286429

TOTAL SIZE OF SYSTEM: .004 [m]

CPU time used in timestep 0 seconds

TIME = 37705.727 DT = 5000.0000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .297945041499985 FE = .517049733111145

NI = .18500522538887

TOTAL SIZE OF SYSTEM: .004 [m]

CPU time used in timestep 0 seconds

TIME = 42705.727 DT = 5000.0000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .29794506795221 FE = .51704961509448

NI = .18500531695331

TOTAL SIZE OF SYSTEM: .004 [m]

CPU time used in timestep 1 seconds

TIME = 47705.727 DT = 5000.0000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .297945044324655 FE = .517049519058708

NI = .185005436616637

TOTAL SIZE OF SYSTEM: .004 [m]

CPU time used in timestep 0 seconds

TIME = 52705.727 DT = 5000.0000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .297945073170377 FE = .517049417655774

NI = .18500550917385

TOTAL SIZE OF SYSTEM: .004 [m]

CPU time used in timestep 0 seconds

TIME = 57705.727 DT = 5000.0000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .297945101278653 FE = .517049327301327

NI = .18500557142002

TOTAL SIZE OF SYSTEM: .004 [m]

CPU time used in timestep 0 seconds

TIME = 62705.727 DT = 5000.0000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: CR = .297945113441899 FE = .517049246325909  
NI = .185005640232191  
TOTAL SIZE OF SYSTEM: .004 [m]  
CPU time used in timestep 0 seconds  
TIME = 67705.727 DT = 5000.0000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: CR = .297945104683444 FE = .517049174072711  
NI = .185005721243846  
TOTAL SIZE OF SYSTEM: .004 [m]  
CPU time used in timestep 1 seconds  
TIME = 72705.727 DT = 5000.0000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: CR = .29794507379698 FE = .517049109192889  
NI = .185005817010131  
TOTAL SIZE OF SYSTEM: .004 [m]  
CPU time used in timestep 0 seconds  
TIME = 77705.727 DT = 5000.0000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: CR = .297945060594546 FE = .517049041582619

output ignored...

... output resumed

U-FRACTION IN SYSTEM: CR = .297944333181282 FE = .51704626318521  
NI = .185009403633508  
TOTAL SIZE OF SYSTEM: .004 [m]  
CPU time used in timestep 0 seconds  
TIME = 607705.73 DT = 5000.0000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: CR = .297944425239856 FE = .517046227417362  
NI = .185009347342782  
TOTAL SIZE OF SYSTEM: .004 [m]  
CPU time used in timestep 0 seconds  
TIME = 612705.73 DT = 5000.0000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: CR = .297944515312297 FE = .517046192225715  
NI = .185009292461987  
TOTAL SIZE OF SYSTEM: .004 [m]  
CPU time used in timestep 0 seconds  
TIME = 617705.73 DT = 5000.0000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: CR = .297944602704325 FE = .517046157760735  
NI = .185009239534939  
TOTAL SIZE OF SYSTEM: .004 [m]  
CPU time used in timestep 0 seconds  
TIME = 622705.73 DT = 5000.0000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: CR = .297944686905369 FE = .517046124128251  
NI = .18500918896638  
TOTAL SIZE OF SYSTEM: .004 [m]  
CPU time used in timestep 0 seconds  
TIME = 627705.73 DT = 5000.0000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: CR = .297944767527865 FE = .517046091404046  
NI = .185009141068089  
TOTAL SIZE OF SYSTEM: .004 [m]  
CPU time used in timestep 1 seconds  
TIME = 632705.73 DT = 5000.0000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: CR = .297944844270216 FE = .517046059642946  
NI = .185009096086838  
TOTAL SIZE OF SYSTEM: .004 [m]  
CPU time used in timestep 0 seconds  
TIME = 637705.73 DT = 5000.0000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: CR = .297944916893067 FE = .51704602888457  
NI = .185009054222363  
TOTAL SIZE OF SYSTEM: .004 [m]  
CPU time used in timestep 0 seconds  
TIME = 642705.73 DT = 5000.0000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: CR = .297944985203518 FE = .517045999157801  
NI = .18500901563868  
TOTAL SIZE OF SYSTEM: .004 [m]  
CPU time used in timestep 0 seconds  
TIME = 647705.73 DT = 5000.0000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: CR = .297945049044104 FE = .517045970483118  
NI = .185008980472778  
TOTAL SIZE OF SYSTEM: .004 [m]  
CPU time used in timestep 0 seconds  
TIME = 652705.73 DT = 5000.0000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: CR = .297945108285015 FE = .517045942874776  
NI = .185008948840209  
TOTAL SIZE OF SYSTEM: .004 [m]  
CPU time used in timestep 0 seconds  
TIME = 657705.73 DT = 5000.0000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: CR = .297945162818325 FE = .517045916342331  
NI = .185008920839345  
TOTAL SIZE OF SYSTEM: .004 [m]  
CPU time used in timestep 0 seconds  
TIME = 662705.73 DT = 5000.0000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: CR = .29794521255387 FE = .517045890891698  
NI = .185008896554432  
TOTAL SIZE OF SYSTEM: .004 [m]  
CPU time used in timestep 0 seconds  
TIME = 667705.73 DT = 5000.0000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: CR = .297945257415957 FE = .517045866526057  
NI = .185008876057986  
TOTAL SIZE OF SYSTEM: .004 [m]  
CPU time used in timestep 0 seconds  
TIME = 672705.73 DT = 5000.0000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: CR = .297945297340851 FE = .517045843246529  
NI = .18500885941262  
TOTAL SIZE OF SYSTEM: .004 [m]  
CPU time used in timestep 0 seconds  
TIME = 677705.73 DT = 5000.0000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: CR = .297945332274807 FE = .517045821052724  
NI = .185008846672469  
TOTAL SIZE OF SYSTEM: .004 [m]  
CPU time used in timestep 0 seconds  
TIME = 682705.73 DT = 5000.0000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: CR = .297945362172496 FE = .517045799943177  
NI = .185008837884327  
TOTAL SIZE OF SYSTEM: .004 [m]  
CPU time used in timestep 1 seconds  
TIME = 687705.73 DT = 5000.0000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: CR = .297945386995732 FE = .517045779915716  
NI = .185008833088553  
TOTAL SIZE OF SYSTEM: .004 [m]  
CPU time used in timestep 0 seconds  
TIME = 692705.73 DT = 5000.0000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: CR = .297945406712412 FE = .51704576096776

```
NI = .185008832319828
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep 0 seconds
TIME = 697705.73 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297945421295774 FE = .517045743096579
NI = .185008835607647
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep 0 seconds
TIME = 702705.73 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297945430723465 FE = .517045726299507
NI = .185008842977028
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep 0 seconds
TIME = 707705.73 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297945434976962 FE = .517045710574128
NI = .18500885444891
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep 0 seconds
TIME = 712705.73 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297945434041613 FE = .517045695917164
NI = .185008870041223
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep 0 seconds
TIME = 717705.73 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297945427905335 FE = .517045682328835
NI = .18500888976583
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep 0 seconds
TIME = 720000.00 DT = 2294.2729 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297945415695563 FE = .517045677674604
NI = .185008906629832
TOTAL SIZE OF SYSTEM: .004 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 0.0000000
DELETING TIME-RECORD FOR TIME 0.10000000E-06
DELETING TIME-RECORD FOR TIME 0.10010000E-03
DELETING TIME-RECORD FOR TIME 477705.73
DELETING TIME-RECORD FOR TIME 707705.73
DELETING TIME-RECORD FOR TIME 712705.73
KEEPING TIME-RECORD FOR TIME 717705.73
AND FOR TIME 720000.00
WORKSPACE RECLAIMED
TIMESTEP AT 720000.000 SELECTED
```

```
DIC>
DIC>
DIC>
DIC>
DIC> set-inter
--OK--
DIC>
```

## exd2a-plot

### DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exd2a\plot.DCM"

DIC>

DIC>

DIC> @@ exd2\_plot.DCM

DIC>

DIC> @@

DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE D2

DIC> @@

DIC> @@ ENTER THE DICTRA MODULE AND SPECIFY THE STORE-RESULT FILE

DIC> @@

DIC> go d-m

TIME STEP AT TIME 7.20000E+05

DIC> read exd2

OK

DIC>

DIC> @@

DIC> @@ ENTER THE DICTRA POST PROCESSOR

DIC> @@

DIC> post

POST PROCESSOR VERSION 1.7

Implemented by Bjorn Jonsson

POST-1:

POST-1:

POST-1: @@

POST-1: @@ LET US SEE HOW THE FRACTION OF FERRITE HAS CHANGED

POST-1: @@ AS A RESULT OF THE DIFFUSION

POST-1: @@

POST-1: s-d-a y npm(bcc)

POST-1: s-d-a x distance global

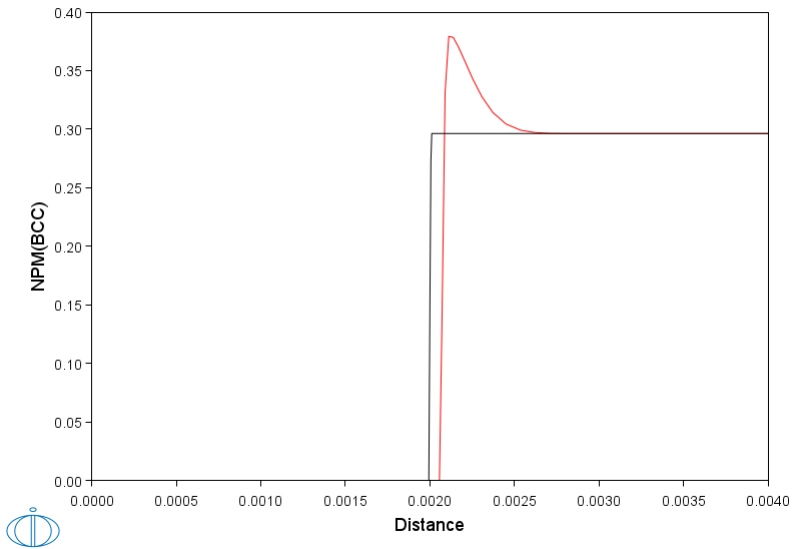
INFO: Distance is set as independent variable

POST-1: s-p-c time 0 720000

POST-1: set-tit Figure D2.1

POST-1: plot

Figure D2.1



POST-1:

POST-1:

POST-1:

POST-1: @@<\_hit\_return\_to\_continue\_>

POST-1: @@

POST-1: @@ NOW PLOT HOW THE AVERAGE Cr-CONCENTRATION VARIES WITH DISTANCE

POST-1: @@

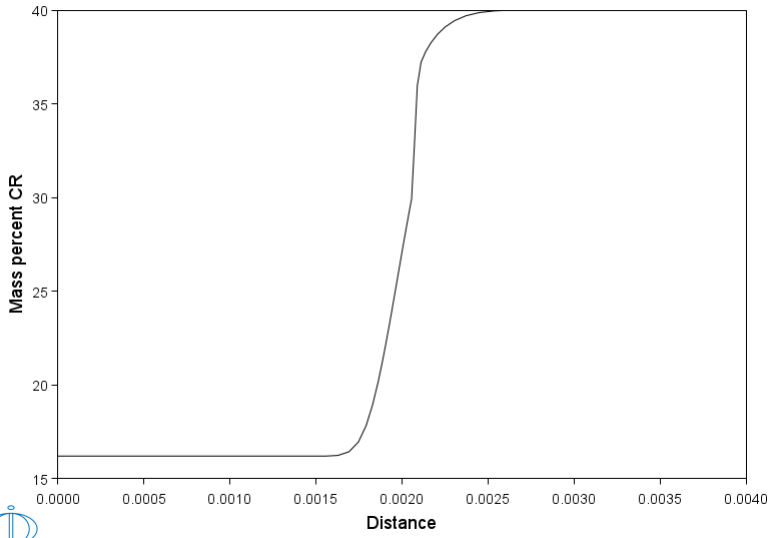
POST-1: s-d-a y w-p cr

POST-1: s-p-c time last

POST-1: set-tit Figure D2.2

POST-1: plot

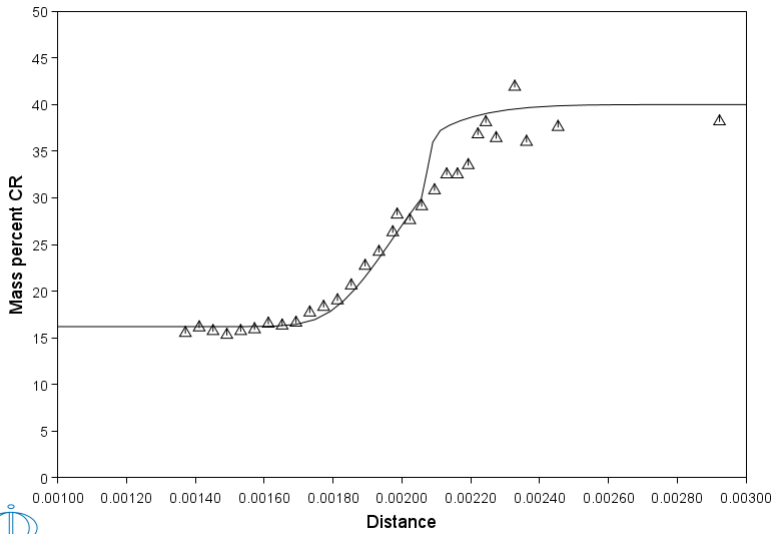
Figure D2.2



```

POST-1:
POST-1:
POST-1:
POST-1: @@<_hit_return_to_continue_>
POST-1: @@
POST-1: @@ NOW SELECT A BETTER SCALING AND APPEND THE EXPERIMENTAL DATA
POST-1: @@
POST-1:
POST-1: app y exd2.exp
PROLOGUE NUMBER: /0/: 1
DATASET NUMBER(s): /-1/: 4
POST-1:
POST-1: s-s-s y n 0 50
POST-1: s-s-s x n 10e-4 30e-4
POST-1:
POST-1: set-tit Figure D2.3
POST-1: plot
    
```

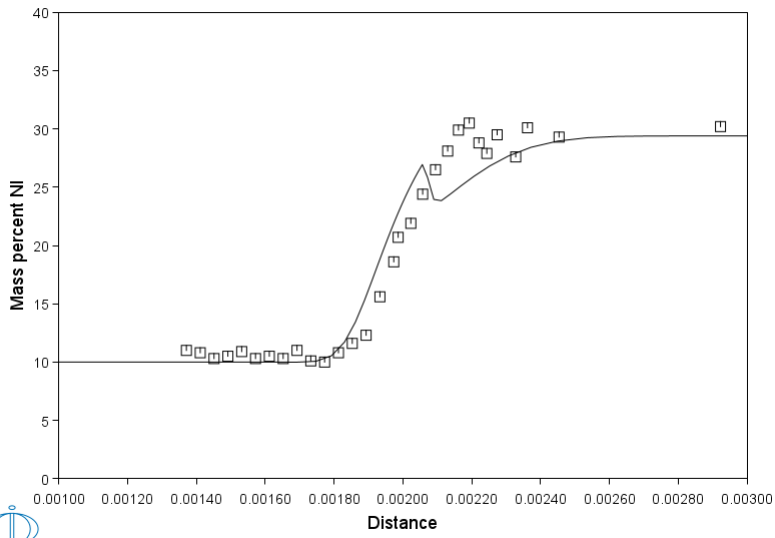
Figure D2.3



```

POST-1:
POST-1:
POST-1:
POST-1: @@<_hit_return_to_continue_>
POST-1: @@
POST-1: @@ NOW WE DO THE SAME FOR NICKEL
POST-1: @@
POST-1:
POST-1: s-d-a y w-p ni
POST-1:
POST-1: app y exd2.exp
PROLOGUE NUMBER: /1/: 1
DATASET NUMBER(s): /-1/: 5
POST-1:
POST-1: s-s-s x n 10e-4 30e-4
POST-1: s-s-s y n 0 40
POST-1:
POST-1: set-tit Figure D2.4
POST-1: plot
    
```

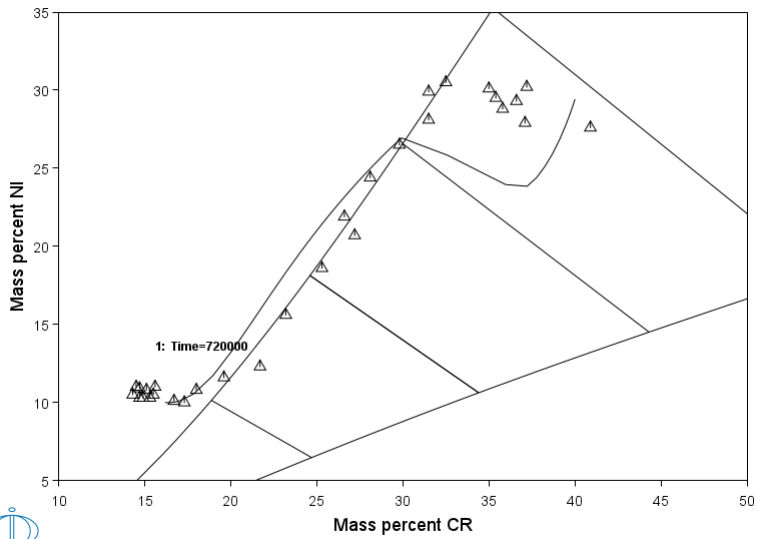
Figure D2.4



```

POST-1:
POST-1:
POST-1:
POST-1: @?<_hit_return_to_continue_>
POST-1: @@
POST-1: @@ LET US PLOT THE DIFFUSION PATH FOR THE COUPLE.
POST-1: @@ WE APPEND THE TERNARY PHASE-DIAGRAM CALCULATED IN THERMO-CALC
POST-1: @@ AND THE EXPERIMENTAL DATA
POST-1: @@
POST-1: s-d-a x w-p cr
POST-1: s-d-a y w-p ni
POST-1: s-i-v dis gl
POST-1: s-p-c time last
POST-1:
POST-1: app y exd2.exp
PROLOGUE NUMBER: /1/: 1
DATASET NUMBER(s): /-1/: 6 7 8
POST-1:
POST-1: s-s-s x n 10 50
POST-1: s-s-s y n 5 35
POST-1:
POST-1: set-tit Figure D2.5
POST-1: plot
    
```

Figure D2.5



```

POST-1:
POST-1:
POST-1:
POST-1:
POST-1: set-interactive
--OK--
POST-1:
    
```

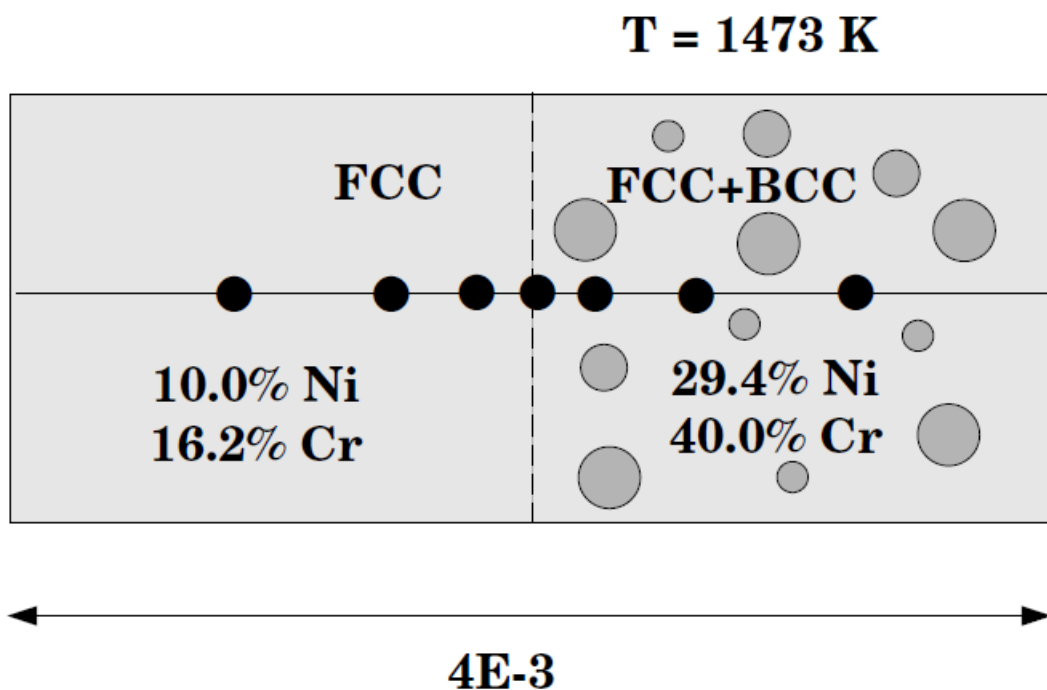


## Example exd2b

### Diffusion couple of Fe-Ni-Cr alloys: Interdiffusion and the Homogenization Model

This example calculates the interdiffusion in a diffusion couple between a two-phase (FCC+BCC) and a single-phase (FCC) Fe-Ni-Cr alloy. Initially it has a step profile. It is similar to exd2a except the default HOMOGENIZATION MODEL is used and then ENTER\_HOMOGENIZATION\_FUNCTION is used instead of ENTER\_LABYRINTH\_FUNCTION.

This case is from A. Engström: Scand. J. Met., vol. 24, 1995, pp.12-20.



## exd2b-setup

### SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,  
Stockholm, Sweden

Software running on Windows 64-bit wordlength  
Compiler: Intel Fortran Compiler 2025.0.0  
License library version: 9.7.0.0036  
Linked: Nov 19 2025 at 14:44:36

```
SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exd2b\setup.DCM"
```

```
SYS: i>:@@
NO SUCH COMMAND, USE HELP
SYS: @@ Diffusion in dispersed systems.
SYS: @@ Diffusion couple of Fe-Cr-Ni alloys: Homogenization model
SYS: @@ This example calculates the interdiffusion in a diffusion
SYS: @@ couple between a two-phase (FCC+BCC) and a single-phase (FCC)
SYS: @@ Fe-Ni-Cr alloy. This case is from A. Engstr m: Scand. J. Met.,
SYS: @@ v. 24, 1995, pp.12-20. This simulation can be run with either
SYS: @@ the DISPERSED SYSTEM MODEL or the HOMOGENIZATION MODEL.
SYS: @@ Here the default HOMOGENIZATION MODEL is used and then
SYS: @@ ENTER HOMOGENIZATION_FUNCTION should be used instead of
SYS: @@ ENTER_LABYRINTH_FUNCTION.
SYS: @@-----
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASE
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\databases\da
ta
Current database: Steels/Fe-Alloys v12.0

VA          /- DEFINED
DICTRA FCC_A1 REJECTED
TDB_TCFE12: sw fedemo
Current database: Iron Demo Database v6.0

VA          /- DEFINED
TDB_FEDEMO: def-sys fe ni cr
FE          NI          CR
DEFINED
TDB_FEDEMO: rej ph * all
GAS:G      LIQUID:L      BCC_A2
C14_LAVES  CBCC_A12     CHI_A12
CUB_A13    FCC_A1       HCP_A3
SIGMA D8B REJECTED
TDB_FEDEMO: res ph fcc,bcc
FCC_A1     BCC_A2 RESTORED
TDB_FEDEMO: get
11:46:38,019 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE MOBILITY DATA
TDB_FEDEMO: @@
TDB_FEDEMO: app mfedemo
Current database: Fe-Alloys Mobility demo database v5.0

VA DEFINED
APP: def-sys fe ni cr
FE          NI          CR
DEFINED
APP: rej ph * all
BCC_A2     FCC_A1       LIQUID:L
REJECTED
APP: res ph fcc,bcc
FCC_A1     BCC_A2 RESTORED
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR
APP: @@
APP: go d-m
NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 1473; * N
DIC>
DIC> @@
DIC> @@ ENTER THE REGION fer
DIC> @@
DIC> enter-region fer
DIC>
```

```

DIC>
DIC> @@
DIC> @@ ENTER GRID INTO THE REGION
DIC> @@
DIC> enter-grid fer 4e-3 auto
DIC>
DIC> @@
DIC> @@ ENTER A MATRIX PHASE IN THE REGION
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act fer matrix fcc
DIC>
DIC> @@
DIC> @@ ENTER THE START COMPOSITION FOR THE MATRIX PHASE
DIC> @@
DIC> enter-composition
REGION NAME : /FER/: fer
PHASE NAME: /FCC_A1/: fcc
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /CR/: cr function 16.2+23.8*HS(x-2e-3);
PROFILE FOR /NI/: ni function 10+19.4*HS(x-2e-3);
DIC>
DIC> @@
DIC> @@ ENTER FERRITE AS THE SPHEROIDAL PHASE IN THE REGION
DIC> @@ SINCE THE FRACTION OF FERRITE IS SMALL, AND THESE APPEAR
DIC> @@ AS ISOLATED PARTICLES, FERRITE IS ENTERED AS A SPHEROIDAL PHASE
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /FER/: fer
PHASE TYPE /MATRIX/: sph
PHASE NAME: /NONE/: bcc
INFO: EQUILIBRIUM COMPOSITION AND FRACTION OF SPHEROID PHASES USED AS DEFAULT
DIC>
DIC> @@
DIC> @@ ENTER THE COMPOSITION FOR THE SPHEROIDAL PHASE
DIC> @@ USE THE EQUILIBRIUM VALUE
DIC> @@
DIC> enter-composition
REGION NAME : /FER/: fer
PHASE NAME: /FCC_A1/: bcc
USE EQUILIBRIUM VALUE /Y/: y
DIC>
DIC> @@ SELECT A HOMOGENIZATION FUNCTION
DIC> @@ IN THIS CASE THE LOWER HASHIN-SHTRIKMAN BOUND
DIC> en-ho 1
SELECTED FUNCTION IS HASHIN-SHTRIKMAN BOUND: GENERAL LOWER
DIC>
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME AND OTHER SIMULATION PARAMETERS
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 720000
AUTOMATIC TIMESTEP CONTROL /YES/: YES
MAX TIMESTEP DURING INTEGRATION /720000/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC> @@
DIC> @@ SAVE THE SETUP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC>
DIC> save exd2 y
DIC>
DIC> set-inter
--OK--
DIC>

```

exd2b-run

DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exd2b\run.DCM"

DIC>

DIC>

DIC> @@ exd2\_run.DCM

DIC>

DIC> @@

DIC> @@ FILE FOR RUNNING THE SIMULATION OF EXAMPLE D2

DIC> @@

DIC>

DIC> @@

DIC> @@ READ THE SETUP FROM FILE AND START THE SIMULATION

DIC> @@

DIC>

DIC> go d-m

TIME STEP AT TIME 0.00000E+00

DIC> read exd2

OK

DIC> sim

INFO: Default responses (if any) will be applied during the simulation. Use "SIMULATE\_REACTION NO" instead for manual input.

Region: FER

geometric 0.980392 dense at 0.20000E-02 27 points

geometric 1.02000 dense at 0.20000E-02 26 points

DEGREE OF IMPLICITY SET TO EULER BACKWARD

INFO: not solving in latticefixed frame of reference

STARTING SIMULATION USING HOMOGENIZATION MODEL

-----

WARNING:BCC\_A2 HAS NO VOLUME FRACTION, CREATING ONE

Starting time-step t0= 0.0000000 dt= 0.10000000E-06

Starting time-step t0= 0.10000000E-06 dt= 0.20000000E-06

Starting time-step t0= 0.30000000E-06 dt= 0.40000000E-06

Starting time-step t0= 0.70000000E-06 dt= 0.80000000E-06

Starting time-step t0= 0.15000000E-05 dt= 0.16000000E-05

Starting time-step t0= 0.31000000E-05 dt= 0.32000000E-05

Starting time-step t0= 0.63000000E-05 dt= 0.64000000E-05

Starting time-step t0= 0.12700000E-04 dt= 0.12800000E-04

Starting time-step t0= 0.25500000E-04 dt= 0.25600000E-04

Starting time-step t0= 0.51100000E-04 dt= 0.51200000E-04

Starting time-step t0= 0.10230000E-03 dt= 0.10240000E-03

Starting time-step t0= 0.20470000E-03 dt= 0.20480000E-03

Starting time-step t0= 0.40950000E-03 dt= 0.40960000E-03

Starting time-step t0= 0.81910000E-03 dt= 0.81920000E-03

Starting time-step t0= 0.16383000E-02 dt= 0.16384000E-02

Starting time-step t0= 0.32767000E-02 dt= 0.32768000E-02

Starting time-step t0= 0.65535000E-02 dt= 0.65536000E-02

Starting time-step t0= 0.13107100E-01 dt= 0.13107200E-01

Starting time-step t0= 0.26214300E-01 dt= 0.26214400E-01

Starting time-step t0= 0.52428700E-01 dt= 0.52428800E-01

Starting time-step t0= 0.10485750 dt= 0.10485760

Starting time-step t0= 0.20971510 dt= 0.20971520

Starting time-step t0= 0.41943030 dt= 0.41943040

Starting time-step t0= 0.83886070 dt= 0.83886080

Starting time-step t0= 1.6777215 dt= 1.6777216

Starting time-step t0= 3.3554431 dt= 3.3554432

Starting time-step t0= 6.7108863 dt= 6.7108864

Starting time-step t0= 13.421773 dt= 13.421773

Starting time-step t0= 26.843545 dt= 26.843546

Starting time-step t0= 53.687091 dt= 53.687091

Starting time-step t0= 107.37418 dt= 107.37418

Starting time-step t0= 214.74836 dt= 214.74836

Starting time-step t0= 429.49673 dt= 429.49673

Starting time-step t0= 858.99346 dt= 858.99346

Starting time-step t0= 1717.9869 dt= 1717.9869

Starting time-step t0= 3435.9738 dt= 3435.9738

Starting time-step t0= 6871.9477 dt= 6871.9477

Starting time-step t0= 13743.895 dt= 13743.895

Starting time-step t0= 27487.791 dt= 27487.791

Starting time-step t0= 54975.581 dt= 54975.581

Starting time-step t0= 109951.162 dt= 109951.162

Starting time-step t0= 219902.324 dt= 219902.324

Starting time-step t0= 439804.648 dt= 439804.648

Starting time-step t0= 879609.296 dt= 879609.296

Starting time-step t0= 1759218.592 dt= 1759218.592

Starting time-step t0= 3518437.184 dt= 3518437.184

Starting time-step t0= 7036874.368 dt= 7036874.368

Starting time-step t0= 14073748.736 dt= 14073748.736

Starting time-step t0= 28147497.472 dt= 28147497.472

Starting time-step t0= 56294994.944 dt= 56294994.944

Starting time-step t0= 112589989.888 dt= 112589989.888

Starting time-step t0= 225179979.776 dt= 225179979.776

Starting time-step t0= 450359959.552 dt= 450359959.552

Starting time-step t0= 900719919.104 dt= 900719919.104

Starting time-step t0= 1801439838.208 dt= 1801439838.208

Starting time-step t0= 3602879676.416 dt= 3602879676.416

Starting time-step t0= 7205759352.832 dt= 7205759352.832

Starting time-step t0= 14411518705.664 dt= 14411518705.664

Starting time-step t0= 28823037411.328 dt= 28823037411.328

Starting time-step t0= 57646074822.656 dt= 57646074822.656

Starting time-step t0= 115292149645.312 dt= 115292149645.312

Starting time-step t0= 230584299290.624 dt= 230584299290.624

Starting time-step t0= 461168598581.248 dt= 461168598581.248

Starting time-step t0= 922337197162.496 dt= 922337197162.496

Starting time-step t0= 1844674354324.992 dt= 1844674354324.992

Starting time-step t0= 3689348708649.984 dt= 3689348708649.984

Starting time-step t0= 7378697417299.968 dt= 7378697417299.968

Starting time-step t0= 14757394834599.936 dt= 14757394834599.936

Starting time-step t0= 29514789669199.872 dt= 29514789669199.872

Starting time-step t0= 59029579338399.744 dt= 59029579338399.744

Starting time-step t0= 118059158676799.488 dt= 118059158676799.488

Starting time-step t0= 236118317353598.976 dt= 236118317353598.976

Starting time-step t0= 472236634707197.952 dt= 472236634707197.952

Starting time-step t0= 944473269414395.904 dt= 944473269414395.904

Starting time-step t0= 1888946538828791.808 dt= 1888946538828791.808

Starting time-step t0= 3777893077657583.616 dt= 3777893077657583.616

Starting time-step t0= 7555786155315167.232 dt= 7555786155315167.232

Starting time-step t0= 15111572310630334.464 dt= 15111572310630334.464

Starting time-step t0= 30223144621260668.928 dt= 30223144621260668.928

Starting time-step t0= 60446289242521337.856 dt= 60446289242521337.856

Starting time-step t0= 120892578485042675.712 dt= 120892578485042675.712

Starting time-step t0= 241785156970085351.424 dt= 241785156970085351.424

Starting time-step t0= 483570313940170702.848 dt= 483570313940170702.848

Starting time-step t0= 967140627880341405.696 dt= 967140627880341405.696

Starting time-step t0= 1934281255760682811.392 dt= 1934281255760682811.392

Starting time-step t0= 3868562511521365622.784 dt= 3868562511521365622.784

Starting time-step t0= 7737125023042731245.568 dt= 7737125023042731245.568

Starting time-step t0= 15474250046085462491.136 dt= 15474250046085462491.136

KEEPING TIME-RECORD FOR TIME 717963.08  
AND FOR TIME 720000.00  
WORKSPACE RECLAIMED

-----  
INTERPOLATION SCHEME USED THIS FRACTION OF  
THE ALLOCATED MEMORY: 5.706238112003934E-003  
EFFICIENCY FACTOR: 3.23110624315444  
-----

DEALLOCATING  
-----

TIMESTEP AT 720000.000 SELECTED

DIC>

DIC>

DIC>

DIC>

DIC> set-inter

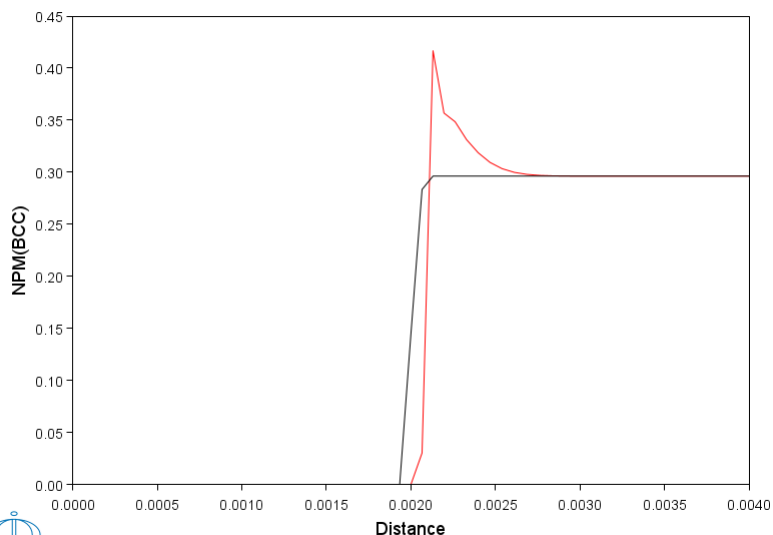
--OK--

DIC>

# exd2b-plot

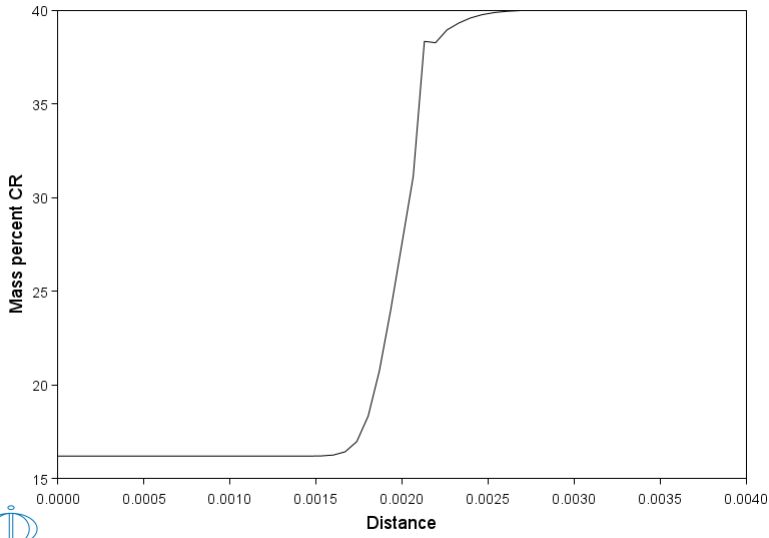
```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exd2b\plot.DCM"
DIC>
DIC>
DIC> @@ exd2_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE D2
DIC> @@
DIC> @@ ENTER THE DICTRA MODULE AND SPECIFY THE STORE-RESULT FILE
DIC> @@
DIC>
DIC> go d-m
TIME STEP AT TIME 7.20000E+05
DIC> read exd2
OK
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA POST PROCESSOR
DIC> @@
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1:
POST-1: @@
POST-1: @@ LET US FIRST SEE HOW THE FRACTION OF FERRITE HAS CHANGED
POST-1: @@ AS A RESULT OF THE DIFFUSION
POST-1: @@
POST-1: s-d-a y npm(bcc)
POST-1: s-d-a x distance global
INFO: Distance is set as independent variable
POST-1: s-p-c time 0 720000
POST-1: set-tit Figure D2.1
POST-1: plot
```

Figure D2.1



```
POST-1:
POST-1:
POST-1:
POST-1: @?<_hit_return_to_continue_>
POST-1: @@
POST-1: @@ LET US NOW PLOT HOW THE AVERAGE CR-CONCENTRATION VARIES WITH DISTANCE
POST-1: @@
POST-1: s-d-a y w-p cr
POST-1: s-p-c time last
POST-1: set-tit Figure D2.2
POST-1: plot
```

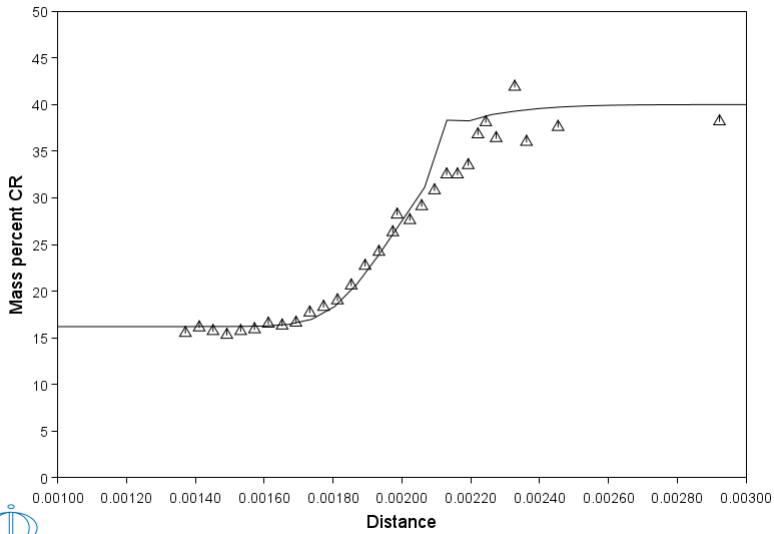
Figure D2.2



```

POST-1:
POST-1:
POST-1:
POST-1: @?<_hit_return_to_continue_>
POST-1: @@
POST-1: @@ WE SELECT A BETTER SCALING AND APPEND EXPERIMENTAL DATA
POST-1: @@
POST-1:
POST-1: app y exd2.exp
PROLOGUE NUMBER: /0/: 1
DATASET NUMBER(s): /-1/: 4
POST-1:
POST-1: s-s-s y n 0 50
POST-1: s-s-s x n 10e-4 30e-4
POST-1:
POST-1: set-tit Figure D2.3
POST-1: plot
    
```

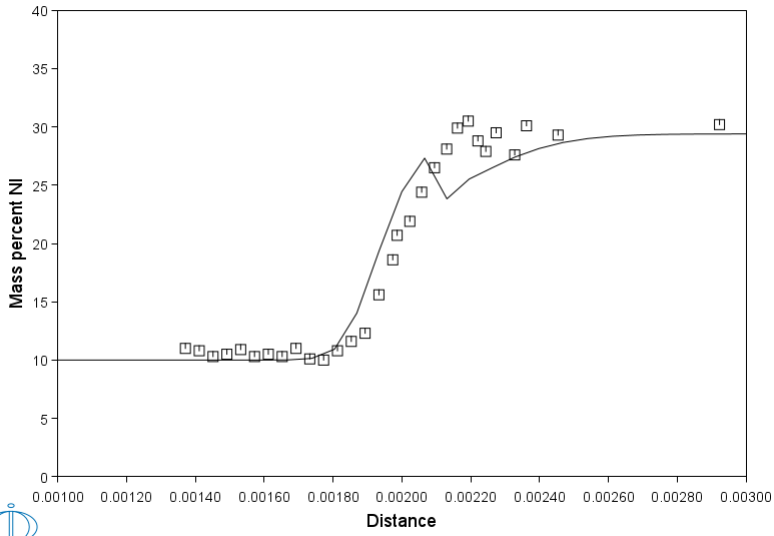
Figure D2.3



```

POST-1:
POST-1:
POST-1:
POST-1: @?<_hit_return_to_continue_>
POST-1: @@
POST-1: @@ NOW WE DO THE SAME FOR NICKEL
POST-1: @@
POST-1:
POST-1: s-d-a y w-p ni
POST-1:
POST-1: app y exd2.exp
PROLOGUE NUMBER: /1/: 1
DATASET NUMBER(s): /-1/: 5
POST-1:
POST-1: s-s-s x n 10e-4 30e-4
POST-1: s-s-s y n 0 40
POST-1:
POST-1: set-tit Figure D2.4
POST-1: plot
    
```

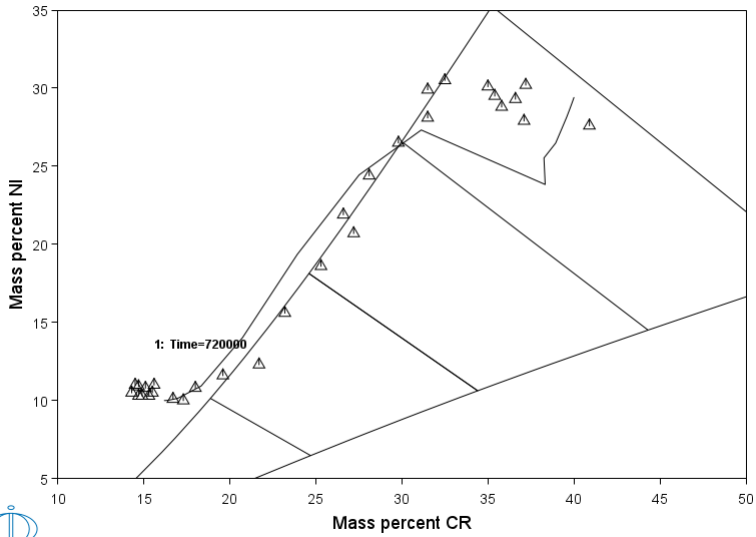
Figure D2.4



```

POST-1:
POST-1:
POST-1:
POST-1: @?<_hit_return_to_continue_>
POST-1: @@
POST-1: @@ LET US PLOT THE DIFFUSION PATH FOR THE COUPLE
POST-1: @@ WE APPEND THE TERNARY PHASE-DIAGRAM CALCULATED IN THERMO-CALC
POST-1: @@ AND THE EXPERIMENTAL DATA
POST-1: @@
POST-1: s-d-a x w-p cr
POST-1: s-d-a y w-p ni
POST-1: s-i-v dis gl
POST-1: s-p-c time last
POST-1:
POST-1: app y exd2.exp
PROLOGUE NUMBER: /1/: 1
DATASET NUMBER(s): /-1/: 6 7 8
POST-1:
POST-1: s-s-s x n 10 50
POST-1: s-s-s y n 5 35
POST-1:
POST-1: set-tit Figure D2.5
POST-1: plot
    
```

Figure D2.5



```

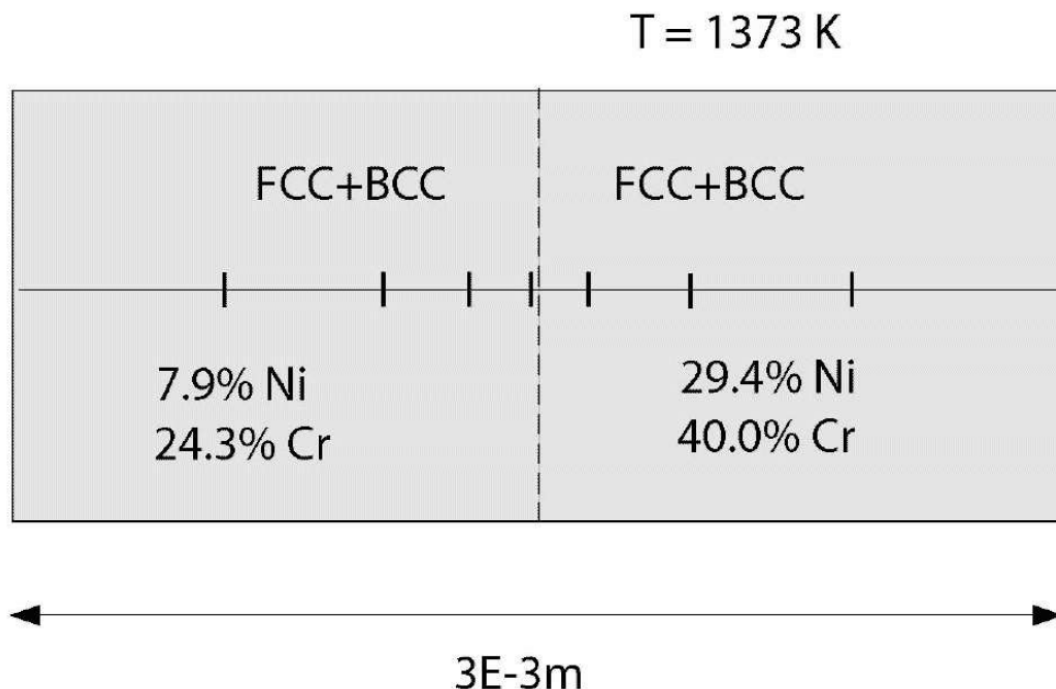
POST-1:
POST-1:
POST-1:
POST-1:
POST-1: set-interactive
--OK--
POST-1:
    
```



## Example exd3

### Diffusion couple of Fe-Ni-Cr alloys: Homogenization Model

This example shows the use of the homogenization model. It is taken from H. Larsson and A. Engström, Acta. Mater. v.54 (2006), pp. 2431-2439. Experimental data from A. Engström, Scand J Metall, 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 will not affect the simulation.



## exd3-setup

### SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,  
Stockholm, Sweden

Software running on Windows 64-bit wordlength  
Compiler: Intel Fortran Compiler 2025.0.0  
License library version: 9.7.0.0036  
Linked: Nov 19 2025 at 14:44:36

```
SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exd3\setup.DCM.test"
```

```
SYS: i>:@@
NO SUCH COMMAND, USE HELP
SYS: @@ Diffusion in dispersed systems.
SYS: @@ Diffusion couple of Fe-Cr-Ni alloys: Homogenization model
SYS: @@ This example uses the homogenization model. It is taken from
SYS: @@ H. Larsson and A. Engstr m, Acta. Mater. v.54 (2006), pp. 2431-2439.
SYS: @@ Experimental data from A. Engstr m, Scand J Metall, v.243 (1995), p.12.
SYS: @@ The homogenization model can be used for multiphase simulations
SYS: @@ like the dispersed system model, but unlike the dispersed system model
SYS: @@ there is no need to have a single continuous matrix phase and, furthermore,
SYS: @@ there is no need to limit the size of time-steps.
SYS: @@ The set-up is performed in the same manner as for the dispersed system
SYS: @@ model, which means that a certain phase is entered as the matrix phase
SYS: @@ and the other phases are entered as spheroidal, but the choice of matrix
SYS: @@ phase will not affect the simulation.
```

```
SYS: @@-----
SYS:
SYS: @@ exd3_setup.DCM
SYS:
SYS:
SYS: go da
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\databases\da
ta
Current database: Steels/Fe-Alloys v12.0
```

```
VA          /- DEFINED
DICTRA FCC_A1 REJECTED
TDB_TCFE12: sw fedemo
Current database: Iron Demo Database v6.0
```

```
VA          /- DEFINED
TDB_FEDEMO: def-sys fe cr ni
FE          CR          NI
DEFINED
TDB_FEDEMO: rej-ph *
GAS:G          LIQUID:L          BCC_A2
C14 LAVES          CBCC_A12          CHI_A12
CUB_A13          FCC_A1          HCP_A3
SIGMA_D8B REJECTED
TDB_FEDEMO: rest-ph bcc,fcc
BCC_A2          FCC_A1 RESTORED
TDB_FEDEMO: get
11:49:42,967 [Thread-0] INFO  JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....
```

Use the command LIST\_REFERENCES to see the list of references for assessed data

```
-OK-
TDB_FEDEMO:
TDB_FEDEMO: app mfedemo
Current database: Fe-Alloys Mobility demo database v5.0
```

```
VA DEFINED
APP: def-sys fe cr ni
FE          CR          NI
DEFINED
APP: rej-ph *
BCC_A2          FCC_A1          LIQUID:L
REJECTED
APP: rest-ph bcc,fcc
BCC_A2          FCC_A1 RESTORED
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....
```

Use the command LIST\_REFERENCES to see the list of references for assessed data

```
-OK-
APP:
APP: go -m
NO TIME STEP DEFINED
DIC>
DIC> set-cond glob T 0 1373.15; * N
DIC>
DIC> ent-geo 0
DIC>
DIC> ent-reg
REGION NAME : fecrni
DIC>
DIC> ent-grid
REGION NAME : /FECRNI/: fecrni
WIDTH OF REGION /1/: 3e-3
TYPE /AUTO/: double
NUMBER OF POINTS /50/: 60
VALUE OF R IN THE GEOMETRICAL SERIE FOR LOWER PART OF REGION: 0.85
```

```
VALUE OF R IN THE GEOMETRICAL SERIE FOR UPPER PART OF REGION: 1.15
DIC>
DIC> ent-ph
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /FECRNI/: fecrni
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC> ent-ph
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /FECRNI/: fecrni
PHASE TYPE /MATRIX/: sph
PHASE NAME: /NONE/: bcc
INFO: EQUILIBRIUM COMPOSITION AND FRACTION OF SPHEROID PHASES USED AS DEFAULT
DIC>
DIC> ent-comp
REGION NAME : /FECRNI/: fecrni
PHASE NAME: /FCC_A1/: fcc#1
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: m-f
PROFILE FOR /CR/: cr
TYPE /LINEAR/: read cr.dat
PROFILE FOR /NI/: ni
TYPE /READ_POINT_BY_POINT/: read ni.dat
DIC>
DIC> ent-comp
REGION NAME : /FECRNI/: fecrni
PHASE NAME: /FCC_A1/: bcc
USE EQUILIBRIUM VALUE /Y/: y
DIC>
DIC> se-si-ti
END TIME FOR INTEGRATION /.1/: 3.6e5
AUTOMATIC TIMESTEP CONTROL /YES/: yes
MAX TIMESTEP DURING INTEGRATION /36000/: 3.6e4
INITIAL TIMESTEP : /1E-07/: 1
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/: 1e-7
DIC>
DIC> @@ SIMULATIONS ARE FASTER WHEN THE RESULTS ARE NOT SAVED
DIC> @@ FOR EVERY TIME STEP
DIC> set-option SAVE_WORKSPACE_ON_FILE 99
DIC>
DIC>
DIC> @@ There are a several options available for the homogenization
DIC> @@ model. There is also an interpolation scheme that may reduce
DIC> @@ simulation times. However, for this example, the default settings
DIC> @@ are kept and the interpolation scheme is turned off.
DIC> @@
DIC> homogen yes yes
INFO: HOMOGENIZATION MODEL ENABLED
DIC>
DIC> @@ There are a large number of homogenization functions
DIC> @@ available. These determine how the average kinetics
DIC> @@ of the multiphase mixture is evaluated. For this example
DIC> @@ the General lower Hashin-Shtrikman bound is a good choice.
DIC> en-ho
ENTER HOMOGENIZATION FUNCTION # /5/: 1
SELECTED FUNCTION IS HASHIN-SHTRIKMAN BOUND: GENERAL LOWER
DIC>
DIC>
DIC>
DIC> save exd3 Y
DIC>
DIC>
DIC> set-inter
--OK--
DIC>
```

exd3-run

DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exd3\run.DCM.test"

DIC>

DIC>

DIC> @@ exd3\_run.DCM

DIC>

DIC> @@

DIC> @@ READ THE SETUP FROM FILE AND START THE SIMULATION

DIC> @@

DIC>

DIC> go d-m

TIME STEP AT TIME 0.00000E+00

DIC> read exd3

OK

DIC>

DIC> sim

INFO: Default responses (if any) will be applied during the simulation. Use "SIMULATE\_REACTION NO" instead for manual input.

DEGREE OF IMPLICIT SET TO EULER BACKWARD

INFO: not solving in latticefixed frame of reference

STARTING SIMULATION USING HOMOGENIZATION MODEL

-----  
WARNING:BCC\_A2 HAS NO VOLUME FRACTION, CREATING ONE  
Starting time-step t0= 0.0000000 dt= 1.0000000  
Starting time-step t0= 1.0000000 dt= 2.0000000  
Starting time-step t0= 3.0000000 dt= 4.0000000  
Starting time-step t0= 7.0000000 dt= 8.0000000  
Starting time-step t0= 15.0000000 dt= 16.0000000  
Starting time-step t0= 31.0000000 dt= 32.0000000  
Starting time-step t0= 63.0000000 dt= 64.0000000  
Starting time-step t0= 127.0000000 dt= 64.0000000  
Starting time-step t0= 191.0000000 dt= 64.0000000  
Starting time-step t0= 255.0000000 dt= 64.0000000  
Starting time-step t0= 319.0000000 dt= 64.0000000  
Starting time-step t0= 383.0000000 dt= 64.0000000  
Starting time-step t0= 447.0000000 dt= 128.0000000  
Starting time-step t0= 575.0000000 dt= 128.0000000  
Starting time-step t0= 703.0000000 dt= 128.0000000  
Starting time-step t0= 831.0000000 dt= 128.0000000  
Starting time-step t0= 959.0000000 dt= 128.0000000  
Starting time-step t0= 1087.0000000 dt= 256.0000000  
Starting time-step t0= 1343.0000000 dt= 256.0000000  
Starting time-step t0= 1599.0000000 dt= 256.0000000  
Starting time-step t0= 1855.0000000 dt= 256.0000000  
Starting time-step t0= 2111.0000000 dt= 256.0000000  
Starting time-step t0= 2367.0000000 dt= 512.0000000  
Starting time-step t0= 2879.0000000 dt= 512.0000000  
Starting time-step t0= 3391.0000000 dt= 512.0000000  
Starting time-step t0= 3903.0000000 dt= 512.0000000  
Starting time-step t0= 4415.0000000 dt= 512.0000000  
Starting time-step t0= 4927.0000000 dt= 1024.0000000  
Starting time-step t0= 5951.0000000 dt= 1024.0000000  
Starting time-step t0= 6975.0000000 dt= 1024.0000000  
Starting time-step t0= 7999.0000000 dt= 1024.0000000  
Starting time-step t0= 9023.0000000 dt= 1024.0000000  
Starting time-step t0= 10047.0000000 dt= 2048.0000000  
Starting time-step t0= 12095.0000000 dt= 2048.0000000  
Starting time-step t0= 14143.0000000 dt= 2048.0000000  
Starting time-step t0= 16191.0000000 dt= 2048.0000000  
Starting time-step t0= 18239.0000000 dt= 2048.0000000  
Starting time-step t0= 20287.0000000 dt= 2048.0000000  
Starting time-step t0= 22335.0000000 dt= 2048.0000000  
Starting time-step t0= 24383.0000000 dt= 4096.0000000  
Starting time-step t0= 28479.0000000 dt= 4096.0000000  
Starting time-step t0= 32575.0000000 dt= 4096.0000000  
Starting time-step t0= 36671.0000000 dt= 4096.0000000  
Starting time-step t0= 40767.0000000 dt= 4096.0000000  
Starting time-step t0= 44863.0000000 dt= 4096.0000000  
Starting time-step t0= 48959.0000000 dt= 4096.0000000  
Starting time-step t0= 53055.0000000 dt= 8192.0000000  
Starting time-step t0= 61247.0000000 dt= 8192.0000000  
Starting time-step t0= 69439.0000000 dt= 8192.0000000  
Starting time-step t0= 77631.0000000 dt= 8192.0000000  
Starting time-step t0= 85823.0000000 dt= 8192.0000000  
Starting time-step t0= 94015.0000000 dt= 8192.0000000  
Starting time-step t0= 102207.0000000 dt= 8192.0000000  
Starting time-step t0= 110399.0000000 dt= 16384.0000000  
Starting time-step t0= 126783.0000000 dt= 16384.0000000  
Starting time-step t0= 143167.0000000 dt= 16384.0000000  
Starting time-step t0= 159551.0000000 dt= 16384.0000000  
Starting time-step t0= 175935.0000000 dt= 16384.0000000  
Starting time-step t0= 192319.0000000 dt= 16384.0000000  
Starting time-step t0= 208703.0000000 dt= 16384.0000000  
Starting time-step t0= 225087.0000000 dt= 16384.0000000  
Starting time-step t0= 241471.0000000 dt= 32768.0000000  
Starting time-step t0= 274239.0000000 dt= 32768.0000000  
Starting time-step t0= 307007.0000000 dt= 32768.0000000  
Starting time-step t0= 339775.0000000 dt= 20225.0000000

MUST SAVE WORKSPACE ON FILE

WORKSPACE SAVED ON FILE

RECLAIMING WORKSPACE

DELETING TIME-RECORD FOR TIME 0.0000000  
DELETING TIME-RECORD FOR TIME 1.0000000  
DELETING TIME-RECORD FOR TIME 383.0000000  
DELETING TIME-RECORD FOR TIME 831.0000000  
DELETING TIME-RECORD FOR TIME 1343.0000000  
DELETING TIME-RECORD FOR TIME 1855.0000000  
DELETING TIME-RECORD FOR TIME 2367.0000000  
DELETING TIME-RECORD FOR TIME 2879.0000000  
DELETING TIME-RECORD FOR TIME 3391.0000000  
DELETING TIME-RECORD FOR TIME 3903.0000000  
DELETING TIME-RECORD FOR TIME 4415.0000000  
DELETING TIME-RECORD FOR TIME 4927.0000000  
DELETING TIME-RECORD FOR TIME 5951.0000000  
DELETING TIME-RECORD FOR TIME 6975.0000000  
DELETING TIME-RECORD FOR TIME 7999.0000000  
DELETING TIME-RECORD FOR TIME 9023.0000000  
DELETING TIME-RECORD FOR TIME 10047.0000000  
DELETING TIME-RECORD FOR TIME 12095.0000000  
DELETING TIME-RECORD FOR TIME 14143.0000000  
DELETING TIME-RECORD FOR TIME 16191.0000000  
DELETING TIME-RECORD FOR TIME 18239.0000000

DELETING TIME-RECORD FOR TIME 20287.000  
DELETING TIME-RECORD FOR TIME 22335.000  
DELETING TIME-RECORD FOR TIME 24383.000  
DELETING TIME-RECORD FOR TIME 28479.000  
DELETING TIME-RECORD FOR TIME 32575.000  
DELETING TIME-RECORD FOR TIME 36671.000  
DELETING TIME-RECORD FOR TIME 40767.000  
DELETING TIME-RECORD FOR TIME 44863.000  
DELETING TIME-RECORD FOR TIME 48959.000  
DELETING TIME-RECORD FOR TIME 53055.000  
DELETING TIME-RECORD FOR TIME 61247.000  
DELETING TIME-RECORD FOR TIME 69439.000  
DELETING TIME-RECORD FOR TIME 77631.000  
DELETING TIME-RECORD FOR TIME 85823.000  
DELETING TIME-RECORD FOR TIME 94015.000  
DELETING TIME-RECORD FOR TIME 102207.00  
DELETING TIME-RECORD FOR TIME 110399.00  
DELETING TIME-RECORD FOR TIME 126783.00  
DELETING TIME-RECORD FOR TIME 143167.00  
DELETING TIME-RECORD FOR TIME 159551.00  
DELETING TIME-RECORD FOR TIME 175935.00  
DELETING TIME-RECORD FOR TIME 192319.00  
DELETING TIME-RECORD FOR TIME 208703.00  
DELETING TIME-RECORD FOR TIME 225087.00  
DELETING TIME-RECORD FOR TIME 241471.00  
DELETING TIME-RECORD FOR TIME 274239.00  
DELETING TIME-RECORD FOR TIME 307007.00

KEEPING TIME-RECORD FOR TIME 339775.00  
AND FOR TIME 360000.00  
WORKSPACE RECLAIMED

-----  
INTERPOLATION SCHEME USED THIS FRACTION OF  
THE ALLOCATED MEMORY: 2.459578209212064E-002  
EFFICIENCY FACTOR: 6.33533796374725  
-----

DEALLOCATING  
-----

TIMESTEP AT 360000.000 SELECTED

DIC>

DIC>

DIC> set-inter

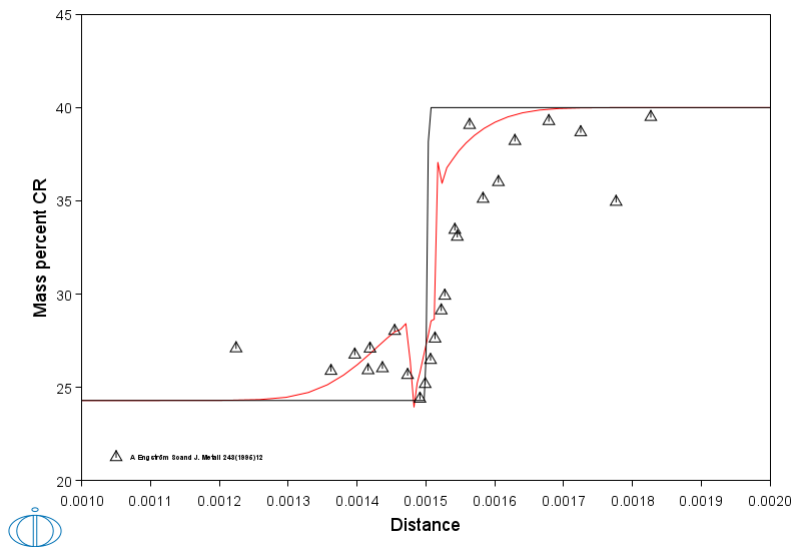
--OK--

DIC>

## exd3-plot

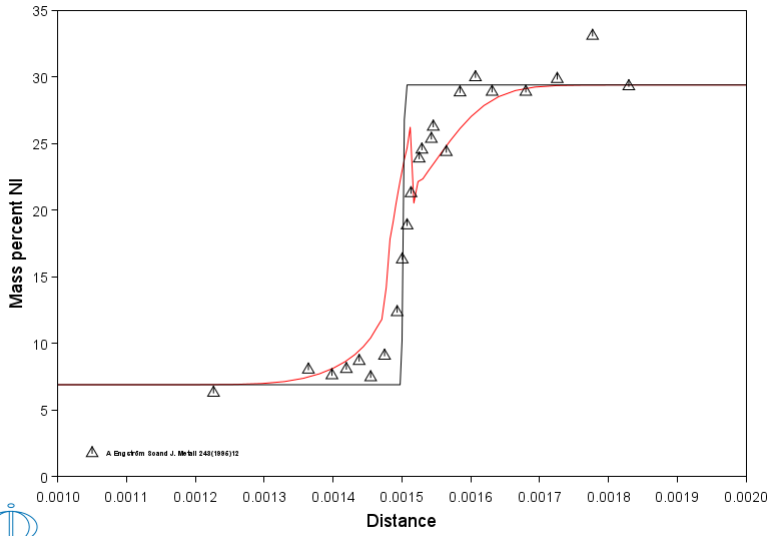
```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exd3\plot.DCM.test"
DIC>
DIC>
DIC> @@ exd3_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE d3
DIC> @@
DIC> @@ ENTER THE DICTRA MODULE AND SPECIFY THE STORE-RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 3.60000E+05
DIC> read exd3
OK
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA POST PROCESSOR
DIC> @@
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1:
POST-1: @@
POST-1: @@ First study the composition profiles of Cr and Ni
POST-1: @@
POST-1: s-d-a x distance global
INFO: Distance is set as independent variable
POST-1: s-d-a y w-p Cr
POST-1: s-p-c time 0 360000
POST-1: set-tit Figure D3.1
POST-1:
POST-1: app yes k5k7cr.exp 0; 1
POST-1:
POST-1: s-s-s x n 1e-3 2e-3
POST-1:
POST-1: s-s-s y n 20 45
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 3
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

Figure D3.1



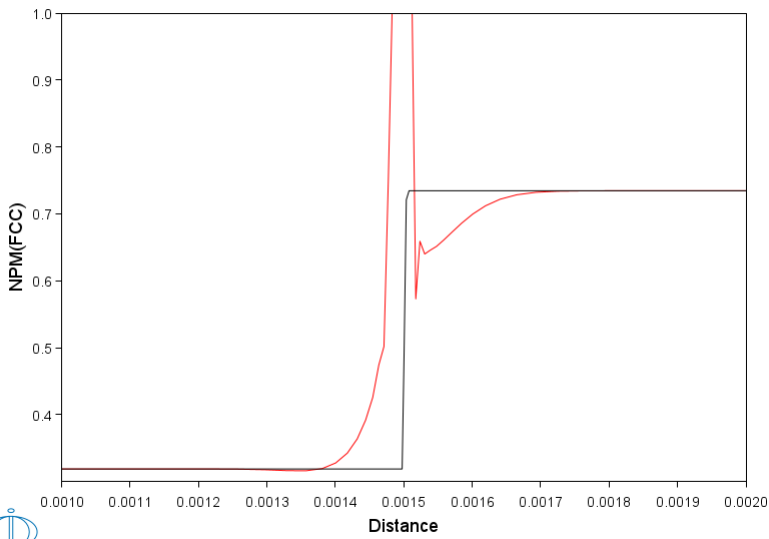
```
POST-1:
POST-1:
POST-1: @?<_hit_return_to_continue_>
POST-1: s-d-a y w-p Ni
POST-1: set-tit Figure D3.2
POST-1:
POST-1: app yes k5k7ni.exp 0; 1
POST-1:
POST-1: s-s-s y n 0 35
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 3
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

Figure D3.2



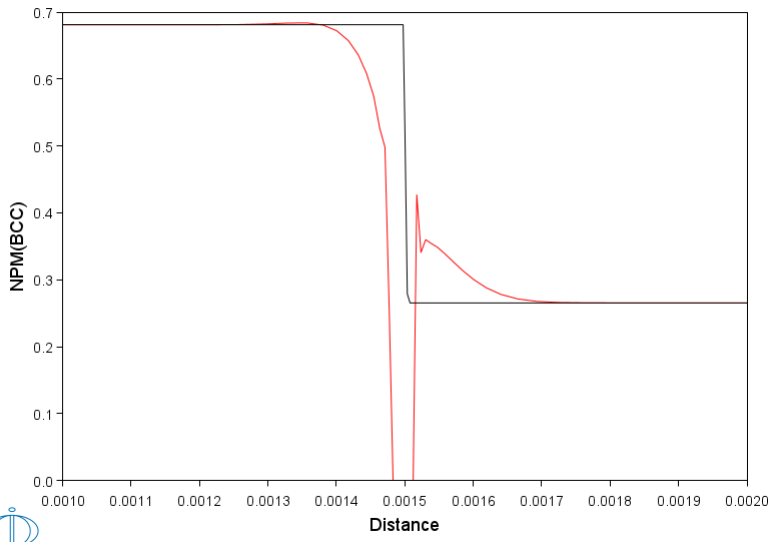
```
POST-1:
POST-1: @?<_hit_return_to_continue_>
POST-1: @@
POST-1: @@ Then study the amount of FCC and BCC
POST-1: @@
POST-1: app no
POST-1: s-d-a y npm(fcc)
POST-1: set-tit Figure D3.3
POST-1:
POST-1: SET_EXP_FILE_FORMAT 3
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

Figure D3.3



```
POST-1:
POST-1: @?<_hit_return_to_continue_>
POST-1: s-d-a y npm(bcc)
POST-1: set-tit Figure D3.4
POST-1:
POST-1: SET_EXP_FILE_FORMAT 3
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

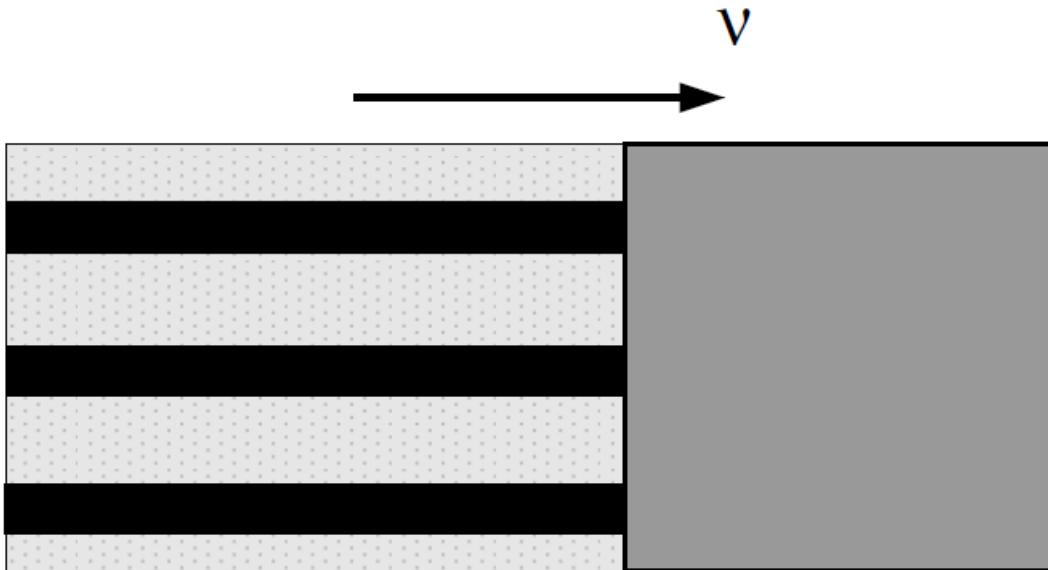
Figure D3.4



POST-1:  
POST-1:  
POST-1: set-interactive  
--OK--  
POST-1:



## Cooperative Growth



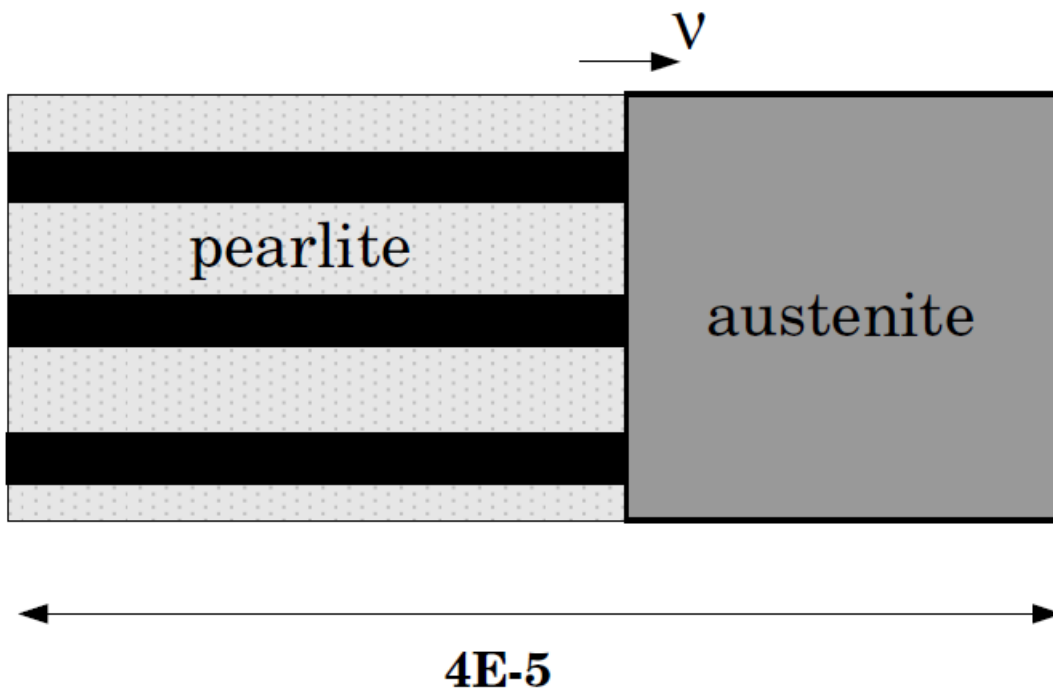


## Example exe1

### Growth of pearlite in an Fe-Mn-C alloy

This is an example of pearlite growth in an Fe-0.50wt%C - 0.91wt%Mn steel.

$$T = 900 - \text{Time} * 10$$



## exe1-setup

### SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,  
Stockholm, Sweden

Software running on Windows 64-bit wordlength  
Compiler: Intel Fortran Compiler 2025.0.0  
License library version: 9.7.0.0036  
Linked: Nov 19 2025 at 14:44:36

```
SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exe1\setup.DCM.test"
```

```
SYS: i>:@@
NO SUCH COMMAND, USE HELP
SYS: @@ Cooperative growth.
SYS: @@ Growth of pearlite in an Fe-Mn-C alloy
SYS: @@ An example of pearlite growth in an Fe-0.50wt%C-0.91wt%Mn steel.
SYS: @@-----
SYS:
SYS: @@ exe1_setup.DCM
SYS:
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASE
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\databases\da
ta
Current database: Steels/Fe-Alloys v12.0

VA                /- DEFINED
DICTRA FCC_A1 REJECTED
TDB_TCFE12: sw FEDEMO
Current database: Iron Demo Database v6.0

VA                /- DEFINED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ DEFINE THE SYSTEM
TDB_FEDEMO: @@
TDB_FEDEMO: def-sys fe c mn
FE                C                MN
DEFINED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ KEEP ONLY THE AUSTENITE, FERRITE AND CEMENTITE PHASES
TDB_FEDEMO: @@
TDB_FEDEMO: rej-ph /all
GAS:G             LIQUID:L             BCC_A2
C14_LAVES         CBCC_A12             CEMENTITE_D011
CUB_A13           DIAMOND_A4             FCC_A1
GRAPHITE_A9       HCP_A3                KSI_CARBIDE
M23C6_D84         M5C2                  M7C3_D101
REJECTED
TDB_FEDEMO: rest-ph fcc,bcc,cem
FCC_A1           BCC_A2             CEMENTITE_D011
RESTORED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ GET THE THERMODYNAMIC DATA
TDB_FEDEMO: @@
TDB_FEDEMO: get
11:52:53,200 [Thread-0] INFO  JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ APPEND THE KINETIC DATA FROM THE MOBILITY DATABASE
TDB_FEDEMO: @@
TDB_FEDEMO: append mfedemo
Current database: Fe-Alloys Mobility demo database v5.0

VA DEFINED
APP: def-sys fe c mn
FE                C                MN
DEFINED
APP: rej-ph /all
BCC_A2           FCC_A1             CEMENTITE_D011
LIQUID:L REJECTED
APP: rest-ph bcc,fcc,cem
BCC_A2           FCC_A1             CEMENTITE_D011
RESTORED
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-
APP:
APP: @@
APP: @@ ALL THE THERMODYNAMIC AND KINETIC DATA HAVE BEEN RETRIEVED.
APP: @@ GO TO THE DICTRA MONITOR TO SET UP YOUR PROBLEM.
APP: @@
```

```

APP: go d-m
NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ SET THE CONDITION FOR TEMPERATURE
DIC> @@
DIC> set-cond glob t 0 900-time*10; * n
DIC>
DIC> @@
DIC> @@ ENTER A REGION
DIC> @@
DIC> enter-reg pearlite
DIC>
DIC> @@
DIC> @@ ENTER A SMALL INITIAL SIZE OF THE GRID IN THE 'PEARLITE' REGION
DIC> @@
DIC> enter-grid pearlite 5e-10 lin 5
DIC>
DIC> @@
DIC> @@ ENTER INTO THE 'PEARLITE' REGION THE PHASES 'BCC' AND 'CEM' AND SPECIFY
DIC> @@ THAT ARE PRESENT IN THE FORM OF A 'LAMELLAR AGGREGATE'. SET THE STATUS
DIC> @@ TO 'ACTIVE'. SEVERAL PROMPTS FOLLOW ABOUT THE VALUES OF THE PARAMETERS
DIC> @@ IN THE PEARLITE GROWTH MODEL, FOR EXAMPLE AS SURFACE TENSION, OPTIMUM
DIC> @@ GROWTH RATE FACTOR, AND BOUNDARY DIFFUSION COEFFICIENTS.
DIC> @@
DIC> @@ CARBON(C) IS TREATED IN A SPECIAL WAY. IF 'AUTOMATIC' IS ENTERED
DIC> @@ THE DIFFUSION OF C IS CALCULATED ACCORDING TO AN EQUATION FOR
DIC> @@ MIXED BOUNDARY AND VOLUME DIFFUSION. YOU CAN CHOOSE BETWEEN
DIC> @@ MANUAL OR AUTOMATIC START VALUES FOR ALL VARIABLES EXCEPT THE GROWTH
DIC> @@ RATE. IN THIS EXAMPLE WE WILL TRY 1E-6
DIC> @@
DIC> @@ FOR MORE INFORMATION ABOUT THE PEARLITE GROWTH MODEL SEE
DIC> @@ B. JÄ-NSSON: TRITA-MAC-0478, 1992 (ROYAL INSTITUTE OF TECHNOLOGY)
DIC> @@ STOCKHOLM, SWEDEN, 1992.
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /PEARLITE/: pearlite
PHASE TYPE /MATRIX/: lam
    Eutectiod reaction is "GAMMA" ==> "ALPHA" + "BETA"
    Enter name of "ALPHA" phase /BCC_A2/: bcc_a2
    Enter name of "BETA" phase /CEMENTITE/: cementite
    Enter name of "GAMMA" phase /FCC_A1/: fcc_a1
    Enter "ALPHA"/"BETA" surface tension
LOW TIME LIMIT /0/: 0
    Surface tension(T,P,TIME)= 1;
HIGH TIME LIMIT /*/: 1000
ANY MORE RANGES /N/: N
    Enter "ALPHA"/"GAMMA" surface tension
LOW TIME LIMIT /0/: 0
    Surface tension(T,P,TIME)= 1;
HIGH TIME LIMIT /*/: 1000
ANY MORE RANGES /N/: N
    Enter "BETA"/"GAMMA" surface tension
LOW TIME LIMIT /0/: 0
    Surface tension(T,P,TIME)= 1;
HIGH TIME LIMIT /*/: 1000
ANY MORE RANGES /N/: N
    Optimum growth condition factor /2/: 2
    Name of dependent element /FE/: fe
INPUT OF DIFFUSION DATA
    Growth model (VOLUME/BOUNDARY/KIRKALDY) for element C /BOUNDARY/: boundary
    DF(C) = /value/AUTOMATIC/MIXED/: auto
    Growth model (VOLUME/BOUNDARY/KIRKALDY) for element MN /BOUNDARY/: boundary
    DF(MN) = /value/MIXED/: 5.4e-14
    DQ(MN): 155000
Automatic start values for the S0 determination /Y/: Y
Growth rate V: 1E-6
Automatic start values on other variables /Y/: Y
DIC>
DIC> @@
DIC> @@ INITIATE THE COMPOSITION RECORDS FOR THE 'PEARLITE'
DIC> @@
DIC> enter-composition
REGION NAME : /PEARLITE/: pearlite
DIC>
DIC> @@
DIC> @@ NOW CONTINUE BY DEFINING A MATRIX PHASE INTO WHICH THE PEARLITE
DIC> @@ WILL GROW. START BY ENTERING A REGION NAME, 'AUSTENITE'
DIC> @@
DIC> enter-region austenite
ATTACH TO REGION NAMED /PEARLITE/:
ATTACHED TO THE RIGHT OF PEARLITE /YES/:
DIC> @@
DIC> @@ SPECIFY WHAT PHASE 'FCC' WILL BE PRESENT IN THE 'AUSTENITE' REGION
DIC> @@ AND WHAT TYPE OF PHASE 'MATRIX' IT IS AND ITS INITIAL STATE 'ACTIVE'
DIC> @@
DIC> enter-phase act austenite matrix fcc
DIC>
DIC> @@
DIC> @@ WE ALSO NEED TO HAVE A SPATIAL GRID IN THE 'AUSTENITE' REGION.
DIC> @@ CHOSE SIZE '4E-5' GRIDTYPE 'GEOMETRICAL', '30' GRIDPOINTS AND '1.5'
DIC> @@ AS VALUES FOR THE GEOMETRICAL FACTOR OF THE GRID.
DIC> @@
DIC> enter-grid austenite 4e-5 geo 30 1.5
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL CONCENTRATION PROFILES IN THE 'FCC' PHASE OF THE
DIC> @@ 'AUSTENITE' REGION. CONCENTRATIONS MUST BE GIVEN IN Y-FRACTIONS.
DIC> @@
DIC> enter-composition
REGION NAME : /AUSTENITE/: austenite
PHASE NAME : /FCC_A1/: fcc
DEPENDENT COMPONENT ? /MN/: fe
COMPOSITION TYPE /MOLE_FRACTION/: site-fraction
PROFILE FOR MN
TYPE /LINEAR/: lin 9.29232973E-3 9.29232973E-3
PROFILE FOR C

```

```
TYPE /LINEAR/: lin 2.3384332E-2 2.3384332E-2
DIC>
DIC> @@
DIC> @@ THE MATRIX PHASE IS NOW COMPLETE.
DIC> @@
DIC>
DIC> @@
DIC> @@ SPECIFY A SPHERICAL '2' GEOMETRY
DIC> @@
DIC> enter-geo 2
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 5
AUTOMATIC TIMESTEP CONTROL /YES/: YES
MAX TIMESTEP DURING INTEGRATION /.5/: 0.1
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exel Y
DIC>
DIC> set-inter
--OK--
DIC>
```

exe1-run

DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exe1\run.DCM.test"

DIC>

DIC>

DIC> @@ exe1\_run.DCM

DIC>

DIC> @@

DIC> @@ FILE FOR RUNNING EXAMPLE e1

DIC> @@

DIC>

DIC> @@

DIC> @@ ENTER THE DICTRA MONITOR

DIC> @@

DIC> go d-m

TIME STEP AT TIME 0.00000E+00

DIC>

DIC> @@

DIC> @@ READ SETUP FROM FILE

DIC> @@

DIC> read exe1

OK

DIC>

DIC> @@

DIC> @@ START THE SIMULATION

DIC> @@

DIC> simulate

INFO: Default responses (if any) will be applied during the simulation. Use "SIMULATE\_REACTION NO" instead for manual input.

DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE

Trying old scheme 4

U-FRACTION IN SYSTEM: C = .0233843320030518 FE = .990707670399293

MN = .0092923297312127

TOTAL SIZE OF SYSTEM: 2.68092626329E-13 [m^3]

U-FRACTION IN SYSTEM: C = .0233843320030518 FE = .990707670399293

MN = .0092923297312127

TOTAL SIZE OF SYSTEM: 2.68092626329E-13 [m^3]

17 GRIDPOINT(S) ADDED TO CELL #1 REGION: AUSTENITE

TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.0000000

CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.77954874E-05 AND 0.77954874E-05

POSITION OF INTERFACE PEARLITE / AUSTENITE IS 0.50077955E-09

U-FRACTION IN SYSTEM: C = .0233843320030518 FE = .990707670399295

MN = .0092923297312127

TOTAL SIZE OF SYSTEM: 2.68092626329E-13 [m^3]

11 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: AUSTENITE

CPU time used in timestep 1 seconds

4 GRIDPOINT(S) ADDED TO CELL #1 REGION: AUSTENITE

TIME = 0.10010000E-03 DT = 0.10000000E-03 SUM OF SQUARES = 0.0000000

CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.77957281E-05 AND 0.77957281E-05

POSITION OF INTERFACE PEARLITE / AUSTENITE IS 0.12803524E-08

U-FRACTION IN SYSTEM: C = .0233843320030518 FE = .990707670399295

MN = .0092923297312127

TOTAL SIZE OF SYSTEM: 2.68092626329E-13 [m^3]

CPU time used in timestep 1 seconds

3 GRIDPOINT(S) REMOVED FROM CELL# 1 REGION # 1

TIME = 0.28379564E-02 DT = 0.27378564E-02 SUM OF SQUARES = 0.0000000

CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.78023193E-05 AND 0.78023193E-05

POSITION OF INTERFACE PEARLITE / AUSTENITE IS 0.22641982E-07

U-FRACTION IN SYSTEM: C = .0233843320030517 FE = .990707670399294

MN = .0092923297312127

TOTAL SIZE OF SYSTEM: 2.68092626329E-13 [m^3]

CPU time used in timestep 0 seconds

2 GRIDPOINT(S) REMOVED FROM CELL# 1 REGION # 1

TIME = 0.83136692E-02 DT = 0.54757128E-02 SUM OF SQUARES = 0.0000000

CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.78155078E-05 AND 0.78155078E-05

POSITION OF INTERFACE PEARLITE / AUSTENITE IS 0.65437458E-07

U-FRACTION IN SYSTEM: C = .0233843320030517 FE = .990707670399294

MN = .0092923297312127

TOTAL SIZE OF SYSTEM: 2.68092626329E-13 [m^3]

CPU time used in timestep 0 seconds

TIME = 0.19265095E-01 DT = 0.10951426E-01 SUM OF SQUARES = 0.0000000

CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.78419091E-05 AND 0.78419091E-05

POSITION OF INTERFACE PEARLITE / AUSTENITE IS 0.15131754E-06

U-FRACTION IN SYSTEM: C = .0233843320030517 FE = .990707670399294

MN = .00929232973121269

TOTAL SIZE OF SYSTEM: 2.68092626329E-13 [m^3]

CPU time used in timestep 0 seconds

TIME = 0.41167946E-01 DT = 0.21902851E-01 SUM OF SQUARES = 0.0000000

CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.78948085E-05 AND 0.78948085E-05

POSITION OF INTERFACE PEARLITE / AUSTENITE IS 0.32423636E-06

U-FRACTION IN SYSTEM: C = .0233843320030517 FE = .990707670399294

MN = .00929232973121268

TOTAL SIZE OF SYSTEM: 2.68092626329E-13 [m^3]

CPU time used in timestep 1 seconds

TIME = 0.84973649E-01 DT = 0.43805702E-01 SUM OF SQUARES = 0.0000000

CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.80009912E-05 AND 0.80009912E-05

POSITION OF INTERFACE PEARLITE / AUSTENITE IS 0.67472540E-06

U-FRACTION IN SYSTEM: C = .0233843320030516 FE = .990707670399294

MN = .00929232973121268

TOTAL SIZE OF SYSTEM: 2.68092626329E-13 [m^3]

CPU time used in timestep 0 seconds

1 GRIDPOINT(S) REMOVED FROM CELL# 1 REGION # 1

TIME = 0.17258505 DT = 0.87611405E-01 SUM OF SQUARES = 0.0000000

CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.82148663E-05 AND 0.82148663E-05

POSITION OF INTERFACE PEARLITE / AUSTENITE IS 0.13944414E-05

U-FRACTION IN SYSTEM: C = .0233843320030516 FE = .990707670399295

MN = .00929232973121267

TOTAL SIZE OF SYSTEM: 2.68092626329E-13 [m^3]

CPU time used in timestep 0 seconds

TIME = 0.27258505 DT = 0.10000000 SUM OF SQUARES = 0.0000000

CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.84613797E-05 AND 0.84613797E-05

POSITION OF INTERFACE PEARLITE / AUSTENITE IS 0.22405793E-05

U-FRACTION IN SYSTEM: C = .0233843320030516 FE = .990707670399295

MN = .00929232973121268

TOTAL SIZE OF SYSTEM: 2.68092626329E-13 [m^3]

CPU time used in timestep 0 seconds

TIME = 0.37258505 DT = 0.10000000 SUM OF SQUARES = 0.0000000

CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.87103605E-05 AND 0.87103605E-05

POSITION OF INTERFACE PEARLITE / AUSTENITE IS 0.31116154E-05

U-FRACTION IN SYSTEM: C = .0233843320030515 FE = .990707670399295

MN = .00929232973121271

TOTAL SIZE OF SYSTEM: 2.68092626329E-13 [m^3]  
CPU time used in timestep 0 seconds  
1 GRIDPOINT(S) REMOVED FROM CELL# 1 REGION # 1  
TIME = 0.47258505 DT = 0.10000000 SUM OF SQUARES = 0.0000000  
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.89617178E-05 AND 0.89617178E-05  
POSITION OF INTERFACE PEARLITE / AUSTENITE IS 0.40077872E-05  
U-FRACTION IN SYSTEM: C = .0233843320030515 FE = .990707670399294  
MN = .00929232973121283  
TOTAL SIZE OF SYSTEM: 2.68092626329E-13 [m^3]  
CPU time used in timestep 1 seconds  
TIME = 0.57258505 DT = 0.10000000 SUM OF SQUARES = 0.0000000

output ignored...

... output resumed

WORKSPACE RECLAIMED  
INFO: CELL 1 REGION AUSTENITE DELETED  
U-FRACTION IN SYSTEM: C = .0233843320030517 FE = .99070767039931  
MN = .0092923297311968  
TOTAL SIZE OF SYSTEM: 2.68082063572E-13 [m^3]  
U-FRACTION IN SYSTEM: C = .0233843320030517 FE = .99070767039931  
MN = .0092923297311968  
TOTAL SIZE OF SYSTEM: 2.68082063572E-13 [m^3]  
TIME = 3.2742064 DT = 0.1000000E-04 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .0233843320030517 FE = .99070767039931  
MN = .0092923297311968  
TOTAL SIZE OF SYSTEM: 2.68082063572E-13 [m^3]  
CPU time used in timestep 0 seconds  
TIME = 3.2842064 DT = 0.10000000E-01 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .0233843320030517 FE = .99070767039931  
MN = .0092923297311968  
TOTAL SIZE OF SYSTEM: 2.68082063572E-13 [m^3]  
CPU time used in timestep 0 seconds  
TIME = 3.3842064 DT = 0.100000000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .0233843320030517 FE = .99070767039931  
MN = .0092923297311968  
TOTAL SIZE OF SYSTEM: 2.68082063572E-13 [m^3]  
CPU time used in timestep 0 seconds  
TIME = 3.4842064 DT = 0.100000000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .0233843320030517 FE = .99070767039931  
MN = .0092923297311968  
TOTAL SIZE OF SYSTEM: 2.68082063572E-13 [m^3]  
CPU time used in timestep 0 seconds  
TIME = 3.5842064 DT = 0.100000000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .0233843320030517 FE = .99070767039931  
MN = .0092923297311968  
TOTAL SIZE OF SYSTEM: 2.68082063572E-13 [m^3]  
CPU time used in timestep 0 seconds  
TIME = 3.6842064 DT = 0.100000000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .0233843320030517 FE = .99070767039931  
MN = .0092923297311968  
TOTAL SIZE OF SYSTEM: 2.68082063572E-13 [m^3]  
CPU time used in timestep 0 seconds  
TIME = 3.7842064 DT = 0.100000000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .0233843320030517 FE = .99070767039931  
MN = .0092923297311968  
TOTAL SIZE OF SYSTEM: 2.68082063572E-13 [m^3]  
CPU time used in timestep 0 seconds  
TIME = 3.8842064 DT = 0.100000000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .0233843320030517 FE = .99070767039931  
MN = .0092923297311968  
TOTAL SIZE OF SYSTEM: 2.68082063572E-13 [m^3]  
CPU time used in timestep 0 seconds  
TIME = 3.9842064 DT = 0.100000000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .0233843320030517 FE = .99070767039931  
MN = .0092923297311968  
TOTAL SIZE OF SYSTEM: 2.68082063572E-13 [m^3]  
CPU time used in timestep 0 seconds  
TIME = 4.0842064 DT = 0.100000000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .0233843320030517 FE = .99070767039931  
MN = .0092923297311968  
TOTAL SIZE OF SYSTEM: 2.68082063572E-13 [m^3]  
CPU time used in timestep 0 seconds  
TIME = 4.1842064 DT = 0.100000000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .0233843320030517 FE = .99070767039931  
MN = .0092923297311968  
TOTAL SIZE OF SYSTEM: 2.68082063572E-13 [m^3]  
CPU time used in timestep 0 seconds  
TIME = 4.2842064 DT = 0.100000000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .0233843320030517 FE = .99070767039931  
MN = .0092923297311968  
TOTAL SIZE OF SYSTEM: 2.68082063572E-13 [m^3]  
CPU time used in timestep 0 seconds  
TIME = 4.3842064 DT = 0.100000000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .0233843320030517 FE = .99070767039931  
MN = .0092923297311968  
TOTAL SIZE OF SYSTEM: 2.68082063572E-13 [m^3]  
CPU time used in timestep 0 seconds  
TIME = 4.4842064 DT = 0.100000000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .0233843320030517 FE = .99070767039931  
MN = .0092923297311968  
TOTAL SIZE OF SYSTEM: 2.68082063572E-13 [m^3]  
CPU time used in timestep 0 seconds  
TIME = 4.5842064 DT = 0.100000000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .0233843320030517 FE = .99070767039931  
MN = .0092923297311968  
TOTAL SIZE OF SYSTEM: 2.68082063572E-13 [m^3]  
CPU time used in timestep 0 seconds  
TIME = 4.6842064 DT = 0.100000000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .0233843320030517 FE = .99070767039931  
MN = .0092923297311968  
TOTAL SIZE OF SYSTEM: 2.68082063572E-13 [m^3]  
CPU time used in timestep 0 seconds  
TIME = 4.7842064 DT = 0.100000000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .0233843320030517 FE = .99070767039931  
MN = .0092923297311968  
TOTAL SIZE OF SYSTEM: 2.68082063572E-13 [m^3]  
CPU time used in timestep 0 seconds  
TIME = 4.8842064 DT = 0.100000000 SUM OF SQUARES = 0.0000000  
U-FRACTION IN SYSTEM: C = .0233843320030517 FE = .99070767039931  
MN = .0092923297311968  
TOTAL SIZE OF SYSTEM: 2.68082063572E-13 [m^3]

```
CPU time used in timestep          0 seconds
TIME = 4.9842064 DT = 0.100000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0233843320030517 FE = .99070767039931
MN = .0092923297311968
TOTAL SIZE OF SYSTEM: 2.68082063572E-13 [m^3]
CPU time used in timestep          0 seconds
TIME = 5.0000000 DT = 0.15793618E-01 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0233843320030517 FE = .99070767039931
MN = .0092923297311968
TOTAL SIZE OF SYSTEM: 2.68082063572E-13 [m^3]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 3.2725851
DELETING TIME-RECORD FOR TIME 3.2741964
DELETING TIME-RECORD FOR TIME 3.2742064
DELETING TIME-RECORD FOR TIME 3.2842064
DELETING TIME-RECORD FOR TIME 3.3842064
DELETING TIME-RECORD FOR TIME 3.4842064
DELETING TIME-RECORD FOR TIME 3.5842064
DELETING TIME-RECORD FOR TIME 3.6842064
DELETING TIME-RECORD FOR TIME 3.7842064
DELETING TIME-RECORD FOR TIME 3.8842064
DELETING TIME-RECORD FOR TIME 3.9842064
DELETING TIME-RECORD FOR TIME 4.0842064
DELETING TIME-RECORD FOR TIME 4.1842064
DELETING TIME-RECORD FOR TIME 4.2842064
DELETING TIME-RECORD FOR TIME 4.3842064
DELETING TIME-RECORD FOR TIME 4.4842064
DELETING TIME-RECORD FOR TIME 4.5842064
DELETING TIME-RECORD FOR TIME 4.6842064
DELETING TIME-RECORD FOR TIME 4.7842064
DELETING TIME-RECORD FOR TIME 4.8842064

KEEPING TIME-RECORD FOR TIME 4.9842064
AND FOR TIME 5.0000000
WORKSPACE RECLAIMED

TIMESTEP AT 5.0000000 SELECTED
```

```
DIC>
DIC> @@
DIC> @@ THE SIMULATION IS FINISHED
DIC> @@
DIC>
DIC> set-inter
--OK--
DIC>
```

## exe1-plot

DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exe1\plot.DCM.test"

DIC>

DIC>

DIC> @@ exe1\_plot.DCM

DIC>

DIC> @@

DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE e1

DIC> @@

DIC>

DIC> @@

DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE

DIC> @@

DIC> go d-m

TIME STEP AT TIME 5.00000E+00

DIC> read exe1

OK

DIC>

DIC> @@

DIC> @@ GO TO THE POST PROCESSOR

DIC> @@

DIC> post

POST PROCESSOR VERSION 1.7

Implemented by Bjorn Jonsson

POST-1:

POST-1: @@

POST-1: @@ PLOT THE TEMPERATURE AS A FUNCTION OF TIME

POST-1: @@

POST-1: s-d-a x time

INFO: Time is set as independent variable

POST-1: s-d-a y t

POST-1: s-p-c interface first

POST-1:

POST-1:

POST-1: SET\_EXP\_FILE\_FORMAT 3

POST-1: MAKE c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\unite\distribution\macroResult.exp Y

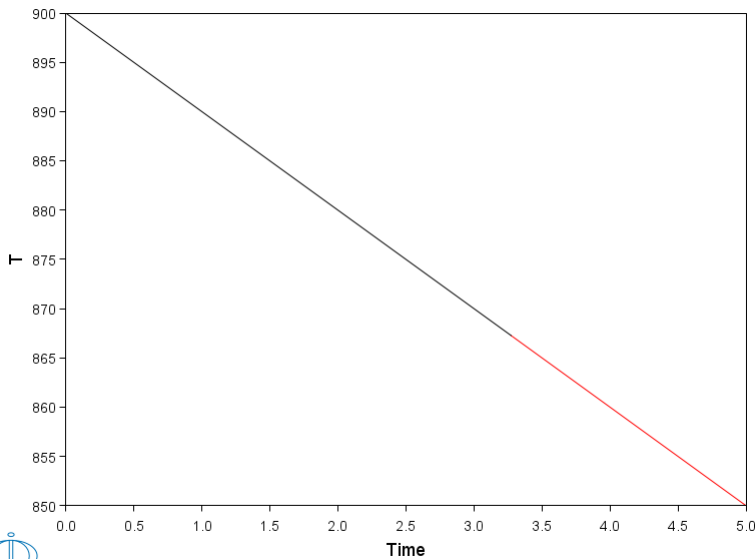
WORKING ...

WORKING ...

OST-1: SET\_EXP\_FILE\_FORMAT 10

POST-1:

POST-1: plot



POST-1:

POST-1:

POST-1:

POST-1:Hit RETURN to continue

POST-1:

POST-1: @@

POST-1: @@ NOW PLOT THE FRACTION OF PEARLITE VS. TIME

POST-1: @@

POST-1: s-d-a y ivv(pearlite)

POST-1:

POST-1:

POST-1: SET\_EXP\_FILE\_FORMAT 3

POST-1: MAKE c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\unite\distribution\macroResult.exp Y

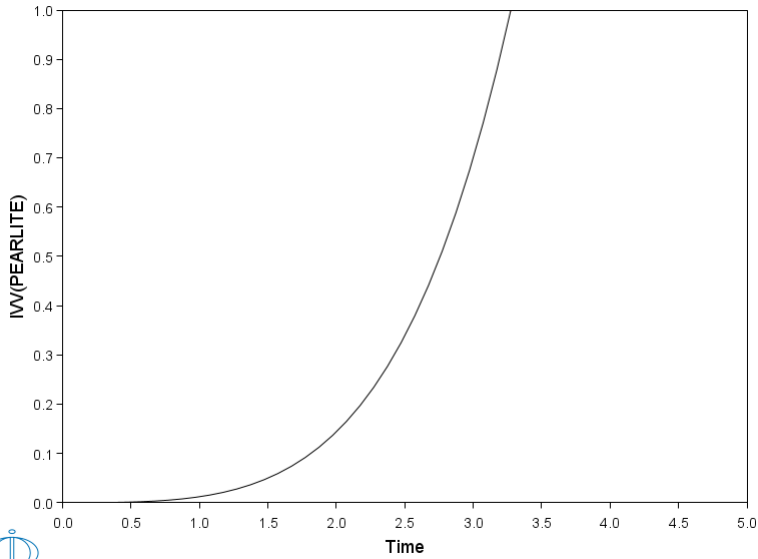
WORKING ...

WORKING ...

OST-1: SET\_EXP\_FILE\_FORMAT 10

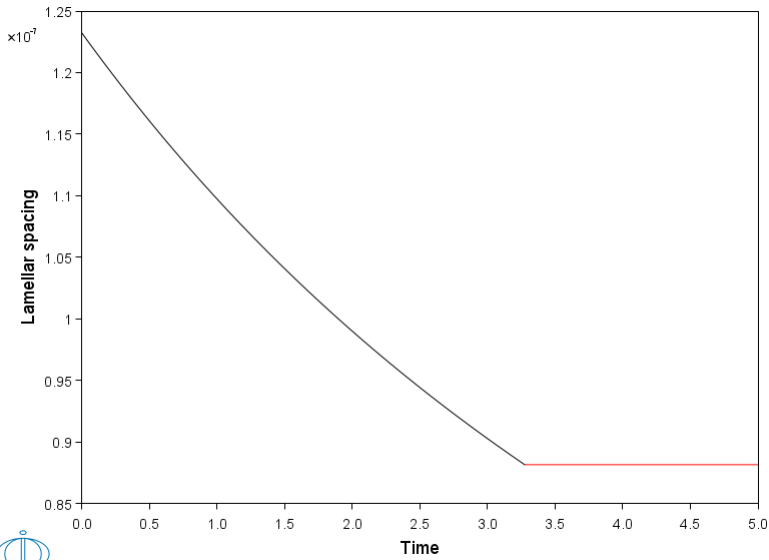
POST-1:

POST-1: plot



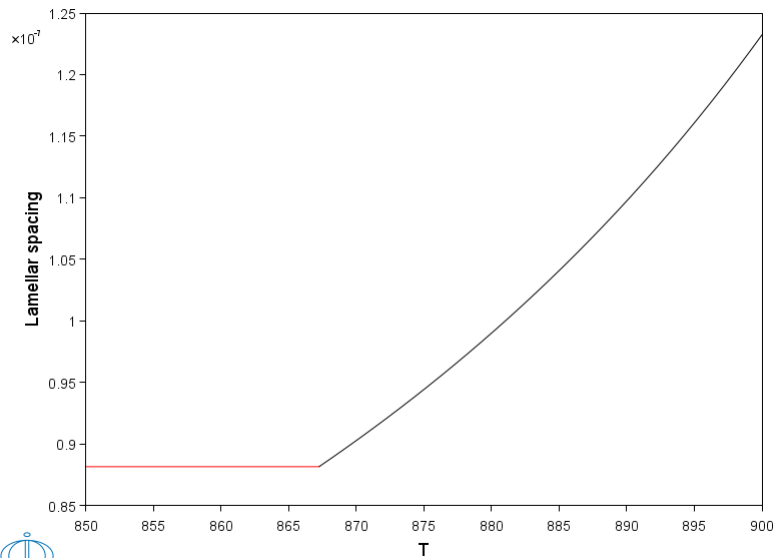
```

POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ PLOT THE LAMELLAR SPACING AS A FUNCTION OF TIME
POST-1: @@
POST-1: s-d-a
AXIS (X, Y OR Z) : y
VARIABLE : lamellar-sp
IN REGION: /*/: pearlite
POST-1:
POST-1: s-p-c
CONDITION /INTEGRAL/: interface
INTERFACE : pearlite
UPPER OR LOWER INTERFACE OF REGION PEARLITE#1 /LOWER/: upper
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 3
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
WORKING ...
WORKING ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
  
```



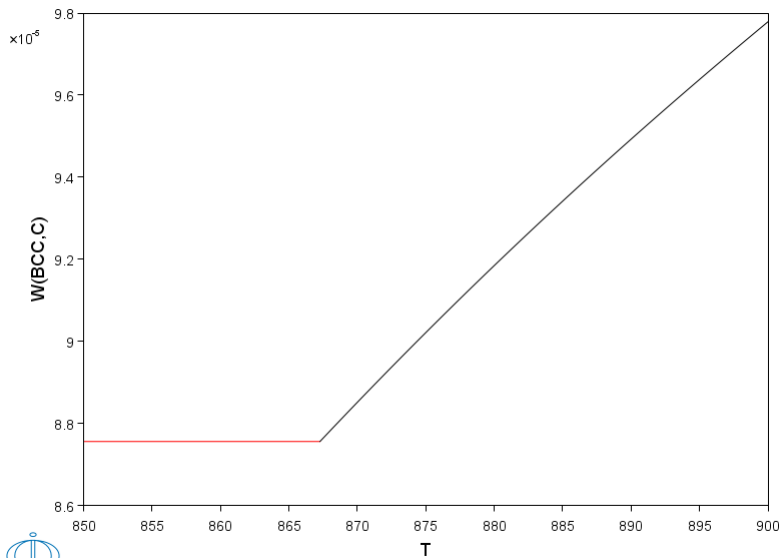
```

POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ LET'S LOOK AT THE LAMELLAR SPACING VS. TEMPERATURE INSTEAD
POST-1: @@
POST-1: s-d-a x t
POST-1:
POST-1: s-p-c interface pearlite upper
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 3
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
WORKING ...
WORKING ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
  
```



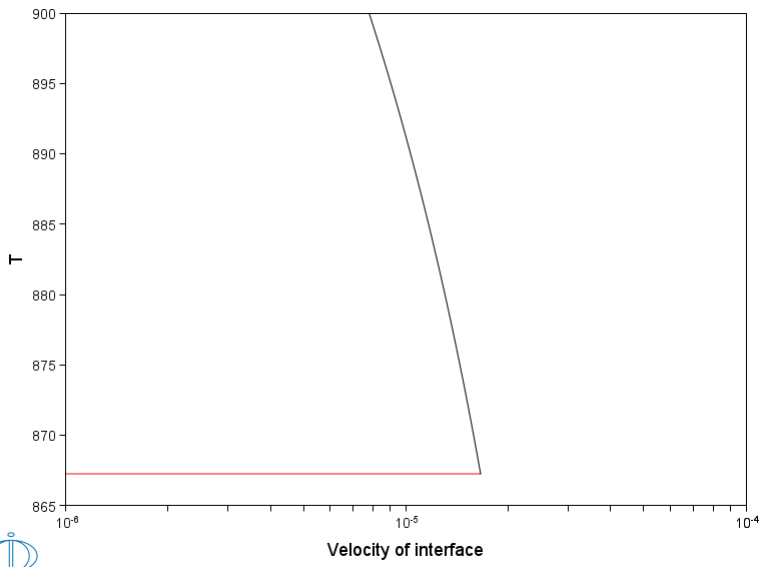
```

POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ AND THE C COMPOSITION IN THE FERRITE VS. TEMP
POST-1: @@
POST-1: s-d-a y w(bcc,c)
POST-1:
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 3
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
WORKING ...
WORKING ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
  
```



```

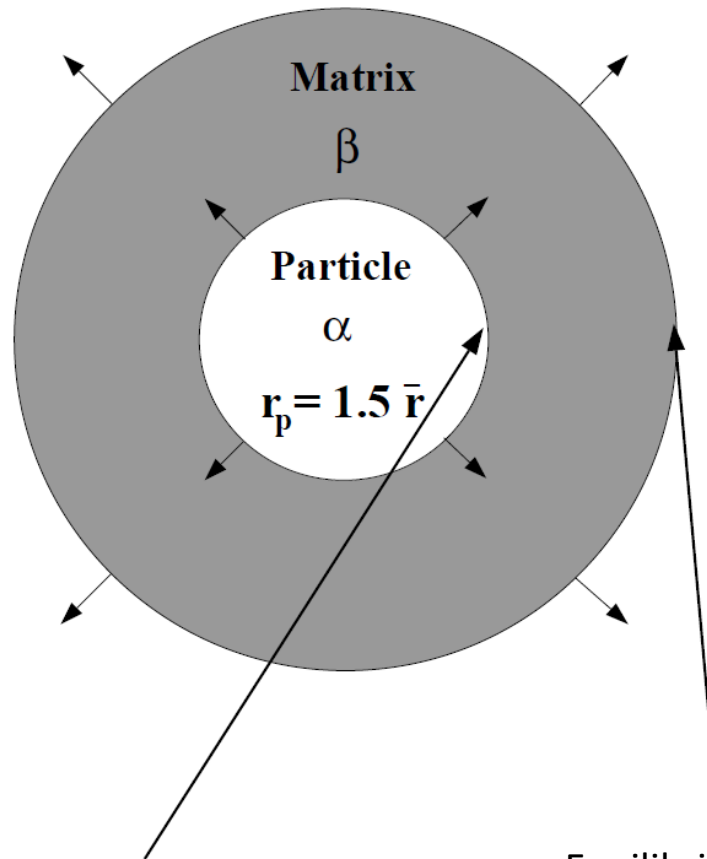
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ FINALLY, LET'S LOOK AT THE VELOCITY OF THE INTERFACE VS. TEMP
POST-1: @@
POST-1: s-d-a y t
POST-1: s-d-a x velocity
INTERFACE : pearlite
UPPER OR LOWER INTERFACE OF REGION PEARLITE#1 /LOWER/: upper
POST-1: set-ax-ty x log
POST-1: s-s-s x n 1e-6 1e-4
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 3
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
WORKING ...
WORKING ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
  
```



```
POST-1:  
POST-1:  
POST-1:  
POST-1:Hit RETURN to continue  
POST-1:  
POST-1:  
POST-1: set-inter  
--OK--  
POST-1:
```



## Coarsening



Moving phase interface  
with  $\alpha$  and  $\beta$  in local  
equilibrium.

$\frac{2\sigma V_m}{r}$  Interfacial energy  
contribution for  $\alpha$  phase

Equilibrium as defined by  
the average composition  
in the system.

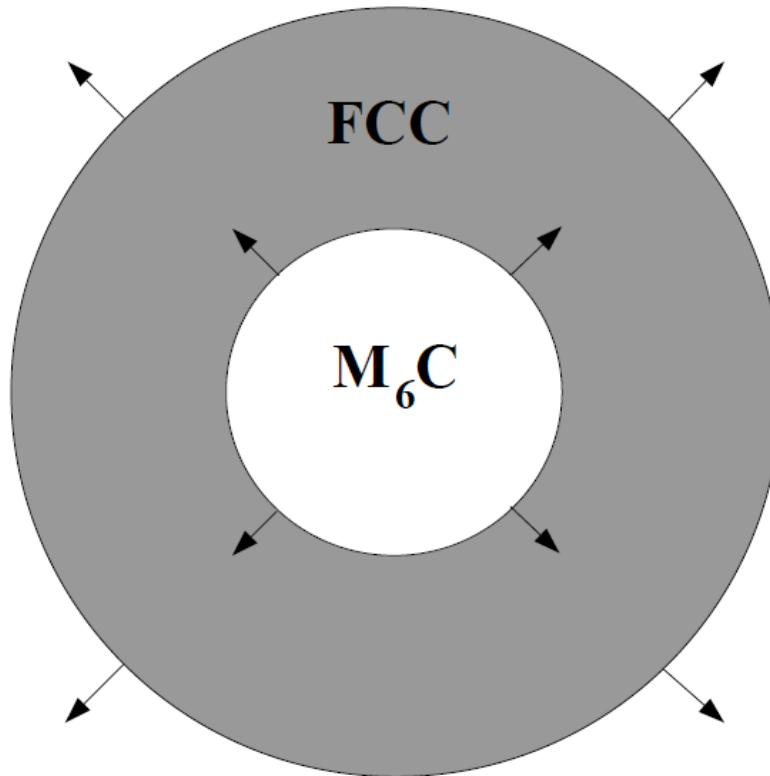
$\frac{2\sigma V_m}{r_p}$  Interfacial energy  
contribution for  $\alpha$  phase



## Example exf1

### Coarsening of an $M_6C$ precipitate in an Fe-Mo-C alloy

This example calculates the Ostwald-ripening of a spherical  $M_6C$  carbide in an austenite matrix.



$$T = 1173K$$

$$r_p = 0.228 \mu m$$

## exfl-setup

### SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,  
Stockholm, Sweden

Software running on Windows 64-bit wordlength  
Compiler: Intel Fortran Compiler 2025.0.0  
License library version: 9.7.0.0036  
Linked: Nov 19 2025 at 14:44:36

```
SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exfl\setup.DCM.test"
```

```
SYS: @@
SYS: @@ Coarsening problem.
SYS: @@ Coarsening of M6C precipitate in an Fe-Mo-C alloy
SYS: @@ This example calculates the Ostwald-ripening of a spherical
SYS: @@ M6C carbide in an austenite matrix.
SYS: @@-----
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASES
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\databases\da
ta
Current database: Steels/Fe-Alloys v12.0

VA                               /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE12: switch TCFE9
Current database: Steels/Fe-Alloys v9.3

VA                               /- DEFINED
L12_FCC                          B2_BCC                          DICTRA_FCC_A1
REJECTED
TDB_TCFE9: def-sys fe mo c
FE                                MO                                C
DEFINED
TDB_TCFE9: rej ph * all
GAS:G                             LIQUID:L                          BCC_A2
FCC_A1                            HCP_A3                            CBCC_A12
CUB_A13                           DIAMOND_FCC_A4                     GRAPHITE
CEMENTITE                          M23C6                              M7C3
M6C                                 M5C2                               M3C2
MC_ETA                             MC_SHP                             KSI_CARBIDE
Z_PHASE                            FE4N_LP1                           FECN_CHI
SIGMA                              MU_PHASE                           P_PHASE
R_PHASE                            CHI_A12                             LAVES_PHASE_C14
AL5FE4 REJECTED
TDB_TCFE9: res ph fcc m6c
FCC_A1                             M6C RESTORED
TDB_TCFE9: get
11:55:56,082 [Thread-0] INFO  JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE MOBILITY DATA
TDB_TCFE9: @@
TDB_TCFE9: app
Use one of these databases

TCFE12 = Steels/Fe-Alloys v12.0
TCFE9  = Steels/Fe-Alloys v9.3
SSUB6  = SGTE Substances v6.0
FEDEMO = Iron Demo Database v6.0
MOB2   = Alloys Mobility v2.7
MOBFE7 = Steels/Fe-Alloys Mobility v7.1
MOBFE4 = Steels/Fe-Alloys Mobility v4.0
MOBFE2 = Steels/Fe-Alloys Mobility v2.0
MFEDMO = Fe-Alloys Mobility demo database v5.0
USER   = User defined Database

DATABASE NAME /TCFE9/: mobfe4
Current database: Steels/Fe-Alloys Mobility v4.0

VA DEFINED
B2_BCC REJECTED
APP: def-sys fe mo c
FE                                MO                                C
DEFINED
APP: rej ph * all
BCC_A2                            CEMENTITE                          FCC_A1
FE4N_LP1                          HCP_A3                              LIQUID:L
REJECTED
APP: res ph fcc m6c
*** ERROR M6C INPUT IGNORED
FCC_A1 RESTORED
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-
APP:
```

```

APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR
APP: @@
APP: go d-m
NO TIME STEP DEFINED
*** ENTERING M6C AS A DIFFUSION NONE PHASE
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> s-cond glob t 0 1173; * N
DIC>
DIC> @@
DIC> @@ ENTER REGIONS part AND aus
DIC> @@
DIC> enter-region
REGION NAME : part
DIC> enter-region aus
ATTACH TO REGION NAMED /PART/:
ATTACHED TO THE RIGHT OF PART /YES/:
DIC> @@
DIC> @@ ENTER GEOMETRICAL GRIDS INTO THE REGIONS
DIC> @@
DIC>
DIC> @@
DIC> @@ THE INITIAL SIZE OF THE CARBIDE PARTICLE IS ASSUMED TO BE KNOWN
DIC> @@ (IN THIS CASE THE VALUE IS FROM NISHIZAWA ET. AL.). THE
DIC> @@ AVERAGE PARTICLE SIZE IS ASSUMED TO BE 0.152E-6 METERS. HOWEVER, THE
DIC> @@ CALCULATIONS ARE PERFORMED ON A MAXIMUM SIZE PARTICLE, WHICH IS ASSUMED
DIC> @@ TO BE 1.5 TIMES THE AVERAGE SIZE. THE SURROUNDING AUSTENITIC MATRIX
DIC> @@ SIZE IS CHOSEN TO MAINTAIN THE AVERAGE COMPOSITION.
DIC> @@
DIC> enter-grid
REGION NAME : /PART/: part
WIDTH OF REGION /1/: 0.228E-6
TYPE /AUTO/: AUTO
DIC>
DIC> enter-grid
REGION NAME : /AUS/: aus
WIDTH OF REGION /1/: 4.53147041E-7
TYPE /AUTO/: AUTO
DIC>
DIC> @@
DIC> @@ ENTER PHASES INTO REGIONS
DIC> @@
DIC> enter-phase active part matrix m6c
DIC>
DIC> enter-phase active aus matrix fcc#1
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITIONS IN THE PHASES
DIC> @@
DIC> enter-composition
REGION NAME : /PART/: part
PHASE NAME: /M6C/: m6c
DEPENDENT COMPONENT ? /MO/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-f
PROFILE FOR /MO/: mo lin 6.20117E-01 6.20117E-01
DIC>
DIC> ent-composition
REGION NAME : /AUS/: aus
PHASE NAME: /FCC_A1/: fcc#1
DEPENDENT COMPONENT ? /MO/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-f
PROFILE FOR /C/: mo lin 1.82099E-02 1.82099E-02
PROFILE FOR /MO/: c lin 2.83351E-03 2.83351E-03
DIC>
DIC>
DIC> @@
DIC> @@ SET A SPHERICAL GEOMETRY
DIC> @@
DIC> ent-geo 2
DIC>
DIC> @@
DIC> @@ ENTER THE SURFACE TENSION ENERGY CONTRIBUTION AS A FUNCTION OF
DIC> @@ THE INTERFACE POSITION (THE RADIUS OF THE PARTICLE).
DIC> @@ ALSO ENTER THE MOLAR VOLUME OF THE PHASE CORRECTED TO BE THE
DIC> @@ MOLAR VOLUME PER SUBSTITUTIONAL ATOM.
DIC> @@
DIC> @@ THE SURFACE TENSION IS 0.7, THE MOLAR VOLUME IS 0.71 AND THE
DIC> @@ TRANSFORMATION TO MOLAR VOLUME PER SUBSTITUTIONAL ATOM IS 7/6.
DIC> @@
DIC> set-surf 2*0.7*0.71*(7/6)/X;
ENTERED FUNCTION :2*.7*.71*7/6/X FOR CELL #1
DIC>
DIC>
DIC> @@
DIC> @@ ENABLE THE SIMPLIFIED MODEL FOR THE COARSENING (OSTWALD-RIPENING)
DIC> @@
DIC> coarse YES
DIC>
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME AND OTHER SIMULATION PARAMETERS
DIC> @@
DIC> set-simulation-time 1E6
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /100000/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exfl Y
DIC>
DIC> set-inter
--OK--

```

exfl-run

DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC-MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exfl\run.DCM.test"

DIC> @@ exfl\_run.DCM

DIC>

DIC> @@

DIC> @@ READ THE SETUP FROM FILE AND START THE SIMULATION

DIC> @@

DIC>

DIC> go d-m

TIME STEP AT TIME 0.00000E+00

\*\*\* ENTERING M6C AS A DIFFUSION NONE PHASE

DIC> read exfl

OK

DIC> sim

INFO: Default responses (if any) will be applied during the simulation. Use "SIMULATE\_REACTION NO" instead for manual input.

Region: PART

geometric 0.833333 dense at 0.228000E-06 58 points

Region: AUS

geometric 1.07691 dense at 0.00000 50 points

DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE

Trying old scheme

GENERATING STARTING VALUES FOR CELL # 1 INTERFACE # 2

DETERMINING INITIAL EQUILIBRIUM VALUES

CALCULATING STARTING VALUES: 9 EQUILIBRIUM CALCULATIONS DONE 6 OUT OF 9

U-FRACTION IN SYSTEM: C = .0190652843033664 FE = .970761291162784

MO = .0292387089677228

TOTAL SIZE OF SYSTEM: 1.32376603026E-18 [m^3]

U-FRACTION IN SYSTEM: C = .0190652843033664 FE = .970761291162784

MO = .0292387089677228

TOTAL SIZE OF SYSTEM: 1.32376603026E-18 [m^3]

0.610221288327387 0.610389365807388 0.610221228974406 2.564831197908535E-002

0.1277067173609035E-004 1.110179678784779E-003 1.288571314577660E-004 5.087173160806686E-

0.1902418902601689E-009 2.197612096648792E-009 3.389027474958636E-009 1.612546345243502E-

0.1467797643373012E-009 1.198076639424611E-009 3.893970602319582E-009 7.387100278506106E-

0.1480396199523241E-010 5.533841114156213E-014 2.946908552531375E-019 TIME = 0.10000000E-06 DT = 0.10000000E-

06 SUM OF SQUARES = 0.25862773E-18

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.55596623E-05 AND -0.55596623E-05

POSITION OF INTERFACE PART / AUS IS 0.22799944E-06

U-FRACTION IN SYSTEM: C = .0190660674474617 FE = .970759033395948

MO = .0292409667345599

TOTAL SIZE OF SYSTEM: 1.32375634647E-18 [m^3]

CPU time used in timestep 2 seconds

7.336609395702361E-005 7.338112766796937E-005 7.335957986077687E-005 2.670017337733632E-007 6.229897846113647E-

012 5.809106788242061E-018 SWITCHING ACTIVITIES FOR INTERFACE #2, CELL #1

FROM: C TO: MO

TIME = 0.30749847E-05 DT = 0.29749847E-05 SUM OF SQUARES = 0.58069418E-17

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.36288005E-08 AND -0.36288005E-08

POSITION OF INTERFACE PART / AUS IS 0.22799943E-06

U-FRACTION IN SYSTEM: C = .0190666386348136 FE = .970759027533689

MO = .0292409725968181

TOTAL SIZE OF SYSTEM: 1.32375615844E-18 [m^3]

CPU time used in timestep 1 seconds

2.185695935725712E-008 2.186215702306940E-008 2.172147907502082E-008 1.720547891277043E-008 1.693387714353585E-

0.1641226441241974E-008 1.534483978746597E-008 1.534396904060139E-008 1.336039376009682E-

0.769677426896860E-009 4.289657206738150E-009 5.954565828722822E-017 TIME = 0.90249540E-05 DT = 0.59499693E-

05 SUM OF SQUARES = 0.56030240E-16

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.51121791E-09 AND -0.51121791E-09

POSITION OF INTERFACE PART / AUS IS 0.22799943E-06

U-FRACTION IN SYSTEM: C = .0190673192325636 FE = .970759026939536

MO = .0292409731909705

TOTAL SIZE OF SYSTEM: 1.32375610546E-18 [m^3]

CPU time used in timestep 0 seconds

3.601337570877803E-010 3.602091327258309E-010 3.672599051884091E-010 3.345891508837517E-010 3.339467367055687E-

0.326641619246723E-010 3.300915214299178E-010 3.304658819517889E-010 3.249906224476215E-

0.148938676185336E-010 2.951917189226764E-010 2.957352342338880E-010 2.576845607481219E-

0.1903221382053056E-010 8.615110006894059E-011 8.655671033214816E-011 6.450748759292848E-

0.3067095562661328E-024 TIME = 0.20924893E-04 DT = 0.11899939E-04 SUM OF SQUARES = 0.30255168E-23

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.10405533E-09 AND -0.10405533E-09

POSITION OF INTERFACE PART / AUS IS 0.22799943E-06

U-FRACTION IN SYSTEM: C = .0190682117489446 FE = .970759027552711

MO = .0292409725777964

TOTAL SIZE OF SYSTEM: 1.32375608389E-18 [m^3]

CPU time used in timestep 1 seconds

1.729121848651809E-011 1.729401856378472E-011 1.960792127235298E-011 1.202596976194040E-011

output ignored...

... output resumed

2.982907503705085E-011 3.070100906912093E-011 3.506346397923557E-011 5.477200960854970E-013 3.033021441276810E-

021 TIME = 602219.69 DT = 100000.00 SUM OF SQUARES = 0.30060556E-20

CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.22957235E-13 AND 0.22957235E-13

POSITION OF INTERFACE PART / AUS IS 0.24250043E-06

U-FRACTION IN SYSTEM: C = .0195537038826586 FE = .970691149042916

MO = .0293088510875911

TOTAL SIZE OF SYSTEM: 1.59273758793E-18 [m^3]

27 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: PART

26 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: AUS

CPU time used in timestep 0 seconds

1.412413308027950E-011 1.460649001349409E-011 1.765314931007403E-011 1.164458062680449E-012 2.808415536120668E-

013 2.617491004750589E-022 TIME = 702219.69 DT = 100000.00 SUM OF SQUARES = 0.16604447E-21

CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.22527562E-13 AND 0.22527562E-13

POSITION OF INTERFACE PART / AUS IS 0.24475319E-06

U-FRACTION IN SYSTEM: C = .0195562807190153 FE = .970693005116594

MO = .0293069950139138

TOTAL SIZE OF SYSTEM: 1.63753938042E-18 [m^3]

26 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: PART

26 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: AUS

CPU time used in timestep 1 seconds

6.794236263390057E-012 6.975596047060683E-012 9.014730015688252E-012 1.950630360650007E-012 1.138878651285509E-

012 1.211029582666416E-013 4.023363645261999E-

023 TIME = 802219.69 DT = 100000.00 SUM OF SQUARES = 0.22394910E-24

CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.22117446E-13 AND 0.22117446E-13

POSITION OF INTERFACE PART / AUS IS 0.24696493E-06

U-FRACTION IN SYSTEM: C = .0195587789271634 FE = .970694791840553

MO = .0293052082899544

TOTAL SIZE OF SYSTEM: 1.68233528236E-18 [m^3]

25 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: PART  
25 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: AUS

CPU time used in timestep 0 seconds  
4.233431109250027E-012 4.186413591946464E-012 5.474903643955341E-012 2.862043336936544E-012 2.318953080738556E-012  
012 1.318033326884503E-012 1.432733061627653E-013 9.446084666324366E-023  
023 TIME = 902219.69 DT = 100000.00 SUM OF SQUARES = 0.42337303E-22  
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.21725491E-13 AND 0.21725491E-13  
POSITION OF INTERFACE PART / AUS IS 0.24913748E-06  
U-FRACTION IN SYSTEM: C = .0195612044532944 FE = .970696534228341  
MO = .0293034659021655  
TOTAL SIZE OF SYSTEM: 1.72712548288E-18 [m^3]  
25 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: PART  
25 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: AUS

CPU time used in timestep 0 seconds  
4.669176704370716E-012 4.334721962902462E-012 4.662041474632528E-012 4.229634314006473E-012 3.695912589217737E-012  
012 2.667649539940000E-012 1.007430824352458E-012 7.827563365531985E-023  
022 TIME = 1000000.0 DT = 97780.306 SUM OF SQUARES = 0.34467205E-22  
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.21354620E-13 AND 0.21354620E-13  
POSITION OF INTERFACE PART / AUS IS 0.25122554E-06  
U-FRACTION IN SYSTEM: C = .0195635706991602 FE = .970698209337135  
MO = .0293017907933725  
TOTAL SIZE OF SYSTEM: 1.77091640814E-18 [m^3]

MUST SAVE WORKSPACE ON FILE  
WORKSPACE SAVED ON FILE  
RECLAIMING WORKSPACE

DELETING TIME-RECORD FOR TIME 0.0000000  
DELETING TIME-RECORD FOR TIME 0.10000000E-06  
DELETING TIME-RECORD FOR TIME 0.30749847E-05  
DELETING TIME-RECORD FOR TIME 0.90249540E-05  
DELETING TIME-RECORD FOR TIME 0.20924893E-04  
DELETING TIME-RECORD FOR TIME 0.44724770E-04  
DELETING TIME-RECORD FOR TIME 0.92324524E-04  
DELETING TIME-RECORD FOR TIME 0.18752403E-03  
DELETING TIME-RECORD FOR TIME 0.37792305E-03  
DELETING TIME-RECORD FOR TIME 0.75872109E-03  
DELETING TIME-RECORD FOR TIME 0.15203172E-02  
DELETING TIME-RECORD FOR TIME 0.30435093E-02  
DELETING TIME-RECORD FOR TIME 0.60898936E-02  
DELETING TIME-RECORD FOR TIME 0.12182662E-01  
DELETING TIME-RECORD FOR TIME 0.24368199E-01  
DELETING TIME-RECORD FOR TIME 0.48739274E-01  
DELETING TIME-RECORD FOR TIME 0.97481422E-01  
DELETING TIME-RECORD FOR TIME 0.19496572  
DELETING TIME-RECORD FOR TIME 0.38993431  
DELETING TIME-RECORD FOR TIME 0.77987150  
DELETING TIME-RECORD FOR TIME 1.5597459  
DELETING TIME-RECORD FOR TIME 3.1194946  
DELETING TIME-RECORD FOR TIME 6.2389921  
DELETING TIME-RECORD FOR TIME 12.477987  
DELETING TIME-RECORD FOR TIME 24.955977  
DELETING TIME-RECORD FOR TIME 49.911957  
DELETING TIME-RECORD FOR TIME 99.823917  
DELETING TIME-RECORD FOR TIME 199.64784  
DELETING TIME-RECORD FOR TIME 399.29568  
DELETING TIME-RECORD FOR TIME 798.59136  
DELETING TIME-RECORD FOR TIME 1597.1827  
DELETING TIME-RECORD FOR TIME 3194.3654  
DELETING TIME-RECORD FOR TIME 6388.7309  
DELETING TIME-RECORD FOR TIME 12777.462  
DELETING TIME-RECORD FOR TIME 25554.924  
DELETING TIME-RECORD FOR TIME 51109.847  
DELETING TIME-RECORD FOR TIME 102219.69  
DELETING TIME-RECORD FOR TIME 202219.69  
DELETING TIME-RECORD FOR TIME 302219.69  
DELETING TIME-RECORD FOR TIME 402219.69  
DELETING TIME-RECORD FOR TIME 502219.69  
DELETING TIME-RECORD FOR TIME 602219.69  
DELETING TIME-RECORD FOR TIME 702219.69  
DELETING TIME-RECORD FOR TIME 802219.69

KEEPING TIME-RECORD FOR TIME 902219.69  
AND FOR TIME 1000000.0  
WORKSPACE RECLAIMED

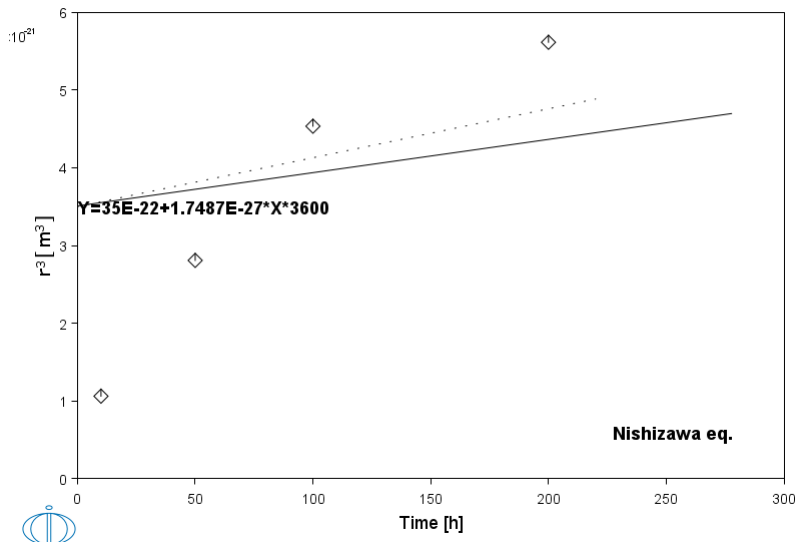
TIMESTEP AT 100000.00 SELECTED

DIC>  
DIC>  
DIC> set-inter  
--OK--  
DIC>

## exfl-plot

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exfl\plot.DCM.test"
DIC> @@ exfl_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE f1
DIC> @@
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 1.00000E+06
*** ENTERING M6C AS A DIFFUSION NONE PHASE
DIC> read exfl
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1: @@
POST-1: @@ PLOT THE AVERAGE PARTICLE SIZE (CUBED) AS THIS ASSUMED TO
POST-1: @@ SCALE LINEARLY WITH TIME. THEN A FUNCTION IS ENTERED SO
POST-1: @@ THIS QUANTITY CAN BE ACCESSED. WE ALSO WANT TO PLOT THIS
POST-1: @@ QUANTITY VERSUS TIME (IN HOURS) SO A FUNCTION IS ENTERED.
POST-1: @@
POST-1: enter-symbol func rr3=(poi(part,u)/1.5)**3;
POST-1: enter-symbol func hours=time/3600;
POST-1: s-d-a x hours
POST-1: s-d-a y rr3
POST-1:
POST-1: @@
POST-1: @@ AS WE ARE PLOTTING FUNCTIONS ON BOTH AXES WE MUST EXPLICITLY
POST-1: @@ DEFINE THE INDEPENDENT VARIABLE AND THE PLOT CONDITION
POST-1: @@
POST-1: s-ind time
POST-1: s-p-c inter
INTERFACE : part upper
POST-1:
POST-1:
POST-1: set-axis-text-status x n
AXIS TEXT : Time [h]
POST-1:
POST-1: @@
POST-1: @@ WHEN THIS IS PLOTTED, THIS AXIS TEXT NOTATION WORKS WELL FOR
POST-1: @@ THE AVERAGE RADIUS CUBED. FOR MORE INFORMATION ABOUT HOW TO
POST-1: @@ ADJUST TEXT IN THE POST PROCESSOR USING THE DATAPLOT LANGUAGE,
POST-1: @@ SEARCH THE ONLINE HELP (FROM THE MAIN MENU -> HELP > ONLINE HELP)
POST-1:
POST-1:
POST-1: set-axis-text-status y n
AXIS TEXT : \latex r^3\, [m^3]
POST-1:
POST-1:
POST-1: @@
POST-1: @@ COMPARE WITH EXPERIMENTAL DATA FROM NISHIZAWA ET AL.
POST-1: @@ TRANS. JPN. INST. MET. VOL. 22 1981 PP. 733-742.
POST-1: @@
POST-1:
POST-1: app y exfl.exp
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 1
POST-1:
POST-1: s-s-s y n 0 6e-21
POST-1:
POST-1: @@
POST-1: @@ SET A TITLE ON THE PLOT
POST-1: @@
POST-1: set-title Figure f1.1
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

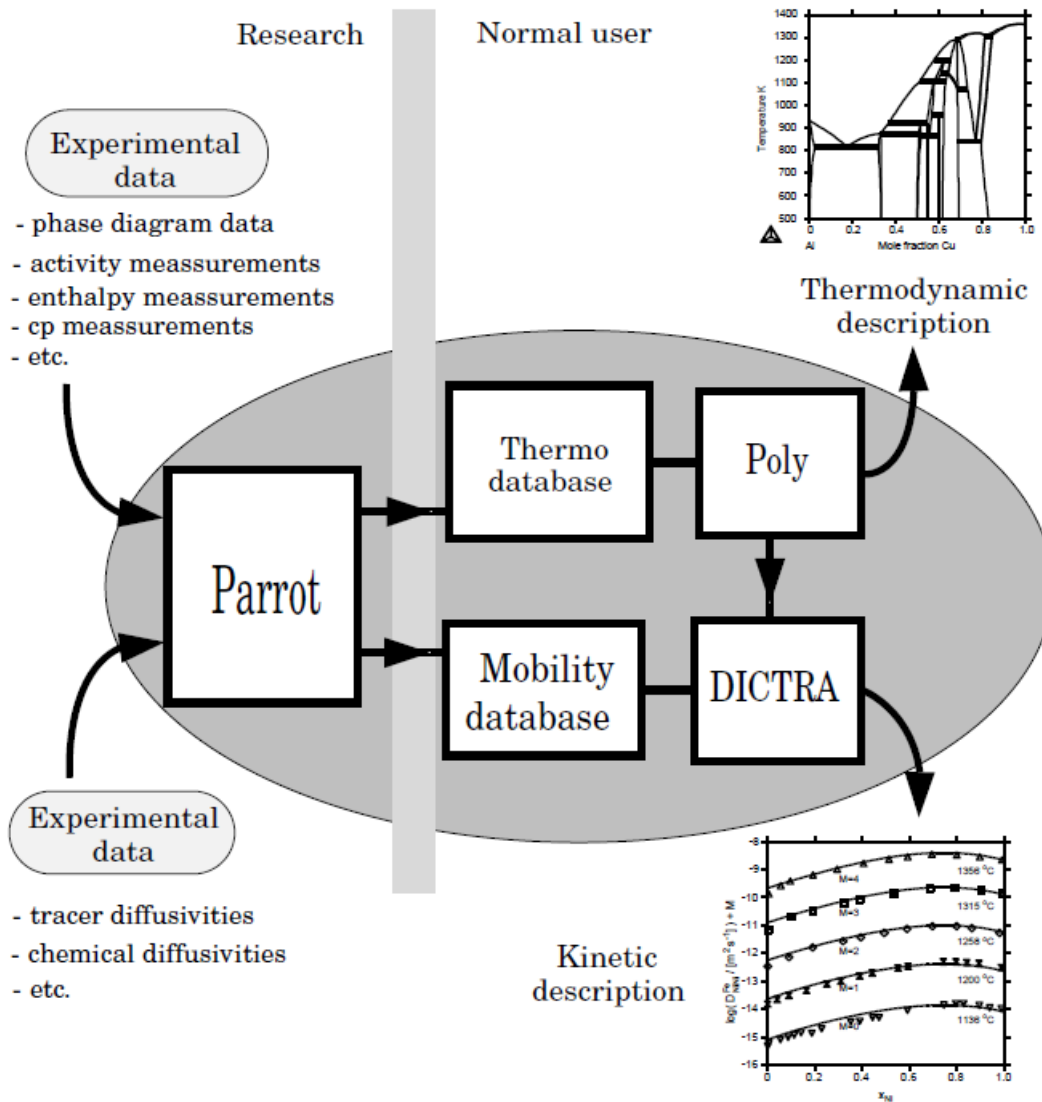
Figure f1.1



```
POST-1:
POST-1:??<_hit_return_to_continue_>
POST-1: @@
POST-1: @@ THE DIFFERENCE BETWEEN THE CALCULATION AND THE EQUATION USED BY
POST-1: @@ NISHIZAWA ET AL. IS MAINLY DUE TO DIFFERENT THERMODYNAMIC
POST-1: @@ DESCRIPTIONS AND DIFFUSIVITIES.
POST-1: @@
POST-1:
POST-1: set-inter
--OK--
POST-1:
```



## Kinetic Data

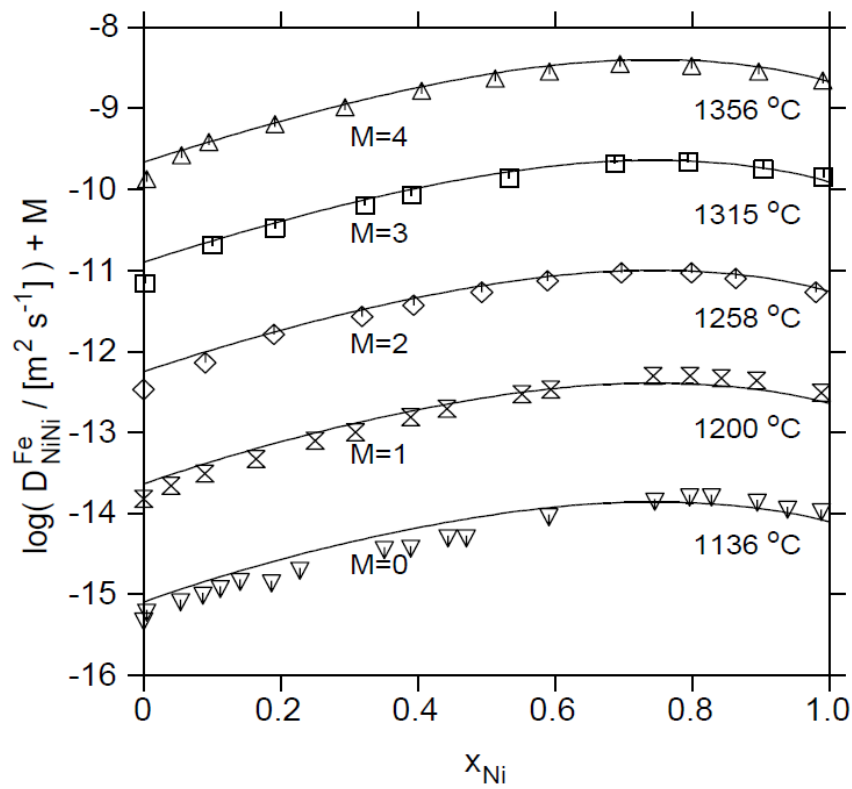




## Example exg1

### Checking diffusivities in an Fe-Ni alloy

This is an example file to check the mobilities and diffusivities in an Fe-Ni alloy.



## exg1-setup

### SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,  
Stockholm, Sweden

Software running on Windows 64-bit wordlength  
Compiler: Intel Fortran Compiler 2025.0.0  
License library version: 9.7.0.0036  
Linked: Nov 19 2025 at 14:44:36

```
SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exg1\setup.DCM.test"
```

```
SYS: @@
SYS: @@ Kinetic data example.
SYS: @@ Checking mobilities and diffusivities in an Fe-Ni alloy
SYS: @@ This is an example file to check the mobilities and diffusivities
SYS: @@ in an Fe-Ni alloy.
SYS: @@-----
SYS:
SYS: @@ exg1_setup.DCM
SYS:
SYS: @@
SYS: @@ START BY GOING TO THE DATABASE MODULE
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\databases\da
ta
Current database: Steels/Fe-Alloys v12.0

VA          /-  DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE12:
TDB_TCFE12: @@
TDB_TCFE12: @@ SELECT A DATABASE FOR THERMODYNAMIC DATA
TDB_TCFE12: @@
TDB_TCFE12: sw fedemo
Current database: Iron Demo Database v6.0

VA          /-  DEFINED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ DEFINE THE SYSTEM TO WORK WITH
TDB_FEDEMO: @@
TDB_FEDEMO: def-sys fe ni
FE          NI  DEFINED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ EXCLUDE THE THERMODYNAMIC DATA FOR THE PHASES THAT ARE NOT NEEDED
TDB_FEDEMO: @@
TDB_FEDEMO: rej ph * all
GAS:G      LIQUID:L      BCC_A2
C14_LAVES  CBCC_A12     CUB_A13
FCC_A1     HCP_A3 REJECTED
TDB_FEDEMO: res ph fcc
FCC_A1 RESTORED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ RETRIEVE DATA FROM THE DATABASE FILE
TDB_FEDEMO: @@
TDB_FEDEMO: get
11:59:11,448 [Thread-0] INFO  JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ MOBILITY/DIFFUSIVITY DATA ARE STORED IN A SEPARATE DATABASE FILE.
TDB_FEDEMO: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE DATA
TDB_FEDEMO: @@
TDB_FEDEMO: app
Use one of these databases

TCFE12 = Steels/Fe-Alloys v12.0
TCFE9  = Steels/Fe-Alloys v9.3
SSUB6  = SGTE Substances v6.0
FEDEMO = Iron Demo Database v6.0
MOB2   = Alloys Mobility v2.7
MOBFE7 = Steels/Fe-Alloys Mobility v7.1
MOBFE4 = Steels/Fe-Alloys Mobility v4.0
MOBFE2 = Steels/Fe-Alloys Mobility v2.0
MFEDEMO = Fe-Alloys Mobility demo database v5.0
USER    = User defined Database

DATABASE NAME /FEDEMO/: mfedemo
Current database: Fe-Alloys Mobility demo database v5.0

VA  DEFINED
APP: def-sys fe ni
FE          NI  DEFINED
APP: rej ph * all
BCC_A2     FCC_A1      LIQUID:L
REJECTED
APP: res ph fcc
FCC_A1 RESTORED
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
```

PARAMETERS ...  
FUNCTIONS ....

Use the command LIST\_REFERENCES to see the list of references for assessed data

-OK-

```
APP: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP
APP: @@
APP: go d-m
      NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ CHECK THE DIFFUSIVITIES
DIC> @@
DIC> check-diffusion-matrix
OUTPUT TO SCREEN OR FILE /SCREEN/:
PHASE NAME : fcc
DEPENDENT COMPONENT ? /NI/: fe
CONCENTRATION OF NI IN U-FRACTION /1/: 0.3
Pressure /100000/: 101325
Temperature /298.15/: 1409
OPTION ( dipbm0ez or * ) /D/: dl

Dkj (reduced n=FE)      [m2/s]
k / j NI
NI      +4.8614E-15

L0kj      [(mole m2)/(J s)]
k / j FE      NI
FE      +3.7712E-19
NI      +1.0011E-19

DIC>
DIC>
DIC>@?<Hit_return_to_continue>
DIC>
DIC> @@
DIC> @@ USE STEPPING IN POLY-3 TO CALCULATE THE DIFFUSIVITIES VS. COMPOSITION
DIC> @@
DIC> go p-3
POLY: s-c t=1409,p=101325,n=1,x(ni)=0.3
POLY: c-e
      Using global minimization procedure
      Calculated      209 grid points in      0.024 s
      Found the set of lowest grid points in      0.001 s
      Calculated solution in      0.029 s using 2 iterations. Total time      0.054 s
POLY:
POLY: s-a-v
Axis number: /1/: 1
Condition /NONE/: x(ni)
Min value /0/: 0
Max value /1/: 1
Increment /.025/: 1e-3
POLY:
POLY: step
Option? /NORMAL/: normal
      No initial equilibrium, using default
      Step will start from axis value      0.300000
...OK

Phase Region from      0.300000      for:
      FCC_A1
Global test at      3.08000E-01      .... OK
Global test at      3.18000E-01      .... OK
Global test at      3.28000E-01      .... OK
Global test at      3.38000E-01      .... OK
Global test at      3.48000E-01      .... OK
Global test at      3.58000E-01      .... OK
Global test at      3.68000E-01      .... OK
Global test at      3.78000E-01      .... OK
Global test at      3.88000E-01      .... OK
Global test at      3.98000E-01      .... OK
Global test at      4.08000E-01      .... OK
Global test at      4.18000E-01      .... OK
Global test at      4.28000E-01      .... OK
Global test at      4.38000E-01      .... OK
Global test at      4.48000E-01      .... OK
Global test at      4.58000E-01      .... OK
Global test at      4.68000E-01      .... OK
Global test at      4.78000E-01      .... OK
Global test at      4.88000E-01      .... OK
Global test at      4.98000E-01      .... OK
Global test at      5.08000E-01      .... OK
Global test at      5.18000E-01      .... OK
Global test at      5.28000E-01      .... OK
Global test at      5.38000E-01      .... OK
Global test at      5.48000E-01      .... OK
Global test at      5.58000E-01      .... OK
Global test at      5.68000E-01      .... OK
Global test at      5.78000E-01      .... OK
Global test at      5.88000E-01      .... OK
Global test at      5.98000E-01      .... OK
Global test at      6.08000E-01      .... OK
Global test at      6.18000E-01      .... OK
Global test at      6.28000E-01      .... OK
Global test at      6.38000E-01      .... OK
Global test at      6.48000E-01      .... OK
Global test at      6.58000E-01      .... OK
Global test at      6.68000E-01      .... OK
Global test at      6.78000E-01      .... OK
Global test at      6.88000E-01      .... OK
Global test at      6.98000E-01      .... OK
Global test at      7.08000E-01      .... OK
Global test at      7.18000E-01      .... OK
Global test at      7.28000E-01      .... OK
Global test at      7.38000E-01      .... OK
Global test at      7.48000E-01      .... OK
Global test at      7.58000E-01      .... OK
Global test at      7.68000E-01      .... OK
Global test at      7.78000E-01      .... OK
Global test at      7.88000E-01      .... OK
```

```

Global test at 7.98000E-01 .... OK
Global test at 8.08000E-01 .... OK
Global test at 8.18000E-01 .... OK
Global test at 8.28000E-01 .... OK
Global test at 8.38000E-01 .... OK
Global test at 8.48000E-01 .... OK
Global test at 8.58000E-01 .... OK
Global test at 8.68000E-01 .... OK
Global test at 8.78000E-01 .... OK
Global test at 8.88000E-01 .... OK
Global test at 8.98000E-01 .... OK
Global test at 9.08000E-01 .... OK
Global test at 9.18000E-01 .... OK
Global test at 9.28000E-01 .... OK
Global test at 9.38000E-01 .... OK
Global test at 9.48000E-01 .... OK
Global test at 9.58000E-01 .... OK
Global test at 9.68000E-01 .... OK
Global test at 9.78000E-01 .... OK
Global test at 9.88000E-01 .... OK
Global test at 9.98000E-01 .... OK
Terminating at 1.00000
Calculated 703 equilibria

```

```

Phase Region from 0.300000 for:
FCC_A1

```

```

Global test at 2.92000E-01 .... OK
Global test at 2.82000E-01 .... OK
Global test at 2.72000E-01 .... OK
Global test at 2.62000E-01 .... OK
Global test at 2.52000E-01 .... OK
Global test at 2.42000E-01 .... OK
Global test at 2.32000E-01 .... OK
Global test at 2.22000E-01 .... OK
Global test at 2.12000E-01 .... OK
Global test at 2.02000E-01 .... OK
Global test at 1.92000E-01 .... OK
Global test at 1.82000E-01 .... OK
Global test at 1.72000E-01 .... OK
Global test at 1.62000E-01 .... OK
Global test at 1.52000E-01 .... OK
Global test at 1.42000E-01 .... OK
Global test at 1.32000E-01 .... OK
Global test at 1.22000E-01 .... OK
Global test at 1.12000E-01 .... OK
Global test at 1.02000E-01 .... OK
Global test at 9.20000E-02 .... OK
Global test at 8.20000E-02 .... OK
Global test at 7.20000E-02 .... OK
Global test at 6.20000E-02 .... OK
Global test at 5.20000E-02 .... OK
Global test at 4.20000E-02 .... OK
Global test at 3.20000E-02 .... OK
Global test at 2.20000E-02 .... OK
Global test at 1.20000E-02 .... OK
Global test at 2.00000E-03 .... OK
Terminating at 0.10000E-11
Calculated 303 equilibria

```

```

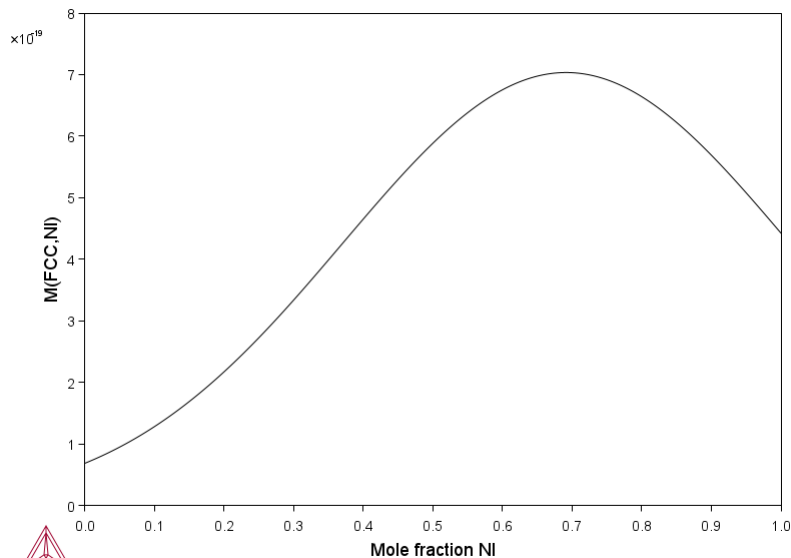
*** Buffer saved on file: C:\Users\azureuser\AppData\Local\Temp\RESULT_002.POLY3

```

```

POLY:
POLY: @@
POLY: @@ ENTER THE POST PROCESSOR AND PLOT THE RESULT
POLY: @@
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2
POST:
POST:
POST:
POST: @@
POST: @@ PLOT THE MOBILITY OF Ni VS. X(Ni)
POST: @@
POST: s-d-a y m(fcc,ni)
POST: s-d-a x m-f ni
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot

```

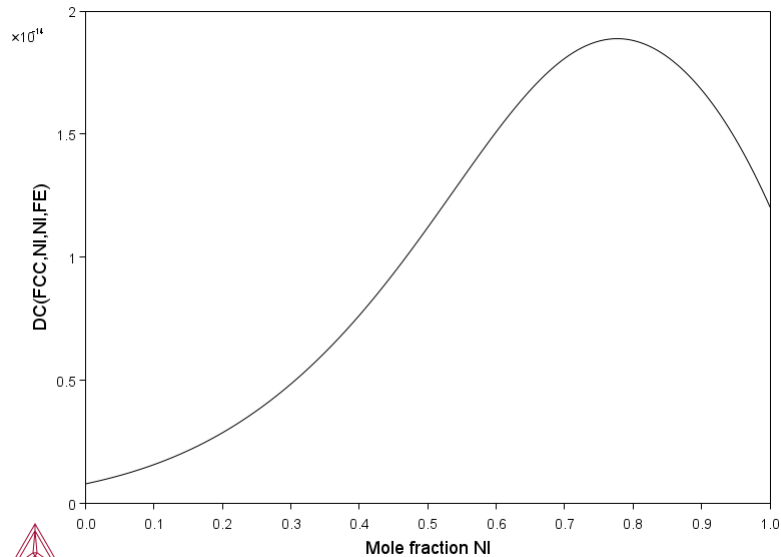


POST:

```

POST:
POST:
POST:@?<Hit_return_to_continue>
POST:
POST: @@
POST: @@ THEN PLOT THE DIFFUSIVITY OF Ni VS. X(Ni)
POST: @@
POST: s-d-a y dc(fcc,ni,ni,fe)
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot

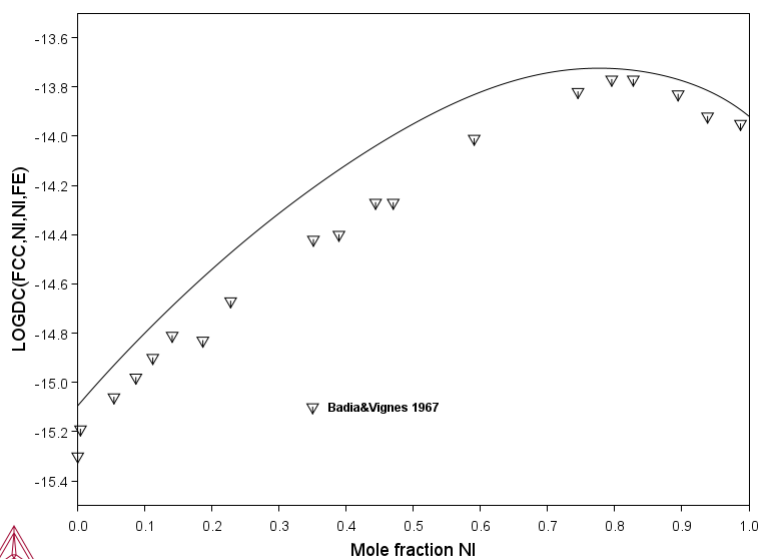
```



```

POST:
POST:
POST:@?<Hit_return_to_continue>
POST:
POST: @@
POST: @@ PLOT THE LOGARITHM OF DC AND APPEND THE EXPERIMENTAL DATA
POST: @@
POST: s-d-a y logdc(fcc,ni,ni,fe)
POST:
POST: app y feni.exp
PROLOGUE NUMBER: /0/: 1
DATASET NUMBER(s): /-1/: 1
POST:
POST: s-s-s y n -15.5 -13.5
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot

```



```

POST:
POST:
POST:@?<Hit_return_to_continue>
POST:
POST: set-inter
POST:

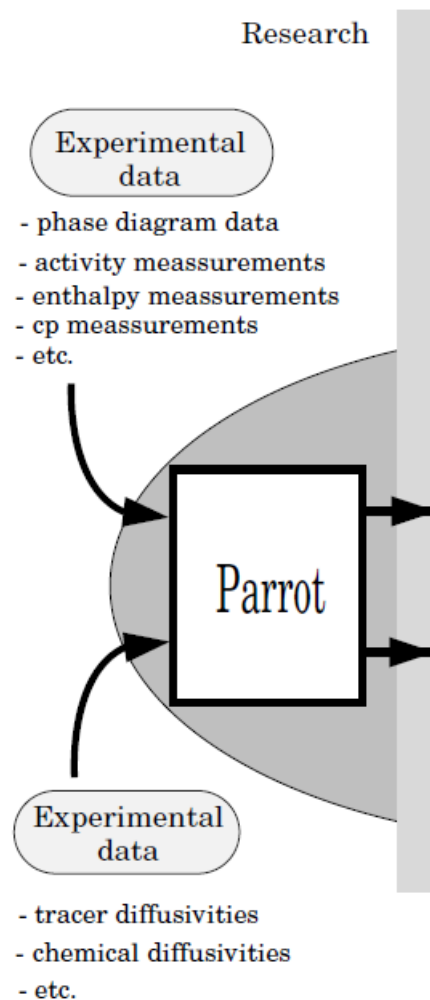
```



## Example exg2

### Optimization of mobilities in Ni-Al fcc alloys

A 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 Z. METALLKUNDE, Feb. 1996).



## exg2-setup

### SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,  
Stockholm, Sweden

Software running on Windows 64-bit wordlength  
Compiler: Intel Fortran Compiler 2025.0.0  
License library version: 9.7.0.0036  
Linked: Nov 19 2025 at 14:44:36

```
SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exg2\setup.DCM.test"
```

```
SYS: i>|@@
NO SUCH COMMAND, USE HELP
SYS: @@ Kinetic data example.
SYS: @@ Optimization of mobilities in Ni-Al fcc alloys
SYS: @@ A file for reading thermodynamic data and setting up the kinetic
SYS: @@ parameters that are needed for an optimization of the FCC phase
SYS: @@ in the binary Ni-Al system.
SYS: @@ See also A. Engström and J. Ågren: ("Assessment of Diffusional
SYS: @@ Mobilities in Face-Centered Cubic Ni-Cr-Al Alloys" in
SYS: @@ Z. Metallkunde, Feb. 1996).
SYS: @@-----
SYS:
SYS: @@ exg2_setup.DCM
SYS:
SYS:
SYS: @@
SYS: @@ EXPLICITLY SELECTING GES VERSION 5 BECAUSE PARAMETER OPTIMIZATION
SYS: @@ IS NOT SUPPORTED IN GES VERSION 6
SYS: @@
SYS: set-ges-version 5
SYS:
SYS: @@
SYS: @@ RETRIEVE THERMODYNAMIC DATA FROM A USER-DEFINED DATABASE
SYS: @@
SYS: go data
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\databases\da
ta
Current database: Steels/Fe-Alloys v12.0

VA
DICTRA_FCC_A1 REJECTED
TDB_TCFE12: sw us tdata.TDB
Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

VA DEFINED
TDB_USER: def-sys al ni
AL NI DEFINED
TDB_USER: rej ph *
LIQUID B2_BCC BCC_A2
FCC_A1 GAMMA_PRIME REJECTED
TDB_USER: rest ph fcc_al
FCC_A1 RESTORED
TDB_USER: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....
-OK-
TDB_USER:
TDB_USER: @@
TDB_USER: @@ APPEND THE KINETIC DATA FROM THE MOBILITY DATABASE IN ORDER TO
TDB_USER: @@ HAVE SOME DUMMY PARAMETERS.
TDB_USER: @@
TDB_USER: app mob2
Current database: Alloys Mobility v2.7

VA DEFINED
GAS:G REJECTED
APP: def-sys al ni
AL NI DEFINED
APP: rej ph *
BCC_A2 FCC_A1 M4N
HCP_A3 LIQUID:L REJECTED
APP: res ph fcc_al
FCC_A1 RESTORED
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-
APP:
APP: @@
APP: @@ GO TO THE DICTRA MODULE AND DEFINE THE KINETIC PARAMETERS. THE
APP: @@ VARIABLES V1,V2,V3 AND V4 ARE TO BE OPTIMIZED. NOTE THAT IF
APP: @@ YOU ARE OPTIMIZING PARAMETERS FOR A PHASE WITH MAGNETIC
APP: @@ CONTRIBUTION. I.E. USING BOTH MF- AND MQ-PARAMETERS, YOU
APP: @@ MIGHT HAVE TO ENTER THE PARROT MODULE AND GO BACK BEFORE
APP: @@ ENTERING PARAMETERS CONTAINING VARIABLES.
APP: @@
APP: go dic_par
PARROT VERSION 5.3d RUNNING ON PC / WINDOWS NT
Developed at the Division of Physical Metallurgy
Royal Institute of Technology Stockholm, Sweden

PARROT:
PARROT:
```

```
PARROT: go d-m
NO TIME STEP DEFINED
DIC>
DIC> @@ MOBILITY OF Al IN Al
DIC> ENTER-MOB-DATA
PARAMETER: MQ(FCC_Al&AL,AL:VA) 298.15 -142000+R*T*LN(1.71E-4); 6000 N
MQ(FCC_Al&AL#1,AL:VA;0)
DIC>
DIC> @@ MOBILITY OF Al IN Ni
DIC> ENTER-MOB-DATA
PARAMETER: MQ(FCC_Al&AL,NI:VA) 298.15 -284000+R*T*LN(7.5E-4); 6000 N
MQ(FCC_Al&AL#1,NI:VA;0)
DIC>
DIC> @@ MOBILITY OF Al INTERACTION BETWEEN Al AND Ni
DIC> ENTER-MOB-DATA
PARAMETER: MQ(FCC_Al&AL,AL,NI:VA;0) 298.15 V1+V2*T; 6000 N
MQ(FCC_Al&AL#1,AL,NI:VA;0)
DIC>
DIC> @@ MOBILITY OF Ni IN Al
DIC> ENTER-MOB-DATA
PARAMETER: MQ(FCC_Al&NI,AL:VA) 298.15 -145900+R*T*LN(4.4E-4); 6000 N
MQ(FCC_Al&NI#1,AL:VA;0)
DIC>
DIC> @@ MOBILITY OF Ni IN Ni
DIC> ENTER-MOB-DATA
PARAMETER: MQ(FCC_Al&NI,NI:VA) 298.15 -287000-69.8*T; 6000 N
MQ(FCC_Al&NI#1,NI:VA;0)
DIC>
DIC> @@ MOBILITY OF Ni INTERACTION BETWEEN Ni AND Al
DIC> ENTER-MOB-DATA
PARAMETER: MQ(FCC_Al&NI,NI,AL:VA;0) 298.15 V3+V4*T; 6000 N
MQ(FCC_Al&NI#1,AL,NI:VA;0)
DIC>
DIC> @@
DIC> @@ GO TO PARROT AND SAVE THE SET UP TO FILE
DIC> @@
DIC> go dic_parrot
PARROT VERSION 5.3d RUNNING ON PC / WINDOWS NT
PARROT: create-new-store-file opt
PARROT:
PARROT: set-inter
--OK--
PARROT:
```

exg2-run

PARROT>About

NO SUCH COMMAND, USE HELP

PARROT:PARROT:MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exg2\run.DCM.test"

PARROT: @@ exg2\_run.DCM

PARROT:

PARROT: @@-----

PARROT: @@ FILE FOR DOING THE OPTIMIZATION IN PARROT

PARROT: @@-----

PARROT:

PARROT: @@

PARROT: @@ GO TO PARROT AND READ THE SETUP

PARROT: @@

PARROT: go dic\_parrot

PARROT VERSION 5.3d RUNNING ON PC / WINDOWS NT

PARROT: set-store-file opt

PARROT:

PARROT:

PARROT: @@

PARROT: @@ COMPILE THE EXPERIMENTAL DATA IN exp.DOP INTO STRUCTURED BINARY DATA.

PARROT: @@

PARROT: compile-experiments exp

OUTPUT TO SCREEN OR FILE /SCREEN/:

INITIATE STORE FILE: /Y/:

-----  
\$ DOP-FILE CONTAINING EXPERIMENTAL INFORMATION USED DURING THE  
\$ OTIMIZATION IN PARROT (COMPARE WITH POP-FILE USED WHEN EVALUATING  
\$ THERMODYNAMIC DATA). THE EXPERIMENTAL DATA HERE STEAM FROM A STUDY BY  
\$ YAMAMOTO ET AL. TRANS. JPN. INST. MET. VOL. 21,NO. 9 (1980), P. 601.  
\$  
\$ CONSULT THE THERMO-CALC USER'S GUIDE TO LEARN MORE ABOUT SYNTAXES  
\$ FOR OPTIMIZATION OF THERMODYNAMIC DATA.  
-----

ENTER CONST P0=101325

TABLE HEAD 10  
CREATE\_NEW 0010,1  
C-S PH FCC=ENT 1  
S-C T=1573,N=1,P=P0  
S-C X(AL)=.01055  
EXPERIMENT LOGDC(FCC\_A1,AL,AL,NI)=-12.6:.1  
CREATE\_NEW 0011,1  
C-S PH FCC=ENT 1  
S-C T=1573,N=1,P=P0  
S-C X(AL)=.02032  
EXPERIMENT LOGDC(FCC\_A1,AL,AL,NI)=-12.56:.1  
CREATE\_NEW 0012,1  
C-S PH FCC=ENT 1  
S-C T=1573,N=1,P=P0  
S-C X(AL)=.02957  
EXPERIMENT LOGDC(FCC\_A1,AL,AL,NI)=-12.65:.1  
CREATE\_NEW 0013,1  
C-S PH FCC=ENT 1  
S-C T=1573,N=1,P=P0  
S-C X(AL)=.03884  
EXPERIMENT LOGDC(FCC\_A1,AL,AL,NI)=-12.52:.1  
CREATE\_NEW 0014,1  
C-S PH FCC=ENT 1  
S-C T=1573,N=1,P=P0  
S-C X(AL)=.03884  
EXPERIMENT LOGDC(FCC\_A1,AL,AL,NI)=-12.52:.1  
CREATE\_NEW 0015,1  
C-S PH FCC=ENT 1  
S-C T=1573,N=1,P=P0  
S-C X(AL)=.04927  
EXPERIMENT LOGDC(FCC\_A1,AL,AL,NI)=-12.48:.1  
CREATE\_NEW 0016,1  
C-S PH FCC=ENT 1  
S-C T=1573,N=1,P=P0  
S-C X(AL)=.06062  
EXPERIMENT LOGDC(FCC\_A1,AL,AL,NI)=-12.43:.1  
CREATE\_NEW 0017,1  
C-S PH FCC=ENT 1  
S-C T=1573,N=1,P=P0  
S-C X(AL)=.07029  
EXPERIMENT LOGDC(FCC\_A1,AL,AL,NI)=-12.41:.1  
CREATE\_NEW 0018,1  
C-S PH FCC=ENT 1  
S-C T=1573,N=1,P=P0  
S-C X(AL)=.08113  
EXPERIMENT LOGDC(FCC\_A1,AL,AL,NI)=-12.37:.1  
CREATE\_NEW 0019,1  
C-S PH FCC=ENT 1  
S-C T=1573,N=1,P=P0  
S-C X(AL)=.09166  
EXPERIMENT LOGDC(FCC\_A1,AL,AL,NI)=-12.32:.1  
CREATE\_NEW 0020,1  
C-S PH FCC=ENT 1  
S-C T=1573,N=1,P=P0  
S-C X(AL)=.09945  
EXPERIMENT LOGDC(FCC\_A1,AL,AL,NI)=-12.28:.1  
CREATE\_NEW 0021,1  
C-S PH FCC=ENT 1  
S-C T=1573,N=1,P=P0  
S-C X(AL)=.1099  
EXPERIMENT LOGDC(FCC\_A1,AL,AL,NI)=-12.24:.1  
CREATE\_NEW 0022,1  
C-S PH FCC=ENT 1  
S-C T=1573,N=1,P=P0  
S-C X(AL)=.1207  
EXPERIMENT LOGDC(FCC\_A1,AL,AL,NI)=-12.2:.1  
CREATE\_NEW 0023,1  
C-S PH FCC=ENT 1  
S-C T=1573,N=1,P=P0  
S-C X(AL)=.129  
EXPERIMENT LOGDC(FCC\_A1,AL,AL,NI)=-12.18:.1  
CREATE\_NEW 0024,1  
C-S PH FCC=ENT 1  
S-C T=1573,N=1,P=P0  
S-C X(AL)=.1392  
EXPERIMENT LOGDC(FCC\_A1,AL,AL,NI)=-12.16:.1

```
CREATE_NEW 0025,1
C-S PH FCC=ENT 1
S-C T=1573,N=1,P=P0
S-C X(AL)=.1503
EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.1:.1
CREATE_NEW 0026,1
C-S PH FCC=ENT 1
S-C T=1573,N=1,P=P0
S-C X(AL)=.1589
EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.08:.1
CREATE_NEW 0027,1
C-S PH FCC=ENT 1
S-C T=1573,N=1,P=P0
```

output ignored...

... output resumed

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V50

VAR.	VALUE	START VALUE	SCALING FACTOR	REL.STAND.DEV
V1	-3.51365596E+04	-3.51365596E+04	-3.51365596E+04	2.46939568E+00
V2	-9.53952154E+01	-9.53952154E+01	-9.53952154E+01	6.29664194E-01
V3	-1.32972461E+05	-1.32959165E+05	-1.32959165E+05	3.97449926E+00
V4	7.81857790E+01	7.81857790E+01	7.81857790E+01	4.46532149E+00

```
NUMBER OF OPTIMIZING VARIABLES : 4
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 2.02977003E+01 TO 2.02976923E+01
DEGREES OF FREEDOM 113. REDUCED SUM OF SQUARES 1.79625595E-01
```

Sorry, LIST-DATA disabled for this database

===== BLOCK NUMBER 1

DEFINED CONSTANTS

P0=101325

10	LOGDC(F... ,AL,NI)=-12.6	-12.56	0.10	4.3827E-02	0.4383
11	LOGDC(F... ,AL,NI)=-12.56	-12.55	0.10	1.2341E-02	0.1234
12	LOGDC(F... ,AL,NI)=-12.65	-12.53	0.10	0.1167	1.167
13	LOGDC(F... ,AL,NI)=-12.52	-12.51	0.10	5.8843E-03	5.8843E-02
14	LOGDC(F... ,AL,NI)=-12.52	-12.51	0.10	5.8843E-03	5.8843E-02
15	LOGDC(F... ,AL,NI)=-12.48	-12.49	0.10	-8.4123E-03	-8.4123E-02
16	LOGDC(F... ,AL,NI)=-12.43	-12.46	0.10	-2.6851E-02	-0.2685
17	LOGDC(F... ,AL,NI)=-12.41	-12.43	0.10	-1.7821E-02	-0.1782
18	LOGDC(F... ,AL,NI)=-12.37	-12.39	0.10	-2.3493E-02	-0.2349
19	LOGDC(F... ,AL,NI)=-12.32	-12.36	0.10	-3.8626E-02	-0.3863
20	LOGDC(F... ,AL,NI)=-12.28	-12.33	0.10	-5.1933E-02	-0.5193
21	LOGDC(F... ,AL,NI)=-12.24	-12.29	0.10	-5.4919E-02	-0.5492
22	LOGDC(F... ,AL,NI)=-12.2	-12.26	0.10	-5.5128E-02	-0.5513
23	LOGDC(F... ,AL,NI)=-12.18	-12.22	0.10	-4.3400E-02	-0.4340
24	LOGDC(F... ,AL,NI)=-12.16	-12.18	0.10	-2.2927E-02	-0.2293
25	LOGDC(F... ,AL,NI)=-12.1	-12.14	0.10	-3.6888E-02	-0.3689
26	LOGDC(F... ,AL,NI)=-12.08	-12.10	0.10	-1.9703E-02	-0.1970
27	LOGDC(F... ,AL,NI)=-12.02	-12.04	0.10	-2.2272E-02	-0.2227
28	LOGDC(F... ,AL,NI)=-11.98	-11.99	0.10	-9.0917E-03	-9.0917E-02
29	LOGDC(F... ,AL,NI)=-11.94	-11.95	0.10	-9.1618E-03	-9.1618E-02
30	LOGDC(F... ,AL,NI)=-13	-12.86	0.10	0.1360	1.360
31	LOGDC(F... ,AL,NI)=-12.96	-12.85	0.10	0.1059	1.059
32	LOGDC(F... ,AL,NI)=-12.92	-12.84	0.10	8.4799E-02	0.8480
33	LOGDC(F... ,AL,NI)=-12.9	-12.82	0.10	8.2549E-02	0.8255
34	LOGDC(F... ,AL,NI)=-12.77	-12.79	0.10	-1.5173E-02	-0.1517
35	LOGDC(F... ,AL,NI)=-12.74	-12.75	0.10	-1.1192E-02	-0.1119
36	LOGDC(F... ,AL,NI)=-12.82	-12.72	0.10	9.5223E-02	0.9522
37	LOGDC(F... ,AL,NI)=-12.82	-12.72	0.10	9.5223E-02	0.9522
38	LOGDC(F... ,AL,NI)=-12.69	-12.68	0.10	5.7856E-03	5.7856E-02
39	LOGDC(F... ,AL,NI)=-12.65	-12.65	0.10	2.6229E-03	2.6229E-02
40	LOGDC(F... ,AL,NI)=-12.64	-12.62	0.10	1.9222E-02	0.1922
41	LOGDC(F... ,AL,NI)=-12.61	-12.58	0.10	2.8492E-02	0.2849
42	LOGDC(F... ,AL,NI)=-12.55	-12.54	0.10	9.2091E-03	9.2091E-02
43	LOGDC(F... ,AL,NI)=-12.53	-12.51	0.10	2.1034E-02	0.2103
44	LOGDC(F... ,AL,NI)=-12.47	-12.47	0.10	2.0402E-03	2.0402E-02
45	LOGDC(F... ,AL,NI)=-12.41	-12.42	0.10	-1.0621E-02	-0.1062
46	LOGDC(F... ,AL,NI)=-12.38	-12.38	0.10	-1.6323E-04	-1.6323E-03
47	LOGDC(F... ,AL,NI)=-12.36	-12.32	0.10	3.6256E-02	0.3626
48	LOGDC(F... ,AL,NI)=-12.36	-12.32	0.10	3.6256E-02	0.3626
49	LOGDC(F... ,AL,NI)=-12.3	-12.27	0.10	3.0494E-02	0.3049
50	LOGDC(F... ,AL,NI)=-13.23	-13.19	0.10	3.8416E-02	0.3842
51	LOGDC(F... ,AL,NI)=-13.23	-13.19	0.10	3.8416E-02	0.3842
52	LOGDC(F... ,AL,NI)=-13.19	-13.18	0.10	1.3209E-02	0.1321
53	LOGDC(F... ,AL,NI)=-13.15	-13.16	0.10	-5.5530E-03	-5.5530E-02
54	LOGDC(F... ,AL,NI)=-13.12	-13.13	0.10	-1.4736E-02	-0.1474
55	LOGDC(F... ,AL,NI)=-13.09	-13.10	0.10	-1.2913E-02	-0.1291
56	LOGDC(F... ,AL,NI)=-13.06	-13.07	0.10	-6.9397E-03	-6.9397E-02
57	LOGDC(F... ,AL,NI)=-13.02	-13.04	0.10	-1.5971E-02	-0.1597
58	LOGDC(F... ,AL,NI)=-12.99	-13.00	0.10	-1.0672E-02	-0.1067
59	LOGDC(F... ,AL,NI)=-12.96	-12.96	0.10	8.0069E-04	8.0069E-03
60	LOGDC(F... ,AL,NI)=-12.91	-12.93	0.10	-2.0470E-02	-0.2047
61	LOGDC(F... ,AL,NI)=-12.88	-12.89	0.10	-7.3947E-03	-7.3947E-02
62	LOGDC(F... ,AL,NI)=-12.86	-12.85	0.10	1.4312E-02	0.1431
63	LOGDC(F... ,AL,NI)=-12.86	-12.85	0.10	1.4312E-02	0.1431
64	LOGDC(F... ,AL,NI)=-12.83	-12.81	0.10	1.7076E-02	0.1708
65	LOGDC(F... ,AL,NI)=-12.8	-12.77	0.10	2.9558E-02	0.2956
66	LOGDC(F... ,AL,NI)=-12.75	-12.72	0.10	2.5293E-02	0.2529
67	LOGDC(F... ,AL,NI)=-12.71	-12.68	0.10	2.6861E-02	0.2686
68	LOGDC(F... ,AL,NI)=-12.67	-12.63	0.10	4.4033E-02	0.4403
70	LOGDC(F... ,AL,NI)=-13.5	-13.54	0.10	-4.2456E-02	-0.4246
71	LOGDC(F... ,AL,NI)=-13.47	-13.53	0.10	-5.5160E-02	-0.5516
72	LOGDC(F... ,AL,NI)=-13.45	-13.50	0.10	-5.0384E-02	-0.5038
73	LOGDC(F... ,AL,NI)=-13.42	-13.48	0.10	-5.6139E-02	-0.5614
74	LOGDC(F... ,AL,NI)=-13.39	-13.44	0.10	-5.3034E-02	-0.5303
75	LOGDC(F... ,AL,NI)=-13.36	-13.40	0.10	-4.3865E-02	-0.4386
76	LOGDC(F... ,AL,NI)=-13.34	-13.37	0.10	-3.0943E-02	-0.3094
77	LOGDC(F... ,AL,NI)=-13.31	-13.33	0.10	-2.0539E-02	-0.2054
78	LOGDC(F... ,AL,NI)=-13.24	-13.29	0.10	-5.0311E-02	-0.5031
79	LOGDC(F... ,AL,NI)=-13.22	-13.26	0.10	-4.1318E-02	-0.4132
80	LOGDC(F... ,AL,NI)=-13.19	-13.22	0.10	-2.6230E-02	-0.2623
81	LOGDC(F... ,AL,NI)=-13.13	-13.17	0.10	-4.3098E-02	-0.4310
82	LOGDC(F... ,AL,NI)=-13.12	-13.14	0.10	-1.9773E-02	-0.1977

83	LOGDC(F...,AL,NI)=-13.08	-13.09	0.10	-1.4457E-02	-0.1446
84	LOGDC(F...,AL,NI)=-13.04	-13.05	0.10	-9.4618E-03	-9.4618E-02
85	LOGDC(F...,AL,NI)=-13.03	-13.01	0.10	2.2404E-02	0.2240
90	LOGDC(F...,AL,NI)=-13.97	-13.92	0.10	5.1241E-02	0.5124
91	LOGDC(F...,AL,NI)=-13.92	-13.90	0.10	2.0497E-02	0.2050
92	LOGDC(F...,AL,NI)=-13.88	-13.87	0.10	9.3920E-03	9.3920E-02
93	LOGDC(F...,AL,NI)=-13.85	-13.84	0.10	5.2264E-03	5.2264E-02
94	LOGDC(F...,AL,NI)=-13.82	-13.81	0.10	1.1044E-02	0.1104
95	LOGDC(F...,AL,NI)=-13.78	-13.77	0.10	1.3352E-02	0.1335
96	LOGDC(F...,AL,NI)=-13.9	-13.74	0.10	0.1640	1.640
97	LOGDC(F...,AL,NI)=-13.85	-13.69	0.10	0.1576	1.576
98	LOGDC(F...,AL,NI)=-13.65	-13.65	0.10	1.5604E-03	1.5604E-02
99	LOGDC(F...,AL,NI)=-13.62	-13.62	0.10	4.9052E-03	4.9052E-02
100	LOGDC(F...,AL,NI)=-13.57	-13.57	0.10	-9.5589E-04	-9.5589E-03
101	LOGDC(F...,AL,NI)=-13.52	-13.53	0.10	-5.4819E-03	-5.4819E-02
102	LOGDC(F...,AL,NI)=-13.47	-13.49	0.10	-2.0262E-02	-0.2026
103	LOGDC(F...,AL,NI)=-13.45	-13.45	0.10	4.9628E-03	4.9628E-02
104	LOGDC(F...,AL,NI)=-13.4	-13.40	0.10	2.8073E-03	2.8073E-02
110	LOGDC(F...,AL,NI)=-14.32	-14.32	0.10	-3.9760E-03	-3.9760E-02
111	LOGDC(F...,AL,NI)=-14.32	-14.30	0.10	1.9307E-02	0.1931
112	LOGDC(F...,AL,NI)=-14.28	-14.27	0.10	1.0664E-02	0.1066
113	LOGDC(F...,AL,NI)=-14.25	-14.24	0.10	8.9412E-03	8.9412E-02
114	LOGDC(F...,AL,NI)=-14.22	-14.20	0.10	1.8329E-02	0.1833
115	LOGDC(F...,AL,NI)=-14.17	-14.16	0.10	1.2994E-02	0.1299
116	LOGDC(F...,AL,NI)=-14.15	-14.12	0.10	3.0489E-02	0.3049
117	LOGDC(F...,AL,NI)=-14.1	-14.07	0.10	2.5593E-02	0.2559
118	LOGDC(F...,AL,NI)=-14.03	-14.03	0.10	-1.4483E-03	-1.4483E-02
119	LOGDC(F...,AL,NI)=-14	-14.00	0.10	2.7074E-03	2.7074E-02
120	LOGDC(F...,AL,NI)=-13.95	-13.95	0.10	-1.9282E-03	-1.9282E-02
121	LOGDC(F...,AL,NI)=-13.9	-13.91	0.10	-5.2349E-03	-5.2349E-02
122	LOGDC(F...,AL,NI)=-13.85	-13.87	0.10	-1.6645E-02	-0.1665
130	LOGDC(F...,AL,NI)=-14.73	-14.76	0.10	-3.0493E-02	-0.3049
131	LOGDC(F...,AL,NI)=-14.71	-14.73	0.10	-2.3757E-02	-0.2376
132	LOGDC(F...,AL,NI)=-14.68	-14.70	0.10	-1.9446E-02	-0.1945
133	LOGDC(F...,AL,NI)=-14.66	-14.67	0.10	-8.5997E-03	-8.5997E-02
134	LOGDC(F...,AL,NI)=-14.61	-14.63	0.10	-1.5314E-02	-0.1531
135	LOGDC(F...,AL,NI)=-14.61	-14.63	0.10	-1.5314E-02	-0.1531
136	LOGDC(F...,AL,NI)=-14.58	-14.58	0.10	3.4408E-03	3.4408E-02
137	LOGDC(F...,AL,NI)=-14.54	-14.54	0.10	3.3897E-03	3.3897E-02
138	LOGDC(F...,AL,NI)=-14.5	-14.49	0.10	9.2113E-03	9.2113E-02
139	LOGDC(F...,AL,NI)=-14.46	-14.44	0.10	1.5390E-02	0.1539
140	LOGDC(F...,AL,NI)=-14.41	-14.41	0.10	1.6005E-03	1.6005E-02
141	LOGDC(F...,AL,NI)=-14.35	-14.36	0.10	-1.1351E-02	-0.1135
142	LOGDC(F...,AL,NI)=-14.27	-14.31	0.10	-4.1487E-02	-0.4149
143	LOGDC(F...,AL,NI)=-14.2	-14.27	0.10	-7.4774E-02	-0.7477

**PARROT:**  
**PARROT:**  
**PARROT:** set-inter  
 --OK--  
**PARROT:**

## exg2-plot

### PARROT>About

NO SUCH COMMAND, USE HELP

PARROT:PARROT:MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exg2\plot.DCM.test"

PARROT: @@ exg2\_plot.DCM

PARROT:

PARROT: @@-----

PARROT: @@ FILE FOR PLOTTING THE RESULT AFTER THE OPTIMIZATION. HERE

PARROT: @@ DIFFUSIVITIES CALCULATED FROM THE OPTIMIZED VARIABLES ARE

PARROT: @@ COMPARED WITH EXPERIMENTALLY MEASURED ONES.

PARROT: @@-----

PARROT:

PARROT: @@

PARROT: @@ GO TO PARROT AND READ THE FILE CONTAINING THE RESULT FROM

PARROT: @@ THE OPTIMIZATION.

PARROT: @@

PARROT: go dic\_parrot

PARROT VERSION 5.3d RUNNING ON PC / WINDOWS NT

PARROT: set-store-file opt

PARROT:

PARROT: @@

PARROT: @@ GO TO POLY3 AND STEP IN X(AL)

PARROT: @@

PARROT: go p-3

POLY: s-c n=1,p=101325,t=1573

POLY: s-c x(al)=.1

POLY: c-e,,,,,

Using global minimization procedure

Calculated 209 grid points in 0.001 s

Found the set of lowest grid points in 0.000 s

Calculated solution in 0.002 s using 2 iterations. Total time 0.003 s

POLY: add,,

POLY:

POLY: s-a-v 1 x(al) 0.0001 .20 0.001,,,,,

POLY: step

Option? /NORMAL/:

Step will start from axis value 0.100000

...OK

Phase Region from 0.100000 for:

FCC\_A1

Global test at 1.08000E-01 .... OK

Global test at 1.18000E-01 .... OK

Global test at 1.28000E-01 .... OK

Global test at 1.38000E-01 .... OK

Global test at 1.48000E-01 .... OK

Global test at 1.58000E-01 .... OK

Global test at 1.68000E-01 .... OK

Global test at 1.78000E-01 .... OK

Global test at 1.88000E-01 .... OK

Global test at 1.98000E-01 .... OK

Terminating at 0.200000

Calculated 103 equilibria

Phase Region from 0.100000 for:

FCC\_A1

Global test at 9.20000E-02 .... OK

Global test at 8.20000E-02 .... OK

Global test at 7.20000E-02 .... OK

Global test at 6.20000E-02 .... OK

Global test at 5.20000E-02 .... OK

Global test at 4.20000E-02 .... OK

Global test at 3.20000E-02 .... OK

Global test at 2.20000E-02 .... OK

Global test at 1.20000E-02 .... OK

Global test at 2.00000E-03 .... OK

Terminating at 0.100000E-03

Calculated 103 equilibria

\*\*\* Buffer saved on file: C:\Users\azureuser\AppData\Local\Temp\RESULT\_002.POLY3

POLY: @@

POLY: @@ REPEATE THE PROCEDURE FOR SOME OTHER TEMPERATURES

POLY: @@

POLY: s-c t=1523,x(al)=.1

POLY: c-e,,,,,

Using global minimization procedure

Calculated 209 grid points in 0.000 s

Found the set of lowest grid points in 0.000 s

Calculated solution in 0.002 s using 2 iterations. Total time 0.002 s

POLY: s-a-v 1 x(al) 0.0001 .20 0.001,,,,,

POLY: step

Option? /NORMAL/:

Step will start from axis value 0.100000

...OK

Phase Region from 0.100000 for:

FCC\_A1

Global test at 1.08000E-01 .... OK

Global test at 1.18000E-01 .... OK

Global test at 1.28000E-01 .... OK

Global test at 1.38000E-01 .... OK

Global test at 1.48000E-01 .... OK

Global test at 1.58000E-01 .... OK

Global test at 1.68000E-01 .... OK

Global test at 1.78000E-01 .... OK

Global test at 1.88000E-01 .... OK

Global test at 1.98000E-01 .... OK

Terminating at 0.200000

Calculated 103 equilibria

Phase Region from 0.100000 for:

FCC\_A1

Global test at 9.20000E-02 .... OK

Global test at 8.20000E-02 .... OK

Global test at 7.20000E-02 .... OK

Global test at 6.20000E-02 .... OK

Global test at 5.20000E-02 .... OK

Global test at 4.20000E-02 .... OK

Global test at 3.20000E-02 .... OK

Global test at 2.20000E-02 .... OK

Global test at 1.20000E-02 .... OK

Global test at 2.00000E-03 .... OK

Terminating at 0.100000E-03

```
Calculated 103 equilibria
*** Buffer saved on file: C:\Users\azureuser\AppData\Local\Temp\RESULT_002.POLY3
POLY: s-c t=1473,x(al)=.1
POLY: c-e,,,,,,,,
Using global minimization procedure
Calculated 209 grid points in 0.001 s
Found the set of lowest grid points in 0.000 s
Calculated solution in 0.002 s using 2 iterations. Total time 0.003 s
POLY: s-a-v 1 x(al) 0.0001 .20 0.001,,,,
POLY: step
Option? /NORMAL/:
Step will start from axis value 0.100000
...OK

Phase Region from 0.100000 for:
FCC_A1
Global test at 1.08000E-01 .... OK
Global test at 1.18000E-01 .... OK
Global test at 1.28000E-01 .... OK
Global test at 1.38000E-01 .... OK
Global test at 1.48000E-01 .... OK
Global test at 1.58000E-01 .... OK
Global test at 1.68000E-01 .... OK
Global test at 1.78000E-01 .... OK
Global test at 1.88000E-01 .... OK
Global test at 1.98000E-01 .... OK
Terminating at 0.200000
Calculated 103 equilibria

Phase Region from 0.100000 for:
FCC_A1
Global test at 9.20000E-02 .... OK
Global test at 8.20000E-02 .... OK
Global test at 7.20000E-02 .... OK
Global test at 6.20000E-02 .... OK
Global test at 5.20000E-02 .... OK
Global test at 4.20000E-02 .... OK
Global test at 3.20000E-02 .... OK
Global test at 2.20000E-02 .... OK
Global test at 1.20000E-02 .... OK
Global test at 2.00000E-03 .... OK
Terminating at 0.100000E-03
Calculated 103 equilibria
*** Buffer saved on file: C:\Users\azureuser\AppData\Local\Temp\RESULT_002.POLY3
POLY: s-c t=1423,x(al)=.1
POLY: c-e,,,,,,,,
Using global minimization procedure
Calculated 209 grid points in 0.001 s
Found the set of lowest grid points in 0.000 s
Calculated solution in 0.002 s using 2 iterations. Total time 0.003 s
POLY: s-a-v 1 x(al) 0.0001 .20 0.001,,,,
POLY: step
Option? /NORMAL/:
Step will start from axis value 0.100000
...OK

Phase Region from 0.100000 for:
FCC_A1
Global test at 1.08000E-01 .... OK
Global test at 1.18000E-01 .... OK
Global test at 1.28000E-01 .... OK
Global test at 1.38000E-01 .... OK
Global test at 1.48000E-01 .... OK
Global test at 1.58000E-01 .... OK
Global test at 1.68000E-01 .... OK
Global test at 1.78000E-01 .... OK
Global test at 1.88000E-01 .... OK
Global test at 1.98000E-01 .... OK
Terminating at 0.200000
Calculated 103 equilibria

Phase Region from 0.100000 for:
FCC_A1
Global test at 9.20000E-02 .... OK
Global test at 8.20000E-02 .... OK
Global test at 7.20000E-02 .... OK
Global test at 6.20000E-02 .... OK
Global test at 5.20000E-02 .... OK
Global test at 4.20000E-02 .... OK
Global test at 3.20000E-02 .... OK
Global test at 2.20000E-02 .... OK
Global test at 1.20000E-02 .... OK
Global test at 2.00000E-03 .... OK
Terminating at 0.100000E-03
Calculated 103 equilibria
*** Buffer saved on file: C:\Users\azureuser\AppData\Local\Temp\RESULT_002.POLY3
POLY: s-c t=1373,x(al)=.1
POLY: c-e,,,,,,,,
Using global minimization procedure
Calculated 209 grid points in 0.000 s
Found the set of lowest grid points in 0.001 s
Calculated solution in 0.001 s using 2 iterations. Total time 0.002 s
POLY: s-a-v 1 x(al) 0.0001 .20 0.001,,,,
POLY: step
Option? /NORMAL/:
Step will start from axis value 0.100000
...OK

Phase Region from 0.100000 for:
FCC_A1
Global test at 1.08000E-01 .... OK
Global test at 1.18000E-01 .... OK
Global test at 1.28000E-01 .... OK
Global test at 1.38000E-01 .... OK
Global test at 1.48000E-01 .... OK
Global test at 1.58000E-01 .... OK
Global test at 1.68000E-01 .... OK
Global test at 1.78000E-01 .... OK
Global test at 1.88000E-01 .... OK
Global test at 1.98000E-01 .... OK
Terminating at 0.200000
Calculated 103 equilibria

Phase Region from 0.100000 for:
FCC_A1
```

```

Global test at 9.20000E-02 .... OK
Global test at 8.20000E-02 .... OK
Global test at 7.20000E-02 .... OK
Global test at 6.20000E-02 .... OK
Global test at 5.20000E-02 .... OK
Global test at 4.20000E-02 .... OK
Global test at 3.20000E-02 .... OK
Global test at 2.20000E-02 .... OK
Global test at 1.20000E-02 .... OK
Global test at 2.00000E-03 .... OK
Terminating at 0.10000E-03
Calculated 103 equilibria
*** Buffer saved on file: C:\Users\azureuser\AppData\Local\Temp\RESULT_002.POLY3
POLY: s-c t=1323,x(al)=.1
POLY: c-e,,,,,,,,
Using global minimization procedure
Calculated 209 grid points in 0.001 s
Found the set of lowest grid points in 0.000 s
Calculated solution in 0.001 s using 2 iterations. Total time 0.002 s
POLY: s-a-v 1 x(al) 0.0001 .20 0.001,,,,
POLY: step
Option? /NORMAL/:
Step will start from axis value 0.100000
...OK

Phase Region from 0.100000 for:
FCC_A1
Global test at 1.08000E-01 .... OK
Global test at 1.18000E-01 .... OK
Global test at 1.28000E-01 .... OK
Global test at 1.38000E-01 .... OK
Global test at 1.48000E-01 .... OK
Global test at 1.58000E-01 .... OK
Global test at 1.68000E-01 .... OK
Global test at 1.78000E-01 .... OK
Global test at 1.88000E-01 .... OK
Global test at 1.98000E-01 .... OK
Terminating at 0.200000
Calculated 103 equilibria

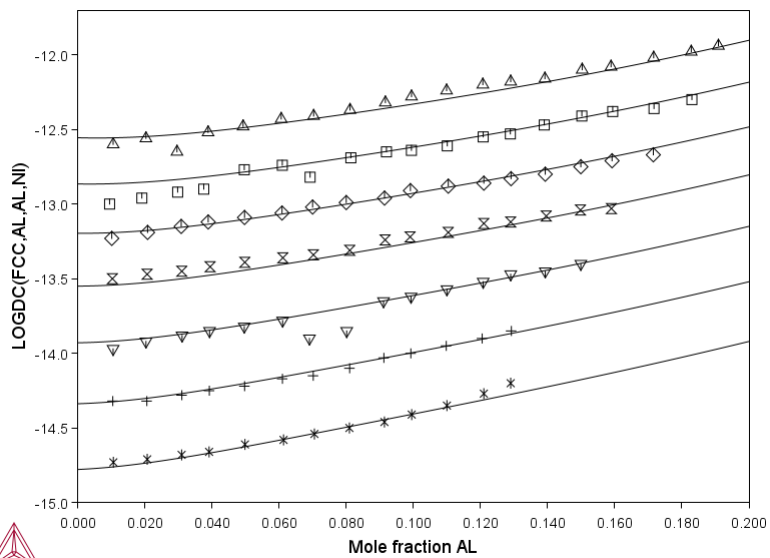
Phase Region from 0.100000 for:
FCC_A1
Global test at 9.20000E-02 .... OK
Global test at 8.20000E-02 .... OK
Global test at 7.20000E-02 .... OK
Global test at 6.20000E-02 .... OK
Global test at 5.20000E-02 .... OK
Global test at 4.20000E-02 .... OK
Global test at 3.20000E-02 .... OK
Global test at 2.20000E-02 .... OK
Global test at 1.20000E-02 .... OK
Global test at 2.00000E-03 .... OK
Terminating at 0.10000E-03
Calculated 103 equilibria
*** Buffer saved on file: C:\Users\azureuser\AppData\Local\Temp\RESULT_002.POLY3
POLY: s-c t=1273,x(al)=.1
POLY: c-e,,,,,,,,
Using global minimization procedure
Calculated 209 grid points in 0.001 s
Found the set of lowest grid points in 0.000 s
Calculated solution in 0.001 s using 2 iterations. Total time 0.002 s
POLY: s-a-v 1 x(al) 0.0001 .20 0.001,,,,
POLY: step
Option? /NORMAL/:
Step will start from axis value 0.100000
...OK

Phase Region from 0.100000 for:
FCC_A1
Global test at 1.08000E-01 .... OK
Global test at 1.18000E-01 .... OK
Global test at 1.28000E-01 .... OK
Global test at 1.38000E-01 .... OK
Global test at 1.48000E-01 .... OK
Global test at 1.58000E-01 .... OK
Global test at 1.68000E-01 .... OK
Global test at 1.78000E-01 .... OK
Global test at 1.88000E-01 .... OK
Global test at 1.98000E-01 .... OK
Terminating at 0.200000
Calculated 103 equilibria

Phase Region from 0.100000 for:
FCC_A1
Global test at 9.20000E-02 .... OK
Global test at 8.20000E-02 .... OK
Global test at 7.20000E-02 .... OK
Global test at 6.20000E-02 .... OK
Global test at 5.20000E-02 .... OK
Global test at 4.20000E-02 .... OK
Global test at 3.20000E-02 .... OK
Global test at 2.20000E-02 .... OK
Global test at 1.20000E-02 .... OK
Global test at 2.00000E-03 .... OK
Terminating at 0.10000E-03
Calculated 103 equilibria
*** Buffer saved on file: C:\Users\azureuser\AppData\Local\Temp\RESULT_002.POLY3
POLY: @@
POLY: @@ ENTER THE POST MODULE, PLOT THE DIFFUSIVITY ON THE Y-AXIS
POLY: @@ AND MOLE-FRACTION A1 ON THE X-AXIS.
POLY: @@
POLY: post
POLY-3 POSTPROCESSOR VERSION 3.2
POST:
POST: s-d-a x m-f al
POST: s-d-a y logdc(fcc,al,al,ni)
POST:
POST: app y yama.exp
PROLOGUE NUMBER: /0/: 1
DATASET NUMBER(s): /-1/: 1 2 3 4 5 6 7
POST:
POST:
POST: s-t-m-s y
COMMAND NOT SUPPORTED IN THIS PLOT DRIVER

```

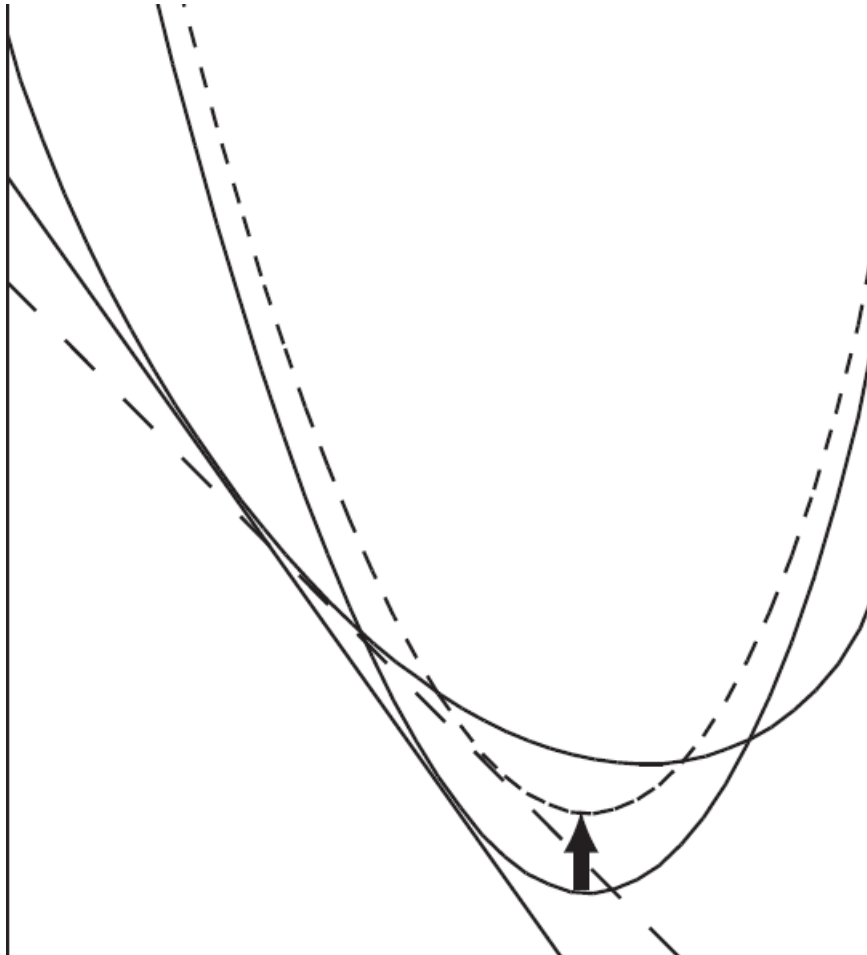
```
POST: s-s-s y n -15 -11.7
POST: s-t-m-s y
      COMMAND NOT SUPPORTED IN THIS PLOT DRIVER
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
```



```
POST:
POST: @?<Hit_return_to_continue>
POST:
POST: set-inter
POST:
```



## Deviation From Local Equilibrium

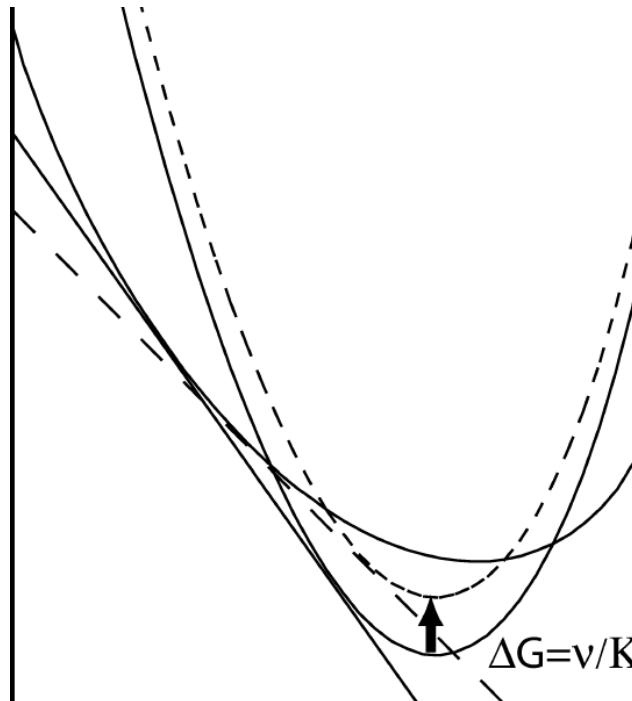




## Example exh1

### $\alpha/\gamma$ diffusion couple with limited interface mobility

This example calculates the growth of ferrite ( $\alpha$ ) into austenite ( $\gamma$ ) with a limited interface mobility. This is achieved by adding a Gibbs-energy contribution to the ferrite using the SET-SURFACE-ENERGY command.



## exh1-setup

### SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,  
Stockholm, Sweden

Software running on Windows 64-bit wordlength  
Compiler: Intel Fortran Compiler 2025.0.0  
License library version: 9.7.0.0036  
Linked: Nov 19 2025 at 14:44:36

```
SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exh1\setup.DCM.test"
```

```
SYS: @@
SYS: @@ Deviation from local equilibrium.
SYS: @@ Ferrite/austenite diffusion couple with interface mobility
SYS: @@ This example calculates the growth of ferrite into austenite with
SYS: @@ a limited interface mobility. this is done by adding a Gibbs-energy
SYS: @@ contribution to the ferrite using the SET-SURFACE-ENERGY command.
SYS: @@-----
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASE
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\databases\da
ta
Current database: Steels/Fe-Alloys v12.0

VA /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE12:
TDB_TCFE12: @@
TDB_TCFE12: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE THE DATA
TDB_TCFE12: @@
TDB_TCFE12: sw FEDEMO
Current database: Iron Demo Database v6.0

VA /- DEFINED
TDB_FEDEMO: def-sys fe c
FE C DEFINED
TDB_FEDEMO: rej ph * all
GAS:G LIQUID:L BCC_A2
C14 LAVES CBCC_A12 CEMENTITE_D011
CUB_A13 DIAMOND_A4 FCC_A1
GRAPHITE_A9 HCP_A3 KSI_CARBIDE
M23C6_D84 M5C2 M7C3_D101
REJECTED
TDB_FEDEMO: res ph bcc fcc
BCC_A2 FCC_A1 RESTORED
TDB_FEDEMO: get
12:03:10,449 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE MOBILITY DATA
TDB_FEDEMO: @@
TDB_FEDEMO: app mfedemo
Current database: Fe-Alloys Mobility demo database v5.0

VA DEFINED
APP: def-sys fe c
FE C DEFINED
APP: rej ph * all
BCC_A2 FCC_A1 CEMENTITE_D011
LIQUID:L REJECTED
APP: res ph bcc fcc
BCC_A2 FCC_A1 RESTORED
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR
APP: @@
APP: go d-m
NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 1000; * N
DIC>
DIC> @@
DIC> @@ START BY ENTERING THE REGIONS ferrite AND austenite WHERE
DIC> @@ THE BCC AND FCC PHASES ARE PUT, RESPECTIVELY. THE FERRITE REGION IS
DIC> @@ ASSUMED INITIALLY TO BE VERY THIN, 1E-9 METERS.
DIC> @@
DIC> enter-region
REGION NAME : ferrite
```

```
DIC>
DIC> enter-region
REGION NAME : austenite
ATTACH TO REGION NAMED /FERRITE/:
ATTACHED TO THE RIGHT OF FERRITE /YES/:
DIC>
DIC> @@
DIC> @@ ENTER GRIDS INTO THE REGIONS
DIC> @@
DIC> enter-grid
REGION NAME : /FERRITE/: ferrite
WIDTH OF REGION /1/: 1e-9
TYPE /AUTO/: AUTO
DIC>
DIC> enter-grid austenite
WIDTH OF REGION /1/: 0.999e-6
TYPE /AUTO/: AUTO
DIC>
DIC> @@
DIC> @@ ENTER THE active PHASES INTO THE REGIONS
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /FERRITE/: ferrite
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: bcc
DIC>
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /AUSTENITE/: austenite
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITION INTO BCC
DIC> @@
DIC> enter-composition
REGION NAME : /FERRITE/: ferrite
PHASE NAME: /BCC_A2/: bcc
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: C
TYPE /LINEAR/: linear
VALUE OF FIRST POINT : 0.019091893
VALUE OF LAST POINT : /1.9091893E-2/: 0.019091893
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITION INTO FCC
DIC> @@
DIC> enter-composition
REGION NAME : /AUSTENITE/: austenite
PHASE NAME: /FCC_A1/: fcc#1
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: C
TYPE /LINEAR/: linear
VALUE OF FIRST POINT : 0.0191
VALUE OF LAST POINT : /1.91E-2/: 0.0191
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exhl y
DIC>
DIC> set-inter
--OK--
DIC>
```

exh1-run

DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exh1\run.DCM.test"

DIC>

DIC>

DIC> @@

DIC> @@ READ THE SETUP FROM FILE AND START THE SIMULATION

DIC> @@

DIC>

DIC> go d-m

TIME STEP AT TIME 0.00000E+00

DIC>

DIC> read exh1

OK

DIC>

DIC> @@

DIC> @@ SET THE SIMULATION TIME

DIC> @@

DIC> set-sim-time

END TIME FOR INTEGRATION /.1/: 2.5E-3

AUTOMATIC TIMESTEP CONTROL /YES/: YES

MAX TIMESTEP DURING INTEGRATION /2.5E-04/:

INITIAL TIMESTEP : /1E-07/: 1E-7

SMALLEST ACCEPTABLE TIMESTEP : /1E-07/: 1E-7

DIC>

DIC>

DIC> @@

DIC> @@ START THE SIMULATION

DIC> @@

DIC> sim

INFO: Default responses (if any) will be applied during the simulation. Use "SIMULATE\_REACTION NO" instead for manual input.

Region: FERRITE

geometric 0.964174 dense at 0.100000E-08 51 points

Region: AUSTENITE

geometric 1.20000 dense at 0.00000 57 points

DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE

Trying old scheme 3

U-FRACTION IN SYSTEM: C = 8.88253285685629E-04 FE = 1

TOTAL SIZE OF SYSTEM: 1E-06 [m]

U-FRACTION IN SYSTEM: C = 8.88253285685629E-04 FE = 1

TOTAL SIZE OF SYSTEM: 1E-06 [m]

6.129174537659537E-004	6.128943047003572E-004	20.3423679232232	6.062437353814954E-004	6.029205751764839E-
004	6.012624196099474E-004	5.996065472035967E-004	5.979331738336693E-004	5.945934417197160E-
004	5.879420347394491E-004	5.747514520154408E-004	5.488192219758681E-004	4.987505814876858E-
004	4.057965014776165E-004	2.486211534522674E-004	4.920170270007913E-	
005	20.3420783723051	4.904901983029824E-005	4.897276737211813E-005	4.893466338715906E-
005	4.891561695582411E-005	4.889657423170352E-005	4.887683398418529E-005	4.883736544564391E-
005	4.875847619481457E-005			

ERROR RETURN FROM NS01A BECAUSE THERE HAVE BEEN 25 CALLS OF CALFUN

RESCALING

5.523048285069478E-007	5.519778703812132E-007	0.203420783672109	5.504891949101719E-007	5.495824990801473E-
007	5.491294314075348E-007	5.488034146754972E-007	5.484774947496821E-007	5.481380356991294E-
007	5.474594328382697E-007	5.461034880773690E-007	5.433966424004828E-007	5.380031264214500E-
007	5.272967959669258E-007	5.062069410695829E-007	4.653184553198548E-007	3.887063800058052E-
007	5.691236797553241E-003	3.875078361397619E-007	3.869092582039349E-007	3.866101427354237E-
007	3.863365989928855E-007	3.860631520567343E-007	3.857798753328794E-007	3.852136337843677E-007

ERROR RETURN FROM NS01A BECAUSE THERE HAVE BEEN 25 CALLS OF CALFUN

\*\*\* ERROR 1890 IN DCNS01: ERROR RETURN FROM NS01A

3.852136337843677E-007	3.852135908235614E-007	3.852136337843677E-007	0.203421591827670	3.852136337843677E-
007	3.841556255321940E-007	3.841556255321940E-007	3.841556255321940E-007	3.836271670063930E-
007	3.836271670063930E-007	3.825713411561884E-007	3.825713411561884E-007	3.804640542594430E-
007	3.804640542594430E-007	3.762669396810266E-007		

output ignored...

... output resumed

1.962025198975442E-007	1.959102902196957E-007	3.432961073906042E-009	1.449257128414354E-010	6.181027321592069E-
013	1.244825784890624E-017	TIME = 0.24605715E-02 DT = 0.21825635E-04	SUM OF SQUARES = 0.12448258E-16	
	CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.32335508E-03 AND 0.32335508E-03			
	POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.70188790E-06			
	U-FRACTION IN SYSTEM: C = 9.16126010458359E-04 FE = 1			
	TOTAL SIZE OF SYSTEM: 1E-06 [m]			
	CPU time used in timestep 0 seconds			
3.359654251512357E-007	3.354817092726576E-007	7.174832030711180E-009	1.343879974221032E-010	6.541437887722555E-
014	6.513306204958121E-019	TIME = 0.24754479E-02 DT = 0.14876355E-04	SUM OF SQUARES = 0.65133062E-18	
	CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.36964318E-03 AND 0.36964318E-03			
	POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.70738685E-06			
	U-FRACTION IN SYSTEM: C = 9.16284230511638E-04 FE = 1			
	TOTAL SIZE OF SYSTEM: 1E-06 [m]			
	CPU time used in timestep 0 seconds			
4.480824841810942E-007	4.473970704295982E-007	3.532271957713549E-009	4.125275023600657E-011	6.019509661976300E-
015	1.076906499891585E-020	TIME = 0.24857463E-02 DT = 0.10298459E-04	SUM OF SQUARES = 0.10769065E-19	
	CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.41477474E-03 AND 0.41477474E-03			
	POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.71165839E-06			
	U-FRACTION IN SYSTEM: C = 9.1695895786688E-04 FE = 1			
	TOTAL SIZE OF SYSTEM: 1E-06 [m]			
	CPU time used in timestep 0 seconds			
7.433870682511251E-007	7.422538887675034E-007	5.180439508320737E-009	5.117681232280809E-011	5.371522465424346E-
015	5.803518179457897E-021	TIME = 0.24926481E-02 DT = 0.69017408E-05	SUM OF SQUARES = 0.58035182E-20	
	CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.46518765E-03 AND 0.46518765E-03			
	POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.71486899E-06			
	U-FRACTION IN SYSTEM: C = 9.16975497122159E-04 FE = 1			
	TOTAL SIZE OF SYSTEM: 1E-06 [m]			
	CPU time used in timestep 1 seconds			
1.502608164374188E-006	1.500645011500603E-006	6.643470397057504E-009	3.748471921331202E-011	1.322133600008516E-
015	2.694768711500598E-022	TIME = 0.24970907E-02 DT = 0.44426453E-05	SUM OF SQUARES = 0.26947687E-21	
	CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.53102356E-03 AND 0.53102356E-03			
	POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.71722814E-06			
	U-FRACTION IN SYSTEM: C = 9.17612807091724E-04 FE = 1			
	TOTAL SIZE OF SYSTEM: 1E-06 [m]			
	CPU time used in timestep 0 seconds			
2.702550154910963E-008	2.699115968916376E-008	8.819804300352050E-011	3.645503558776434E-013	6.411839505507341E-
018	TIME = 0.24997240E-02 DT = 0.26333071E-05	SUM OF SQUARES = 0.64118395E-17		
	CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.60758572E-03 AND 0.60758572E-03			

POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.71882810E-06  
U-FRACTION IN SYSTEM: C = 9.18427804299815E-04 FE = 1  
TOTAL SIZE OF SYSTEM: 1E-06 [m]  
CPU time used in timestep 0 seconds  
1.191723590417681E-006 1.191408793300165E-006 1.881599553681577E-009 3.489617124379390E-012 1.216770543076059E-017  
TIME = 0.25000000E-02 DT = 0.27597876E-06 SUM OF SQUARES = 0.12167705E-16  
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.10657228E-02 AND 0.10657228E-02  
POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.71912222E-06  
U-FRACTION IN SYSTEM: C = 9.19856765262792E-04 FE = 1  
TOTAL SIZE OF SYSTEM: 1E-06 [m]  
MUST SAVE WORKSPACE ON FILE  
WORKSPACE SAVED ON FILE  
RECLAIMING WORKSPACE  
DELETING TIME-RECORD FOR TIME 0.0000000  
DELETING TIME-RECORD FOR TIME 0.10000000E-06  
DELETING TIME-RECORD FOR TIME 0.30000000E-06  
DELETING TIME-RECORD FOR TIME 0.70000000E-06  
DELETING TIME-RECORD FOR TIME 0.15000000E-05  
DELETING TIME-RECORD FOR TIME 0.31000000E-05  
DELETING TIME-RECORD FOR TIME 0.63000000E-05  
DELETING TIME-RECORD FOR TIME 0.75544080E-05  
DELETING TIME-RECORD FOR TIME 0.10063224E-04  
DELETING TIME-RECORD FOR TIME 0.15080856E-04  
DELETING TIME-RECORD FOR TIME 0.25023807E-04  
DELETING TIME-RECORD FOR TIME 0.44909710E-04  
DELETING TIME-RECORD FOR TIME 0.80648021E-04  
DELETING TIME-RECORD FOR TIME 0.13180785E-03  
DELETING TIME-RECORD FOR TIME 0.19798464E-03  
DELETING TIME-RECORD FOR TIME 0.27942201E-03  
DELETING TIME-RECORD FOR TIME 0.37639362E-03  
DELETING TIME-RECORD FOR TIME 0.48934339E-03  
DELETING TIME-RECORD FOR TIME 0.61915242E-03  
DELETING TIME-RECORD FOR TIME 0.76215067E-03  
DELETING TIME-RECORD FOR TIME 0.90545598E-03  
DELETING TIME-RECORD FOR TIME 0.10492878E-02  
DELETING TIME-RECORD FOR TIME 0.11937426E-02  
DELETING TIME-RECORD FOR TIME 0.13387337E-02  
DELETING TIME-RECORD FOR TIME 0.14842001E-02  
DELETING TIME-RECORD FOR TIME 0.16306187E-02  
DELETING TIME-RECORD FOR TIME 0.17788612E-02  
DELETING TIME-RECORD FOR TIME 0.19290777E-02  
DELETING TIME-RECORD FOR TIME 0.20812340E-02  
DELETING TIME-RECORD FOR TIME 0.22089892E-02  
DELETING TIME-RECORD FOR TIME 0.22991889E-02  
DELETING TIME-RECORD FOR TIME 0.23623992E-02  
DELETING TIME-RECORD FOR TIME 0.24071859E-02  
DELETING TIME-RECORD FOR TIME 0.24387459E-02  
DELETING TIME-RECORD FOR TIME 0.24605715E-02  
DELETING TIME-RECORD FOR TIME 0.24754479E-02  
DELETING TIME-RECORD FOR TIME 0.24857463E-02  
DELETING TIME-RECORD FOR TIME 0.24926481E-02  
DELETING TIME-RECORD FOR TIME 0.24970907E-02  
  
KEEPING TIME-RECORD FOR TIME 0.24997240E-02  
AND FOR TIME 0.25000000E-02  
WORKSPACE RECLAIMED  
  
TIMESTEP AT 0.25000000E-02 SELECTED

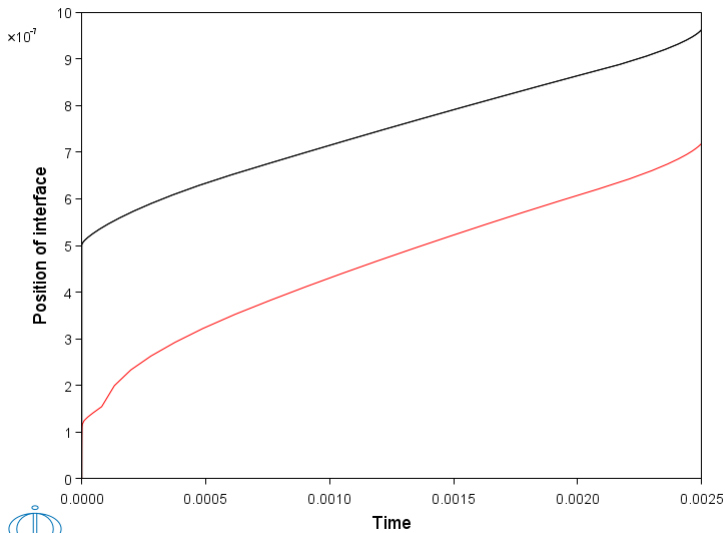
DIC>  
DIC>  
DIC> set-inter  
--OK--  
DIC>

# exh1-plot

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exh1\plot.DCM.test"
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 2.50000E-03
DIC>
DIC> read exh1
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1: @@
POST-1: @@ SET THE DATA APPENDED FROM THE "EXP" FILE TO BE READ
POST-1: @@
POST-1: set-col for for red
COMMAND NOT SUPPORTED IN THIS PLOT DRIVER
POST-1:
POST-1: @@
POST-1: @@ COMPARE THE POSITION OF THE INTERFACE AS A FUNCTION OF TIME
POST-1: @@
POST-1: s-d-a x time
INFO: Time is set as independent variable
POST-1: s-d-a y posi aus low
POST-1:
POST-1: @@
POST-1: @@ APPEND THE SIMULATION (WITHOUT THE ENERGY CONTRIBUTION) FROM FILE
POST-1: @@
POST-1: app y noadd.exp 1; 1
POST-1:
POST-1: @@
POST-1: @@ SET A TITLE ON THE PLOT
POST-1: @@
POST-1: set-title Figure h1
POST-1:
POST-1: @@
POST-1: @@ PLOT THE RESULTS
POST-1: @@
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
WORKING ...
WORKING ... OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

Figure h1

CELL # 1



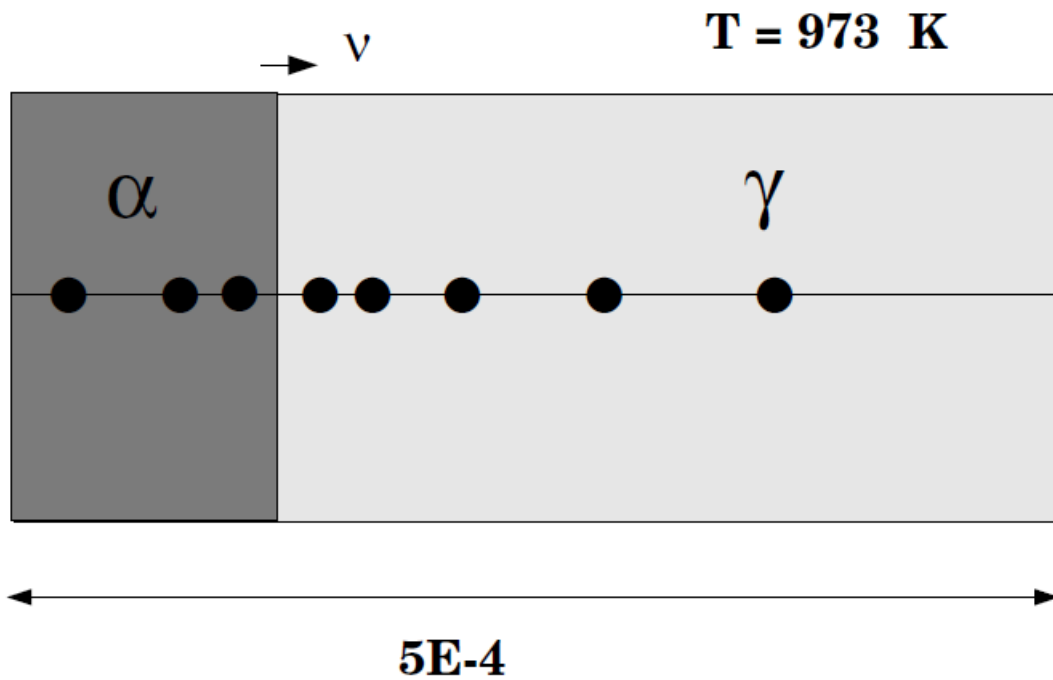
```
POST-1:
POST-1:
POST-1: set-inter
--OK--
POST-1:
```



## Example exh2

### $\alpha/\gamma$ para-equilibrium in an Fe-Ni-C alloy

This example calculates the growth of ferrite ( $\alpha$ ) into austenite ( $\gamma$ ) 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." *Met. Mat. Trans A* 35.4 (2004): 1211-1221.



## exh2-setup

### SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,  
Stockholm, Sweden

Software running on Windows 64-bit wordlength  
Compiler: Intel Fortran Compiler 2025.0.0  
License library version: 9.7.0.0036  
Linked: Nov 19 2025 at 14:44:36

```
SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exh2\setup.DCM.test"
```

```
SYS: @@
SYS: @@ Deviation from local equilibrium.
SYS: @@ Ferrite/austenite para-equilibrium in an Fe-Ni-C alloy
SYS: @@ This example calculates the growth of ferrite into austenite
SYS: @@ in an Fe-2.02%Ni-0.0885%C alloy using the para-equilibrium model.
SYS: @@ The results are compared with experimental information from
SYS: @@ Hutchinson, C. R., A. Fuchsmann, and Yves Brechet. "The diffusional
SYS: @@ formation of ferrite from austenite in Fe-C-Ni alloys." Metall.
SYS: @@ Mat. Trans. A 35.4 (2004): 1211-1221.
SYS: @@-----
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASE
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\databases\da
ta
Current database: Steels/Fe-Alloys v12.0

VA /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE12:
TDB_TCFE12: @@
TDB_TCFE12: @@ SELECT A DATABASE FOR THERMODYNAMIC DATA
TDB_TCFE12: @@
TDB_TCFE12: sw fedemo
Current database: Iron Demo Database v6.0

VA /- DEFINED
TDB_FEDEMO: def-sys fe ni c
FE NI C
DEFINED
TDB_FEDEMO: rej ph * all
GAS:G LIQUID:L BCC_A2
C14 LAVES CBCC_A12 CEMENTITE_D011
CUB_A13 DIAMOND_A4 FCC_A1
GRAPHITE_A9 HCP_A3 KSI_CARBIDE
M23C6_D84 MSC2 M7C3_D101
REJECTED
TDB_FEDEMO: res ph bcc fcc
BCC_A2 FCC_A1 RESTORED
TDB_FEDEMO: get
12:06:37,741 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE MOBILITY DATA
TDB_FEDEMO: @@
TDB_FEDEMO: app mfedemo
Current database: Fe-Alloys Mobility demo database v5.0

VA DEFINED
APP: def-sys fe ni c
FE NI C
DEFINED
APP: rej ph * all
BCC_A2 FCC_A1 CEMENTITE_D011
LIQUID:L REJECTED
APP: res ph bcc fcc
BCC_A2 FCC_A1 RESTORED
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR
APP: @@
APP: go d-m
NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 973; * N
DIC>
DIC> @@
DIC> @@ START BY ENTERING THE REGIONS ferrite AND austenite WHERE THE
```

```
DIC> @@ BCC AND FCC PHASES ARE PUT, RESPECTIVELY. THE FERRITE REGION IS
DIC> @@ ASSUMED INITIALLY TO BE VERY THIN, 1E-9 METERS.
DIC> @@
DIC> enter-region
REGION NAME : ferrite
DIC>
DIC> enter-region
REGION NAME : austenite
ATTACH TO REGION NAMED /FERRITE/:
ATTACHED TO THE RIGHT OF FERRITE /YES/:
DIC>
DIC> @@
DIC> @@ ENTER GRIDS INTO THE REGIONS
DIC> @@
DIC> enter-grid
REGION NAME : /FERRITE/: ferrite
WIDTH OF REGION /1/: 1e-9
TYPE /AUTO/: AUTO
DIC>
DIC> enter-grid austenite
WIDTH OF REGION /1/: 50e-6
TYPE /AUTO/: AUTO
DIC>
DIC> @@
DIC> @@ ENTER active PHASES INTO THE REGIONS
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /FERRITE/: ferrite
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: bcc
DIC>
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /AUSTENITE/: austenite
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITION INTO BCC
DIC> @@
DIC> enter-composition
REGION NAME : /FERRITE/: ferrite
PHASE NAME: /BCC_A2/: bcc
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: c
TYPE /LINEAR/: linear
VALUE OF FIRST POINT : 0.0885
VALUE OF LAST POINT : /8.85E-2/: 0.0885
PROFILE FOR /NI/: ni
TYPE /LINEAR/: linear
VALUE OF FIRST POINT : 2.02
VALUE OF LAST POINT : /2.02/: 2.02
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITION INTO FCC
DIC> @@
DIC> enter-composition
REGION NAME : /AUSTENITE/: austenite
PHASE NAME: /FCC_A1/: fcc#1
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: c
TYPE /LINEAR/: linear
VALUE OF FIRST POINT : 0.0885
VALUE OF LAST POINT : /8.85E-2/: 0.0885
PROFILE FOR /NI/: ni
TYPE /LINEAR/: linear
VALUE OF FIRST POINT : 2.02
VALUE OF LAST POINT : /2.02/: 2.02
DIC>
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exh2 y
DIC>
DIC> set-inter
--OK--
DIC>
```

exh2-run

DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exh2\run.DCM.test"

DIC>

DIC>

DIC>

DIC> @@

DIC> @@ FILE TO RUN EXAMPLE exh2

DIC> @@

DIC>

DIC> @@

DIC> @@ READ THE SETUP FROM FILE

DIC> @@

DIC>

DIC> go d-m

TIME STEP AT TIME 0.00000E+00

DIC>

DIC> read exh2

OK

DIC>

DIC> @@

DIC> @@ SET THE SIMULATION TIME

DIC> @@

DIC> set-sim-time 50,,,,,,,,,,

DIC>

DIC>

DIC> @@

DIC> @@ ENABLE THE PARA-EQUILIBRIUM MODEL

DIC> @@

DIC> para

ENABLE PARAEQ : /NO/: YES

U-FRACTION OF COMPONENT FE /AUTO/: AUTO

U-FRACTION OF COMPONENT NI /AUTO/: AUTO

DIC>

DIC> @@

DIC> @@ START THE SIMULATION

DIC> @@

DIC> sim

INFO: Default responses (if any) will be applied during the simulation. Use "SIMULATE\_REACTION NO" instead for manual input.

Region: FERRITE

geometric 0.964171 dense at 0.100000E-08 51 points

Region: AUSTENITE

geometric 1.20000 dense at 0.00000 57 points

DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE

Trying old scheme 4

GENERATING STARTING VALUES FOR CELL # 1 INTERFACE # 2

DETERMINING INITIAL EQUILIBRIUM VALUES

CALCULATING STARTING VALUES: 9 EQUILIBRIUM CALCULATIONS DONE 6 OUT OF 9

DETERMINED ACTIVITIES ACR(C) .161541295585

UNABLE TO OBTAIN GOOD STARTING VALUE USING THE OLD SCHEME

Trying new scheme

GENERATING STARTING VALUES FOR CELL # 1 INTERFACE # 2

DETERMINING INITIAL EQUILIBRIUM VALUES

CALCULATING STARTING VALUES: 18 EQUILIBRIUM CALCULATIONS DONE 1 OUT OF 18

U-FRACTION IN SYSTEM: C = .00412262676333 FE = .980742621143593

NI = .0192573788564064

TOTAL SIZE OF SYSTEM: 5.0001E-05 [m]

U-FRACTION IN SYSTEM: C = .00412262676333 FE = .980742621143593

NI = .0192573788564064

TOTAL SIZE OF SYSTEM: 5.0001E-05 [m]

2232.10933123601 2232.10933123118 2228.18553675641 2.32388314928639 1.991496426446273E-

003 8.452960099771964E-003 4.785304810655034E-005 1.932479770378503E-003 4.194261193685144E-

005 3.202374887548627E-005 1.619456673150708E-005 1.959968179465662E-003 5.697674549899568E-

007 1.328945618892549E-017 TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.42881043E-20

CELL # 1 VELOCITY AT INTERFACE # 2 IS 3.1432820 AND 3.1432820

POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.31532820E-06

U-FRACTION IN SYSTEM: C = .00413396129130636 FE = .980742621143594

NI = .0192573788564064

TOTAL SIZE OF SYSTEM: 5.0001E-05 [m]

46 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: FERRITE

CPU time used in timestep 3 seconds

2189.02053454150 2189.02053456980 2185.12797661083 2.22502445772034 1.912761745800095E-

003 7.928642173764768E-003 7.405444038852032E-005 1.965446429817397E-003

output ignored...

... output resumed

1192.63240703101 1189.62544886548 0.586696638545274 2.470345208986976E-004 1.628948379719393E-

006 7.424235330307716E-010 2.065845559790816E-003 5.084320359545113E-

019 TIME = 36.593206 DT = 5.0000000 SUM OF SQUARES = 0.50843153E-18

CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.20310173E-06 AND 0.20310173E-06

POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.11911120E-04

U-FRACTION IN SYSTEM: C = .00414772184447735 FE = .980742621143593

NI = .0192573788564067

TOTAL SIZE OF SYSTEM: 5.0001E-05 [m]

20 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: FERRITE

CPU time used in timestep 1 seconds

1169.39662305032 1169.39662305223 1166.41547026096 0.562252748964268 2.317822579808669E-

004 1.486139663754339E-006 6.540072287920605E-010 2.068868732339013E-003 4.878910704123769E-

019 TIME = 41.593206 DT = 5.0000000 SUM OF SQUARES = 0.48789098E-18

CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.19170532E-06 AND 0.19170532E-06

POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.12869647E-04

U-FRACTION IN SYSTEM: C = .00414851113638844 FE = .980742621143593

NI = .0192573788564067

TOTAL SIZE OF SYSTEM: 5.0001E-05 [m]

15 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: FERRITE

CPU time used in timestep 1 seconds

1146.60821566302 1146.60821566340 1143.65269377647 0.538840294099288 2.174785349378767E-

004 1.441568849099777E-006 6.240080177561884E-010 2.071959967181790E-003 4.777796568753878E-

019 TIME = 46.593206 DT = 5.0000000 SUM OF SQUARES = 0.47777952E-18

CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.18195627E-06 AND 0.18195627E-06

POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.13779428E-04

U-FRACTION IN SYSTEM: C = .00414912963525125 FE = .980742621143593

NI = .0192573788564067

TOTAL SIZE OF SYSTEM: 5.0001E-05 [m]  
10 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: FERRITE

CPU time used in timestep 1 seconds  
1124.25873624323 1124.25873624031 1121.32867092848 0.516415094017740 2.040662887025250E-  
004 7.872234679590309E-005 3.067898117565920E-008 2.162134064338327E-011 2.058540750034059E-  
003 1.529953261058165E-020 TIME = 49.384484 DT = 2.7912777 SUM OF SQUARES = 0.15299533E-19  
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.20010318E-06 AND 0.20010318E-06  
POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.14337972E-04  
U-FRACTION IN SYSTEM: C = .00415071769735891 FE = .980742621143593  
NI = .0192573788564068  
TOTAL SIZE OF SYSTEM: 5.0001E-05 [m]  
8 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: FERRITE

CPU time used in timestep 1 seconds  
1102.33989364269 1102.33989364416 1099.43511073552 0.494935036536964 1.915026073437086E-  
004 8.105440426900372E-004 2.829100764335205E-008 2.063250973221209E-003 2.484685044519068E-  
009 7.341481014364588E-016 TIME = 50.000000 DT = 0.61551595 SUM OF SQUARES = 0.18428261E-16  
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.25861680E-06 AND 0.25861680E-06  
POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.14497155E-04  
U-FRACTION IN SYSTEM: C = .00415225389931968 FE = .980742621143593  
NI = .0192573788564068  
TOTAL SIZE OF SYSTEM: 5.0001E-05 [m]

MUST SAVE WORKSPACE ON FILE  
WORKSPACE SAVED ON FILE

RECLAIMING WORKSPACE

DELETING TIME-RECORD FOR TIME 0.0000000  
DELETING TIME-RECORD FOR TIME 0.10000000E-06  
DELETING TIME-RECORD FOR TIME 0.20000000E-06  
DELETING TIME-RECORD FOR TIME 0.39649286E-06  
DELETING TIME-RECORD FOR TIME 0.78947858E-06  
DELETING TIME-RECORD FOR TIME 0.15754500E-05  
DELETING TIME-RECORD FOR TIME 0.31473929E-05  
DELETING TIME-RECORD FOR TIME 0.62912787E-05  
DELETING TIME-RECORD FOR TIME 0.12579050E-04  
DELETING TIME-RECORD FOR TIME 0.25154593E-04  
DELETING TIME-RECORD FOR TIME 0.50305679E-04  
DELETING TIME-RECORD FOR TIME 0.10060785E-03  
DELETING TIME-RECORD FOR TIME 0.20121220E-03  
DELETING TIME-RECORD FOR TIME 0.40242089E-03  
DELETING TIME-RECORD FOR TIME 0.80483826E-03  
DELETING TIME-RECORD FOR TIME 0.16096730E-02  
DELETING TIME-RECORD FOR TIME 0.32193425E-02  
DELETING TIME-RECORD FOR TIME 0.64386816E-02  
DELETING TIME-RECORD FOR TIME 0.12877360E-01  
DELETING TIME-RECORD FOR TIME 0.25754716E-01  
DELETING TIME-RECORD FOR TIME 0.51509428E-01  
DELETING TIME-RECORD FOR TIME 0.10301885  
DELETING TIME-RECORD FOR TIME 0.20603770  
DELETING TIME-RECORD FOR TIME 0.41207540  
DELETING TIME-RECORD FOR TIME 0.82415080  
DELETING TIME-RECORD FOR TIME 1.6483016  
DELETING TIME-RECORD FOR TIME 3.2966032  
DELETING TIME-RECORD FOR TIME 6.5932063  
DELETING TIME-RECORD FOR TIME 11.593206  
DELETING TIME-RECORD FOR TIME 16.593206  
DELETING TIME-RECORD FOR TIME 21.593206  
DELETING TIME-RECORD FOR TIME 26.593206  
DELETING TIME-RECORD FOR TIME 31.593206  
DELETING TIME-RECORD FOR TIME 36.593206  
DELETING TIME-RECORD FOR TIME 41.593206  
DELETING TIME-RECORD FOR TIME 46.593206

KEEPING TIME-RECORD FOR TIME 49.384484  
AND FOR TIME 50.000000  
WORKSPACE RECLAIMED

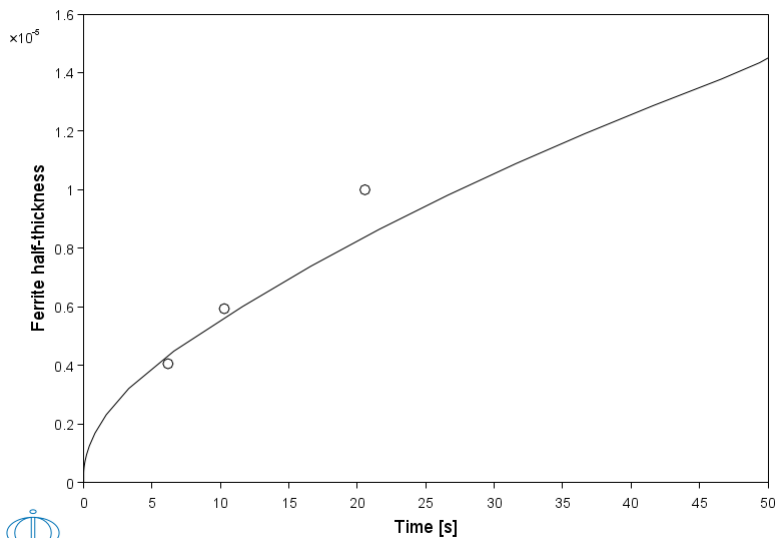
TIMESTEP AT 50.000000 SELECTED

DIC>  
DIC>  
DIC> set-inter  
--OK--  
DIC>

## exh2-plot

```
DIC>About
NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exh2\plot.DCM.test"
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 5.00000E+01
DIC>
DIC> read exh2
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1:
POST-1:
POST-1: @@
POST-1: @@ WE WANT TO PLOT THE POSITION OF THE INTERFACE AS A FUNCTION OF TIME
POST-1: @@ I.E. THE FERRITE HALF-THICKNESS
POST-1: @@
POST-1: s-d-a x time
INFO: Time is set as independent variable
POST-1: s-d-a y posi aus low
POST-1:
POST-1: @@
POST-1: @@ APPEND THE EXPERIMENTAL INFORMATION
POST-1: @@
POST-1: app y exh2.exp 1; 1
POST-1:
POST-1: @@
POST-1: @@ SET A TITLE ON THE PLOT
POST-1: @@
POST-1: set-title Figure h2
POST-1:
POST-1: @@
POST-1: @@ RENAME THE AXIS LABELS
POST-1: @@
POST-1: set-axis-text-status
AXIS (X, Y OR Z) : x
AUTOMATIC AXIS TEXT (Y OR N) /N/: NO
AXIS TEXT : Time [s]
POST-1:
POST-1: set-axis-text-status
AXIS (X, Y OR Z) : y
AUTOMATIC AXIS TEXT (Y OR N) /N/: NO
AXIS TEXT : Ferrite half-thickness
POST-1:
POST-1: @@
POST-1: @@ PLOT THE RESULTS
POST-1: @@
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

Figure h2



```
POST-1:
POST-1:
POST-1:
POST-1: set-inter
--OK--
POST-1:
```

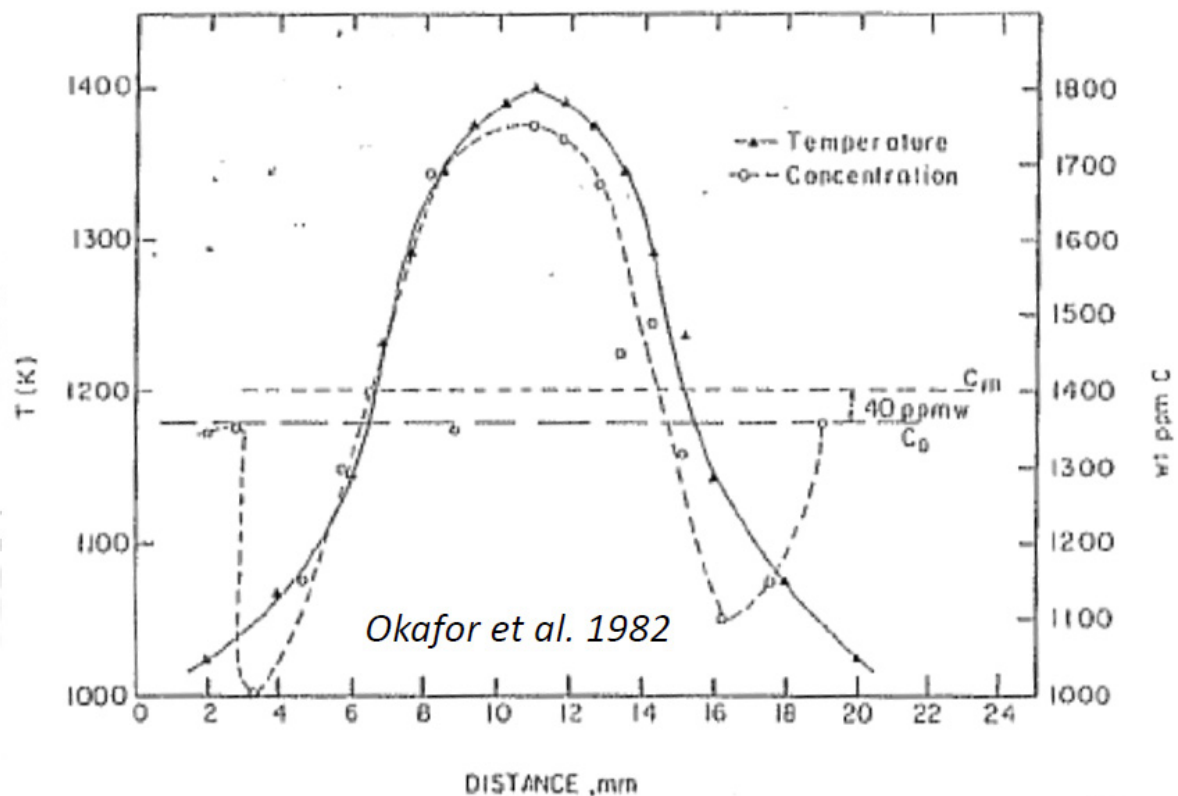


### Example exh3

#### Diffusion induced by a temperature gradient (thermomigration)

This calculation shows how a temperature gradient induces diffusion.

$$J_C = -\frac{u_C}{V_s} y_{Va} M_{CVa} \left( \frac{\partial \mu_C}{\partial x} + \frac{Q_C^*}{T} \frac{\partial T}{\partial x} \right)$$



## exh3-setup

### SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,  
Stockholm, Sweden

Software running on Windows 64-bit wordlength  
Compiler: Intel Fortran Compiler 2025.0.0  
License library version: 9.7.0.0036  
Linked: Nov 19 2025 at 14:44:36

```
SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exh3\setup.DCM.test"
```

```
SYS: @@
SYS: @@ Deviation from local equilibrium.
SYS: @@ Diffusion induced by a temperature gradient (thermomigration)
SYS: @@ This calculation shows how a temperature gradient induces
SYS: @@ diffusion.
SYS: @@-----
SYS:
SYS: go da
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\databases\da
ta
Current database: Steels/Fe-Alloys v12.0

VA          /-  DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE12: sw fedemo
Current database: Iron Demo Database v6.0

VA          /-  DEFINED
TDB_FEDEMO: def-sys fe ni c
FE          NI          C
          DEFINED
TDB_FEDEMO: rej ph * all
GAS:G          LIQUID:L          BCC_A2
C14_LAVES          CBCC_A12          CEMENTITE_D011
CUB_A13          DIAMOND_A4          FCC_A1
GRAPHITE_A9          HCP_A3          KSI_CARBIDE
M23C6_D84          MSC2          M7C3_D101
          REJECTED
TDB_FEDEMO: res ph fcc graph
FCC_A1          GRAPHITE_A9 RESTORED
TDB_FEDEMO: get
12:09:59,549 [Thread-0] INFO  JavaWrapper: *** Invoking Gibbs Energy System v6 ***
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....
```

Use the command LIST\_REFERENCES to see the list of references for assessed data

-OK-

```
TDB_FEDEMO: app mfedemo
Current database: Fe-Alloys Mobility demo database v5.0
```

```
VA  DEFINED
APP: def-sys fe ni c
FE          NI          C
          DEFINED
APP: rej ph * all
          BCC_A2          FCC_A1          CEMENTITE_D011
          LIQUID:L REJECTED
APP: res ph fcc
FCC_A1 RESTORED
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....
```

Use the command LIST\_REFERENCES to see the list of references for assessed data

-OK-

```
APP: go d-m
NO TIME STEP DEFINED
*** ENTERING GRAPHITE_A9 AS A DIFFUSION NONE PHASE
DIC>
DIC> @@ ENTER A GAUSSIAN-SHAPED TEMPERATURE GRADIENT
DIC> set-cond glob T 0 1000+400*exp(-3.35074E4*(x-11e-3)**2); * N
DIC>
DIC> set-ref C grap,,,,,,,,,
DIC>
DIC> ent-reg aus,,,,,
DIC>
DIC> ent-grid aus 25e-3 auto
DIC>
DIC> ent-pha act aus matrix fcc#1
DIC>
DIC> ent-comp aus fcc#1 fe w-p
PROFILE FOR /C/: c lin 0.14 0.14
PROFILE FOR /NI/: ni lin 32.5 32.5
DIC>
DIC> s-s-time 5E7,,,,,,,,,
DIC>
DIC> @@ ENTER THE HEAT OF TRANSFER PARAMETER FOR CARBON
DIC> ent-heat-tra-p
HEAT TRANSFER PARAMETER FOR PHASE: fcc
ELEMENT: C
PARAMETER /O/: -42000
DIC>
DIC>
```

```
DIC> save exh3 y
DIC>
DIC> set-inter
--OK--
DIC>
```

exh3-run

DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exh3\run.DCM.test"

DIC>

DIC> go d-m

TIME STEP AT TIME 0.00000E+00

\*\*\* ENTERING GRAPHITE\_A9 AS A DIFFUSION NONE PHASE

DIC>

DIC> read exh3

OK

DIC>

DIC> sim

INFO: Default responses (if any) will be applied during the simulation. Use "SIMULATE\_REACTION NO" instead for manual input.

Region: AUS

linear 50 points

DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE

U-FRACTION IN SYSTEM: C = .00662305741857946 FE = .685349154604931  
NI = .31465084539507

TOTAL SIZE OF SYSTEM: .025 [m]

U-FRACTION IN SYSTEM: C = .00662305741857946 FE = .685349154604931  
NI = .31465084539507

TOTAL SIZE OF SYSTEM: .025 [m]

TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00662305741857946 FE = .685349154604931  
NI = .31465084539507

TOTAL SIZE OF SYSTEM: .025 [m]

CPU time used in timestep 0 seconds

TIME = 0.10010000E-03 DT = 0.10000000E-03 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00662305741857946 FE = .685349154604931  
NI = .31465084539507

TOTAL SIZE OF SYSTEM: .025 [m]

CPU time used in timestep 0 seconds

TIME = 0.40010010 DT = 0.40000000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00662305741857947 FE = .685349154604931  
NI = .31465084539507

TOTAL SIZE OF SYSTEM: .025 [m]

CPU time used in timestep 1 seconds

TIME = 1627.0525 DT = 1626.6524 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00662305741857947 FE = .68534915460493  
NI = .31465084539507

TOTAL SIZE OF SYSTEM: .025 [m]

CPU time used in timestep 0 seconds

TIME = 170014.89 DT = 168387.83 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00662305741834655 FE = .685349154604931  
NI = .31465084539507

TOTAL SIZE OF SYSTEM: .025 [m]

CPU time used in timestep 1 seconds

TIME = 506790.55 DT = 336775.67 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00662305741835073 FE = .685349154604931  
NI = .31465084539507

TOTAL SIZE OF SYSTEM: .025 [m]

CPU time used in timestep 0 seconds

TIME = 1180341.9 DT = 673551.33 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00662305741835076 FE = .68534915460493  
NI = .31465084539507

TOTAL SIZE OF SYSTEM: .025 [m]

CPU time used in timestep 0 seconds

TIME = 2527444.6 DT = 1347102.7 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00662305741835495 FE = .68534915460493  
NI = .31465084539507

TOTAL SIZE OF SYSTEM: .025 [m]

CPU time used in timestep 1 seconds

TIME = 5221649.9 DT = 2694205.3 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00662305741836956 FE = .68534915460493  
NI = .31465084539507

TOTAL SIZE OF SYSTEM: .025 [m]

CPU time used in timestep 0 seconds

TIME = 10221650. DT = 5000000.0 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00662305741846215 FE = .68534915460493  
NI = .31465084539507

TOTAL SIZE OF SYSTEM: .025 [m]

CPU time used in timestep 0 seconds

TIME = 14360595. DT = 4138945.1 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00662305741847918 FE = .68534915460493  
NI = .31465084539507

TOTAL SIZE OF SYSTEM: .025 [m]

CPU time used in timestep 0 seconds

TIME = 18263542. DT = 3902946.9 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00662305741849128 FE = .68534915460493  
NI = .314650845395069

TOTAL SIZE OF SYSTEM: .025 [m]

CPU time used in timestep 1 seconds

TIME = 22078920. DT = 3815377.7 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00662305741849863 FE = .685349154604931  
NI = .31465084539507

TOTAL SIZE OF SYSTEM: .025 [m]

CPU time used in timestep 0 seconds

TIME = 25858793. DT = 3779873.2 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00662305741850394 FE = .68534915460493  
NI = .314650845395069

TOTAL SIZE OF SYSTEM: .025 [m]

CPU time used in timestep 0 seconds

TIME = 29624578. DT = 3765785.5 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00662305741807207 FE = .68534915460493  
NI = .31465084539507

TOTAL SIZE OF SYSTEM: .025 [m]

CPU time used in timestep 0 seconds

TIME = 33385416. DT = 3760837.2 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00662305741776046 FE = .685349154604931  
NI = .31465084539507

TOTAL SIZE OF SYSTEM: .025 [m]

CPU time used in timestep 0 seconds

TIME = 37145195. DT = 3759779.4 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00662305741702901 FE = .68534915460493  
NI = .31465084539507

TOTAL SIZE OF SYSTEM: .025 [m]

CPU time used in timestep 1 seconds

TIME = 40905511. DT = 3760316.4 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00662305741643541 FE = .68534915460493  
NI = .31465084539507

TOTAL SIZE OF SYSTEM: .025 [m]

CPU time used in timestep 0 seconds

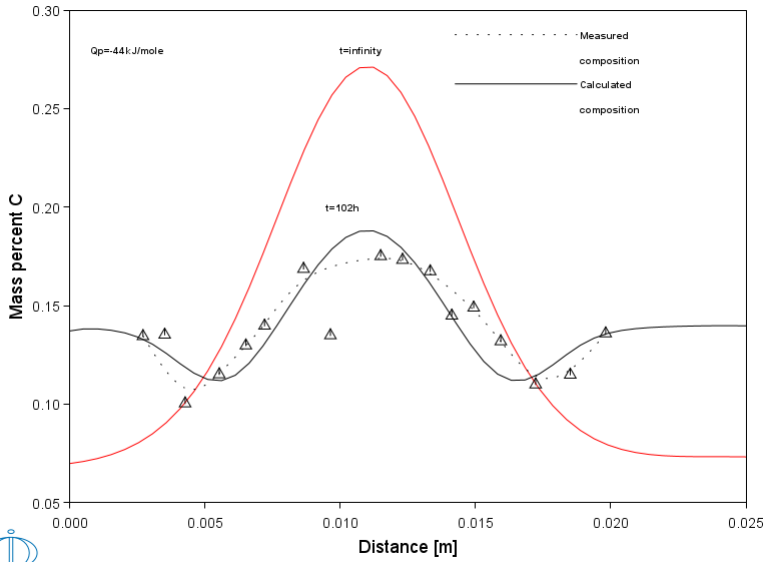
```
TIME = 44294168. DT = 3388657.1 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741601727 FE = .68534915460493
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep 0 seconds
TIME = 46438546. DT = 2144377.3 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741583866 FE = .68534915460493
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep 0 seconds
TIME = 47961210. DT = 1522664.7 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741574719 FE = .68534915460493
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep 0 seconds
TIME = 49233541. DT = 1272330.7 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741568699 FE = .68534915460493
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep 1 seconds
TIME = 49869706. DT = 636165.36 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741567134 FE = .68534915460493
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep 0 seconds
TIME = 50000000. DT = 130293.61 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741567247 FE = .68534915460493
NI = .314650845395069
TOTAL SIZE OF SYSTEM: .025 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 0.0000000
DELETING TIME-RECORD FOR TIME 0.100000000E-06
DELETING TIME-RECORD FOR TIME 0.100100000E-03
DELETING TIME-RECORD FOR TIME 0.40010010
DELETING TIME-RECORD FOR TIME 1627.0525
DELETING TIME-RECORD FOR TIME 170014.89
DELETING TIME-RECORD FOR TIME 506790.55
DELETING TIME-RECORD FOR TIME 1180341.9
DELETING TIME-RECORD FOR TIME 2527444.6
DELETING TIME-RECORD FOR TIME 5221649.9
DELETING TIME-RECORD FOR TIME 10221650.
DELETING TIME-RECORD FOR TIME 14360595.
DELETING TIME-RECORD FOR TIME 18263542.
DELETING TIME-RECORD FOR TIME 22078920.
DELETING TIME-RECORD FOR TIME 25858793.
DELETING TIME-RECORD FOR TIME 29624578.
DELETING TIME-RECORD FOR TIME 33385416.
DELETING TIME-RECORD FOR TIME 37145195.
DELETING TIME-RECORD FOR TIME 40905511.
DELETING TIME-RECORD FOR TIME 44294168.
DELETING TIME-RECORD FOR TIME 46438546.
DELETING TIME-RECORD FOR TIME 47961210.
DELETING TIME-RECORD FOR TIME 49233541.
KEEPING TIME-RECORD FOR TIME 49869706.
AND FOR TIME 50000000.
WORKSPACE RECLAIMED
TIMESTEP AT 50000000.0 SELECTED
```

```
DIC>
DIC> set-inter
--OK--
DIC>
```

exh3-plot

DIC>About

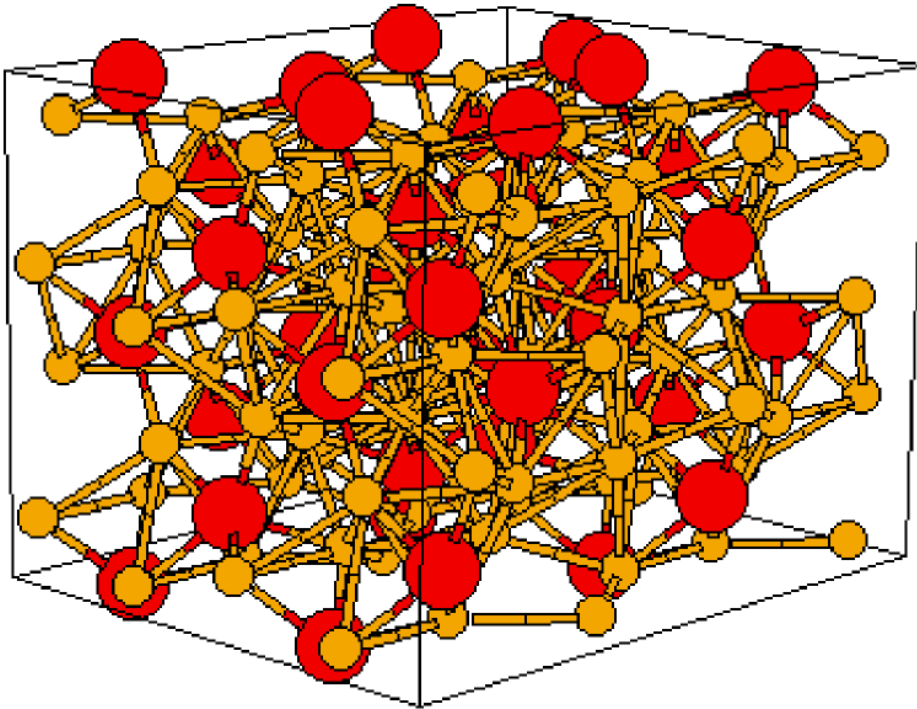
```
NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exh3\plot.DCM.test"
DIC> go d-m
TIME STEP AT TIME 5.00000E+07
*** ENTERING GRAPHITE_A9 AS A DIFFUSION NONE PHASE
DIC>
DIC>
DIC> read exh3
OK
DIC>
DIC> post
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
POST-1: s-d-a x dist glob
INFO: Distance is set as independent variable
POST-1: s-d-a y w-p c
POST-1: s-p-c time 367200 5E7
POST-1: s-s-s y n 0.1 0.18
POST-1: s-s-s y y
POST-1: app y exh3.exp 0; 1 3;
POST-1: s-p-o n y y n y n n,,,,,,,,,
POST-1:
POST-1: set-ax-text-st x
AUTOMATIC AXIS TEXT (Y OR N) /N/: n
AXIS TEXT : Distance [m]
POST-1:
POST-1: set-ax-text-st y
AUTOMATIC AXIS TEXT (Y OR N) /N/: n
AXIS TEXT : Mass percent C
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```



```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1: set-inter
--OK--
POST-1:
```



## **Diffusion in Complex Phases**

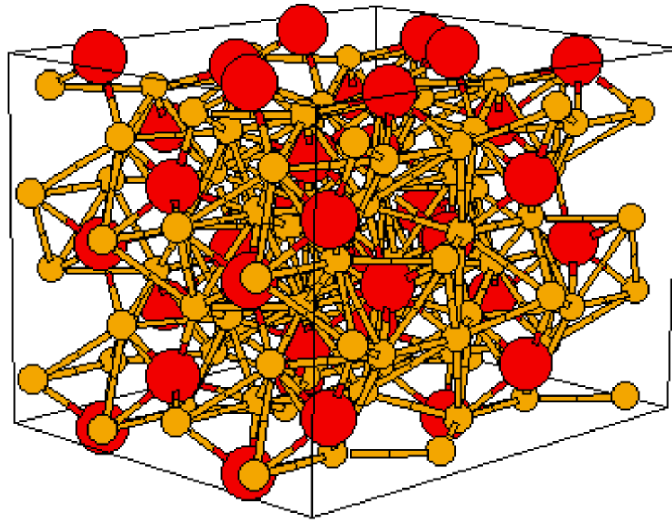




## Example exi1

### Diffusion in system with B2 ordering

Diffusion including effects from chemical ordering. In this example folder, there is also a datafile `AlFeNi-data.TDB`, which contains both a thermodynamic and kinetic description for the ordered and disordered bcc.



## exil-setup

### SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,  
Stockholm, Sweden

Software running on Windows 64-bit wordlength  
Compiler: Intel Fortran Compiler 2025.0.0  
License library version: 9.7.0.0036  
Linked: Nov 19 2025 at 14:44:36

```
SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exil\setup.DCM.test"
```

```
SYS: @@
```

```
SYS: @@ Diffusion in complex phases.
```

```
SYS: @@ Diffusion in a system with B2 ordering
```

```
SYS: @@ This example shows diffusion in a system with B2 ordering.
```

```
SYS: @@ The datafile AlFeNi-data.TDB contains both a thermodynamic
```

```
SYS: @@ and kinetic description for the ordered and disordered BCC.
```

```
SYS: @@-----
```

```
SYS:
```

```
SYS: @@ exil_setup.DCM
```

```
SYS:
```

```
SYS:
```

```
SYS: go da
```

```
THERMODYNAMIC DATABASE module
```

```
Database folder:
```

```
C:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\databases\da
```

```
ta
```

```
Current database: Steels/Fe-Alloys v12.0
```

```
VA /- DEFINED
```

```
DICTRA FCC_A1 REJECTED
```

```
TDB_TCFE12: sw user AlFeNi-data.TDB
```

```
Current database: User defined Database
```

```
This database does not support the DATABASE_INFORMATION command
```

```
VA DEFINED
```

```
12:13:00,632 [Thread-0] INFO TDBFileParser: USER_1695849785_22, number of lines read: 609
```

```
12:13:01,043 [Thread-0] INFO DatabaseUtils: Parsing of USER_1695849785_22 completed in 486 ms
```

```
TDB_USER: def-sys fe al ni
```

```
FE AL NI
```

```
DEFINED
```

```
TDB_USER: rej ph *
```

```
B2_BCC BCC_DIS B2_ORD
```

```
REJECTED
```

```
TDB_USER: res ph bcc_dis b2_ord
```

```
BCC_DIS B2_ORD RESTORED
```

```
TDB_USER: get
```

```
12:13:01,235 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***
```

```
ELEMENTS .....
```

```
SPECIES .....
```

```
PHASES .....
```

```
PARAMETERS ...
```

```
FUNCTIONS ....
```

```
INFO: Forcing option USE_POLY3 for complex phase B2_ORD
```

```
-OK-
```

```
TDB_USER: go -m
```

```
NO TIME STEP DEFINED
```

```
DIC> set-cond glob T 0 1277; * N
```

```
DIC>
```

```
DIC> enter-region beta
```

```
DIC>
```

```
DIC> enter-grid beta
```

```
WIDTH OF REGION /1/: 2e-3
```

```
TYPE /AUTO/: double
```

```
NUMBER OF POINTS /50/: 50
```

```
VALUE OF R IN THE GEOMETRICAL SERIE FOR LOWER PART OF REGION: 0.85
```

```
VALUE OF R IN THE GEOMETRICAL SERIE FOR UPPER PART OF REGION: 1.1765
```

```
DIC>
```

```
DIC> enter-phase
```

```
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
```

```
REGION NAME : /BETA/: beta
```

```
PHASE TYPE /MATRIX/: matrix
```

```
PHASE NAME: /NONE/: b2_ord
```

```
DIC>
```

```
DIC> enter-composition
```

```
REGION NAME : /BETA/: beta
```

```
PHASE NAME: /B2_ORD/: b2_ord
```

```
DEPENDENT COMPONENT ? /NI/: fe
```

```
COMPOSITION TYPE /MOLE_FRACTION/: mole-fraction
```

```
PROFILE FOR /AL/: ni
```

```
TYPE /LINEAR/: function
```

```
Function F(X)= 0.28-0.277*erf((x-1e-3)/3e-6);
```

```
PROFILE FOR /NI/: al
```

```
TYPE /FUNCTION/: function
```

```
Function F(X)= 0.4295-0.0105*erf((x-1e-3)/3e-6);
```

```
12:13:02,359 [Thread-0] INFO Database: Preparing system for use: USER_1695849785_22
```

```
12:13:02,996 [Thread-0] INFO Phase: Preparing phase for use: B2_ORD
```

```
12:13:03,194 [Thread-0] INFO Phase: Preparing phase for use: BCC_DIS
```

```
DIC>
```

```
DIC> set-simulation-time
```

```
END TIME FOR INTEGRATION /.1/: 345600
```

```
AUTOMATIC TIMESTEP CONTROL /YES/:
```

```
MAX TIMESTEP DURING INTEGRATION /34560/:
```

```
INITIAL TIMESTEP : /1E-07/:
```

```
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
```

```
DIC> s-a-s-v
```

```
AUTOMATIC STARTING VALUES FOR PHASE COMPOSITIONS /YES/: no
```

```
START VALUES FOR PHASES IN REGION BETA
```

```
PHASE: B2_ORD
```

```
MAJOR CONSTITUENTS IN PHASE B2_ORD: NI;AL
```

```
DIC>
```

```
DIC>
```

```
DIC>
```

```
DIC>
```

```
DIC>
```

```
DIC>
```

```
DIC> save ex11 yes
DIC>
DIC> set-inter
--OK--
DIC>
```

exil-run

DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exil\run.DCM.test"

DIC>

DIC>

DIC> @@ exil\_run.DCM

DIC>

DIC> @@

DIC> @@ FILE FOR RUNNING EXAMPLE i1

DIC> @@

DIC>

DIC> @@

DIC> @@ ENTER THE DICTRA MONITOR AND READ THE STORE RESULT FILE

DIC> @@

DIC> go d-m

TIME STEP AT TIME 0.00000E+00

DIC> read exil

OK

DIC>

DIC> @@

DIC> @@ START THE SIMULATION

DIC> @@

DIC> sim

INFO: Default responses (if any) will be applied during the simulation. Use "SIMULATE\_REACTION NO" instead for manual input.

DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE

INFO: FORCED STARTING VALUES TURNED ON

U-FRACTION IN SYSTEM: AL = .429499345639258 FE = .290517917020317

NI = .279982737340425

TOTAL SIZE OF SYSTEM: .002 [m]

U-FRACTION IN SYSTEM: AL = .429499345639258 FE = .290517917020317

NI = .279982737340425

TOTAL SIZE OF SYSTEM: .002 [m]

6 GRIDPOINT(S) ADDED TO CELL #1 REGION: BETA

TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: AL = .429499345639258 FE = .290517917020317

NI = .279982737340425

TOTAL SIZE OF SYSTEM: .002 [m]

CPU time used in timestep 5 seconds

TIME = 0.10010000E-03 DT = 0.10000000E-03 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: AL = .429499345639258 FE = .290517917020317

NI = .279982737340425

TOTAL SIZE OF SYSTEM: .002 [m]

CPU time used in timestep 1 seconds

TIME = 0.40010010 DT = 0.400000000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: AL = .429499345639258 FE = .290517917020317

NI = .279982737340425

TOTAL SIZE OF SYSTEM: .002 [m]

CPU time used in timestep 1 seconds

TIME = 513.08856 DT = 512.68846 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: AL = .429499345639247 FE = .290517917020327

NI = .279982737340426

TOTAL SIZE OF SYSTEM: .002 [m]

CPU time used in timestep 1 seconds

TIME = 1538.4655 DT = 1025.3769 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: AL = .429499345639233 FE = .290517917020342

NI = .279982737340425

TOTAL SIZE OF SYSTEM: .002 [m]

CPU time used in timestep 1 seconds

TIME = 3589.2193 DT = 2050.7538 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: AL = .429499345639231 FE = .290517917020345

NI = .279982737340424

TOTAL SIZE OF SYSTEM: .002 [m]

CPU time used in timestep 2 seconds

TIME = 7690.7270 DT = 4101.5077 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: AL = .429499345639227 FE = .290517917020346

NI = .279982737340428

TOTAL SIZE OF SYSTEM: .002 [m]

CPU time used in timestep 1 seconds

TIME = 15893.742 DT = 8203.0154 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: AL = .429499345639233 FE = .290517917020342

NI = .279982737340426

TOTAL SIZE OF SYSTEM: .002 [m]

CPU time used in timestep 2 seconds

TIME = 32299.773 DT = 16406.031 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: AL = .42949934563921 FE = .290517917020363

NI = .279982737340427

TOTAL SIZE OF SYSTEM: .002 [m]

CPU time used in timestep 1 seconds

TIME = 65111.835 DT = 32812.062 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: AL = .429499345639174 FE = .290517917020383

NI = .279982737340444

TOTAL SIZE OF SYSTEM: .002 [m]

CPU time used in timestep 2 seconds

TIME = 99671.835 DT = 34560.000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: AL = .429499345639088 FE = .290517917020497

NI = .279982737340415

TOTAL SIZE OF SYSTEM: .002 [m]

CPU time used in timestep 2 seconds

TIME = 134231.83 DT = 34560.000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: AL = .429499345639131 FE = .290517917020483

NI = .279982737340386

TOTAL SIZE OF SYSTEM: .002 [m]

CPU time used in timestep 1 seconds

TIME = 168791.83 DT = 34560.000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: AL = .429499345639167 FE = .290517917020446

NI = .279982737340387

TOTAL SIZE OF SYSTEM: .002 [m]

CPU time used in timestep 2 seconds

TIME = 203351.83 DT = 34560.000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: AL = .429499345639157 FE = .290517917020456

NI = .279982737340388

TOTAL SIZE OF SYSTEM: .002 [m]

CPU time used in timestep 1 seconds

TIME = 237911.83 DT = 34560.000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: AL = .429499345639151 FE = .290517917020441

NI = .279982737340408

TOTAL SIZE OF SYSTEM: .002 [m]

CPU time used in timestep 1 seconds

TIME = 272471.83 DT = 34560.000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: AL = .429499345639151 FE = .290517917020425

NI = .279982737340423

TOTAL SIZE OF SYSTEM: .002 [m]

```
CPU time used in timestep          2 seconds
TIME = 307031.83      DT = 34560.000      SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: AL = .429499345639159 FE = .290517917020413
NI = .279982737340428
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep          1 seconds
TIME = 341591.83      DT = 34560.000      SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: AL = .429499345639172 FE = .290517917020402
NI = .279982737340426
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep          1 seconds
TIME = 345600.00      DT = 4008.1652      SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: AL = .429499345639172 FE = .290517917020402
NI = .279982737340426
TOTAL SIZE OF SYSTEM: .002 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME      0.0000000
DELETING TIME-RECORD FOR TIME      0.10000000E-06
DELETING TIME-RECORD FOR TIME      0.10010000E-03
DELETING TIME-RECORD FOR TIME      0.40010010
DELETING TIME-RECORD FOR TIME      513.08856
DELETING TIME-RECORD FOR TIME      1538.4655
DELETING TIME-RECORD FOR TIME      3589.2193
DELETING TIME-RECORD FOR TIME      7690.7270
DELETING TIME-RECORD FOR TIME      15893.742
DELETING TIME-RECORD FOR TIME      32299.773
DELETING TIME-RECORD FOR TIME      65111.835
DELETING TIME-RECORD FOR TIME      99671.835
DELETING TIME-RECORD FOR TIME      134231.83
DELETING TIME-RECORD FOR TIME      168791.83
DELETING TIME-RECORD FOR TIME      203351.83
DELETING TIME-RECORD FOR TIME      237911.83
DELETING TIME-RECORD FOR TIME      272471.83
DELETING TIME-RECORD FOR TIME      307031.83

KEEPING TIME-RECORD FOR TIME      341591.83
AND FOR TIME                      345600.00
WORKSPACE RECLAIMED

TIMESTEP AT      345600.000      SELECTED
```

```
DIC>
DIC> set-inter
--OK--
DIC>
```

# exil-plot

## DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exil\plot.DCM.test"

DIC>

DIC> @@ exil\_plot.DCM

DIC>

DIC> @@

DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE i1

DIC> @@

DIC>

DIC> @@

DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE

DIC> @@

DIC> go d-m

TIME STEP AT TIME 3.45600E+05

DIC> read exil

OK

DIC>

DIC> @@

DIC> @@ ENTER THE POST PROCESSOR

DIC> @@

DIC> post

POST PROCESSOR VERSION 1.7

Implemented by Bjorn Jonsson

POST-1:

POST-1: s-d-a x dist glob

INFO: Distance is set as independent variable

POST-1:

POST-1: s-d-a y m-f al

POST-1:

POST-1: s-p-c time last

POST-1:

POST-1:

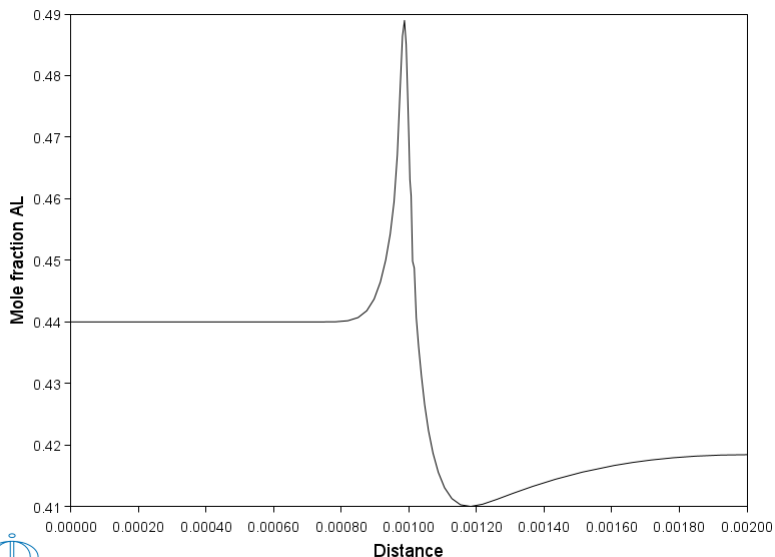
POST-1: SET\_EXP\_FILE\_FORMAT 5

POST-1: MAKE c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\unite\distribution\macroResult.exp Y

POST-1: SET\_EXP\_FILE\_FORMAT 10

POST-1:

POST-1: plot



POST-1:

POST-1: @?<Hit\_return\_to\_continue>

POST-1:

POST-1: ent tab prof

Variable(s) x(al) x(ni)

POST-1:

POST-1: ent fun rdist

FUNCTION: 1e6\*(gd-10e-4)

&

POST-1: s-d-a y prof

COLUMN NUMBER /\*/: 1 2

POST-1:

POST-1: s-d-a x rdist

POST-1:

POST-1:

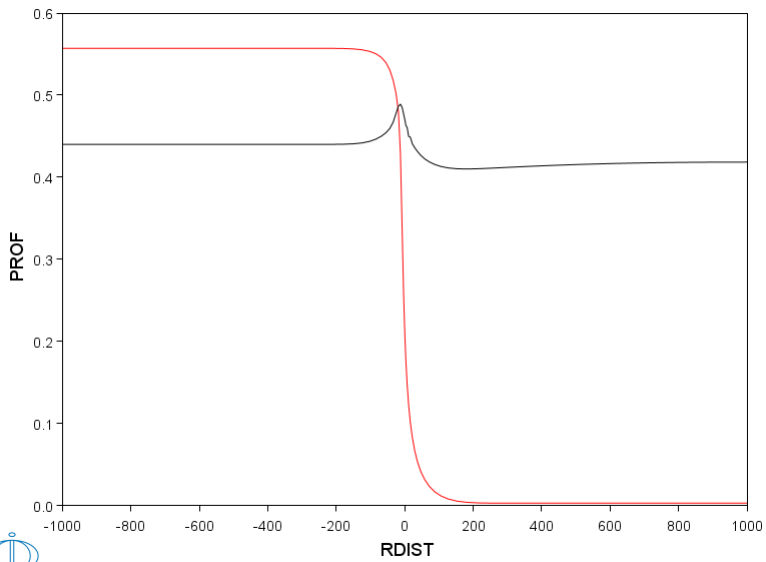
POST-1: SET\_EXP\_FILE\_FORMAT 5

POST-1: MAKE c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\unite\distribution\macroResult.exp Y

POST-1: SET\_EXP\_FILE\_FORMAT 10

POST-1:

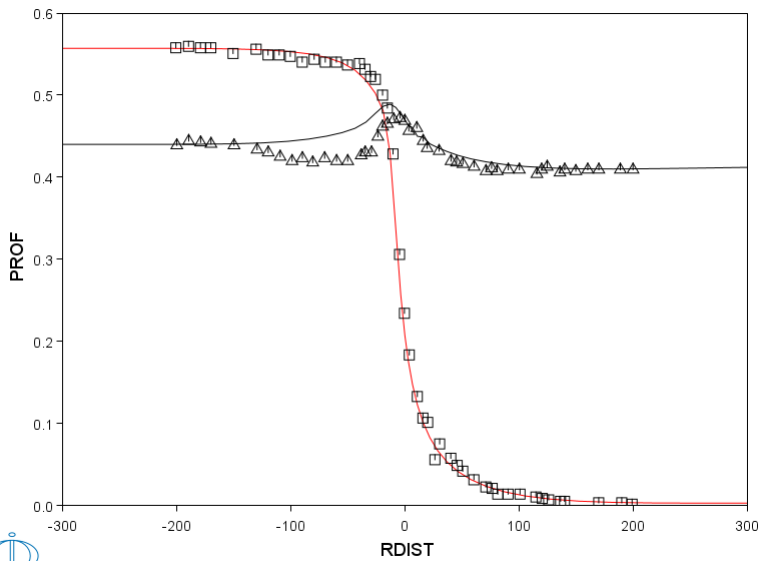
POST-1: plot



```

POST-1:
POST-1:
POST-1: @?<Hit_return_to_continue>
POST-1:
POST-1: app y exil.exp
PROLOGUE NUMBER: /0/: 1
DATASET NUMBER(s): /-1/: 1
POST-1:
POST-1: s-s-s x n -300 300
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

```



```

POST-1:
POST-1:
POST-1: set-inter
--OK--
POST-1:

```



## Example exi2

### 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., *Met. Trans A*, vol 13A (1982), pp. 1871-1873.

$$J \sim \Delta\mu$$

## exi2-setup

### SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,  
Stockholm, Sweden

Software running on Windows 64-bit wordlength  
Compiler: Intel Fortran Compiler 2025.0.0  
License library version: 9.7.0.0036  
Linked: Nov 19 2025 at 14:44:36

```
SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exi2\setup.DCM.test"
```

```
SYS: @@  
SYS: @@ Diffusion in complex phases.  
SYS: @@ Diffusion of carbon in cementite  
SYS: @@ This example demonstrates the use of the model for calculation of  
SYS: @@ diffusion through a stoichiometric phase. The flux of a component in  
SYS: @@ the stoichiometric phase is assumed to be proportional to the  
SYS: @@ difference in chemical potential at each side of the stoichiometric  
SYS: @@ phase multiplied with the mobility for the component in the phase. The  
SYS: @@ mobility is assessed from experimental information and is basically  
SYS: @@ the tracer diffusivity for the component.  
SYS: @@  
SYS: @@ This calculation is compared with experimental data where a sample of  
SYS: @@ pure iron has been exposed to a gas atmosphere with a certain carbon  
SYS: @@ activity. The weight gain is then measured as a function of time.  
SYS: @@ The experimental data is obtained from Ozturk B., Fearing V. L.,  
SYS: @@ Ruth A. Jr. and Simkovich G., Met. Trans A, vol 13A (1982), pp. 1871-1873.  
SYS: @@-----
```

```
SYS: @@  
SYS: @@ RETRIEVE DATA FROM THE DATABASES  
SYS: @@  
SYS: go da  
THERMODYNAMIC DATABASE module  
Database folder:  
C:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\databases\da  
ta  
Current database: Steels/Fe-Alloys v12.0
```

```
VA /- DEFINED  
DICTRA_FCC_A1 REJECTED
```

```
TDB_TCFE12: @@  
TDB_TCFE12: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA  
TDB_TCFE12: @@  
TDB_TCFE12: switch FEDEMO  
Current database: Iron Demo Database v6.0
```

```
VA /- DEFINED  
TDB_FEDEMO: def-sys fe c  
FE C DEFINED  
TDB_FEDEMO: rej ph * all  
GAS:G LIQUID:L BCC_A2  
C14 LAVES CBCC_A12 CEMENTITE_D011  
CUB_A13 DIAMOND_A4 FCC_A1  
GRAPHITE_A9 HCP_A3 KSI_CARBIIDE  
M23C6_D84 M5C2 M7C3_D101  
REJECTED
```

```
TDB_FEDEMO: res ph bcc fcc cementite grap  
BCC_A2 FCC_A1 CEMENTITE_D011  
GRAPHITE_A9 RESTORED
```

```
TDB_FEDEMO: get  
12:16:24,231 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***  
REINITIATING GES .....  
ELEMENTS .....  
SPECIES .....  
PHASES .....  
PARAMETERS ...  
FUNCTIONS ....
```

Use the command LIST\_REFERENCES to see the list of references for assessed data

```
-OK-  
TDB_FEDEMO:  
TDB_FEDEMO: @@  
TDB_FEDEMO: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE MOBILITY DATA  
TDB_FEDEMO: @@  
TDB_FEDEMO: app MFEDEMO  
Current database: Fe-Alloys Mobility demo database v5.0
```

```
VA DEFINED  
APP: def-sys fe c  
FE C DEFINED  
APP: rej ph * all  
BCC_A2 FCC_A1 CEMENTITE_D011  
LIQUID:L REJECTED  
APP: res ph fcc bcc cementite  
FCC_A1 BCC_A2 CEMENTITE_D011  
RESTORED  
APP: get  
ELEMENTS .....  
SPECIES .....  
PHASES .....  
PARAMETERS ...  
FUNCTIONS ....
```

Use the command LIST\_REFERENCES to see the list of references for assessed data

```
-OK-  
APP:  
APP: @@  
APP: @@ ENTER THE DICTRA MONITOR  
APP: @@  
APP: go d-m  
NO TIME STEP DEFINED  
*** ENTERING GRAPHITE_A9 AS A DIFFUSION NONE PHASE
```

```

DIC>
DIC> set-ref c grap,,,,,,,,,
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob t 0 723; * n
DIC>
DIC> @@
DIC> @@ ENTER THE REGIONS carb AND fer
DIC> @@
DIC> enter-region
REGION NAME : fer
DIC>
DIC> enter-region
REGION NAME : carb
ATTACH TO REGION NAMED /FER/:
ATTACHED TO THE RIGHT OF FER /YES/:
DIC> @@
DIC> @@ ENTER LINEAR GRIDS INTO THE REGIONS
DIC> @@
DIC> @@
DIC> @@ ENTER A SIZE FOR THE FERRITE
DIC> @@
DIC> enter-grid
REGION NAME : /FER/: fer
WIDTH OF REGION /1/: 3.3E-6
TYPE /AUTO/: AUTO
DIC>
DIC> @@
DIC> @@ ENTER A SIZE (VERY SMALL) FOR THE CEMENTITE LAYER
DIC> @@
DIC> @@
DIC> enter-grid
REGION NAME : /CARB/: carb
WIDTH OF REGION /1/: 1E-12
TYPE /AUTO/: AUTO
DIC>
DIC>
DIC> @@
DIC> @@ ENTER PHASES INTO THE REGIONS
DIC> @@
DIC> enter-phase act carb matrix cementite
COMPOSITION RECORD FOR STOICHIOMETRIC PHASE CEMENTITE_D011 IN REGION CARB CREATED
DIC> enter-phase act fer matrix bcc#1
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITIONS IN THE PHASES
DIC> @@
DIC> enter-composition
REGION NAME : /FER/: carb
PHASE NAME: /CEMENTITE_D011/: cementite
DIC>
DIC> enter-composition
REGION NAME : /FER/: fer
PHASE NAME: /BCC_A2/: bcc#1
COMPOSITION TYPE /MOLE_FRACTION/: weig-fraction
PROFILE FOR /C/: C lin 1E-5 1E-5
DIC>
DIC> set-cond bound upp
CONDITION TYPE /CLOSED_SYSTEM/: mix
Dependent substitutional element:FE
Dependent interstitial element:VA
LOW TIME LIMIT /0/: 0
ACR(C)(TIME)= 9;
HIGH TIME LIMIT /*/: *
ANY MORE RANGES /N/: N
DIC>
DIC>
DIC> @@
DIC> @@ SIMULATE FOR 150 MINUTES
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 9000
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /900/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exi2 Y
DIC>
DIC> set-inter
--OK--
DIC>

```

exi2-run

DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exi2\run.DCM.test"

DIC>

DIC>

DIC> @@ exi2\_run.DCM

DIC>

DIC> @@

DIC> @@ FILE FOR RUNNING EXAMPLE i2

DIC> @@

DIC>

DIC> @@

DIC> @@ ENTER THE DICTRA MONITOR AND READ THE STORE RESULT FILE

DIC> @@

DIC> go d-m

TIME STEP AT TIME 0.00000E+00

\*\*\* ENTERING GRAPHITE\_A9 AS A DIFFUSION NONE PHASE

DIC> read exi2

OK

DIC>

DIC> @@

DIC> @@ START THE SIMULATION

DIC> @@

DIC> sim

INFO: Default responses (if any) will be applied during the simulation. Use "SIMULATE\_REACTION NO" instead for manual input.

Region: FER

geometric 0.833333 dense at 0.330000E-05 58 points

Region: CARB

geometric 1.03732 dense at 0.00000 27 points

geometric 0.964027 dense at 0.100000E-11 28 points

DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE

Trying old scheme 3

U-FRACTION IN SYSTEM: C = 4.6598005784384E-05 FE = 1

TOTAL SIZE OF SYSTEM: 3.300001E-06 [m]

U-FRACTION IN SYSTEM: C = 4.6598005784384E-05 FE = 1

TOTAL SIZE OF SYSTEM: 3.300001E-06 [m]

0.111094398574294 0.111116618523482 1.492608521054145E-021 TIME = 0.10000000E-06 DT = 0.10000000E-

06 SUM OF SQUARES = 0.14926085E-20

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.18662795E-05 AND -0.18662795E-05

POSITION OF INTERFACE FER / CARB IS 0.32999998E-05

U-FRACTION IN SYSTEM: C = 4.65902910647489E-05 FE = 1

TOTAL SIZE OF SYSTEM: 3.300001E-06 [m]

CPU time used in timestep 0 seconds

3.323893769823795E-005 3.324596706135781E-005 7.233236589042160E-019 TIME = 0.42041248E-04 DT = 0.41941248E-

04 SUM OF SQUARES = 0.72332366E-18

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.99189833E-07 AND -0.99189833E-07

POSITION OF INTERFACE FER / CARB IS 0.32999957E-05

U-FRACTION IN SYSTEM: C = 4.69866088811509E-05 FE = 1

TOTAL SIZE OF SYSTEM: 3.300001E-06 [m]

43 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: CARB

CPU time used in timestep 0 seconds

5.940110999669561E-006 5.941690376777649E-006 2.104117988379031E-021 TIME = 0.12592374E-03 DT = 0.83882496E-

04 SUM OF SQUARES = 0.21041180E-20

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.24081889E-07 AND -0.24081889E-07

POSITION OF INTERFACE FER / CARB IS 0.32999936E-05

U-FRACTION IN SYSTEM: C = 4.71625228459343E-05 FE = 1

TOTAL SIZE OF SYSTEM: 3.300001E-06 [m]

CPU time used in timestep 1 seconds

4.461608160703778E-006 4.464931782486729E-006 1.636372192861907E-024 TIME = 0.29368874E-03 DT = 0.16776499E-

03 SUM OF SQUARES = 0.16363722E-23

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.17262907E-07 AND -0.17262907E-07

POSITION OF INTERFACE FER / CARB IS 0.32999907E-05

U-FRACTION IN SYSTEM: C = 4.74178764530576E-05 FE = 1

TOTAL SIZE OF SYSTEM: 3.300001E-06 [m]

2 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: CARB

CPU time used in timestep 0 seconds

2.345403980549840E-006 2.347131404695197E-006 9.284327548873648E-025 TIME = 0.62921872E-03 DT = 0.33552998E-

03 SUM OF SQUARES = 0.92843275E-24

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.12322827E-07 AND -0.12322827E-07

POSITION OF INTERFACE FER / CARB IS 0.32999866E-05

U-FRACTION IN SYSTEM: C = 4.77844661736849E-05 FE = 1

TOTAL SIZE OF SYSTEM: 3.300001E-06 [m]

46 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: CARB

CPU time used in timestep 0 seconds

1.221304081916776E-006 1.222193895137852E-006 3.101453521948746E-025 TIME = 0.13002787E-02 DT = 0.67105997E-

03 SUM OF SQUARES = 0.31014535E-24

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.87607071E-08 AND -0.87607071E-08

POSITION OF INTERFACE FER / CARB IS 0.32999807E-05

U-FRACTION IN SYSTEM: C = 4.83070921370174E-05 FE = 1

TOTAL SIZE OF SYSTEM: 3.300001E-06 [m]

17 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: CARB

CPU time used in timestep 0 seconds

6.255421686500668E-007 6.259949039541144E-007 1.800510303087057E-025 TIME = 0.26423986E-02 DT = 0.13421199E-

02 SUM OF SQUARES = 0.18005103E-24

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.62125570E-08 AND -0.62125570E-08

POSITION OF INTERFACE FER / CARB IS 0.32999724E-05

U-FRACTION IN SYSTEM: C = 4.90492847126159E-05 FE = 1

TOTAL SIZE OF SYSTEM: 3.300001E-06 [m]

41 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: CARB

CPU time used in timestep 0 seconds

3.168643734259357E-007 3.170928724322179E-007

output ignored...

... output resumed

1.301364867290735E-007 1.302712141808378E-007 1.843534117375387E-

028 TIME = 3207.3147 DT = 900.00000 SUM OF SQUARES = 0.18435341E-27

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.45187270E-11 AND -0.45187270E-11

POSITION OF INTERFACE FER / CARB IS 0.32713661E-05

U-FRACTION IN SYSTEM: C = .00291788309545735 FE = 1

TOTAL SIZE OF SYSTEM: 3.300001E-06 [m]

21 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: CARB

CPU time used in timestep 0 seconds

```

3.377659190387827E-008      3.383086688779757E-008      1.961189739094106E-
029      TIME = 4107.3147      DT = 900.00000      SUM OF SQUARES = 0.19611897E-28
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.38769576E-11 AND -0.38769576E-11
POSITION OF INTERFACE FER / CARB IS 0.32678768E-05
U-FRACTION IN SYSTEM: C = .00327030650759308 FE = 1
TOTAL SIZE OF SYSTEM: 3.300001E-06 [m]
15 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: CARB

CPU time used in timestep      0 seconds
1.311342784028283E-008      1.314244738346602E-008      3.302723518027951E-
030      TIME = 5007.3147      DT = 900.00000      SUM OF SQUARES = 0.33027235E-29
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.34558504E-11 AND -0.34558504E-11
POSITION OF INTERFACE FER / CARB IS 0.32647666E-05
U-FRACTION IN SYSTEM: C = .00358445040429918 FE = 1
TOTAL SIZE OF SYSTEM: 3.300001E-06 [m]
12 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: CARB

CPU time used in timestep      0 seconds
6.184494689289238E-009      6.202261928651467E-009      2.840823780400587E-
031      TIME = 5907.3147      DT = 900.00000      SUM OF SQUARES = 0.28408238E-30
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.31507905E-11 AND -0.31507905E-11
POSITION OF INTERFACE FER / CARB IS 0.32619309E-05
U-FRACTION IN SYSTEM: C = .00387086373221729 FE = 1
TOTAL SIZE OF SYSTEM: 3.300001E-06 [m]
24 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: CARB

CPU time used in timestep      0 seconds
3.274215435456154E-009      3.286004107096795E-009      4.286971591269478E-
031      TIME = 6807.3147      DT = 900.00000      SUM OF SQUARES = 0.42869716E-30
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.29160992E-11 AND -0.29160992E-11
POSITION OF INTERFACE FER / CARB IS 0.32593064E-05
U-FRACTION IN SYSTEM: C = .00413594313662343 FE = 1
TOTAL SIZE OF SYSTEM: 3.300001E-06 [m]
10 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: CARB

CPU time used in timestep      0 seconds
1.870097337252293E-007      1.878344674571135E-007      1.264643842388650E-
029      TIME = 7707.3147      DT = 900.00000      SUM OF SQUARES = 0.12646438E-28
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.27280333E-11 AND -0.27280333E-11
POSITION OF INTERFACE FER / CARB IS 0.32568511E-05
U-FRACTION IN SYSTEM: C = .00438392696890556 FE = 1
TOTAL SIZE OF SYSTEM: 3.300001E-06 [m]
9 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: CARB

CPU time used in timestep      0 seconds
1.125755556993257E-007      1.131743110018835E-007      3.856145082900733E-
030      TIME = 8607.3147      DT = 900.00000      SUM OF SQUARES = 0.38561451E-29
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.25728080E-11 AND -0.25728080E-11
POSITION OF INTERFACE FER / CARB IS 0.32545356E-05
U-FRACTION IN SYSTEM: C = .00461780050542361 FE = 1
TOTAL SIZE OF SYSTEM: 3.300001E-06 [m]
7 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: CARB

CPU time used in timestep      0 seconds
7.034765029309732E-008      7.079414981850979E-008      2.601088760516486E-
031      TIME = 9000.0000      DT = 392.68528      SUM OF SQUARES = 0.26010888E-30
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.24417764E-11 AND -0.24417764E-11
POSITION OF INTERFACE FER / CARB IS 0.32535768E-05
U-FRACTION IN SYSTEM: C = .00471464650795351 FE = 1
TOTAL SIZE OF SYSTEM: 3.300001E-06 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 0.0000000
DELETING TIME-RECORD FOR TIME 0.10000000E-06
DELETING TIME-RECORD FOR TIME 0.42041248E-04
DELETING TIME-RECORD FOR TIME 0.12592374E-03
DELETING TIME-RECORD FOR TIME 0.29368874E-03
DELETING TIME-RECORD FOR TIME 0.62921872E-03
DELETING TIME-RECORD FOR TIME 0.13002787E-02
DELETING TIME-RECORD FOR TIME 0.26423986E-02
DELETING TIME-RECORD FOR TIME 0.53266385E-02
DELETING TIME-RECORD FOR TIME 0.10695118E-01
DELETING TIME-RECORD FOR TIME 0.21432078E-01
DELETING TIME-RECORD FOR TIME 0.42905997E-01
DELETING TIME-RECORD FOR TIME 0.85853835E-01
DELETING TIME-RECORD FOR TIME 0.17174951
DELETING TIME-RECORD FOR TIME 0.34354086
DELETING TIME-RECORD FOR TIME 0.68712357
DELETING TIME-RECORD FOR TIME 1.3742890
DELETING TIME-RECORD FOR TIME 2.7486198
DELETING TIME-RECORD FOR TIME 5.4972814
DELETING TIME-RECORD FOR TIME 10.994605
DELETING TIME-RECORD FOR TIME 21.989251
DELETING TIME-RECORD FOR TIME 43.978544
DELETING TIME-RECORD FOR TIME 87.957130
DELETING TIME-RECORD FOR TIME 175.91430
DELETING TIME-RECORD FOR TIME 351.82865
DELETING TIME-RECORD FOR TIME 703.65734
DELETING TIME-RECORD FOR TIME 1407.3147
DELETING TIME-RECORD FOR TIME 2307.3147
DELETING TIME-RECORD FOR TIME 3207.3147
DELETING TIME-RECORD FOR TIME 4107.3147
DELETING TIME-RECORD FOR TIME 5007.3147
DELETING TIME-RECORD FOR TIME 5907.3147
DELETING TIME-RECORD FOR TIME 6807.3147
DELETING TIME-RECORD FOR TIME 7707.3147

KEEPING TIME-RECORD FOR TIME 8607.3147
AND FOR TIME 9000.0000
WORKSPACE RECLAIMED

TIMESTEP AT 9000.0000 SELECTED

```

```

DIC>
DIC> set-inter
--OK--
DIC>

```

## exi2-plot

DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exi2\plot.DCM.test"

DIC>

DIC> @@ exi2\_plot.DCM

DIC>

DIC> @@

DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE i2

DIC> @@

DIC>

DIC> @@

DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE

DIC> @@

DIC> go d-m

TIME STEP AT TIME 9.00000E+03

\*\*\* ENTERING GRAPHITE\_A9 AS A DIFFUSION NONE PHASE

DIC>

DIC>

DIC> read exi2 Y

OK

DIC>

DIC>

DIC> @@

DIC> @@ PLOT THE SIZE OF THE CEMENTITE LAYER AS A FUNCTION OF TIME

DIC> @@

DIC> post

POST PROCESSOR VERSION 1.7

Implemented by Bjorn Jonsson

POST-1:

POST-1: ent-symb func csize

FUNCTION: 1e6\*(poi(car,u)-poi(car,l));

POST-1:

POST-1: ent-symb func minutes

FUNCTION: time/60;

POST-1:

POST-1: s-d-a x minutes

POST-1: s-d-a y csize

POST-1:

POST-1: s-p-c inter first

POST-1:

POST-1: s-a-t-s x n Time [min]

POST-1: s-a-t-s y n Distance [i;µm]

POST-1:

POST-1:

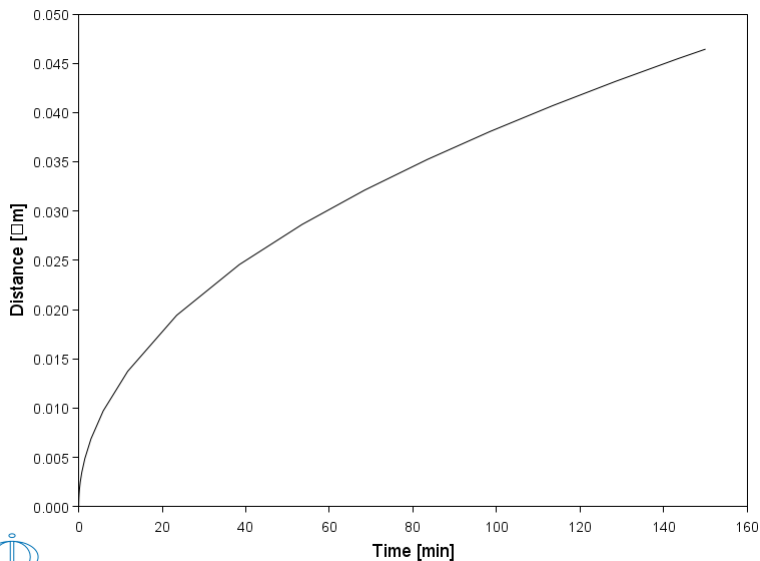
POST-1: SET\_EXP\_FILE\_FORMAT 5

POST-1: MAKE c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\unite\distribution\macroResult.exp Y

OST-1: SET\_EXP\_FILE\_FORMAT 10

POST-1:

POST-1: plot



POST-1:

POST-1: @?<\_hit\_return\_to\_continue\_>

POST-1:

POST-1:

POST-1: @@

POST-1: @@ ASSUME A CERTAIN TIME FOR NUCLEATION OF THE CEMENTITE LAYER

POST-1: @@

POST-1: ent-symb func cortim

FUNCTION: (time+1400)/60;

POST-1:

POST-1: @@

POST-1: @@ PLOT THE WEIGHT GAIN AS A FUNCTION OF TIME

POST-1: @@

POST-1: ent-symb func cwei

FUNCTION: 1e12\*(poi(car,u)-poi(car,l)-1E-12)\*12.01/2.33E-5\*1e-4)\*\*2;

POST-1:

POST-1:

POST-1: s-d-a x cortim

POST-1: s-d-a y cwei

POST-1:

POST-1: @@

POST-1: @@ COMPARE WITH EXPERIMENTAL DATA

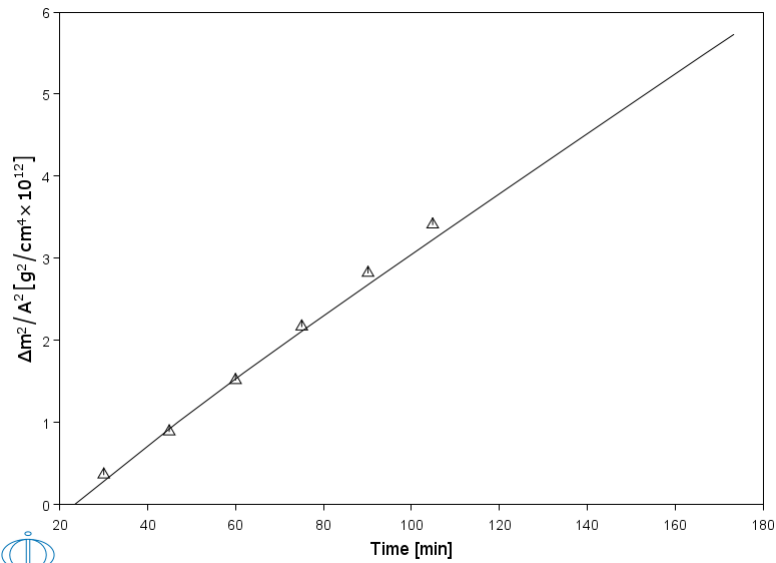
POST-1: @@

POST-1: app y exi2.exp 0; 1

POST-1:

POST-1:

```
POST-1: s-a-t-s x n Time [min]
POST-1: s-a-t-s y n \latex \Delta m^2/A^2, [g^2/cm^4\times 10^{12}]
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```



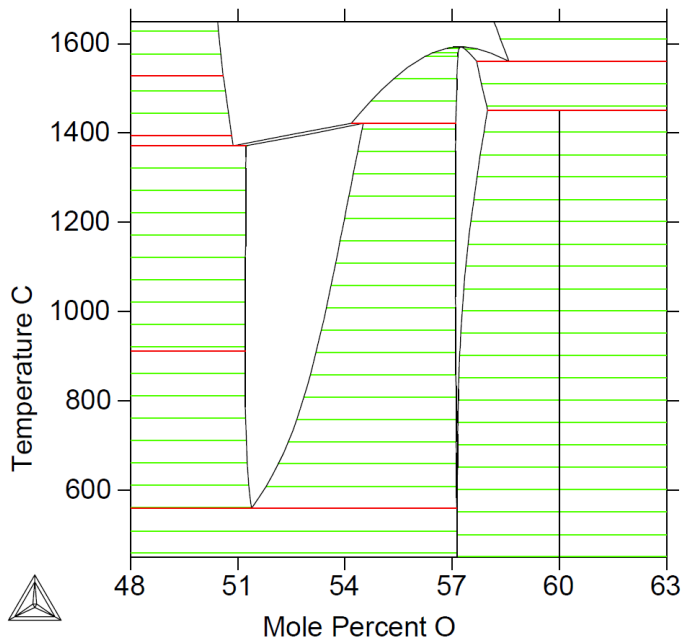
```
POST-1:
POST-1:
POST-1: set-inter
--OK--
POST-1:
```



## Example exi3a

### Diffusion in iron oxide (FeO)

This example shows the oxidation of an iron sample and the consequent growth of an oxide layer using the grain boundary diffusion contribution model.



## exi3a-setup

### SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,  
Stockholm, Sweden

Software running on Windows 64-bit wordlength  
Compiler: Intel Fortran Compiler 2025.0.0  
License library version: 9.7.0.0036  
Linked: Nov 19 2025 at 14:44:36

```
SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exi3a\setup.DCM.test"
```

```
SYS: @@  
SYS: @@ Diffusion in complex phases.  
SYS: @@ Diffusion in iron oxide (FeO)  
SYS: @@ This example shows the oxidation of an iron sample and the  
SYS: @@ consequent growth of an oxide layer.  
SYS: @@-----  
SYS:  
SYS: @@ exi3_setup.DCM  
SYS:  
SYS: @@  
SYS: @@ START BY GOING TO THE DATABASE MODULE  
SYS: @@  
SYS: go da  
THERMODYNAMIC DATABASE module  
Database folder:  
C:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\databases\da  
ta  
Current database: Steels/Fe-Alloys v12.0
```

```
VA /- DEFINED  
DICTRA_FCC_A1 REJECTED  
TDB_TCFE12:  
TDB_TCFE12: @@  
TDB_TCFE12: @@ SELECT A USER DATABASE FOR READING THE THERMODYNAMIC DATA  
TDB_TCFE12: @@  
TDB_TCFE12: sw user FeO.TDB  
Current database: User defined Database  
This database does not support the DATABASE_INFORMATION command  
  
VA /- DEFINED  
12:19:22,508 [Thread-0] INFO TDBFileParser: USER_190315336_22, number of lines read: 217  
12:19:22,759 [Thread-0] INFO DatabaseUtils: Parsing of USER_190315336_22 completed in 337 ms  
TDB_USER: def-sys fe o  
FE O DEFINED  
TDB_USER: rej sp *  
/- VA FE  
O FE+2 FE+3  
FE+4 FE2O3 FEO  
FEO3/2 O-2 O2  
REJECTED  
TDB_USER: res sp fe fe+2 fe+3 o o2 o-2 va  
FE FE+2 FE+3  
O O2 O-2  
VA RESTORED  
TDB_USER: rej ph * all  
GAS:G BCC_A2 SPINEL:I  
REJECTED  
TDB_USER: res ph bcc spinel gas  
BCC_A2 SPINEL:I GAS:G  
RESTORED  
TDB_USER:  
TDB_USER: get  
12:19:22,900 [Thread-0] INFO JavaWrapper: *** Invoking Gibbs Energy System v6 ***  
ELEMENTS .....  
SPECIES .....  
PHASES .....  
PARAMETERS ...  
FUNCTIONS ....
```

Use the command LIST\_REFERENCES to see the list of references for assessed data

-OK-

\*\*\* WARNING: One or more elements have been rejected only as species but not as elements. This is not allowed with GES6, temporarily reverting

```
TDB_USER:  
TDB_USER: @@  
TDB_USER: @@ SWITCH TO A USER-DEFINED MOBILITY DATABASE TO RETRIEVE MOBILITY DATA  
TDB_USER: @@  
TDB_USER: app user FeOmob.TDB  
Current database: User defined Database  
test database  
  
VA /- O  
DEFINED  
12:19:23,230 [Thread-0] INFO TDBFileParser: USER_1269960560_22, number of lines read: 129  
12:19:23,267 [Thread-0] INFO DatabaseUtils: Parsing of USER_1269960560_22 completed in 37 ms  
TDB_APP: def-sys fe o  
FE DEFINED  
TDB_APP: rej sp *  
/- VA FE  
O FE+2 FE+3  
FE2O3 FEO FEO3/2  
O-2 O2 REJECTED  
TDB_APP: res sp fe fe+2 fe+3 o o2 o-2 va  
FE FE+2 FE+3  
O O2 O-2  
VA RESTORED  
TDB_APP: rej ph * all  
SPINEL:I GAS:G BCC_A2  
REJECTED  
TDB_APP: res ph bcc spinel gas  
BCC_A2 SPINEL:I GAS:G  
RESTORED  
TDB_APP:  
TDB_APP: get
```

```

ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
*** ERROR 2018 IN DESHPH: DIFFUSION DATA NOT POSSIBLE FOR GAS PHASE
*** ERROR 2018 IN DESHPH: DIFFUSION DATA NOT POSSIBLE FOR GAS PHASE
FUNCTIONS ....
-OK-
TDB_APP:
TDB_APP:
TDB_APP: @@
TDB_APP: @@ ENTER THE DICTRA MONITOR
TDB_APP: @@
TDB_APP: go d-m
NO TIME STEP DEFINED
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 823; * N
DIC>
DIC>
DIC> @@
DIC> @@ SET THE REFERENCE STATE FOR O TO O2 (GAS)
DIC> @@
DIC> set-ref o gas,,,,,,,,
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE REGIONS fer AND sp
DIC> @@
DIC> ent-reg fer
DIC> ent-reg sp,,,,,,,,
DIC>
DIC>
DIC> @@
DIC> @@ ENTER PHASES INTO THE REGIONS
DIC> @@
DIC> ent-phase act fer matrix bcc#1
DIC> ent-phase act sp matrix spinel
DIC>
DIC>
DIC> @@
DIC> @@ ENTER GRIDS INTO THE REGIONS
DIC> @@
DIC>
DIC> @@
DIC> @@ ENTER A SIZE FOR THE FERRITE
DIC> @@
DIC> @@
DIC> ent-grid fer 4.99999e-3 AUTO
DIC>
DIC>
DIC> @@
DIC> @@ ENTER A THIN INITIAL SIZE FOR THE OXIDE
DIC> @@
DIC> @@
DIC> ent-grid sp 1.00e-10 AUTO
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITIONS IN BCC
DIC> @@
DIC> ent-comp fer bcc#1 m-f
PROFILE FOR /O/: o lin 1e-9 1e-9
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITIONS IN THE OXIDE
DIC> @@
DIC> ent-comp sp spinel m-f
this is a phase with charged species
with more than 2 sublattices
PROFILE FOR /FE/: FE lin 4.28771E-01 4.28549E-01
DIC>
DIC>
DIC> @@
DIC> @@ ENTER A BOUNDARY CONDITION "GAS" ON THE UPPER (RIGHT-MOST) INTERFACE
DIC> @@ OF THE OXIDE. THIS ALLOWS THE SYSTEM TO EXPAND AND THE OXIDE LAYER
DIC> @@ TO GROW EXTERNALLY. FOR THIS EXAMPLE AN OXYGEN ACTIVITY IS SPECIFIED
DIC> @@ THAT IS LOW ENOUGH NOT TO FORM CORUNDUM (FE2O3). WE ALSO SPECIFY
DIC> @@ THAT THERE IS NO FLUX OF Fe ACROSS THIS INTERFACE, I.E. NO Fe
DIC> @@ IS ALLOWED TO ENTER OR LEAVE THE SYSTEM.
DIC> @@
DIC> set-cond boundary upper gas
TYPE OF CONDITION FOR COMPONENT FE /ZERO_FLUX/: zero-flux
TYPE OF CONDITION FOR COMPONENT O /ZERO_FLUX/: act
LOW TIME LIMIT /O/: 0 4.5e-4; * N
DIC>
DIC>
DIC> @@
DIC> @@ ENTER START VALUES FOR THE INITIAL INTERFACE VELOCITIES
DIC> @@
DIC> s-a-s-v -1e-5 1e-5 yes
STARTING VALUES WILL BE TAKEN FROM PROFILES
DIC>
DIC>
DIC> @@
DIC> @@ SIMULATE FOR 24 HOURS
DIC> @@
DIC> s-s-time 86400,,,,
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC> @@
DIC> @@ SPECIFY THAT POTENTIALS AND NOT ACTIVITIES ARE VARIED AT THE PHASE
DIC> @@ INTERFACE. ALSO USE A FULLY IMPLICIT SCHEME FOR TIME INTEGRATION.
DIC> @@
DIC> set-option DEGREE_OF_IMPLICITY 1.0
DIC> set-option VARY_POTENTIALS_OR_ACTIVITIES POT
RELEASING OLD STARTING VALUES

```

```
DIC>  
DIC> @@  
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT  
DIC> @@  
DIC> save exi3.DIC Y  
DIC>  
DIC> set-inter  
--OK--  
DIC>
```

exi3a-run

DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exi3a\run.DCM.test"

DIC>

DIC>

DIC> @@ exi3\_run.DCM

DIC>

DIC> @@

DIC> @@ FILE FOR RUNNING EXAMPLE i3

DIC> @@

DIC>

DIC> @@

DIC> @@ ENTER THE DICTRA MONITOR AND READ THE STORE RESULT FILE

DIC> @@

DIC> go d-m

TIME STEP AT TIME 0.00000E+00

DIC> read exi3

OK

DIC>

DIC> @@

DIC> @@ START THE SIMULATION

DIC> @@

DIC> sim y

INFO: Default responses (if any) will be applied during the simulation. Use "SIMULATE\_REACTION NO" instead for manual input.

Region: FER

geometric 0.833333 dense at 0.499999E-02 58 points

Region: SP

geometric 1.03726 dense at 0.00000 27 points

geometric 0.964075 dense at 0.100000E-09 28 points

Trying old scheme 3

U-FRACTION IN SYSTEM: FE = 0.99999999500542 O = 2.10000395011622E-08

TOTAL SIZE OF SYSTEM: .0049999901 [m]

U-FRACTION IN SYSTEM: FE = 0.99999999500542 O = 2.10000395011622E-08

TOTAL SIZE OF SYSTEM: .0049999901 [m]

0.349081609858999 0.349080835531550 0.349081007853904 4.642752747505995E-002 1.120690054913772E-

022 TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.90194335E-22

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.39716422E-03 AND 0.0000000

POSITION OF INTERFACE FER / SP IS 0.49999900E-02

CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.67173966E-03 AND 0.0000000

POSITION OF INTERFACE SP / gas interface IS 0.49999901E-02

U-FRACTION IN SYSTEM: FE = 0.99999998952496 O = 3.46904751690148E-08

TOTAL SIZE OF SYSTEM: .00499999012746 [m]

2 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: SP

CPU time used in timestep 4 seconds

1.517028292176161E-005 1.517215069608089E-005 1.517300764370686E-005 2.265990420845123E-007 5.697661555441296E-

031 TIME = 0.30000000E-06 DT = 0.20000000E-06 SUM OF SQUARES = 0.56975558E-30

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.14930286E-03 AND 0.0000000

POSITION OF INTERFACE FER / SP IS 0.49999899E-02

CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.20336879E-03 AND 0.0000000

POSITION OF INTERFACE SP / gas interface IS 0.49999901E-02

U-FRACTION IN SYSTEM: FE = 0.99999998714832 O = 4.28252475791112E-08

TOTAL SIZE OF SYSTEM: .00499999013827 [m]

7 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: SP

CPU time used in timestep 1 seconds

1.514037495171659E-008 1.513166981068657E-008 1.510830032176752E-008 2.795568792863825E-011 9.864748592100637E-

033 TIME = 0.70000000E-06 DT = 0.40000000E-06 SUM OF SQUARES = 0.98630559E-32

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.14929887E-03 AND 0.0000000

POSITION OF INTERFACE FER / SP IS 0.49999899E-02

CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.21700179E-03 AND 0.0000000

POSITION OF INTERFACE SP / gas interface IS 0.49999902E-02

U-FRACTION IN SYSTEM: FE = 0.99999998166679 O = 6.01854379777001E-08

TOTAL SIZE OF SYSTEM: .00499999016535 [m]

44 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: SP

CPU time used in timestep 0 seconds

5.663774818837994E-007 5.665323146073978E-007 5.665310409931821E-007 2.246879451473522E-010 1.332775494962310E-

034 TIME = 0.15000000E-05 DT = 0.80000000E-06 SUM OF SQUARES = 0.85693538E-35

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.93408704E-04 AND 0.0000000

POSITION OF INTERFACE FER / SP IS 0.49999898E-02

CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.13329938E-03 AND 0.0000000

POSITION OF INTERFACE SP / gas interface IS 0.49999902E-02

U-FRACTION IN SYSTEM: FE = 0.99999997507896 O = 8.15134066057134E-08

TOTAL SIZE OF SYSTEM: .00499999019726 [m]

19 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: SP

CPU time used in timestep 1 seconds

8.058821561752016E-006 8.062619089474481E-006 8.062238357193631E-006 1.165684182191291E-008 2.052996181733722E-

032 TIME = 0.31000000E-05 DT = 0.16000000E-05 SUM OF SQUARES = 0.87750183E-32

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.70802777E-04 AND 0.0000000

POSITION OF INTERFACE FER / SP IS 0.49999897E-02

CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.10188903E-03 AND 0.0000000

POSITION OF INTERFACE SP / gas interface IS 0.49999902E-02

U-FRACTION IN SYSTEM: FE = 0.99999996490286 O = 1.14118010001096E-07

TOTAL SIZE OF SYSTEM: .004999990247 [m]

32 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: SP

CPU time used in timestep 0 seconds

8.132098852618615E-006 8.134925573841666E-006 8.134787791164075E-006 7.243073328920213E-009 2.777807879241706E-

031 TIME = 0.63000000E-05 DT = 0.32000000E-05 SUM OF SQUARES = 0.27354901E-30

output ignored...

... output resumed

POSITION OF INTERFACE FER / SP IS 0.49497155E-02

CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.85407152E-09 AND 0.0000000

POSITION OF INTERFACE SP / gas interface IS 0.50215844E-02

U-FRACTION IN SYSTEM: FE = .995603829359565 O = .0143121645761789

TOTAL SIZE OF SYSTEM: .00502158440342 [m]

27 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: SP

CPU time used in timestep 0 seconds

2.790409294570028E-007 2.794910911415554E-007 2.794508894727145E-007 3.803336758548622E-010 1.691959548799568E-

033 TIME = 56943.895 DT = 8640.0000 SUM OF SQUARES = 0.13910330E-32

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.54744068E-09 AND 0.0000000

POSITION OF INTERFACE FER / SP IS 0.49449857E-02

CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.78319159E-09 AND 0.0000000

POSITION OF INTERFACE SP / gas interface IS 0.50236213E-02

U-FRACTION IN SYSTEM: FE = .995197138119411 O = .0156533528957594  
TOTAL SIZE OF SYSTEM: .00502362129123 [m]  
14 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: SP

CPU time used in timestep 1 seconds  
1.594434870751020E-007 1.597546086899677E-007 1.597282693767137E-007 2.020570951031568E-010 8.380804523622581E-  
034 TIME = 65583.895 DT = 8640.0000 SUM OF SQUARES = 0.81927254E-33  
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.50752276E-09 AND 0.0000000  
POSITION OF INTERFACE FER / SP IS 0.49406007E-02  
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.72678065E-09 AND 0.0000000  
POSITION OF INTERFACE SP / gas interface IS 0.50255157E-02  
U-FRACTION IN SYSTEM: FE = .994819677334695 O = .0168969527422597  
TOTAL SIZE OF SYSTEM: .00502551567938 [m]  
14 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: SP

CPU time used in timestep 0 seconds  
9.565003039175641E-008 9.587316942933162E-008 9.585506335686136E-008 1.148735197124206E-010 4.521421471002847E-  
034 TIME = 74223.895 DT = 8640.0000 SUM OF SQUARES = 0.43333424E-33  
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.47496539E-09 AND 0.0000000  
POSITION OF INTERFACE FER / SP IS 0.49364970E-02  
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.68063741E-09 AND 0.0000000  
POSITION OF INTERFACE SP / gas interface IS 0.50272927E-02  
U-FRACTION IN SYSTEM: FE = .994466192093075 O = .0180607362911242  
TOTAL SIZE OF SYSTEM: .00502729268569 [m]  
13 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: SP

CPU time used in timestep 1 seconds  
5.967303039175641E-008 5.973203651930760E-008 5.971910347031317E-008 6.870509385067094E-011 1.113428249098871E-  
034 TIME = 82863.895 DT = 8640.0000 SUM OF SQUARES = 0.10833356E-33  
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.44780139E-09 AND 0.0000000  
POSITION OF INTERFACE FER / SP IS 0.49326280E-02  
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.64205364E-09 AND 0.0000000  
POSITION OF INTERFACE SP / gas interface IS 0.50289710E-02  
U-FRACTION IN SYSTEM: FE = .994132791227442 O = .0191577859112694  
TOTAL SIZE OF SYSTEM: .00502897102519 [m]  
10 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: SP

CPU time used in timestep 0 seconds  
1.009711694759717E-008 1.004042487447079E-008 1.016247011600812E-008 1.115235233007664E-011 5.115751414778595E-  
034 TIME = 86400.000 DT = 3536.1047 SUM OF SQUARES = 0.50856588E-33  
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.44532653E-09 AND 0.0000000  
POSITION OF INTERFACE FER / SP IS 0.49310532E-02  
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.61782693E-09 AND 0.0000000  
POSITION OF INTERFACE SP / gas interface IS 0.50295810E-02  
U-FRACTION IN SYSTEM: FE = .994011770932698 O = .0195898327439478  
TOTAL SIZE OF SYSTEM: .00502958100464 [m]

MUST SAVE WORKSPACE ON FILE

WORKSPACE SAVED ON FILE

RECLAIMING WORKSPACE

DELETING TIME-RECORD FOR TIME 0.0000000  
DELETING TIME-RECORD FOR TIME 0.10000000E-06  
DELETING TIME-RECORD FOR TIME 0.30000000E-06  
DELETING TIME-RECORD FOR TIME 0.70000000E-06  
DELETING TIME-RECORD FOR TIME 0.15000000E-05  
DELETING TIME-RECORD FOR TIME 0.31000000E-05  
DELETING TIME-RECORD FOR TIME 0.63000000E-05  
DELETING TIME-RECORD FOR TIME 0.12700000E-04  
DELETING TIME-RECORD FOR TIME 0.25500000E-04  
DELETING TIME-RECORD FOR TIME 0.51100000E-04  
DELETING TIME-RECORD FOR TIME 0.10230000E-03  
DELETING TIME-RECORD FOR TIME 0.20470000E-03  
DELETING TIME-RECORD FOR TIME 0.40950000E-03  
DELETING TIME-RECORD FOR TIME 0.81910000E-03  
DELETING TIME-RECORD FOR TIME 0.16383000E-02  
DELETING TIME-RECORD FOR TIME 0.32767000E-02  
DELETING TIME-RECORD FOR TIME 0.65535000E-02  
DELETING TIME-RECORD FOR TIME 0.13107100E-01  
DELETING TIME-RECORD FOR TIME 0.26214300E-01  
DELETING TIME-RECORD FOR TIME 0.52428700E-01  
DELETING TIME-RECORD FOR TIME 0.10485750  
DELETING TIME-RECORD FOR TIME 0.20971510  
DELETING TIME-RECORD FOR TIME 0.41943030  
DELETING TIME-RECORD FOR TIME 0.83886070  
DELETING TIME-RECORD FOR TIME 1.6777215  
DELETING TIME-RECORD FOR TIME 3.3554431  
DELETING TIME-RECORD FOR TIME 6.7108863  
DELETING TIME-RECORD FOR TIME 13.421773  
DELETING TIME-RECORD FOR TIME 26.843545  
DELETING TIME-RECORD FOR TIME 53.687091  
DELETING TIME-RECORD FOR TIME 107.37418  
DELETING TIME-RECORD FOR TIME 214.74836  
DELETING TIME-RECORD FOR TIME 429.49673  
DELETING TIME-RECORD FOR TIME 858.99346  
DELETING TIME-RECORD FOR TIME 1717.9869  
DELETING TIME-RECORD FOR TIME 3435.9738  
DELETING TIME-RECORD FOR TIME 6871.9477  
DELETING TIME-RECORD FOR TIME 13743.895  
DELETING TIME-RECORD FOR TIME 22383.895  
DELETING TIME-RECORD FOR TIME 31023.895  
DELETING TIME-RECORD FOR TIME 39663.895  
DELETING TIME-RECORD FOR TIME 48303.895  
DELETING TIME-RECORD FOR TIME 56943.895  
DELETING TIME-RECORD FOR TIME 65583.895  
DELETING TIME-RECORD FOR TIME 74223.895

KEEPING TIME-RECORD FOR TIME 82863.895  
AND FOR TIME 86400.000

WORKSPACE RECLAIMED

TIMESTEP AT 86400.0000 SELECTED

DIC>  
DIC> set-inter  
--OK--  
DIC>

## exi3a-plot

### DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exi3a\plot.DCM.test"

DIC>

DIC> @@ exi3\_plot.DCM

DIC>

DIC> @@

DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE i3

DIC> @@

DIC>

DIC> @@

DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE

DIC> @@

DIC> go d-m

TIME STEP AT TIME 8.64000E+04

DIC> read exi3

OK

DIC>

DIC> @@

DIC> @@ ENTER THE POST PROCESSOR

DIC> @@

DIC> post

POST PROCESSOR VERSION 1.7

Implemented by Bjorn Jonsson

POST-1:

POST-1: @@

POST-1: @@ PLOT THE THICKNESS OF THE OXIDE LAYER GROWING AT THE SURFACE.

POST-1: @@ FOR THIS WE NEED TO ENTER A FUNCTION ACCORDING TO THE FOLLOWING.

POST-1: ent func oxideth

FUNCTION: poi(sp,upper)-poi(sp,lower)

&

POST-1: @@

POST-1: @@ PUT THIS FUNCTION ON THE Y-AXIS

POST-1: @@

POST-1: s-d-a y oxideth

POST-1:

POST-1: @@

POST-1: @@ AND PLOT THE OXIDE THICKNESS VERSUS TIME

POST-1: @@

POST-1: s-d-a x time

INFO: Time is set as independent variable

POST-1:

POST-1: @@

POST-1: @@ SINCE WE ARE PLOTTING A FUNCTION, SPECIFY A PLOT CONDITION

POST-1: @@

POST-1: s-p-c interface sp upper

POST-1:

POST-1:

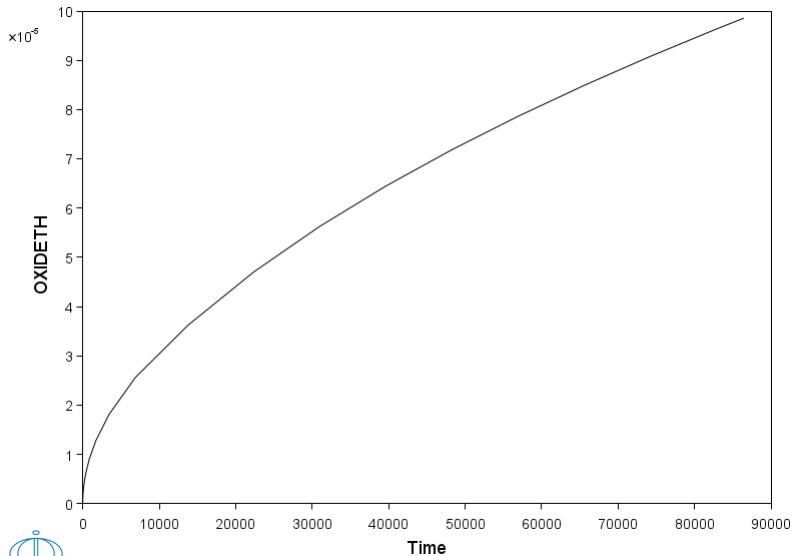
POST-1: SET\_EXP\_FILE\_FORMAT 5

POST-1: MAKE c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\unite\distribution\macroResult.exp Y

OST-1: SET\_EXP\_FILE\_FORMAT 10

POST-1:

POST-1: plot



POST-1:

POST-1: @?<Hit\_return\_to\_continue>

POST-1:

POST-1: @@

POST-1: @@ NOW PLOT THE MOBILITY IN A SPINEL FOR Fe+2 ON THE SECOND SUBLATTICE

POST-1: @@

POST-1: s-d-a y logm(sp,fe+2#2)

POST-1:

POST-1: @@

POST-1: @@ LIMIT THE PLOT TO THE SPINEL PHASE

POST-1: @@

POST-1: s-d-a x dis local sp

INFO: Distance is set as independent variable

POST-1:

POST-1: s-p-c time 86400

POST-1:

POST-1:

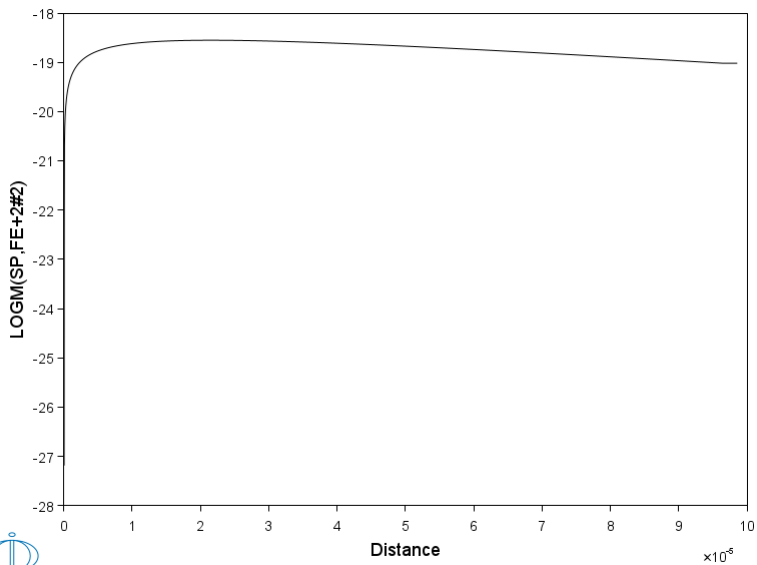
POST-1: SET\_EXP\_FILE\_FORMAT 5

POST-1: MAKE c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\unite\distribution\macroResult.exp Y

POST-1: SET\_EXP\_FILE\_FORMAT 10

POST-1:

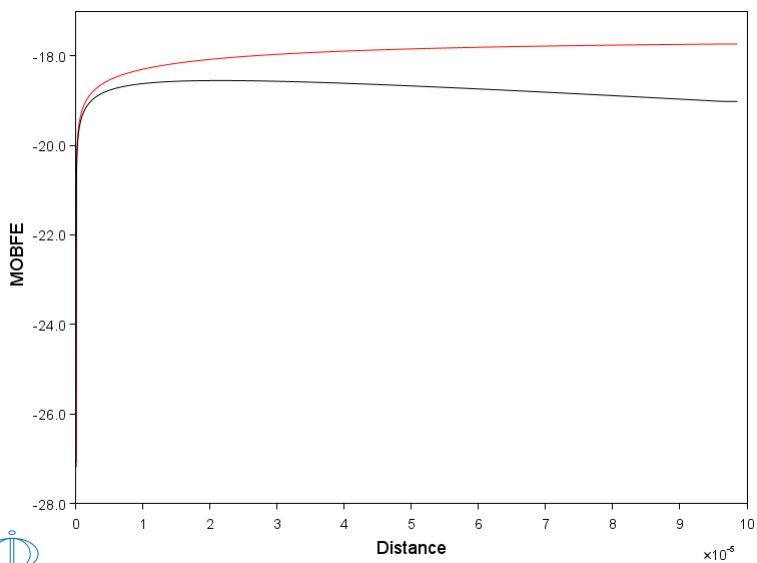
POST-1: plot



```

POST-1:
POST-1:
POST-1: @?<Hit_return_to_continue>
POST-1:
POST-1: @@
POST-1: @@ COMPARE MOBILITIES IN A SPINEL FOR Fe+2 AND Fe+3 SPECIES PRESENT ON THE
POST-1: @@ SECOND SUBLATTICE. FOR THIS WE NEED TO ENTER A TABLE.
POST-1: @@
POST-1: ent table mobfe
Variable(s) logm(sp,fe+2#2) logm(sp,fe+3#2)
POST-1:
POST-1: s-d-a y mobfe
COLUMN NUMBER /*/:
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

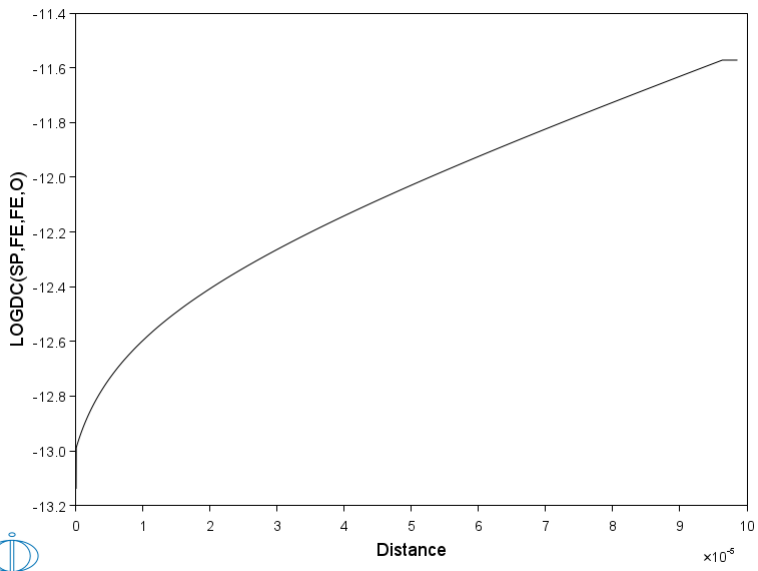
```



```

POST-1:
POST-1:
POST-1: @?<Hit_return_to_continue>
POST-1: @@
POST-1: @@ NOW PLOT THE INTERDIFFUSION COEFFICIENT OF Fe IN A SPINEL
POST-1: @@
POST-1: s-d-a y logdc(sp,fe,fe,o)
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\unite\distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

```



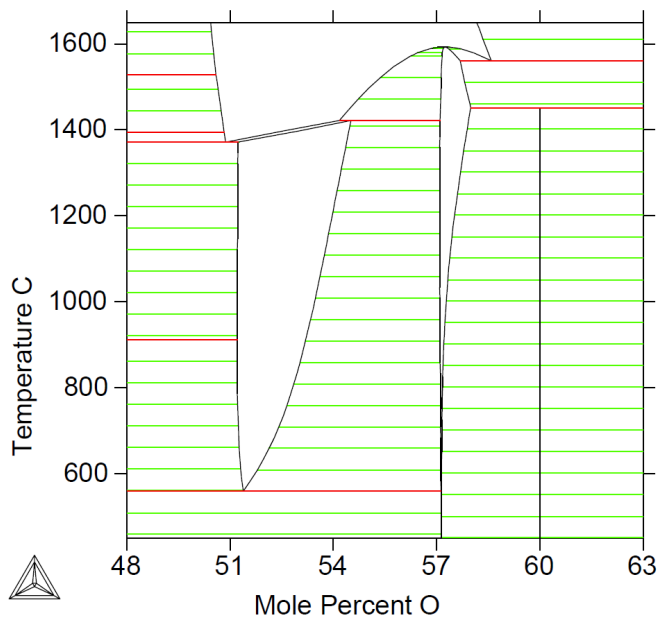
POST-1:  
POST-1:  
POST-1: set-inter  
--OK--  
POST-1:



## Example i3b

### Diffusion in iron oxide (FeO) with grain boundary contribution

Oxidation of iron sample and consequent growth of an oxide layer using the grain boundary diffusion contribution model.



## exi3b-setup

### SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,  
Stockholm, Sweden

Software running on Windows 64-bit wordlength  
Compiler: Intel Fortran Compiler 2025.0.0  
License library version: 9.7.0.0036  
Linked: Nov 19 2025 at 14:44:36

```
SYS:SYS:MACRO "c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\examples\exi3b\setup.DCM.test"
```

```
SYS: @@
SYS: @@ Diffusion in complex phases.
SYS: @@ Diffusion in iron oxide (FeO) with a grain boundary contribution
SYS: @@ This example shows the oxidation of an iron sample and consequent
SYS: @@ growth of an oxide layer using the grain boundary diffusion
SYS: @@ contribution model.
SYS: @@-----
SYS:
SYS: @@ exi3_setup.DCM
SYS:
SYS: @@
SYS: @@ START BY GOING TO THE DATABASE MODULE
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Database folder:
C:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples\databases\da
ta
Current database: Steels/Fe-Alloys v12.0

VA          /-  DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE12:
TDB_TCFE12: @@
TDB_TCFE12: @@ SELECT A USER DATABASE TO READ THE THERMODYNAMIC DATA
TDB_TCFE12: @@
TDB_TCFE12: sw user FeO.TDB
Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

VA          /-  DEFINED
12:22:49,105 [Thread-0] INFO  TDBFileParser: USER_1997769799_22, number of lines read: 217
12:22:49,361 [Thread-0] INFO  DatabaseUtils: Parsing of USER_1997769799_22 completed in 346 ms
TDB_USER: def-sys fe o
FE          O  DEFINED
TDB_USER: rej sp *
/-          VA          FE
O           FE+2       FE+3
FE+4       FE2O3      FEO
FE03/2     O-2        O2
REJECTED
TDB_USER: res sp fe fe+2 fe+3 o o2 o-2 va
FE          FE+2       FE+3
O           O2         O-2
VA RESTORED
TDB_USER: rej ph * all
GAS:G      BCC_A2      SPINEL:I
REJECTED
TDB_USER: res ph bcc spinel gas
BCC_A2     SPINEL:I    GAS:G
RESTORED
TDB_USER:
TDB_USER: get
12:22:49,475 [Thread-0] INFO  JavaWrapper: *** Invoking Gibbs Energy System v6 ***
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

Use the command LIST_REFERENCES to see the list of references for assessed data

-OK-

*** WARNING: One or more elements have been rejected only as species but not as elements. This is not allowed with GES6, temporarily reverting

TDB_USER:
TDB_USER: @@
TDB_USER: @@ SWITCH TO A USER-DEFINED MOBILITY DATABASE TO RETRIEVE MOBILITY DATA
TDB_USER: @@
TDB_USER: app user FeOmob.TDB
Current database: User defined Database
test database

VA          /-  O
DEFINED
12:22:49,859 [Thread-0] INFO  TDBFileParser: USER_1399043279_22, number of lines read: 128
12:22:49,900 [Thread-0] INFO  DatabaseUtils: Parsing of USER_1399043279_22 completed in 42 ms
TDB_APP: def-sys fe o
FE          DEFINED
TDB_APP: rej sp *
/-          VA          FE
O           FE+2       FE+3
FE2O3      FEO         FEO3/2
O-2        O2 REJECTED
TDB_APP: res sp fe fe+2 fe+3 o o2 o-2 va
FE          FE+2       FE+3
O           O2         O-2
VA RESTORED
TDB_APP: rej ph * all
SPINEL:I   GAS:G      BCC_A2
REJECTED
TDB_APP: res ph bcc spinel gas
BCC_A2     SPINEL:I    GAS:G
RESTORED
TDB_APP:
```

```

TDB_APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
*** ERROR 2018 IN DESHPH: DIFFUSION DATA NOT POSSIBLE FOR GAS PHASE
*** ERROR 2018 IN DESHPH: DIFFUSION DATA NOT POSSIBLE FOR GAS PHASE
FUNCTIONS ....
-OK-
TDB_APP:
TDB_APP:
TDB_APP: @@
TDB_APP: @@ ENTER THE DICTRA MONITOR
TDB_APP: @@
TDB_APP: go d-m
NO TIME STEP DEFINED
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 823; * N
DIC>
DIC>
DIC> @@
DIC> @@ SET THE REFERENCE STATE FOR O TO O2 (GAS)
DIC> @@
DIC> set-ref o gas,,,,,,,,
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE REGIONS fer AND sp
DIC> @@
DIC> ent-reg fer
DIC> ent-reg sp,,,,,,,,
DIC>
DIC>
DIC> @@
DIC> @@ ENTER PHASES INTO THE REGIONS
DIC> @@
DIC> ent-phase act fer matrix bcc#1
DIC> ent-phase act sp matrix spinel
DIC>
DIC>
DIC> @@
DIC> @@ ENTER GRIDS INTO THE REGIONS
DIC> @@
DIC>
DIC> @@
DIC> @@ ENTER A SIZE FOR THE FERRITE
DIC> @@
DIC>
DIC> ent-grid fer 4.99999e-3 AUTO
DIC>
DIC> @@
DIC> @@ ENTER A THIN INITIAL SIZE FOR THE OXIDE
DIC> @@
DIC>
DIC> ent-grid sp 1.00e-10 AUTO
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITIONS IN BCC
DIC> @@
DIC> ent-comp fer bcc#1 m-f
PROFILE FOR /O/: o lin 1e-9 1e-9
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITIONS IN THE OXIDE
DIC> @@
DIC> ent-comp sp spinel m-f
this is a phase with charged species
with more than 2 sublattices
PROFILE FOR /FE/: FE lin 4.28771E-01 4.28549E-01
DIC>
DIC>
DIC> @@
DIC> @@ ENTER A BOUNDARY CONDITION "GAS" ON THE UPPER (RIGHT-MOST) INTERFACE
DIC> @@ OF THE OXIDE. THIS ALLOWS THE SYSTEM TO EXPAND AND THE OXIDE LAYER
DIC> @@ TO GROW EXTERNALLY. FOR THIS EXAMPLE AN OXYGEN ACTIVITY IS SPECIFIED
DIC> @@ THAT IS LOW ENOUGH NOT TO FORM CORUNDUM (FE2O3). ALSO SPECIFY THAT
DIC> @@ THERE IS NO FLUX OF Fe ACROSS THIS INTERFACE, I.E. NO Fe IS
DIC> @@ ALLOWED TO ENTER OR LEAVE THE SYSTEM.
DIC> @@
DIC> set-cond boundary upper gas
TYPE OF CONDITION FOR COMPONENT FE /ZERO_FLUX/: zero-flux
TYPE OF CONDITION FOR COMPONENT O /ZERO_FLUX/: act
LOW TIME LIMIT /O/: 0 4.5e-4; * N
DIC>
DIC>
DIC> @@
DIC> @@ ENTER START VALUES FOR THE INITIAL INTERFACE VELOCITIES
DIC> @@
DIC> s-a-s-v -1e-5 1e-5 yes
STARTING VALUES WILL BE TAKEN FROM PROFILES
DIC>
DIC>
DIC> @@
DIC> @@ SIMULATE FOR 24 HOURS
DIC> @@
DIC> s-s-time 86400,,,,
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC> @@
DIC> @@ SPECIFY THAT POTENTIALS AND NOT ACTIVITIES ARE VARIED AT THE PHASE
DIC> @@ INTERFACE. ALSO USE A FULLY IMPLICIT SCHEME FOR TIME INTEGRATION.
DIC> @@
DIC> set-option DEGREE_OF_IMPLICITY 1.0
DIC> set-option VARY_POTENTIALS_OR_ACTIVITIES POT

```

```
RELEASING OLD STARTING VALUES
DIC>
DIC> @@ ENABLE THE GRAIN BOUNDARY DIFFUSION CONTRIBUTION MODEL
DIC> GB
REGION NAME : /SP/: SP
PHASE NAME: /SPINEL/: SPINEL
Enable model for grainboundary contribution to diffusion /YES/: YES
Grainboundary thickness /5E-10/: 5e-10
Grainsize(T,P,TIME)= 10.0e-6;
Bulkdiffusion activation energy multiplier /.5/: 0.333333
Enable model for dislocation contribution to diffusion /YES/: NO
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exi3b.DIC Y
DIC>
DIC>
DIC>
DIC> set-inter
--OK--
DIC>
```

exi3b-run

DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exi3b\run.DCM.test"

DIC>

DIC>

DIC> @@ exi3\_run.DCM

DIC>

DIC> @@

DIC> @@ FILE FOR RUNNING EXAMPLE I3

DIC> @@

DIC>

DIC> @@

DIC> @@ ENTER THE DICTRA MONITOR AND READ THE STORE RESULT FILE

DIC> @@

DIC> go d-m

TIME STEP AT TIME 0.00000E+00

DIC> read exi3b

OK

DIC>

DIC> @@

DIC> @@ START THE SIMULATION

DIC> @@

DIC> sim y

INFO: Default responses (if any) will be applied during the simulation. Use "SIMULATE\_REACTION NO" instead for manual input.

Region: FER

geometric 0.833333 dense at 0.499999E-02 58 points

Region: SP

geometric 1.03726 dense at 0.00000 27 points

geometric 0.964075 dense at 0.100000E-09 28 points

Trying old scheme 3

U-FRACTION IN SYSTEM: FE = 0.99999999500542 O = 2.10000395011622E-08

TOTAL SIZE OF SYSTEM: .0049999901 [m]

U-FRACTION IN SYSTEM: FE = 0.99999999500542 O = 2.10000395011622E-08

TOTAL SIZE OF SYSTEM: .0049999901 [m]

0.292908950472656 0.292908246928952 0.292908395685021 3.918702200652587E-002 9.367735717507752E-

023 TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.74972824E-22

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.36177235E-03 AND 0.0000000

POSITION OF INTERFACE FER / SP IS 0.49999900E-02

CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.61983704E-03 AND 0.0000000

POSITION OF INTERFACE SP / gas interface IS 0.49999901E-02

U-FRACTION IN SYSTEM: FE = 0.99999998985525 O = 3.36524206707485E-08

TOTAL SIZE OF SYSTEM: .00499999012581 [m]

3 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: SP

CPU time used in timestep 1 seconds

3.143617040855247E-006 3.144236471659743E-006 3.144881466811322E-006 4.076561546982120E-008 7.212645257549425E-

032 TIME = 0.30000000E-06 DT = 0.20000000E-06 SUM OF SQUARES = 0.60465361E-31

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.26719690E-03 AND 0.0000000

POSITION OF INTERFACE FER / SP IS 0.49999899E-02

CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.37865989E-03 AND 0.0000000

POSITION OF INTERFACE SP / gas interface IS 0.49999901E-02

U-FRACTION IN SYSTEM: FE = 0.99999998519419 O = 4.87988508687407E-08

TOTAL SIZE OF SYSTEM: .0049999901481 [m]

33 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: SP

CPU time used in timestep 2 seconds

8.582625080322057E-007 8.586191088743216E-007 8.585770780586650E-007 1.725688368190803E-009 1.121891808424791E-

034 TIME = 0.70000000E-06 DT = 0.40000000E-06 SUM OF SQUARES = 0.16974138E-34

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.19377424E-03 AND 0.0000000

POSITION OF INTERFACE FER / SP IS 0.49999898E-02

CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.27792398E-03 AND 0.0000000

POSITION OF INTERFACE SP / gas interface IS 0.49999902E-02

U-FRACTION IN SYSTEM: FE = 0.99999997826752 O = 7.10328257106202E-08

TOTAL SIZE OF SYSTEM: .00499999018176 [m]

25 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: SP

CPU time used in timestep 1 seconds

6.515892209006579E-007 6.518089521559404E-007 6.517960973641674E-007 7.160515018440124E-010 1.726801201357940E-

033 TIME = 0.15000000E-05 DT = 0.80000000E-06 SUM OF SQUARES = 0.16974138E-32

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.13205341E-03 AND 0.0000000

POSITION OF INTERFACE FER / SP IS 0.49999897E-02

CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.18888697E-03 AND 0.0000000

POSITION OF INTERFACE SP / gas interface IS 0.49999902E-02

U-FRACTION IN SYSTEM: FE = 0.99999996888748 O = 1.01254825184996E-07

TOTAL SIZE OF SYSTEM: .00499999022723 [m]

25 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: SP

CPU time used in timestep 2 seconds

2.443476937795328E-007 2.444400502254134E-007 2.444331403409376E-007 3.133477941735192E-010 6.757329275701920E-

034 TIME = 0.31000000E-05 DT = 0.16000000E-05 SUM OF SQUARES = 0.35181370E-33

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.93735802E-04 AND 0.0000000

POSITION OF INTERFACE FER / SP IS 0.49999896E-02

CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.13437817E-03 AND 0.0000000

POSITION OF INTERFACE SP / gas interface IS 0.49999903E-02

U-FRACTION IN SYSTEM: FE = 0.9999999551222 O = 1.44255972784647E-07

TOTAL SIZE OF SYSTEM: .00499999029225 [m]

29 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: SP

CPU time used in timestep 3 seconds

1.350156100676961E-005 1.350641195995434E-005 1.350610187182701E-005 1.525413798364827E-008 2.200149266547059E-

032 TIME = 0.63000000E-05 DT = 0.32000000E-05 SUM OF SQUARES = 0.21998483E-31

output ignored...

... output resumed

POSITION OF INTERFACE FER / SP IS 0.49344229E-02

CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.10984395E-08 AND 0.0000000

POSITION OF INTERFACE SP / gas interface IS 0.50281239E-02

U-FRACTION IN SYSTEM: FE = .994278667446015 O = .0186355570646506

TOTAL SIZE OF SYSTEM: .00502812390109 [m]

28 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: SP

CPU time used in timestep 3 seconds

4.810881384903808E-007 4.818502687534282E-007 4.817787239929768E-007 6.672711984601621E-010 2.745954803520864E-

033 TIME = 56943.895 DT = 8640.0000 SUM OF SQUARES = 0.26188133E-32

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.70318910E-09 AND 0.0000000

POSITION OF INTERFACE FER / SP IS 0.49283473E-02

CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.10060063E-08 AND 0.0000000

POSITION OF INTERFACE SP / gas interface IS 0.50307402E-02

U-FRACTION IN SYSTEM: FE = .993757761568711 O = .0203536215381767  
TOTAL SIZE OF SYSTEM: .00503074024138 [m]  
16 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: SP

CPU time used in timestep 2 seconds  
2.759410377008257E-007 2.764666912549018E-007 2.764223294828198E-007 3.498157980721660E-010 4.393527685633382E-  
034 TIME = 65583.895 DT = 8640.0000 SUM OF SQUARES = 0.36412113E-33  
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.65102059E-09 AND 0.0000000  
POSITION OF INTERFACE FER / SP IS 0.49227225E-02  
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.93227325E-09 AND 0.0000000  
POSITION OF INTERFACE SP / gas interface IS 0.50331703E-02  
U-FRACTION IN SYSTEM: FE = .993275042334175 O = .0219441459344009  
TOTAL SIZE OF SYSTEM: .00503317026435 [m]  
11 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: SP

CPU time used in timestep 3 seconds  
1.589276677386145E-007 1.592978117430478E-007 1.592654678748259E-007 1.906234424384614E-010 1.195581198289139E-  
032 TIME = 74223.895 DT = 8640.0000 SUM OF SQUARES = 0.11943775E-31  
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.60902394E-09 AND 0.0000000  
POSITION OF INTERFACE FER / SP IS 0.49174605E-02  
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.87303127E-09 AND 0.0000000  
POSITION OF INTERFACE SP / gas interface IS 0.50354513E-02  
U-FRACTION IN SYSTEM: FE = .992822785564275 O = .0234321821932705  
TOTAL SIZE OF SYSTEM: .00503545128769 [m]  
14 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: SP

CPU time used in timestep 2 seconds  
9.8810726236609520E-008 9.888140217383175E-008 9.886219594631730E-008 1.117162369142064E-010 2.204287006661954E-  
034 TIME = 82863.895 DT = 8640.0000 SUM OF SQUARES = 0.21741944E-33  
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.57420070E-09 AND 0.0000000  
POSITION OF INTERFACE FER / SP IS 0.49124995E-02  
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.82330959E-09 AND 0.0000000  
POSITION OF INTERFACE SP / gas interface IS 0.50376036E-02  
U-FRACTION IN SYSTEM: FE = .992396693735749 O = .0248342299540171  
TOTAL SIZE OF SYSTEM: .00503760358843 [m]  
10 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: SP

CPU time used in timestep 2 seconds  
1.759128687822074E-008 1.751684888645274E-008 1.771652447788329E-008 1.534273091642826E-011 1.339123164456750E-  
033 TIME = 86400.000 DT = 3536.1047 SUM OF SQUARES = 0.13270861E-32  
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.56935899E-09 AND 0.0000000  
POSITION OF INTERFACE FER / SP IS 0.49104861E-02  
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.78982165E-09 AND 0.0000000  
POSITION OF INTERFACE SP / gas interface IS 0.50383832E-02  
U-FRACTION IN SYSTEM: FE = .992242570130794 O = .0253847103980189  
TOTAL SIZE OF SYSTEM: .00503838316747 [m]

MUST SAVE WORKSPACE ON FILE  
WORKSPACE SAVED ON FILE  
RECLAIMING WORKSPACE

DELETING TIME-RECORD FOR TIME 0.0000000  
DELETING TIME-RECORD FOR TIME 0.10000000E-06  
DELETING TIME-RECORD FOR TIME 0.30000000E-06  
DELETING TIME-RECORD FOR TIME 0.70000000E-06  
DELETING TIME-RECORD FOR TIME 0.15000000E-05  
DELETING TIME-RECORD FOR TIME 0.31000000E-05  
DELETING TIME-RECORD FOR TIME 0.63000000E-05  
DELETING TIME-RECORD FOR TIME 0.12700000E-04  
DELETING TIME-RECORD FOR TIME 0.25500000E-04  
DELETING TIME-RECORD FOR TIME 0.51100000E-04  
DELETING TIME-RECORD FOR TIME 0.10230000E-03  
DELETING TIME-RECORD FOR TIME 0.20470000E-03  
DELETING TIME-RECORD FOR TIME 0.40950000E-03  
DELETING TIME-RECORD FOR TIME 0.81910000E-03  
DELETING TIME-RECORD FOR TIME 0.16383000E-02  
DELETING TIME-RECORD FOR TIME 0.32767000E-02  
DELETING TIME-RECORD FOR TIME 0.65535000E-02  
DELETING TIME-RECORD FOR TIME 0.13107100E-01  
DELETING TIME-RECORD FOR TIME 0.26214300E-01  
DELETING TIME-RECORD FOR TIME 0.52428700E-01  
DELETING TIME-RECORD FOR TIME 0.10485750  
DELETING TIME-RECORD FOR TIME 0.20971510  
DELETING TIME-RECORD FOR TIME 0.41943030  
DELETING TIME-RECORD FOR TIME 0.83886070  
DELETING TIME-RECORD FOR TIME 1.6777215  
DELETING TIME-RECORD FOR TIME 3.3554431  
DELETING TIME-RECORD FOR TIME 6.7108863  
DELETING TIME-RECORD FOR TIME 13.421773  
DELETING TIME-RECORD FOR TIME 26.843545  
DELETING TIME-RECORD FOR TIME 53.687091  
DELETING TIME-RECORD FOR TIME 107.37418  
DELETING TIME-RECORD FOR TIME 214.74836  
DELETING TIME-RECORD FOR TIME 429.49673  
DELETING TIME-RECORD FOR TIME 858.99346  
DELETING TIME-RECORD FOR TIME 1717.9869  
DELETING TIME-RECORD FOR TIME 3435.9738  
DELETING TIME-RECORD FOR TIME 6871.9477  
DELETING TIME-RECORD FOR TIME 13743.895  
DELETING TIME-RECORD FOR TIME 22383.895  
DELETING TIME-RECORD FOR TIME 31023.895  
DELETING TIME-RECORD FOR TIME 39663.895  
DELETING TIME-RECORD FOR TIME 48303.895  
DELETING TIME-RECORD FOR TIME 56943.895  
DELETING TIME-RECORD FOR TIME 65583.895  
DELETING TIME-RECORD FOR TIME 74223.895

KEEPING TIME-RECORD FOR TIME 82863.895  
AND FOR TIME 86400.000  
WORKSPACE RECLAIMED

TIMESTEP AT 86400.0000 SELECTED

DIC>  
DIC> set-inter  
--OK--  
DIC>

## exi3b-plot

DIC>About

NO SUCH COMMAND, USE HELP

DIC>DIC>MACRO "c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\examples\exi3b\plot.DCM.test"

DIC>

DIC> @@ exi3\_plot.DCM

DIC>

DIC> @@

DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE i3

DIC> @@

DIC>

DIC> @@

DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE

DIC> @@

DIC> go d-m

TIME STEP AT TIME 8.64000E+04

DIC> read exi3b

OK

DIC>

DIC> @@

DIC> @@ ENTER THE POST PROCESSOR

DIC> @@

DIC> post

POST PROCESSOR VERSION 1.7

Implemented by Bjorn Jonsson

POST-1:

POST-1: @@

POST-1: @@ PLOT THE THICKNESS OF THE OXIDE LAYER GROWING AT THE SURFACE.

POST-1: @@ FOR THIS WE NEED TO ENTER A FUNCTION ACCORDING TO THE FOLLOWING.

POST-1: ent func oxideth

FUNCTION: poi(sp,upper)-poi(sp,lower)

&

POST-1: @@

POST-1: @@ PUT THIS FUNCTION ON THE Y-AXIS

POST-1: @@

POST-1: s-d-a y oxideth

POST-1: @@

POST-1: @@ AND PLOT THE OXIDE THICKNESS VERSUS TIME

POST-1: @@

POST-1: s-d-a x time

INFO: Time is set as independent variable

POST-1: @@

POST-1: @@

POST-1: @@ SINCE WE ARE PLOTTING A FUNCTION, SPECIFY A PLOT CONDITION

POST-1: @@

POST-1: s-p-c interface sp upper

POST-1: @@

POST-1: app y exi3a.exp 0; 1;

POST-1: @@

POST-1: @@

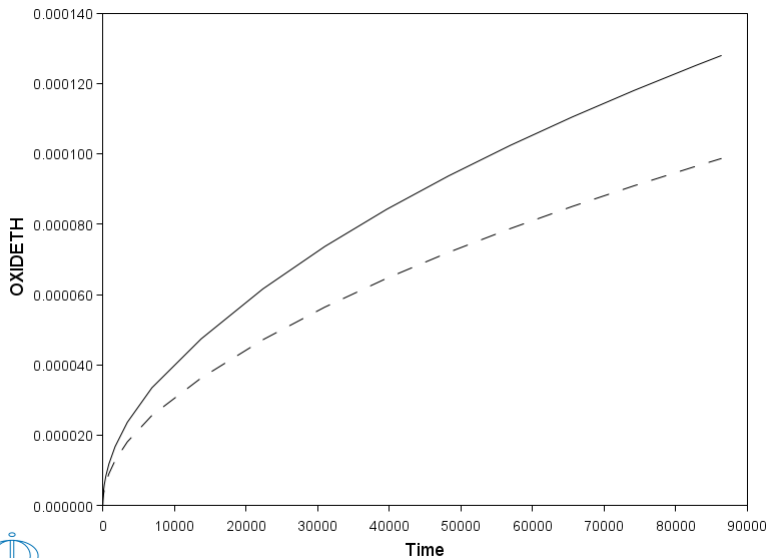
POST-1: SET\_EXP\_FILE\_FORMAT 4

POST-1: MAKE c:\jenkins\workspace\dev\_pipeline\generate\_dictra\_console\_examples\unite\distribution\macroResult.exp Y

OST-1: SET\_EXP\_FILE\_FORMAT 10

POST-1:

POST-1: plot



POST-1:

POST-1:

POST-1: set-inter

--OK--

POST-1: