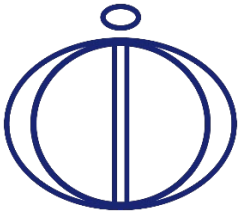
Diffusion Module (DICTRA) Example Macros

Thermo-Calc Version 2025a



Thermo-Calc Software

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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

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. Kikichi: 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 cannon 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 WidmannstÃ¤tten 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. HÃ¶glund and J. Ã…gren: 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. HÃ¶glund, B. JÃ¶nsson and J. Ã…gren: 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. EngstrÃ¶m, L. HÃ¶glund and J. Ã…gren: 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. EngstrÃ¶m, L. HÃ¶glund and J. Ã…gren: 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. EngstrÃ¶m: 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. EngstrÃ¶m: 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. EngstrÃ¶m, Acta. Mater. v.54 (2006), pp. 2431-2439. Experimental data from A. EngstrÃ¶m, 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. EngstrÃ¶m and J. Ã…gren: ("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

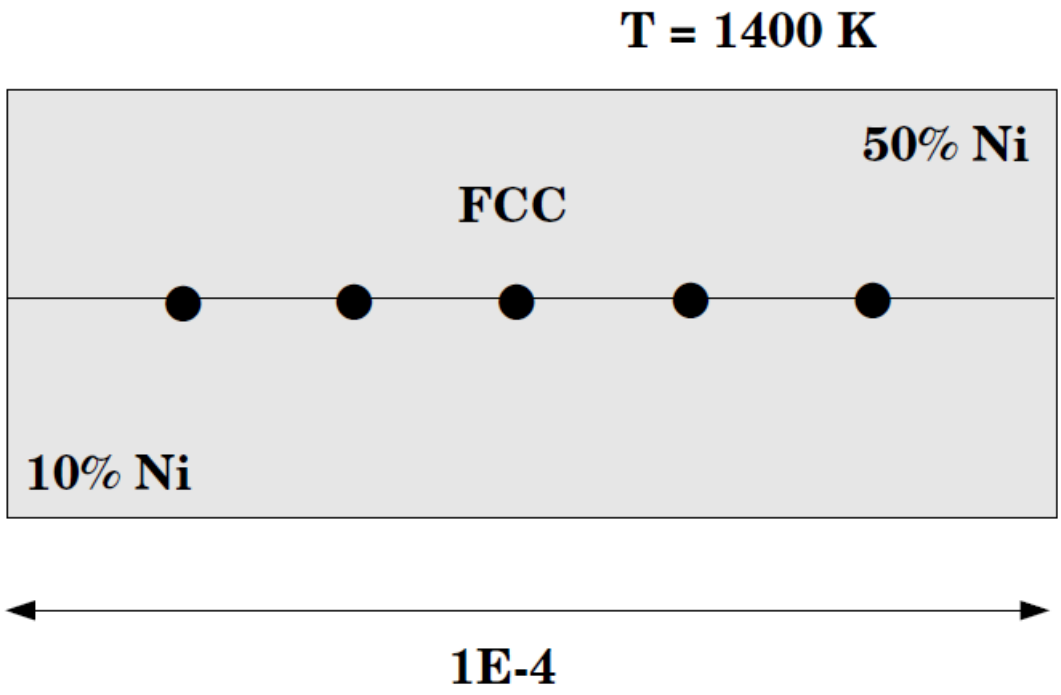
Diffusion in complex phases. Diffusion in iron oxide (FeO) with a grain boundary contribution This example shows the oxidation of an iron sample and consequent growth of an oxide layer using the grain boundary diffusion contribution model.

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

exa1-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: unknown compiler
 License library version: 9.7.0.0036
 Linked: Fri Oct 18 11:32:56 2024


SYS:SYS:MACRO exa1\setup.DCM
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: ----------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@
SYS: @@ START BY GOING TO THE DATABASE MODULE
SYS: @@
SYS: goto_module
MODULE NAME: data
12:27:19,968 [Thread-0] INFO  LicenseManager: Initializing user: jenkins.integrationtest@thermocalc.se
12:27:19,983 [Thread-0] INFO  LicenseController: Running License Spring in DEV environment.
12:27:21,177 [Thread-0] INFO  LicenseManager: There is an activated standalone license for jenkins.integrationtest@thermocalc.se for TC-
Application
 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 v5.0
 MOB2    =  Alloys Mobility  v2.7
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBFE7  =  Steels/Fe-Alloys Mobility  v7.1
 MFEDEMO =  Fe-Alloys Mobility demo database v4.0
 USER    =  User defined Database

DATABASE NAME /TCFE12/: fedemo
 Current database: Iron Demo Database v5.0

 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: *
 BCC_A2                 CBCC_A12               CUB_A13
 FCC_A1                 GAS:G                  HCP_A3
 LAVES_PHASE_C14        LIQUID:L  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
12:27:22,288 [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 v5.0
 MOB2    =  Alloys Mobility  v2.7
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBFE7  =  Steels/Fe-Alloys Mobility  v7.1
 MFEDEMO =  Fe-Alloys Mobility demo database v4.0
 USER    =  User defined Database

DATABASE NAME /FEDEMO/: mfedemo
 Current database: Fe-Alloys Mobility demo database v4.0

 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
12:27:22,862 [Thread-0] INFO  StandaloneLicenseController: Checking out license for: Diffusion (DICTRA)
 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 /LINEAR/: 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 exa1 Y
DIC>
DIC> set_interactive
 --OK---
DIC>
```

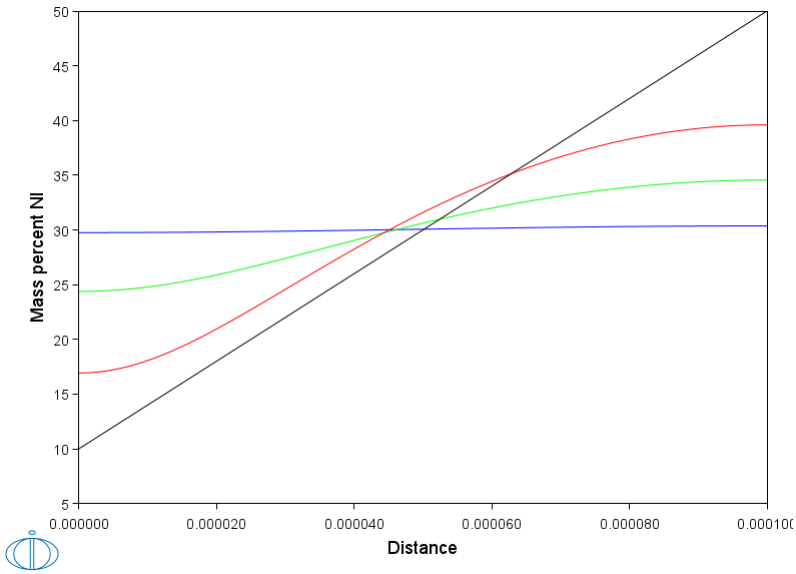
exa1-run

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exa1\run.DCM DIC>
DIC>
DIC> @@ exa1_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 exa1
 OK
DIC>
DIC> @@
DIC> @@ Start the simulation
DIC> @@
DIC> simulate_reaction
 Region: AUSTENITE
 linear    75 points
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
 U-FRACTION IN SYSTEM:  FE = .709680136600384  NI = .290319863399616
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 U-FRACTION IN SYSTEM:  FE = .709680136600384  NI = .290319863399616
 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 = .709680136600384  NI = .290319863399616
 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 = .709680136600384  NI = .290319863399616
 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 = .709680136600384  NI = .290319863399616
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =   183.71515     DT =   183.31505     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .709680136600384  NI = .290319863399616
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =   550.34526     DT =   366.63011     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .709680136600384  NI = .290319863399616
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =   1283.6055     DT =   733.26022     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .709680136600384  NI = .290319863399616
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =   2750.1259     DT =   1466.5204     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .709680136600385  NI = .290319863399616
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    1  seconds
 TIME =   5683.1668     DT =   2933.0409     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .709680136600385  NI = .290319863399616
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =   11549.249     DT =   5866.0817     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .709680136600384  NI = .290319863399616
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =   23281.412     DT =   11732.163     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .709680136600384  NI = .290319863399616
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =   46745.739     DT =   23464.327     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .709680136600384  NI = .290319863399616
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =   93674.393     DT =   46928.654     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .709680136600384  NI = .290319863399616
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =   187531.70     DT =   93857.308     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .709680136600385  NI = .290319863399615
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =   287531.70     DT =   100000.00     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .709680136600385  NI = .290319863399615
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =   387531.70     DT =   100000.00     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .709680136600385  NI = .290319863399615
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =   487531.70     DT =   100000.00     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .709680136600383  NI = .290319863399616
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =   587531.70     DT =   100000.00     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .709680136600385  NI = .290319863399616
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =   687531.70     DT =   100000.00     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .709680136600385  NI = .290319863399615
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =   787531.70     DT =   100000.00     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .709680136600385  NI = .290319863399615
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =   887531.70     DT =   100000.00     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .709680136600385  NI = .290319863399615
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =   987531.70     DT =   100000.00     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .709680136600385  NI = .290319863399615
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
```

```
 TIME =   1000000.0     DT =   12468.299     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .709680136600385  NI = .290319863399615
 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    183.71515
 DELETING TIME-RECORD FOR TIME    550.34526
 DELETING TIME-RECORD FOR TIME    1283.6055
 DELETING TIME-RECORD FOR TIME    2750.1259
 DELETING TIME-RECORD FOR TIME    5683.1668
 DELETING TIME-RECORD FOR TIME    11549.249
 DELETING TIME-RECORD FOR TIME    23281.412
 DELETING TIME-RECORD FOR TIME    46745.739
 DELETING TIME-RECORD FOR TIME    93674.393
 DELETING TIME-RECORD FOR TIME    187531.70
 DELETING TIME-RECORD FOR TIME    287531.70
 DELETING TIME-RECORD FOR TIME    387531.70
 DELETING TIME-RECORD FOR TIME    487531.70
 DELETING TIME-RECORD FOR TIME    587531.70
 DELETING TIME-RECORD FOR TIME    687531.70
 DELETING TIME-RECORD FOR TIME    787531.70
 DELETING TIME-RECORD FOR TIME    887531.70

 KEEPING TIME-RECORD FOR TIME    987531.70
 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>
```

exa1-plot

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exa1\plot.DCM DIC>
DIC>
DIC> @@ exa1_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 exa1
 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
```

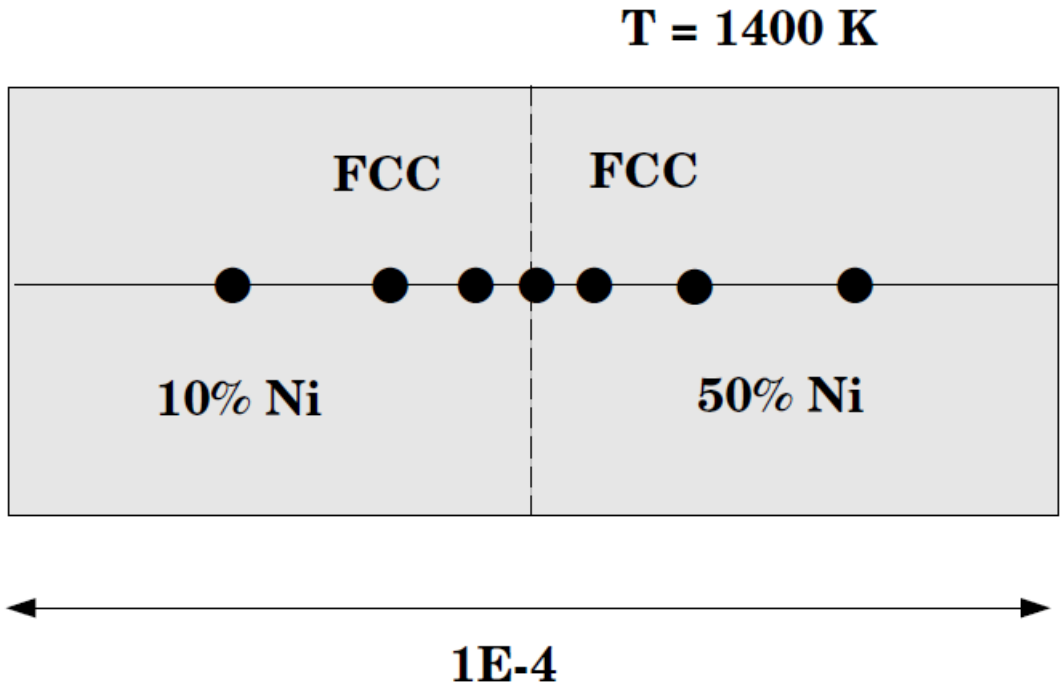



```
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: set_interactive
 --OK---
POST-1:
```

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: unknown compiler
 License library version: 9.7.0.0036
 Linked: Fri Oct 18 11:32:56 2024


SYS:SYS:MACRO exa2a\setup.DCM
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: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
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
12:30:17,226 [Thread-0] INFO  LicenseManager: Initializing user: jenkins.integrationtest@thermocalc.se
12:30:17,248 [Thread-0] INFO  LicenseController: Running License Spring in DEV environment.
12:30:18,364 [Thread-0] INFO  LicenseManager: There is an activated standalone license for jenkins.integrationtest@thermocalc.se for TC-
Application
 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 v5.0

 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
 BCC_A2                   CBCC_A12                 CUB_A13
 FCC_A1                   GAS:G                    HCP_A3
 LAVES_PHASE_C14          LIQUID:L  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
12:30:19,578 [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 v5.0
 MOB2    =  Alloys Mobility  v2.7
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBFE7  =  Steels/Fe-Alloys Mobility  v7.1
 MFEDEMO =  Fe-Alloys Mobility demo database v4.0
 USER    =  User defined Database

DATABASE NAME /FEDEMO/: mfedemo
 Current database: Fe-Alloys Mobility demo database v4.0

 VA  DEFINED
APP: def-sys fe ni
   ... the command in full is DEFINE_SYSTEM
 FE                    NI  DEFINED
APP: rej ph * all
   ... the command in full is REJECT
 BCC_A2                FCC_A1                LIQUID:L
   REJECTED
APP: res ph fcc
   ... the command in full is RESTORE
 FCC_A1  RESTORED
APP: get
   ... the command in full is 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: go d-m
   ... the command in full is GOTO_MODULE
12:30:20,070 [Thread-0] INFO  StandaloneLicenseController: Checking out license for: Diffusion (DICTRA)
 NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond
   ... the command in full is SET_CONDITION
GLOBAL OR BOUNDARY CONDITION /GLOBAL/: glob
VARIABLE : T
LOW TIME LIMIT /0/: 0
T(TIME,X)= 1400;
HIGH TIME LIMIT /*/: *
ANY MORE RANGES /N/: N
DIC>
DIC> @@
DIC> @@ ENTER A REGION
DIC> @@
DIC> enter-region
REGION NAME : austenite
DIC>
DIC> @@
DIC> @@ ENTER A GRID INTO THE REGION.
DIC> @@ IN THIS CASE WE WANT SEVERAL POINTS IN THE MIDDLE OF THE REGION,
DIC> @@ SO A DOUBLE GEOMETRIC GRID IS CONSTRUCTED.
DIC> @@
DIC> enter-grid
   ... the command in full is ENTER_GRID_COORDINATES
REGION NAME : /AUSTENITE/: austenite
WIDTH OF REGION /1/: 1e-4
TYPE /LINEAR/: double
NUMBER OF POINTS /50/: 60
VALUE OF R IN THE GEOMETRICAL SERIE FOR LOWER PART OF REGION: 0.9
VALUE OF R IN THE GEOMETRICAL SERIE FOR UPPER PART OF REGION: 1.11
DIC>
DIC> @@
DIC> @@ ENTER THE active PHASES INTO THE REGIONS
DIC> @@
DIC> enter-phase
   ... the command in full is ENTER_PHASE_IN_REGION
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /AUSTENITE/: austenite
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL Ni COMPOSITION INTO THE PHASE. READ DATA FROM
DIC> @@ THE FILE ni.dat WHICH CONTAINS THE Ni-PROFILE.
DIC> @@
DIC> enter-composition
   ... the command in full is ENTER_COMPOSITIONS
REGION NAME : /AUSTENITE/: austenite
PHASE NAME: /FCC_A1/: fcc#1
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /NI/: ni
TYPE /LINEAR/: read a2ani.dat
   ... the command in full is CREATE_NEW_EQUILIBRIUM
   ... the command in full is COMPUTE_EQUILIBRIUM
   ... the command in full is COMPUTE_EQUILIBRIUM
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    ... the command in full is COMPUTE_EQUILIBRIUM
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 exa2a Y
   ... the command in full is SAVE_WORKSPACES
DIC>
DIC> set-inter
   ... the command in full is SET_INTERACTIVE
 --OK---
DIC>
```

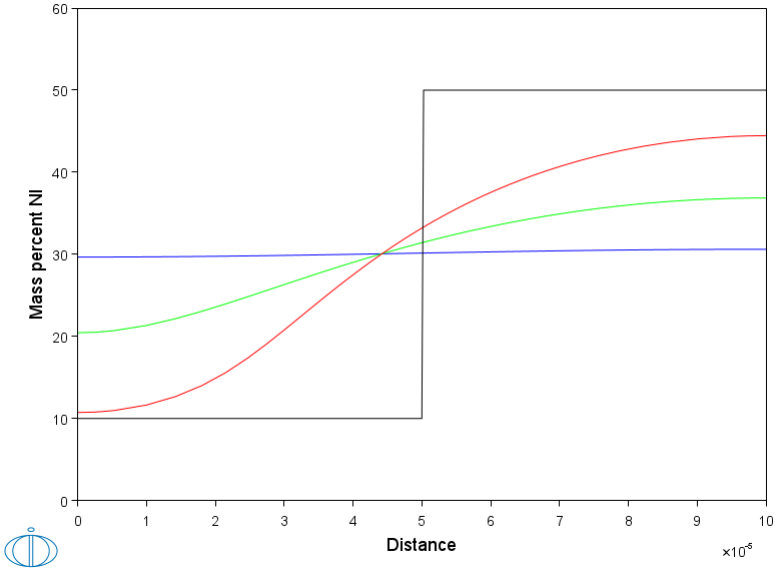
exa2a-run

```
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> @@ LET US DEFINE A LOG-FILE FOR THIS EXAMPLE
DIC> @@
DIC> @@set-log-file run
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
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
   ... the command in full is SET_NUMERICAL_LIMITS
 U-FRACTION IN SYSTEM:  FE = .708888245406169  NI = .29111175459383
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 U-FRACTION IN SYSTEM:  FE = .708888245406169  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 = .291111754593831
 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 = .291111754593831
 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 = .291111754593831
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =   54.850849     DT =   31.114714     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 =   117.08028     DT =   62.229428     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 =   241.53913     DT =   124.45886     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 =   490.45684     DT =   248.91771     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 =   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 = .291111754593831
 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 = .708888245406169  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 = .708888245406169  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 = .708888245406169  NI = .291111754593831
 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 = .708888245406169  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 = .708888245406172  NI = .291111754593828
 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 = .708888245406173  NI = .291111754593827
 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 = .708888245406176  NI = .291111754593824
 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 = .70888824540618  NI = .29111175459382
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    1  seconds
 TIME =   627438.49     DT =   100000.00     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .708888245406177  NI = .291111754593823
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =   727438.49     DT =   100000.00     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .708888245406175  NI = .291111754593825
 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 = .708888245406173  NI = .291111754593826
 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 = .708888245406173  NI = .291111754593827
 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 = .708888245406174  NI = .291111754593826
 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    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 exa2a\plot.DCM
   ... 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> @@ LET US DEFINE A LOG-FILE FOR THIS EXAMPLE
DIC> @@
DIC> set-log-file plot
 AMBIGUOUS COMMAND, USE HELP
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
```

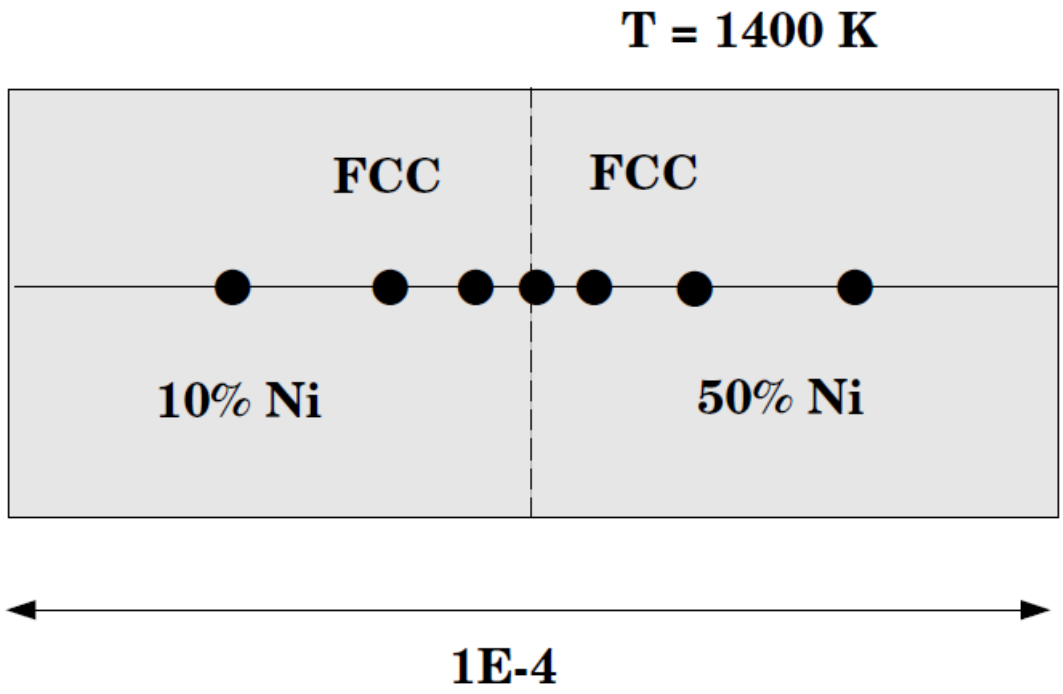



```
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
 --OK---
POST-1:
```

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: unknown compiler
 License library version: 9.7.0.0036
 Linked: Fri Oct 18 11:32:56 2024


SYS:SYS:MACRO exa2b\setup.DCM
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: ----------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
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
12:33:13,716 [Thread-0] INFO  LicenseManager: Initializing user: jenkins.integrationtest@thermocalc.se
12:33:13,736 [Thread-0] INFO  LicenseController: Running License Spring in DEV environment.
12:33:14,897 [Thread-0] INFO  LicenseManager: There is an activated standalone license for jenkins.integrationtest@thermocalc.se for TC-
Application
 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 v5.0

 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
 BCC_A2                   CBCC_A12                 CUB_A13
 FCC_A1                   GAS:G                    HCP_A3
 LAVES_PHASE_C14          LIQUID:L  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
12:33:15,963 [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 v5.0
 MOB2    =  Alloys Mobility  v2.7
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBFE7  =  Steels/Fe-Alloys Mobility  v7.1
```

```
 MFEDEMO =  Fe-Alloys Mobility demo database v4.0
 USER    =  User defined Database

DATABASE NAME /FEDEMO/: mfedemo
 Current database: Fe-Alloys Mobility demo database v4.0

 VA  DEFINED
APP: def-sys fe ni
   ... the command in full is DEFINE_SYSTEM
 FE                       NI  DEFINED
APP: rej ph * all
   ... the command in full is REJECT
 BCC_A2                   FCC_A1                   LIQUID:L
   REJECTED
APP: res ph fcc
   ... the command in full is RESTORE
 FCC_A1  RESTORED
APP: get
   ... the command in full is 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: go d-m
   ... the command in full is GOTO_MODULE
12:33:16,474 [Thread-0] INFO  StandaloneLicenseController: Checking out license for: Diffusion (DICTRA)
 NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond
   ... the command in full is SET_CONDITION
GLOBAL OR BOUNDARY CONDITION /GLOBAL/: glob
VARIABLE : T
LOW TIME LIMIT /0/: 0
T(TIME,X)= 1400;
HIGH TIME LIMIT /*/: *
ANY MORE RANGES /N/: N
DIC>
DIC> @@
DIC> @@ ENTER A REGION
DIC> @@
DIC> enter-region
REGION NAME : austenite
DIC>
DIC> @@
DIC> @@ ENTER A GRID INTO THE REGION.
DIC> @@ AS IN EXAMPLE a2a WE WANT SEVERAL POINTS IN THE MIDDLE OF THE REGION,
DIC> @@ SO A DOUBLE GEOMETRIC GRID IS ALSO CONSTRUCTED IN THIS EXAMPLE.
DIC> @@
DIC> enter-grid
   ... the command in full is ENTER_GRID_COORDINATES
REGION NAME : /AUSTENITE/: austenite
WIDTH OF REGION /1/: 1e-4
TYPE /LINEAR/: double
NUMBER OF POINTS /50/: 60
VALUE OF R IN THE GEOMETRICAL SERIE FOR LOWER PART OF REGION: 0.9
VALUE OF R IN THE GEOMETRICAL SERIE FOR UPPER PART OF REGION: 1.11
DIC>
DIC> @@
DIC> @@ ENTER ACTIVE PHASES INTO THE REGIONS
DIC> @@
DIC> enter-phase
   ... the command in full is ENTER_PHASE_IN_REGION
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /AUSTENITE/: austenite
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL Ni COMPOSITION INTO THE PHASE. READ DATA FROM
DIC> @@ THE FILE ni.dat WHICH CONTAINS THE Ni-PROFILE.
DIC> @@
DIC> enter-composition
   ... the command in full is ENTER_COMPOSITIONS
REGION NAME : /AUSTENITE/: austenite
PHASE NAME: /FCC_A1/: fcc#1
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /NI/: ni
TYPE /LINEAR/: read a2bni.dat
   ... the command in full is CREATE_NEW_EQUILIBRIUM
   ... the command in full is COMPUTE_EQUILIBRIUM
   ... the command in full is COMPUTE_EQUILIBRIUM
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    ... the command in full is COMPUTE_EQUILIBRIUM
    ... the command in full is COMPUTE_EQUILIBRIUM
    ... the command in full is COMPUTE_EQUILIBRIUM
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    ... the command in full is COMPUTE_EQUILIBRIUM
    ... the command in full is COMPUTE_EQUILIBRIUM
    ... the command in full is COMPUTE_EQUILIBRIUM
    ... the command in full is COMPUTE_EQUILIBRIUM
DIC>
DIC> @@
DIC> @@ THE BOUNDARY CONDITION IS A CLOSED SYSTEM AS WE DO NOT SPECIFY
DIC> @@ ANYTHING ELSE
DIC> @@
DIC>
DIC> @@
DIC> @@ AFTER THE SIMULATION IN exa2a THE PROFILES HAVE SOME FLUCTUATIONS. WE
DIC> @@ NOW TRY TO GET RID OF THESE USING IMPLICIT (1) TIME INTEGRATION
DIC> @@ INSTEAD OF THE MORE ACCURATE (BUT LESS STABLE) TRAPETZOIDAL METHOD
DIC> @@ (THE DEFAULT).
DIC> @@
DIC> s-s-c
    ... the command in full is SET_SIMULATION_CONDITION
NS01A PRINT CONTROL : /0/:
```

```
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /AUTO/:
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -> 1): /AUTO/: 1.0
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/: @@
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/: @@ 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 exa2b Y
   ... the command in full is SAVE_WORKSPACES
DIC>
DIC> set-inter
   ... the command in full is SET_INTERACTIVE
 --OK---
DIC>
```

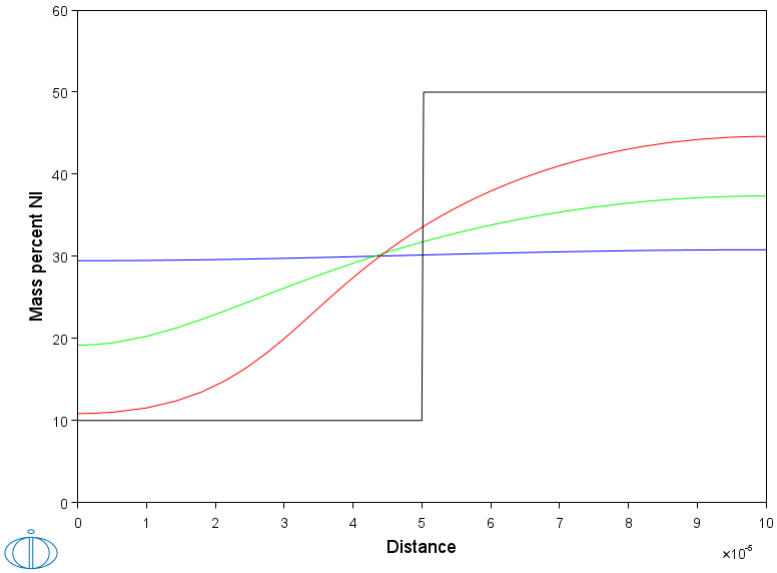
exa2b-run

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exa2b\run.DCM
   ... 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> @@ LET US DEFINE A LOG-FILE FOR THIS EXAMPLE
DIC> @@
DIC> set-log-file run
 AMBIGUOUS COMMAND, USE HELP
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
   ... the command in full is SET_NUMERICAL_LIMITS
 U-FRACTION IN SYSTEM:  FE = .708888245406169  NI = .29111175459383
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 U-FRACTION IN SYSTEM:  FE = .708888245406169  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 = .708888245406169  NI = .29111175459383
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =   8.1713545     DT =   7.7712544     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 =   23.713863     DT =   15.542509     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 =   54.798881     DT =   31.085018     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 =   116.96892     DT =   62.170036     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 =   241.30899     DT =   124.34007     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .70888824540617  NI = .291111754593831
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =   489.98913     DT =   248.68014     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 =   987.34941     DT =   497.36028     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 =   1982.0700     DT =   994.72057     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 =   3971.5111     DT =   1989.4411     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 =   7950.3934     DT =   3978.8823     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 =   15908.158     DT =   7957.7646     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 =   31823.687     DT =   15915.529     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 =   63654.745     DT =   31831.058     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 =   127316.86     DT =   63662.116     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .708888245406172  NI = .291111754593829
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =   227316.86     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 =   327316.86     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 =   427316.86     DT =   100000.00     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .708888245406158  NI = .291111754593842
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =   527316.86     DT =   100000.00     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .708888245406155  NI = .291111754593845
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =   627316.86     DT =   100000.00     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .708888245406153  NI = .291111754593847
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =   727316.86     DT =   100000.00     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .708888245406152  NI = .291111754593848
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =   827316.86     DT =   100000.00     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .708888245406153  NI = .291111754593847
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =   927316.86     DT =   100000.00     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .70888824540615  NI = .29111175459385
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =   1000000.0     DT =   72683.138     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .708888245406151  NI = .291111754593849
 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    8.1713545
 DELETING TIME-RECORD FOR TIME    23.713863
 DELETING TIME-RECORD FOR TIME    54.798881
 DELETING TIME-RECORD FOR TIME    116.96892
 DELETING TIME-RECORD FOR TIME    241.30899
 DELETING TIME-RECORD FOR TIME    489.98913
 DELETING TIME-RECORD FOR TIME    987.34941
 DELETING TIME-RECORD FOR TIME    1982.0700
 DELETING TIME-RECORD FOR TIME    3971.5111
 DELETING TIME-RECORD FOR TIME    7950.3934
 DELETING TIME-RECORD FOR TIME    15908.158
 DELETING TIME-RECORD FOR TIME    31823.687
 DELETING TIME-RECORD FOR TIME    63654.745
 DELETING TIME-RECORD FOR TIME    127316.86
 DELETING TIME-RECORD FOR TIME    227316.86
 DELETING TIME-RECORD FOR TIME    327316.86
 DELETING TIME-RECORD FOR TIME    427316.86
 DELETING TIME-RECORD FOR TIME    527316.86
 DELETING TIME-RECORD FOR TIME    627316.86
 DELETING TIME-RECORD FOR TIME    727316.86
 DELETING TIME-RECORD FOR TIME    827316.86

 KEEPING TIME-RECORD FOR TIME    927316.86
 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 exa2b\plot.DCM
   ... 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> @@ LET US DEFINE A LOG-FILE FOR THIS EXAMPLE
DIC> @@
DIC> set-log-file plot
 AMBIGUOUS COMMAND, USE HELP
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
```



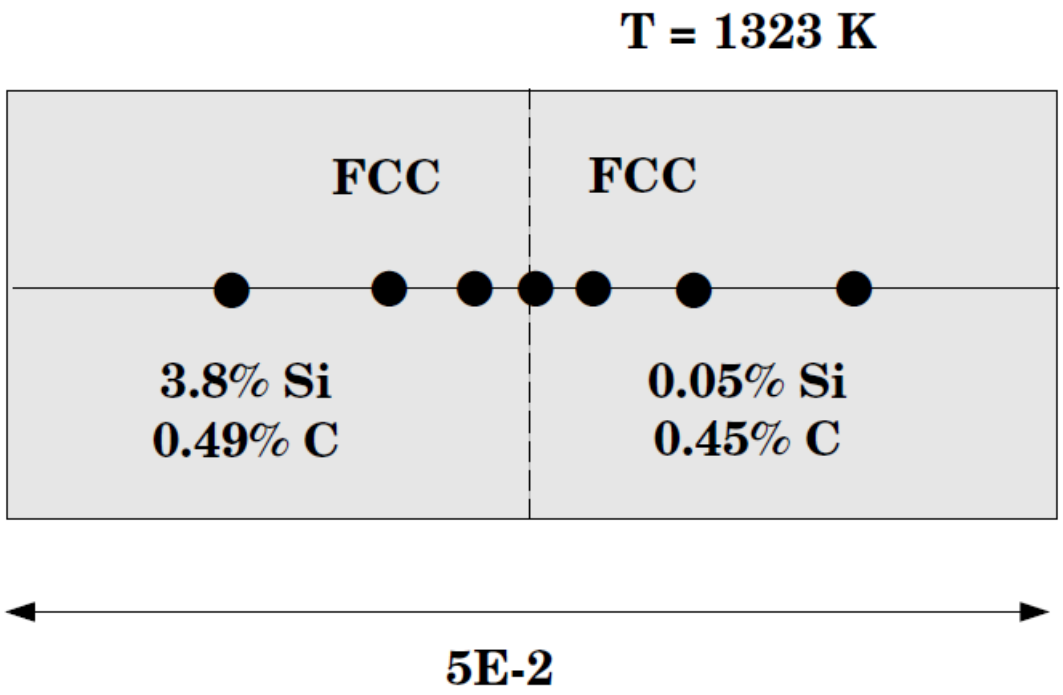

```
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
 --OK---
POST-1:
```

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: unknown compiler
 License library version: 9.7.0.0036
 Linked: Fri Oct 18 11:32:56 2024


SYS:SYS:MACRO exa3\setup.DCM
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: ------------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
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
12:36:09,339 [Thread-0] INFO  LicenseManager: Initializing user: jenkins.integrationtest@thermocalc.se
12:36:09,350 [Thread-0] INFO  LicenseController: Running License Spring in DEV environment.
12:36:10,484 [Thread-0] INFO  LicenseManager: There is an activated standalone license for jenkins.integrationtest@thermocalc.se for TC-
Application
 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
12:36:11,923 [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: @@
APP: @@ ENTER THE DICTRA MONITOR
APP: @@
APP: go d-m
12:36:13,912 [Thread-0] INFO  StandaloneLicenseController: Checking out license for: Diffusion (DICTRA)
 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 /LINEAR/: 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 exa3\run.DCM 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
 Region: AUSTENITE

 geometric   0.775567     dense at   0.250000E-01   62 points
 geometric    1.28938     dense at   0.250000E-01   61 points
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
 U-FRACTION IN SYSTEM:  C = .0215351645464253  FE = .962915638654286
                        SI = .0370843613457149
 TOTAL SIZE OF SYSTEM:  .05 [m]
 U-FRACTION IN SYSTEM:  C = .0215351645464253  FE = .962915638654286
                        SI = .0370843613457149
 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 = .0370843613457149
 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 = .0370843613457149
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.57710924E-02 DT =  0.56709924E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351645464254  FE = .962915638654286
                        SI = .0370843613457149
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.17113077E-01 DT =  0.11341985E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351645464254  FE = .962915638654286
                        SI = .0370843613457149
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    1  seconds
 TIME =  0.39797047E-01 DT =  0.22683970E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351645464254  FE = .962915638654286
                        SI = .0370843613457149
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.85164986E-01 DT =  0.45367939E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351645464254  FE = .962915638654286
                        SI = .0370843613457149
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.17590086     DT =  0.90735878E-01 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 =  0.35737262     DT =  0.18147176     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 =  0.72031613     DT =  0.36294351     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351645464256  FE = .962915638654286
                        SI = .0370843613457148
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    0  seconds
 TIME =   1.4462032     DT =  0.72588703     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351645464256  FE = .962915638654286
                        SI = .0370843613457149
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    0  seconds
 TIME =   2.8979772     DT =   1.4517741     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351645464256  FE = .962915638654286
                        SI = .0370843613457148
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    0  seconds
 TIME =   5.8015253     DT =   2.9035481     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351645464256  FE = .962915638654286
                        SI = .0370843613457149
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    0  seconds
 TIME =   11.608622     DT =   5.8070962     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351645464255  FE = .962915638654286
                        SI = .0370843613457148
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    0  seconds
 TIME =   23.222814     DT =   11.614192     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351645464233  FE = .962915638654286
                        SI = .0370843613457149
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    0  seconds
 TIME =   46.451199     DT =   23.228385     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351645464232  FE = .962915638654286
                        SI = .0370843613457149
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    0  seconds
 TIME =   92.907969     DT =   46.456770     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351645464234  FE = .962915638654286
                        SI = .0370843613457149
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    0  seconds
 TIME =   185.82151     DT =   92.913539     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351645464241  FE = .962915638654286
```

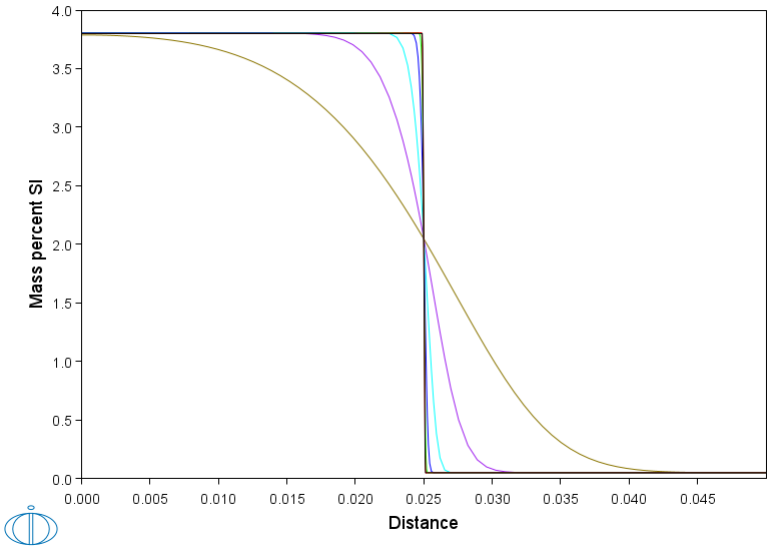
```
                        SI = .0370843613457149
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    0  seconds
 TIME =   371.64859     DT =   185.82708     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351645464243  FE = .962915638654286
                        SI = .0370843613457148
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    0  seconds
 TIME =   743.30274     DT =   371.65416     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351645464246  FE = .962915638654286
                        SI = .0370843613457148
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    1  seconds
 TIME =   1486.6111     DT =   743.30832     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351645464242  FE = .962915638654286
                        SI = .0370843613457148
 TOTAL SIZE OF SYSTEM:  .05 [m]


output ignored...



... output resumed

                        SI = .0370843613457148
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    0  seconds
 TIME =   12178363.     DT =   6089181.7     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351645457843  FE = .962915638654285
                        SI = .0370843613457148
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    0  seconds
 TIME =   24356727.     DT =   12178363.     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351645454141  FE = .962915638654285
                        SI = .0370843613457148
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    0  seconds
 TIME =   48713454.     DT =   24356727.     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .021535164545032  FE = .962915638654285
                        SI = .0370843613457148
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    0  seconds
 TIME =   97426908.     DT =   48713454.     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351645439542  FE = .962915638654285
                        SI = .0370843613457148
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    1  seconds
 TIME =  0.19485382E+09 DT =   97426908.     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351645439467  FE = .962915638654285
                        SI = .0370843613457149
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.38970763E+09 DT =  0.19485382E+09 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351645444974  FE = .962915638654286
                        SI = .0370843613457147
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.77941526E+09 DT =  0.38970763E+09 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351645457158  FE = .962915638654286
                        SI = .0370843613457144
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.15588305E+10 DT =  0.77941526E+09 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351645372402  FE = .962915638654286
                        SI = .0370843613457147
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.25588305E+10 DT =  0.10000000E+10 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351645333891  FE = .962915638654286
                        SI = .0370843613457145
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.35588305E+10 DT =  0.10000000E+10 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351645298693  FE = .962915638654285
                        SI = .0370843613457146
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.45588305E+10 DT =  0.10000000E+10 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351645156433  FE = .962915638654286
                        SI = .0370843613457133
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.55588305E+10 DT =  0.10000000E+10 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351645015361  FE = .962915638654286
                        SI = .0370843613457136
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.65588305E+10 DT =  0.10000000E+10 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351644959889  FE = .962915638654288
                        SI = .0370843613457118
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    1  seconds
 TIME =  0.75588305E+10 DT =  0.10000000E+10 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351645028132  FE = .962915638654288
                        SI = .0370843613457113
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.85588305E+10 DT =  0.10000000E+10 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351645129319  FE = .962915638654289
                        SI = .037084361345711
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.95588305E+10 DT =  0.10000000E+10 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351645148812  FE = .96291563865429
                        SI = .0370843613457108
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.10000000E+11 DT =  0.44116948E+09 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .021535164519554  FE = .962915638654289
                        SI = .0370843613457113
 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   0.57710924E-02
 DELETING TIME-RECORD FOR TIME   0.17113077E-01
 DELETING TIME-RECORD FOR TIME   0.39797047E-01
 DELETING TIME-RECORD FOR TIME   0.85164986E-01
 DELETING TIME-RECORD FOR TIME   0.17590086
 DELETING TIME-RECORD FOR TIME   0.35737262
 DELETING TIME-RECORD FOR TIME   0.72031613
 DELETING TIME-RECORD FOR TIME    1.4462032
 DELETING TIME-RECORD FOR TIME    2.8979772
 DELETING TIME-RECORD FOR TIME    5.8015253
 DELETING TIME-RECORD FOR TIME    11.608622
 DELETING TIME-RECORD FOR TIME    23.222814
 DELETING TIME-RECORD FOR TIME    46.451199
 DELETING TIME-RECORD FOR TIME    92.907969
 DELETING TIME-RECORD FOR TIME    185.82151
 DELETING TIME-RECORD FOR TIME    371.64859
 DELETING TIME-RECORD FOR TIME    743.30274
 DELETING TIME-RECORD FOR TIME    1486.6111
 DELETING TIME-RECORD FOR TIME    2973.2277
 DELETING TIME-RECORD FOR TIME    5946.4610
 DELETING TIME-RECORD FOR TIME    11892.927
 DELETING TIME-RECORD FOR TIME    23785.861
 DELETING TIME-RECORD FOR TIME    47571.727
 DELETING TIME-RECORD FOR TIME    95143.459
 DELETING TIME-RECORD FOR TIME    190286.92
 DELETING TIME-RECORD FOR TIME    380573.85
 DELETING TIME-RECORD FOR TIME    761147.71
 DELETING TIME-RECORD FOR TIME    1522295.4
 DELETING TIME-RECORD FOR TIME    3044590.9
 DELETING TIME-RECORD FOR TIME    6089181.7
 DELETING TIME-RECORD FOR TIME    12178363.
 DELETING TIME-RECORD FOR TIME    24356727.
 DELETING TIME-RECORD FOR TIME    48713454.
 DELETING TIME-RECORD FOR TIME    97426908.
 DELETING TIME-RECORD FOR TIME   0.19485382E+09
 DELETING TIME-RECORD FOR TIME   0.38970763E+09
 DELETING TIME-RECORD FOR TIME   0.77941526E+09
 DELETING TIME-RECORD FOR TIME   0.15588305E+10
 DELETING TIME-RECORD FOR TIME   0.25588305E+10
 DELETING TIME-RECORD FOR TIME   0.35588305E+10
 DELETING TIME-RECORD FOR TIME   0.45588305E+10
 DELETING TIME-RECORD FOR TIME   0.55588305E+10
 DELETING TIME-RECORD FOR TIME   0.65588305E+10
 DELETING TIME-RECORD FOR TIME   0.75588305E+10
 DELETING TIME-RECORD FOR TIME   0.85588305E+10

 KEEPING TIME-RECORD FOR TIME   0.95588305E+10
 AND FOR TIME                   0.10000000E+11
 WORKSPACE RECLAIMED

 TIMESTEP AT    0.100000000E+11 SELECTED

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

exa3-plot

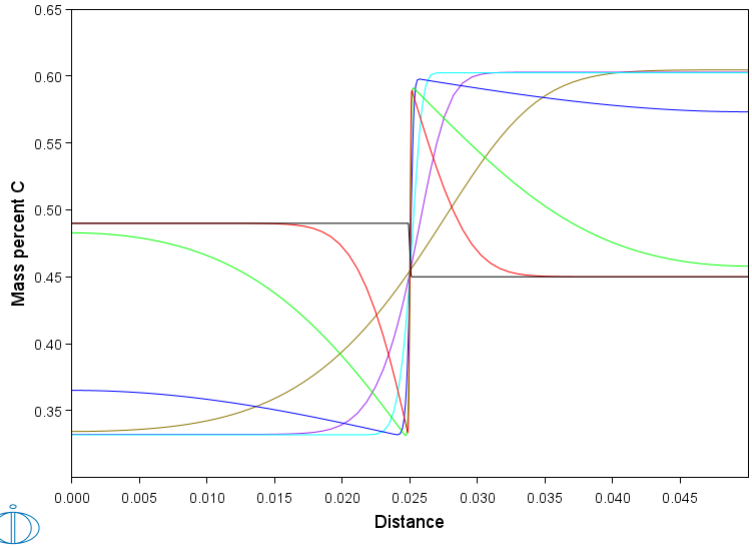
```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exa3\plot.DCM DIC>
DIC>
DIC> @@ darken_plot.DCM
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA MODULE AND SPECIFY THE STORE-RESULT FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  1.00000E+10
DIC> read exa3
 OK
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA POST PROCESSOR
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:
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



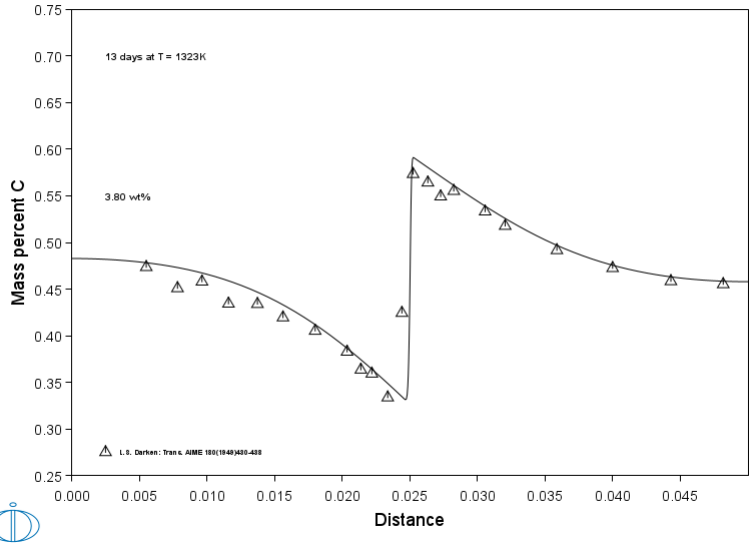

```
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1: @@
POST-1: @@ PLOT THE CONCENTRATION PROFILES FOR C
POST-1: @@
POST-1: @@ WE ONLY NEED TO CHANGE THE Y-AXIS
POST-1: @@
POST-1: set-diagram-axis y w-p c
POST-1: set-title Figure a3.2
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples/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

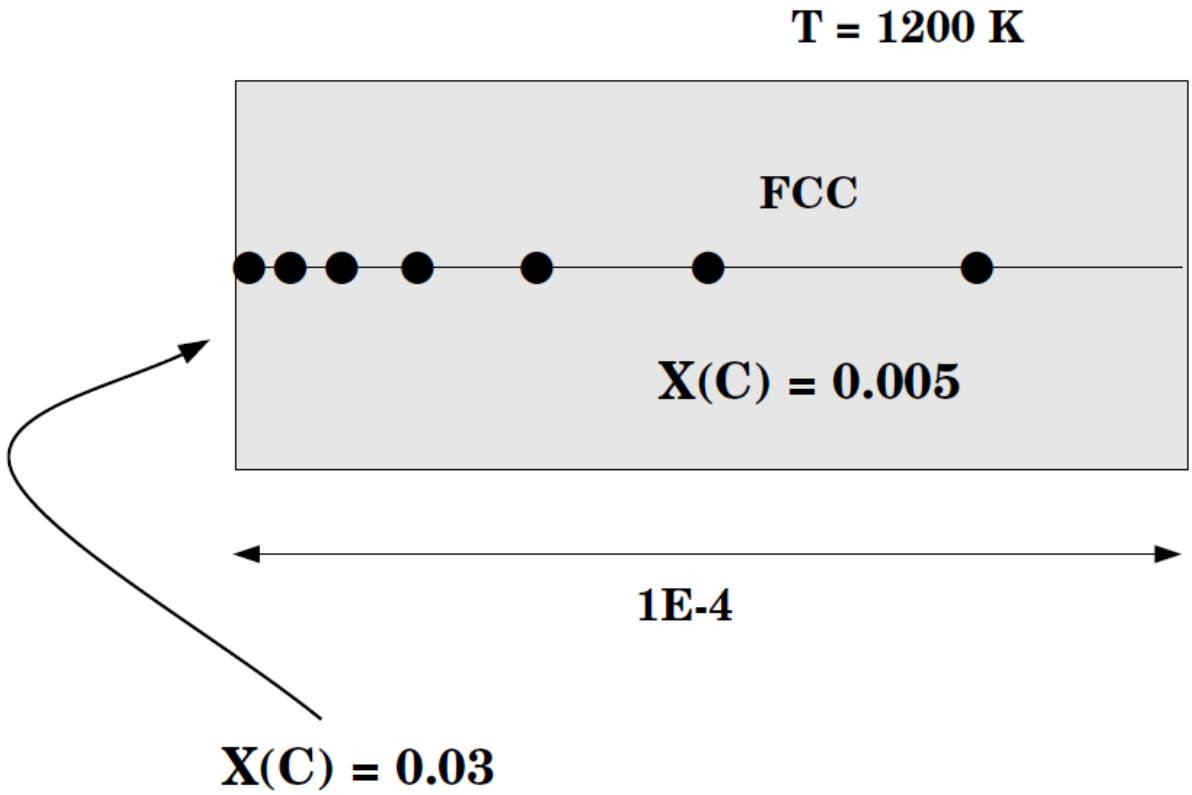



```
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1: set-inter
 --OK---
POST-1:
```

Example 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: unknown compiler
 License library version: 9.7.0.0036
 Linked: Fri Oct 18 11:32:56 2024


SYS:SYS:MACRO exa4\setup.DCM
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: ----------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exa4_setup.DCM
SYS:
SYS:
SYS: @@
SYS: @@ READ THE DATA FROM THE DATABASES
SYS: @@
SYS: go da
12:39:14,903 [Thread-0] INFO  LicenseManager: Initializing user: jenkins.integrationtest@thermocalc.se
12:39:14,921 [Thread-0] INFO  LicenseController: Running License Spring in DEV environment.
12:39:15,987 [Thread-0] INFO  LicenseManager: There is an activated standalone license for jenkins.integrationtest@thermocalc.se for TC-
Application
 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 v5.0

 VA                       /-  DEFINED
TDB_FEDEMO: def-system fe,c
 FE                       C  DEFINED
TDB_FEDEMO: rej-ph *
 BCC_A2                   CBCC_A12                 CEMENTITE
 CUB_A13                  DIAMOND_FCC_A4           FCC_A1
 GAS:G                    GRAPHITE                 HCP_A3
 KSI_CARBIDE              LAVES_PHASE_C14          LIQUID:L
 M23C6                    M5C2                     M7C3
   REJECTED
TDB_FEDEMO: rest-ph fcc
 FCC_A1  RESTORED
TDB_FEDEMO: get
12:39:17,090 [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
12:39:17,517 [Thread-0] INFO  TDBFileParser: USER_1068030556_19, number of lines read: 29
12:39:17,603 [Thread-0] INFO  DatabaseUtils: Parsing of USER_1068030556_19 completed in 136 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
12:39:17,691 [Thread-0] INFO  Database: Preparing system for use: USER_1068030556_19
 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
12:39:18,738 [Thread-0] INFO  StandaloneLicenseController: Checking out license for: Diffusion (DICTRA)
 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 /LINEAR/: 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
12:39:19,172 [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>
```

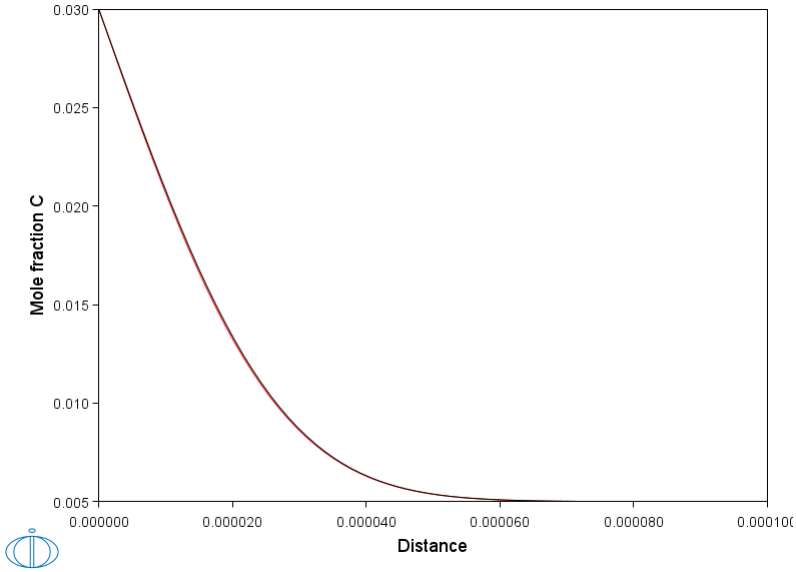
exa4-run

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exa4\run.DCM 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
 Region: STEEL
 geometric     1.25105      dense at     0.00000        94 points
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
 U-FRACTION IN SYSTEM:  C = .0050251256281407  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 U-FRACTION IN SYSTEM:  C = .0050251256281407  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 = .00502617509162927  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.37956667E-05 DT =  0.36956667E-05 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00502708779555048  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.11187000E-04 DT =  0.73913334E-05 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00502817020604311  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.25969667E-04 DT =  0.14782667E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0050296038735483  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.55535000E-04 DT =  0.29565333E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00503157393095319  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.11466567E-03 DT =  0.59130667E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00503432266150507  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.23292700E-03 DT =  0.11826133E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00503818457565281  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.46944967E-03 DT =  0.23652267E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00504362854755978  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.94249500E-03 DT =  0.47304534E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00505131516064607  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.18885857E-02 DT =  0.94609067E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00506217699893383  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.37807670E-02 DT =  0.18921813E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00507753183894502  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.75651297E-02 DT =  0.37843627E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00509924254027779  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.15133855E-01 DT =  0.75687254E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00512994305448753  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.30271306E-01 DT =  0.15137451E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0051733579791448  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.60546207E-01 DT =  0.30274901E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00523475442805027  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.12109601     DT =  0.60549803E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00532158103955812  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.24219562     DT =  0.12109961     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00544437164798843  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.48439483     DT =  0.24219921     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00561802316451053  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.96879325     DT =  0.48439842     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00586359475094639  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =   1.9375901     DT =  0.96879685     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00621077816889617  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =   3.8751838     DT =   1.9375937     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00670148793819335  FE = 1
```

```
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =   7.7503712     DT =   3.8751874     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00739523402893566  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =   15.500746     DT =   7.7503748     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00837631081644418  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    1  seconds
 TIME =   25.500746     DT =   10.000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0093213064061285  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =   35.500746     DT =   10.000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0100925061409116  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =   45.500746     DT =   10.000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0107609822959055  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =   55.500746     DT =   10.000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0113593595275401  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =   65.500746     DT =   10.000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0119059374456757  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =   75.500746     DT =   10.000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0124122120385256  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =   85.500746     DT =   10.000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0128859665829032  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =   95.500746     DT =   10.000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0133327602484627  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =   100.00000     DT =   4.4992540     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0135261063630477  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   0.37956667E-05
 DELETING TIME-RECORD FOR TIME   0.11187000E-04
 DELETING TIME-RECORD FOR TIME   0.25969667E-04
 DELETING TIME-RECORD FOR TIME   0.55535000E-04
 DELETING TIME-RECORD FOR TIME   0.11466567E-03
 DELETING TIME-RECORD FOR TIME   0.23292700E-03
 DELETING TIME-RECORD FOR TIME   0.46944967E-03
 DELETING TIME-RECORD FOR TIME   0.94249500E-03
 DELETING TIME-RECORD FOR TIME   0.18885857E-02
 DELETING TIME-RECORD FOR TIME   0.37807670E-02
 DELETING TIME-RECORD FOR TIME   0.75651297E-02
 DELETING TIME-RECORD FOR TIME   0.15133855E-01
 DELETING TIME-RECORD FOR TIME   0.30271306E-01
 DELETING TIME-RECORD FOR TIME   0.60546207E-01
 DELETING TIME-RECORD FOR TIME   0.12109601
 DELETING TIME-RECORD FOR TIME   0.24219562
 DELETING TIME-RECORD FOR TIME   0.48439483
 DELETING TIME-RECORD FOR TIME   0.96879325
 DELETING TIME-RECORD FOR TIME    1.9375901
 DELETING TIME-RECORD FOR TIME    3.8751838
 DELETING TIME-RECORD FOR TIME    7.7503712
 DELETING TIME-RECORD FOR TIME    15.500746
 DELETING TIME-RECORD FOR TIME    25.500746
 DELETING TIME-RECORD FOR TIME    35.500746
 DELETING TIME-RECORD FOR TIME    45.500746
 DELETING TIME-RECORD FOR TIME    55.500746
 DELETING TIME-RECORD FOR TIME    65.500746
 DELETING TIME-RECORD FOR TIME    75.500746
 DELETING TIME-RECORD FOR TIME    85.500746

 KEEPING TIME-RECORD FOR TIME    95.500746
 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>
```

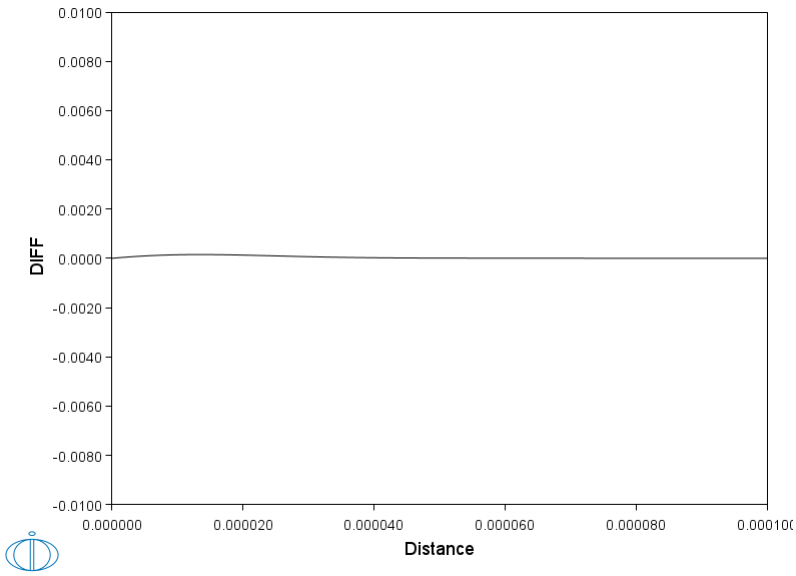
exa4-plot

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exa4\plot.DCM 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 ERFSOL
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
```

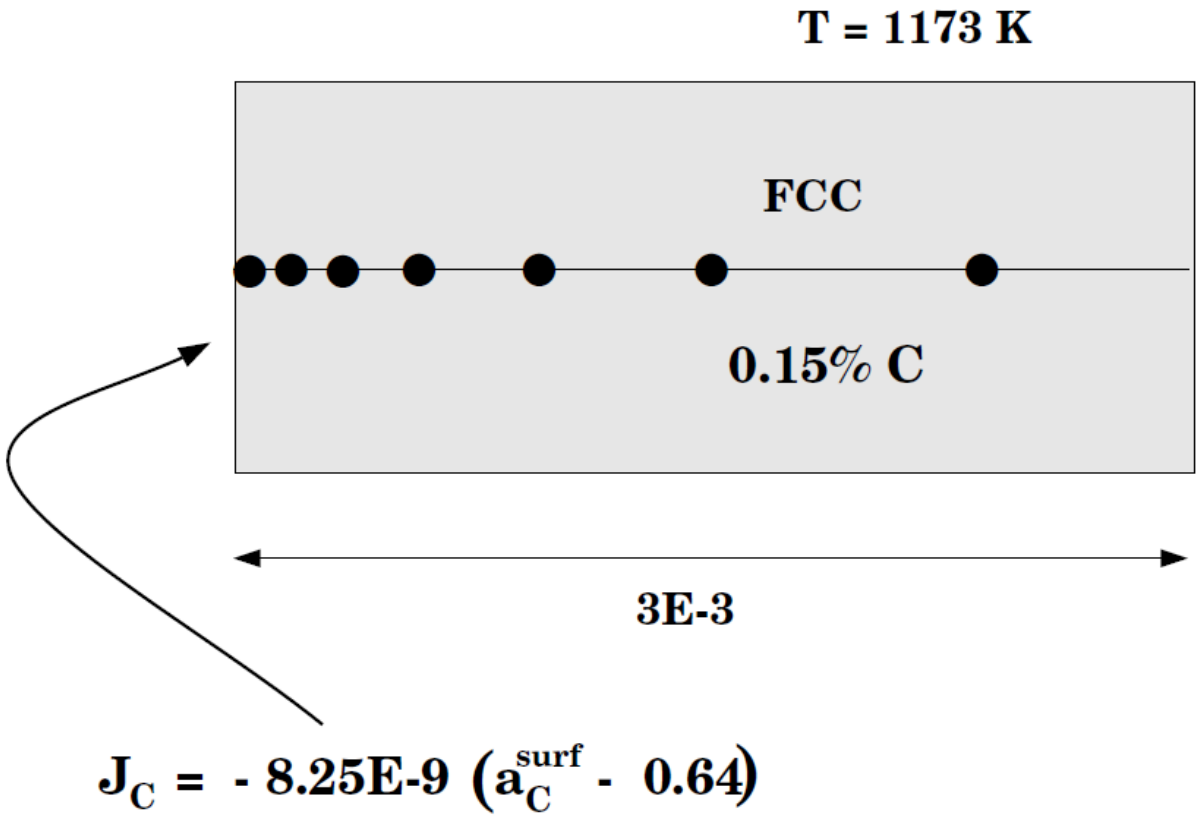



```
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: set-interactive
 --OK---
POST-1:
```

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% N2 and 60% cracked methanol is used as carrier gas. The carburizing "carbon potential" in the gas is 0.85 wt%.



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: unknown compiler
 License library version: 9.7.0.0036
 Linked: Fri Oct 18 11:32:56 2024


SYS:SYS:MACRO exa5\setup.DCM
SYS: ï»¿@@
 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: ----------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exa5_setup.DCM
SYS:
SYS: @@
SYS: @@ GO TO THE DATABASES AND READ THE THERMODYNAMIC AND KINETIC DATA
SYS: @@
SYS: go da
12:42:13,056 [Thread-0] INFO  LicenseManager: Initializing user: jenkins.integrationtest@thermocalc.se
12:42:13,068 [Thread-0] INFO  LicenseController: Running License Spring in DEV environment.
12:42:14,181 [Thread-0] INFO  LicenseManager: There is an activated standalone license for jenkins.integrationtest@thermocalc.se for TC-
Application
 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 v5.0

 VA                       /-  DEFINED
TDB_FEDEMO: def-sys fe,c
 FE                       C  DEFINED
TDB_FEDEMO: rej-ph *
 BCC_A2                   CBCC_A12                 CEMENTITE
 CUB_A13                  DIAMOND_FCC_A4           FCC_A1
 GAS:G                    GRAPHITE                 HCP_A3
 KSI_CARBIDE              LAVES_PHASE_C14          LIQUID:L
 M23C6                    M5C2                     M7C3
   REJECTED
TDB_FEDEMO: rest-ph fcc graphite
 FCC_A1                   GRAPHITE  RESTORED
TDB_FEDEMO: get
12:42:15,265 [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 v5.0
 MOB2    =  Alloys Mobility  v2.7
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBFE7  =  Steels/Fe-Alloys Mobility  v7.1
 MFEDEMO =  Fe-Alloys Mobility demo database v4.0
 USER    =  User defined Database

DATABASE NAME /FEDEMO/: mfedemo
 Current database: Fe-Alloys Mobility demo database v4.0

 VA  DEFINED
APP: def-sys fe,c
 FE                       C  DEFINED
APP: rej-ph *
 BCC_A2                   FCC_A1                   CEMENTITE
 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
```

```
12:42:15,814 [Thread-0] INFO  StandaloneLicenseController: Checking out license for: Diffusion (DICTRA)
 NO TIME STEP DEFINED
 *** ENTERING GRAPHITE 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 /LINEAR/: 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> @@
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> @@                k      k
DIC> @@
DIC> @@                                  N
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> @@
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 Ã…gren (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 Ã…gren's paper.
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 Ã…gren'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:
                              N
   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>
```

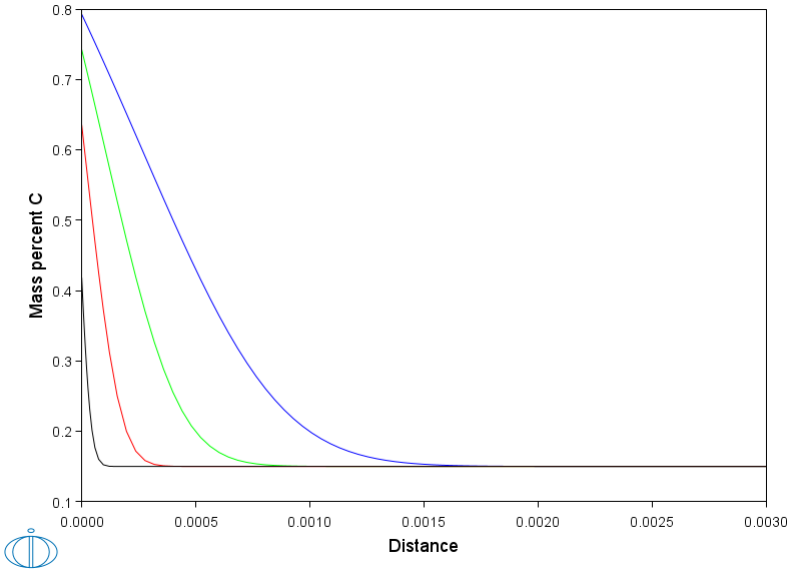
exa5-run

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exa5\run.DCM 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 AS A DIFFUSION NONE PHASE
DIC> read exa5
 OK
DIC>
DIC> @@
DIC> @@ Start the simulation
DIC> @@
DIC> sim
 Region: STEEL
 geometric    1.27936     dense at    0.00000       95 points
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
 U-FRACTION IN SYSTEM:  C = .00698495916383109  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
 U-FRACTION IN SYSTEM:  C = .00698495916383109  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
 TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =   0.0000000

 U-FRACTION IN SYSTEM:  C = .00698495916398349  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1  seconds
 TIME =  0.95299491E-03 DT =  0.95289491E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698496061502291  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.28587847E-02 DT =  0.19057898E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698496351399744  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.66703643E-02 DT =  0.38115796E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698496930531781  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1  seconds
 TIME =  0.14293524E-01 DT =  0.76231592E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698498087073359  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.29539842E-01 DT =  0.15246318E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698500395469351  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1  seconds
 TIME =  0.60032479E-01 DT =  0.30492637E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698504999274662  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.12101775     DT =  0.60985274E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698514170641631  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1  seconds
 TIME =  0.24298830     DT =  0.12197055     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698532412013541  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.48692940     DT =  0.24394110     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698568611535581  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.97481159     DT =  0.48788219     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698640221700123  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1  seconds
 TIME =   1.9505760     DT =  0.97576438     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698781256430923  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0  seconds
 TIME =   3.9021047     DT =   1.9515288     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00699057318697584  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1  seconds
 TIME =   7.8051623     DT =   3.9030575     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00699593118623284  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0  seconds
 TIME =   15.611277     DT =   7.8061151     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00700621054657889  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1  seconds
 TIME =   31.223507     DT =   15.612230     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00702562665925562  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0  seconds
 TIME =   62.447968     DT =   31.224460     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00706155638240379  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1  seconds
 TIME =   124.89689     DT =   62.448921     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00712632808815366  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1  seconds
 TIME =   249.79473     DT =   124.89784     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00723942185480152  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0  seconds
 TIME =   499.59041     DT =   249.79568     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00742975463683524  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1  seconds
 TIME =   999.18178     DT =   499.59136     SUM OF SQUARES =   0.0000000
```

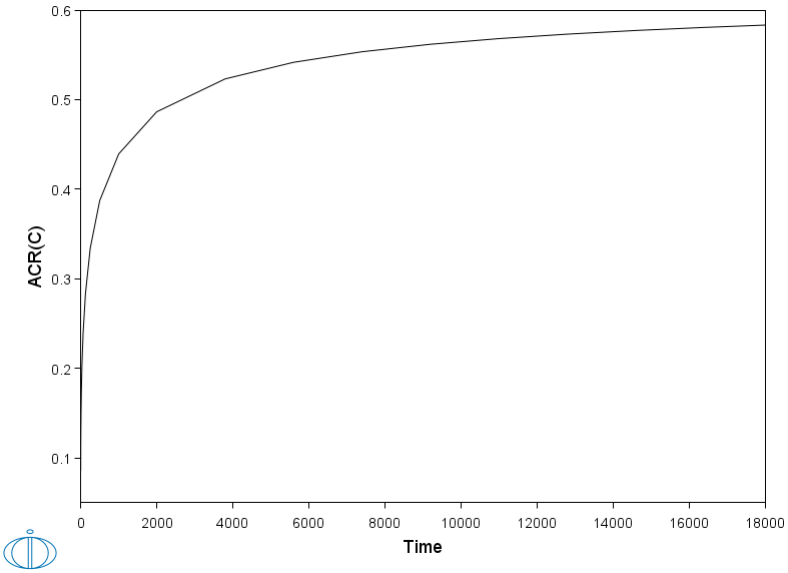
```
 U-FRACTION IN SYSTEM:  C = .00773776331980571  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0  seconds
 TIME =   1998.3645     DT =   999.18273     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00821761065515563  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1  seconds
 TIME =   3798.3645     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00887750840101946  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0  seconds
 TIME =   5598.3645     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00940738002428763  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1  seconds
 TIME =   7398.3645     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00986378023700771  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0  seconds
 TIME =   9198.3645     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0102709311131761  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1  seconds
 TIME =   10998.365     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0106420492512965  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1  seconds
 TIME =   12798.365     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0109853092783316  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0  seconds
 TIME =   14598.365     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0113061900988817  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1  seconds
 TIME =   16398.365     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0116085766431791  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0  seconds
 TIME =   18000.000     DT =   1601.6355     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0118644277553409  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   0.95299491E-03
 DELETING TIME-RECORD FOR TIME   0.28587847E-02
 DELETING TIME-RECORD FOR TIME   0.66703643E-02
 DELETING TIME-RECORD FOR TIME   0.14293524E-01
 DELETING TIME-RECORD FOR TIME   0.29539842E-01
 DELETING TIME-RECORD FOR TIME   0.60032479E-01
 DELETING TIME-RECORD FOR TIME   0.12101775
 DELETING TIME-RECORD FOR TIME   0.24298830
 DELETING TIME-RECORD FOR TIME   0.48692940
 DELETING TIME-RECORD FOR TIME   0.97481159
 DELETING TIME-RECORD FOR TIME    1.9505760
 DELETING TIME-RECORD FOR TIME    3.9021047
 DELETING TIME-RECORD FOR TIME    7.8051623
 DELETING TIME-RECORD FOR TIME    15.611277
 DELETING TIME-RECORD FOR TIME    31.223507
 DELETING TIME-RECORD FOR TIME    62.447968
 DELETING TIME-RECORD FOR TIME    124.89689
 DELETING TIME-RECORD FOR TIME    249.79473
 DELETING TIME-RECORD FOR TIME    499.59041
 DELETING TIME-RECORD FOR TIME    999.18178
 DELETING TIME-RECORD FOR TIME    1998.3645
 DELETING TIME-RECORD FOR TIME    3798.3645
 DELETING TIME-RECORD FOR TIME    5598.3645
 DELETING TIME-RECORD FOR TIME    7398.3645
 DELETING TIME-RECORD FOR TIME    9198.3645
 DELETING TIME-RECORD FOR TIME    10998.365
 DELETING TIME-RECORD FOR TIME    12798.365
 DELETING TIME-RECORD FOR TIME    14598.365

 KEEPING TIME-RECORD FOR TIME    16398.365
 AND FOR TIME                    18000.000
 WORKSPACE RECLAIMED

 TIMESTEP AT     18000.0000     SELECTED

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

exa5-plot

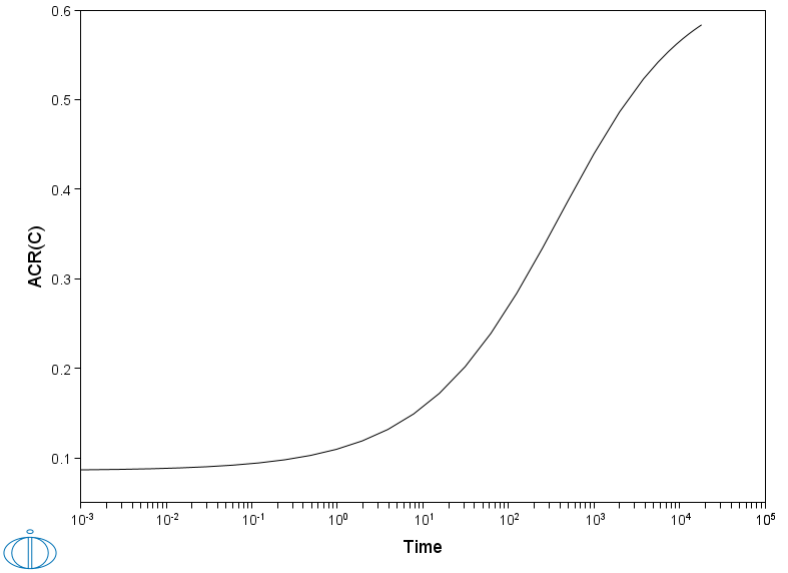
```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exa5\plot.DCM DIC>
DIC>
DIC> @@ exa5_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE a5
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  1.80000E+04
*** ENTERING GRAPHITE 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
```



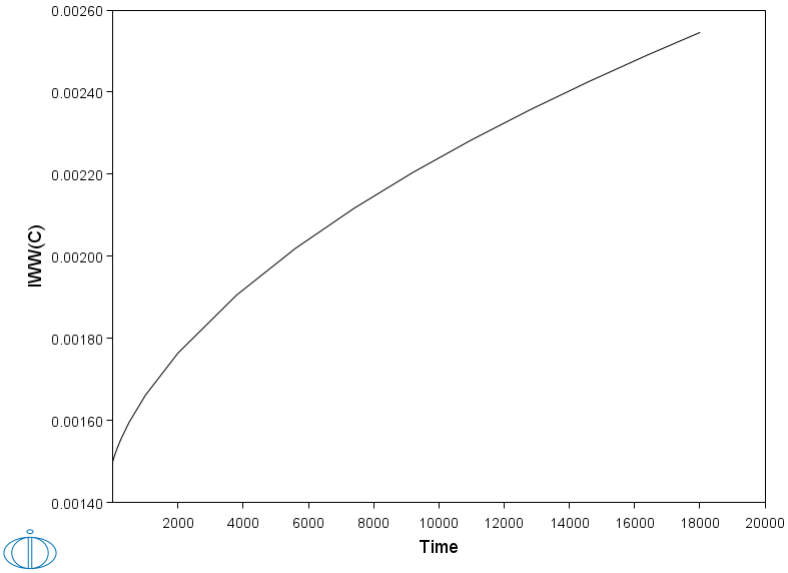

```
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: @@
POST-1: @@ PLOT THE VARIATION OF THE C ACTIVITY AT THE SURFACE
POST-1: @@
POST-1: s-d-a y acr(c)
POST-1:
POST-1: s-d-a x time
  INFO: Time is set as independent variable
POST-1:
POST-1: s-p-c
CONDITION /TIME/: interface
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
AXIS (X, Y OR Z) : x
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
AXIS (X, Y OR Z) : x
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
     OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

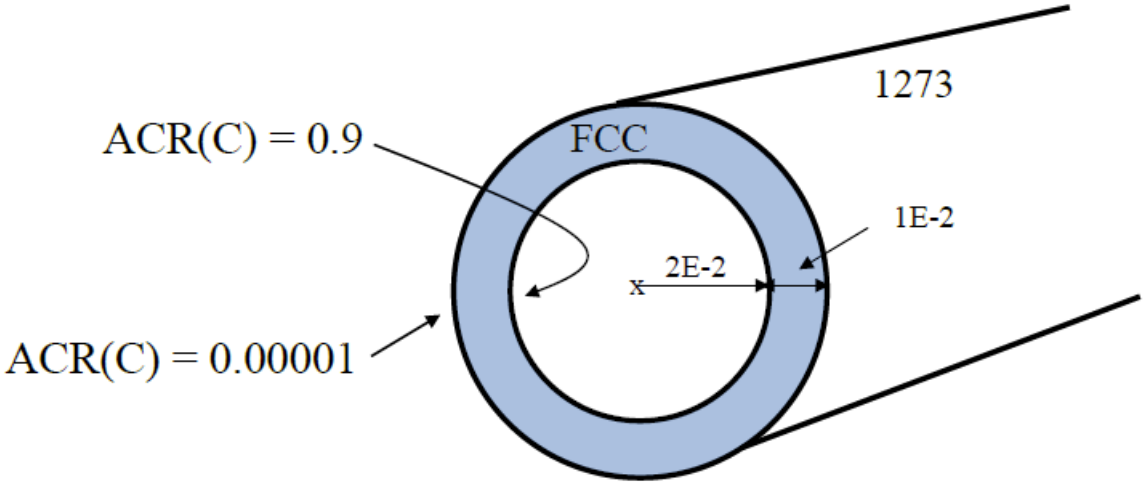



```
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1:
POST-1: set-inter
 --OK---
POST-1:
```

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: unknown compiler
 License library version: 9.7.0.0036
 Linked: Fri Oct 18 11:32:56 2024


SYS:SYS:MACRO exa6\setup.DCM
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: ----------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ setup.DCM
SYS:
SYS:
SYS: @@
SYS: @@ GO TO THE DATABASE MODULE
SYS: @@
SYS: go da
12:45:24,234 [Thread-0] INFO  LicenseManager: Initializing user: jenkins.integrationtest@thermocalc.se
12:45:24,246 [Thread-0] INFO  LicenseController: Running License Spring in DEV environment.
12:45:25,315 [Thread-0] INFO  LicenseManager: There is an activated standalone license for jenkins.integrationtest@thermocalc.se for TC-
Application
 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
 L12_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
 FESI2_H                FESI2_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
12:45:26,778 [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_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ SWITCH TO A MOBILITY DATABASE TO RETRIVE 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 v5.0
 MOB2    =  Alloys Mobility  v2.7
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBFE7  =  Steels/Fe-Alloys Mobility  v7.1
 MFEDEMO =  Fe-Alloys Mobility demo database v4.0
 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
12:45:28,732 [Thread-0] INFO  StandaloneLicenseController: Checking out license for: Diffusion (DICTRA)
 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 /LINEAR/: 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_a1#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

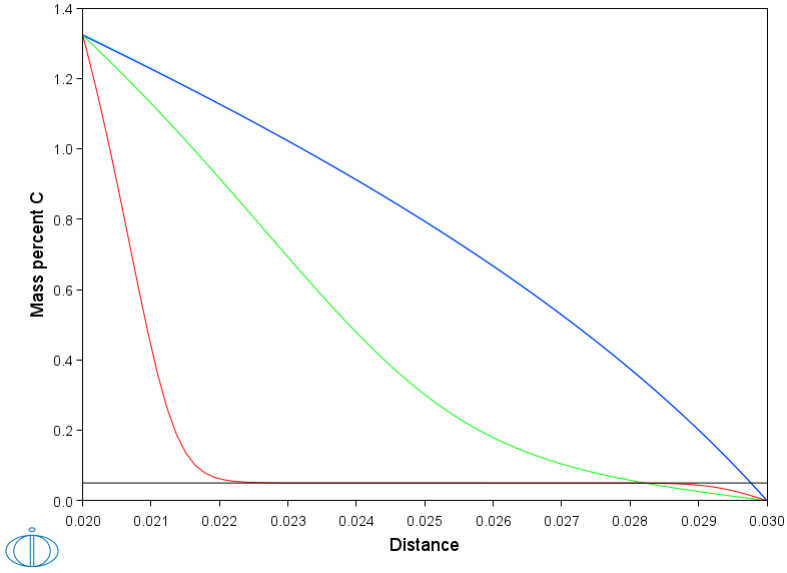
```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exa6\run.DCM DIC>
DIC>
DIC> @@ run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING exa6
DIC> @@
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  0.00000E+00
*** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
DIC> read exa6
 OK
DIC>
DIC> @@
DIC> @@ Start the simulation
DIC> @@
DIC> simulate
 Region: AUS

 geometric    1.27604     dense at    0.00000       60 points
 geometric   0.783674     dense at   0.100000E-01   61 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 = .00115512673207609  FE = .490055682684517
                        MN = .00302988813183617  SI = .00691442924890043
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0  seconds
 TIME =  0.56872581E-03 DT =  0.56862581E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00115539046454592  FE = .490055682684517
                        MN = .00302988813183617  SI = .00691442924890043
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    1  seconds
 TIME =  0.17059774E-02 DT =  0.11372516E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00115567510064984  FE = .490055682684517
                        MN = .00302988813183617  SI = .00691442924890043
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0  seconds
 TIME =  0.39804807E-02 DT =  0.22745033E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0011560487094729  FE = .490055682684517
                        MN = .00302988813183617  SI = .00691442924890043
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0  seconds
 TIME =  0.85294872E-02 DT =  0.45490065E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00115655912635867  FE = .490055682684517
                        MN = .00302988813183617  SI = .00691442924890043
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0  seconds
 TIME =  0.17627500E-01 DT =  0.90980130E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00115727073516779  FE = .490055682684517
                        MN = .00302988813183617  SI = .00691442924890043
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    1  seconds
 TIME =  0.35823526E-01 DT =  0.18196026E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0011582703950613  FE = .490055682684517
                        MN = .00302988813183617  SI = .00691442924890043
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0  seconds
 TIME =  0.72215578E-01 DT =  0.36392052E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00115967961028044  FE = .490055682684517
                        MN = .00302988813183617  SI = .00691442924890043
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0  seconds
 TIME =  0.14499968     DT =  0.72784104E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00116166951188139  FE = .490055682684517
                        MN = .00302988813183617  SI = .00691442924890043
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0  seconds
 TIME =  0.29056789     DT =  0.14556821     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00116448166788345  FE = .490055682684517
                        MN = .00302988813183617  SI = .00691442924890044
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0  seconds
 TIME =  0.58170431     DT =  0.29113642     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00116845744539901  FE = .490055682684517
                        MN = .00302988813183617  SI = .00691442924890045
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    1  seconds
 TIME =   1.1639771     DT =  0.58227283     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00117407951438293  FE = .490055682684517
                        MN = .00302988813183616  SI = .0069144292489005
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0  seconds
 TIME =   2.3285228     DT =   1.1645457     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0011820305728604  FE = .490055682684517
                        MN = .00302988813183615  SI = .0069144292489006
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0  seconds
 TIME =   4.6576141     DT =   2.3290913     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00119327652565352  FE = .490055682684517
                        MN = .00302988813183613  SI = .00691442924890082
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0  seconds
 TIME =   9.3157968     DT =   4.6581827     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00120918436056017  FE = .490055682684516
                        MN = .00302988813183609  SI = .00691442924890128
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0  seconds
 TIME =   18.632162     DT =   9.3163653     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00123168907416774  FE = .490055682684515
                        MN = .00302988813183599  SI = .00691442924890222
```

```
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    1  seconds
 TIME =   37.264893     DT =   18.632731     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0012635303688526  FE = .490055682684514
                        MN = .00302988813318358  SI = .00691442924890 41
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0  seconds
 TIME =   74.530354     DT =   37.265461     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00130859024666678  FE = .49005568268451
                        MN = .00302988813183541  SI = .00691442924890786
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0  seconds
 TIME =   149.06128     DT =   74.530923     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00137237416492751  FE = .490055682684503


output ignored...



... output resumed

 TIME =   4510975.0     DT =   2068745.7     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .016525523457144  FE = .490055682687858
                        MN = .00302988813213476  SI = .00691442924526043
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    1  seconds
 TIME =   7984253.8     DT =   3473278.8     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165254508590697  FE = .490055682692971
                        MN = .00302988813259319  SI = .00691442923968928
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0  seconds
 TIME =   14356039.     DT =   6371785.0     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165252154821963  FE = .490055682706394
                        MN = .00302988813380114  SI = .00691442922505839
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0  seconds
 TIME =   27099609.     DT =   12743570.     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165248326666943  FE = .490055682744166
                        MN = .00302988813721716  SI = .00691442918387045
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    1  seconds
 TIME =   52586749.     DT =   25487140.     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165245057734572  FE = .490055682840343
                        MN = .00302988814633 77  SI = .00691442907857307
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0  seconds
 TIME =  0.10356103E+09 DT =   50974280.     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165244338589318  FE = .490055683043849
                        MN = .00302988816787848  SI = .00691442885352646
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    1  seconds
 TIME =  0.20356103E+09 DT =  0.10000000E+09 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165251143593027  FE = .490055683399 03
                        MN = .00302988821068092  SI = .00691442845554229
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0  seconds
 TIME =  0.30356103E+09 DT =  0.10000000E+09 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165294065728479  FE = .490055683698864
                        MN = .00302988825007241  SI = .00691442811631683
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0  seconds
 TIME =  0.40356103E+09 DT =  0.10000000E+09 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165328554141336  FE = .4900556839606
                        MN = .00302988828597 52  SI = .00691442781867839
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    1  seconds
 TIME =  0.50356103E+09 DT =  0.10000000E+09 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165359337862441  FE = .490055684195043
                        MN = .00302988831898553  SI = .00691442755122457
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0  seconds
 TIME =  0.60356103E+09 DT =  0.10000000E+09 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165387963870418  FE = .490055684408837
                        MN = .00302988834962401  SI = .00691442730679207
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0  seconds
 TIME =  0.70356103E+09 DT =  0.10000000E+09 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165415123631262  FE = .490055684606355
                        MN = .00302988837829336  SI = .00691442708060457
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    1  seconds
 TIME =  0.80356103E+09 DT =  0.10000000E+09 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165441188639461  FE = .490055684790642
                        MN = .00302988840530221  SI = .00691442686930959
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0  seconds
 TIME =  0.90356103E+09 DT =  0.10000000E+09 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165466383340927  FE = .49005568496391
                        MN = .00302988843089012  SI = .00691442667045363
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    1  seconds
 TIME =  0.99821067E+09 DT =   94649637.     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165491221039358  FE = .490055685119269
                        MN = .00302988845397132  SI = .00691442649201306
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0  seconds
 TIME =  0.10000000E+10 DT =   1789334.3     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165517598390004  FE = .490055685122132
                        MN = .0030298884543974  SI = .00691442648872354
 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   0.56872581E-03
 DELETING TIME-RECORD FOR TIME   0.17059774E-02
 DELETING TIME-RECORD FOR TIME   0.39804807E-02
 DELETING TIME-RECORD FOR TIME   0.85294872E-02
 DELETING TIME-RECORD FOR TIME   0.17627500E-01
 DELETING TIME-RECORD FOR TIME   0.35823526E-01
 DELETING TIME-RECORD FOR TIME   0.72215578E-01
 DELETING TIME-RECORD FOR TIME   0.14499968
 DELETING TIME-RECORD FOR TIME   0.29056789
 DELETING TIME-RECORD FOR TIME   0.58170431
```

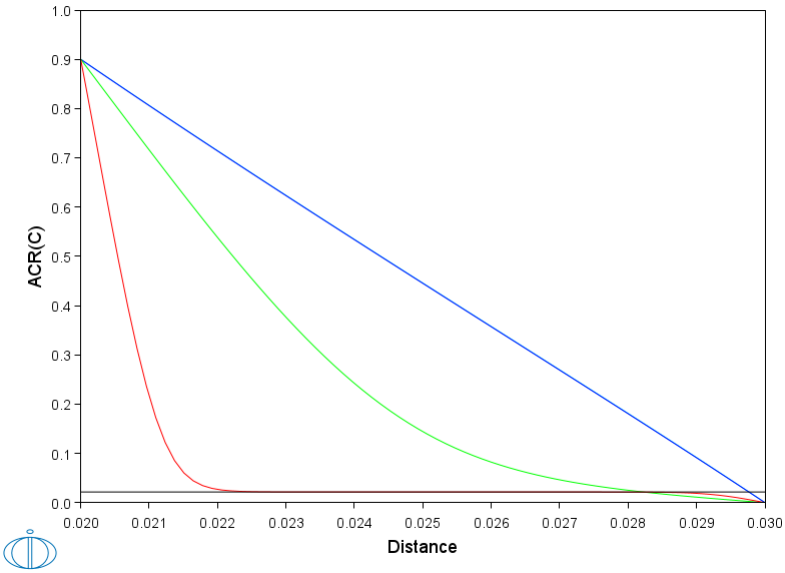
```
 DELETING TIME-RECORD FOR TIME    1.1639771
 DELETING TIME-RECORD FOR TIME    2.3285228
 DELETING TIME-RECORD FOR TIME    4.6576141
 DELETING TIME-RECORD FOR TIME    9.3157968
 DELETING TIME-RECORD FOR TIME    18.632162
 DELETING TIME-RECORD FOR TIME    37.264893
 DELETING TIME-RECORD FOR TIME    74.530354
 DELETING TIME-RECORD FOR TIME    149.06128
 DELETING TIME-RECORD FOR TIME    298.12312
 DELETING TIME-RECORD FOR TIME    596.24681
 DELETING TIME-RECORD FOR TIME    1192.4942
 DELETING TIME-RECORD FOR TIME    2384.9890
 DELETING TIME-RECORD FOR TIME    4769.9785
 DELETING TIME-RECORD FOR TIME    9539.9575
 DELETING TIME-RECORD FOR TIME    19079.916
 DELETING TIME-RECORD FOR TIME    38159.832
 DELETING TIME-RECORD FOR TIME    76319.664
 DELETING TIME-RECORD FOR TIME    152639.33
 DELETING TIME-RECORD FOR TIME    305278.66
 DELETING TIME-RECORD FOR TIME    610557.32
 DELETING TIME-RECORD FOR TIME    1221114.6
 DELETING TIME-RECORD FOR TIME    2442229.3
 DELETING TIME-RECORD FOR TIME    4510975.0
 DELETING TIME-RECORD FOR TIME    7984253.8
 DELETING TIME-RECORD FOR TIME    14356039.
 DELETING TIME-RECORD FOR TIME    27099609.
 DELETING TIME-RECORD FOR TIME    52586749.
 DELETING TIME-RECORD FOR TIME   0.10356103E+09
 DELETING TIME-RECORD FOR TIME   0.20356103E+09
 DELETING TIME-RECORD FOR TIME   0.30356103E+09
 DELETING TIME-RECORD FOR TIME   0.40356103E+09
 DELETING TIME-RECORD FOR TIME   0.50356103E+09
 DELETING TIME-RECORD FOR TIME   0.60356103E+09
 DELETING TIME-RECORD FOR TIME   0.70356103E+09
 DELETING TIME-RECORD FOR TIME   0.80356103E+09
 DELETING TIME-RECORD FOR TIME   0.90356103E+09

 KEEPING TIME-RECORD FOR TIME   0.99821067E+09
 AND FOR TIME                   0.10000000E+10
 WORKSPACE RECLAIMED

 TIMESTEP AT    0.100000000E+10 SELECTED

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

exa6-plot

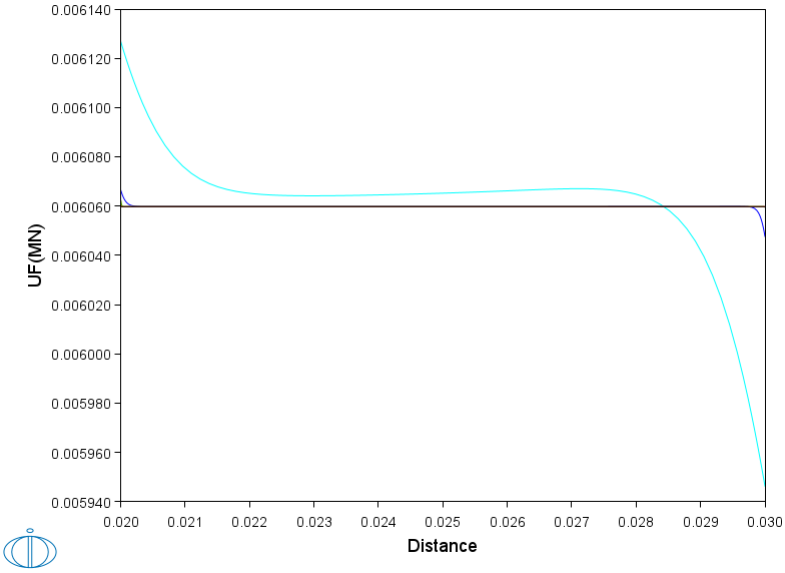
```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exa6\plot.DCM DIC>
DIC>
DIC> @@ exa6_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE exa6
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  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
```



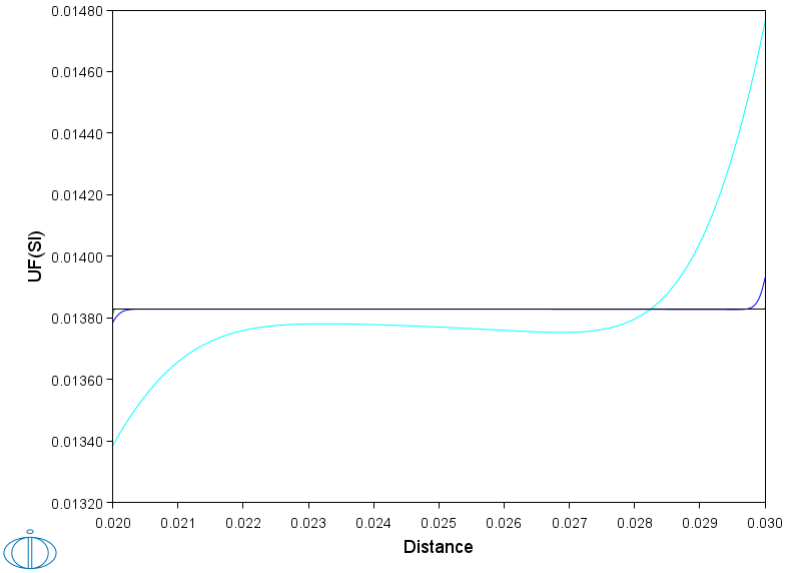

```
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ PLOT THE ACTIVITY OF C
POST-1: @@
POST-1:
POST-1: s-d-a y acr(c)
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```



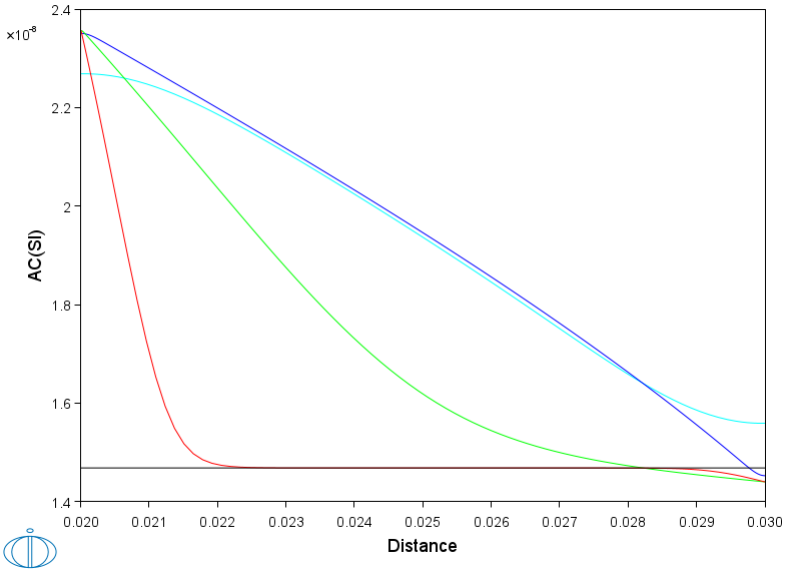

```
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ LET US LOOK AT THE MN AND SI PROFILES
POST-1: @@
POST-1: @@ WE PLOT THE U-FRACTION OF MN AND SI WHICH WILL BE INDEPENDENT
POST-1: @@ OF THE C-CONCENTRATION.
POST-1: @@
POST-1: s-d-a y u-f mn
POST-1:
POST-1:
POST-1: 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:
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
```



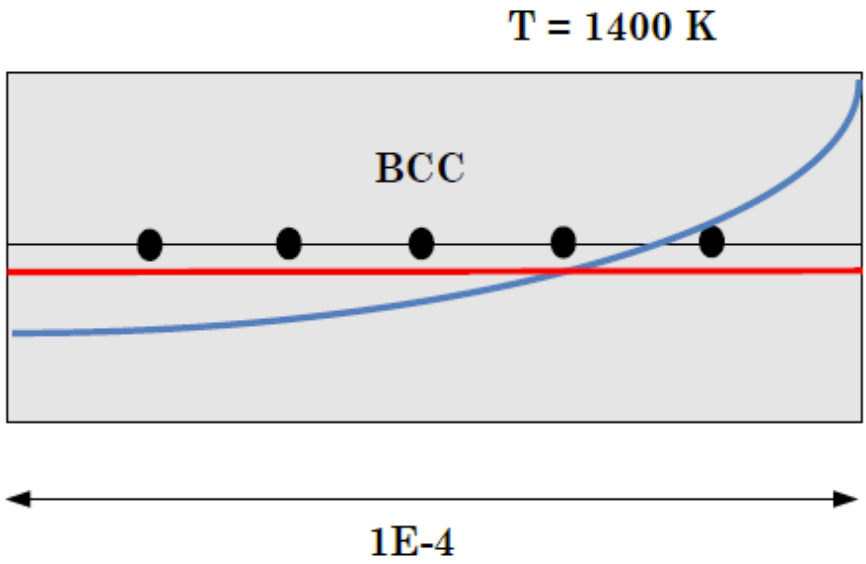

```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: set-inter
 --OK---
POST-1:
```

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.



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: unknown compiler
 License library version: 9.7.0.0036
 Linked: Fri Oct 18 11:32:56 2024


SYS:SYS:MACRO exa7\setup.DCM
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: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ In this example only a single phase, ferrite, is entered in the simulation
SYS: go da
12:49:54,262 [Thread-0] INFO  LicenseManager: Initializing user: jenkins.integrationtest@thermocalc.se
12:49:54,275 [Thread-0] INFO  LicenseController: Running License Spring in DEV environment.
12:49:55,375 [Thread-0] INFO  LicenseManager: There is an activated standalone license for jenkins.integrationtest@thermocalc.se for TC-
Application
 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 v5.0

 VA                       /-  DEFINED
TDB_FEDEMO: def-sys fe cr ni mn
 FE                       CR                       NI
 MN  DEFINED
TDB_FEDEMO: rej ph *
 BCC_A2                   CBCC_A12                 CHI_A12
 CUB_A13                  DIAMOND_FCC_A4           FCC_A1
 GAS:G                    HCP_A3                   LAVES_PHASE_C14
 LIQUID:L                 SIGMA  REJECTED
TDB_FEDEMO: rest ph bcc
 BCC_A2  RESTORED
TDB_FEDEMO: get
12:49:56,469 [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 v4.0

 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
12:49:57,034 [Thread-0] INFO  StandaloneLicenseController: Checking out license for: Diffusion (DICTRA)
 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>
```

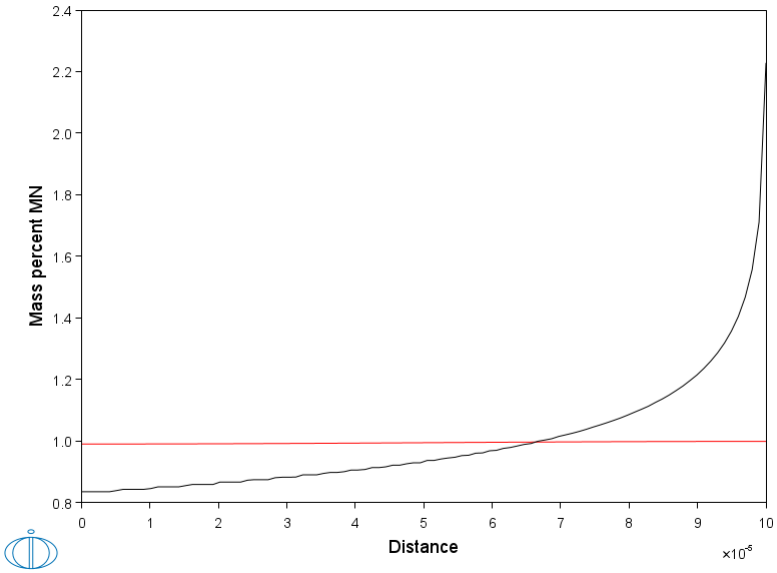
exa7-run

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exa7\run.DCM DIC> go dict-mon
 TIME STEP AT TIME  0.00000E+00
DIC>
DIC> read exa7
 OK
DIC>
DIC> sim
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
 U-FRACTION IN SYSTEM:  CR = .180420497424242  FE = .796498787878788
                        MN = .00999016878282828  NI = .0130905459141415
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 U-FRACTION IN SYSTEM:  CR = .180420497424242  FE = .796498787878788
                        MN = .00999016878282828  NI = .0130905459141415
 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 = .796498787878787

                        MN = .00999016878282828  NI = .0130905459141415
 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:  CR = .180420497424242  FE = .796498787878788
                        MN = .00999016878282828  NI = .0130905459141415
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    1  seconds
 TIME =  0.43088419     DT =  0.43078409     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .180420497424242  FE = .796498787878788
                        MN = .00999016878282828  NI = .0130905459141415
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =   1.2924524     DT =  0.86156818     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .180420497424242  FE = .796498787878788
                        MN = .00999016878282829  NI = .0130905459141415
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    1  seconds
 TIME =   3.0155887     DT =   1.7231364     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .180420497424242  FE = .796498787878787
                        MN = .00999016878282902  NI = .0130905459141415
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =   6.4618615     DT =   3.4462727     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .180420497424241  FE = .796498787878781
                        MN = .00999016878283681  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 = .00999016878287913  NI = .0130905459141425
 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 = .0099901687828793  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 = .0130905459141338
 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 = .00999016878288081  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 = .796498787878951
                        MN = .00999016878288575  NI = .0130905459141089
 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 = .00999016878289932  NI = .0130905459140991
 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 = .180420497423903  FE = .796498787879085
                        MN = .00999016878291501  NI = .0130905459140973
 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 = .180420497423884  FE = .796498787879096
                        MN = .00999016878292102  NI = .0130905459140985
 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 = .180420497423871  FE = .796498787879108
                        MN = .00999016878292249  NI = .0130905459140987
 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 = .00999016878292205  NI = .0130905459140981
 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 = .180420497424025  FE = .796498787878919
                        MN = .00999016878295026  NI = .0130905459141059
 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 = .00999016878297177  NI = .0130905459141178
 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 = .180420497424307  FE = .796498787878573
                        MN = .00999016878299042  NI = .0130905459141295
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
```

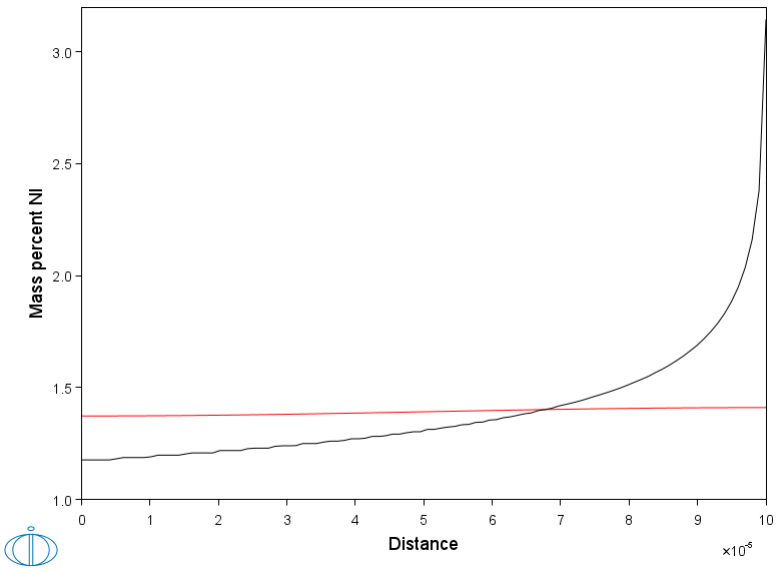
```
 TIME =   3320.6922     DT =   360.00000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .180420497424408  FE = .796498787878447
                        MN = .00999016878300547  NI = .0130905459141397
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =   3600.0000     DT =   279.30777     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .180420497424463  FE = .796498787878379
                        MN = .00999016878301348  NI = .0130905459141452
 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   0.43088419
 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     3600.00000     SELECTED

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

exa7-plot

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exa7\plot.DCM 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
```

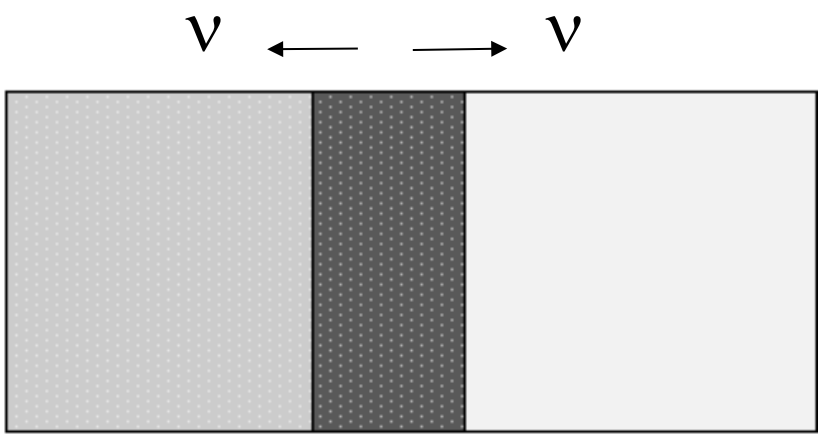



```
POST-1:
POST-1: @@ Hit enter for the next plot
POST-1:@?
POST-1:
POST-1: s-d-a y w-p ni
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```




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

Moving Boundary Problems

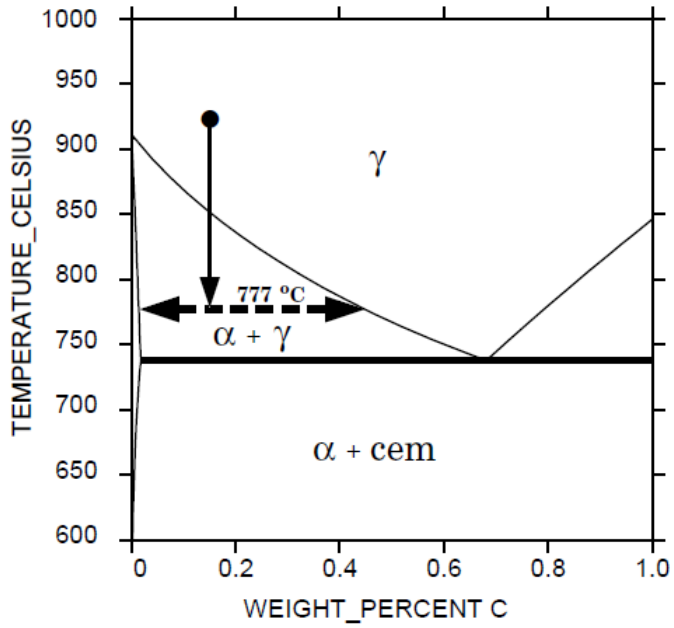


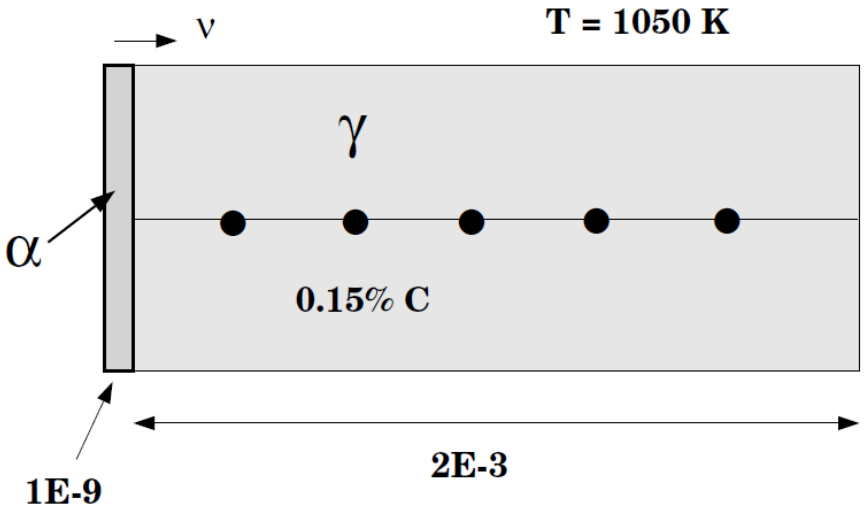
Example exb1a

γ to α 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





exb1a-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: unknown compiler
 License library version: 9.7.0.0036
 Linked: Fri Oct 18 11:32:56 2024


SYS:SYS:MACRO exb1a\setup.DCM
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: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exb1a_setup.DCM
SYS:
SYS:
SYS: @@
SYS: @@ START BY GOING TO THE DATABASE MODULE
SYS: @@
SYS: go da
12:52:52,972 [Thread-0] INFO  LicenseManager: Initializing user: jenkins.integrationtest@thermocalc.se
12:52:52,986 [Thread-0] INFO  LicenseController: Running License Spring in DEV environment.
12:52:54,174 [Thread-0] INFO  LicenseManager: There is an activated standalone license for jenkins.integrationtest@thermocalc.se for TC-
Application
 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 v5.0

 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
 BCC_A2                   CBCC_A12                 CEMENTITE
 CUB_A13                  DIAMOND_FCC_A4           FCC_A1
 GAS:G                    GRAPHITE                 HCP_A3
 KSI_CARBIDE              LAVES_PHASE_C14          LIQUID:L
 M23C6                    M5C2                     M7C3
   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
12:52:55,250 [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 v5.0
 MOB2    =  Alloys Mobility  v2.7
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBFE7  =  Steels/Fe-Alloys Mobility  v7.1
 MFEDEMO =  Fe-Alloys Mobility demo database v4.0
 USER    =  User defined Database
```

```
DATABASE NAME /FEDEMO/: MFEDEMO
 Current database: Fe-Alloys Mobility demo database v4.0

 VA  DEFINED
APP: def-sys fe c
 FE                     C  DEFINED
APP: rej ph * all
 BCC_A2                 FCC_A1                 CEMENTITE
 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
12:52:55,811 [Thread-0] INFO  StandaloneLicenseController: Checking out license for: Diffusion (DICTRA)
 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 /LINEAR/: linear
NUMBER OF POINTS /50/: 10
DIC>
DIC> enter-grid austenite
WIDTH OF REGION /1/: 20e-4
TYPE /LINEAR/: geo
NUMBER OF POINTS /50/: 100
VALUE OF R IN THE GEOMETRICAL SERIE : 1.05
DIC>
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> @@
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> s-s-c
NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /AUTO/:
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -> 1): /AUTO/: 1.0
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/:
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exb1a Y
DIC>
DIC> set-inter
 --OK---
DIC>
```

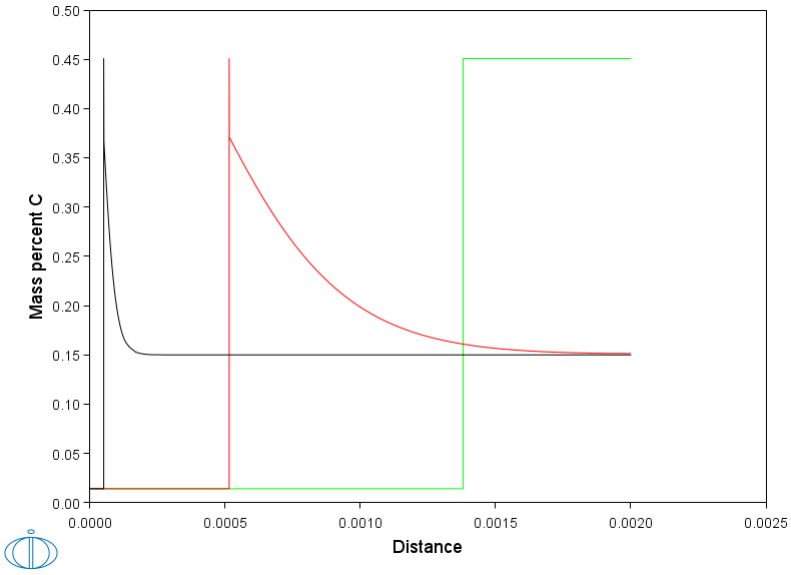
exb1a-run

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exb1a\run.DCM DIC>
DIC>
DIC> @@ exb1a_run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING EXAMPLE b1a
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 exb1a
 OK
DIC>
DIC> @@
DIC> @@ START THE SIMULATION
DIC> @@
DIC> simulate
  Trying old scheme                     3
 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
  11  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUSTENITE

  CPU time used in timestep                    0  seconds
 3.924867797204817E-003        3.925632782423393E-003        2.584529361849211E-005        1.486336344159754E-005        1.819317210163107E-
006        2.382917723735793E-009        8.205871875161355E-010        1.188244165235047E-010        1.385519086981538E-
021       TIME =  0.30000000E-06 DT =  0.20000000E-06 SUM OF SQUARES =  0.13855191E-20
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.39725751E-05 AND   0.39725751E-05
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.97260514E-06
 U-FRACTION IN SYSTEM:  C = .00698493868664155  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]
  CPU time used in timestep                    0  seconds
 3.647318307917246E-009        3.609056395668418E-009        4.074137743669682E-013        7.916095759688517E-019       TIME =  0.70000000E-
06 DT =  0.40000000E-06 SUM OF SQUARES =  0.79160958E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.39679416E-05 AND   0.39679416E-05
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.97260672E-06
 U-FRACTION IN SYSTEM:  C = .00698493868663974  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]
  CPU time used in timestep                    0  seconds
 4.098767961292138E-009        4.058526202268376E-009        5.738226457801994E-014        8.116782232718016E-019       TIME =  0.15000000E-
05 DT =  0.80000000E-06 SUM OF SQUARES =  0.81167822E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.39678978E-05 AND   0.39678978E-05
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.97260990E-06
 U-FRACTION IN SYSTEM:  C = .00698493868663611  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: FERRITE

  CPU time used in timestep                    0  seconds
 4.094059438948623E-009        4.053917868450578E-009        1.401585421709595E-014        2.793920640065191E-019       TIME =  0.31000000E-
05 DT =  0.16000000E-05 SUM OF SQUARES =  0.27939206E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.39678105E-05 AND   0.39678105E-05
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.97261625E-06
 U-FRACTION IN SYSTEM:  C = .00698493868662885  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: FERRITE

  CPU time used in timestep                    0  seconds
 4.084396637429527E-009        4.044353044689921E-009        1.349116878101177E-015        1.815171265344652E-019       TIME =  0.63000000E-
05 DT =  0.32000000E-05 SUM OF SQUARES =  0.18151713E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.39676284E-05 AND   0.39676284E-05
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.97262894E-06
 U-FRACTION IN SYSTEM:  C = .00698493868661436  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: FERRITE

  CPU time used in timestep                    0  seconds
 4.066830175766578E-009

output ignored...



... output resumed

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

  CPU time used in timestep                    0  seconds
 2.735324850049158E-005        2.735765105064528E-005        2.857135237040981E-
019       TIME =  0.61258999E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.28571352E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.50076134E-16 AND  -0.50076134E-16
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.13801532E-02
 U-FRACTION IN SYSTEM:  C = .00697876327235651  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUSTENITE

  CPU time used in timestep                    0  seconds
 5.162392166619635E-006        5.161937365686040E-006        2.879944878831782E-
022       TIME =  0.71258999E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.28799449E-21
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.16048019E-15 AND  -0.16048019E-15
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.13801372E-02
 U-FRACTION IN SYSTEM:  C = .00697892692000533  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUSTENITE
```

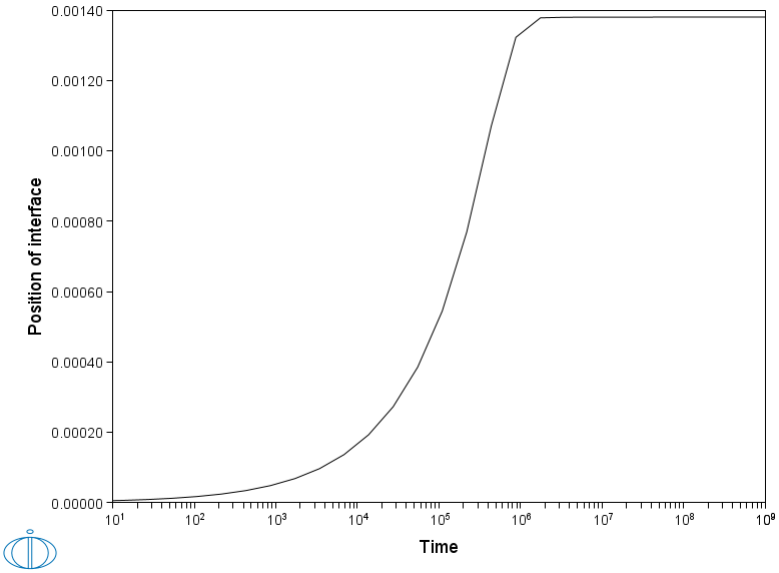
```
  CPU time used in timestep                    0  seconds
 1.643370810140709E-004        1.643453047522188E-004        3.581749652560398E-
021       TIME =  0.81258999E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.35817497E-20
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.47129302E-15 AND   0.47129302E-15
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.13801843E-02
 U-FRACTION IN SYSTEM:  C = .00697844632489939  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]
  32  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: FERRITE

  CPU time used in timestep                    0  seconds
 1.435574617094120E-004        1.435800350381092E-004        2.993167413804371E-
019       TIME =  0.91258999E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.29931674E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.12561450E-15 AND  -0.12561450E-15
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.13801718E-02
 U-FRACTION IN SYSTEM:  C = .00697857441870352  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUSTENITE

  CPU time used in timestep                    0  seconds
 1.107002687003183E-005        1.107169759564005E-005        1.286992003239478E-
022       TIME =  0.10000000E+10 DT =   87410009.     SUM OF SQUARES =  0.12869920E-21
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.40036032E-16 AND   0.40036032E-16
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.13801753E-02
 U-FRACTION IN SYSTEM:  C = .0069785387324832  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    0.100000000E+10 SELECTED

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

exb1a-plot

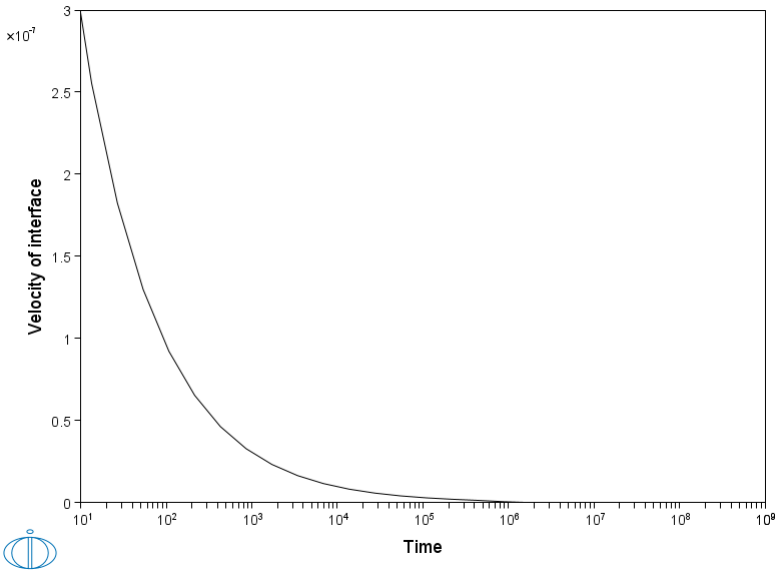
```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exb1a\plot.DCM DIC>
DIC>
DIC> @@ exb1a_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE b1a
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  1.00000E+09
DIC> read exb1a
 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: @@
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
        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
```

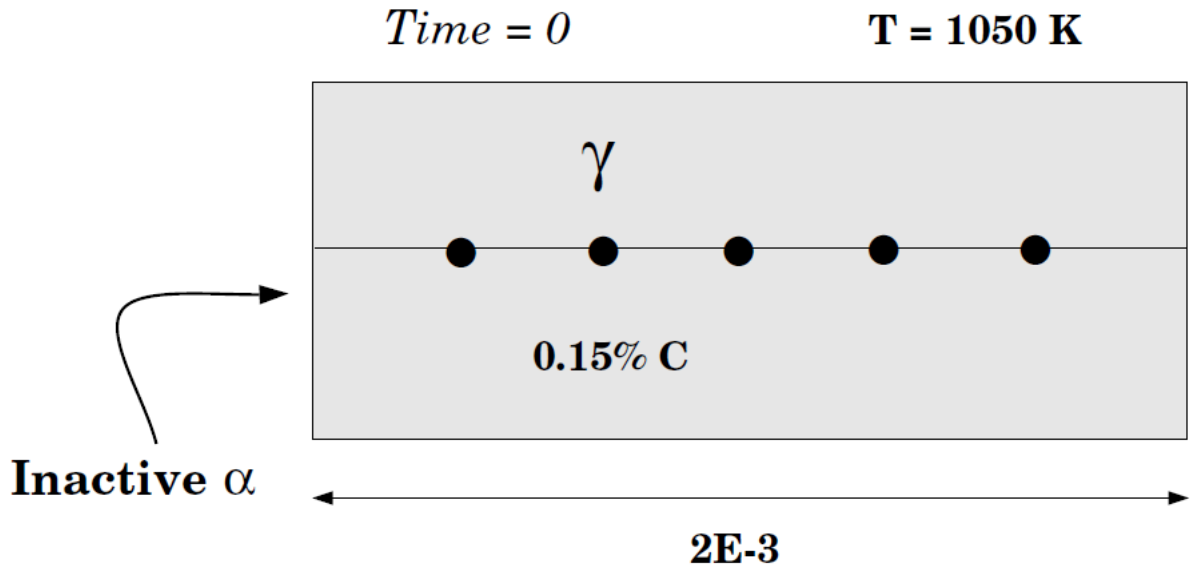


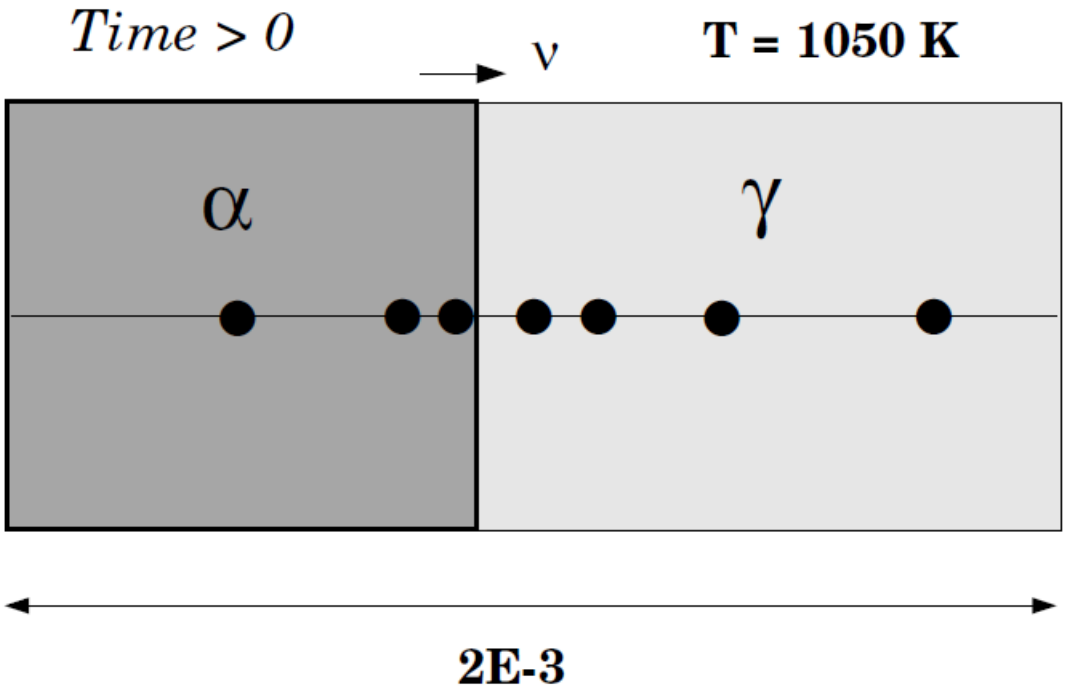

```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1: set-inter
 --OK---
POST-1:
```

Example exb1b

γ to α transformation in a binary Fe-C alloy: Inactive α

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





exb1b-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: unknown compiler
 License library version: 9.7.0.0036
 Linked: Fri Oct 18 11:32:56 2024


SYS:SYS:MACRO exb1b\setup.DCM
SYS: @@
SYS: @@ Moving boundary problem.
SYS: @@ Austenite to ferrite transformation in a binary Fe-C alloy
SYS: @@ This is the same example as in exb1a but now the problem is with
SYS: @@ ferrite as an inactive phase adjacent to the initial austenite.
SYS: ----------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exb1b_setup.DCM
SYS:
SYS: @@
SYS: @@ START BY GOING TO THE DATABASE MODULE
SYS: @@
SYS: go da
12:55:53,165 [Thread-0] INFO  LicenseManager: Initializing user: jenkins.integrationtest@thermocalc.se
12:55:53,179 [Thread-0] INFO  LicenseController: Running License Spring in DEV environment.
12:55:54,275 [Thread-0] INFO  LicenseManager: There is an activated standalone license for jenkins.integrationtest@thermocalc.se for TC-
Application
 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 v5.0

 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
 BCC_A2                   CBCC_A12                 CEMENTITE
 CUB_A13                  DIAMOND_FCC_A4           FCC_A1
 GAS:G                    GRAPHITE                 HCP_A3
 KSI_CARBIDE              LAVES_PHASE_C14          LIQUID:L
 M23C6                    M5C2                     M7C3
   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
12:55:55,359 [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 v5.0
 MOB2    =  Alloys Mobility  v2.7
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBFE7  =  Steels/Fe-Alloys Mobility  v7.1
 MFEDEMO =  Fe-Alloys Mobility demo database v4.0
 USER    =  User defined Database

DATABASE NAME /FEDEMO/: MFEDEMO
 Current database: Fe-Alloys Mobility demo database v4.0

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

```
 BCC_A2                  FCC_A1                  CEMENTITE
 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
12:55:55,930 [Thread-0] INFO  StandaloneLicenseController: Checking out license for: Diffusion (DICTRA)
 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 /LINEAR/: 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 /100000000/:
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> s-s-c
NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /AUTO/:
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -> 1): /AUTO/: 1.0
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/:
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exb1b Y
DIC>
DIC> set-inter
 --OK---
DIC>
```

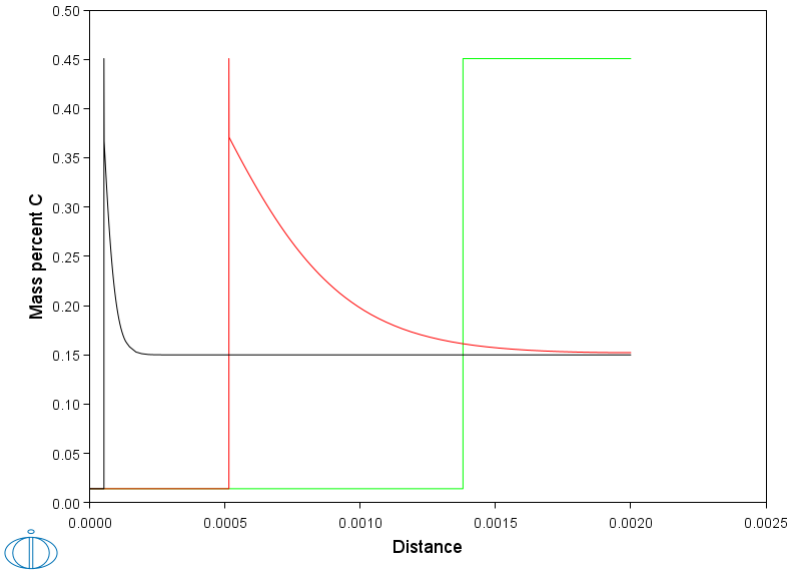
exb1b-run

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exb1b\run.DCM DIC>
DIC>
DIC> @@ exb1b_run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING EXAMPLE b1b
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 exb1b
 OK
DIC>
DIC> @@
DIC> @@ START THE SIMULATION
DIC> @@
DIC> sim y
 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
 ------------------------------------------------------------
  11  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
 0.117127671162496        0.117128128916191        114.061414554258        0.114375906495099        0.105392179153623        9.205187129929521
002        7.158223425194700E-002        3.558703799368233E-002        2.021962344783487E-003        1.121278826080358E-
005        1.860868025616069E-009        2.256092380280181E-017       TIME =  0.12500000E-06 DT =  0.10000000E-
06 SUM OF SQUARES =  0.22560924E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS    9.7403076     AND    9.7403076
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.19740308E-05
 U-FRACTION IN SYSTEM:  C = .00698153921639083  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
 3.652284725189946E-003        3.653015065433610E-003        1.677079944016108E-009        1.228084622293129E-009        1.389993134483879E-
010        4.649723520377790E-013        1.267493235033127E-013        3.414712501203870E-010        4.430338059554130E-
014        3.552205617644033E-010        1.573580480434683E-014        3.633799792715740E-010        5.640475590130512E-
015        3.682534413947552E-010        2.032658495300786E-015        3.711749961653276E-010        7.348303612434650E-
016        3.729301850465035E-010        2.661514781502254E-016        3.739859956060369E-010        9.650751384447345E-
017       TIME =  0.39382734E-04 DT =  0.39257734E-04 SUM OF SQUARES =  0.96507514E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.96405057E-05 AND   0.96405057E-05
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.19744092E-05
 U-FRACTION IN SYSTEM:  C = .00698153902316687  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                  0  seconds
  19  GRIDPOINT(S) ADDED   TO   CELL #1   REGION: R_BCC_A2
 7.164143207225419E-007        7.177059646506402E-007        1.189358796820148E-017       TIME =  0.11789820E-03 DT =  0.78515467E-
04 SUM OF SQUARES =  0.11893588E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.83991846E-05 AND   0.83991846E-05
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.19750687E-05
 U-FRACTION IN SYSTEM:  C = .00698153902253604  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                  0  seconds
 1.345442012049659E-008        1.330048750117228E-008        1.695166636025482E-018       TIME =  0.27492913E-03 DT =  0.15703093E-
03 SUM OF SQUARES =  0.16951666E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.83746772E-05 AND   0.83746772E-05
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.19763838E-05
 U-FRACTION IN SYSTEM:  C = .00698153902148981  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]


output ignored...



... output resumed

 U-FRACTION IN SYSTEM:  C = .00698157462623608  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  18  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_BCC_A2

  CPU time used in timestep                  0  seconds
 4.707447715678769E-006        4.708755015542431E-006        9.607583886739340E-
020       TIME =  0.67265734E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.96075839E-19
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.41324439E-16 AND   0.41324439E-16
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13798810E-02
 U-FRACTION IN SYSTEM:  C = .00698153248614061  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  4  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_BCC_A2

  CPU time used in timestep                  0  seconds
 1.350425355123420E-003        1.350486059745406E-003        1.661527465599188E-
```

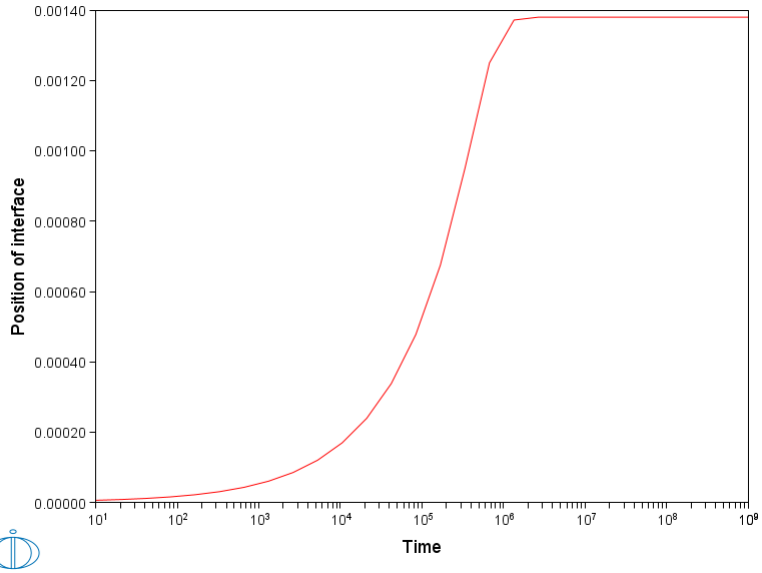
```
025       TIME =  0.77265734E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.16615275E-24
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.13968626E-15 AND  -0.13968626E-15
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13798670E-02
 U-FRACTION IN SYSTEM:  C = .00698167492951646  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUSTENITE

  CPU time used in timestep                    0  seconds
 3.448265292765822E-005        3.448593190930922E-005        2.473994942960656E-
022       TIME =  0.87265734E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.24739949E-21
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.15103406E-15 AND   0.15103406E-15
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13798821E-02
 U-FRACTION IN SYSTEM:  C = .00698152091436651  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  14  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_BCC_A2

  CPU time used in timestep                    0  seconds
 4.041394345259142E-005        4.041778163291770E-005        8.212628118198100E-
019       TIME =  0.97265734E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.82126281E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.16369403E-15 AND  -0.16369403E-15
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13798658E-02
 U-FRACTION IN SYSTEM:  C = .00698168783937385  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUSTENITE

  CPU time used in timestep                    0  seconds
 2.619383545337222E-005        2.619718449745630E-005        1.833020171535089E-
019       TIME =  0.10000000E+10 DT =   27342662.     SUM OF SQUARES =  0.18330202E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.90526284E-16 AND   0.90526284E-16
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13798682E-02
 U-FRACTION IN SYSTEM:  C = .00698166259852017  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   0.39382734E-04
 DELETING TIME-RECORD FOR TIME   0.11789820E-03
 DELETING TIME-RECORD FOR TIME   0.27492913E-03
 DELETING TIME-RECORD FOR TIME   0.58899100E-03
 DELETING TIME-RECORD FOR TIME   0.12171147E-02
 DELETING TIME-RECORD FOR TIME   0.24733622E-02
 DELETING TIME-RECORD FOR TIME   0.49858572E-02
 DELETING TIME-RECORD FOR TIME   0.10010847E-01
 DELETING TIME-RECORD FOR TIME   0.20060827E-01
 DELETING TIME-RECORD FOR TIME   0.40160786E-01
 DELETING TIME-RECORD FOR TIME   0.80360705E-01
 DELETING TIME-RECORD FOR TIME   0.16076054
 DELETING TIME-RECORD FOR TIME   0.32156022
 DELETING TIME-RECORD FOR TIME   0.64315957
 DELETING TIME-RECORD FOR TIME    1.2863583
 DELETING TIME-RECORD FOR TIME    2.5727557
 DELETING TIME-RECORD FOR TIME    5.1455505
 DELETING TIME-RECORD FOR TIME    10.291140
 DELETING TIME-RECORD FOR TIME    20.582319
 DELETING TIME-RECORD FOR TIME    41.164678
 DELETING TIME-RECORD FOR TIME    82.329395
 DELETING TIME-RECORD FOR TIME    164.65883
 DELETING TIME-RECORD FOR TIME    329.31770
 DELETING TIME-RECORD FOR TIME    658.63544
 DELETING TIME-RECORD FOR TIME    1317.2709
 DELETING TIME-RECORD FOR TIME    2634.5419
 DELETING TIME-RECORD FOR TIME    5269.0838
 DELETING TIME-RECORD FOR TIME    10538.168
 DELETING TIME-RECORD FOR TIME    21076.335
 DELETING TIME-RECORD FOR TIME    42152.670
 DELETING TIME-RECORD FOR TIME    84305.341
 DELETING TIME-RECORD FOR TIME    168610.68
 DELETING TIME-RECORD FOR TIME    337221.36
 DELETING TIME-RECORD FOR TIME    674442.73
 DELETING TIME-RECORD FOR TIME    1348885.5
 DELETING TIME-RECORD FOR TIME    2697770.9
 DELETING TIME-RECORD FOR TIME    5395541.8
 DELETING TIME-RECORD FOR TIME    10791084.
 DELETING TIME-RECORD FOR TIME    21582167.
 DELETING TIME-RECORD FOR TIME    43164334.
 DELETING TIME-RECORD FOR TIME    86328669.
 DELETING TIME-RECORD FOR TIME   0.17265734E+09
 DELETING TIME-RECORD FOR TIME   0.27265734E+09
 DELETING TIME-RECORD FOR TIME   0.37265734E+09
 DELETING TIME-RECORD FOR TIME   0.47265734E+09
 DELETING TIME-RECORD FOR TIME   0.57265734E+09
 DELETING TIME-RECORD FOR TIME   0.67265734E+09
 DELETING TIME-RECORD FOR TIME   0.77265734E+09
 DELETING TIME-RECORD FOR TIME   0.87265734E+09

 KEEPING TIME-RECORD FOR TIME   0.97265734E+09
 AND FOR TIME                   0.10000000E+10
 WORKSPACE RECLAIMED

 TIMESTEP AT    0.100000000E+10 SELECTED

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

exb1b-plot

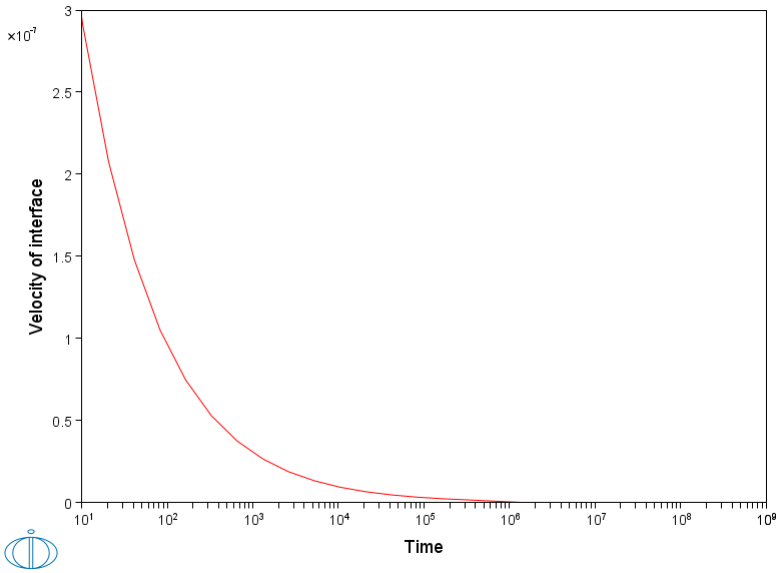
```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exb1b\plot.DCM DIC>
DIC>
DIC> @@ exb1b_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE b1b
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  1.00000E+09
DIC> read exb1b
 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
ORKING ...          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
ORKING ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

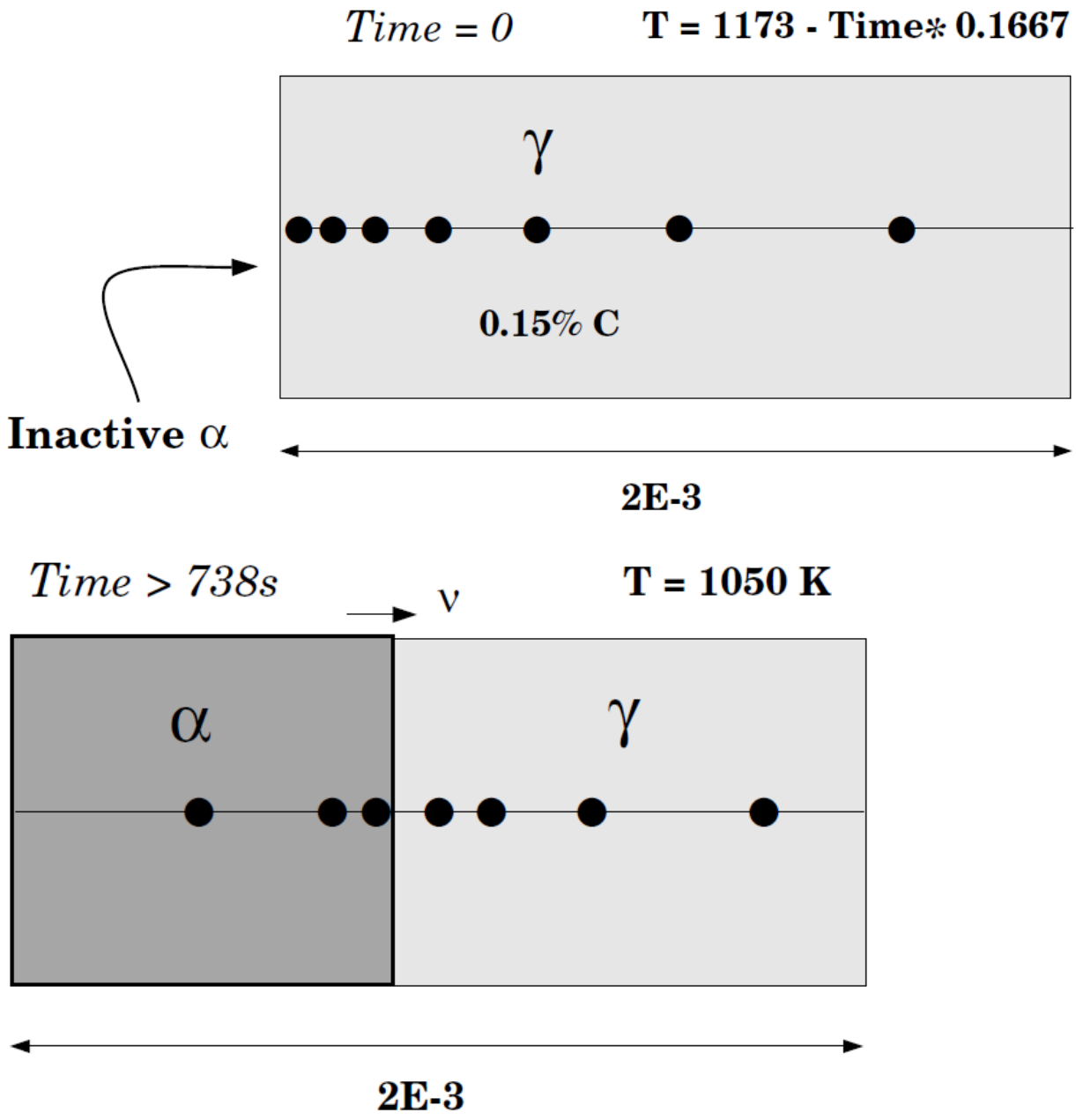



```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1: set-inter
 --OK---
POST-1:
```

Example exb1c

γ to α 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.



exb1c-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: unknown compiler
 License library version: 9.7.0.0036
 Linked: Fri Oct 18 11:32:56 2024


SYS:SYS:MACRO exb1c\setup.DCM
SYS: @@
SYS: @@ Moving boundary problem.
SYS: @@ Austenite to ferrite transformation in a binary Fe-C alloy
SYS: @@ This is the same example as in exb1a and exb1b 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 exb1b ferrite is an inactive
SYS: @@ phase adjacent to the initial austenite.
SYS: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exb1c_setup.DCM
SYS:
SYS: @@
SYS: @@ START BY GOING TO THE DATABASE MODULE
SYS: @@
SYS: go da
12:58:52,584 [Thread-0] INFO  LicenseManager: Initializing user: jenkins.integrationtest@thermocalc.se
12:58:52,596 [Thread-0] INFO  LicenseController: Running License Spring in DEV environment.
12:58:53,725 [Thread-0] INFO  LicenseManager: There is an activated standalone license for jenkins.integrationtest@thermocalc.se for TC-
Application
 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 v5.0

 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
 BCC_A2                   CBCC_A12                 CEMENTITE
 CUB_A13                  DIAMOND_FCC_A4           FCC_A1
 GAS:G                    GRAPHITE                 HCP_A3
 KSI_CARBIDE              LAVES_PHASE_C14          LIQUID:L
 M23C6                    M5C2                     M7C3
   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
12:58:54,798 [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 v5.0
 MOB2    =  Alloys Mobility  v2.7
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBFE7  =  Steels/Fe-Alloys Mobility  v7.1
 MFEDEMO =  Fe-Alloys Mobility demo database v4.0
 USER    =  User defined Database

DATABASE NAME /FEDEMO/: MFEDEMO
 Current database: Fe-Alloys Mobility demo database v4.0
```

```
 VA  DEFINED
APP: def-sys fe c
 FE                    C  DEFINED
APP: rej ph * all
 BCC_A2                FCC_A1                CEMENTITE
 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
12:58:55,379 [Thread-0] INFO  StandaloneLicenseController: Checking out license for: Diffusion (DICTRA)
 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 /LINEAR/: 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> s-s-c
NS01A PRINT CONTROL : /0/:
```

```
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /AUTO/:
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -> 1): /AUTO/: 1.0
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/:
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exb1c Y
DIC>
DIC> set-inter
 --OK---
DIC>
```

exb1c-run

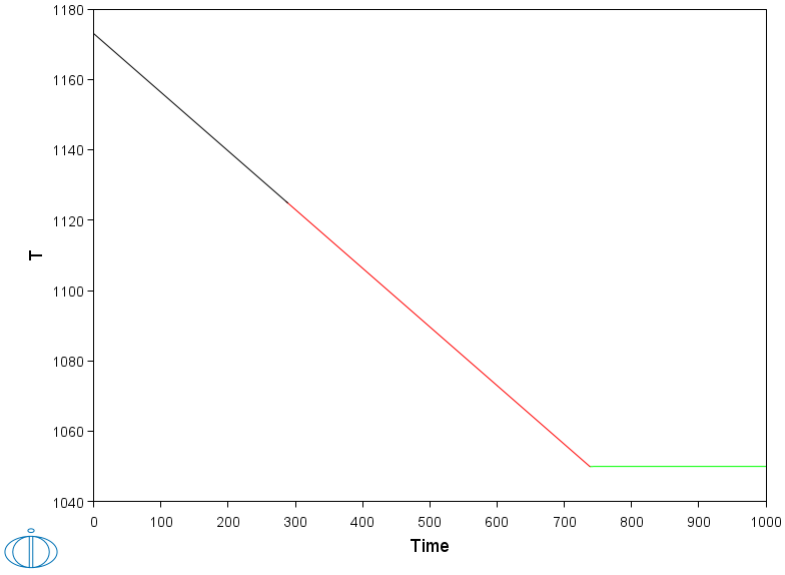
```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exb1c\run.DCM DIC>
DIC>
DIC> @@ exb1c_run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING EXAMPLE exb1c
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  0.00000E+00
DIC> read exb1c
 OK
DIC>
DIC> @@
DIC> @@ START THE SIMULATION
DIC> @@
DIC> sim
 Region: AUSTENITE
 geometric    1.27617     dense at    0.00000       95 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 =  0.49553997E-03 DT =  0.49543997E-03 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 =  0.14864199E-02 DT =  0.99087994E-03 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 =  0.34681798E-02 DT =  0.19817599E-02 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 =  0.74316996E-02 DT =  0.39635198E-02 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 =  0.15358739E-01 DT =  0.79270396E-02 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 =  0.31212818E-01 DT =  0.15854079E-01 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 =  0.62920977E-01 DT =  0.31708158E-01 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 =  0.12633729     DT =  0.63416316E-01 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 =  0.25316993     DT =  0.12683263     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698495916383109  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    1  seconds
 TIME =  0.50683519     DT =  0.25366527     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 =   1.0141657     DT =  0.50733053     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 =   2.0288268     DT =   1.0146611     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 =   4.0581489     DT =   2.0293221     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 =   8.1167932     DT =   4.0586443     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 =   16.234082     DT =   8.1172885     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 =   32.468659     DT =   16.234577     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 =   64.937813     DT =   32.469154     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 =   101.83781     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 =   138.73781     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 =   175.63781     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 =   212.53781     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 =   249.43781     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 =   286.33781     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
 INFO: PHASE BCC_A2 IS SCHEDULED TO APPEAR
 INFO: BACKTRACING WITH SMALLER TIMESTEP   9.2250
 INFO: PHASE BCC_A2 IS SCHEDULED TO APPEAR
   REGION STATUS CHANGE, ITERATING: TIME=   290.95031
   REGION STATUS CHANGE, ITERATING: TIME=   288.64406
   REGION STATUS CHANGE, ITERATING: TIME=   289.79719
   REGION STATUS CHANGE, ITERATING: TIME=   289.22063
   REGION STATUS CHANGE, ITERATING: TIME=   288.93234
   REGION STATUS CHANGE, ITERATING: TIME=   288.78820


output ignored...



... output resumed

TIME =  0.44460949E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.42672657E-20
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.99771874E-16 AND   0.99771874E-16
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13792031E-02
 U-FRACTION IN SYSTEM:  C = .00698844524809282  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  9  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_BCC_A2

  CPU time used in timestep                    0  seconds
 6.300181379980967E-005        6.300497946320894E-005        4.491936266715634E-
027       TIME =  0.54460949E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.44919363E-26
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.29141025E-15 AND  -0.29141025E-15
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13791740E-02
 U-FRACTION IN SYSTEM:  C = .00698874241016547  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUSTENITE

  CPU time used in timestep                    0  seconds
 2.245720080822418E-005        2.246272137854412E-005        3.328976115222247E-
022       TIME =  0.64460949E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.33289761E-21
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.53223173E-16 AND  -0.53223173E-16
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13791686E-02
 U-FRACTION IN SYSTEM:  C = .00698879668385231  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUSTENITE

  CPU time used in timestep                    0  seconds
 1.325572924315520E-005        1.325650385393237E-005        5.894036172117351E-
021       TIME =  0.74460949E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.58940362E-20
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.12635981E-15 AND   0.12635981E-15
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13791813E-02
 U-FRACTION IN SYSTEM:  C = .00698866782996929  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  11  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_BCC_A2

  CPU time used in timestep                    0  seconds
 1.604064290660115E-005        1.604266596376776E-005        1.298441436334128E-
027       TIME =  0.84460949E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.12984414E-26
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.72545164E-16 AND  -0.72545164E-16
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13791740E-02
 U-FRACTION IN SYSTEM:  C = .00698874180702061  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUSTENITE

  CPU time used in timestep                    0  seconds
 2.797201818780974E-006        2.797686843430792E-006        7.359769241521117E-
023       TIME =  0.94460949E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.73597692E-22
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.10911310E-16 AND   0.10911310E-16
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13791751E-02
 U-FRACTION IN SYSTEM:  C = .00698873068034426  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
 2.871867831218063E-006        2.871128724184850E-006        3.651360553371141E-
017       TIME =  0.10000000E+10 DT =   55390509.     SUM OF SQUARES =  0.36513606E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.19002339E-16 AND   0.19002339E-16
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13791762E-02
 U-FRACTION IN SYSTEM:  C = .00698871994710342  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    755.23871
 DELETING TIME-RECORD FOR TIME    789.71613
 DELETING TIME-RECORD FOR TIME    858.67096
 DELETING TIME-RECORD FOR TIME    996.58063
 DELETING TIME-RECORD FOR TIME    1272.4000
 DELETING TIME-RECORD FOR TIME    1824.0387
 DELETING TIME-RECORD FOR TIME    2927.3160
 DELETING TIME-RECORD FOR TIME    5133.8707
 DELETING TIME-RECORD FOR TIME    9546.9802
 DELETING TIME-RECORD FOR TIME    18373.199
 DELETING TIME-RECORD FOR TIME    36025.637
 DELETING TIME-RECORD FOR TIME    71330.512
 DELETING TIME-RECORD FOR TIME    141940.26
 DELETING TIME-RECORD FOR TIME    283159.77
 DELETING TIME-RECORD FOR TIME    565598.77
 DELETING TIME-RECORD FOR TIME    1130476.8
 DELETING TIME-RECORD FOR TIME    2260232.8
 DELETING TIME-RECORD FOR TIME    4519744.8
 DELETING TIME-RECORD FOR TIME    9038768.9
 DELETING TIME-RECORD FOR TIME    18076817.
 DELETING TIME-RECORD FOR TIME    36152913.
 DELETING TIME-RECORD FOR TIME    72305106.
 DELETING TIME-RECORD FOR TIME   0.14460949E+09
 DELETING TIME-RECORD FOR TIME   0.24460949E+09
 DELETING TIME-RECORD FOR TIME   0.34460949E+09
 DELETING TIME-RECORD FOR TIME   0.44460949E+09
 DELETING TIME-RECORD FOR TIME   0.54460949E+09
```

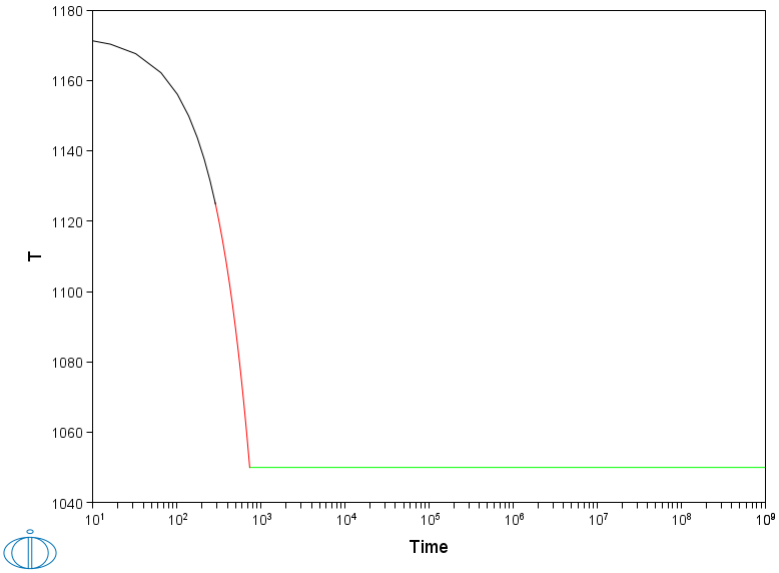
```
 DELETING TIME-RECORD FOR TIME    0.64460949E+09
 DELETING TIME-RECORD FOR TIME    0.74460949E+09
 DELETING TIME-RECORD FOR TIME    0.84460949E+09

 KEEPING TIME-RECORD FOR TIME    0.94460949E+09
 AND FOR TIME                    0.10000000E+10
 WORKSPACE RECLAIMED

 TIMESTEP AT    0.100000000E+10 SELECTED

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

exb1c-plot

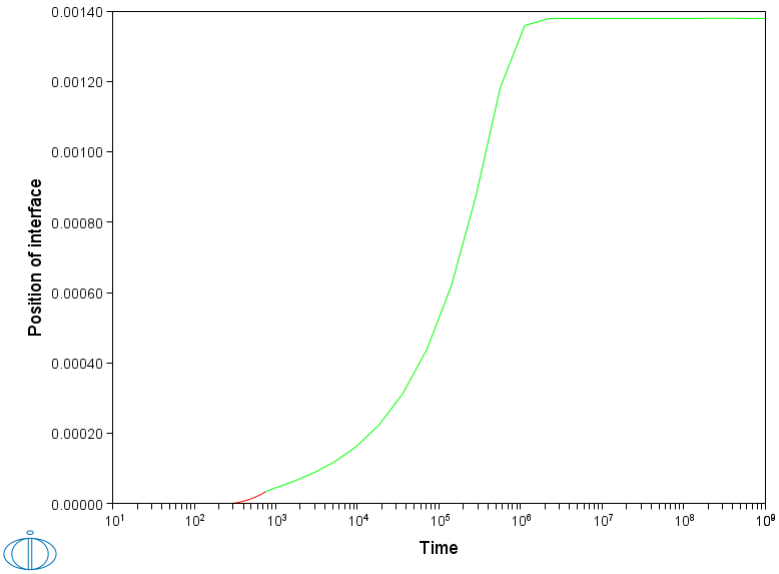
```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exb1c\plot.DCM DIC>
DIC>
DIC> @@ exb1c_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE b1c
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  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
ORKING ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```



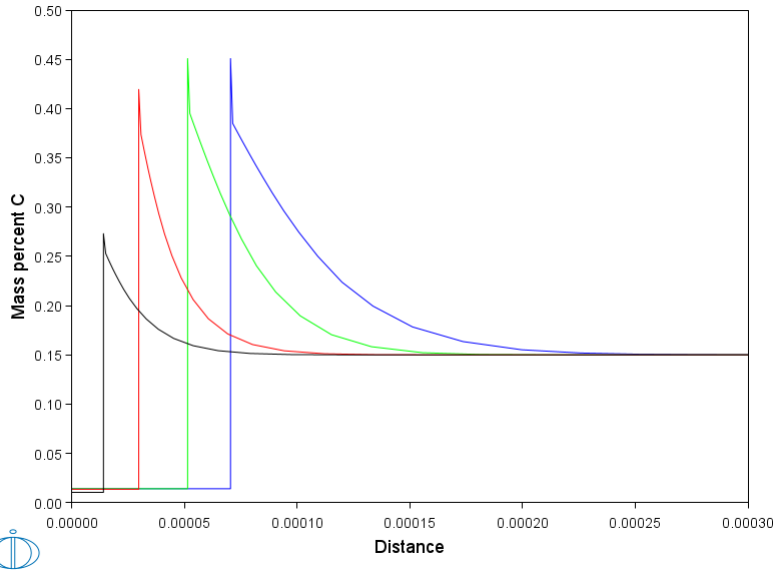

```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: @@
POST-1: @@ PLOT VS. LOG TIME
POST-1: @@
POST-1: set-axis-type x log
POST-1: s-s-s x n 10 1e9
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples/unite/distribution\macroResult.exp 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
ORKING ...          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 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
ORKING ...OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

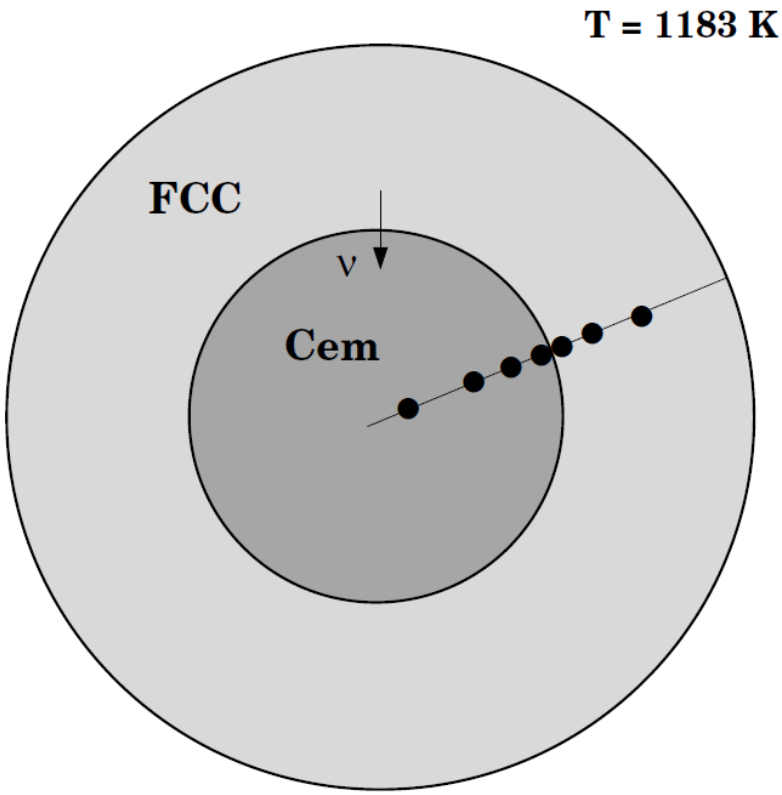



```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1: set-inter
 --OK---
POST-1:
```

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: unknown compiler
 License library version: 9.7.0.0036
 Linked: Fri Oct 18 11:32:56 2024


SYS:SYS:MACRO exb2\setup.DCM
SYS: SET_GES_VERSION
USE GES VERSION 5 OR 6 /6/: 5
SYS: GO DA
13:01:53,100 [Thread-0] INFO  LicenseManager: Initializing user: jenkins.integrationtest@thermocalc.se
13:01:53,115 [Thread-0] INFO  LicenseController: Running License Spring in DEV environment.
13:01:54,224 [Thread-0] INFO  LicenseManager: There is an activated standalone license for jenkins.integrationtest@thermocalc.se for TC-
Application
 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 v5.0

 VA                        /-  DEFINED
TDB_FEDEMO: DE-E FE CR C
 FE                        CR                        C
   DEFINED
TDB_FEDEMO: REJ PH *
 BCC_A2                    CBCC_A12                  CEMENTITE
 CHI_A12                   CUB_A13                   DIAMOND_FCC_A4
 FCC_A1                    GAS:G                     GRAPHITE
 HCP_A3                    KSI_CARBIDE               LAVES_PHASE_C14
 LIQUID:L                  M23C6                     M3C2
 M5C2                      M7C3                      SIGMA
   REJECTED
TDB_FEDEMO: RES PH FCC_A1 CEMENTITE
 FCC_A1                    CEMENTITE  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: APP MFEDEMO
 Current database: Fe-Alloys Mobility demo database v4.0

 VA  DEFINED
APP: DE-E FE CR C
 FE                        CR                        C
   DEFINED
APP: REJ PH *
 BCC_A2                    FCC_A1                    CEMENTITE
 LIQUID:L  REJECTED
APP: RES PH FCC_A1 CEMENTITE
 FCC_A1                    CEMENTITE  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: GO D-M
13:01:55,173 [Thread-0] INFO  StandaloneLicenseController: Checking out license for: Diffusion (DICTRA)
 NO TIME STEP DEFINED
DIC> SET_CONDITION GLOBAL T 0 1183; * N
DIC> ENTER_REGION
REGION NAME : CARB
DIC> ENTER_REGION
REGION NAME : AUS
ATTACH TO REGION NAMED /CARB/: CARB
ATTACHED TO THE RIGHT OF CARB /YES/: YES
DIC> ,
DIC> ,
DIC> ENTER_GRID
REGION NAME : /CARB/: CARB
WIDTH OF REGION /1/: 5.255E-7
TYPE /LINEAR/: AUTO
DIC> ,
DIC> ,
DIC> ENTER_GRID
REGION NAME : /AUS/: AUS
WIDTH OF REGION /1/: 5.3924863E-7
TYPE /LINEAR/: AUTO
DIC> ,
DIC> ,
DIC> ENTER_PHASE
ACTIVE OR INACTIVE PHASE /ACTIVE/: ACTIVE
REGION NAME : /CARB/: CARB
PHASE TYPE /MATRIX/: MATRIX
```

```
PHASE NAME: /NONE/: CEMENTITE
DIC> ,
DIC> ,
DIC> ENTER_PHASE
ACTIVE OR INACTIVE PHASE /ACTIVE/: ACTIVE
REGION NAME : /AUS/: AUS
PHASE TYPE /MATRIX/: MATRIX
PHASE NAME: /NONE/: FCC_A1#1
DIC> ,
DIC> ,
DIC> ENTER_COMPOSITION
REGION NAME : /CARB/: AUS
PHASE NAME: /FCC_A1#1/: FCC_A1#1
DEPENDENT COMPONENT ? /FE/: FE
COMPOSITION TYPE /MOLE_FRACTION/: WEIGHT_FRACTION
PROFILE FOR /C/: CR
TYPE /LINEAR/: LINEAR
VALUE OF FIRST POINT : 4.4332285E-3
VALUE OF LAST POINT : /4.4332285E-3/: 4.4332285E-3
PROFILE FOR /CR/: C
TYPE /LINEAR/: LINEAR
VALUE OF FIRST POINT : 1.510215E-4
VALUE OF LAST POINT : /1.510215E-4/: 1.510215E-4
DIC> ,
DIC> ,
DIC> ENTER_COMPOSITION
REGION NAME : /CARB/: CARB
PHASE NAME: /CEMENTITE/: CEMENTITE
DEPENDENT COMPONENT ? /FE/: FE
COMPOSITION TYPE /MOLE_FRACTION/: WEIGHT_FRACTION
PROFILE FOR /CR/: CR
TYPE /LINEAR/: LINEAR
VALUE OF FIRST POINT : 0.12423326
VALUE OF LAST POINT : /0.12423326/: 0.12423326
DIC> ,
DIC> ,
DIC> ENTER_GEOMETRICAL_EXPONENT
GEOMETRICAL EXPONENT /0/: 2
DIC> ,
DIC> SET_SIMULATION_TIME
END TIME FOR INTEGRATION /.1/: 10000
AUTOMATIC TIMESTEP CONTROL /YES/: YES
MAX TIMESTEP DURING INTEGRATION /1000/: 1000
INITIAL TIMESTEP : /1E-07/: 1E-7
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/: 1E-7
DIC> ,
DIC> save exb2 Y
DIC> ,
DIC> go sys
13:01:55,539 [Thread-0] INFO  StandaloneLicenseController: Releasing license for: Diffusion (DICTRA)
SYS: ,
SYS: set-inter
SYS:
```

exb2-run

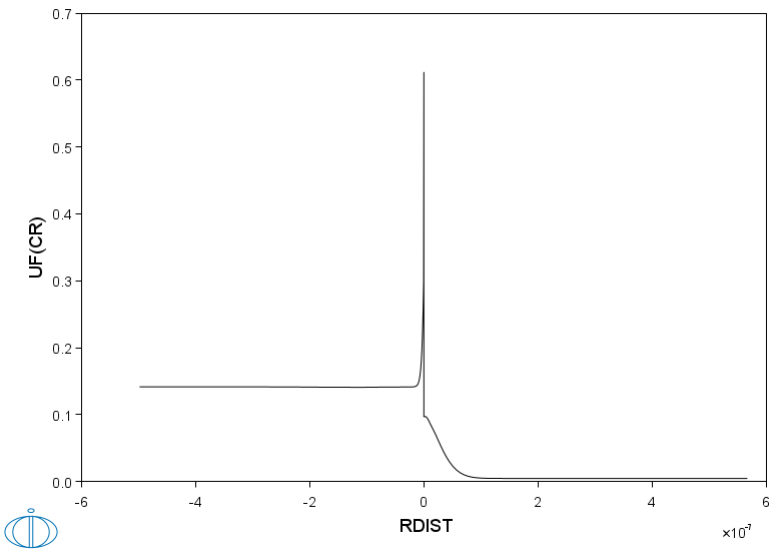
```
SYS:About

 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: unknown compiler
 License library version: 9.7.0.0036
 Linked: Fri Oct 18 11:32:56 2024


SYS:SYS:MACRO exb2\run.DCM SYS:
SYS:
SYS: @@ exb2_run.DCM
SYS:
SYS: @@
SYS: @@ READ THE SET UP FROM FILE AND START THE SIMULATION
SYS: @@
SYS:
SYS: go d-m
13:02:50,596 [Thread-0] INFO  StandaloneLicenseController: Checking out license for: Diffusion (DICTRA) TIME STEP
AT TIME  0.00000E+00
DIC> read exb2
 OK
DIC> sim
 Region: CARB
 geometric   0.863418     dense at   0.525500E-06   89 points
 Region: AUS

 geometric    1.05932     dense at    0.00000       77 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                                                      DONE     9 OUT OF     9
04
 U-FRACTION IN SYSTEM:  C = .0406910188248198  CR = .0212231529163473
                        FE = .97877684721416
 TOTAL SIZE OF SYSTEM:  5.05626560299E-18 [m^3]
 U-FRACTION IN SYSTEM:  C = .0406910188248198  CR = .0212231529163473
                        FE = .97877684721416
 TOTAL SIZE OF SYSTEM:  5.05626560299E-18 [m^3]
 0.174822717043676        0.174863837612061        0.174822771086727        2.939400104982828E-003        7.6968843548002 50E-
005        4.225962411887480E-006        7.656587621861788E-007        2.590564756771282E-007        2.348148112734887E-
007        9.395228943647151E-008        9.382517841505027E-008        9.389398638366630E-008        9.400589727934374E-
008        9.357681914045472E-008        9.348651968420604E-008        9.330573159708859E-008        9.426358202409885E-
008        9.294475213757037E-008        9.222441942374784E-008        9.079026418008753E-008        9.174093735752857E-
008        8.794822416905559E-008        8.237139194169516E-008        7.166242566737878E-008        7.255844999865708E-
008        5.213969419673716E-008        2.158835323044197E-008        6.101933678032568E-011        2.489855334703457E-
014        1.371431124655254E-018       TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =  0.30620986E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.26976638E-02 AND  -0.26976638E-02
 POSITION OF INTERFACE CARB / AUS IS   0.52523023E-06
 U-FRACTION IN SYSTEM:  C = .040714955890211  CR = .0212232168337605
                        FE = .978776783296747
 TOTAL SIZE OF SYSTEM:  5.05626560299E-18 [m^3]
  CPU time used in timestep                0  seconds
 5.514933385228125E-005        5.516153468651187E-005        5.514938159541911E-005        1.136420092484870E-007        9.218164484133925E-
008        5.597898588726280E-008        2.406298821136314E-008        4.685533549623942E-012        5.734137919518977E-
016        5.396694224780842E-019       TIME =  0.30000000E-06 DT =  0.20000000E-06 SUM OF SQUARES =  0.18699240E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.18416544E-03 AND  -0.18416544E-03
 POSITION OF INTERFACE CARB / AUS IS   0.52519340E-06
 U-FRACTION IN SYSTEM:  C = .0407166662839749  CR = .0212232252013087
                        FE = .978776774929198
 TOTAL SIZE OF SYSTEM:  5.05626560299E-18 [m^3]
  CPU time used in timestep                0  seconds
 1.438532416880551E-006        1.438824451051302E-006        1.438488901269197E-006        1.368039299432932E-006        1.344280446388578E-
006        1.295548565872077E-006        1.195687998709032E-006        1.195641429660763E-006        1.011439800288802E-
006        6.864779768666986E-007        2.285005172906121E-007        5.404066553397666E-011        1.525748519234987E-
015        4.232122551495736E-019       TIME =  0.70000000E-06 DT =  0.40000000E-06 SUM OF SQUARES =  0.11431872E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.13849267E-03 AND  -0.13849267E-03
 POSITION OF INTERFACE CARB / AUS IS   0.52513800E-06
 U-FRACTION IN SYSTEM:  C = .0407166334238572  CR = .0212232371896216
                        FE = .978776762940886
 TOTAL SIZE OF SYSTEM:  5.05626560299E-18 [m^3]


output ignored...



... output resumed

 5.999886001935909E-008        2.365830515028872E-008        3.355564225533292E-012        1.944450955620792E-
016       TIME =   6035.9209     DT =   1000.0000     SUM OF SQUARES =  0.29949941E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.14805943E-10 AND  -0.14805943E-10
 POSITION OF INTERFACE CARB / AUS IS   0.26810926E-06
 U-FRACTION IN SYSTEM:  C = .0407464748437476  CR = .0212228243988234
                        FE = .978777175731684
 TOTAL SIZE OF SYSTEM:  5.05626560299E-18 [m^3]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUS

  CPU time used in timestep                1  seconds
 1.198927168684437E-007        1.201701907986178E-007        1.199354136940520E-007        3.800479812019265E-008        1.558661364261345E-
008        1.286704745119868E-012        2.362131528309901E-016        3.872322492480993E-
018       TIME =   7035.9209     DT =   1000.0000     SUM OF SQUARES =  0.38703445E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.13004088E-10 AND  -0.13004088E-10
 POSITION OF INTERFACE CARB / AUS IS   0.25510517E-06
 U-FRACTION IN SYSTEM:  C = .0407465862824098  CR = .021222822126755
                        FE = .978777178003752
 TOTAL SIZE OF SYSTEM:  5.05626560299E-18 [m^3]
  CPU time used in timestep                2  seconds
 5.225209238433798E-008        5.240492700616315E-008        5.227548559262851E-008        2.121750331796429E-008        9.585949013895591E-
009        4.729687144392894E-013        9.527987036771062E-
017       TIME =   8035.9209     DT =   1000.0000     SUM OF SQUARES =  0.90213274E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.11718729E-10 AND  -0.11718729E-10
 POSITION OF INTERFACE CARB / AUS IS   0.24338645E-06
 U-FRACTION IN SYSTEM:  C = .0407466565900236  CR = .0212228205419725
```

```
                      FE = .978777179588534
 TOTAL SIZE OF SYSTEM:  5.05626560299E-18 [m^3]
  CPU time used in timestep                    1  seconds
 2.026205430686269E-008        2.034121653237753E-008        2.027098933011042E-008        1.012909882398464E-008        5.233950919097625E-
009        1.132974763153268E-013        5.220699332671211E-
018       TIME =   9035.9209     DT =   1000.0000     SUM OF SQUARES =  0.47592982E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.10826664E-10 AND  -0.10826664E-10
 POSITION OF INTERFACE CARB / AUS IS   0.23255978E-06
 U-FRACTION IN SYSTEM:  C = .0407466962479669  CR = .0212228193844846
                      FE = .978777180746022
 TOTAL SIZE OF SYSTEM:  5.05626560299E-18 [m^3]
  CPU time used in timestep                    1  seconds
 1.455653723700638E-008        1.454807449291241E-008        1.450007706644325E-008        8.387586322423751E-009        4.531346365416658E-
009        1.022107285456354E-014        8.998524401118482E-
017       TIME =   10000.000     DT =   964.07913     SUM OF SQUARES =  0.89949661E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.10215839E-10 AND  -0.10215839E-10
 POSITION OF INTERFACE CARB / AUS IS   0.22271090E-06
 U-FRACTION IN SYSTEM:  C = .0407467174738084  CR = .0212228185233998
                      FE = .978777181607107
 TOTAL SIZE OF SYSTEM:  5.05626560299E-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    0.70000000E-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    0.10029595E-03
 DELETING TIME-RECORD FOR TIME    0.18748734E-03
 DELETING TIME-RECORD FOR TIME    0.33543544E-03
 DELETING TIME-RECORD FOR TIME    0.57835846E-03
 DELETING TIME-RECORD FOR TIME    0.95749442E-03
 DELETING TIME-RECORD FOR TIME    0.15304571E-02
 DELETING TIME-RECORD FOR TIME    0.23679917E-02
 DELETING TIME-RECORD FOR TIME    0.35511488E-02
 DELETING TIME-RECORD FOR TIME    0.51733881E-02
 DELETING TIME-RECORD FOR TIME    0.73237753E-02
 DELETING TIME-RECORD FOR TIME    0.10103564E-01
 DELETING TIME-RECORD FOR TIME    0.13647423E-01
 DELETING TIME-RECORD FOR TIME    0.18227586E-01
 DELETING TIME-RECORD FOR TIME    0.24220302E-01
 DELETING TIME-RECORD FOR TIME    0.32222097E-01
 DELETING TIME-RECORD FOR TIME    0.43283483E-01
 DELETING TIME-RECORD FOR TIME    0.59469160E-01
 DELETING TIME-RECORD FOR TIME    0.85515267E-01
 DELETING TIME-RECORD FOR TIME    0.13484423
 DELETING TIME-RECORD FOR TIME    0.23350215
 DELETING TIME-RECORD FOR TIME    0.42032578
 DELETING TIME-RECORD FOR TIME    0.75799508
 DELETING TIME-RECORD FOR TIME     1.3381135
 DELETING TIME-RECORD FOR TIME     2.3269768
 DELETING TIME-RECORD FOR TIME     4.0419404
 DELETING TIME-RECORD FOR TIME     6.9712858
 DELETING TIME-RECORD FOR TIME     12.031708
 DELETING TIME-RECORD FOR TIME     21.055606
 DELETING TIME-RECORD FOR TIME     37.776149
 DELETING TIME-RECORD FOR TIME     69.974366
 DELETING TIME-RECORD FOR TIME     134.37080
 DELETING TIME-RECORD FOR TIME     263.16367
 DELETING TIME-RECORD FOR TIME     520.74940
 DELETING TIME-RECORD FOR TIME     1035.9209
 DELETING TIME-RECORD FOR TIME     2035.9209
 DELETING TIME-RECORD FOR TIME     3035.9209
 DELETING TIME-RECORD FOR TIME     4035.9209
 DELETING TIME-RECORD FOR TIME     5035.9209
 DELETING TIME-RECORD FOR TIME     6035.9209
 DELETING TIME-RECORD FOR TIME     7035.9209
 DELETING TIME-RECORD FOR TIME     8035.9209

 KEEPING TIME-RECORD FOR TIME     9035.9209
 AND FOR TIME                     10000.000
 WORKSPACE RECLAIMED

 TIMESTEP AT     10000.0000     SELECTED

DIC> ,
DIC> ,
DIC> go sys
13:04:48,366 [Thread-0] INFO  StandaloneLicenseController: Releasing license for: Diffusion (DICTRA)
SYS: ,
SYS: set-inter
SYS:
```

exb2-plot

```
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: unknown compiler
 License library version: 9.7.0.0036
 Linked: Fri Oct 18 11:32:56 2024


SYS:SYS:MACRO exb2\plot.DCM SYS:
SYS:
SYS: @@ exb2_plot.DCM
SYS:
SYS: @@
SYS: @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE b2
SYS: @@
SYS:
SYS: @@
SYS: @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
SYS: @@
SYS: go d-m
13:05:43,444 [Thread-0] INFO  StandaloneLicenseController: Checking out license for: Diffusion (DICTRA)
TIME STEP AT TIME  1.00000E+04
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
```

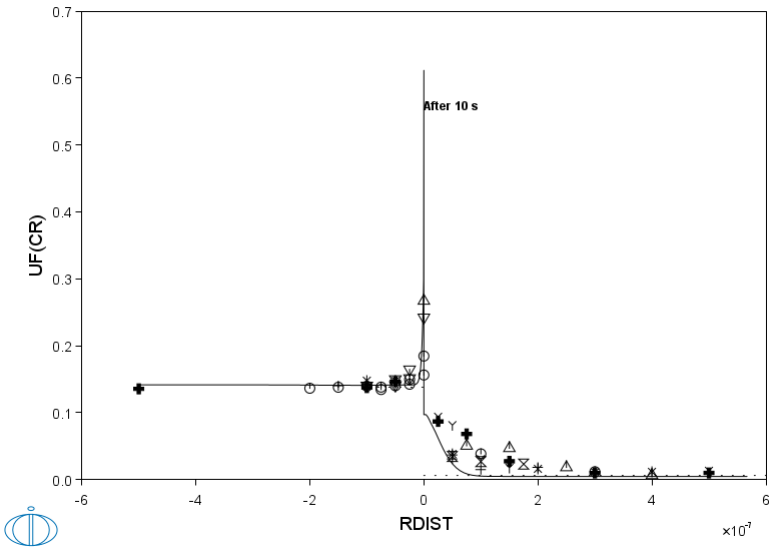
Figure b2.1




```
POST-1:
```

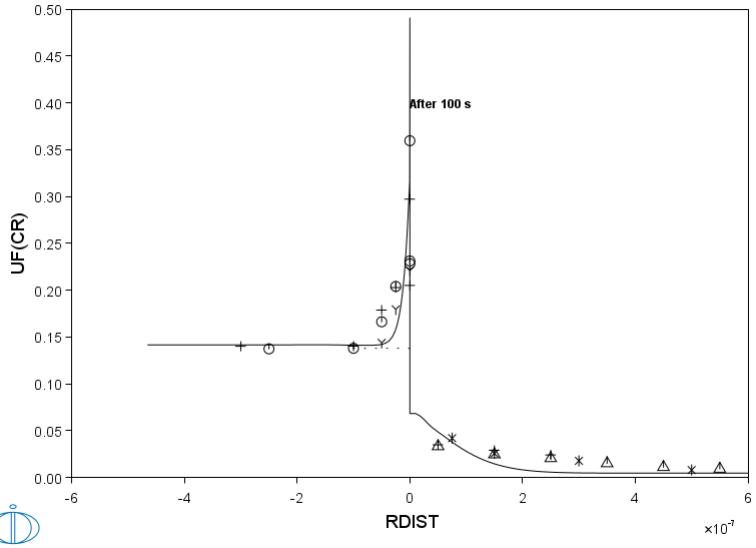
```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: @@
POST-1: @@ INCLUDE EXPERIMENTAL DATA POINTS ON THE PLOT FOR COMPARISION
POST-1: @@
POST-1: @@ FIRST LIST DATASETS
POST-1: @@
POST-1: app y exb2.exp
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: -1
 DATASET 1 CONCENTRATION 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



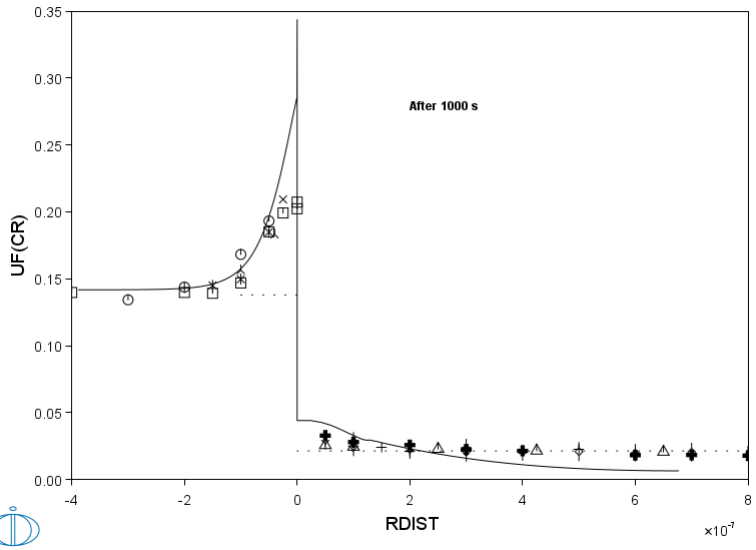

```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: @@
POST-1: @@ PLOT ALSO FOR 100, 1000 AND 10000 seconds
POST-1: @@
POST-1:
POST-1: s-p-c time 100
POST-1:
POST-1: app y exb2.exp
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 2
POST-1:
POST-1: set-title Figure 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



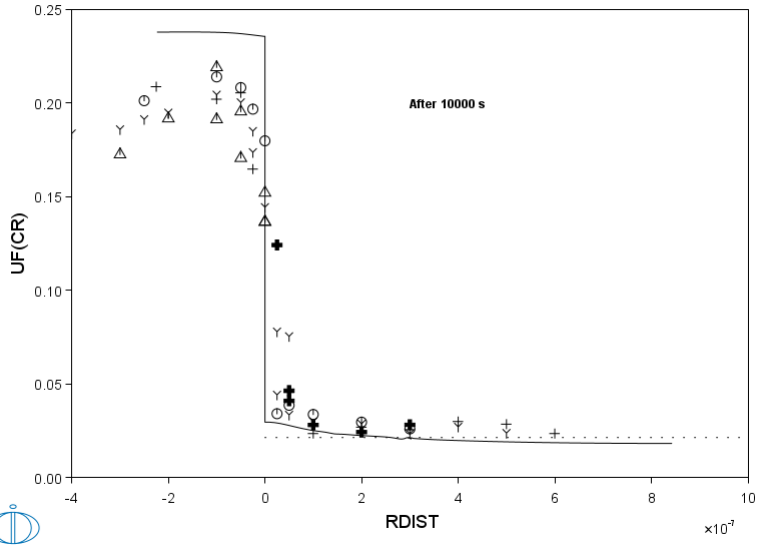

```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1:
POST-1: s-p-c time 1000
POST-1:
POST-1: app y exb2.exp
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 3
POST-1:
POST-1: set-title Figure b2.4
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

Figure b2.4



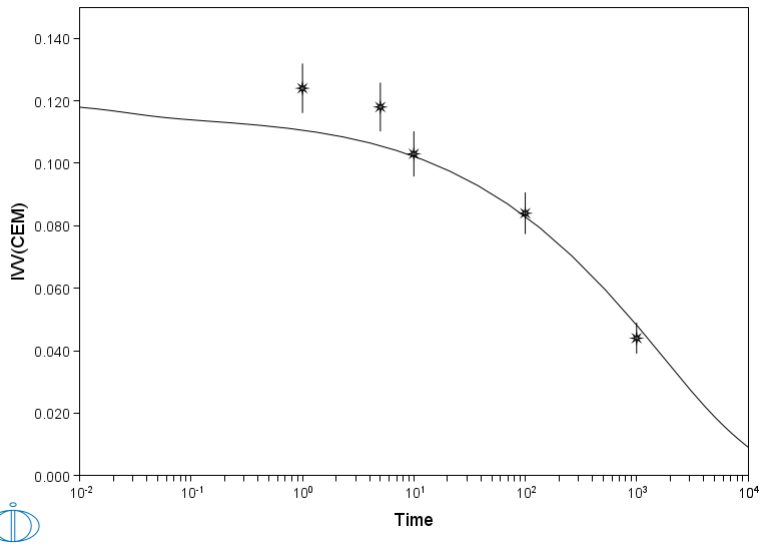

```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: s-p-c time 10000
POST-1:
POST-1: app y exb2.exp
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 4
POST-1:
POST-1: set-title Figure b2.5
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples/unite/distribution\macroResult.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
```

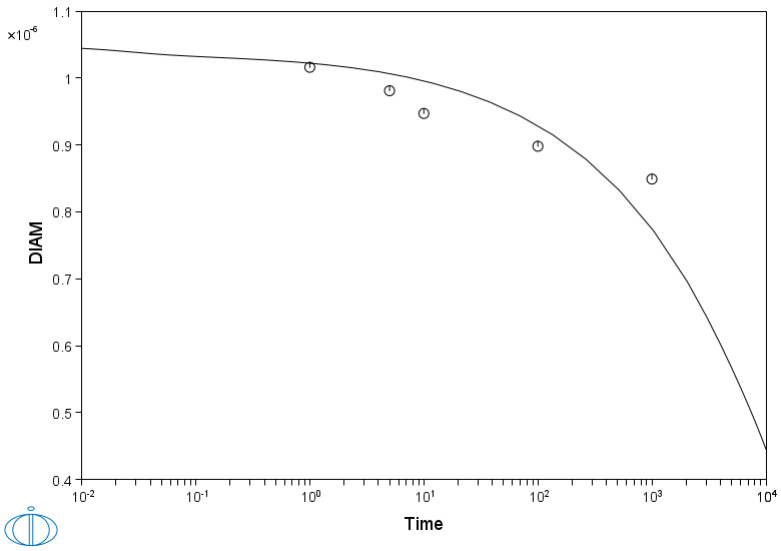
Figure b2.6




```
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

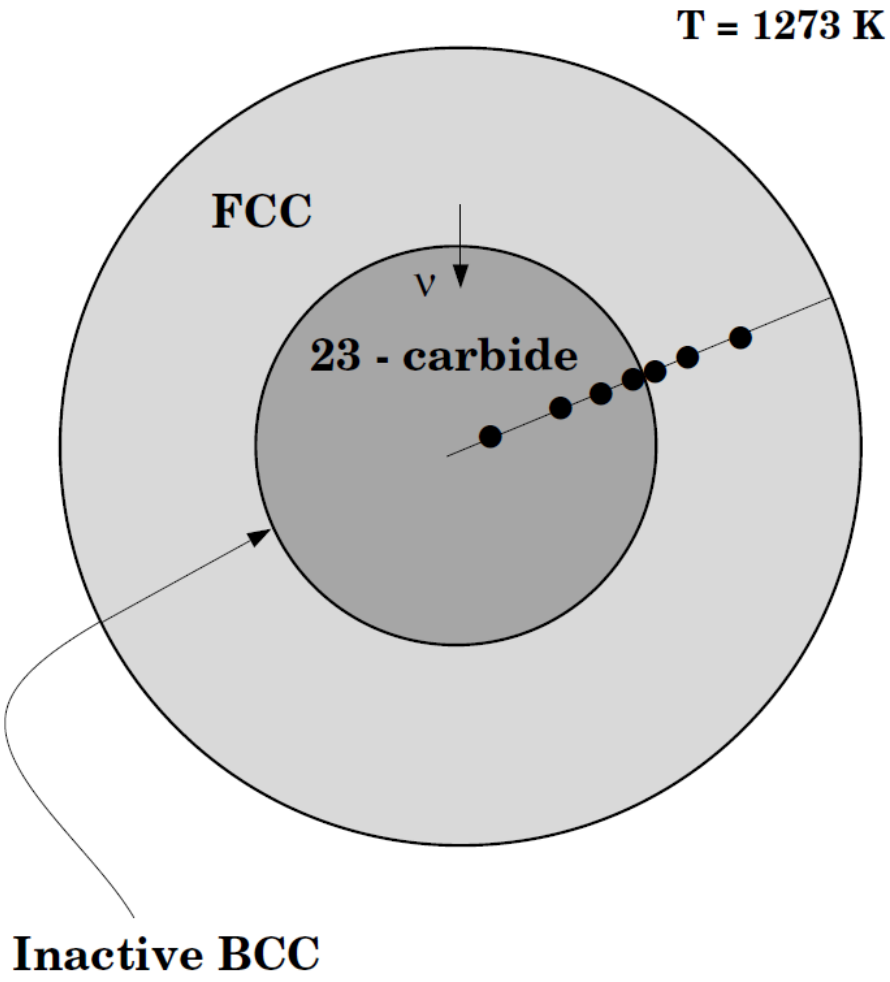



```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: set-inter
 --OK---
POST-1:
```

Example exb3

Dissolution of 23-carbide in an austenitic matrix

This example calculates the dissolution of an M23C6 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: unknown compiler
 License library version: 9.7.0.0036
 Linked: Fri Oct 18 11:32:56 2024


SYS:SYS:MACRO exb3\setup.DCM
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: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASES
SYS: @@
SYS: go da
13:06:49,488 [Thread-0] INFO  LicenseManager: Initializing user: jenkins.integrationtest@thermocalc.se
13:06:49,510 [Thread-0] INFO  LicenseController: Running License Spring in DEV environment.
13:06:50,585 [Thread-0] INFO  LicenseManager: There is an activated standalone license for jenkins.integrationtest@thermocalc.se for TC-
Application
 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 v5.0

 VA                        /-  DEFINED
TDB_FEDEMO: def-sys fe c cr
 FE                        C                         CR
   DEFINED
TDB_FEDEMO: rej ph *
 BCC_A2                    CBCC_A12                  CEMENTITE
 CHI_A12                   CUB_A13                   DIAMOND_FCC_A4
 FCC_A1                    GAS:G                     GRAPHITE
 HCP_A3                    KSI_CARBIDE               LAVES_PHASE_C14
 LIQUID:L                  M23C6                     M3C2
 M5C2                      M7C3                      SIGMA
   REJECTED
TDB_FEDEMO: res ph fcc bcc m23
 FCC_A1                    BCC_A2                    M23C6
   RESTORED
TDB_FEDEMO: get
13:06:51,682 [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 v4.0

 VA  DEFINED
APP: def-sys c cr fe
 C                         CR                        FE
   DEFINED
APP: rej ph *
 BCC_A2                    FCC_A1                    CEMENTITE
 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
13:06:52,235 [Thread-0] INFO  StandaloneLicenseController: Checking out license for: Diffusion (DICTRA)
 NO TIME STEP DEFINED
 *** ENTERING M23C6 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;
DIC>
DIC> ent-mob-est M23 cr
M[M23,CR](T)= 3e-11*exp(-278000/8.3145/T);
DIC>
DIC> ent-mob-est M23 fe
M[M23,FE](T)= 1e-11*exp(-275000/8.3145/T);
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/: 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

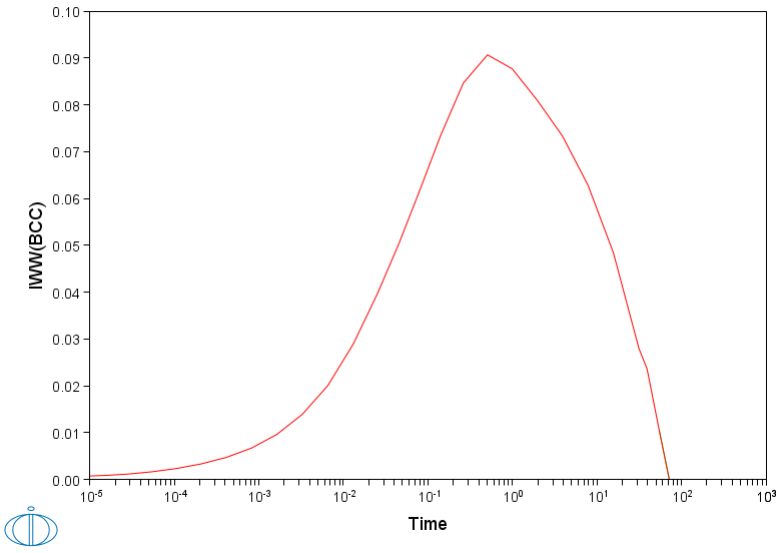
```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exb3\run.DCM DIC>
DIC>
DIC> @@ exb3_run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING EXAMPLE b3
DIC> @@
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA MONITOR AND READ THE SET UP FROM FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  0.00000E+00
DIC> read exb3
 OK
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> @@
DIC> @@ START THE SIMULATION
DIC> @@
DIC> sim yes
 Region: CARBIDE
 geometric   0.951339     dense at   0.500000E-06   77 points
 Region: MATRIX

 geometric    1.05169     dense at    0.00000       76 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]
 0.563752609069994        0.563886381801045        0.563753419684951        1.010018006844779E-002        2.780813598052816E-
004        1.635894637965996E-005        2.440981321434799E-006        1.172555947057629E-006        1.044792964976161E-
006        3.760898454198118E-008        3.342218624125184E-008        2.629923475732254E-008        3.034711864167112E-
008        2.004518858259055E-008        1.009871947004566E-008        3.416640135483140E-010        2.489505896789105E-
015        2.068224477270468E-019       TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =  0.24116107E-20
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.95403058E-03 AND  -0.95403058E-03
 POSITION OF INTERFACE CARBIDE / MATRIX IS   0.49990460E-06
 U-FRACTION IN SYSTEM:  C = .0278707541966487  CR = .149918419393047
                        FE = .850081580737459
 TOTAL SIZE OF SYSTEM:  4.93068569406E-18 [m^3]
  CPU time used in timestep                    6  seconds
 3.091422033659211E-005        3.092050575384746E-005        3.091377535205507E-005        4.589585444380703E-008        2.465668827679773E-
009        1.391159927091919E-013        3.099374147112224E-019       TIME =  0.30000000E-06 DT =  0.20000000E-
06 SUM OF SQUARES =  0.11438838E-24
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.76187577E-04 AND  -0.76187577E-04
 POSITION OF INTERFACE CARBIDE / MATRIX IS   0.49988936E-06
 U-FRACTION IN SYSTEM:  C = .0278707747843359  CR = .149918434415919
                        FE = .850081565714588
 TOTAL SIZE OF SYSTEM:  4.93068569406E-18 [m^3]
  CPU time used in timestep                    1  seconds
 6.261408986312320E-006        6.263527127090957E-006        6.260430758664788E-006        3.647101708655316E-007        1.742120613995579E-
008        6.315584692073077E-013        9.338327823766821E-020       TIME =  0.70000000E-06 DT =  0.40000000E-
06 SUM OF SQUARES =  0.11193404E-19
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.56147679E-04 AND  -0.56147679E-04
 POSITION OF INTERFACE CARBIDE / MATRIX IS   0.49986690E-06
 U-FRACTION IN SYSTEM:  C = .0278707698920309  CR = .14991845638382
                        FE = .850081543746687
 TOTAL SIZE OF SYSTEM:  4.93068569406E-18 [m^3]
  CPU time used in timestep                    1  seconds
 2.733933653436332E-006        2.734994742537779E-006        2.733627730264119E-006        7.812754924423405E-008        8.217982627279895E-
010        1.150208381607498E-014        1.326827369940729E-019       TIME =  0.15000000E-05 DT =  0.80000000E-
06 SUM OF SQUARES =  0.50845866E-21
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.36264148E-04 AND  -0.36264148E-04
 POSITION OF INTERFACE CARBIDE / MATRIX IS   0.49983789E-06


output ignored...



... output resumed

 3.848727789223281E-017       TIME =   5414.0440     DT =   800.00000     SUM OF SQUARES =  0.57858246E-20
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.72900969E-12 AND  -0.72900969E-12
 POSITION OF INTERFACE CARBIDE / MATRIX IS   0.39316223E-06
 U-FRACTION IN SYSTEM:  C = .0277946065031215  CR = .149744698962975
                        FE = .850255301167532
 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
 7.074492777311735E-008        7.076558198024483E-008        7.067455474730985E-008        4.486201921988812E-008        3.525643246477608E-
008        1.826839039672797E-008        7.326529197427166E-010        1.127210479588651E-015        2.611008031666860E-
020       TIME =   6214.0440     DT =   800.00000     SUM OF SQUARES =  0.26038926E-19
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.30174470E-12 AND  -0.30174470E-12
 POSITION OF INTERFACE CARBIDE / MATRIX IS   0.39292084E-06
 U-FRACTION IN SYSTEM:  C = .0277946082551446  CR = .149744699030401
                        FE = .850255301100106
 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
 2.405855489176618E-008        2.406353003440865E-008        2.401645372839490E-008        1.580345707638346E-008        1.454204197734934E-
008        1.154009764476587E-008        6.948497823183423E-009        6.943517519327478E-009        1.110460413301649E-
009        3.567404147438633E-016        3.410122322972613E-
020       TIME =   7014.0440     DT =   800.00000     SUM OF SQUARES =  0.34082180E-19
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.57991657E-13 AND  -0.57991657E-13
```

```
 POSITION OF INTERFACE CARBIDE / MATRIX IS   0.39287444E-06
 U-FRACTION IN SYSTEM:  C = .0277946106453739  CR = .149744699168333
                        FE = .850255300962174
 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
 8.116675096638794E-009        8.117228710356137E-009        8.091633720786405E-009        5.253059272457056E-009        5.176613838896075E-
009        4.956826873906181E-009        4.595987155851478E-009        4.593911157356757E-009        3.855841350083578E-
009        2.619303792106272E-009        8.493378448306802E-010        1.346961182970850E-013        8.901441933572719E-
019       TIME =   7814.0440     DT =   800.00000     SUM OF SQUARES =  0.88664377E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.81119329E-13 AND   0.81119329E-13
 POSITION OF INTERFACE CARBIDE / MATRIX IS   0.39293934E-06
 U-FRACTION IN SYSTEM:  C = .0277946087826722  CR = .149744699170268
                        FE = .850255300960239
 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
 6.155821593874212E-008        6.155660501105446E-008        6.185686103610645E-008        2.734231152305422E-008        2.701316892278625E-
008        2.636588815453615E-008        2.507970657849227E-008        2.507992375104873E-008        2.262021366932725E-
008        1.806387677252107E-008        1.049849691355771E-008        1.050196753923910E-008        1.484510701263905E-
009        2.013102824586105E-017       TIME =   8000.0000     DT =   185.95599     SUM OF SQUARES =  0.12316557E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.38173009E-12 AND   0.38173009E-12
 POSITION OF INTERFACE CARBIDE / MATRIX IS   0.39301032E-06
 U-FRACTION IN SYSTEM:  C = .0277946070127407  CR = .149744699172284
                        FE = .850255300958223
 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    54.786203
 DELETING TIME-RECORD FOR TIME    71.866744
 DELETING TIME-RECORD FOR TIME    71.866754
 DELETING TIME-RECORD FOR TIME    71.866774
 DELETING TIME-RECORD FOR TIME    71.866814
 DELETING TIME-RECORD FOR TIME    71.866894
 DELETING TIME-RECORD FOR TIME    71.867054
 DELETING TIME-RECORD FOR TIME    71.867374
 DELETING TIME-RECORD FOR TIME    71.868014
 DELETING TIME-RECORD FOR TIME    71.869294
 DELETING TIME-RECORD FOR TIME    71.871854
 DELETING TIME-RECORD FOR TIME    71.876974
 DELETING TIME-RECORD FOR TIME    71.887214
 DELETING TIME-RECORD FOR TIME    71.907694
 DELETING TIME-RECORD FOR TIME    71.948654
 DELETING TIME-RECORD FOR TIME    72.030574
 DELETING TIME-RECORD FOR TIME    72.194414
 DELETING TIME-RECORD FOR TIME    72.522094
 DELETING TIME-RECORD FOR TIME    73.177454
 DELETING TIME-RECORD FOR TIME    74.488174
 DELETING TIME-RECORD FOR TIME    77.109614
 DELETING TIME-RECORD FOR TIME    82.352494
 DELETING TIME-RECORD FOR TIME    92.838254
 DELETING TIME-RECORD FOR TIME    113.80977
 DELETING TIME-RECORD FOR TIME    155.75281
 DELETING TIME-RECORD FOR TIME    239.63889
 DELETING TIME-RECORD FOR TIME    407.41105
 DELETING TIME-RECORD FOR TIME    742.95537
 DELETING TIME-RECORD FOR TIME    1414.0440
 DELETING TIME-RECORD FOR TIME    2214.0440
 DELETING TIME-RECORD FOR TIME    3014.0440
 DELETING TIME-RECORD FOR TIME    3814.0440
 DELETING TIME-RECORD FOR TIME    4614.0440
 DELETING TIME-RECORD FOR TIME    5414.0440
 DELETING TIME-RECORD FOR TIME    6214.0440
 DELETING TIME-RECORD FOR TIME    7014.0440

 KEEPING TIME-RECORD FOR TIME    7814.0440
 AND FOR TIME                    8000.0000
 WORKSPACE RECLAIMED

 TIMESTEP AT     8000.00000     SELECTED

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

exb3-plot

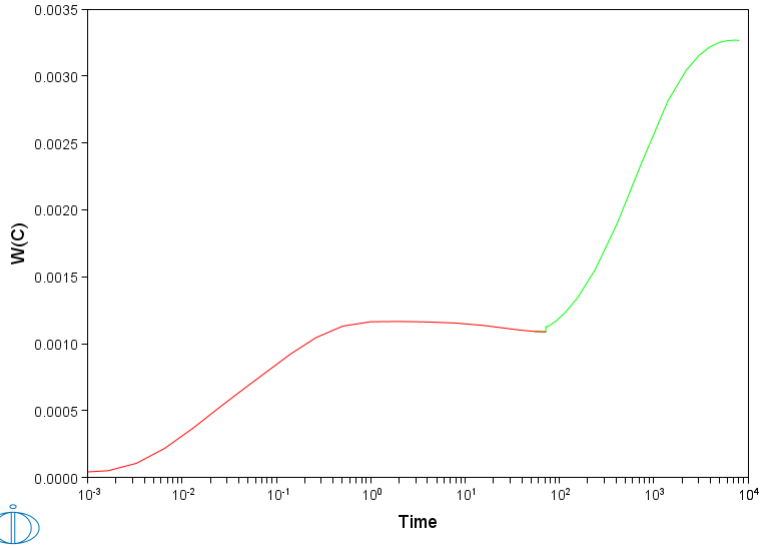
```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exb3\plot.DCM DIC>
DIC>
DIC> @@ exb3_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE b3
DIC> @@
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA MODULE AND SPECIFY THE STORE RESULT FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  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 iww(bcc)
POST-1: s-d-a x time

  INFO: Time is set as independent variable
POST-1: s-ax-typ 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
ORKING ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

Figure b3.1



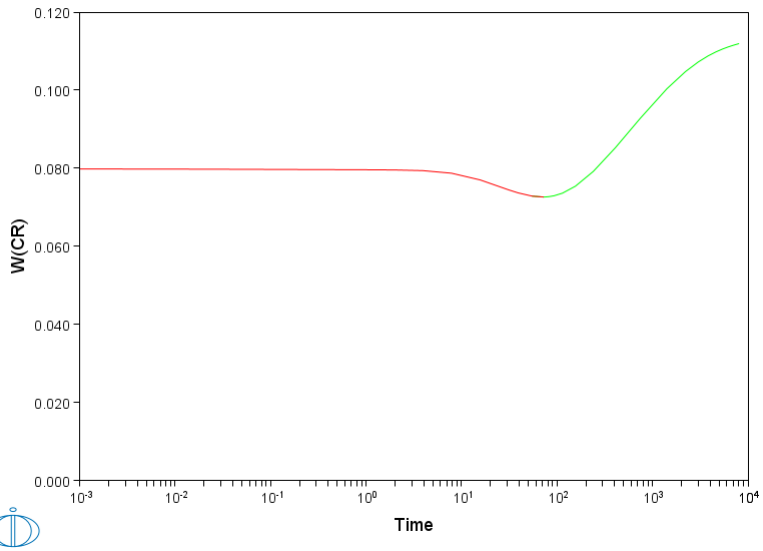

```
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: @@
POST-1: @@ NOW LOOK AT THE ALLOYING ELEMENTS AT THE UPPER BOUND OF THE SYSTEM
POST-1: @@
POST-1: s-d-a y w(c)
POST-1: s-s-s x n 1E-3 1E4
POST-1: s-p-c interface last
POST-1:
POST-1: set-tit Figure b3.2
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples/unite/distribution\macroResult.exp Y
ORKING ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

Figure b3.2



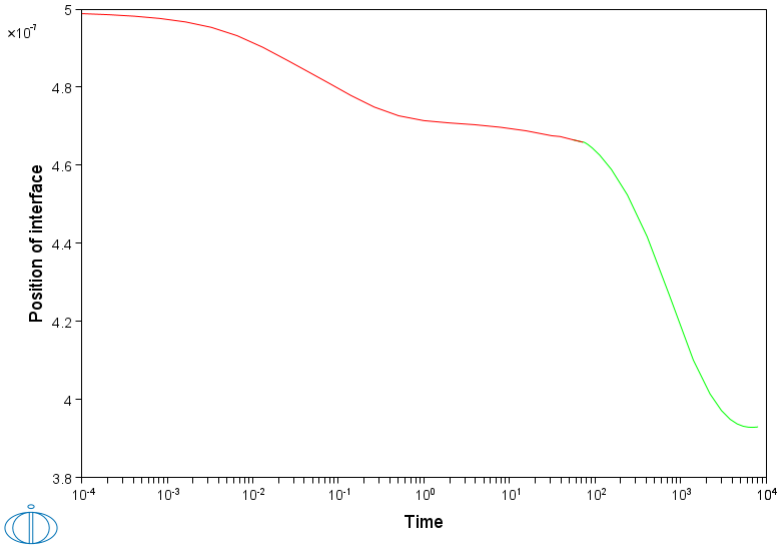

```
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: s-d-a y w(cr)
POST-1: s-s-s y n 0 0.12
POST-1:
POST-1: set-tit Figure b3.3
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples/unite/distribution\macroResult.exp Y
ORKING ...          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
ORKING ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

Figure b3.4

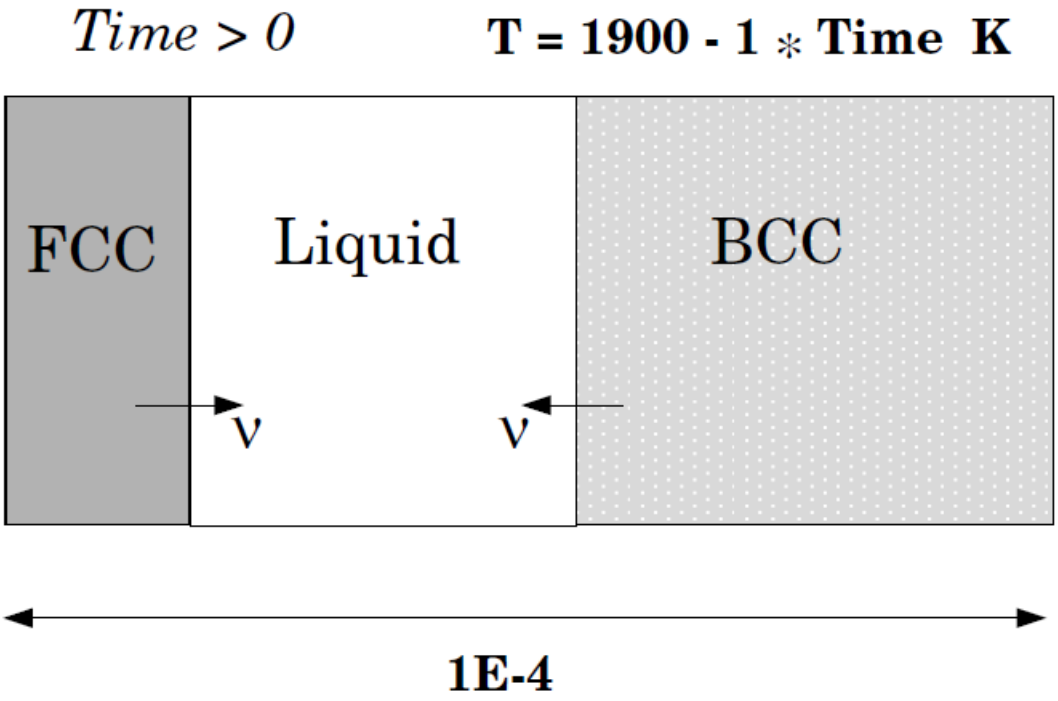



```
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1:
POST-1: set-inter
 --OK---
POST-1:
```

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 -> 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.



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: unknown compiler
 License library version: 9.7.0.0036
 Linked: Fri Oct 18 11:32:56 2024


SYS:SYS:MACRO exb4a\setup.DCM
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: ----------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exb4a_setup.DCM
SYS:
SYS:
SYS: @@
SYS: @@ START BY GOING TO THE DATABASE MODULE
SYS: @@
SYS: go da
13:15:02,325 [Thread-0] INFO  LicenseManager: Initializing user: jenkins.integrationtest@thermocalc.se
13:15:02,342 [Thread-0] INFO  LicenseController: Running License Spring in DEV environment.
13:15:03,512 [Thread-0] INFO  LicenseManager: There is an activated standalone license for jenkins.integrationtest@thermocalc.se for TC-
Application
 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
13:15:05,150 [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_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 v5.0
 MOB2    =  Alloys Mobility  v2.7
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBFE7  =  Steels/Fe-Alloys Mobility  v7.1
 MFEDEMO =  Fe-Alloys Mobility demo database v4.0
 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
13:15:07,470 [Thread-0] INFO  StandaloneLicenseController: Checking out license for: Diffusion (DICTRA)
 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 /LINEAR/: 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> s-s-c
NS01A PRINT CONTROL : /0/:
```

```
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /AUTO/: AUTO
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -> 1): /AUTO/:
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/:
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

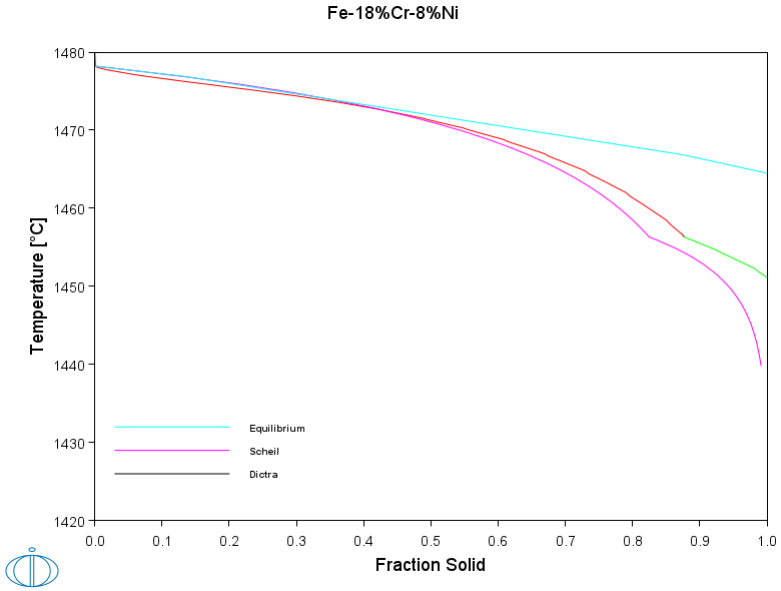
```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exb4a\run.DCM DIC>
DIC>
DIC> @@ exb4a_run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING EXAMPLE b4a
DIC> @@
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA MONITOR AND READ THE SET UP FROM FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  0.00000E+00
DIC> read exb4a
 OK
DIC>
DIC> @@
DIC> @@ START THE SIMULATION
DIC> @@
DIC> sim yes
 Region: SMALTA
 geometric     1.13113      dense at     0.00000        53 points
 geometric    0.884075      dense at    0.100000E-03    54 points
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
 INFO: TIMESTEP IS CONTROLLED BY INTERFACE POSITION
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                         NI = .0754116207882254
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                         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 = .733068011219291
                                                          NI = .0754116207882254
                                                TOTAL SIZE OF SYSTEM:  1E-04 [m]

  CPU time used in timestep                    2  seconds
 TIME =  0.75536897E-06 DT =  0.65536897E-06 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                                                          NI = .0754116207882254
                                                TOTAL SIZE OF SYSTEM:  1E-04 [m]

  CPU time used in timestep                    0  seconds
 TIME =  0.20661069E-05 DT =  0.13107379E-05 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                                                          NI = .0754116207882254
                                                TOTAL SIZE OF SYSTEM:  1E-04 [m]

  CPU time used in timestep                    0  seconds
 TIME =  0.46875828E-05 DT =  0.26214759E-05 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                                                          NI = .0754116207882254
                                                TOTAL SIZE OF SYSTEM:  1E-04 [m]

  CPU time used in timestep                    0  seconds
 TIME =  0.99305345E-05 DT =  0.52429517E-05 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                                                          NI = .0754116207882254
                                                TOTAL SIZE OF SYSTEM:  1E-04 [m]

  CPU time used in timestep                    0  seconds
 TIME =  0.20416438E-04 DT =  0.10485903E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                                                          NI = .0754116207882254
                                                TOTAL SIZE OF SYSTEM:  1E-04 [m]

  CPU time used in timestep                    1  seconds
 TIME =  0.41388245E-04 DT =  0.20971807E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                                                          NI = .0754116207882254
                                                TOTAL SIZE OF SYSTEM:  1E-04 [m]

  CPU time used in timestep                    0  seconds
 TIME =  0.83331859E-04 DT =  0.41943614E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                                                          NI = .0754116207882254
                                                TOTAL SIZE OF SYSTEM:  1E-04 [m]

  CPU time used in timestep                    0  seconds
 TIME =  0.16721909E-03 DT =  0.83887228E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                                                          NI = .0754116207882254
                                                TOTAL SIZE OF SYSTEM:  1E-04 [m]

  CPU time used in timestep                    0  seconds
 TIME =  0.33499354E-03 DT =  0.16777446E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                                                          NI = .0754116207882254
                                                TOTAL SIZE OF SYSTEM:  1E-04 [m]

  CPU time used in timestep                    0  seconds
 TIME =  0.67054245E-03 DT =  0.33554891E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                                                          NI = .0754116207882254
                                                TOTAL SIZE OF SYSTEM:  1E-04 [m]

  CPU time used in timestep                    0  seconds
 TIME =  0.13416403E-02 DT =  0.67109782E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                                                          NI = .0754116207882254
                                                TOTAL SIZE OF SYSTEM:  1E-04 [m]

  CPU time used in timestep                    0  seconds
 TIME =  0.26838359E-02 DT =  0.13421956E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                                                          NI = .0754116207882254
                                                TOTAL SIZE OF SYSTEM:  1E-04 [m]

  CPU time used in timestep                    0  seconds
 TIME =  0.53682272E-02 DT =  0.26843913E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                                                          NI = .0754116207882254
                                                TOTAL SIZE OF SYSTEM:  1E-04 [m]

  CPU time used in timestep                    0  seconds
 TIME =  0.10737010E-01 DT =  0.53687826E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                                                          NI = .0754116207882253
                                                TOTAL SIZE OF SYSTEM:  1E-04 [m]

  CPU time used in timestep                    1  seconds
 TIME =  0.21474575E-01 DT =  0.10737565E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292

                         NI = .0754116207882253
```

```
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.42949705E-01 DT =  0.21475130E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882253
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.85899966E-01 DT =  0.42950261E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992481  FE = .733068011219293
                        NI = .0754116207882251
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.17180049     DT =  0.85900521E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992481  FE = .733068011219294


output ignored...



... output resumed

 5.514020082822429E-006        5.514911388132715E-006        5.510290592157270E-006        7.037616795618768E-010        4.755837981267047E-
013        4.290884673935608E-018       TIME =   178.37675     DT =   1.3107200     SUM OF SQUARES =  0.42892806E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.59586298E-07 AND  -0.59586298E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.70733312E-05
 U-FRACTION IN SYSTEM:  CR = .191500140553765  FE = .733101749908671
                        NI = .0753981095375642
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_BCC_A2

  CPU time used in timestep                    1  seconds
 1.084827053979186E-005        1.084821676825446E-005        1.084216322806263E-005        3.719115206553259E-007        3.455230208942483E-
011        4.177969770244869E-016        7.425690863980879E-
021       TIME =   180.99819     DT =   2.6214400     SUM OF SQUARES =  0.74196435E-20
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.43677839E-07 AND  -0.43677839E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.69588324E-05
 U-FRACTION IN SYSTEM:  CR = .191500140472994  FE = .733101750092071
                        NI = .0753981094349351
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  2  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_BCC_A2

  CPU time used in timestep                    2  seconds
 7.952600143322148E-006        7.952743903473148E-006        7.949263215758215E-006        9.909657496450635E-007        1.840177300178130E-
007        1.409168481699029E-012        9.369477747928810E-
017       TIME =   186.24107     DT =   5.2428800     SUM OF SQUARES =  0.92185218E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.17541386E-07 AND  -0.17541386E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.68668650E-05
 U-FRACTION IN SYSTEM:  CR = .191500140397143  FE = .733101750328692
                        NI = .0753981092741656
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_BCC_A2

  CPU time used in timestep                    1  seconds
 5.746576534691800E-006        5.746728479242748E-006        5.745076598210180E-006        2.360343713990736E-006        1.577169620638083E-
006        3.829962161134910E-007        4.339238583290681E-011        4.703447843004499E-015        6.367717166966128E-
019       TIME =   196.72683     DT =   10.485760     SUM OF SQUARES =  0.50954620E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.21895465E-07 AND   0.21895465E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.70964556E-05
 U-FRACTION IN SYSTEM:  CR = .191500140395396  FE = .733101750358394
                        NI = .0753981092462106
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    2  seconds
 1.321138207086155E-005        1.321159776785756E-005        1.320626573830183E-005        7.851089475818431E-008        2.076707210837201E-
011        7.867668154367367E-017       TIME =   200.00000     DT =   3.2731716     SUM OF SQUARES =  0.13982197E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.13968010E-07 AND   0.13968010E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.71421753E-05
 U-FRACTION IN SYSTEM:  CR = .191500140391685  FE = .733101750377513
                        NI = .0753981092308021
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 MUST SAVE WORKSPACE ON FILE
 WORKSPACE SAVED ON FILE
 RECLAIMING WORKSPACE
 DELETING TIME-RECORD FOR TIME    175.56687
 DELETING TIME-RECORD FOR TIME    175.75532
 DELETING TIME-RECORD FOR TIME    175.75533
 DELETING TIME-RECORD FOR TIME    175.75535
 DELETING TIME-RECORD FOR TIME    175.75539
 DELETING TIME-RECORD FOR TIME    175.75547
 DELETING TIME-RECORD FOR TIME    175.75563
 DELETING TIME-RECORD FOR TIME    175.75595
 DELETING TIME-RECORD FOR TIME    175.75659
 DELETING TIME-RECORD FOR TIME    175.75787
 DELETING TIME-RECORD FOR TIME    175.76043
 DELETING TIME-RECORD FOR TIME    175.76555
 DELETING TIME-RECORD FOR TIME    175.77579
 DELETING TIME-RECORD FOR TIME    175.79627
 DELETING TIME-RECORD FOR TIME    175.83723
 DELETING TIME-RECORD FOR TIME    175.91915
 DELETING TIME-RECORD FOR TIME    176.08299
 DELETING TIME-RECORD FOR TIME    176.41067
 DELETING TIME-RECORD FOR TIME    177.06603
 DELETING TIME-RECORD FOR TIME    178.37675
 DELETING TIME-RECORD FOR TIME    180.99819
 DELETING TIME-RECORD FOR TIME    186.24107

 KEEPING TIME-RECORD FOR TIME    196.72683
 AND FOR TIME                    200.00000
 WORKSPACE RECLAIMED

 TIMESTEP AT     200.000000     SELECTED

DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ THE SIMULATION IS FINISHED
```

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

exb4a-plot

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exb4a\plot.DCM DIC>
DIC>
DIC> @@ exb4a_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE b4a
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 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 exb4.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
ORKING ...orking ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

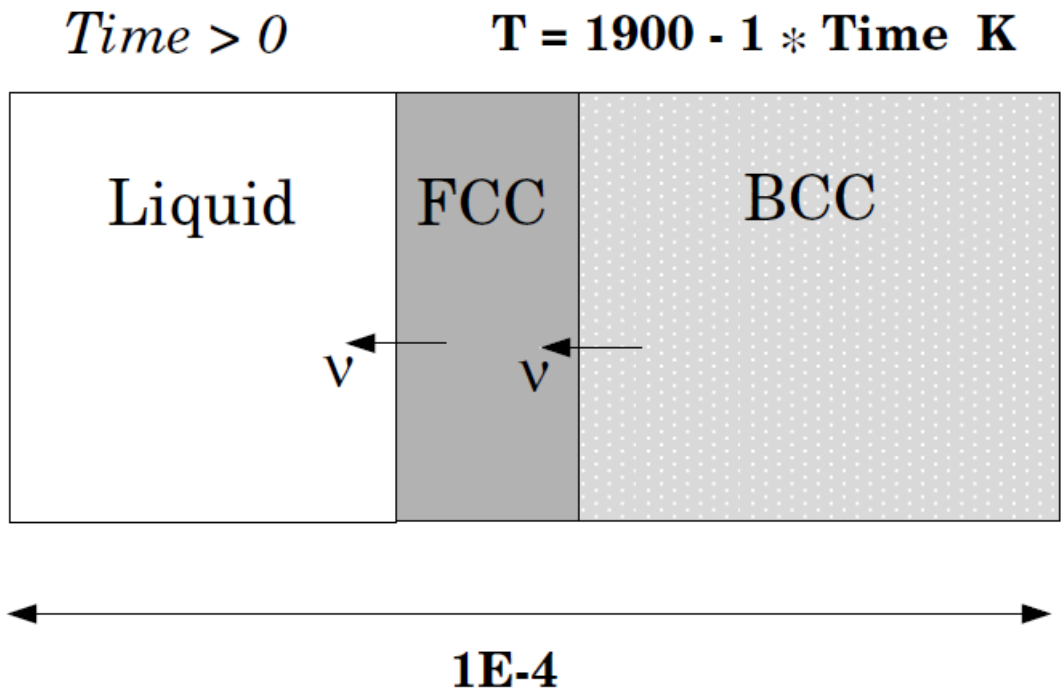



```
POST-1:
POST-1:
POST-1: set-inter
 --OK---
POST-1:
```

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 -> FCC. Hence the FCC region should appear in between the LIQUID and the BCC. Comparison is made with both a Scheil-Gulliver simulation and equilibrium solidification conditions, both made with Thermo-Calc.



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: unknown compiler
 License library version: 9.7.0.0036
 Linked: Fri Oct 18 11:32:56 2024


SYS:SYS:MACRO exb4b\setup.DCM
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: ----------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exb4b_setup.DCM
SYS:
SYS:
SYS: @@
SYS: @@ START BY GOING TO THE DATABASE MODULE
SYS: @@
SYS: go da
13:20:30,482 [Thread-0] INFO  LicenseManager: Initializing user: jenkins.integrationtest@thermocalc.se
13:20:30,493 [Thread-0] INFO  LicenseController: Running License Spring in DEV environment.
13:20:31,591 [Thread-0] INFO  LicenseManager: There is an activated standalone license for jenkins.integrationtest@thermocalc.se for TC-
Application
 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 v5.0

 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
 BCC_A2                   CBCC_A12                 CHI_A12
 CUB_A13                  FCC_A1                   GAS:G
 HCP_A3                   LAVES_PHASE_C14          LIQUID:L
 SIGMA  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
13:20:32,676 [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 v5.0
 MOB2    =  Alloys Mobility  v2.7
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBFE7  =  Steels/Fe-Alloys Mobility  v7.1
 MFEDEMO =  Fe-Alloys Mobility demo database v4.0
 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: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP
APP: @@
APP: go d-m
13:20:33,514 [Thread-0] INFO  StandaloneLicenseController: Checking out license for: Diffusion (DICTRA)
 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 /LINEAR/: 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> s-s-c
NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /AUTO/: yes
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
```

```
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -> 1): /AUTO/:
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/: @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exb4b Y
DIC>
DIC> set-inter
 --OK---
DIC>
```

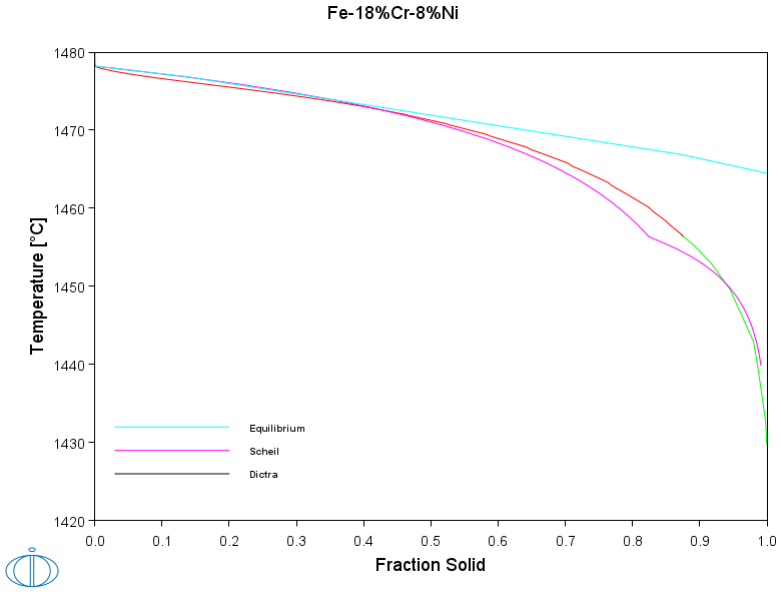
exb4b-run

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exb4b\run.DCM 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
 Region: SMALTA
 geometric   0.866196     dense at   0.100000E-03   89 points
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                         NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                         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 =  0.94776182E-06 DT =  0.84776182E-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 =  0.26432855E-05 DT =  0.16955236E-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 =  0.60343328E-05 DT =  0.33910473E-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 =  0.12816427E-04 DT =  0.67820946E-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 =  0.26380616E-04 DT =  0.13564189E-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 =  0.53508995E-04 DT =  0.27128378E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992482  FE = .733068011219292
                                                                NI = .0754116207882255
                                                TOTAL SIZE OF SYSTEM:  1E-04 [m]

  CPU time used in timestep                     0  seconds
 TIME =  0.10776575E-03 DT =  0.54256757E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992482  FE = .733068011219292
                                                                NI = .0754116207882255
                                                TOTAL SIZE OF SYSTEM:  1E-04 [m]

  CPU time used in timestep                     0  seconds
 TIME =  0.21627926E-03 DT =  0.10851351E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992482  FE = .733068011219292
                                                                NI = .0754116207882255
                                                TOTAL SIZE OF SYSTEM:  1E-04 [m]

  CPU time used in timestep                     0  seconds
 TIME =  0.43330629E-03 DT =  0.21702703E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992482  FE = .733068011219292
                                                                NI = .0754116207882255
                                                TOTAL SIZE OF SYSTEM:  1E-04 [m]

  CPU time used in timestep                     1  seconds
 TIME =  0.86736034E-03 DT =  0.43405405E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992482  FE = .733068011219292
                                                                NI = .0754116207882255
                                                TOTAL SIZE OF SYSTEM:  1E-04 [m]

  CPU time used in timestep                     0  seconds
 TIME =  0.17354684E-02 DT =  0.86810811E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992482  FE = .733068011219292
                                                                NI = .0754116207882255
                                                TOTAL SIZE OF SYSTEM:  1E-04 [m]

  CPU time used in timestep                     0  seconds
 TIME =  0.34716847E-02 DT =  0.17362162E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992482  FE = .733068011219292
                                                                NI = .0754116207882255
                                                TOTAL SIZE OF SYSTEM:  1E-04 [m]

  CPU time used in timestep                     0  seconds
 TIME =  0.69441171E-02 DT =  0.34724324E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992482  FE = .733068011219292
                                                                NI = .0754116207882255
                                                TOTAL SIZE OF SYSTEM:  1E-04 [m]

  CPU time used in timestep                     0  seconds
 TIME =  0.13888982E-01 DT =  0.69448648E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992482  FE = .733068011219292
                                                                NI = .0754116207882255
                                                TOTAL SIZE OF SYSTEM:  1E-04 [m]

  CPU time used in timestep                     0  seconds
 TIME =  0.27778712E-01 DT =  0.13889730E-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 =  0.55558171E-01 DT =  0.27779459E-01 SUM OF SQUARES =   0.0000000
```

```
 U-FRACTION IN SYSTEM:  CR = .191520367992482  FE = .733068011219292
                        NI = .0754116207882254
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.11111709     DT =  0.55558919E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992482  FE = .733068011219292
                        NI = .0754116207882258
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.22223493     DT =  0.11111784     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .19152036799248  FE = .733068011219295
                        NI = .0754116207882249
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.44447060     DT =  0.22223567     SUM OF SQUARES =   0.0000000


output ignored...



... output resumed

  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_BCC_A2

  CPU time used in timestep                    2  seconds
 5.139565407027669E-008        5.140798655414667E-008        5.100322508121547E-008        2.851224761501404E-009        2.680774736474247E-
009        2.318513389013127E-009        1.711478567270615E-009        1.706278419027410E-009        7.403855487205554E-
010        7.491643237007726E-013        1.153552695658592E-
018       TIME =   198.43707     DT =  0.65536000     SUM OF SQUARES =  0.11486045E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.26044384E-08 AND  -0.26044384E-08
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.10556331E-04
 U-FRACTION IN SYSTEM:  CR = .19111014993086  FE = .733547209684841
                        NI = .0753426403842982
 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
 1.304182173387704E-007        1.304255357083201E-007        1.306083691992910E-007        1.230192701597723E-007        1.224896417598367E-
007        1.214349182789879E-007        1.193032692179761E-007        1.192993044981165E-007        1.151292873099127E-
007        1.069683415179910E-007        9.156880683330858E-008        9.157798616109581E-008        6.430879629455531E-
008        2.433804659619870E-008        7.623826756464617E-016        8.803709551680435E-
025       TIME =   199.74779     DT =   1.3107200     SUM OF SQUARES =  0.48113915E-24
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.66244255E-08 AND   0.66244255E-08
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.10565014E-04
 U-FRACTION IN SYSTEM:  CR = .191110149932036  FE = .733547209684699
                        NI = .0753426403832655
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  29  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_FCC_A1

  CPU time used in timestep                    2  seconds
 1.465895759291694E-009        1.466040185758873E-009        1.474708087365044E-009        1.158914552248960E-009        1.147413217103301E-
009        1.123679375944863E-009        1.077741106712051E-009        1.077529964704765E-009        9.879986406216589E-
010        8.208524162988330E-010        5.325399542727353E-010        5.326722687166035E-010        1.425091607267353E-
010        3.216187787669356E-017       TIME =   200.00000     DT =  0.25221463     SUM OF SQUARES =  0.26698122E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.24230933E-08 AND  -0.24230933E-08
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.10564403E-04
 U-FRACTION IN SYSTEM:  CR = .191110149932011  FE = .733547209684735
                        NI = .0753426403832543
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 MUST SAVE WORKSPACE ON FILE
 WORKSPACE SAVED ON FILE
 RECLAIMING WORKSPACE
 DELETING TIME-RECORD FOR TIME    193.98930
 DELETING TIME-RECORD FOR TIME    197.12636
 DELETING TIME-RECORD FOR TIME    197.12637
 DELETING TIME-RECORD FOR TIME    197.12639
 DELETING TIME-RECORD FOR TIME    197.12643
 DELETING TIME-RECORD FOR TIME    197.12651
 DELETING TIME-RECORD FOR TIME    197.12667
 DELETING TIME-RECORD FOR TIME    197.12699
 DELETING TIME-RECORD FOR TIME    197.12763
 DELETING TIME-RECORD FOR TIME    197.12891
 DELETING TIME-RECORD FOR TIME    197.13147
 DELETING TIME-RECORD FOR TIME    197.13659
 DELETING TIME-RECORD FOR TIME    197.14683
 DELETING TIME-RECORD FOR TIME    197.16731
 DELETING TIME-RECORD FOR TIME    197.20827
 DELETING TIME-RECORD FOR TIME    197.29019
 DELETING TIME-RECORD FOR TIME    197.45403
 DELETING TIME-RECORD FOR TIME    197.78171
 DELETING TIME-RECORD FOR TIME    198.43707

 KEEPING TIME-RECORD FOR TIME    199.74779
 AND FOR TIME                    200.00000
 WORKSPACE RECLAIMED

 TIMESTEP AT     200.000000     SELECTED

DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
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>
```

exb4b-plot

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exb4b\plot.DCM DIC>
DIC>
DIC> @@ exb4b_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE b4b
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 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
ORKING ...orking ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

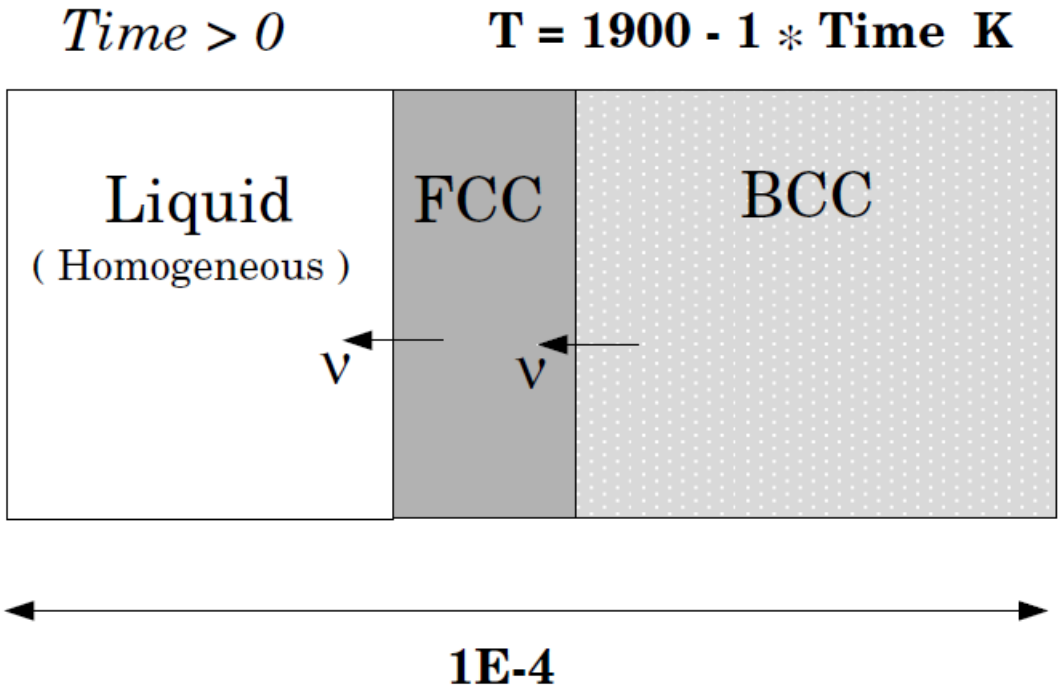



```
POST-1:
POST-1:
POST-1:
POST-1: set-inter
 --OK---
POST-1:
```

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.



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: unknown compiler
 License library version: 9.7.0.0036
 Linked: Fri Oct 18 11:32:56 2024


SYS:SYS:MACRO exb4c\setup.DCM
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: ----------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exb4c_setup.DCM
SYS:
SYS: @@
SYS: @@ START BY GOING TO THE DATABASE MODULE
SYS: @@
SYS: go da
13:27:12,659 [Thread-0] INFO  LicenseManager: Initializing user: jenkins.integrationtest@thermocalc.se
13:27:12,674 [Thread-0] INFO  LicenseController: Running License Spring in DEV environment.
13:27:13,803 [Thread-0] INFO  LicenseManager: There is an activated standalone license for jenkins.integrationtest@thermocalc.se for TC-
Application
 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
13:27:15,248 [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 v5.0
 MOB2    =  Alloys Mobility  v2.7
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBFE7  =  Steels/Fe-Alloys Mobility  v7.1
 MFEDEMO =  Fe-Alloys Mobility demo database v4.0
 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
13:27:17,523 [Thread-0] INFO  StandaloneLicenseController: Checking out license for: Diffusion (DICTRA)
 NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ LIST THE MOBILITIES IN THE LIQUID
DIC> @@
DIC> list-mobility-data
 Sorry, LIST-DATA disabled for this database
DIC>
DIC>
DIC> liquid
 NO SUCH COMMAND, USE HELP
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

13:27:18,586 [Thread-0] INFO  Database: Preparing system for use: MOBFE4_MODIFIED_172925803791016
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> li-mob
 AMBIGUOUS COMMAND, USE HELP
DIC>
DIC>
DIC> liquid
 NO SUCH COMMAND, USE HELP
DIC>
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 /LINEAR/: 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
13:27:20,346 [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> s-s-c
NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /AUTO/: yes
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -> 1): /AUTO/:
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/: @@
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

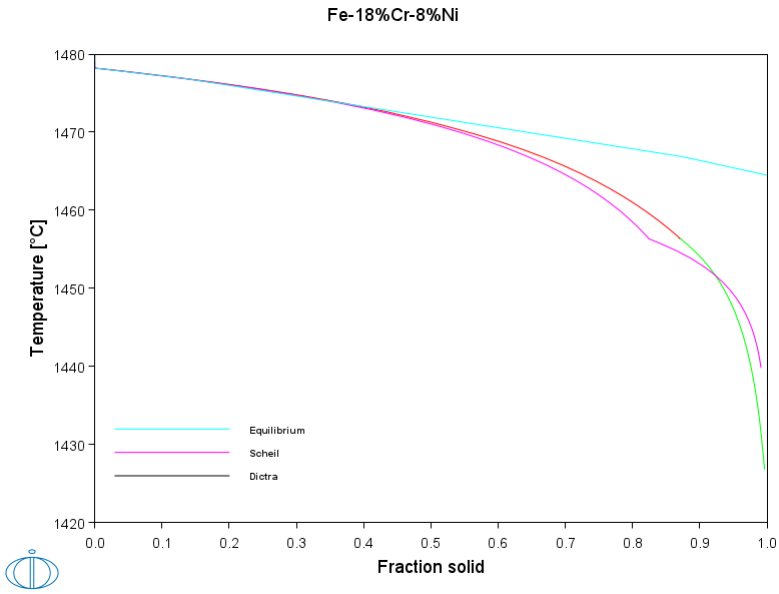
```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exb4c\run.DCM DIC>
DIC> @@ exb4c_run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING EXAMPLE b4b
DIC> @@
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA MONITOR AND READ THE SET UP FROM FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  0.00000E+00
DIC> read exb4c
 OK
DIC>
DIC> @@
DIC> @@ START THE SIMULATION
DIC> @@
DIC> sim yes
 Region: SMALTA
 geometric   0.866196     dense at   0.100000E-03   89 points
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                                    NI = .0754116207882255
                                TOTAL SIZE OF SYSTEM:  1E-04 [m]
                          13:28:16,632 [Thread-0] INFO  Phase: Preparing phase for use: BCC_A2
                          13:28:17,266 [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 = .0754116207882255
                                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 = .733068011219291
                                    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                     0  seconds
                       TIME =  0.31000000E-05 DT =  0.16000000E-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 =  0.63000000E-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 = .0754116207882254
                                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 = .0754116207882254
                                TOTAL SIZE OF SYSTEM:  1E-04 [m]
                              CPU time used in timestep                     1  seconds
                       TIME =  0.51100000E-04 DT =  0.25600000E-04 SUM OF SQUARES =   0.0000000
                          U-FRACTION IN SYSTEM:  CR = .191520367992482  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 = .191520367992482  FE = .733068011219292
                                    NI = .0754116207882255
                                TOTAL SIZE OF SYSTEM:  1E-04 [m]
                              CPU time used in timestep                     0  seconds
                       TIME =  0.20470000E-03 DT =  0.10240000E-03 SUM OF SQUARES =   0.0000000
                          U-FRACTION IN SYSTEM:  CR = .191520367992484  FE = .733068011219291
                                    NI = .075411620788225
                                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 = .733068011219292
                                    NI = .0754116207882248
                                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 = .191520367992482  FE = .733068011219292
                                    NI = .0754116207882257
                                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 = .191520367992479  FE = .733068011219297
                                    NI = .075411620788224
                                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 = .191520367992469  FE = .7330680112193
                        NI = .0754116207882307
 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 = .191520367992498  FE = .73306801121927
                        NI = .0754116207882329
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
```

```
  CPU time used in timestep                    0  seconds
 TIME =  0.13107100E-01 DT =  0.65536000E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992459  FE = .733068011219317
                        NI = .0754116207882242
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.26214300E-01 DT =  0.13107200E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992559  FE = .733068011219251
                        NI = .07541162078819
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    1  seconds
 TIME =  0.52428700E-01 DT =  0.26214400E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992416  FE = .733068011219469
                        NI = .0754116207881154
 TOTAL SIZE OF SYSTEM:  1E-04 [m]


output ignored...



... output resumed

  CPU time used in timestep                   16  seconds
 4.509651198700606E-006        4.511260885404113E-006        4.509651887737562E-006        4.507366005391236E-006        4.509637147969166E-
006        1.004336069264140E-006        1.052123826763307E-007        3.875379970159113E-008        4.424547553276597E-
008        4.595926357264435E-009        5.073323317415209E-009        4.576715692224007E-009        4.583146950301550E-
009        6.359913201032690E-010        1.438326148310476E-010        6.666994662417487E-012        7.328043382444014E-
014        1.044307780792139E-014        1.739706625579858E-014        7.014781421083336E-014        2.565754961527261E-
013        4.494204505827981E-015        1.180738388783807E-015        2.672613145122565E-016       TIME =   200.00000     DT =  0.88751250E-
01 SUM OF SQUARES =  0.14938741E-29
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.50590492E-07 AND  -0.50590492E-07
 POSITION OF INTERFACE SMALTA / R_FCC_A1 IS   0.37316501E-06
 CELL # 1 VELOCITY AT INTERFACE # 3 IS  -0.15074363E-08 AND  -0.15074363E-08
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.10989155E-04
 U-FRACTION IN SYSTEM:  CR = .191197404753821  FE = .733444988283428
                        NI = .0753576069627509
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 MUST SAVE WORKSPACE ON FILE
 WORKSPACE SAVED ON FILE
 RECLAIMING WORKSPACE
 DELETING TIME-RECORD FOR TIME    170.37562
 DELETING TIME-RECORD FOR TIME    170.48353
 DELETING TIME-RECORD FOR TIME    170.48353
 DELETING TIME-RECORD FOR TIME    170.48353
 DELETING TIME-RECORD FOR TIME    170.48353
 DELETING TIME-RECORD FOR TIME    170.48353
 DELETING TIME-RECORD FOR TIME    170.48353
 DELETING TIME-RECORD FOR TIME    170.48353
 DELETING TIME-RECORD FOR TIME    170.48354
 DELETING TIME-RECORD FOR TIME    170.48355
 DELETING TIME-RECORD FOR TIME    170.48358
 DELETING TIME-RECORD FOR TIME    170.48363
 DELETING TIME-RECORD FOR TIME    170.48373
 DELETING TIME-RECORD FOR TIME    170.48394
 DELETING TIME-RECORD FOR TIME    170.48435
 DELETING TIME-RECORD FOR TIME    170.48517
 DELETING TIME-RECORD FOR TIME    170.48680
 DELETING TIME-RECORD FOR TIME    170.49008
 DELETING TIME-RECORD FOR TIME    170.49663
 DELETING TIME-RECORD FOR TIME    170.50974
 DELETING TIME-RECORD FOR TIME    170.53596
 DELETING TIME-RECORD FOR TIME    170.58838
 DELETING TIME-RECORD FOR TIME    170.69324
 DELETING TIME-RECORD FOR TIME    170.90296
 DELETING TIME-RECORD FOR TIME    171.32239
 DELETING TIME-RECORD FOR TIME    172.16125
 DELETING TIME-RECORD FOR TIME    173.16125
 DELETING TIME-RECORD FOR TIME    174.16125
 DELETING TIME-RECORD FOR TIME    175.16125
 DELETING TIME-RECORD FOR TIME    176.16125
 DELETING TIME-RECORD FOR TIME    177.16125
 DELETING TIME-RECORD FOR TIME    178.16125
 DELETING TIME-RECORD FOR TIME    179.16125
 DELETING TIME-RECORD FOR TIME    180.16125
 DELETING TIME-RECORD FOR TIME    181.16125
 DELETING TIME-RECORD FOR TIME    182.16125
 DELETING TIME-RECORD FOR TIME    183.16125
 DELETING TIME-RECORD FOR TIME    184.16125
 DELETING TIME-RECORD FOR TIME    185.16125
 DELETING TIME-RECORD FOR TIME    186.16125
 DELETING TIME-RECORD FOR TIME    187.16125
 DELETING TIME-RECORD FOR TIME    188.16125
 DELETING TIME-RECORD FOR TIME    189.16125
 DELETING TIME-RECORD FOR TIME    190.16125
 DELETING TIME-RECORD FOR TIME    191.16125
 DELETING TIME-RECORD FOR TIME    192.16125
 DELETING TIME-RECORD FOR TIME    193.16125
 DELETING TIME-RECORD FOR TIME    194.16125
 DELETING TIME-RECORD FOR TIME    195.16125
 DELETING TIME-RECORD FOR TIME    196.16125
 DELETING TIME-RECORD FOR TIME    196.41125
 DELETING TIME-RECORD FOR TIME    196.91125
 DELETING TIME-RECORD FOR TIME    197.91125
 DELETING TIME-RECORD FOR TIME    198.91125

 KEEPING TIME-RECORD FOR TIME    199.91125
 AND FOR TIME                    200.00000
 WORKSPACE RECLAIMED

 TIMESTEP AT     200.000000     SELECTED

DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
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 exb4c\plot.DCM 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 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
ORKING ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

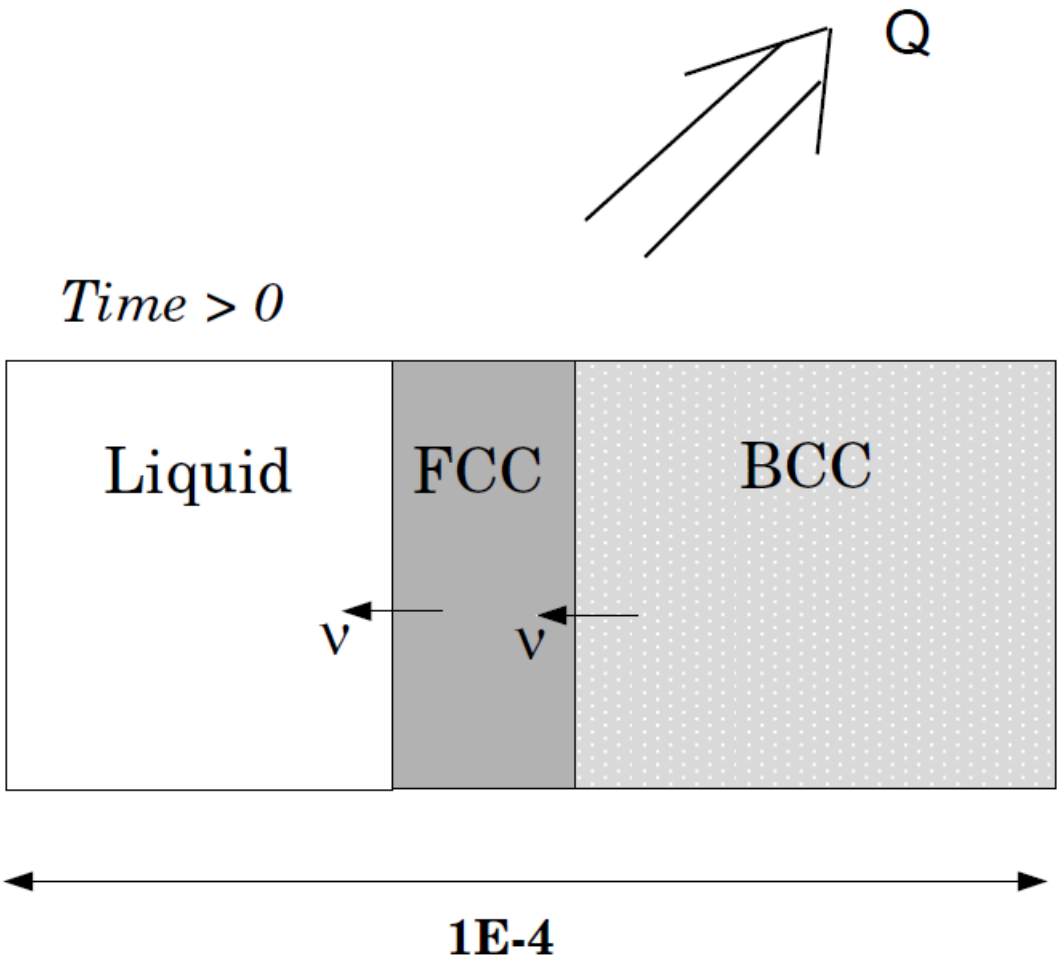



```
POST-1:
POST-1:
POST-1:
POST-1: set-inter
 --OK---
POST-1:
```

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: unknown compiler
 License library version: 9.7.0.0036
 Linked: Fri Oct 18 11:32:56 2024


SYS:SYS:MACRO exb4d\setup.DCM
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: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exb4d_setup.DCM
SYS:
SYS: @@
SYS: @@ START BY GOING TO THE DATABASE MODULE
SYS: @@
SYS: go da
13:34:19,261 [Thread-0] INFO  LicenseManager: Initializing user: jenkins.integrationtest@thermocalc.se
13:34:19,273 [Thread-0] INFO  LicenseController: Running License Spring in DEV environment.
13:34:20,573 [Thread-0] INFO  LicenseManager: There is an activated standalone license for jenkins.integrationtest@thermocalc.se for TC-
Application
 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 v5.0

 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
 BCC_A2                  CBCC_A12                CHI_A12
 CUB_A13                 FCC_A1                  GAS:G
 HCP_A3                  LAVES_PHASE_C14         LIQUID:L
 SIGMA  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
13:34:21,633 [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 v5.0
 MOB2    =  Alloys Mobility  v2.7
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBFE7  =  Steels/Fe-Alloys Mobility  v7.1
 MFEDEMO =  Fe-Alloys Mobility demo database v4.0
 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
13:34:22,263 [Thread-0] INFO  StandaloneLicenseController: Checking out license for: Diffusion (DICTRA)
 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 /LINEAR/: 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> @@
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> s-s-c
NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /AUTO/: yes
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/: no
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -> 1): /AUTO/:
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/: @@
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 exb4d\run.DCM 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

 Region: SMALTA
 geometric   0.866196     dense at   0.100000E-03   89 points
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
 TEMPERATURE:   1900.0000     ENTHALPY:   73940.238
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 TEMPERATURE:   1900.0000     ENTHALPY:   73940.238
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 3.863918610029206E-003        3.864691456615999E-003        3.844149509874589E-012        3.828409457237947E-021       TIME =  0.10000000E-
06 DT =  0.10000000E-06 SUM OF SQUARES =  0.38284095E-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
 3.863369715420627E-003        3.864142409529244E-003        3.862638941968515E-012        3.868991631399091E-021       TIME =  0.39902696E-
05 DT =  0.38902696E-05 SUM OF SQUARES =  0.38689916E-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
 1.545211263951873E-004        1.545520343606063E-004        5.894633261884094E-015        5.894633261884094E-015        1.742256102296206E-
012        1.927921854525490E-026       TIME =  0.11770809E-04 DT =  0.77805392E-05 SUM OF SQUARES =  0.19279219E-25
 TEMPERATURE:   1900.0000     ENTHALPY:   73940.237
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                        NI = .0754116207882254
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 1.544972738489654E-004        1.545281794262292E-004        6.073550732438570E-015        6.073550732438570E-015        1.745310903714427E-
012        9.779385076896095E-026       TIME =  0.27331887E-04 DT =  0.15561078E-04 SUM OF SQUARES =  0.97793851E-25
 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
 1.544495742888185E-004        1.544804750956444E-004        6.066058931563158E-015        6.066058931563158E-015        1.745184034580139E-
012        1.226458563556245E-027       TIME =  0.58454044E-04 DT =  0.31122157E-04 SUM OF SQUARES =  0.12264586E-26
 TEMPERATURE:   1899.9999     ENTHALPY:   73940.233
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882254
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 1.543541972360844E-004        1.543850885000752E-004        6.174007254643545E-015        6.174007254643545E-015        1.747006864638327E-
012        2.536232115065987E-027       TIME =  0.12069836E-03 DT =  0.62244313E-04 SUM OF SQUARES =  0.25362321E-26
 TEMPERATURE:   1899.9998     ENTHALPY:   73940.227
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    1  seconds
 1.541635314850205E-004        1.541944036628519E-004        6.424058632672412E-015        6.424058632672412E-015        1.751173664497199E-
012        6.567707885373491E-027       TIME =  0.24518698E-03 DT =  0.12448863E-03 SUM OF SQUARES =  0.65677079E-26
 TEMPERATURE:   1899.9995     ENTHALPY:   73940.216
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds


output ignored...



... output resumed

 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.47764828E-05
 TEMPERATURE:   1706.9084     ENTHALPY:   56074.266
 U-FRACTION IN SYSTEM:  CR = .191388019855254  FE = .73323061492677
                        NI = .0753813652179764
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  11  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_FCC_A1

  CPU time used in timestep                    2  seconds
 2.130458036905798E-002        2.130451540948964E-002        2.130460957846459E-002        2.130415108071696E-002        8.353426849076627E-
005        2.459206461248073E-008        3.595916556164513E-013        4.362031520114629E-016        2.146715375118808E-
019       TIME =   197.47105     DT =   1.0007812     SUM OF SQUARES =  0.15188542E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.72964603E-07 AND   0.72964603E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.48495044E-05
 TEMPERATURE:   1704.7324     ENTHALPY:   55983.005
 U-FRACTION IN SYSTEM:  CR = .19138801985558  FE = .733230614927052
                        NI = .0753813652173677
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  8  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_FCC_A1

  CPU time used in timestep                    1  seconds
 9.357932626071368E-002        9.357897868205686E-002        9.357940509128312E-002        9.357842606617575E-002        6.849361962962038E-
004        1.339537295123986E-006        1.349225278427375E-009        4.690734499869817E-014        8.357276456085232E-
```

```
017       TIME =   199.47261     DT =   2.0015625     SUM OF SQUARES =  0.45657814E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.93944999E-07 AND   0.93944999E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.50375412E-05
 TEMPERATURE:   1700.3967      ENTHALPY:   55800.483
 U-FRACTION IN SYSTEM:  CR = .19138801985286  FE = .733230614928366
                        NI = .0753813652187737
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  67  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_FCC_A1

  CPU time used in timestep                      1  seconds
 4.855056974966846E-003        4.855030126256783E-003        4.855065973426648E-003        4.854851374321911E-003        1.015066445619968E-
007        1.883684902605120E-011        1.326228119110918E-
017       TIME =   200.00000     DT =  0.52738619     SUM OF SQUARES =  0.76517871E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.83133043E-07 AND   0.83133043E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.50813844E-05
 TEMPERATURE:   1699.2506      ENTHALPY:   55752.390
 U-FRACTION IN SYSTEM:  CR = .191388019853196  FE = .73323061492652
                        NI = .0753813652202836
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 MUST SAVE WORKSPACE ON FILE
 WORKSPACE SAVED ON FILE
 RECLAIMING WORKSPACE
 DELETING TIME-RECORD FOR TIME    194.90655
 DELETING TIME-RECORD FOR TIME    195.53204
 DELETING TIME-RECORD FOR TIME    195.59459
 DELETING TIME-RECORD FOR TIME    195.71968
 DELETING TIME-RECORD FOR TIME    195.96988
 DELETING TIME-RECORD FOR TIME    196.47027
 DELETING TIME-RECORD FOR TIME    197.47105

 KEEPING TIME-RECORD FOR TIME    199.47261
 AND FOR TIME                    200.00000
 WORKSPACE RECLAIMED

 TIMESTEP AT     200.000000     SELECTED

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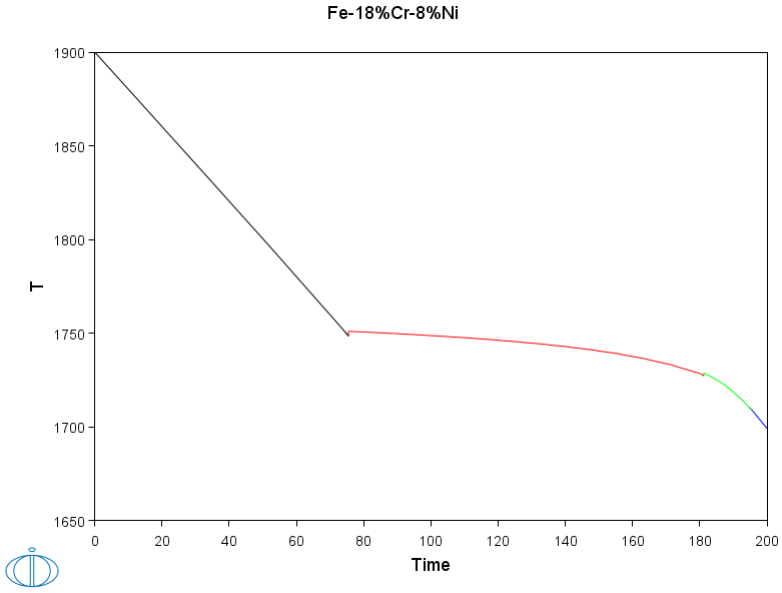
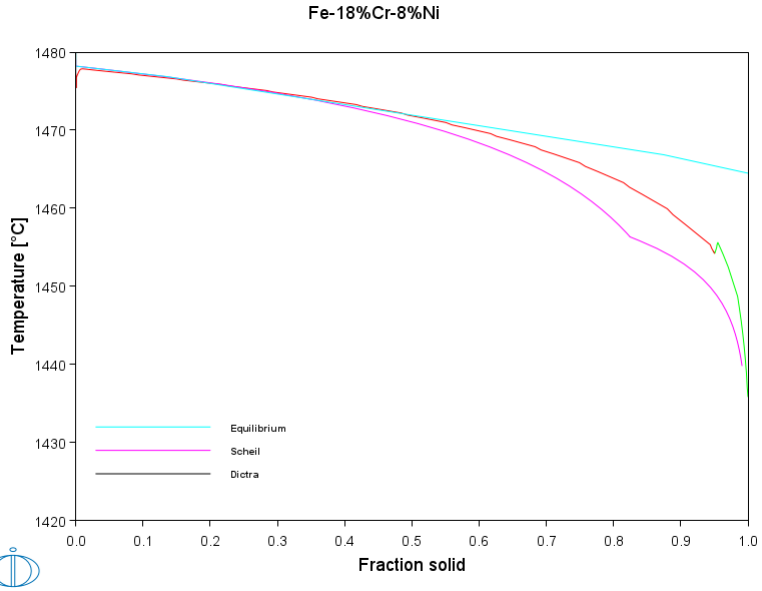

exb4d-plot

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exb4d\plot.DCM DIC>
DIC>
DIC> @@ exb4d_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE b4b
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 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
ORKING ...orking ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```




```
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
ORKING ...orking ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

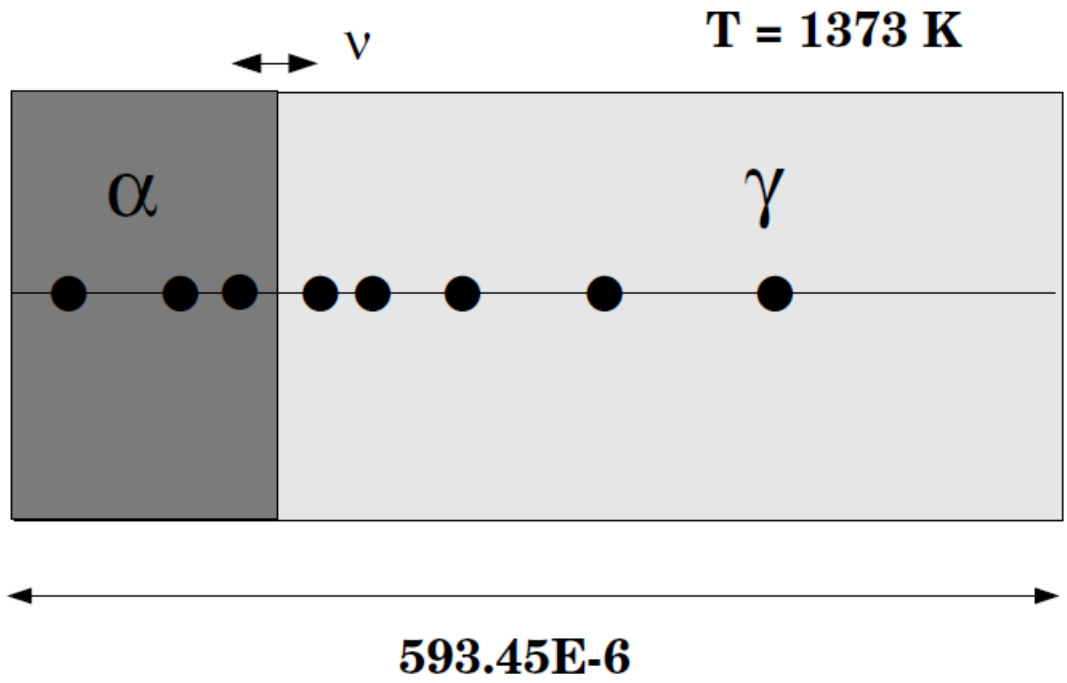



```
POST-1:
POST-1:
POST-1:
POST-1: set-inter
 --OK---
POST-1:
```

Example exb5

γ/α/γ diffusion couple of Fe-Ni-Cr alloys

This example demonstrates the evaluation of a ternary Fe-Cr-Ni diffusion couple. A thin slice of α phase (38%Cr, 0%Ni) is clamped between two thicker slices of γ 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. Kikichi: 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: unknown compiler
 License library version: 9.7.0.0036
 Linked: Fri Oct 18 11:32:56 2024


SYS:SYS:MACRO exb5\setup.DCM 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. Kikichi: Acta Metall.Mater.

SYS: @@ 41 (1993), pp.2045-2059.
SYS: ----------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exb5_setup.DCM
SYS:
SYS: @@
SYS: @@ GO TO A DATABASE AND READ THE THERMODYNAMIC AND KINETIC DATA
SYS: @@
SYS: go da
13:41:02,829 [Thread-0] INFO  LicenseManager: Initializing user: jenkins.integrationtest@thermocalc.se
13:41:02,842 [Thread-0] INFO  LicenseController: Running License Spring in DEV environment.
13:41:03,964 [Thread-0] INFO  LicenseManager: There is an activated standalone license for jenkins.integrationtest@thermocalc.se for TC-
Application
 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 v5.0

 VA                       /-  DEFINED
TDB_FEDEMO: def-sys cr fe ni
 CR                       FE                       NI
   DEFINED
TDB_FEDEMO: rej-ph /all
 BCC_A2                   CBCC_A12                 CHI_A12
 CUB_A13                  FCC_A1                   GAS:G
 HCP_A3                   LAVES_PHASE_C14          LIQUID:L
 SIGMA  REJECTED
TDB_FEDEMO: res-ph bcc,fcc
 BCC_A2                   FCC_A1  RESTORED
TDB_FEDEMO: get
13:41:05,034 [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 v5.0
 MOB2    =  Alloys Mobility  v2.7
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBFE7  =  Steels/Fe-Alloys Mobility  v7.1
 MFEDEMO =  Fe-Alloys Mobility demo database v4.0
 USER    =  User defined Database

DATABASE NAME /FEDEMO/: mfedemo
 Current database: Fe-Alloys Mobility demo database v4.0

 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
13:41:05,635 [Thread-0] INFO  StandaloneLicenseController: Checking out license for: Diffusion (DICTRA)
 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>
```

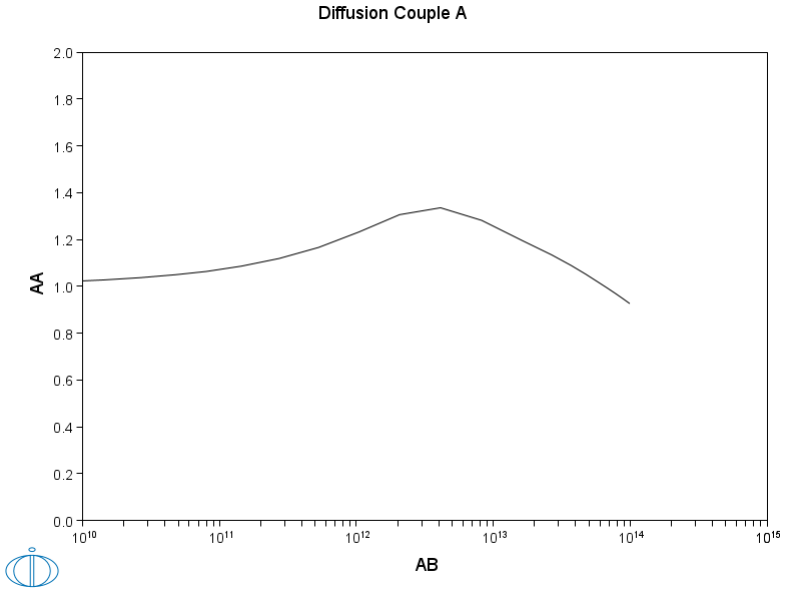
exb5-run

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exb5\run.DCM 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  0.00000E+00
DIC> read exb5
 OK
DIC>
DIC> @@
DIC> @@ START THE SIMULATION
DIC> @@
DIC> simulate
 Region: ALPHA
 geometric   0.787882     dense at   0.934500E-04   96 points
 Region: GAMMA

 geometric    1.29714     dense at    0.00000       96 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
 *** ERROR  1611 IN QTHISS: TOO MANY ITERATIONS
 Give the command INFO TROUBLE for help
 *** 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                     2  failed
  try                   3  failed
 DETERMINED ACTIVITIES  ACR(CR) .002753312066 73
  UNABLE TO OBTAIN GOOD STARTING VALUE USING THE OLD SCHEME
USE NEW SCHEME /YES/:
  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 = .223047485172707
 TOTAL SIZE OF SYSTEM:  5.9345E-04 [m]
 U-FRACTION IN SYSTEM:  CR = .305280432605602  FE = .471672082221692
                        NI = .223047485172707
 TOTAL SIZE OF SYSTEM:  5.9345E-04 [m]
 4.488884160223573E-002        4.489776407263253E-002        4.488891917919257E-002        1.471050192950912E-006        1.464677834307632E-
006        1.243977133126083E-006        1.170195125865789E-006        1.169001090850043E-006        1.083386197007612E-
006        9.864742289915659E-007        8.052169527572799E-007        8.052423220412046E-007        4.986100731405504E-
007        1.057999935685297E-007        1.652274749409299E-012        1.782496945994161E-015        1.182857587009230E-
019       TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =  0.84860606E-19
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.48679045E-02 AND  -0.48679045E-02
 POSITION OF INTERFACE ALPHA / GAMMA IS   0.93449513E-04
 U-FRACTION IN SYSTEM:  CR = .305280432608531  FE = .471672082224247
                        NI = .223047485167223
 TOTAL SIZE OF SYSTEM:  5.9345E-04 [m]
  4  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: ALPHA
  7  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: GAMMA

  CPU time used in timestep                  2  seconds
 1.221735332554993E-004        1.221979858387549E-004        1.221738014890116E-004        2.506137660420502E-009        2.642826838933915E-
009        2.592777103781170E-009        2.744557993368463E-009        2.501610069763879E-009        2.487606484145803E-
009        2.473994138346345E-009        2.466074004269576E-009        2.461667319106754E-009        2.432579464786101E-
009        2.377952074471541E-009        2.270799215119537E-009        2.272804240977707E-009        2.064511250792881E-
009        1.684673403283288E-009        1.054908849181801E-009        1.060485960619613E-009        2.520474454714755E-
010        4.111299423752579E-012

output ignored...



... output resumed

                       NI = .223047486070157
 TOTAL SIZE OF SYSTEM:  5.9345E-04 [m]
  6  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: GAMMA

  CPU time used in timestep                  1  seconds
 4.569323491456198E-007        4.580952500205198E-007        4.546624601431393E-007        2.468122161489763E-009        8.454658411949928E-
006        1.119820853062559E-007        2.537710393776061E-008        6.843991441769256E-009        2.460616074302035E-
009        2.315780378716773E-009        2.102444568563490E-009        2.110147047992171E-009        1.789053202091259E-
009        1.171415782728415E-009        8.454399206600982E-006        7.494170187562310E-006        3.276788793681825E-
009        1.682466448224741E-009        1.279470231844726E-009        1.171546040007228E-009        1.202735641658811E-
009        1.177691695956214E-009        1.171119199067579E-009        1.163448170584850E-009        1.164031690959471E-
009        1.158126542479074E-009        1.146319738099367E-009        1.123031316316353E-009        1.128379153490799E-
009        1.088191523632150E-009        9.896260383493083E-010        8.297109973060340E-010        8.224513635991282E-
010        5.338335562052021E-010        1.464007865482157E-010        1.227920148238415E-012        3.160213171796849E-
021       TIME =   3093553.9     DT =   360000.00     SUM OF SQUARES =  0.24673120E-21
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.56677189E-11 AND  -0.56677189E-11
 POSITION OF INTERFACE ALPHA / GAMMA IS   0.88531853E-04
 U-FRACTION IN SYSTEM:  CR = .305280433847308  FE = .471672080074342
                        NI = .22304748607835
 TOTAL SIZE OF SYSTEM:  5.9345E-04 [m]
  5  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: GAMMA

  CPU time used in timestep                  4  seconds
 3.147840586150086E-007        3.156726038865369E-007        3.129253452827497E-007        2.089865868762208E-009        4.625962631295723E-
010        1.608998746556003E-013        4.259008830667696E-
019       TIME =   3453553.9     DT =   360000.00     SUM OF SQUARES =  0.24726341E-21
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.52006922E-11 AND  -0.52006922E-11
 POSITION OF INTERFACE ALPHA / GAMMA IS   0.86659604E-04
 U-FRACTION IN SYSTEM:  CR = .305280433861286  FE = .471672080046809
                        NI = .223047486091905
```

```
 TOTAL SIZE OF SYSTEM:  5.9345E-04 [m]
  4  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: GAMMA

  CPU time used in timestep                    1  seconds
 5.962264523568051E-007        5.961610382142017E-007        5.968778615376425E-007        6.683872292146301E-009        1.633351510636594E-
013        7.734104188364651E-021       TIME =   3600000.0     DT =   146446.07     SUM OF SQUARES =  0.33972481E-20
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.46233102E-11 AND  -0.46233102E-11
 POSITION OF INTERFACE ALPHA / GAMMA IS   0.85982539E-04
 U-FRACTION IN SYSTEM:  CR = .305280433868743  FE = .471672080031609
                        NI = .223047486099649
 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   0.35977533E-04
 DELETING TIME-RECORD FOR TIME   0.10773260E-03
 DELETING TIME-RECORD FOR TIME   0.25124273E-03
 DELETING TIME-RECORD FOR TIME   0.53826299E-03
 DELETING TIME-RECORD FOR TIME   0.11123035E-02
 DELETING TIME-RECORD FOR TIME   0.22603846E-02
 DELETING TIME-RECORD FOR TIME   0.45565466E-02
 DELETING TIME-RECORD FOR TIME   0.72719533E-02
 DELETING TIME-RECORD FOR TIME   0.12702767E-01
 DELETING TIME-RECORD FOR TIME   0.21279333E-01
 DELETING TIME-RECORD FOR TIME   0.27251790E-01
 DELETING TIME-RECORD FOR TIME   0.31615384E-01
 DELETING TIME-RECORD FOR TIME   0.40342574E-01
 DELETING TIME-RECORD FOR TIME   0.57796952E-01
 DELETING TIME-RECORD FOR TIME   0.92705708E-01
 DELETING TIME-RECORD FOR TIME   0.16252322
 DELETING TIME-RECORD FOR TIME   0.30215825
 DELETING TIME-RECORD FOR TIME   0.51935812
 DELETING TIME-RECORD FOR TIME   0.88820140
 DELETING TIME-RECORD FOR TIME    1.6258880
 DELETING TIME-RECORD FOR TIME    3.1012611
 DELETING TIME-RECORD FOR TIME    4.6067718
 DELETING TIME-RECORD FOR TIME    7.6177933
 DELETING TIME-RECORD FOR TIME    13.639836
 DELETING TIME-RECORD FOR TIME    17.807173
 DELETING TIME-RECORD FOR TIME    26.141846
 DELETING TIME-RECORD FOR TIME    36.344698
 DELETING TIME-RECORD FOR TIME    52.233308
 DELETING TIME-RECORD FOR TIME    84.010526
 DELETING TIME-RECORD FOR TIME    147.56496
 DELETING TIME-RECORD FOR TIME    271.40526
 DELETING TIME-RECORD FOR TIME    503.69187
 DELETING TIME-RECORD FOR TIME    922.75233
 DELETING TIME-RECORD FOR TIME    1673.3008
 DELETING TIME-RECORD FOR TIME    2792.4410
 DELETING TIME-RECORD FOR TIME    5030.7213
 DELETING TIME-RECORD FOR TIME    9507.2820
 DELETING TIME-RECORD FOR TIME    18460.403
 DELETING TIME-RECORD FOR TIME    36366.646
 DELETING TIME-RECORD FOR TIME    72179.132
 DELETING TIME-RECORD FOR TIME    143804.10
 DELETING TIME-RECORD FOR TIME    287054.04
 DELETING TIME-RECORD FOR TIME    573553.93
 DELETING TIME-RECORD FOR TIME    933553.93
 DELETING TIME-RECORD FOR TIME    1293553.9
 DELETING TIME-RECORD FOR TIME    1653553.9
 DELETING TIME-RECORD FOR TIME    2013553.9
 DELETING TIME-RECORD FOR TIME    2373553.9
 DELETING TIME-RECORD FOR TIME    2733553.9
 DELETING TIME-RECORD FOR TIME    3093553.9

 KEEPING TIME-RECORD FOR TIME    3453553.9
 AND FOR TIME                    3600000.0
 WORKSPACE RECLAIMED

 TIMESTEP AT     3600000.00     SELECTED

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

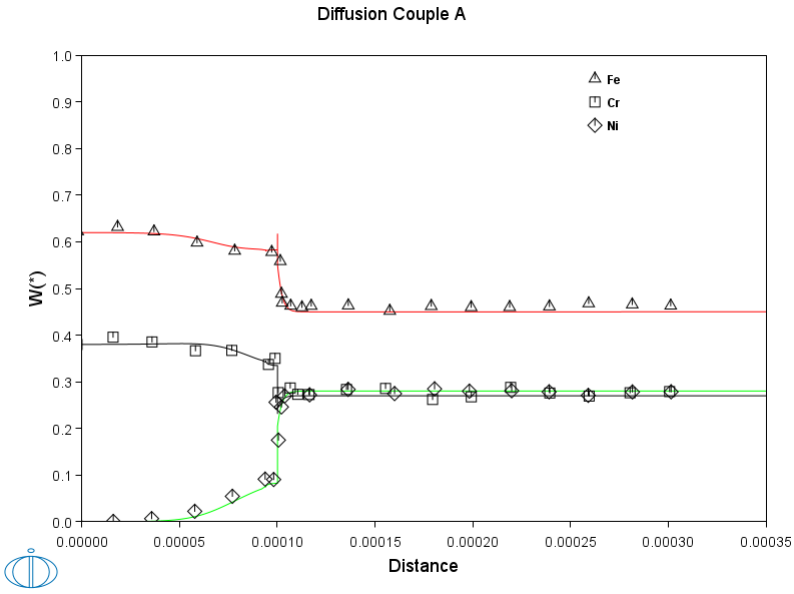
exb5-plot

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exb5\plot.DCM 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: @@ l0 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)/l0;
POST-1: enter func ab=time/l0**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
```

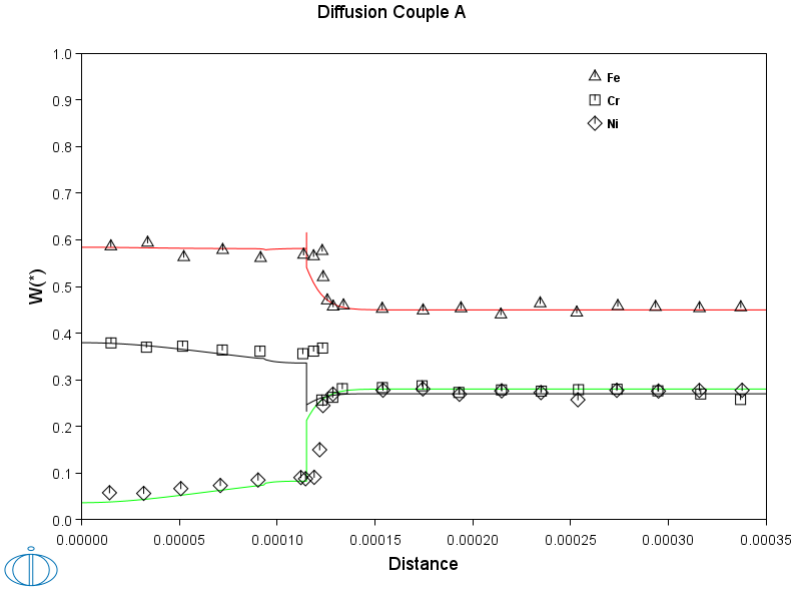



```
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ PLOT THE CONCENTRATION PROFILES FOR DIFFERENT ANNEALING TIMES
POST-1: @@
POST-1: s-d-a x dist glo
  INFO: Distance is set as independent variable
POST-1: s-ax-ty x lin
POST-1: s-s-s x n 0 350e-6
POST-1:
POST-1: s-d-a y w(*)
POST-1: s-s-s y n 0 1
POST-1:
POST-1: s-p-c time 3600
POST-1:
```

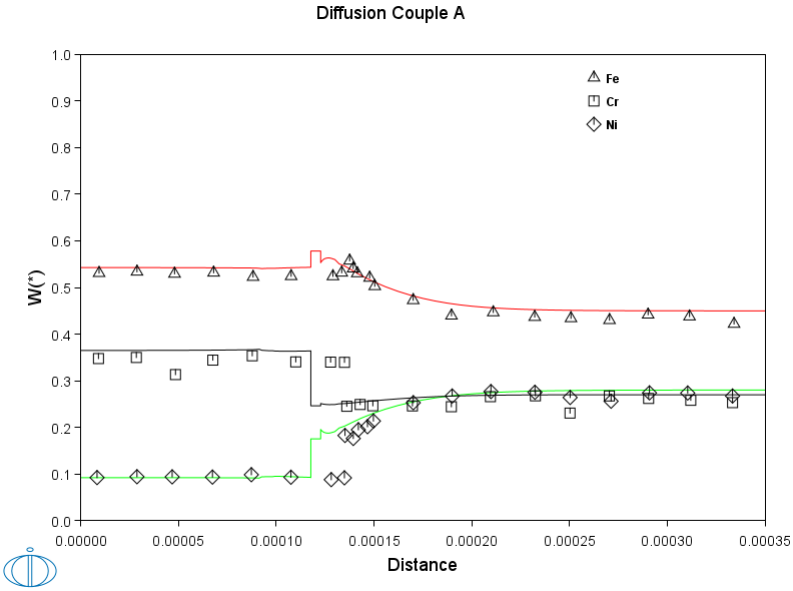
```
POST-1: app y exb5.exp 0; 1
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```



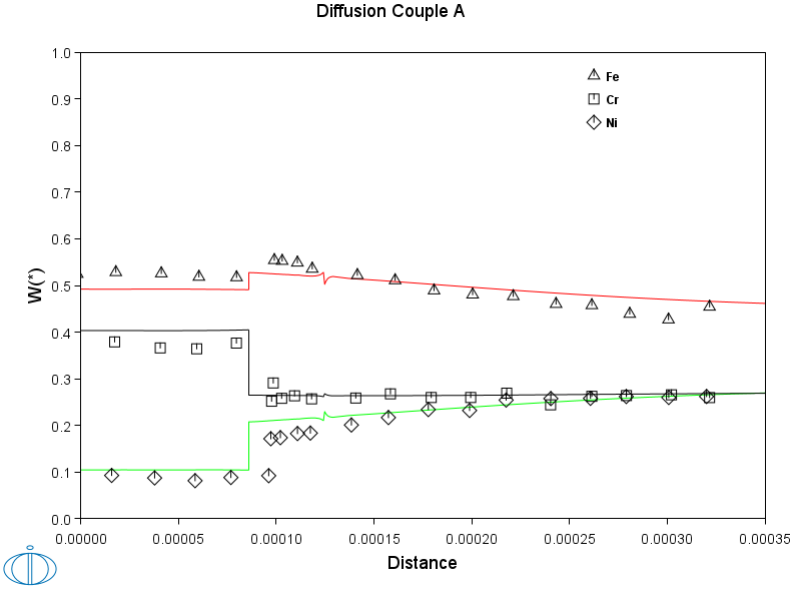

```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: s-p-c time 36000
POST-1: app y exb5.exp 0; 2
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```



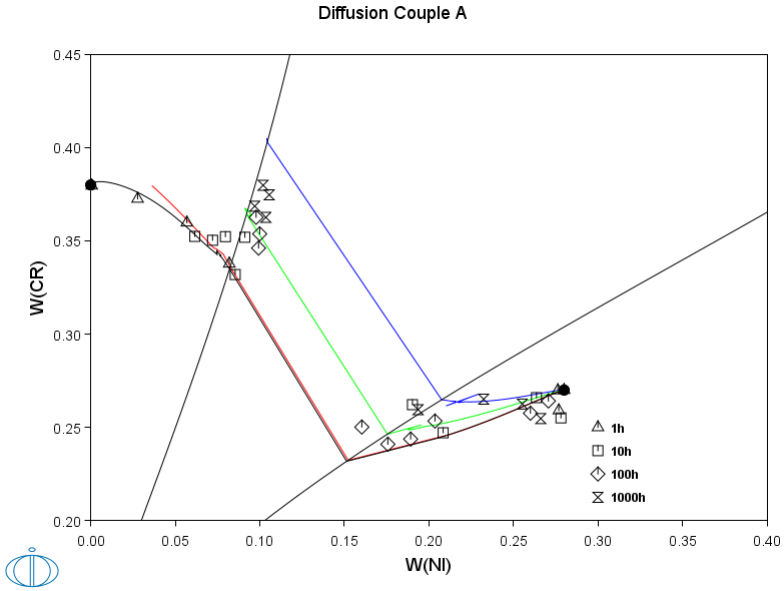

```
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: s-p-c time 360000
POST-1: app y exb5.exp 0; 3
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```




```
POST-1:
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
```




```
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
```

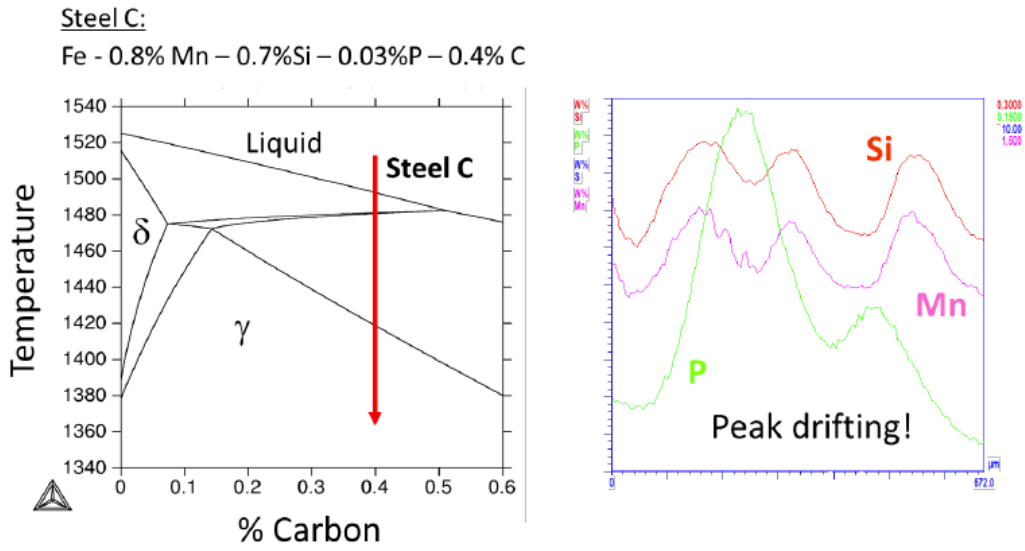


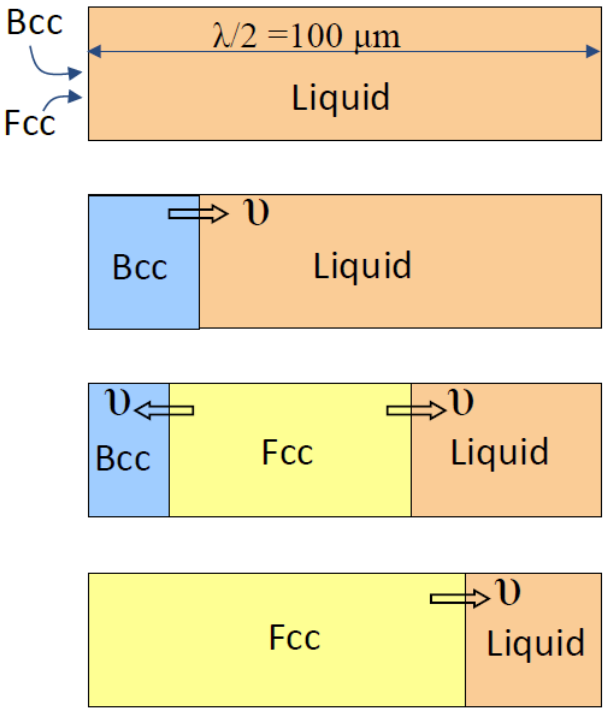

```
POST-1:
POST-1:
POST-1:
POST-1: set-inter
 --OK---
POST-1:
```

Example exb6

Micro-segregation of phosphorus

This example illustrates the effect of microsegregation of phosphorus during peritectic solidification in steel.





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: unknown compiler
 License library version: 9.7.0.0036
 Linked: Fri Oct 18 11:32:56 2024


SYS:SYS:MACRO exb6\setup.DCM
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: ----------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@
SYS: @@ START BY GOING TO THE DATABASE MODULE
SYS: @@
SYS: go da
13:45:11,804 [Thread-0] INFO  LicenseManager: Initializing user: jenkins.integrationtest@thermocalc.se
13:45:11,818 [Thread-0] INFO  LicenseController: Running License Spring in DEV environment.
13:45:13,037 [Thread-0] INFO  LicenseManager: There is an activated standalone license for jenkins.integrationtest@thermocalc.se for TC-
Application
 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
13:45:14,521 [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 v5.0
 MOB2    =  Alloys Mobility  v2.7
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBFE7  =  Steels/Fe-Alloys Mobility  v7.1
 MFEDEMO =  Fe-Alloys Mobility demo database v4.0
 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
13:45:16,782 [Thread-0] INFO  StandaloneLicenseController: Checking out license for: Diffusion (DICTRA)
 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 /1/: 1e-4
TYPE /LINEAR/: 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> @@
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> s-s-c
NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /AUTO/: yes
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -> 1): /AUTO/:
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/:
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exb6 Y
DIC>
DIC> set-inter
 --OK---
DIC>
```

exb6-run

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exb6\run.DCM 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
 Region: SMALTA
 geometric     1.15279      dense at     0.00000        88 points
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
 U-FRACTION IN SYSTEM:  C = .0185375871047351  FE = .977481861209079
                        MN = .00810568126669964  P = 5.39133528237326E-04
                                    SI = .0138733239959839
                                TOTAL SIZE OF SYSTEM:  1E-04 [m]
                    U-FRACTION IN SYSTEM:  C = .0185375871047351  FE = .977481861209079
                        MN = .00810568126669964  P = 5.39133528237326E-04
                                    SI = .0138733239959839
                                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 = .977481861209079
                    MN = .00810568126669965  P = 5.39133528237326E-04
 SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    1  seconds
 TIME =  0.79252098E-06 DT =  0.69252098E-06 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .018537587104735  FE = .977481861209079
                    MN = .00810568126669965  P = 5.39133528237326E-04
 SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    1  seconds
 TIME =  0.21775630E-05 DT =  0.13850420E-05 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .018537587104735  FE = .977481861209079
                    MN = .00810568126669964  P = 5.39133528237326E-04
 SI = .0138733239959839
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.49476469E-05 DT =  0.27700839E-05 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .018537587104735  FE = .977481861209079
                    MN = .00810568126669965  P = 5.39133528237326E-04
 SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    1  seconds
 TIME =  0.10487815E-04 DT =  0.55401679E-05 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .018537587104735  FE = .977481861209079
                    MN = .00810568126669964  P = 5.39133528237327E-04
 SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.21568150E-04 DT =  0.11080336E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .018537587104735  FE = .977481861209079
                    MN = .00810568126669964  P = 5.39133528237327E-04
 SI = .0138733239959839
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.43728822E-04 DT =  0.22160671E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .018537587104735  FE = .977481861209079
                    MN = .00810568126669964  P = 5.39133528237326E-04
 SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    1  seconds
 TIME =  0.88050165E-04 DT =  0.44321343E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .018537587104735  FE = .977481861209079
                    MN = .00810568126669964  P = 5.39133528237327E-04
 SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.17669285E-03 DT =  0.88642686E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .018537587104735  FE = .977481861209079
                    MN = .00810568126669964  P = 5.39133528237327E-04
 SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.35397822E-03 DT =  0.17728537E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .018537587104735  FE = .977481861209079
                    MN = .00810568126669964  P = 5.39133528237326E-04
 SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    1  seconds
 TIME =  0.70854897E-03 DT =  0.35457074E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .018537587104735  FE = .977481861209079
                    MN = .00810568126669964  P = 5.39133528237326E-04
 SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.14176905E-02 DT =  0.70914149E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .018537587104735  FE = .977481861209079
                    MN = .00810568126669964  P = 5.39133528237326E-04
 SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.28359734E-02 DT =  0.14182830E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .018537587104735  FE = .977481861209079
                    MN = .00810568126669964  P = 5.39133528237326E-04
 SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.56725394E-02 DT =  0.28365659E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .018537587104735  FE = .977481861209079
                    MN = .00810568126669964  P = 5.39133528237326E-04
 SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.11345671E-01 DT =  0.56731319E-02 SUM OF SQUARES =   0.0000000
```

```
 U-FRACTION IN SYSTEM:  C = .018537587104735  FE = .977481861209079
                        MN = .00810568126669964  P = 5.39133528237326E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.22691935E-01 DT =  0.11346264E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .018537587104735  FE = .977481861209079
                        MN = .00810568126669965  P = 5.39133528237326E-04
                        SI = .0138733239959839
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.45384463E-01 DT =  0.22692528E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .018537587104735  FE = .977481861209079
                        MN = .00810568126669965  P = 5.39133528237324E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0  seconds
 TIME =  0.90769518E-01 DT =  0.45385055E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .018537587104735  FE = .977481861209079
                        MN = .00810568126669962  P = 5.39133528237323E-04
                        SI = .0138733239959838


output ignored...



... output resumed

 DELETING TIME-RECORD FOR TIME    920.11031
 DELETING TIME-RECORD FOR TIME    935.11031
 DELETING TIME-RECORD FOR TIME    950.11031
 DELETING TIME-RECORD FOR TIME    965.11031
 DELETING TIME-RECORD FOR TIME    980.11031
 DELETING TIME-RECORD FOR TIME    995.11031
 DELETING TIME-RECORD FOR TIME    1010.1103
 DELETING TIME-RECORD FOR TIME    1025.1103
 DELETING TIME-RECORD FOR TIME    1040.1103
 DELETING TIME-RECORD FOR TIME    1055.1103
 DELETING TIME-RECORD FOR TIME    1070.1103
 DELETING TIME-RECORD FOR TIME    1085.1103
 DELETING TIME-RECORD FOR TIME    1100.1103
 DELETING TIME-RECORD FOR TIME    1115.1103
 DELETING TIME-RECORD FOR TIME    1130.1103
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 DELETING TIME-RECORD FOR TIME    1175.1103
 DELETING TIME-RECORD FOR TIME    1190.1103
 DELETING TIME-RECORD FOR TIME    1205.1103
 DELETING TIME-RECORD FOR TIME    1220.1103
 DELETING TIME-RECORD FOR TIME    1235.1103
 DELETING TIME-RECORD FOR TIME    1250.1103
 DELETING TIME-RECORD FOR TIME    1265.1103
 DELETING TIME-RECORD FOR TIME    1280.1103
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 DELETING TIME-RECORD FOR TIME    1505.1103
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 DELETING TIME-RECORD FOR TIME    1880.1103
 DELETING TIME-RECORD FOR TIME    1895.1103
 DELETING TIME-RECORD FOR TIME    1910.1103
 DELETING TIME-RECORD FOR TIME    1925.1103
 DELETING TIME-RECORD FOR TIME    1940.1103
 DELETING TIME-RECORD FOR TIME    1955.1103
 DELETING TIME-RECORD FOR TIME    1970.1103
 DELETING TIME-RECORD FOR TIME    1985.1103
 DELETING TIME-RECORD FOR TIME    2000.1103
 DELETING TIME-RECORD FOR TIME    2015.1103
 DELETING TIME-RECORD FOR TIME    2030.1103
 DELETING TIME-RECORD FOR TIME    2045.1103
 DELETING TIME-RECORD FOR TIME    2060.1103
 DELETING TIME-RECORD FOR TIME    2075.1103
 DELETING TIME-RECORD FOR TIME    2090.1103
 DELETING TIME-RECORD FOR TIME    2105.1103
 DELETING TIME-RECORD FOR TIME    2120.1103
 DELETING TIME-RECORD FOR TIME    2135.1103
 DELETING TIME-RECORD FOR TIME    2150.1103
 DELETING TIME-RECORD FOR TIME    2165.1103
 DELETING TIME-RECORD FOR TIME    2180.1103
 DELETING TIME-RECORD FOR TIME    2195.1103
 DELETING TIME-RECORD FOR TIME    2210.1103
```

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 DELETING TIME-RECORD FOR TIME    2225.1103
 DELETING TIME-RECORD FOR TIME    2240.1103
 DELETING TIME-RECORD FOR TIME    2255.1103
 DELETING TIME-RECORD FOR TIME    2270.1103
 DELETING TIME-RECORD FOR TIME    2285.1103
 DELETING TIME-RECORD FOR TIME    2300.1103
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 DELETING TIME-RECORD FOR TIME    2495.1103
 DELETING TIME-RECORD FOR TIME    2510.1103
 DELETING TIME-RECORD FOR TIME    2525.1103
 DELETING TIME-RECORD FOR TIME    2540.1103
 DELETING TIME-RECORD FOR TIME    2555.1103
 DELETING TIME-RECORD FOR TIME    2570.1103
 DELETING TIME-RECORD FOR TIME    2585.1103
 DELETING TIME-RECORD FOR TIME    2600.1103
 DELETING TIME-RECORD FOR TIME    2615.1103
 DELETING TIME-RECORD FOR TIME    2630.1103
 DELETING TIME-RECORD FOR TIME    2645.1103
 DELETING TIME-RECORD FOR TIME    2660.1103
 DELETING TIME-RECORD FOR TIME    2675.1103
 DELETING TIME-RECORD FOR TIME    2690.1103
 DELETING TIME-RECORD FOR TIME    2705.1103
 DELETING TIME-RECORD FOR TIME    2720.1103
 DELETING TIME-RECORD FOR TIME    2735.1103
 DELETING TIME-RECORD FOR TIME    2750.1103
 DELETING TIME-RECORD FOR TIME    2765.1103
 DELETING TIME-RECORD FOR TIME    2780.1103
 DELETING TIME-RECORD FOR TIME    2795.1103
 DELETING TIME-RECORD FOR TIME    2810.1103
 DELETING TIME-RECORD FOR TIME    2825.1103
 DELETING TIME-RECORD FOR TIME    2840.1103
 DELETING TIME-RECORD FOR TIME    2855.1103
 DELETING TIME-RECORD FOR TIME    2870.1103
 DELETING TIME-RECORD FOR TIME    2885.1103
 DELETING TIME-RECORD FOR TIME    2900.1103
 DELETING TIME-RECORD FOR TIME    2915.1103
 DELETING TIME-RECORD FOR TIME    2930.1103
 DELETING TIME-RECORD FOR TIME    2945.1103
 DELETING TIME-RECORD FOR TIME    2960.1103
 DELETING TIME-RECORD FOR TIME    2975.1103

 KEEPING TIME-RECORD FOR TIME    2990.1103
 AND FOR TIME                    3000.0000
 WORKSPACE RECLAIMED

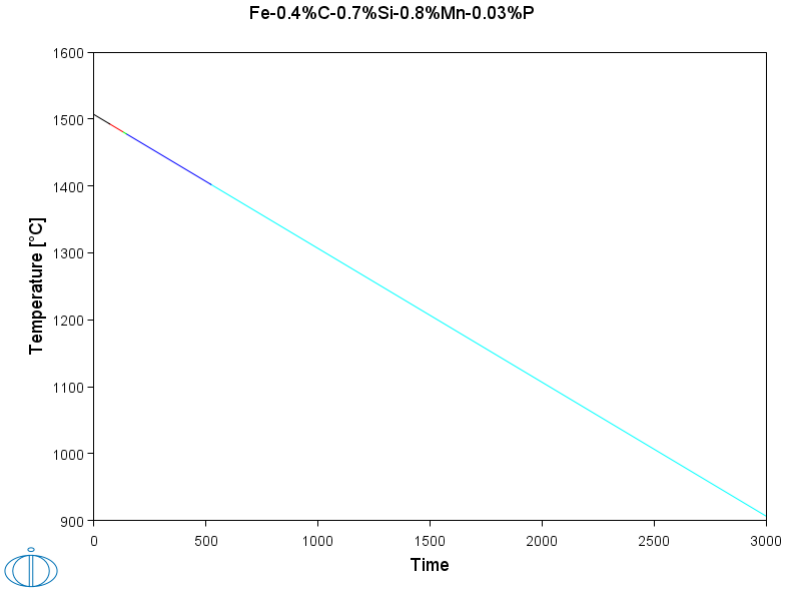
 TIMESTEP AT     3000.00000     SELECTED

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

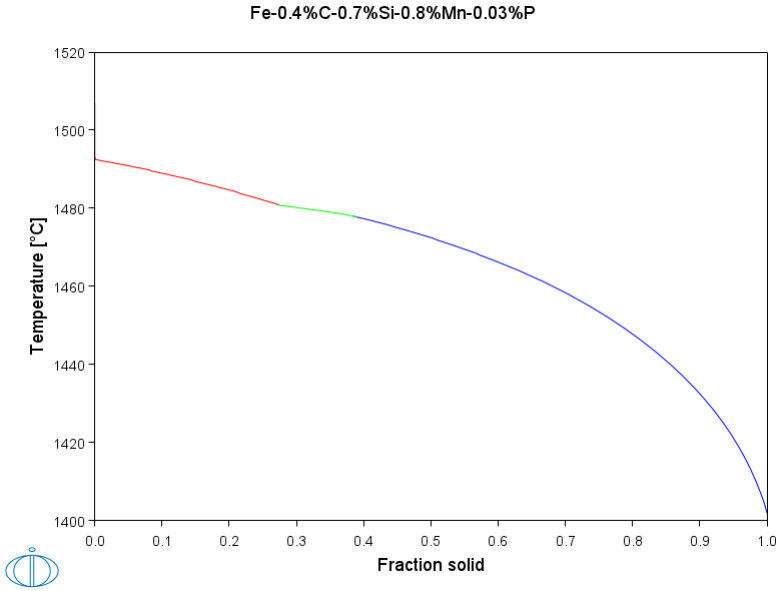
exb6-plot

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exb6\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  3.00000E+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

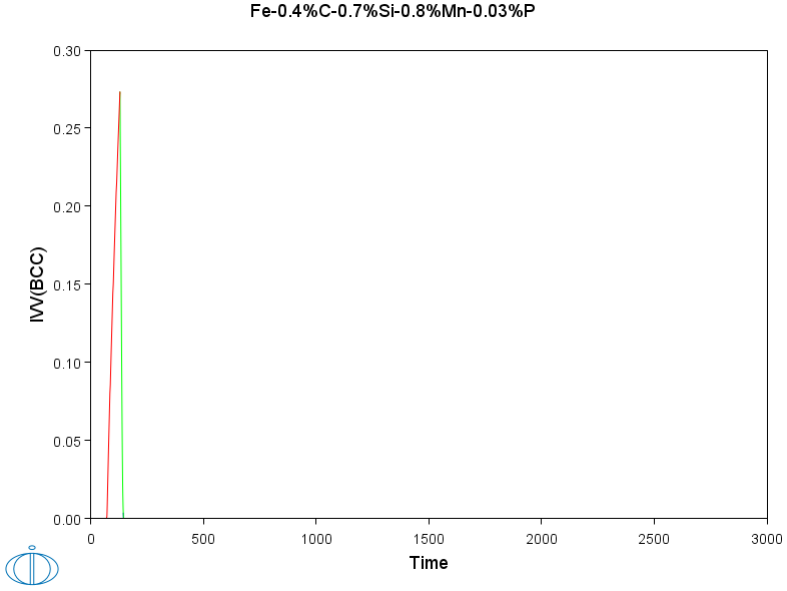
  INFO: Time is set as independent variable
POST-1: s-p-c interf first
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples/unite/distribution\macroResult.exp Y
ORKING ...orking ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```



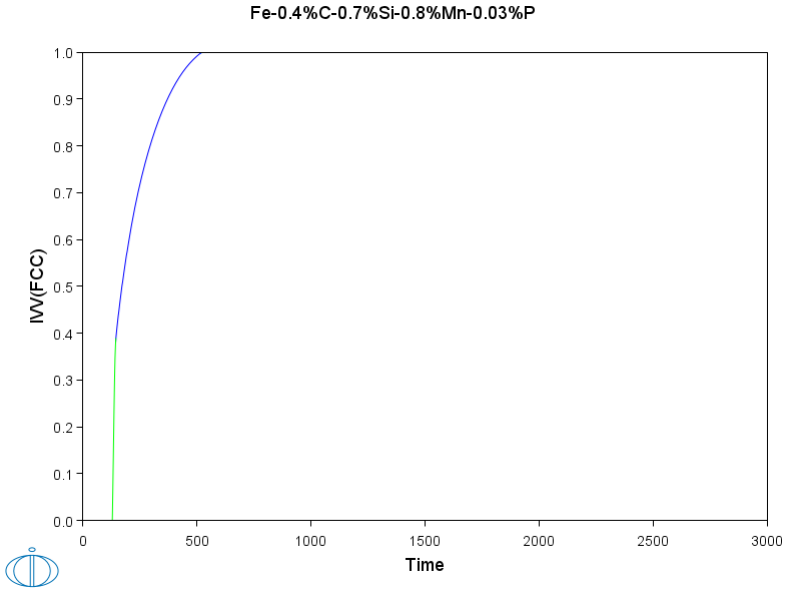

```
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ PLOT THE FRACTION OF SOLID
POST-1: @@
POST-1: enter func fs=1-ivv(liq);
POST-1: s-d-a x fs
POST-1: s-s-s x n 0 1
POST-1: s-ax-te x n Fraction solid
POST-1:
POST-1: s-d-a y t-c
POST-1:
POST-1:
POST-1: s-p-c interf smalta lower
POST-1:
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
ORKING ...orking ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```



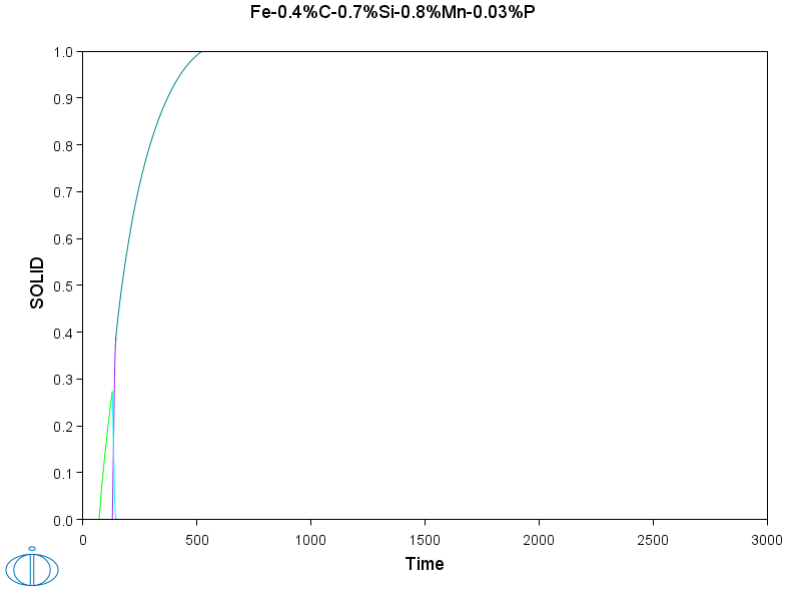

```
POST-1:
POST-1:Hit RETURN to continue
POST-1: s-d-a y ivv(bcc)
POST-1: s-d-a x time
  INFO: Time is set as independent variable
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples/unite/distribution\macroResult.exp Y
ORKING ...orking ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```



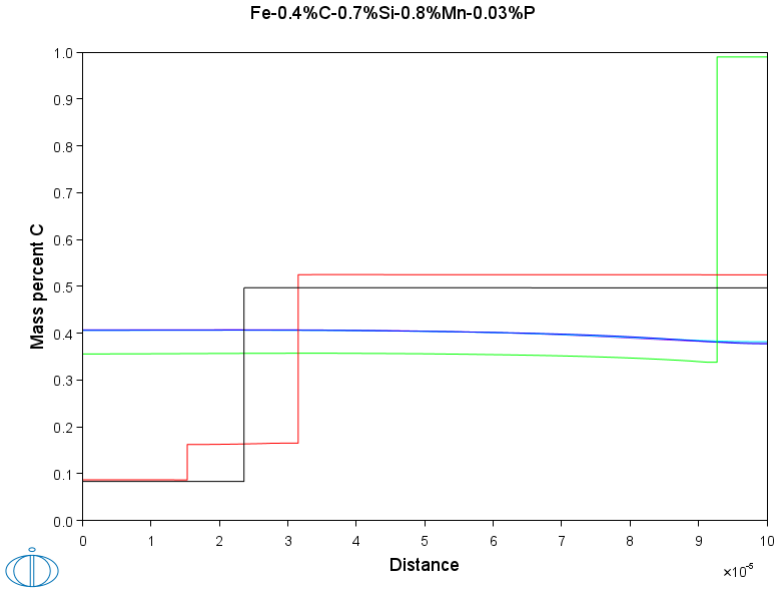

```
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: s-d-a y ivv(fcc)
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples/unite/distribution\macroResult.exp Y
ORKING ...orking ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```



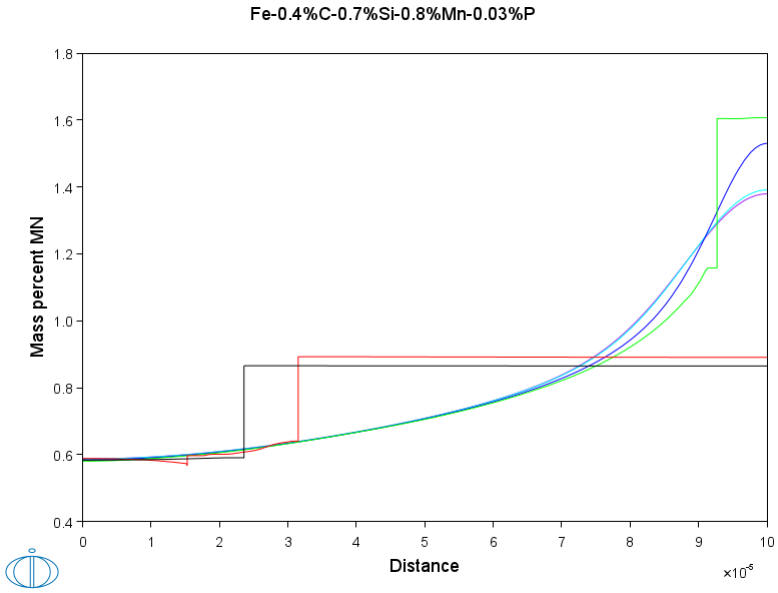

```
POST-1:
POST-1:Hit RETURN to continue
POST-1: ent table solid
Variable(s) ivv(bcc) ivv(fcc)
POST-1:
POST-1: s-d-a y solid
COLUMN NUMBER /*/:
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples/unite/distribution\macroResult.exp Y
ORKING ...orking ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```



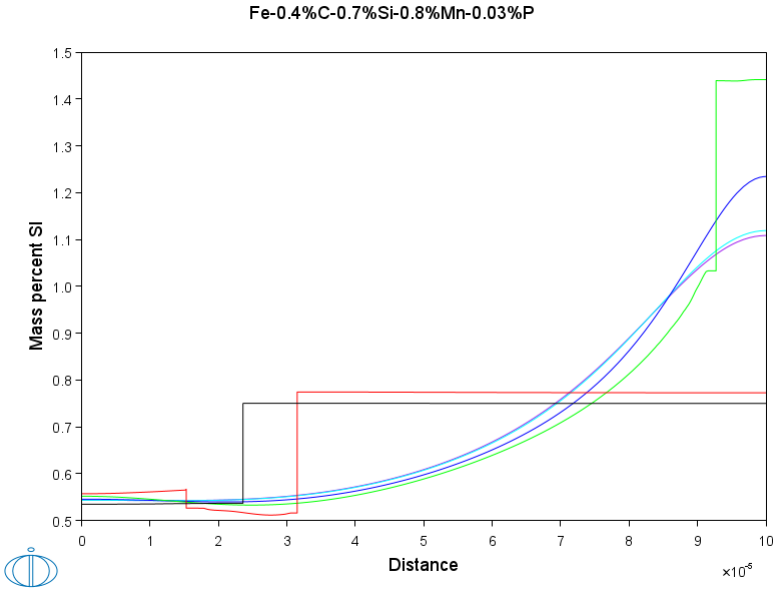

```
POST-1:
POST-1:Hit RETURN to continue
POST-1: s-d-a y w-p c
POST-1: s-d-a x dis gl
  INFO: Distance is set as independent variable
POST-1: s-p-c time 120,135,400,700,1500,3000
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples/unite/distribution\macroResult.exp Y
ORKING ...orking ...OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```



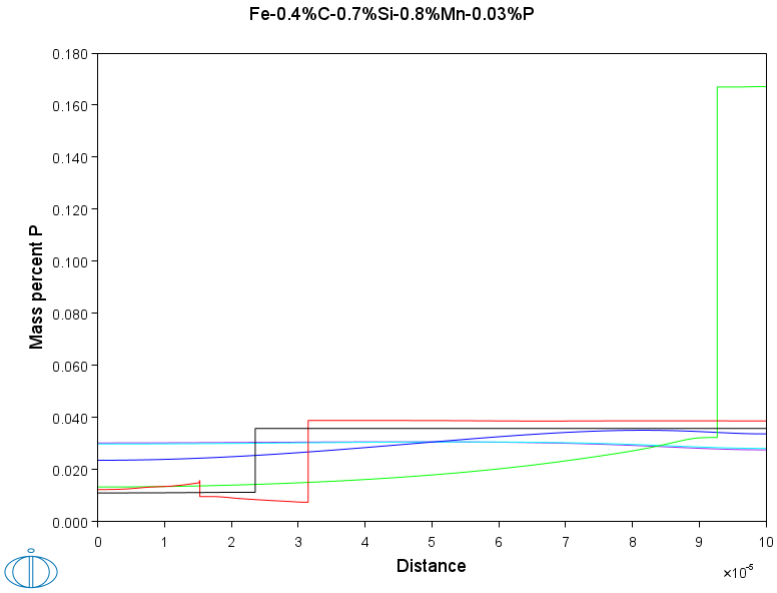

```
POST-1:
POST-1:Hit RETURN to continue
POST-1: s-d-a y w-p mn
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples/unite/distribution\macroResult.exp Y
ORKING ...orking ...OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```



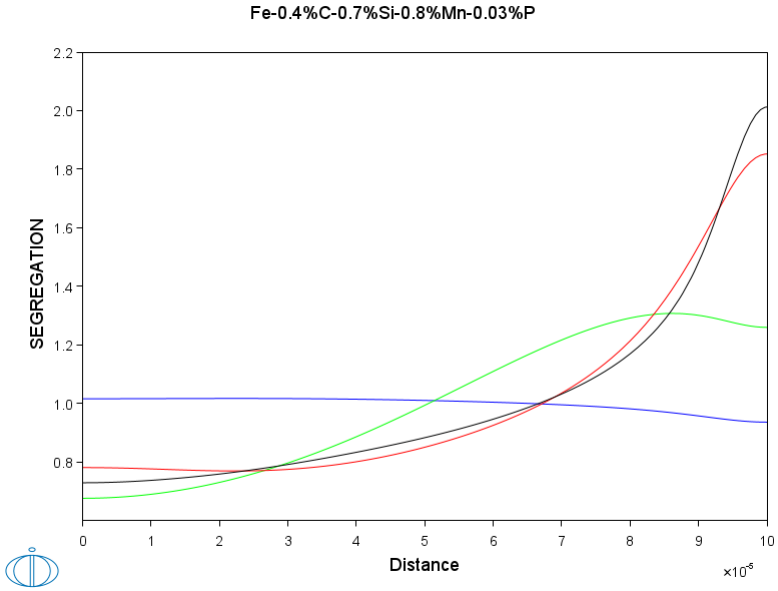

```
POST-1:
POST-1:Hit RETURN to continue
POST-1: s-d-a y w-p si
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples/unite/distribution\macroResult.exp Y
ORKING ...orking ...OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```



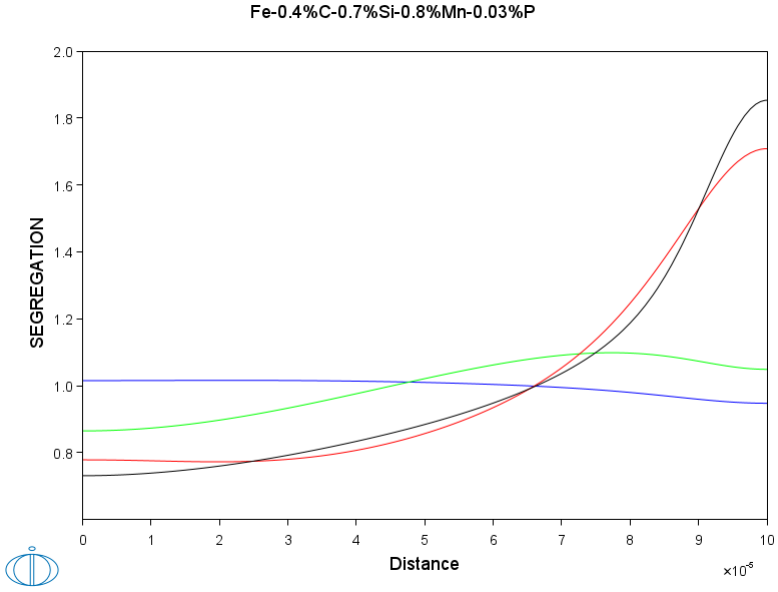

```
POST-1:
POST-1:Hit RETURN to continue
POST-1: s-d-a y w-p p
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples/unite/distribution\macroResult.exp Y
ORKING ...orking ...OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```



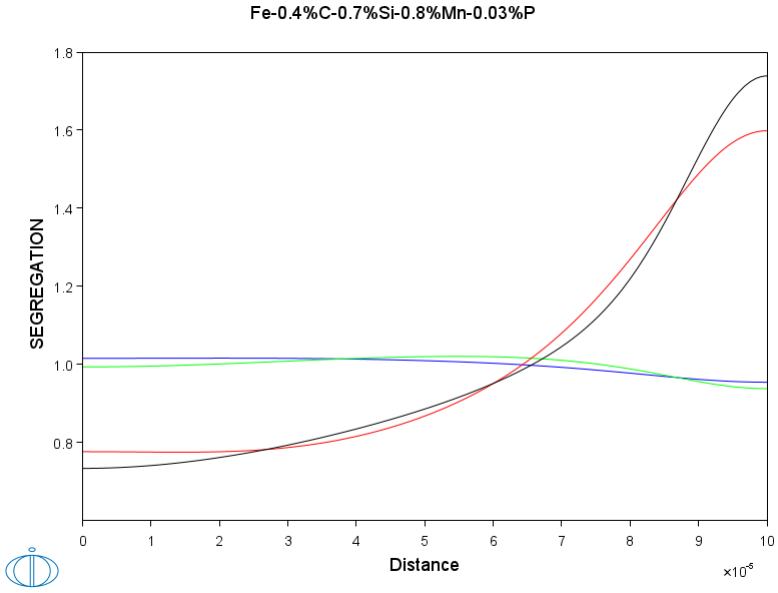

```
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: ent function mnn
FUNCTION: w(mn)/0.008
&
POST-1: ent function sin
FUNCTION: w(si)/0.007
&
POST-1: ent function pn
FUNCTION: w(p)/0.0003
&
POST-1: ent function cn
FUNCTION: w(c)/0.004
&
POST-1: ent tabel segregation
Variable(s) mnn sin pn cn
POST-1:
POST-1:
POST-1: s-d-a y segregation
COLUMN NUMBER /*/:
POST-1:
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
```



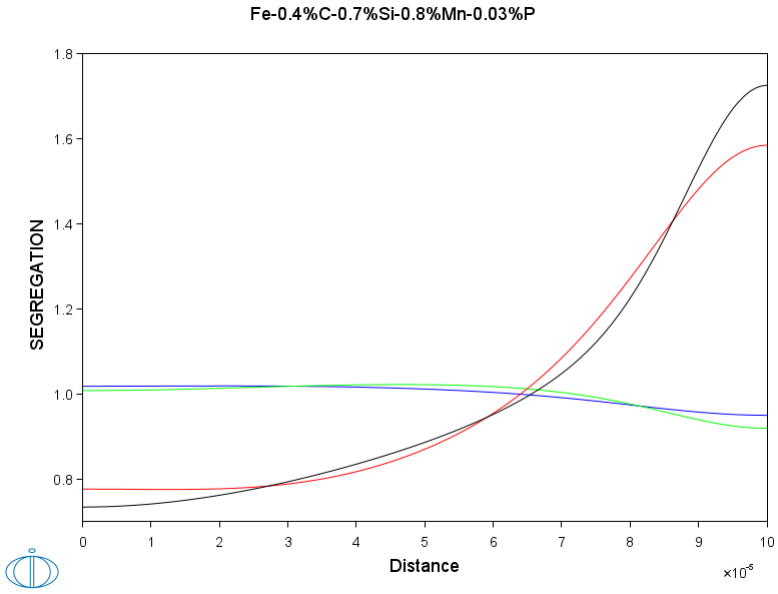

```
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: s-p-c time 800
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```




```
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
```




```
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
```

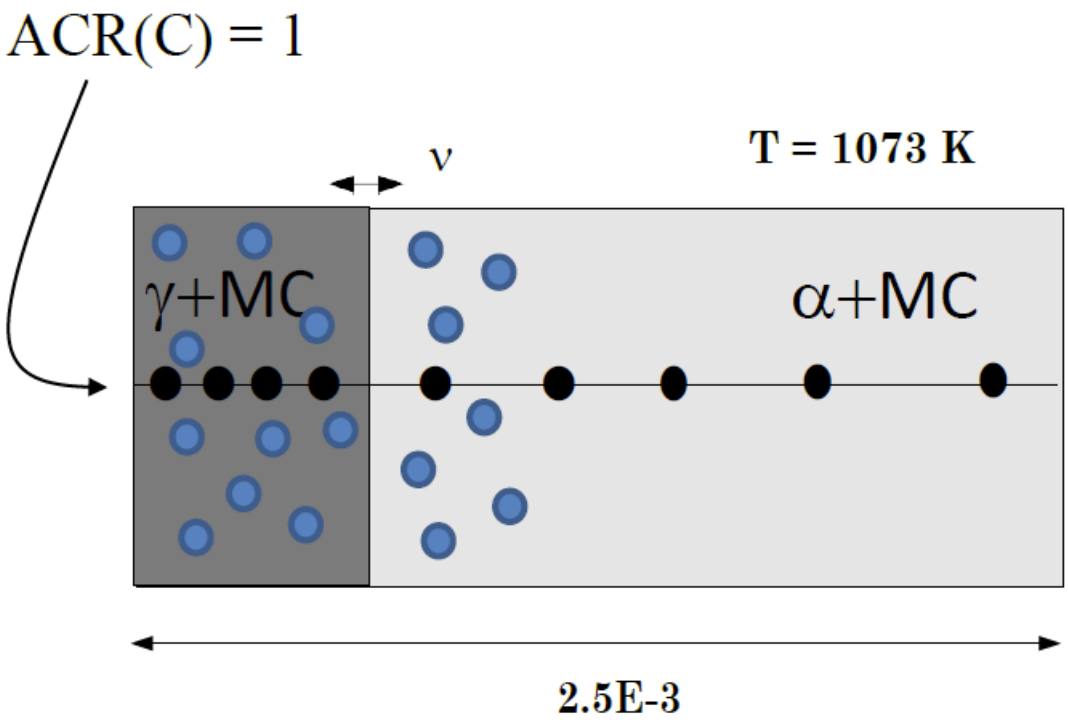



```
POST-1:
POST-1:Hit RETURN to continue
POST-1: set-inter
 --OK---
POST-1:
```

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: unknown compiler
 License library version: 9.7.0.0036
 Linked: Fri Oct 18 11:32:56 2024


SYS:SYS:MACRO 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: ------------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASE
SYS: @@
SYS: go da
14:30:41,567 [Thread-0] INFO  LicenseManager: Initializing user: jenkins.integrationtest@thermocalc.se
14:30:41,579 [Thread-0] INFO  LicenseController: Running License Spring in DEV environment.
14:30:42,638 [Thread-0] INFO  LicenseManager: There is an activated standalone license for jenkins.integrationtest@thermocalc.se for TC-
Application
 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
 L12_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                C1FE3_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: @@
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
14:30:44,861 [Thread-0] INFO  StandaloneLicenseController: Checking out license for: Diffusion (DICTRA)
 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 /LINEAR/: AUTO
DIC>
DIC>
DIC> enter-grid
REGION NAME : /AUS/: aus
WIDTH OF REGION /1/: 1e-9
TYPE /LINEAR/: 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> @@
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> @@
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> @@
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 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
 Region: AUS
 geometric    1.01184                 0.00000       38 points
                          dense at
 geometric   0.988299     dense at   0.100000E-08   39 points
 Region: FERR
 geometric    1.11821     dense at    0.00000       84 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_A1#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=  0.24414063E-11 dt=  0.24414063E-11
Starting time-step t0=  0.48828125E-11 dt=  0.48828125E-11
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=  0.15625000E-09
Starting time-step t0=  0.46875000E-09 dt=  0.15625000E-09
Starting time-step t0=  0.62500000E-09 dt=  0.15625000E-09
Starting time-step t0=  0.78125000E-09 dt=  0.15625000E-09
Starting time-step t0=  0.93750000E-09 dt=  0.31250000E-09
Starting time-step t0=  0.12500000E-08 dt=  0.31250000E-09
Starting time-step t0=  0.15625000E-08 dt=  0.31250000E-09
Starting time-step t0=  0.18750000E-08 dt=  0.31250000E-09
Starting time-step t0=  0.21875000E-08 dt=  0.62500000E-09
Starting time-step t0=  0.28125000E-08 dt=  0.62500000E-09
Starting time-step t0=  0.34375000E-08 dt=  0.12500000E-08
Starting time-step t0=  0.46875000E-08 dt=  0.25000000E-08
Starting time-step t0=  0.71875000E-08 dt=  0.50000000E-08
Starting time-step t0=  0.12187500E-07 dt=  0.10000000E-07
Starting time-step t0=  0.22187500E-07 dt=  0.10000000E-07
Starting time-step t0=  0.32187500E-07 dt=  0.10000000E-07
Starting time-step t0=  0.42187500E-07 dt=  0.10000000E-07
Starting time-step t0=  0.52187500E-07 dt=  0.20000000E-07
Starting time-step t0=  0.72187500E-07 dt=  0.20000000E-07
Starting time-step t0=  0.92187500E-07 dt=  0.20000000E-07
Starting time-step t0=  0.11218750E-06 dt=  0.40000000E-07
Starting time-step t0=  0.15218750E-06 dt=  0.40000000E-07
Starting time-step t0=  0.19218750E-06 dt=  0.80000000E-07
Starting time-step t0=  0.27218750E-06 dt=  0.80000000E-07
Starting time-step t0=  0.35218750E-06 dt=  0.16000000E-06
Starting time-step t0=  0.51218750E-06 dt=  0.32000000E-06
Starting time-step t0=  0.83218750E-06 dt=  0.64000000E-06
Starting time-step t0=  0.14721875E-05 dt=  0.12800000E-05
Starting time-step t0=  0.27521875E-05 dt=  0.25600000E-05
Starting time-step t0=  0.53121875E-05 dt=  0.51200000E-05
Starting time-step t0=  0.10432188E-04 dt=  0.10240000E-04
Starting time-step t0=  0.20672188E-04 dt=  0.20480000E-04
Starting time-step t0=  0.41152187E-04 dt=  0.40960000E-04
Starting time-step t0=  0.82112187E-04 dt=  0.81920000E-04
Starting time-step t0=  0.16403219E-03 dt=  0.16384000E-03
Starting time-step t0=  0.32787219E-03 dt=  0.32768000E-03
Starting time-step t0=  0.65555219E-03 dt=  0.65536000E-03
Starting time-step t0=  0.13109122E-02 dt=  0.13107200E-02
Starting time-step t0=  0.26216322E-02 dt=  0.26214400E-02
Starting time-step t0=  0.52430722E-02 dt=  0.52428800E-02
Starting time-step t0=  0.10485952E-01 dt=  0.52428800E-02
Starting time-step t0=  0.15728832E-01 dt=  0.10485760E-01
Starting time-step t0=  0.26214592E-01 dt=  0.10485760E-01
Starting time-step t0=  0.36700352E-01 dt=  0.10485760E-01
Starting time-step t0=  0.47186112E-01 dt=  0.20971520E-01
Starting time-step t0=  0.68157632E-01 dt=  0.20971520E-01
Starting time-step t0=  0.89129152E-01 dt=  0.20971520E-01
 Error                    408
Starting time-step t0=  0.89784512E-01 dt=  0.65536000E-03
Starting time-step t0=  0.90439872E-01 dt=  0.65536000E-03
Starting time-step t0=  0.91095232E-01 dt=  0.65536000E-03
Starting time-step t0=  0.91750592E-01 dt=  0.65536000E-03
Starting time-step t0=  0.92405952E-01 dt=  0.65536000E-03
Starting time-step t0=  0.93061312E-01 dt=  0.65536000E-03
Starting time-step t0=  0.93716672E-01 dt=  0.65536000E-03
Starting time-step t0=  0.94372032E-01 dt=  0.65536000E-03
Starting time-step t0=  0.95027392E-01 dt=  0.65536000E-03
Starting time-step t0=  0.95682752E-01 dt=  0.13107200E-02
Starting time-step t0=  0.96993472E-01 dt=  0.13107200E-02
Starting time-step t0=  0.98304192E-01 dt=  0.13107200E-02
Starting time-step t0=  0.99614912E-01 dt=  0.13107200E-02
Starting time-step t0=  0.10092563     dt=  0.13107200E-02
Starting time-step t0=  0.10223635     dt=  0.13107200E-02
Starting time-step t0=  0.10354707     dt=  0.13107200E-02
Starting time-step t0=  0.10485779     dt=  0.26214400E-02
```

```
Starting time-step t0=  0.10747923     dt=  0.26214400E-02
Starting time-step t0=  0.11010067     dt=  0.26214400E-02
Starting time-step t0=  0.11272211     dt=  0.52428800E-02
Starting time-step t0=  0.11796499     dt=  0.52428800E-02
Starting time-step t0=  0.12320787     dt=  0.52428800E-02
Starting time-step t0=  0.12845075     dt=  0.10485760E-01
Starting time-step t0=  0.13893651     dt=  0.10485760E-01
Starting time-step t0=  0.14942227     dt=  0.10485760E-01
Starting time-step t0=  0.15990803     dt=  0.10485760E-01
Starting time-step t0=  0.17039379     dt=  0.10485760E-01
Starting time-step t0=  0.18087955     dt=  0.10485760E-01
Starting time-step t0=  0.19136531     dt=  0.20971520E-01
Starting time-step t0=  0.21233683     dt=  0.20971520E-01
Starting time-step t0=  0.23330835     dt=  0.20971520E-01
Starting time-step t0=  0.25427987     dt=  0.20971520E-01
Starting time-step t0=  0.27525139     dt=  0.20971520E-01
Starting time-step t0=  0.29622291     dt=  0.20971520E-01
Starting time-step t0=  0.31719443     dt=  0.20971520E-01
Starting time-step t0=  0.33816595     dt=  0.20971520E-01
Starting time-step t0=  0.35913747     dt=  0.20971520E-01
Starting time-step t0=  0.38010899     dt=  0.20971520E-01
Starting time-step t0=  0.40108051     dt=  0.41943040E-01
Starting time-step t0=  0.44302355     dt=  0.83886080E-01
Starting time-step t0=  0.52690963     dt=  0.83886080E-01
Starting time-step t0=  0.61079571     dt=  0.83886080E-01


output ignored...


... output resumed

 DELETING TIME-RECORD FOR TIME    26673.784
 DELETING TIME-RECORD FOR TIME    26716.733
 DELETING TIME-RECORD FOR TIME    26759.683
 DELETING TIME-RECORD FOR TIME    26802.633
 DELETING TIME-RECORD FOR TIME    26845.582
 DELETING TIME-RECORD FOR TIME    26888.532
 DELETING TIME-RECORD FOR TIME    26952.957
 DELETING TIME-RECORD FOR TIME    26995.906
 DELETING TIME-RECORD FOR TIME    27038.856
 DELETING TIME-RECORD FOR TIME    27081.806
 DELETING TIME-RECORD FOR TIME    27124.755
 DELETING TIME-RECORD FOR TIME    27167.705
 DELETING TIME-RECORD FOR TIME    27210.655
 DELETING TIME-RECORD FOR TIME    27253.604
 DELETING TIME-RECORD FOR TIME    27296.554
 DELETING TIME-RECORD FOR TIME    27339.504
 DELETING TIME-RECORD FOR TIME    27382.453
 DELETING TIME-RECORD FOR TIME    27425.403
 DELETING TIME-RECORD FOR TIME    27468.353
 DELETING TIME-RECORD FOR TIME    27522.040
 DELETING TIME-RECORD FOR TIME    27564.989
 DELETING TIME-RECORD FOR TIME    27607.939
 DELETING TIME-RECORD FOR TIME    27650.889
 DELETING TIME-RECORD FOR TIME    27693.839
 DELETING TIME-RECORD FOR TIME    27736.788
 DELETING TIME-RECORD FOR TIME    27779.738
 DELETING TIME-RECORD FOR TIME    27822.688
 DELETING TIME-RECORD FOR TIME    27865.637
 DELETING TIME-RECORD FOR TIME    27908.587
 DELETING TIME-RECORD FOR TIME    27951.537
 DELETING TIME-RECORD FOR TIME    27994.486
 DELETING TIME-RECORD FOR TIME    28037.436
 DELETING TIME-RECORD FOR TIME    28080.386
 DELETING TIME-RECORD FOR TIME    28123.335
 DELETING TIME-RECORD FOR TIME    28177.022
 DELETING TIME-RECORD FOR TIME    28219.972
 DELETING TIME-RECORD FOR TIME    28262.922
 DELETING TIME-RECORD FOR TIME    28305.871
 DELETING TIME-RECORD FOR TIME    28348.821
 DELETING TIME-RECORD FOR TIME    28391.771
 DELETING TIME-RECORD FOR TIME    28434.720
 DELETING TIME-RECORD FOR TIME    28477.670
 DELETING TIME-RECORD FOR TIME    28520.620
 DELETING TIME-RECORD FOR TIME    28563.569
 DELETING TIME-RECORD FOR TIME    28606.519
 DELETING TIME-RECORD FOR TIME    28649.469
 DELETING TIME-RECORD FOR TIME    28692.418
 DELETING TIME-RECORD FOR TIME    28735.368
 DELETING TIME-RECORD FOR TIME    28799.793
 DELETING TIME-RECORD FOR TIME    28842.742
 DELETING TIME-RECORD FOR TIME    28885.692
 DELETING TIME-RECORD FOR TIME    28939.379
 DELETING TIME-RECORD FOR TIME    28982.329
 DELETING TIME-RECORD FOR TIME    29025.278
 DELETING TIME-RECORD FOR TIME    29068.228
 DELETING TIME-RECORD FOR TIME    29111.178
 DELETING TIME-RECORD FOR TIME    29164.865
 DELETING TIME-RECORD FOR TIME    29207.814
 DELETING TIME-RECORD FOR TIME    29250.764
 DELETING TIME-RECORD FOR TIME    29293.714
 DELETING TIME-RECORD FOR TIME    29336.663
 DELETING TIME-RECORD FOR TIME    29390.351
 DELETING TIME-RECORD FOR TIME    29433.300
 DELETING TIME-RECORD FOR TIME    29497.725
 DELETING TIME-RECORD FOR TIME    29540.674
 DELETING TIME-RECORD FOR TIME    29583.624
 DELETING TIME-RECORD FOR TIME    29626.574
 DELETING TIME-RECORD FOR TIME    29669.523
 DELETING TIME-RECORD FOR TIME    29712.473
 DELETING TIME-RECORD FOR TIME    29776.898
 DELETING TIME-RECORD FOR TIME    29819.847
 DELETING TIME-RECORD FOR TIME    29862.797
 DELETING TIME-RECORD FOR TIME    29905.747
 DELETING TIME-RECORD FOR TIME    29948.696
 DELETING TIME-RECORD FOR TIME    29991.646
 DELETING TIME-RECORD FOR TIME    30034.596
 DELETING TIME-RECORD FOR TIME    30077.545
 DELETING TIME-RECORD FOR TIME    30120.495
 DELETING TIME-RECORD FOR TIME    30163.445
 DELETING TIME-RECORD FOR TIME    30206.394
 DELETING TIME-RECORD FOR TIME    30249.344
 DELETING TIME-RECORD FOR TIME    30292.294
 DELETING TIME-RECORD FOR TIME    30335.243
```

```
 DELETING TIME-RECORD FOR TIME    30378.193
 DELETING TIME-RECORD FOR TIME    30421.143
 DELETING TIME-RECORD FOR TIME    30464.092
 DELETING TIME-RECORD FOR TIME    30507.042
 DELETING TIME-RECORD FOR TIME    30549.992
 DELETING TIME-RECORD FOR TIME    30592.941
 DELETING TIME-RECORD FOR TIME    30635.891
 DELETING TIME-RECORD FOR TIME    30700.316
 DELETING TIME-RECORD FOR TIME    30743.265
 DELETING TIME-RECORD FOR TIME    30818.427
 DELETING TIME-RECORD FOR TIME    30861.377
 DELETING TIME-RECORD FOR TIME    30904.327
 DELETING TIME-RECORD FOR TIME    30947.276
 DELETING TIME-RECORD FOR TIME    30990.226
 DELETING TIME-RECORD FOR TIME    31033.176
 DELETING TIME-RECORD FOR TIME    31076.125
 DELETING TIME-RECORD FOR TIME    31119.075
 DELETING TIME-RECORD FOR TIME    31162.025
 DELETING TIME-RECORD FOR TIME    31204.974
 DELETING TIME-RECORD FOR TIME    31247.924
 DELETING TIME-RECORD FOR TIME    31290.874
 DELETING TIME-RECORD FOR TIME    31333.823
 DELETING TIME-RECORD FOR TIME    31376.773
 DELETING TIME-RECORD FOR TIME    31441.197
 DELETING TIME-RECORD FOR TIME    31484.147
 DELETING TIME-RECORD FOR TIME    31527.097
 DELETING TIME-RECORD FOR TIME    31570.046
 DELETING TIME-RECORD FOR TIME    31612.996
 DELETING TIME-RECORD FOR TIME    31655.946
 DELETING TIME-RECORD FOR TIME    31731.108
 DELETING TIME-RECORD FOR TIME    31774.057
 DELETING TIME-RECORD FOR TIME    31817.007
 DELETING TIME-RECORD FOR TIME    31859.957
 DELETING TIME-RECORD FOR TIME    31902.906
 DELETING TIME-RECORD FOR TIME    31945.856
 DELETING TIME-RECORD FOR TIME    31988.806
 DELETING TIME-RECORD FOR TIME    32031.755
 DELETING TIME-RECORD FOR TIME    32074.705
 DELETING TIME-RECORD FOR TIME    32117.655
 DELETING TIME-RECORD FOR TIME    32160.604
 DELETING TIME-RECORD FOR TIME    32203.554
 DELETING TIME-RECORD FOR TIME    32246.504
 DELETING TIME-RECORD FOR TIME    32289.454
 DELETING TIME-RECORD FOR TIME    32332.403

 KEEPING TIME-RECORD FOR TIME    32375.353
 AND FOR TIME                    32400.000
 WORKSPACE RECLAIMED
 -------------------------------------------------
 INTERPOLATION SCHEME USED THIS FRACTION OF
 THE ALLOCATED MEMORY:   0.131836825520669
 EFFICIENCY FACTOR:    33.3314025122010
 MEMORY FRACTION USAGE PER BRANCH:
  0.195780311406258
  8.808639892001351E-002
  9.254160181970550E-002
 -------------------------------------------------
 DEALLOCATING
 -------------------------------------------------

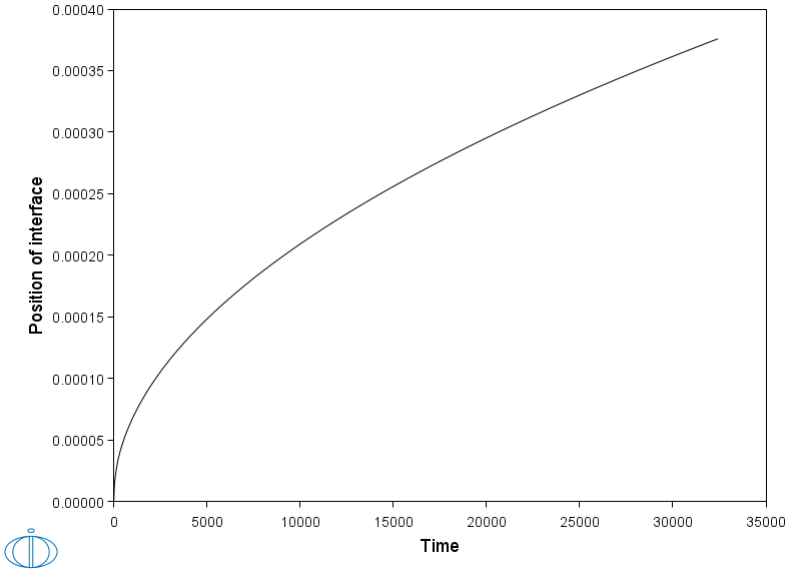
 TIMESTEP AT     32400.0000     SELECTED

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

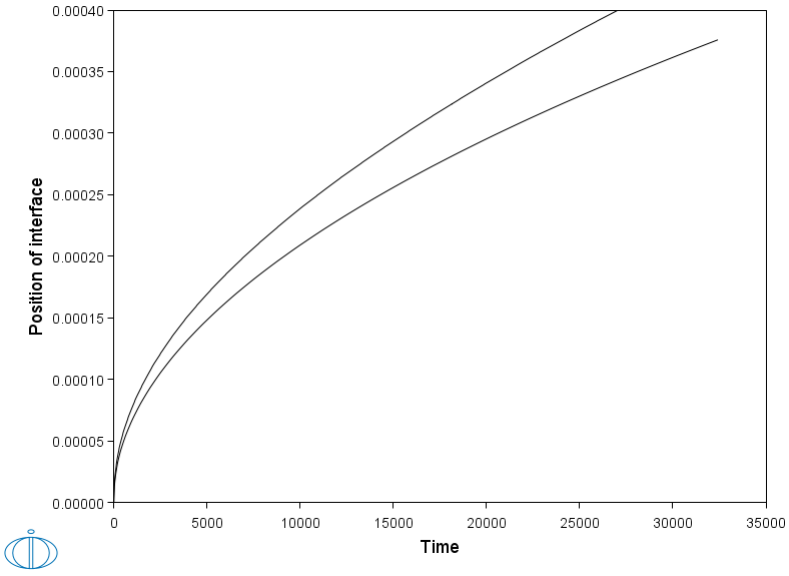
exb7-plot

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO 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 C1NB1_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
```



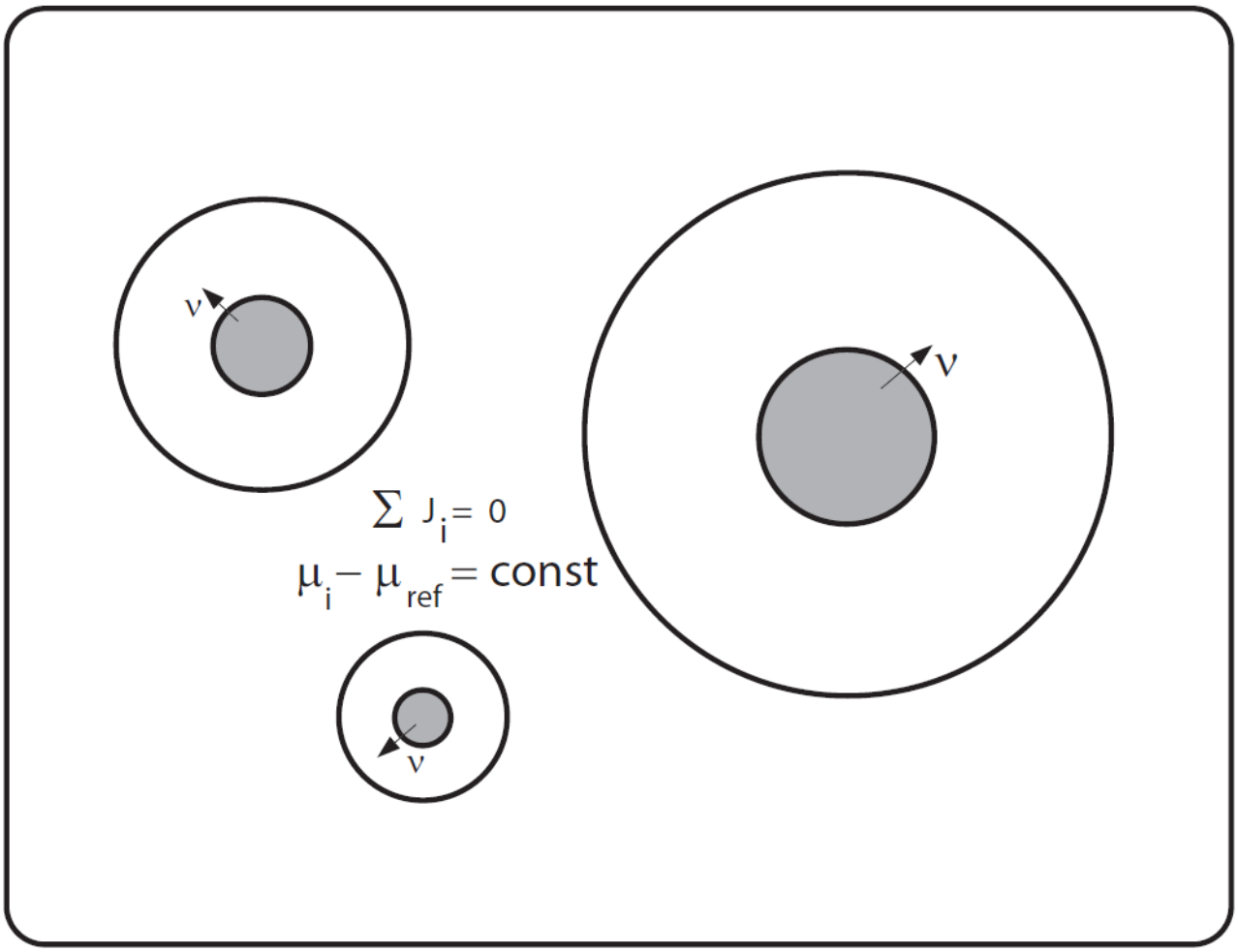

```
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ APPEND DATA FROM A CORRESPONDING SIMULATION
POST-1: @@ WITHOUT NIOBIUM
POST-1: @@
POST-1:
POST-1: app y fec.exp 0
DATASET NUMBER(s): /-1/: 1
POST-1:
POST-1: plot
```




```
POST-1:
```

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

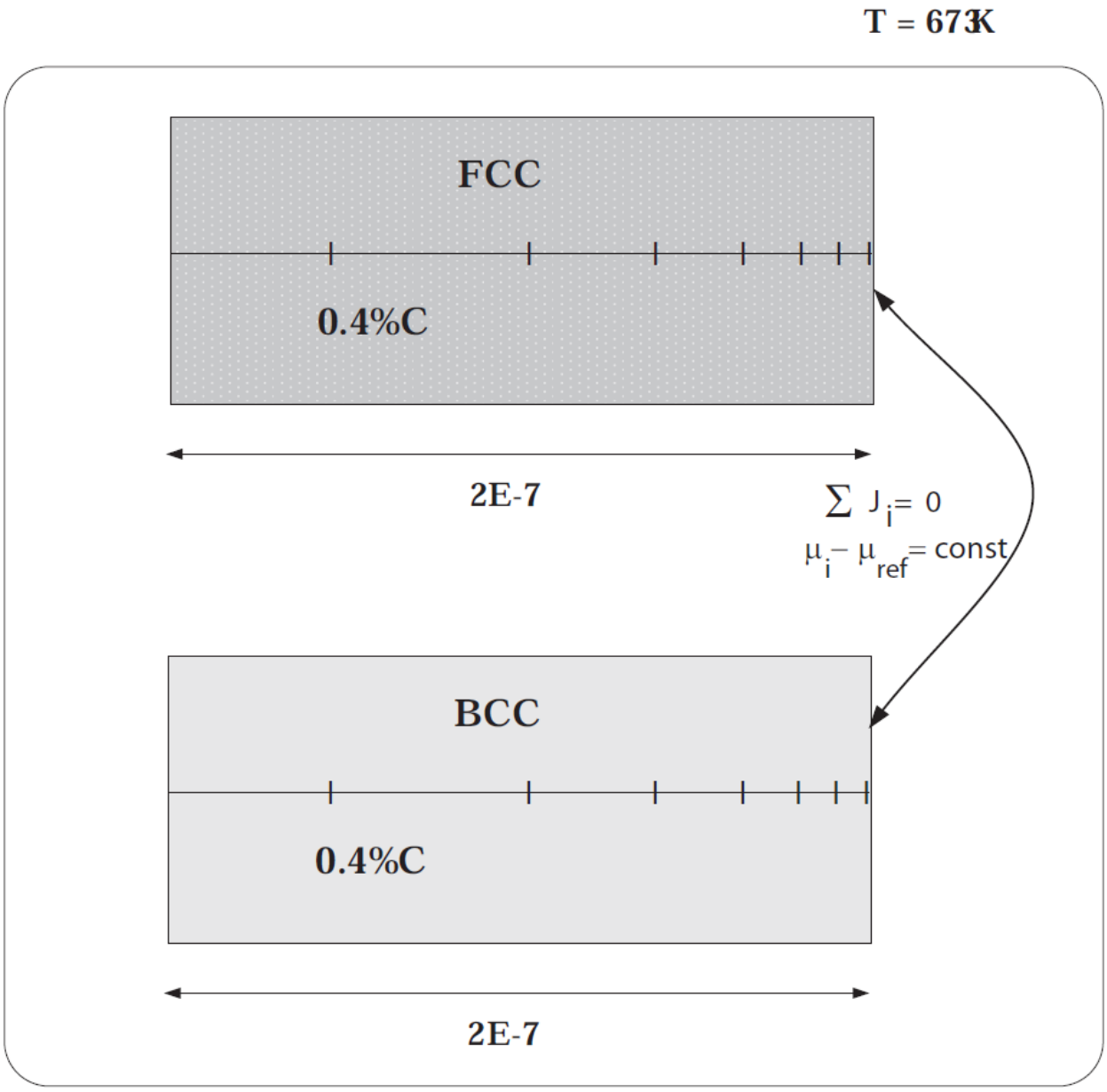
Cell Calculations



Example exc1

'Carbon cannon' in α/γ 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.



exc1-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: unknown compiler
 License library version: 9.7.0.0036
 Linked: Fri Oct 18 11:32:56 2024


SYS:SYS:MACRO exc1\setup.DCM
SYS: ï»¿@@
 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 WidmannstÃ¤tten
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. HÃ¶glund and J. Ã…gren: Acta Metall. Mater. 41 (1993), pp.1951-1957.
SYS: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exc1_setup.DCM
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASE
SYS: @@
SYS: go da
14:37:52,080 [Thread-0] INFO  LicenseManager: Initializing user: jenkins.integrationtest@thermocalc.se
14:37:52,090 [Thread-0] INFO  LicenseController: Running License Spring in DEV environment.
14:37:53,178 [Thread-0] INFO  LicenseManager: There is an activated standalone license for jenkins.integrationtest@thermocalc.se for TC-
Application
 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 v5.0

 VA                       /-  DEFINED
TDB_FEDEMO: def-sys fe c
 FE                       C  DEFINED
TDB_FEDEMO: rej ph * all
 BCC_A2                   CBCC_A12                 CEMENTITE
 CUB_A13                  DIAMOND_FCC_A4           FCC_A1
 GAS:G                    GRAPHITE                 HCP_A3
 KSI_CARBIDE              LAVES_PHASE_C14          LIQUID:L
 M23C6                    M5C2                     M7C3
   REJECTED
TDB_FEDEMO: res ph fcc,bcc
 FCC_A1                   BCC_A2  RESTORED
TDB_FEDEMO: get
14:37:54,261 [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 v4.0

 VA  DEFINED
APP: def-sys fe c
 FE                       C  DEFINED
APP: rej ph * all
 BCC_A2                   FCC_A1                   CEMENTITE
 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
```

```
14:37:54,748 [Thread-0] INFO  StandaloneLicenseController: Checking out license for: Diffusion (DICTRA)
 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-simulation-cond
NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /AUTO/:
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -> 1): /AUTO/: 1.0
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/:
DIC-2> @@
DIC-2> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC-2> @@
DIC-2> save exc1 Y
DIC-2>
DIC-2> set-inter
 --OK---
DIC-2>
```

exc1-run

```
DIC-2>About
 NO SUCH COMMAND, USE HELP
DIC-2>DIC-2>MACRO exc1\run.DCM DIC-2>
DIC-2>
DIC-2> @@ exc1_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 exc1
 OK
DIC> sim
 Region: AUS
 geometric   0.807790     dense at   0.200000E-06   94 points
 Region: FER
 geometric   0.902995     dense at   0.200000E-06   84 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]
  135307.642815820         135301.527756833         2262.52030312600         27.0263371728539        4.079916077775184E-
003        7.622433292833595E-009        2.128570473283522E-018       TIME =  0.10000000E-06 DT =  0.10000000E-
06 SUM OF SQUARES =  0.21285705E-17
 U-FRACTION IN SYSTEM:  C = .018673311178274  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    0  seconds
  208816.034890406         208822.265430346         5072.20638557645         182.384319733901        0.270385769468413        1.592497675668544
005        1.417906187461779E-012       TIME =  0.30000000E-06 DT =  0.20000000E-06 SUM OF SQUARES =  0.14179062E-11
 U-FRACTION IN SYSTEM:  C = .0186733111782859  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    1  seconds
  1814854.68882182         1814793.74342137         46429.6905806392         779.865577579337        0.2444667991630O2        1.350142054712660
006        2.323634829480956E-015       TIME =  0.70000000E-06 DT =  0.40000000E-06 SUM OF SQUARES =  0.23236348E-14
 U-FRACTION IN SYSTEM:  C = .0186733111782858  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    0  seconds
  160981.695992437         160966.298643037         473.094715618747         1.20596610124271        7.950968550466077E-
006        1.345267246846770E-013       TIME =  0.15000000E-05 DT =  0.80000000E-06 SUM OF SQUARES =  0.13452672E-12
 U-FRACTION IN SYSTEM:  C = .0186733111782873  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    1  seconds
  98750.8619683812         98742.4697568137         373.098136997977         1.20077816375018        1.265620984540425E-
005        4.329806129952154E-013       TIME =  0.31000000E-05 DT =  0.16000000E-05 SUM OF SQUARES =  0.43298061E-12
 U-FRACTION IN SYSTEM:  C = .0186733111782925  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    1  seconds
  44587.8325289803         44583.8234072530         150.768304019182        0.438221743816040        3.757794245626230E-
006        9.437999994062030E-014       TIME =  0.63000000E-05 DT =  0.32000000E-05 SUM OF SQUARES =  0.94380000E-13
 U-FRACTION IN SYSTEM:  C = .0186733111782975  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    0  seconds
  21859.5994961233         21857.6129647661         72.2612290402324        0.205632792775804        1.689336117715827E-
006        3.978453188056322E-014       TIME =  0.12700000E-04 DT =  0.64000000E-05 SUM OF SQUARES =  0.39784532E-13
 U-FRACTION IN SYSTEM:  C = .0186733111783038  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    1  seconds
  10786.8377482087         10785.8505057635         35.1458415974932        9.867370023610589E-002        7.895969513889057E-
007        1.786779594455915E-014       TIME =  0.25500000E-04 DT =  0.12800000E-04 SUM OF SQUARES =  0.17867796E-13
 U-FRACTION IN SYSTEM:  C = .0186733111783124  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    0  seconds
  535369.675221392         535320.456989284         1731.44143349908         4.82682529900785        3.807517348056760E-
005        8.431126112574533E-013       TIME =  0.51100000E-04 DT =  0.25600000E-04 SUM OF SQUARES =  0.84311261E-12
 U-FRACTION IN SYSTEM:  C = .0186733111783241  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    0  seconds


output ignored...



... output resumed

TIME =  0.19085954     DT =  0.21069509E-01 SUM OF SQUARES =  0.13303619E-14
 U-FRACTION IN SYSTEM:  C = .0186733111787198  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    1  seconds
  4108.02803301117         4102.19302144178         4.056696676418507E-002        3.572873504583514E-007        2.452762234536281E-
017       TIME =  0.21376470     DT =  0.22905157E-01 SUM OF SQUARES =  0.24527622E-16
 U-FRACTION IN SYSTEM:  C = .0186733111787186  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    0  seconds
  571.074978481085         569.214487629745         2.707313231531283E-003        5.592515824767624E-010        5.623363624507712E-
017       TIME =  0.23956620     DT =  0.25801504E-01 SUM OF SQUARES =  0.56233636E-16
 U-FRACTION IN SYSTEM:  C = .0186733111787191  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    1  seconds
  102143.643501521         102350.463526968         0.181390032353163        1.492899557896823E-006        1.232275590545007E-
015       TIME =  0.27042983     DT =  0.30863623E-01 SUM OF SQUARES =  0.12322756E-14
 U-FRACTION IN SYSTEM:  C = .0186733111787202  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    0  seconds
  930479.460779709         930975.816610817         46.8812006728164        1.326573692200910E-003        1.239404901396882E-
008        6.409750094701172E-002        1.457419367127132E-015       TIME =  0.31031413     DT =  0.39884302E-
01 SUM OF SQUARES =  0.14574194E-14
 U-FRACTION IN SYSTEM:  C = .01867331117872  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    1  seconds
  1154275.19089850         1154716.10722486         113.748788592907        1.340252896755056E-002        1.435200845092451E-
010        4.036177260803351E-002        5.124799607593372E-016       TIME =  0.36031413     DT =  0.50000000E-
01 SUM OF SQUARES =  0.51247996E-15
 U-FRACTION IN SYSTEM:  C = .0186733111787201  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    0  seconds
  65808.5506106695         65901.6294261245         0.287193529275020        3.200184478134127E-006        2.405550535687920E-
016       TIME =  0.41031413     DT =  0.50000000E-01 SUM OF SQUARES =  0.24055505E-15
 U-FRACTION IN SYSTEM:  C = .0186733111787206  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
```

```
  CPU time used in timestep                    1  seconds
  65692.0897194078         65608.0917072953        0.836823312294995        4.522513737505278E-006        1.639092376263767E-
016       TIME =  0.46031413     DT =  0.50000000E-01 SUM OF SQUARES =  0.16390924E-15
 U-FRACTION IN SYSTEM:  C = .0186733111787208  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    0  seconds
  1458259.21771608         1457851.95148816         234.482126471522        8.616621045424688E-002        4.028484572131457E-
006        3.685335293257121E-016       TIME =  0.50000000     DT =  0.39685871E-01 SUM OF SQUARES =  0.36853353E-15
 U-FRACTION IN SYSTEM:  C = .0186733111787212  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    0.0000000
 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   0.44751337E-01
 DELETING TIME-RECORD FOR TIME   0.60463644E-01
 DELETING TIME-RECORD FOR TIME   0.77981816E-01
 DELETING TIME-RECORD FOR TIME   0.95020874E-01
 DELETING TIME-RECORD FOR TIME   0.11287366
 DELETING TIME-RECORD FOR TIME   0.13105170
 DELETING TIME-RECORD FOR TIME   0.14998839
 DELETING TIME-RECORD FOR TIME   0.16979003
 DELETING TIME-RECORD FOR TIME   0.19085954
 DELETING TIME-RECORD FOR TIME   0.21376470
 DELETING TIME-RECORD FOR TIME   0.23956620
 DELETING TIME-RECORD FOR TIME   0.27042983
 DELETING TIME-RECORD FOR TIME   0.31031413
 DELETING TIME-RECORD FOR TIME   0.36031413
 DELETING TIME-RECORD FOR TIME   0.41031413

 KEEPING TIME-RECORD FOR TIME   0.46031413
 AND FOR TIME                   0.50000000
 WORKSPACE RECLAIMED

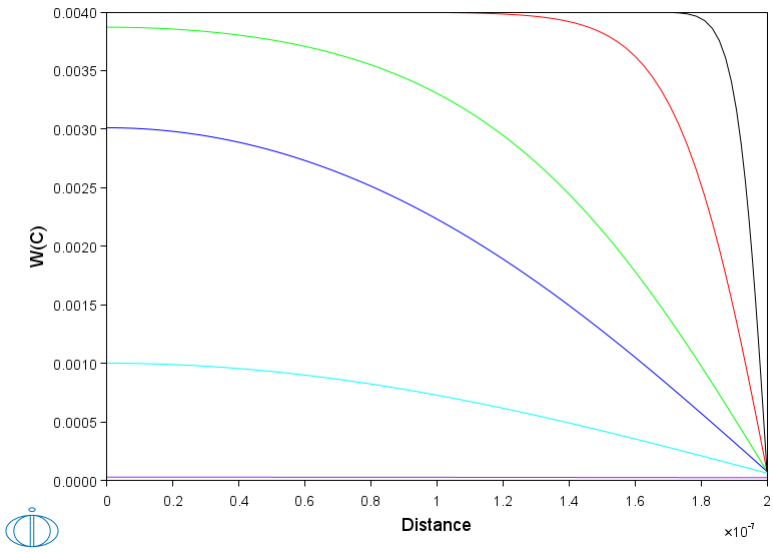
 TIMESTEP AT    0.500000000     SELECTED

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

exc1-plot

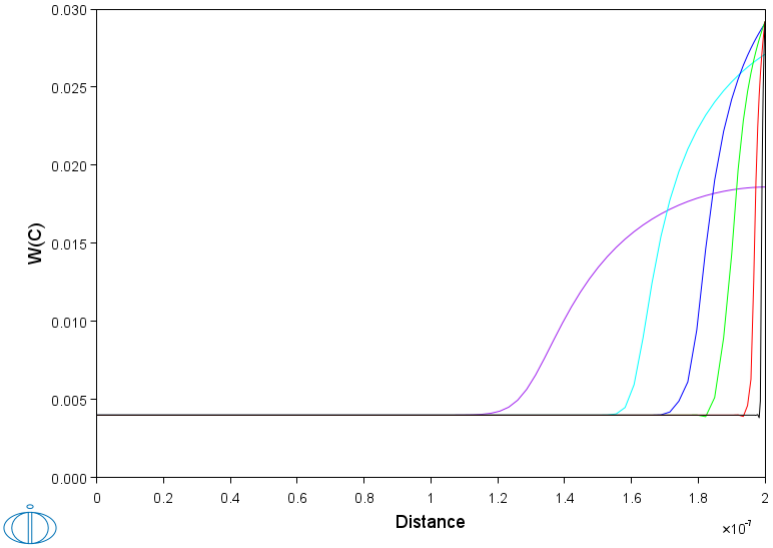
```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exc1\plot.DCM DIC>
DIC>
DIC> @@ exc1_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE c1
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  5.00000E-01
DIC> read exc1
 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



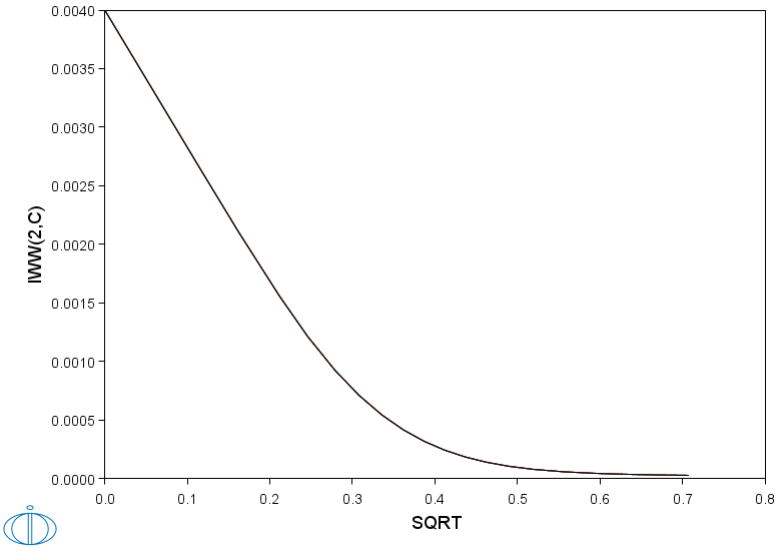

```
POST-2:
POST-2:
POST-2:
POST-2:@?<_hit_return_to_continue_>
POST-2:
POST-2: @@
POST-2: @@ DO THE SAME THING FOR THE AUSTENITE (CELL-1)
POST-2: @@
POST-2: select-cell
Number /NEXT/: 1
 CELL   1 SELECTED
POST-1: set-title Figure c1.2
POST-1: plot
```

Figure c1.2



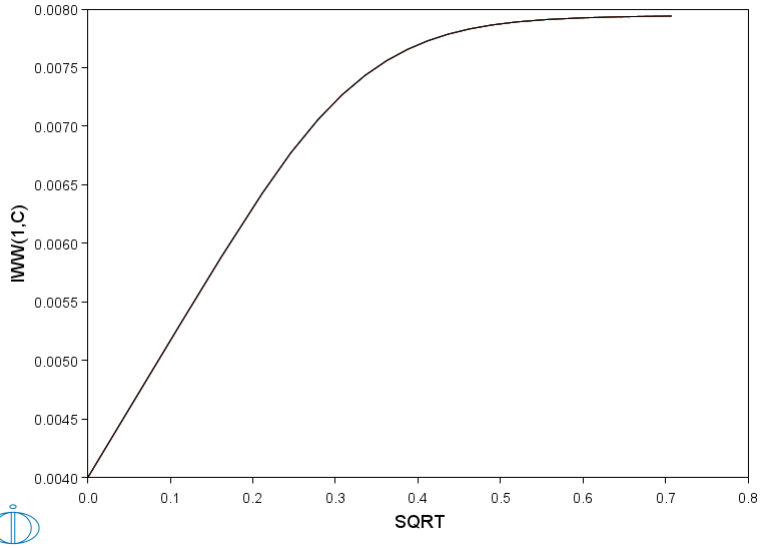

```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: @@
POST-1: @@ PLOT THE AVARAGE WEIGHT FRACTION OF CARBON IN FERRITE VS. SQUARE ROOT
POST-1: @@ OF TIME. START BY DEFINING A "SQUARE-ROOT-OF-TIME" FUNCTION.
POST-1: @@
POST-1: sel-cell 2
 CELL    2 SELECTED
POST-2: enter func sqrt=sqrt(time);
POST-2: s-d-a x sqrt
POST-2: s-d-a y iww(2,c)
POST-2: s-i-v time
POST-2: set-title Figure c1.3
POST-2: plot
```

Figure c1.3



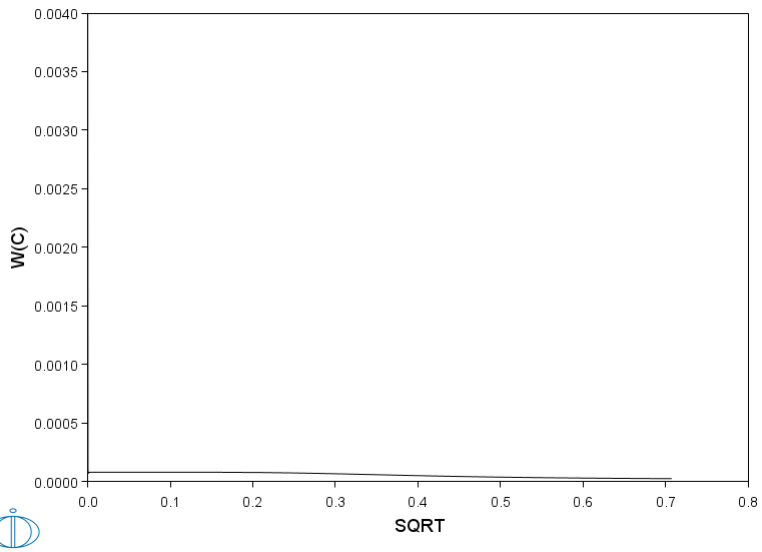

```
POST-2:
POST-2:
POST-2:
POST-2:@?<_hit_return_to_continue_>
POST-2:
POST-2: @@
POST-2: @@ DO THE SAME THING FOR THE AUSTENITE
POST-2: @@
POST-2: sel-cell 1
 CELL    1 SELECTED
POST-1: s-d-a y iww(1,c)
POST-1: set-title Figure c1.4
POST-1: plot
```

Figure c1.4



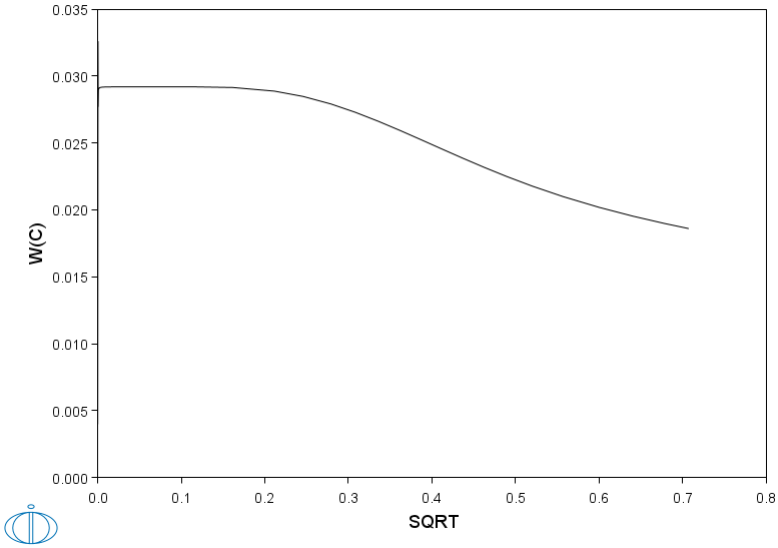

```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: @@
POST-1: @@ PLOT HOW THE CONCENTRATION IN FERRITE AT THE FERRITE/AUSTENITE BOUNDARY
POST-1: @@ V.S SQUARE ROOT OF TIME. THE  FERRITE/AUSTENITE BOUNDARY IS REPRESENTED
POST-1: @@ BY THE CELL BOUNDARY I.E. THE "LAST" INTERFACE.
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

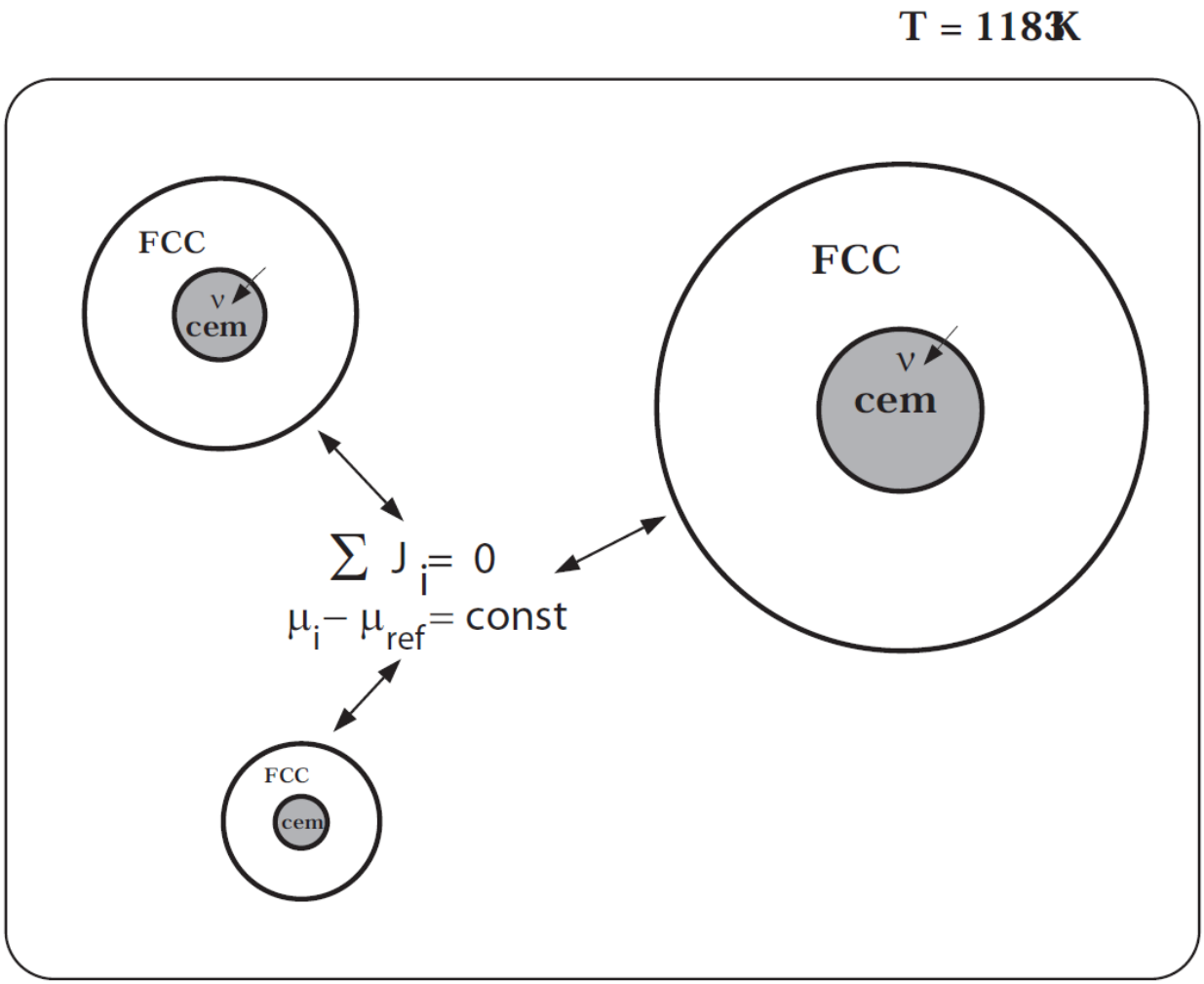



```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: set-inter
 --OK---
POST-1:
```

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.



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: unknown compiler
 License library version: 9.7.0.0036
 Linked: Fri Oct 18 11:32:56 2024


SYS:SYS:MACRO exc2\setup.DCM
SYS: ï»¿@@
 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. HÃ¶glund, B. JÃ¶nsson and J. Ã…gren:
SYS: @@ Metall.Trans.A, v. 22A (1991), pp. 1745-1752.
SYS: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exc2_setup.DCM
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASE
SYS: @@
SYS: go da
14:41:07,913 [Thread-0] INFO  LicenseManager: Initializing user: jenkins.integrationtest@thermocalc.se
14:41:07,926 [Thread-0] INFO  LicenseController: Running License Spring in DEV environment.
14:41:09,037 [Thread-0] INFO  LicenseManager: There is an activated standalone license for jenkins.integrationtest@thermocalc.se for TC-
Application
 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 v5.0

 VA                        /-  DEFINED
TDB_FEDEMO: def-sys fe cr c
 FE                        CR                        C
   DEFINED
TDB_FEDEMO: rej ph * all
 BCC_A2                    CBCC_A12                  CEMENTITE
 CHI_A12                   CUB_A13                   DIAMOND_FCC_A4
 FCC_A1                    GAS:G                     GRAPHITE
 HCP_A3                    KSI_CARBIDE               LAVES_PHASE_C14
 LIQUID:L                  M23C6                     M3C2
 M5C2                      M7C3                      SIGMA
   REJECTED
TDB_FEDEMO: res ph fcc cementite
 FCC_A1                    CEMENTITE  RESTORED
TDB_FEDEMO: get
14:41:10,098 [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 v4.0

 VA  DEFINED
APP: def-sys fe cr c
 FE                        CR                        C
   DEFINED
APP: rej ph * all
 BCC_A2                    FCC_A1                    CEMENTITE
 LIQUID:L  REJECTED
APP: res ph fcc cementite
 FCC_A1                    CEMENTITE  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
14:41:10,650 [Thread-0] INFO  StandaloneLicenseController: Checking out license for: Diffusion (DICTRA)
 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 GEOMTRICAL 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 /LINEAR/: 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 /LINEAR/: 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-2>
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 GEOMTRICAL 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 GEOMTRICAL 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> @@
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 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>
DIC-3> go d-m
 TIME STEP AT TIME  0.00000E+00
DIC-3> read exc2
 OK
DIC> sim yes
 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
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        3.626488639510962E-006        3.511997011626638E-
006        3.402323193205779E-006        3.207385177398647E-006        3.013575760567609E-006        3.034833370691419E-
006        2.666125028219394E-006        2.602539804322142E-006        2.328375229025504E-006        1.750312349012622E-
006        1.749273203708094E-006        4.075236873032249E-004        6.106453349196179E-003        1.770380341798807E-
006        1.242048115818841E-006        5.483515721600652E-007        5.480043529846149E-007        1.327553301765130E-
007        2.382230520986728E-008        1.323331856029851E-008        5.542161996842264E-009        1.039982722406221E-
009        2.958858956725420E-010        7.697419519572880E-010        4.032279949869757E-010        2.166092460141906E-
012        6.687099630271476E-017       TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =  0.18286937E-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 = .0407183318974313  CR = .0214509582219593
                        FE = .978549041908548
 TOTAL SIZE OF SYSTEM:  2.30050996865E-17 [m^3]
  CPU time used in timestep                4  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
 0.720078253871663        0.720078268703713

output ignored...



... output resumed

 2.283830655729331E-002        2.283830676606915E-002        2.283830676057919E-002        2.283981643379663E-002        2.283995210532048E-
002        2.283448945308952E-002        2.283761255679290E-002        1.491842558976137E-003        3.865918918098311E-
006        9.200378920785326E-009        3.610158102196856E-012        1.062570776420941E-
017       TIME =   7227.0921     DT =   1000.0000     SUM OF SQUARES =  0.32928424E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.13080917E-10 AND  -0.13080917E-10
 POSITION OF INTERFACE CARB / AUS IS   0.42001679E-06
 CELL # 3 VELOCITY AT INTERFACE # 2 IS  -0.14333666E-10 AND  -0.14333666E-10
 POSITION OF INTERFACE CARB / AUS IS   0.23556611E-06
 U-FRACTION IN SYSTEM:  C = .0407429546789286  CR = .0215435267682685
                        FE = .978456473362238
 TOTAL SIZE OF SYSTEM:  2.30050996865E-17 [m^3]
  CPU time used in timestep                4  seconds
 3.400641895705857E-002        3.400641909216802E-002        3.400641906530464E-002        3.400815939702265E-002        3.400827680084697E-
002        3.400197279404037E-002        3.400548308609514E-002        2.366747763705887E-003        3.426599279548059E-
006        7.975520190435769E-010        1.957790690260421E-013        7.278377336561062E-
017       TIME =   8227.0921     DT =   1000.0000     SUM OF SQUARES =  0.24458446E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.11666052E-10 AND  -0.11666052E-10
 POSITION OF INTERFACE CARB / AUS IS   0.40835074E-06
 CELL # 3 VELOCITY AT INTERFACE # 2 IS  -0.13193820E-10 AND  -0.13193820E-10
 POSITION OF INTERFACE CARB / AUS IS   0.22237229E-06
 U-FRACTION IN SYSTEM:  C = .0407430021762649  CR = .021543182536694
                        FE = .978456817593813
 TOTAL SIZE OF SYSTEM:  2.30050996865E-17 [m^3]
  1  GRIDPOINT(S) REMOVED FROM CELL #3   REGION: AUS

  CPU time used in timestep                4  seconds
 3.733423912304688E-002        3.733423922061026E-002        3.733423917931009E-002        3.733593882041732E-002        3.733601936768893E-
002        3.732983448688868E-002        3.733310444812683E-002        3.202648072836520E-003        4.772199214248983E-
006        1.840130679366424E-009        9.353573705619087E-013        3.896529718912137E-
016       TIME =   9227.0921     DT =   1000.0000     SUM OF SQUARES =  0.12300445E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.10556470E-10 AND  -0.10556470E-10
```

```
 POSITION OF INTERFACE CARB / AUS IS   0.39779427E-06
 CELL # 3 VELOCITY AT INTERFACE # 2 IS  -0.12565889E-10 AND  -0.12565889E-10
 POSITION OF INTERFACE CARB / AUS IS   0.20980640E-06
 U-FRACTION IN SYSTEM:  C = .0407430209895106  CR = .021542936786108
                        FE = .978457063344399
 TOTAL SIZE OF SYSTEM:  2.30050996865E-17 [m^3]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUS

  CPU time used in timestep                    4  seconds
 4.867871177422172E-002        4.867871186568649E-002        4.867871184964485E-002        4.868040586309015E-002        4.868045479179083E-
002        4.867410613974811E-002        4.867677352966204E-002        5.134103772368011E-003        8.770123685446737E-
006        6.885304062766576E-009        1.714954977841026E-012        8.043798167157075E-016        2.019731221193595E-
013        8.895510636691113E-019       TIME =   10000.000     DT =   772.90786     SUM OF SQUARES =  0.43787502E-20
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.96123190E-11 AND  -0.96123190E-11
 POSITION OF INTERFACE CARB / AUS IS   0.39036483E-06
 CELL # 3 VELOCITY AT INTERFACE # 2 IS  -0.11916200E-10 AND  -0.11916200E-10
 POSITION OF INTERFACE CARB / AUS IS   0.20059627E-06
 U-FRACTION IN SYSTEM:  C = .0407430131956872  CR = .0215427799692041
                        FE = .978457220161303
 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    2679.6081
 DELETING TIME-RECORD FOR TIME    2884.9149
 DELETING TIME-RECORD FOR TIME    2884.9149
 DELETING TIME-RECORD FOR TIME    2884.9149
 DELETING TIME-RECORD FOR TIME    2884.9149
 DELETING TIME-RECORD FOR TIME    2884.9150
 DELETING TIME-RECORD FOR TIME    2884.9152
 DELETING TIME-RECORD FOR TIME    2884.9155
 DELETING TIME-RECORD FOR TIME    2884.9161
 DELETING TIME-RECORD FOR TIME    2884.9174
 DELETING TIME-RECORD FOR TIME    2884.9200
 DELETING TIME-RECORD FOR TIME    2884.9251
 DELETING TIME-RECORD FOR TIME    2884.9353
 DELETING TIME-RECORD FOR TIME    2884.9558
 DELETING TIME-RECORD FOR TIME    2884.9968
 DELETING TIME-RECORD FOR TIME    2885.0787
 DELETING TIME-RECORD FOR TIME    2885.2425
 DELETING TIME-RECORD FOR TIME    2885.5702
 DELETING TIME-RECORD FOR TIME    2886.2256
 DELETING TIME-RECORD FOR TIME    2887.5363
 DELETING TIME-RECORD FOR TIME    2890.1577
 DELETING TIME-RECORD FOR TIME    2895.4006
 DELETING TIME-RECORD FOR TIME    2905.8864
 DELETING TIME-RECORD FOR TIME    2926.8579
 DELETING TIME-RECORD FOR TIME    2968.8009
 DELETING TIME-RECORD FOR TIME    3052.6870
 DELETING TIME-RECORD FOR TIME    3220.4592
 DELETING TIME-RECORD FOR TIME    3556.0035
 DELETING TIME-RECORD FOR TIME    4227.0921
 DELETING TIME-RECORD FOR TIME    5227.0921
 DELETING TIME-RECORD FOR TIME    6227.0921
 DELETING TIME-RECORD FOR TIME    7227.0921
 DELETING TIME-RECORD FOR TIME    8227.0921

 KEEPING TIME-RECORD FOR TIME    9227.0921
 AND FOR TIME                    10000.000
 WORKSPACE RECLAIMED

 TIMESTEP AT     10000.0000     SELECTED

DIC> ,
DIC> ,
DIC> go sys
14:58:44,423 [Thread-0] INFO  StandaloneLicenseController: Releasing license for: Diffusion (DICTRA)
SYS: ,
SYS: set-inter
SYS:
```

exc2-plot

```
SYS:About

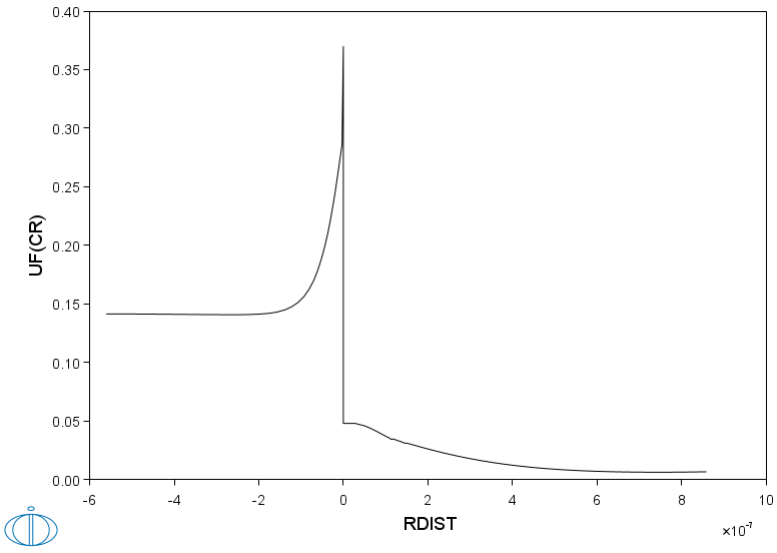
 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software running on Windows 64-bit wordlength
 Compiler: unknown compiler
 License library version: 9.7.0.0036
 Linked: Fri Oct 18 11:32:56 2024


SYS:SYS:MACRO exc2\plot.DCM SYS:
SYS:
SYS: @@ exc2_plot.DCM
SYS:
SYS: @@
SYS: @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE c2
SYS: @@
SYS:
SYS: @@
SYS: @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
SYS: @@
SYS: go d-m
14:59:39,516 [Thread-0] INFO  StandaloneLicenseController: Checking out license for: Diffusion (DICTRA) 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
```

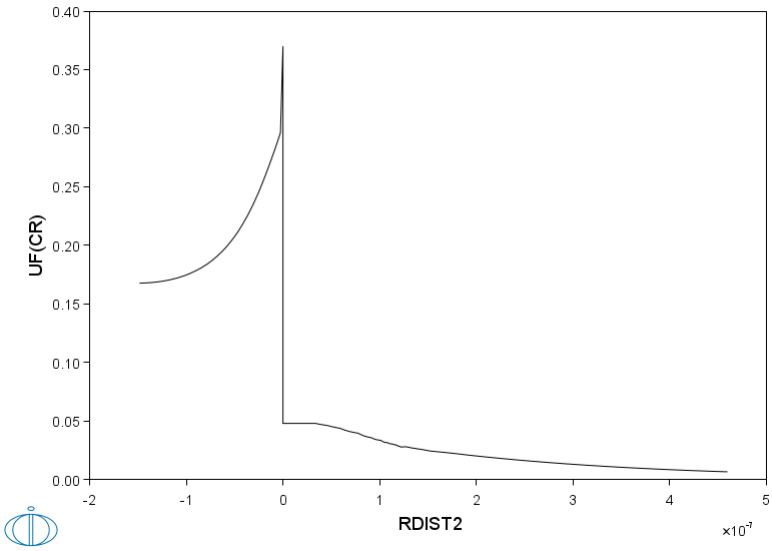
Figure C2.1




```
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: @@
POST-1: @@ SELECT CELL 2
POST-1: @@
POST-1: select-cell
Number /NEXT/: 2
```

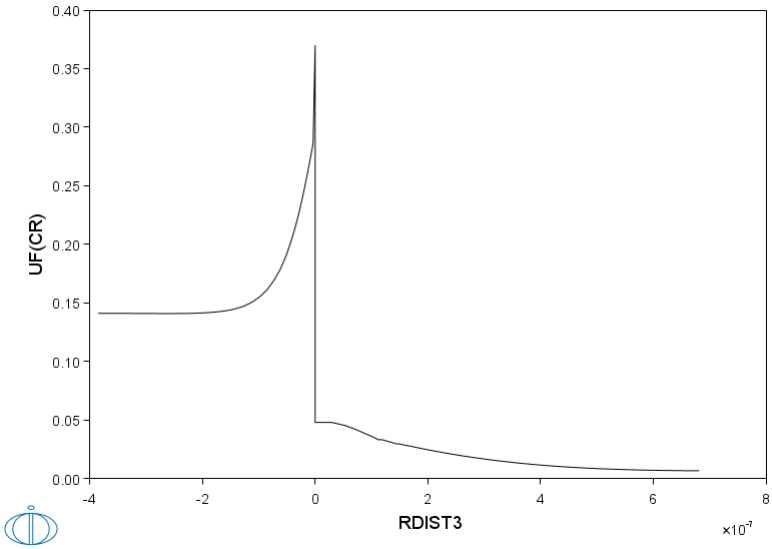
```
 CELL    2 SELECTED
POST-2:
POST-2: enter-symb
Function or table /FUNCTION/: func
NAME: rdist2
FUNCTION: gd-poi(carb,u);
POST-2:
POST-2: s-d-a x rdist2
POST-2:
POST-2: set-title Figure C2.2
POST-2: plot
```

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
```

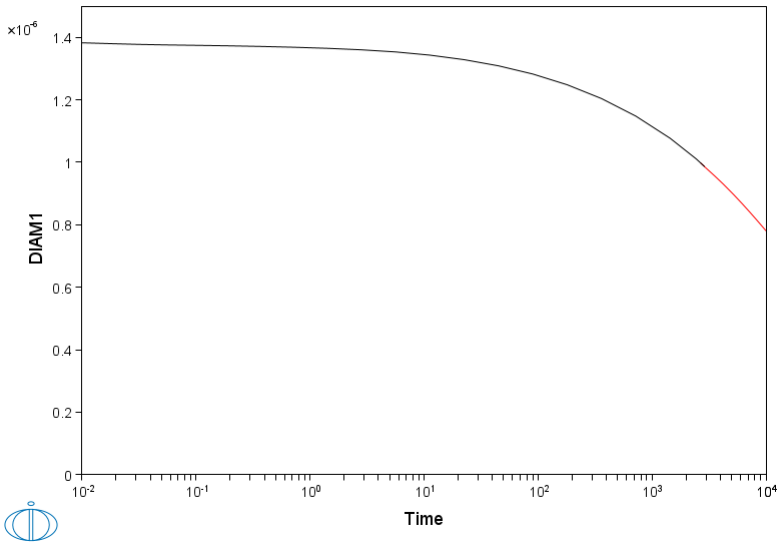
Figure C2.3




```
POST-3:
POST-3:
POST-3:
POST-3:
POST-3:@?<_hit_return_to_continue_>
POST-3:
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: @@
POST-3: @@ SELECT THE FIRST CELL
POST-3: @@
POST-3: sel-cell 1
```

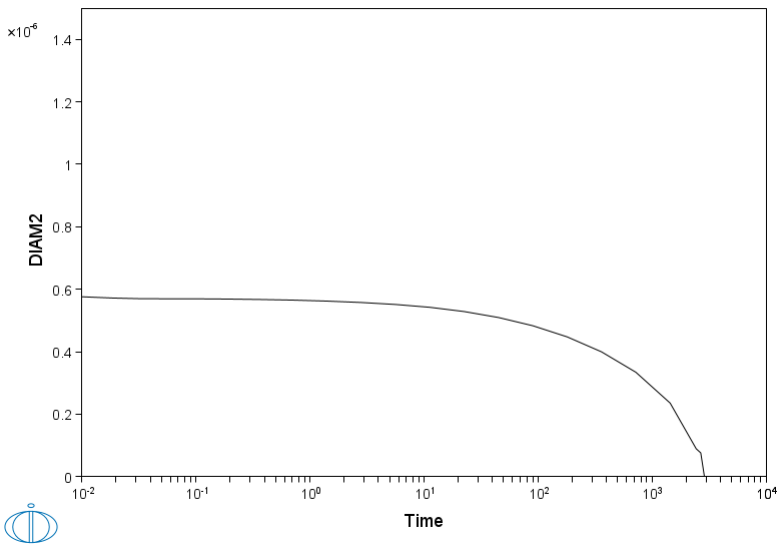
```
 CELL   1 SELECTED
POST-1:
POST-1: s-d-a x time
  INFO: Time is set as independent variable
POST-1: s-s-s x n .01 10000
POST-1: set-axis-type x log
POST-1:
POST-1: enter func diam1=2*poi(carb,u);
POST-1: s-d-a y diam1
POST-1: s-s-s y n 0 1.5e-6
POST-1:
POST-1: s-p-c interf carb upp
POST-1:
POST-1: app n
POST-1: set-title Figure C2.4
POST-1: plot
```

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
```

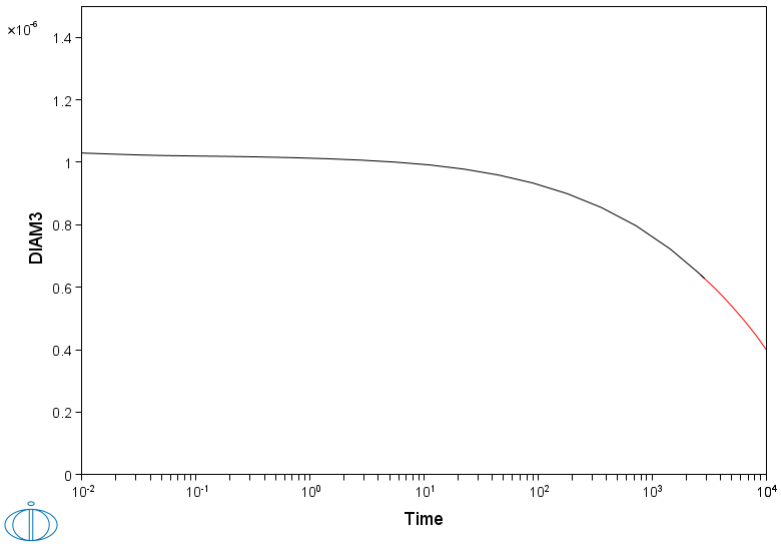
Figure C2.5




```
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
```

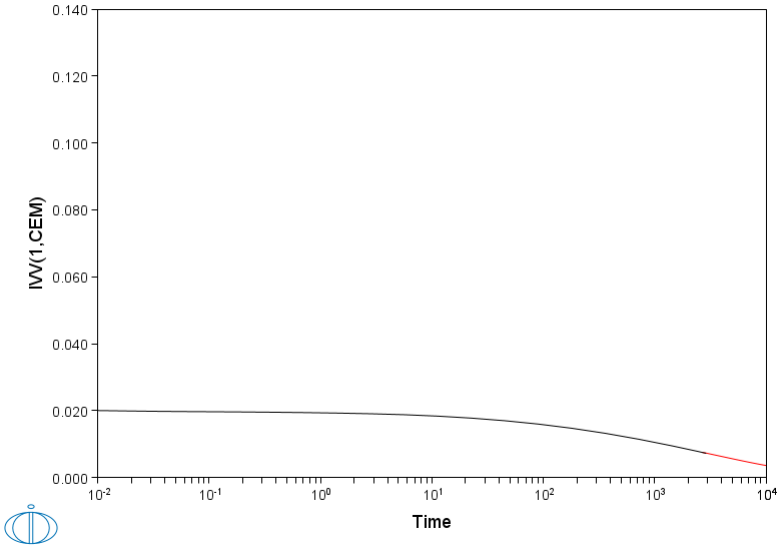
```
 CELL   3 SELECTED
POST-3:
POST-3: enter func diam3=2*poi(carb,u);
POST-3: s-d-a y diam3
POST-3: s-s-s y n 0 1.5e-6
POST-3:
POST-3: s-p-c interf carb upp
POST-3:
POST-3: set-title Figure C2.6
POST-3:
POST-3: plot
```

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
```

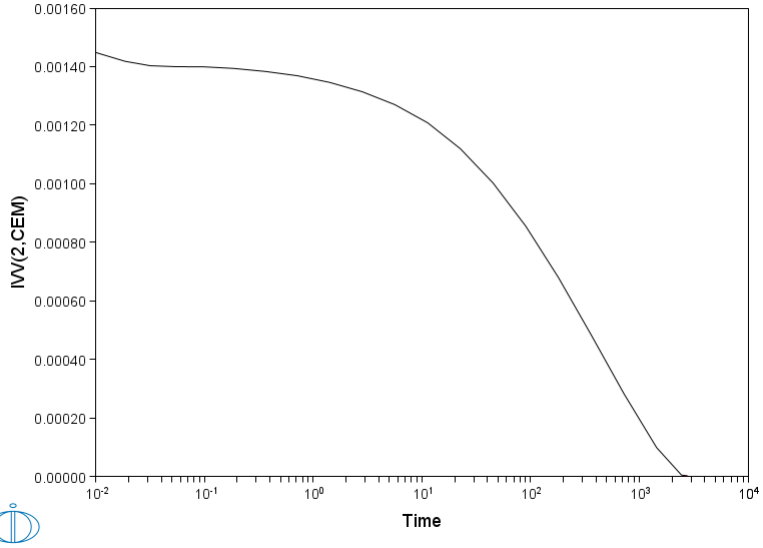
Figure C2.7




```
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
```

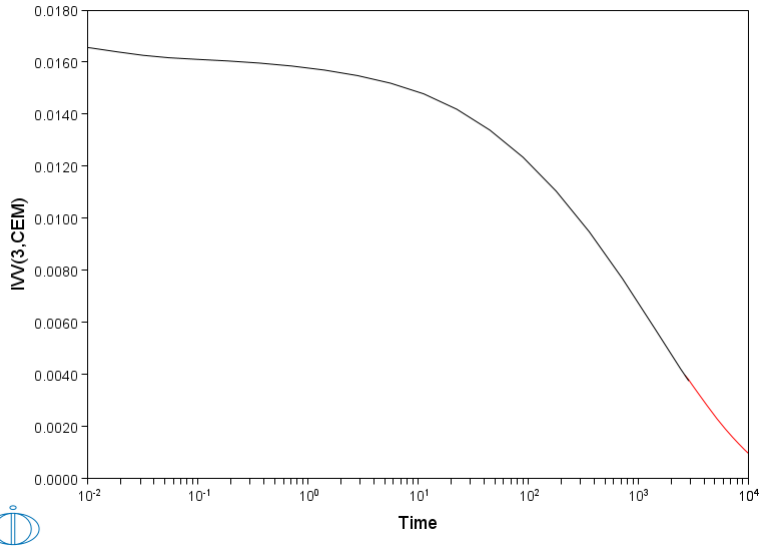
```
POST-3: plot
```

Figure C2.8



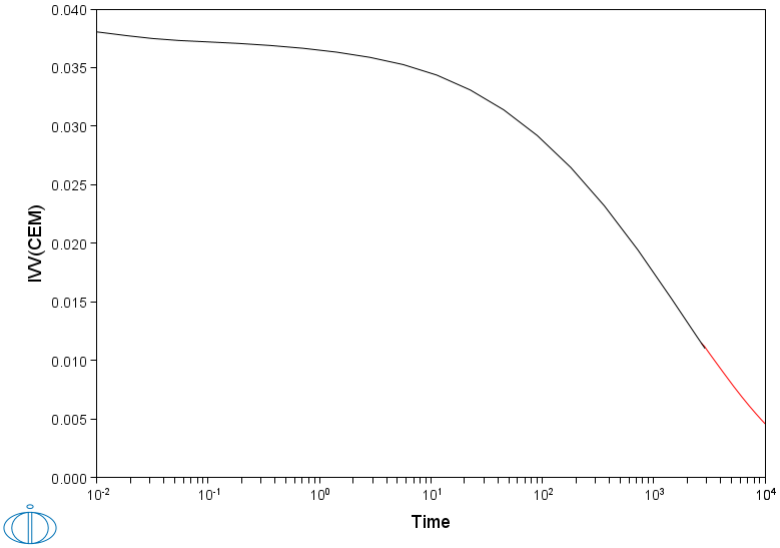

```
POST-3:
POST-3:
POST-3:
POST-3:
POST-3:@?<_hit_return_to_continue_>
POST-3:
POST-3: @@
POST-3: @@ CELL 3
POST-3: @@
POST-3: s-d-a y ivv(3,cem)
POST-3:
POST-3: set-title Figure C2.9
POST-3: plot
```

Figure C2.9



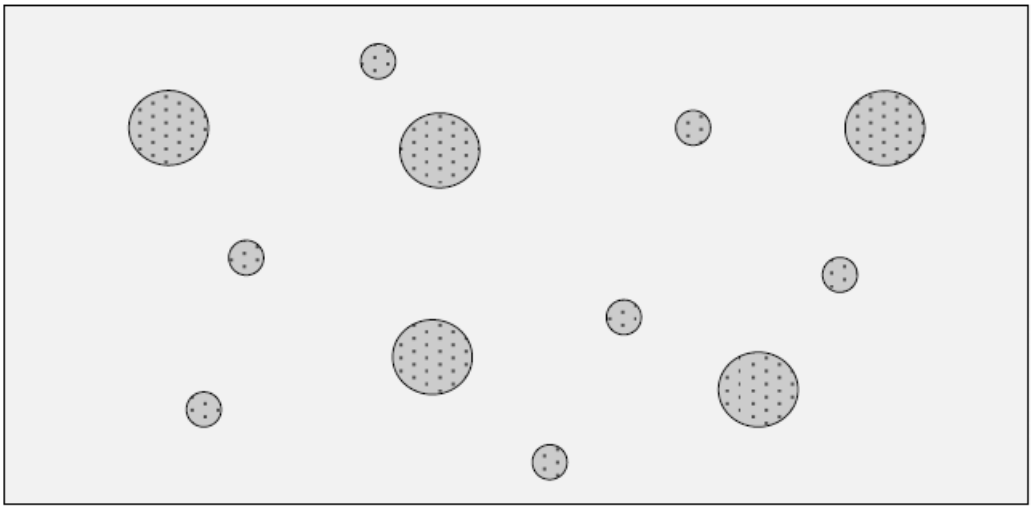

```
POST-3:
POST-3:
POST-3:
POST-3:
POST-3:@?<_hit_return_to_continue_>
POST-3:
POST-3: @@
POST-3: @@ FINALLY, PLOT HOW THE TOTAL VOLUME FRACTION OF CEMENTITE
POST-3: @@ VARIES WITH TIME.
POST-3: @@
POST-3: s-d-a y ivv(cem)
POST-3:
POST-3: set-title Figure C2.10
POST-3: plot
```

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:
```

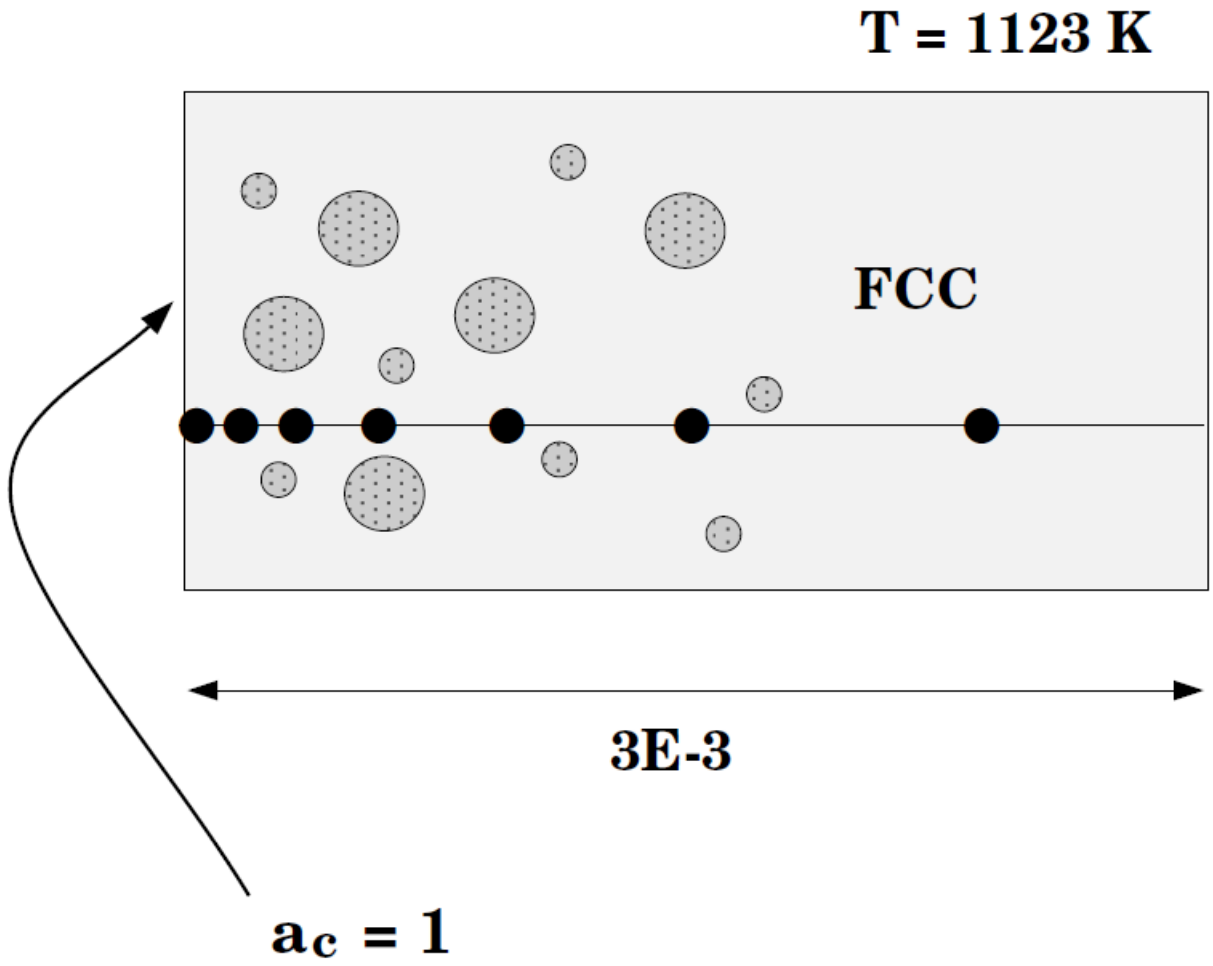
Diffusion in Dispersed Systems



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 M3C2 and M7C3 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.



exd1a-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: unknown compiler
 License library version: 9.7.0.0036
 Linked: Fri Oct 18 11:32:56 2024


SYS:SYS:MACRO exd1a\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. EngstrÃ¶m, L. HÃ¶glund and J. Ã…gren:
SYS: @@ Metall.Trans.A v. 25A (1994), pp. 1127-1134.
SYS: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exd1_setup.DCM
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASE
SYS: @@
SYS: go da
15:00:54,047 [Thread-0] INFO  LicenseManager: Initializing user: jenkins.integrationtest@thermocalc.se
15:00:54,063 [Thread-0] INFO  LicenseController: Running License Spring in DEV environment.
15:00:55,138 [Thread-0] INFO  LicenseManager: There is an activated standalone license for jenkins.integrationtest@thermocalc.se for TC-
Application
 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 v5.0

 VA                       /-  DEFINED
TDB_FEDEMO: def-sys ni cr c
 NI                       CR                       C
   DEFINED
TDB_FEDEMO: rej ph * all
 BCC_A2                   CBCC_A12                 CEMENTITE
 CHI_A12                  CUB_A13                  DIAMOND_FCC_A4
 FCC_A1                   GAS:G                    GRAPHITE
 HCP_A3                   KSI_CARBIDE              LAVES_PHASE_C14
 LIQUID:L                 M23C6                    M3C2
 M7C3                     SIGMA  REJECTED
TDB_FEDEMO: res ph fcc,m7c3,m3c2,grap
 FCC_A1                   M7C3                     M3C2
 GRAPHITE  RESTORED
TDB_FEDEMO: get
15:00:56,204 [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 v4.0

 VA  DEFINED
APP: def-sys ni c cr
 NI                       C                        CR
   DEFINED
APP: rej ph * all
 BCC_A2                   FCC_A1                   CEMENTITE
 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: @@
APP: @@ ENTER THE DICTRA MONITOR
APP: @@
APP: go d-m
15:00:56,678 [Thread-0] INFO  StandaloneLicenseController: Checking out license for: Diffusion (DICTRA)
 NO TIME STEP DEFINED
 *** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
 *** ENTERING M3C2 AS A DIFFUSION NONE PHASE
 *** ENTERING M7C3 AS A DIFFUSION NONE PHASE
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 1123; * N
DIC>
DIC> @@
DIC> @@ SET THE REFERENCE STATE FOR CARBON
DIC> @@
DIC> set-reference-state
Component: C
Reference state: grap
Temperature /*/: *
Pressure /100000/: 101325
DIC>
DIC> @@
DIC> @@ ENTER THE REGION aus
DIC> @@
DIC> enter-region aus
DIC>
DIC> @@
DIC> @@ ENTER A GEOMETRICAL GRID INTO THE REGION
DIC> @@
DIC> enter-grid aus 3e-3 geo 100 1.02
DIC>
DIC> @@
DIC> @@ ENTER A MATRIX PHASE IN THE REGION
DIC> @@
DIC> enter-phase act aus matrix fcc_a1#1
DIC>
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> @@
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> @@
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>
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> @@
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> @@
DIC> @@ ENTER THE LABYRINTH FACTOR
DIC> @@
```

```
DIC> enter-lab
REGION NAME : aus
f(T,P,VOLFR,X)= volfr**2;
DIC>
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 SO 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-simulation-condition
NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /AUTO/:
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/: 99
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -> 1): /AUTO/:
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/:
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>
```

exd1a-run

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exd1a\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 AS A DIFFUSION NONE PHASE
 *** ENTERING M3C2 AS A DIFFUSION NONE PHASE
 *** ENTERING M7C3 AS A DIFFUSION NONE PHASE
DIC> read exd1
 OK
DIC> sim
 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 HAS NO VOLUME FRACTION, CREATING ONE
  WARNING:M3C2 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 = 8.3223382995161E-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 = 1.14491977930612E-04  CR = .273386452547545
                        NI = .726613547452455
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1  seconds
 TIME =  0.40010010     DT =  0.40000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = 1.34397531949335E-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 = 1.73234190866319E-04  CR = .273386451404806
                        NI = .726613548595194
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0  seconds
 TIME =   136.73132     DT =   75.504702     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = 2.15195361346136E-04  CR = .273386450378639
                        NI = .726613549621361
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0  seconds
 TIME =   246.77986     DT =   110.04854     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = 2.65132773423406E-04  CR = .273386449367934
                        NI = .726613550632066
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1  seconds
 TIME =   417.73078     DT =   170.95092     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = 3.26703519714743E-04  CR = .273386448427441
                        NI = .72661355157256
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0  seconds
 TIME =   700.87762     DT =   283.14684     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = 4.03852183677248E-04  CR = .273386447458975
                        NI = .726613552541025
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0  seconds
 TIME =   1196.7621     DT =   495.88443     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = 5.03958315340985E-04  CR = .273386446322885
                        NI = .726613553677115
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1  seconds
 TIME =   2136.4660     DT =   939.70399     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = 6.43012086810223E-04  CR = .273386444988437
                        NI = .726613555011563
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0  seconds
 TIME =   3936.4660     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = 8.38519749163073E-04  CR = .273386443511134
                        NI = .726613556488866
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0  seconds
 TIME =   5736.4660     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0010173697033215  CR = .273386442681224
                        NI = .726613557318776
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0  seconds
 TIME =   7536.4660     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00118296902880157  CR = .273386442066142
                        NI = .726613557933858
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0  seconds
 TIME =   9336.4660     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00133879540957735  CR = .273386441011293
                        NI = .726613558988706
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1  seconds
 TIME =   11136.466     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00148538430057558  CR = .27338643927903
                        NI = .72661356072097
 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 = .00162329996141555  CR = .273386436825667
                        NI = .726613563174333
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0  seconds
 TIME =   14736.466     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00175666371078121  CR = .273386434544898
                        NI = .726613565455102
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0  seconds
```

```
 TIME =   16509.560     DT =   1773.0939     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00188419698676038  CR = .273386432317815
                        NI = .726613567682185
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0  seconds
 TIME =   18202.529     DT =   1692.9692     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00200374370728573  CR = .273386430131716
                        NI = .726613569868284
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1  seconds
 TIME =   19871.496     DT =   1668.9668     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00212043403493914  CR = .273386427985689
                        NI = .726613572014311
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0  seconds
 TIME =   21585.287     DT =   1713.7913     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00223651041851037  CR = .273386426227076
                        NI = .726613573772924
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0  seconds
 TIME =   23385.287     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00235302551823151  CR = .273386424970864


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 = .031453798352627  CR = .27338632521063
                        NI = .726613674789370
 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 = .0314617329030152  CR = .273386325190173
                        NI = .726613674809828
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0  seconds
 TIME =   3567585.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0314696650642585  CR = .273386325169498
                        NI = .726613674830502
 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 = .0314775948480471  CR = .273386325148606
                        NI = .726613674851394
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1  seconds
 TIME =   3571185.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0314855222664734  CR = .273386325127497
                        NI = .726613674872503
 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 = .031493447332012  CR = .27338632510617
                        NI = .726613674893830
 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 = .0315013700574988  CR = .273386325084625
                        NI = .726613674915375
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0  seconds
 TIME =   3576585.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0315092904561124  CR = .273386325062862
                        NI = .726613674937138
 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 = .0315172085413542  CR = .273386325040881
                        NI = .726613674959119
 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 = .0315251243270304  CR = .273386325018682
                        NI = .726613674981318
 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 = .0315330378272337  CR = .273386324996264
                        NI = .726613675003736
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0  seconds
 TIME =   3583785.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0315409490563256  CR = .273386324973628
                        NI = .726613675026373
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1  seconds
 TIME =   3585585.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0315488580289199  CR = .273386324950772
                        NI = .726613675049228
 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 = .0315567647598656  CR = .273386324927698
                        NI = .726613675072303
 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 = .0315646692642313  CR = .273386324904404
                        NI = .726613675095596
 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 = .0315725715572896  CR = .273386324880891
                        NI = .726613675119109
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0  seconds
 TIME =   3592785.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0315804716545022  CR = .273386324857158
                        NI = .726613675142842
 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 = .0315883695715051  CR = .273386324833206
                        NI = .726613675166795
 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 = .0315962653240952  CR = .273386324809033
                        NI = .726613675190967
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1  seconds
 TIME =   3598185.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0316041589282164  CR = .27338632478464
                        NI = .72661367521536
 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 = .0316120503999466  CR = .273386324760027
                        NI = .726613675239973
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0  seconds
 TIME =   3600000.0     DT =   14.712794     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0316121157454992  CR = .273386324759815
                        NI = .726613675240185
 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

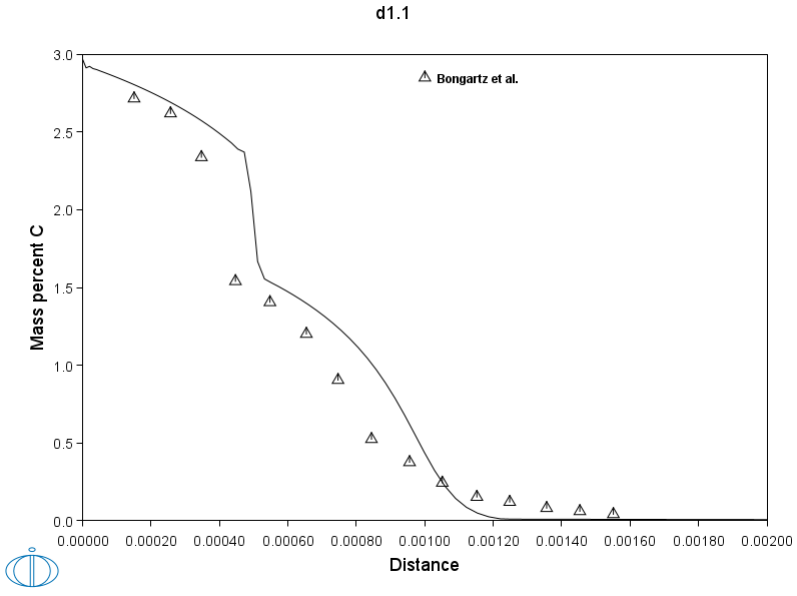
 TIMESTEP AT     3600000.00     SELECTED

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

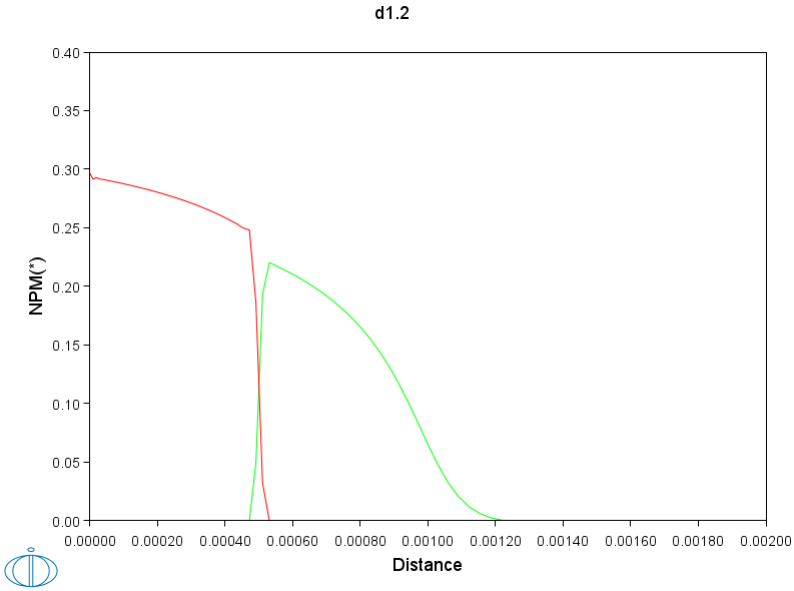
exd1a-plot

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exd1a\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 AS A DIFFUSION NONE PHASE
 *** ENTERING M3C2 AS A DIFFUSION NONE PHASE
 *** ENTERING M7C3 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
```




```
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
```

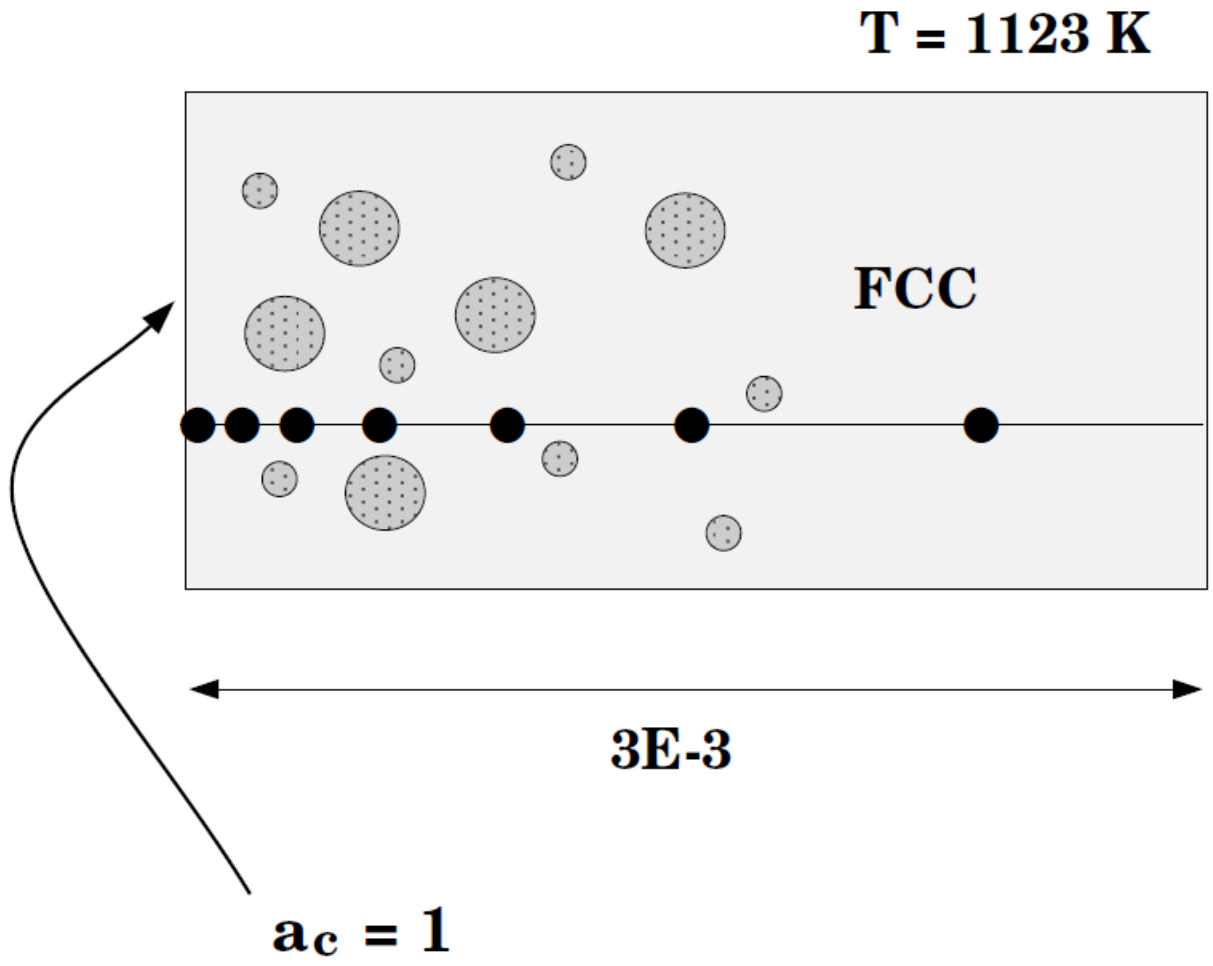



```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: set-inter
 --OK---
POST-1:
```

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.



exd1b-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: unknown compiler
 License library version: 9.7.0.0036
 Linked: Fri Oct 18 11:32:56 2024


SYS:SYS:MACRO exd1b\setup.DCM
SYS: ï»¿@@
 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. EngstrÃ¶m, L. HÃ¶glund and J. Ã…gren: 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: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exd1b_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
15:08:46,043 [Thread-0] INFO  LicenseManager: Initializing user: jenkins.integrationtest@thermocalc.se
15:08:46,055 [Thread-0] INFO  LicenseController: Running License Spring in DEV environment.
15:08:47,155 [Thread-0] INFO  LicenseManager: There is an activated standalone license for jenkins.integrationtest@thermocalc.se for TC-
Application
 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 v5.0

 VA                       /-  DEFINED
TDB_FEDEMO: def-sys ni cr c
 NI                       CR                       C
   DEFINED
TDB_FEDEMO: rej ph * all
 BCC_A2                   CBCC_A12                 CEMENTITE
 CHI_A12                  CUB_A13                  DIAMOND_FCC_A4
 FCC_A1                   GAS:G                    GRAPHITE
 HCP_A3                   KSI_CARBIDE              LAVES_PHASE_C14
 LIQUID:L                 M23C6                    M3C2
 M7C3                     SIGMA  REJECTED
TDB_FEDEMO: res ph fcc,m7c3,m3c2,grap
 FCC_A1                   M7C3                     M3C2
 GRAPHITE  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 v4.0

 VA  DEFINED
APP: def-sys ni c cr
 NI                       C                        CR
   DEFINED
APP: rej ph * all
 BCC_A2                   FCC_A1                   CEMENTITE
 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: @@
APP: @@ ENTER THE DICTRA MONITOR
APP: @@
APP: go d-m
15:08:48,098 [Thread-0] INFO  StandaloneLicenseController: Checking out license for: Diffusion (DICTRA)
 NO TIME STEP DEFINED
 *** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
 *** ENTERING M3C2 AS A DIFFUSION NONE PHASE
 *** ENTERING M7C3 AS A DIFFUSION NONE PHASE
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 1123; * N
DIC>
DIC> @@
DIC> @@ SET THE REFERENCE STATE FOR CARBON
DIC> @@
DIC> set-reference-state
Component: C
Reference state: grap
Temperature /*/: *
Pressure /100000/: 101325
DIC>
DIC> @@
DIC> @@ ENTER THE REGION aus
DIC> @@
DIC> enter-region aus
DIC>
DIC> @@
DIC> @@ ENTER A GEOMETRICAL GRID INTO THE REGION
DIC> @@
DIC> enter-grid aus 3e-3 geo 100 1.02
DIC>
DIC> @@
DIC> @@ ENTER A MATRIX PHASE IN THE REGION
DIC> @@
DIC> enter-phase act aus matrix fcc_a1#1
DIC>
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> @@
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> @@
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>
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> @@
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> @@
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-simulation-condition
NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /AUTO/:
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/: 99
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -> 1): /AUTO/:
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/:
DIC>
DIC> @@
DIC> @@ SAVE THE SETUP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exd1 y
DIC>
DIC> set-inter
 --OK---
DIC>
```

exd1b-run

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exd1b\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 AS A DIFFUSION NONE PHASE
 *** ENTERING M3C2 AS A DIFFUSION NONE PHASE
 *** ENTERING M7C3 AS A DIFFUSION NONE PHASE
DIC> read exd1
 OK
DIC> sim
 DEGREE OF IMPLICITY 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 HAS NO VOLUME FRACTION, CREATING ONE
WARNING:M3C2 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
Starting time-step t0=   90.439680     dt=   3.3554432


output ignored...


... output resumed

 DELETING TIME-RECORD FOR TIME    2287724.2
 DELETING TIME-RECORD FOR TIME    2294596.2
 DELETING TIME-RECORD FOR TIME    2301468.1
 DELETING TIME-RECORD FOR TIME    2308340.1
 DELETING TIME-RECORD FOR TIME    2315212.0
 DELETING TIME-RECORD FOR TIME    2322084.0
 DELETING TIME-RECORD FOR TIME    2328955.9
 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    2593525.9
 DELETING TIME-RECORD FOR TIME    2600397.9
 DELETING TIME-RECORD FOR TIME    2607269.8
 DELETING TIME-RECORD FOR TIME    2614141.8
 DELETING TIME-RECORD FOR TIME    2621013.7
 DELETING TIME-RECORD FOR TIME    2627885.6
 DELETING TIME-RECORD FOR TIME    2634757.6
 DELETING TIME-RECORD FOR TIME    2641629.5
 DELETING TIME-RECORD FOR TIME    2648501.5
 DELETING TIME-RECORD FOR TIME    2655373.4
 DELETING TIME-RECORD FOR TIME    2662245.4
 DELETING TIME-RECORD FOR TIME    2669117.3
 DELETING TIME-RECORD FOR TIME    2675989.3
 DELETING TIME-RECORD FOR TIME    2682861.2
 DELETING TIME-RECORD FOR TIME    2689733.2
 DELETING TIME-RECORD FOR TIME    2696605.1
 DELETING TIME-RECORD FOR TIME    2703477.1
 DELETING TIME-RECORD FOR TIME    2710349.0
 DELETING TIME-RECORD FOR TIME    2717221.0
 DELETING TIME-RECORD FOR TIME    2724092.9
 DELETING TIME-RECORD FOR TIME    2730964.9
 DELETING TIME-RECORD FOR TIME    2737836.8
 DELETING TIME-RECORD FOR TIME    2744708.8
 DELETING TIME-RECORD FOR TIME    2758452.7
 DELETING TIME-RECORD FOR TIME    2772196.6
 DELETING TIME-RECORD FOR TIME    2785940.4
 DELETING TIME-RECORD FOR TIME    2799684.3
 DELETING TIME-RECORD FOR TIME    2813428.2
 DELETING TIME-RECORD FOR TIME    2827172.1
 DELETING TIME-RECORD FOR TIME    2840916.0
 DELETING TIME-RECORD FOR TIME    2854659.9
 DELETING TIME-RECORD FOR TIME    2868403.8
 DELETING TIME-RECORD FOR TIME    2875275.8
 DELETING TIME-RECORD FOR TIME    2882147.7
 DELETING TIME-RECORD FOR TIME    2895891.6
 DELETING TIME-RECORD FOR TIME    2909635.5
 DELETING TIME-RECORD FOR TIME    2923379.4
 DELETING TIME-RECORD FOR TIME    2937123.3
 DELETING TIME-RECORD FOR TIME    2950867.2
 DELETING TIME-RECORD FOR TIME    2964611.1
 DELETING TIME-RECORD FOR TIME    2978355.0
 DELETING TIME-RECORD FOR TIME    2992098.9
```

```
 DELETING TIME-RECORD FOR TIME    3005842.8
 DELETING TIME-RECORD FOR TIME    3019586.7
 DELETING TIME-RECORD FOR TIME    3033330.6
 DELETING TIME-RECORD FOR TIME    3047074.5
 DELETING TIME-RECORD FOR TIME    3060818.4
 DELETING TIME-RECORD FOR TIME    3074562.2
 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    3239489.0
 DELETING TIME-RECORD FOR TIME    3253232.9
 DELETING TIME-RECORD FOR TIME    3266976.8
 DELETING TIME-RECORD FOR TIME    3280720.7
 DELETING TIME-RECORD FOR TIME    3294464.6
 DELETING TIME-RECORD FOR TIME    3308208.5
 DELETING TIME-RECORD FOR TIME    3321952.4
 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    3567624.5
 DELETING TIME-RECORD FOR TIME    3572349.0
 DELETING TIME-RECORD FOR TIME    3582656.9

 KEEPING TIME-RECORD FOR TIME    3596400.8
 AND FOR TIME                    3600000.0
 WORKSPACE RECLAIMED
 -------------------------------------------------
 INTERPOLATION SCHEME USED THIS FRACTION OF
 THE ALLOCATED MEMORY:   5.119531976024998E-002
 EFFICIENCY FACTOR:    65.7005540833534
 -------------------------------------------------
 DEALLOCATING
 -------------------------------------------------

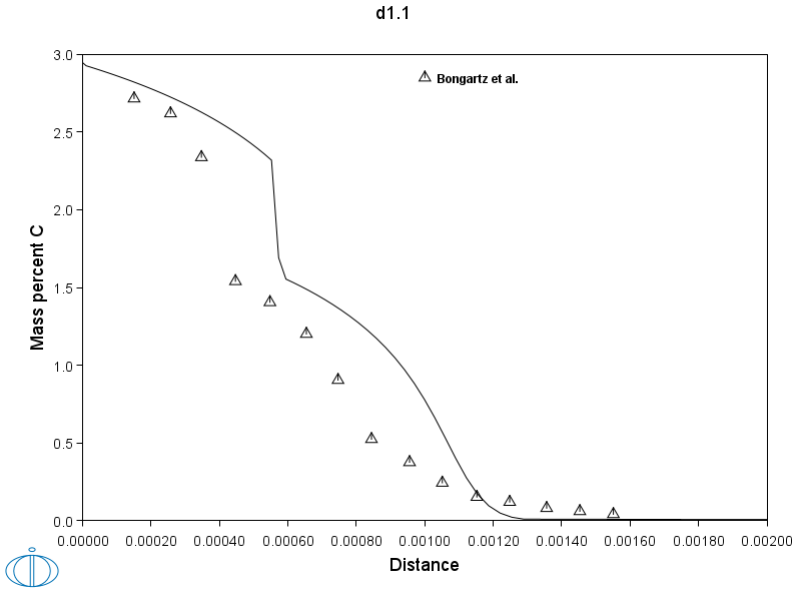
 TIMESTEP AT     3600000.00     SELECTED

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

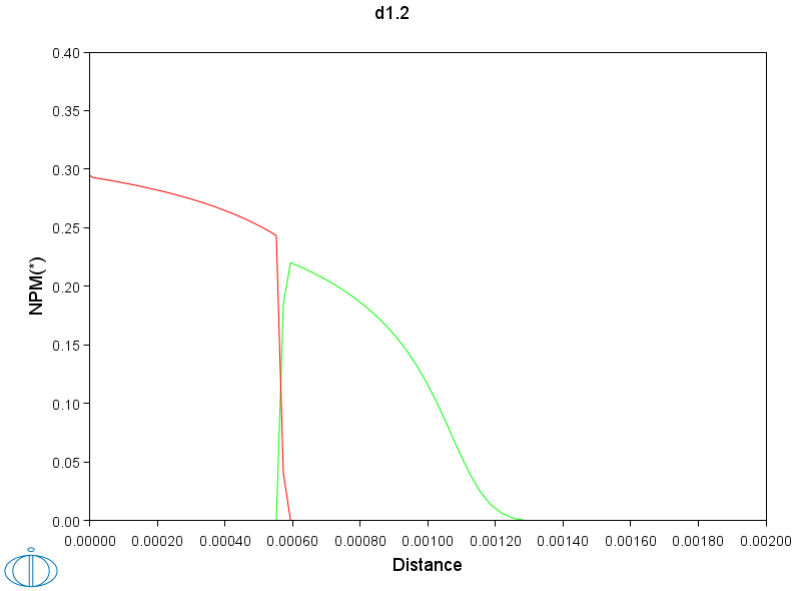
exd1b-plot

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exd1b\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 AS A DIFFUSION NONE PHASE
 *** ENTERING M3C2 AS A DIFFUSION NONE PHASE
 *** ENTERING M7C3 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
```




```
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: plot
```



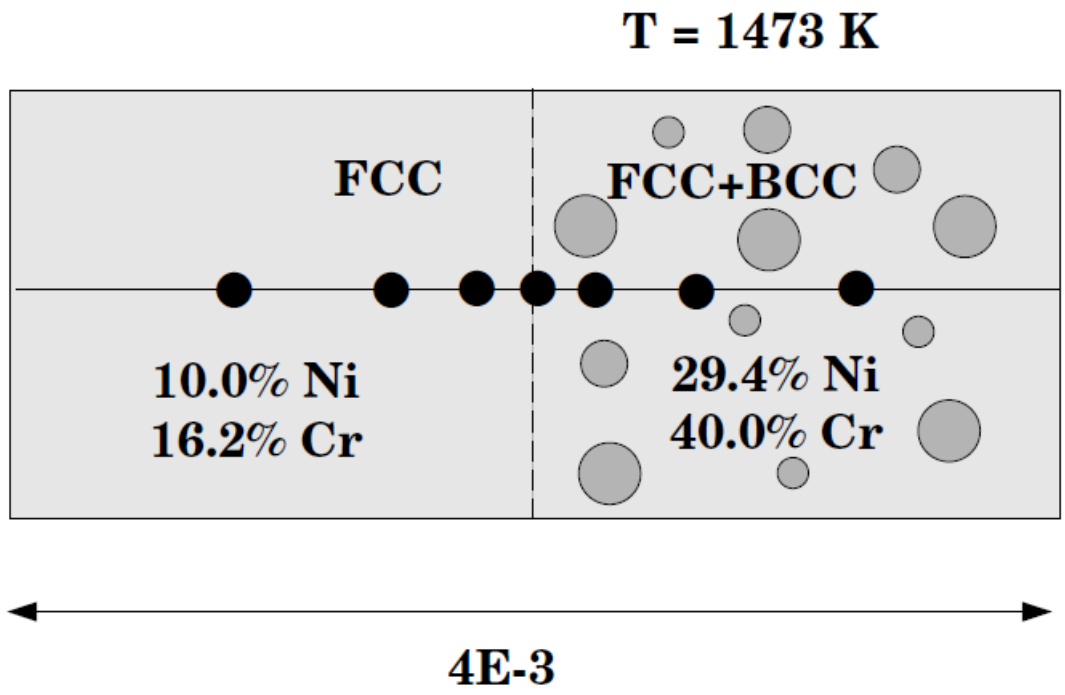

```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: set-inter
 --OK---
POST-1:
```

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: unknown compiler
 License library version: 9.7.0.0036
 Linked: Fri Oct 18 11:32:56 2024


SYS:SYS:MACRO 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. EngstrÃ¶m: 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: ------------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exd2_setup.DCM
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASE
SYS: @@
SYS: go da
15:13:08,706 [Thread-0] INFO  LicenseManager: Initializing user: jenkins.integrationtest@thermocalc.se
15:13:08,719 [Thread-0] INFO  LicenseController: Running License Spring in DEV environment.
15:13:09,777 [Thread-0] INFO  LicenseManager: There is an activated standalone license for jenkins.integrationtest@thermocalc.se for TC-
Application
 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 v5.0

 VA                        /-  DEFINED
TDB_FEDEMO: def-sys fe ni cr
 FE                        NI                        CR
   DEFINED
TDB_FEDEMO: rej ph * all
 BCC_A2                    CBCC_A12                  CHI_A12
 CUB_A13                   FCC_A1                    GAS:G
 HCP_A3                    LAVES_PHASE_C14           LIQUID:L
 SIGMA  REJECTED
TDB_FEDEMO: res ph fcc,bcc
 FCC_A1                    BCC_A2  RESTORED
TDB_FEDEMO: get
15:13:10,867 [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 v4.0

 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
15:13:11,406 [Thread-0] INFO  StandaloneLicenseController: Checking out license for: Diffusion (DICTRA)
 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 A DOUBLE GEOMETRICAL GRID INTO THE REGION
DIC> @@ THIS GIVES A SHORT DISTANCE BETWEEN THE GRIDPOINTS
DIC> @@ IN THE MIDDLE OF THE REGION WHERE THE INITIAL INTERFACE IS
DIC> @@
DIC> enter-grid fer
WIDTH OF REGION /1/: 4e-3
TYPE /LINEAR/: double
NUMBER OF POINTS /50/: 200
VALUE OF R IN THE GEOMETRICAL SERIE FOR LOWER PART OF REGION: 0.97
VALUE OF R IN THE GEOMETRICAL SERIE FOR UPPER PART OF REGION: 1.03093
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 FROM FILES
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
TYPE /LINEAR/: read d2cr.dat
PROFILE FOR /NI/: ni
TYPE /LINEAR/: read d2ni.dat
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-simulation-condition
NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /AUTO/:
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/: 99
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -> 1): /AUTO/:
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/:
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 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
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
 U-FRACTION IN SYSTEM:  CR = .297842647391914  FE = .517227320517284
                                                                    NI = .184930032090802
                                                  TOTAL SIZE OF SYSTEM:  .004 [m]
  WARNING:BCC_A2 HAS NO VOLUME FRACTION, CREATING ONE
 U-FRACTION IN SYSTEM:  CR = .297842647391914  FE = .517227320517284
                        NI = .184930032090802
 TOTAL SIZE OF SYSTEM:  .004 [m]
 TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .29784264735407  FE = .517227320607451
                                                                    NI = .184930032038479
                                                  TOTAL SIZE OF SYSTEM:  .004 [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:  CR = .297842648053526  FE = .51722731894091

                        NI = .184930033005564
 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 = .297842678638828  FE = .517227246207373
                        NI = .184930075153799
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0  seconds
 TIME =   271.88387     DT =   271.48377     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297847795079484  FE = .51721624145468
                        NI = .184935963465835
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    1  seconds
 TIME =   814.85142     DT =   542.96755     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297849638822154  FE = .517212917841346
                        NI = .184937443336499
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0  seconds
 TIME =   1900.7865     DT =   1085.9351     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297850567224199  FE = .517211425368537
                        NI = .184938007407264
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0  seconds
 TIME =   4072.6567     DT =   2171.8702     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297851129181218  FE = .517210587708858
                        NI = .184938283109924
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    1  seconds
 TIME =   8416.3971     DT =   4343.7404     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297851499665049  FE = .517210052695751
                        NI = .1849384476392
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0  seconds
 TIME =   13416.397     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297851736213304  FE = .517209776489761
                        NI = .184938487296936
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0  seconds
 TIME =   18416.397     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297851886304404  FE = .517209625386024
                        NI = .184938488309573
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    1  seconds
 TIME =   23416.397     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297851977716567  FE = .517209529914972
                        NI = .184938492368462
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0  seconds
 TIME =   28416.397     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852026282483  FE = .517209463841181
                        NI = .184938509876335
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0  seconds
 TIME =   33416.397     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852041585337  FE = .517209416417482
                        NI = .184938541997181
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    1  seconds
 TIME =   38416.397     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852041308091  FE = .517209383465791
                        NI = .184938575226117
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0  seconds
 TIME =   43416.397     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852052435151  FE = .517209358433594
                        NI = .184938589131255
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0  seconds
 TIME =   48416.397     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852064191602  FE = .517209339986068
                        NI = .18493859582233
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0  seconds
 TIME =   53416.397     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852067109212  FE = .517209327487742
                        NI = .184938605403047
 TOTAL SIZE OF SYSTEM:  .004 [m]
```

```
 CPU time used in timestep                    0  seconds
 TIME =   58416.397     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852077817661  FE = .517209313736656
                        NI = .184938608445684
 TOTAL SIZE OF SYSTEM:  .004 [m]
 CPU time used in timestep                    0  seconds
 TIME =   63416.397     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852087274147  FE = .517209300962537
                        NI = .184938611763317
 TOTAL SIZE OF SYSTEM:  .004 [m]
 CPU time used in timestep                    1  seconds
 TIME =   68416.397     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852090608974  FE = .517209290212186
                        NI = .18493861917884
 TOTAL SIZE OF SYSTEM:  .004 [m]
 CPU time used in timestep                    0  seconds
 TIME =   73416.397     DT =   5000.0000     SUM OF SQUARES =   0.0000000


output ignored...



... output resumed

 U-FRACTION IN SYSTEM:  CR = .297852053448001  FE = .517209174262072
                        NI = .184938772289927
 TOTAL SIZE OF SYSTEM:  .004 [m]
 CPU time used in timestep                    0  seconds
 TIME =   608416.40     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852057961433  FE = .517209173665085
                        NI = .184938768373483
 TOTAL SIZE OF SYSTEM:  .004 [m]
 CPU time used in timestep                    0  seconds
 TIME =   613416.40     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852061283561  FE = .51720917357851
                        NI = .184938765137929
 TOTAL SIZE OF SYSTEM:  .004 [m]
 CPU time used in timestep                    1  seconds
 TIME =   618416.40     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852063346543  FE = .517209173965083
                        NI = .184938762688374
 TOTAL SIZE OF SYSTEM:  .004 [m]
 CPU time used in timestep                    0  seconds
 TIME =   623416.40     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852063998468  FE = .517209174903867
                        NI = .184938761097665
 TOTAL SIZE OF SYSTEM:  .004 [m]
 CPU time used in timestep                    0  seconds
 TIME =   628416.40     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852063172889  FE = .517209176410902
                        NI = .184938760416209
 TOTAL SIZE OF SYSTEM:  .004 [m]
 CPU time used in timestep                    0  seconds
 TIME =   633416.40     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852061575864  FE = .517209175951883
                        NI = .184938762472253
 TOTAL SIZE OF SYSTEM:  .004 [m]
 CPU time used in timestep                    0  seconds
 TIME =   638416.40     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852058357297  FE = .517209176189083
                        NI = .18493876545362
 TOTAL SIZE OF SYSTEM:  .004 [m]
 CPU time used in timestep                    0  seconds
 TIME =   643416.40     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852053514545  FE = .517209177039924
                        NI = .184938769445531
 TOTAL SIZE OF SYSTEM:  .004 [m]
 CPU time used in timestep                    1  seconds
 TIME =   648416.40     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852047033294  FE = .517209178463695
                        NI = .184938774503011
 TOTAL SIZE OF SYSTEM:  .004 [m]
 CPU time used in timestep                    0  seconds
 TIME =   653416.40     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852038894178  FE = .517209180441844
                        NI = .184938780663978
 TOTAL SIZE OF SYSTEM:  .004 [m]
 CPU time used in timestep                    0  seconds
 TIME =   658416.40     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852029075284  FE = .517209182967747
                        NI = .184938787956969
 TOTAL SIZE OF SYSTEM:  .004 [m]
 CPU time used in timestep                    0  seconds
 TIME =   663416.40     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852023970342  FE = .517209184577063
                        NI = .184938791452595
 TOTAL SIZE OF SYSTEM:  .004 [m]
 CPU time used in timestep                    0  seconds
 TIME =   668416.40     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852026842133  FE = .517209184685555
                        NI = .184938788472312
 TOTAL SIZE OF SYSTEM:  .004 [m]
 CPU time used in timestep                    1  seconds
 TIME =   673416.40     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852032363208  FE = .517209184531521
                        NI = .184938783105271
 TOTAL SIZE OF SYSTEM:  .004 [m]
 CPU time used in timestep                    0  seconds
 TIME =   678416.40     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852039304553  FE = .517209182207698
                        NI = .184938778487749
 TOTAL SIZE OF SYSTEM:  .004 [m]
 CPU time used in timestep                    0  seconds
 TIME =   683416.40     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852046052987  FE = .517209180294763
                        NI = .18493877365225
 TOTAL SIZE OF SYSTEM:  .004 [m]
 CPU time used in timestep                    0  seconds
 TIME =   688416.40     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852052167002  FE = .51720917880267
                        NI = .184938769030328
 TOTAL SIZE OF SYSTEM:  .004 [m]
 CPU time used in timestep                    0  seconds
 TIME =   693416.40     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852057386756  FE = .517209177738875
```

```
                        NI = .184938764874369
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0  seconds
 TIME =   698416.40     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852061547184  FE = .517209177111162
                        NI = .184938761341654
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    1  seconds
 TIME =   703416.40     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .29785206453641  FE = .517209176928112
                        NI = .184938758535478
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0  seconds
 TIME =   708416.40     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852066274022  FE = .517209177198911
                        NI = .184938756527066
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0  seconds
 TIME =   713416.40     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852066699118  FE = .517209177933359
                        NI = .184938755367522
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0  seconds
 TIME =   718416.40     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852065827036  FE = .517209179079285
                        NI = .184938755093679
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0  seconds
 TIME =   720000.00     DT =   1583.6029     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852062178807  FE = .517209180265847
                        NI = .184938757555346
 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    468416.40
 DELETING TIME-RECORD FOR TIME    708416.40
 DELETING TIME-RECORD FOR TIME    713416.40

 KEEPING TIME-RECORD FOR TIME    718416.40
 AND FOR TIME                    720000.00
 WORKSPACE RECLAIMED

 TIMESTEP AT     720000.000     SELECTED

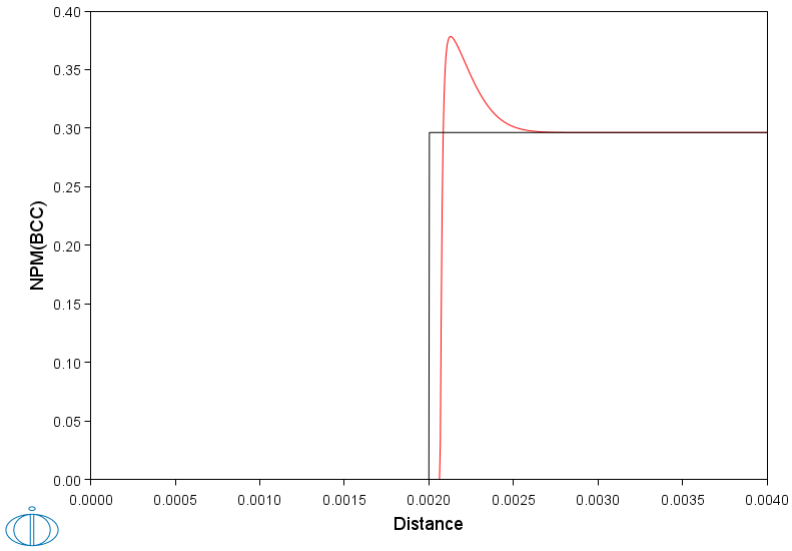
DIC>
DIC>
DIC>
DIC>
DIC> set-inter
 --OK---
DIC>
```

exd2a-plot

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO 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>
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

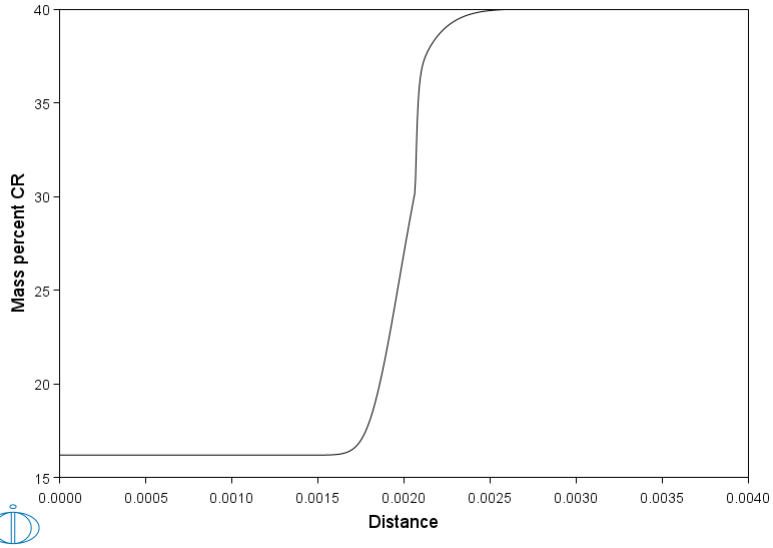
  INFO: Distance is set as independent variable
POST-1: s-p-c time 0 720000
POST-1: set-tit Figure D2.1
POST-1: plot
```

Figure D2.1



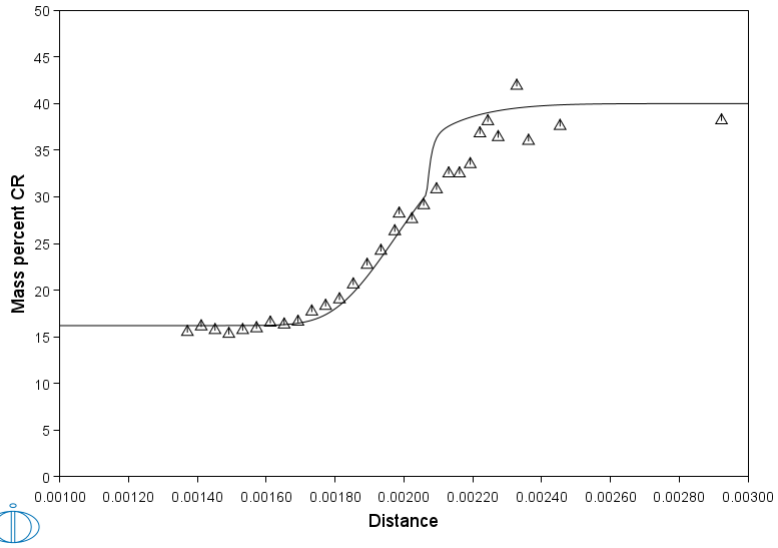

```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1: @@
POST-1: @@ NOW PLOT HOW THE AVERAGE Cr-CONCENTRATION VARIES WITH DISTANCE
POST-1: @@
POST-1: s-d-a y w-p cr
POST-1: s-p-c time last
POST-1: set-tit Figure D2.2
POST-1: plot
```

Figure D2.2



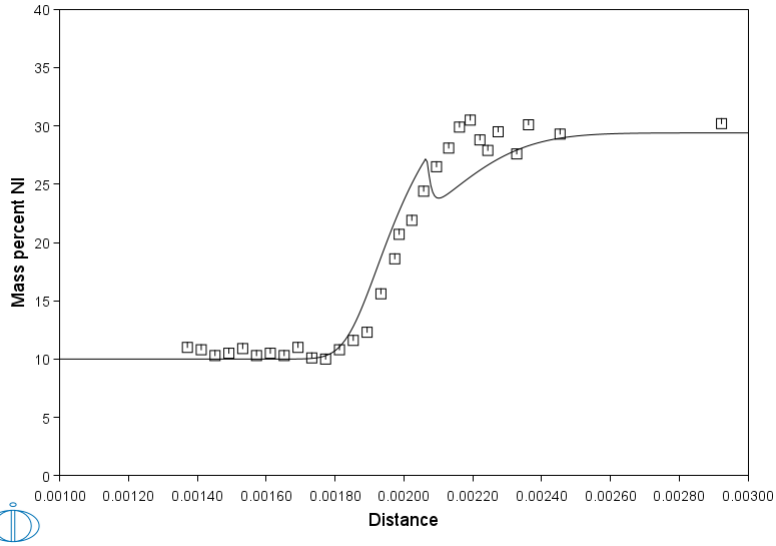

```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1: @@
POST-1: @@ NOW SELECT A BETTER SCALING AND APPEND THE EXPERIMENTAL DATA
POST-1: @@
POST-1:
POST-1: app y exd2.exp
PROLOGUE NUMBER: /0/: 1
DATASET NUMBER(s): /-1/: 4
POST-1:
POST-1: s-s-s y n 0 50
POST-1: s-s-s x n 10e-4 30e-4
POST-1:
POST-1: set-tit Figure D2.3
POST-1: plot
```

Figure D2.3



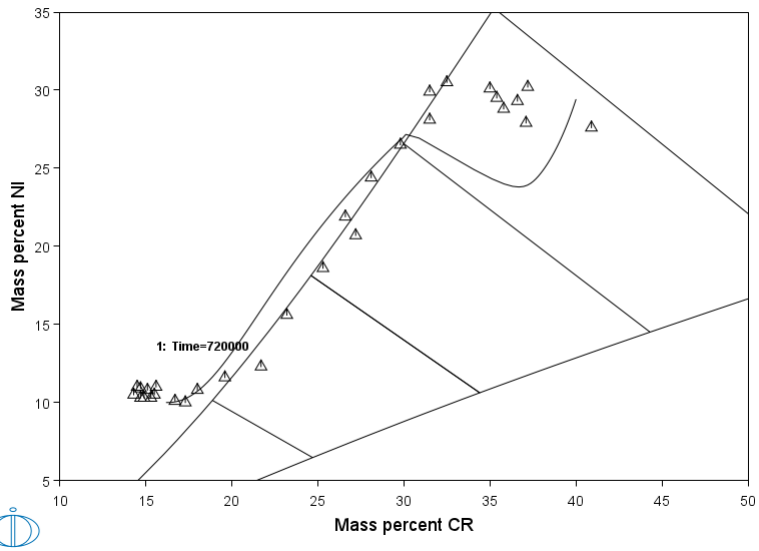

```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1: @@
POST-1: @@ NOW WE DO THE SAME FOR NICKEL
POST-1: @@
POST-1:
POST-1: s-d-a y w-p ni
POST-1:
POST-1: app y exd2.exp
PROLOGUE NUMBER: /1/: 1
DATASET NUMBER(s): /-1/: 5
POST-1:
POST-1: s-s-s x n 10e-4 30e-4
POST-1: s-s-s y n 0 40
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



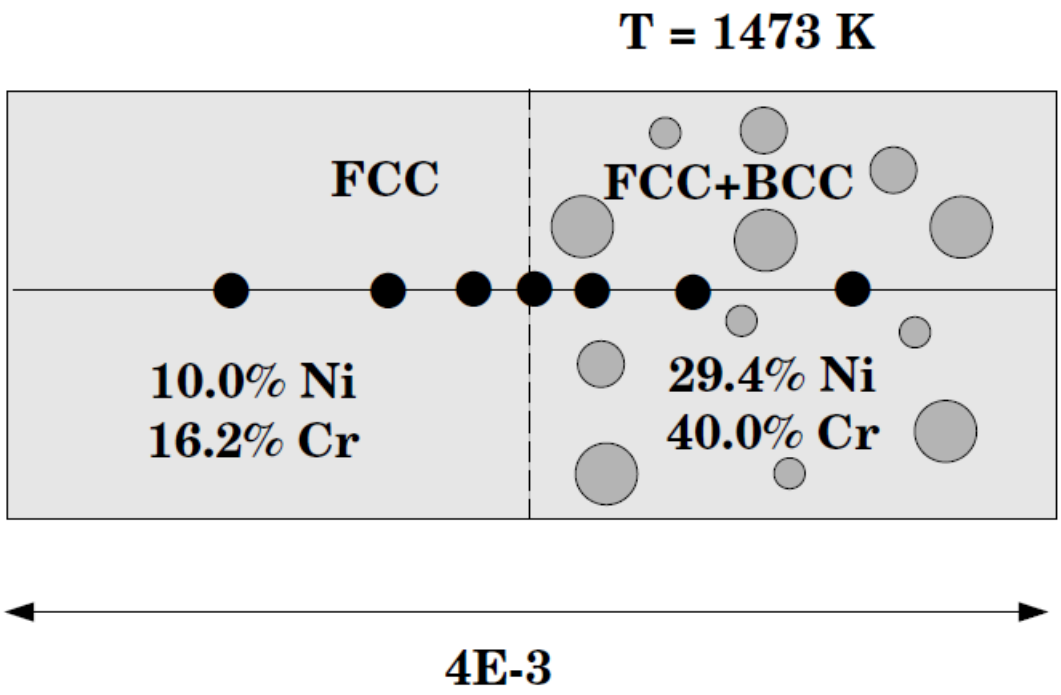

```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1: set-interactive
 --OK---
POST-1:
```

Example exd2b

Diffusion couple of Fe-Ni-Cr alloys: 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: unknown compiler
 License library version: 9.7.0.0036
 Linked: Fri Oct 18 11:32:56 2024


SYS:SYS:MACRO exd2b\setup.DCM
SYS: ï»¿@@
 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. EngstrÃ¶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: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASE
SYS: @@
SYS: go da
15:16:28,186 [Thread-0] INFO  LicenseManager: Initializing user: jenkins.integrationtest@thermocalc.se
15:16:28,199 [Thread-0] INFO  LicenseController: Running License Spring in DEV environment.
15:16:29,285 [Thread-0] INFO  LicenseManager: There is an activated standalone license for jenkins.integrationtest@thermocalc.se for TC-
Application
 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 v5.0

 VA                       /-  DEFINED
TDB_FEDEMO: def-sys fe ni cr
 FE                       NI                       CR
   DEFINED
TDB_FEDEMO: rej ph * all
 BCC_A2                   CBCC_A12                 CHI_A12
 CUB_A13                  FCC_A1                   GAS:G
 HCP_A3                   LAVES_PHASE_C14          LIQUID:L
 SIGMA  REJECTED
TDB_FEDEMO: res ph fcc,bcc
 FCC_A1                   BCC_A2  RESTORED
TDB_FEDEMO: get
15:16:30,365 [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 v4.0

 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
15:16:31,018 [Thread-0] INFO  StandaloneLicenseController: Checking out license for: Diffusion (DICTRA)
 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 A DOUBLE-GEOMETRICAL GRID INTO THE REGION
DIC> @@ THIS GIVES A SHORT DISTANCE BETWEEN THE GRIDPOINTS
DIC> @@ IN THE MIDDLE OF THE REGION WHERE THE INITIAL INTERFACE IS
DIC> @@
DIC> enter-grid fer
WIDTH OF REGION /1/: 4e-3
TYPE /LINEAR/: double
NUMBER OF POINTS /50/: 200
VALUE OF R IN THE GEOMETRICAL SERIE FOR LOWER PART OF REGION: 0.97
VALUE OF R IN THE GEOMETRICAL SERIE FOR UPPER PART OF REGION: 1.03093
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 FROM FILES
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
TYPE /LINEAR/: read d2cr.dat
PROFILE FOR /NI/: ni
TYPE /LINEAR/: read d2ni.dat
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 /72000/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC> set-simulation-condition
NS01A PRINT CONTROL : /0/: 0
FLUX CORRECTION FACTOR : /1/: 1
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/: 2
CHECK INTERFACE POSITION /AUTO/: n
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/: act
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/: y
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/: 99
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -> 1): /AUTO/: 1
MAX TIMESTEP CHANGE PER TIMESTEP : /2/: 2
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/: n
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/: y
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/: n
DIC>
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 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: 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=   26.843546
Starting time-step t0=   80.530637     dt=   26.843546
Starting time-step t0=   107.37418     dt=   26.843546
Starting time-step t0=   134.21773     dt=   26.843546
Starting time-step t0=   161.06127     dt=   26.843546
Starting time-step t0=   187.90482     dt=   26.843546
Starting time-step t0=   214.74836     dt=   53.687091
Starting time-step t0=   268.43546     dt=   53.687091
Starting time-step t0=   322.12255     dt=   53.687091
Starting time-step t0=   375.80964     dt=   53.687091
Starting time-step t0=   429.49673     dt=   53.687091
Starting time-step t0=   483.18382     dt=   53.687091
Starting time-step t0=   536.87091     dt=   53.687091
Starting time-step t0=   590.55800     dt=   107.37418
Starting time-step t0=   697.93219     dt=   107.37418
Starting time-step t0=   805.30637     dt=   107.37418
Starting time-step t0=   912.68055     dt=   107.37418
Starting time-step t0=   1020.0547     dt=   107.37418
Starting time-step t0=   1127.4289     dt=   214.74836
Starting time-step t0=   1342.1773     dt=   214.74836
Starting time-step t0=   1556.9256     dt=   214.74836
Starting time-step t0=   1771.6740     dt=   214.74836
Starting time-step t0=   1986.4224     dt=   214.74836
Starting time-step t0=   2201.1707     dt=   214.74836
Starting time-step t0=   2415.9191     dt=   214.74836
Starting time-step t0=   2630.6675     dt=   429.49673
Starting time-step t0=   3060.1642     dt=   429.49673
Starting time-step t0=   3489.6609     dt=   429.49673
Starting time-step t0=   3919.1577     dt=   429.49673
Starting time-step t0=   4348.6544     dt=   429.49673
Starting time-step t0=   4778.1511     dt=   429.49673
Starting time-step t0=   5207.6478     dt=   858.99346
Starting time-step t0=   6066.6413     dt=   858.99346
Starting time-step t0=   6925.6348     dt=   858.99346
Starting time-step t0=   7784.6282     dt=   858.99346
Starting time-step t0=   8643.6217     dt=   858.99346
Starting time-step t0=   9502.6151     dt=   858.99346
Starting time-step t0=   10361.609     dt=   858.99346
Starting time-step t0=   11220.602     dt=   858.99346
Starting time-step t0=   12079.596     dt=   1717.9869
Starting time-step t0=   13797.582     dt=   1717.9869
Starting time-step t0=   15515.569     dt=   1717.9869
Starting time-step t0=   17233.556     dt=   1717.9869
Starting time-step t0=   18951.543     dt=   1717.9869
Starting time-step t0=   20669.530     dt=   1717.9869
Starting time-step t0=   22387.517     dt=   3435.9738
Starting time-step t0=   25823.491     dt=   3435.9738
Starting time-step t0=   29259.465     dt=   3435.9738
Starting time-step t0=   32695.439     dt=   3435.9738
Starting time-step t0=   36131.412     dt=   3435.9738
Starting time-step t0=   39567.386     dt=   3435.9738
Starting time-step t0=   43003.360     dt=   3435.9738
Starting time-step t0=   46439.334     dt=   6871.9477
Starting time-step t0=   53311.282     dt=   6871.9477
Starting time-step t0=   60183.229     dt=   6871.9477
Starting time-step t0=   67055.177     dt=   6871.9477
Starting time-step t0=   73927.125     dt=   6871.9477
Starting time-step t0=   80799.072     dt=   6871.9477
Starting time-step t0=   87671.020     dt=   6871.9477
```

```
Starting time-step t0=   94542.968     dt=   6871.9477
Starting time-step t0=   101414.92     dt=   13743.895
Starting time-step t0=   115158.81     dt=   13743.895
Starting time-step t0=   122030.76     dt=   6871.9477
Starting time-step t0=   128902.71     dt=   13743.895
Starting time-step t0=   142646.60     dt=   13743.895
Starting time-step t0=   149518.55     dt=   13743.895
Starting time-step t0=   163262.44     dt=   13743.895
Starting time-step t0=   177006.34     dt=   13743.895
Starting time-step t0=   183878.29     dt=   13743.895
Starting time-step t0=   197622.18     dt=   13743.895
Starting time-step t0=   211366.08     dt=   27487.791
Starting time-step t0=   238853.87     dt=   27487.791
Starting time-step t0=   266341.66     dt=   27487.791
Starting time-step t0=   293829.45     dt=   27487.791
Starting time-step t0=   321317.24     dt=   27487.791
Starting time-step t0=   335061.14     dt=   27487.791
Starting time-step t0=   348805.03     dt=   13743.895
Starting time-step t0=   362548.93     dt=   27487.791
Starting time-step t0=   390036.72     dt=   27487.791
Starting time-step t0=   396908.67     dt=   13743.895
Starting time-step t0=   410652.56     dt=   13743.895
Starting time-step t0=   424396.46     dt=   27487.791
Starting time-step t0=   451884.25     dt=   27487.791
Starting time-step t0=   465628.14     dt=   27487.791
Starting time-step t0=   479372.04     dt=   13743.895
Starting time-step t0=   493115.93     dt=   27487.791
Starting time-step t0=   520603.72     dt=   54975.581
Starting time-step t0=   548091.51     dt=   27487.791
Starting time-step t0=   575579.30     dt=   54975.581
Starting time-step t0=   630554.89     dt=   54975.581
Starting time-step t0=   658042.68     dt=   27487.791
Starting time-step t0=   685530.47     dt=   34469.532
 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    805.30637
 DELETING TIME-RECORD FOR TIME    1556.9256
 DELETING TIME-RECORD FOR TIME    2415.9191
 DELETING TIME-RECORD FOR TIME    3489.6609
 DELETING TIME-RECORD FOR TIME    4348.6544
 DELETING TIME-RECORD FOR TIME    5207.6478
 DELETING TIME-RECORD FOR TIME    6066.6413
 DELETING TIME-RECORD FOR TIME    6925.6348
 DELETING TIME-RECORD FOR TIME    7784.6282
 DELETING TIME-RECORD FOR TIME    8643.6217
 DELETING TIME-RECORD FOR TIME    9502.6151
 DELETING TIME-RECORD FOR TIME    10361.609
 DELETING TIME-RECORD FOR TIME    11220.602
 DELETING TIME-RECORD FOR TIME    12079.596
 DELETING TIME-RECORD FOR TIME    13797.582
 DELETING TIME-RECORD FOR TIME    15515.569
 DELETING TIME-RECORD FOR TIME    17233.556
 DELETING TIME-RECORD FOR TIME    18951.543
 DELETING TIME-RECORD FOR TIME    20669.530
 DELETING TIME-RECORD FOR TIME    22387.517
 DELETING TIME-RECORD FOR TIME    25823.491
 DELETING TIME-RECORD FOR TIME    29259.465
 DELETING TIME-RECORD FOR TIME    32695.439
 DELETING TIME-RECORD FOR TIME    36131.412
 DELETING TIME-RECORD FOR TIME    39567.386
 DELETING TIME-RECORD FOR TIME    43003.360
 DELETING TIME-RECORD FOR TIME    46439.334
 DELETING TIME-RECORD FOR TIME    53311.282
 DELETING TIME-RECORD FOR TIME    60183.229
 DELETING TIME-RECORD FOR TIME    67055.177
 DELETING TIME-RECORD FOR TIME    73927.125
 DELETING TIME-RECORD FOR TIME    80799.072
 DELETING TIME-RECORD FOR TIME    87671.020
 DELETING TIME-RECORD FOR TIME    94542.968
 DELETING TIME-RECORD FOR TIME    101414.92
 DELETING TIME-RECORD FOR TIME    115158.81
 DELETING TIME-RECORD FOR TIME    122030.76
 DELETING TIME-RECORD FOR TIME    128902.71
 DELETING TIME-RECORD FOR TIME    142646.60
 DELETING TIME-RECORD FOR TIME    149518.55
 DELETING TIME-RECORD FOR TIME    163262.44
 DELETING TIME-RECORD FOR TIME    177006.34
 DELETING TIME-RECORD FOR TIME    183878.29
 DELETING TIME-RECORD FOR TIME    197622.18
 DELETING TIME-RECORD FOR TIME    211366.08
 DELETING TIME-RECORD FOR TIME    238853.87
 DELETING TIME-RECORD FOR TIME    266341.66
 DELETING TIME-RECORD FOR TIME    293829.45
 DELETING TIME-RECORD FOR TIME    321317.24
 DELETING TIME-RECORD FOR TIME    335061.14
 DELETING TIME-RECORD FOR TIME    348805.03
 DELETING TIME-RECORD FOR TIME    362548.93
 DELETING TIME-RECORD FOR TIME    390036.72
 DELETING TIME-RECORD FOR TIME    396908.67
 DELETING TIME-RECORD FOR TIME    410652.56
 DELETING TIME-RECORD FOR TIME    424396.46
 DELETING TIME-RECORD FOR TIME    451884.25
 DELETING TIME-RECORD FOR TIME    465628.14
 DELETING TIME-RECORD FOR TIME    479372.04
 DELETING TIME-RECORD FOR TIME    493115.93
 DELETING TIME-RECORD FOR TIME    520603.72
 DELETING TIME-RECORD FOR TIME    548091.51
 DELETING TIME-RECORD FOR TIME    575579.30
 DELETING TIME-RECORD FOR TIME    630554.89
 DELETING TIME-RECORD FOR TIME    658042.68

 KEEPING TIME-RECORD FOR TIME    685530.47
 AND FOR TIME                    720000.00
 WORKSPACE RECLAIMED
 -------------------------------------------------
 INTERPOLATION SCHEME USED THIS FRACTION OF
 THE ALLOCATED MEMORY:   3.445374607681511E-002
 EFFICIENCY FACTOR:    25.1644713836111
 -------------------------------------------------
 DEALLOCATING
 -------------------------------------------------

 TIMESTEP AT     720000.000     SELECTED
```

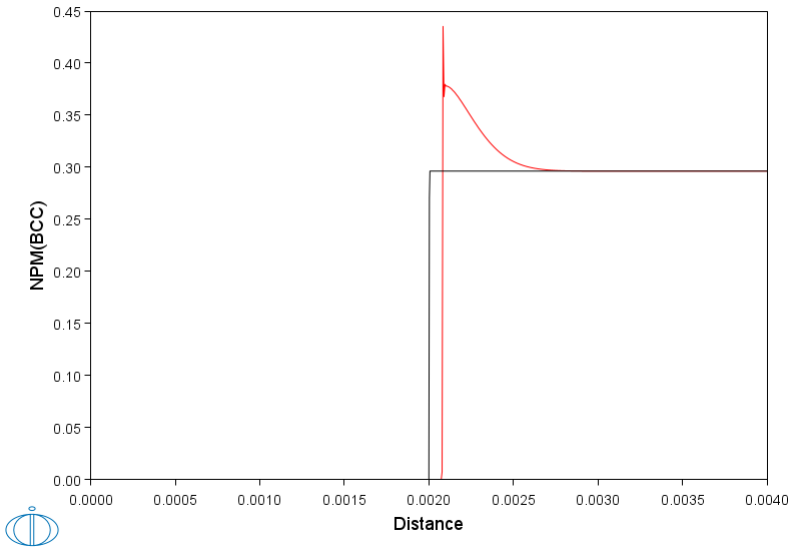
```
DIC>
DIC>
DIC>
DIC>
DIC> set-inter
 --OK---
DIC>
```

exd2b-plot

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO 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

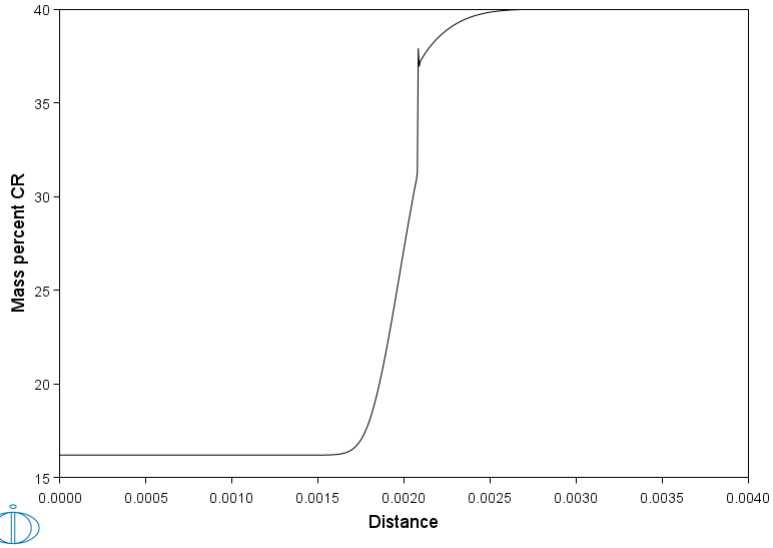
  INFO: Distance is set as independent variable
POST-1: s-p-c time 0 720000
POST-1: set-tit Figure D2.1
POST-1: plot
```

Figure D2.1



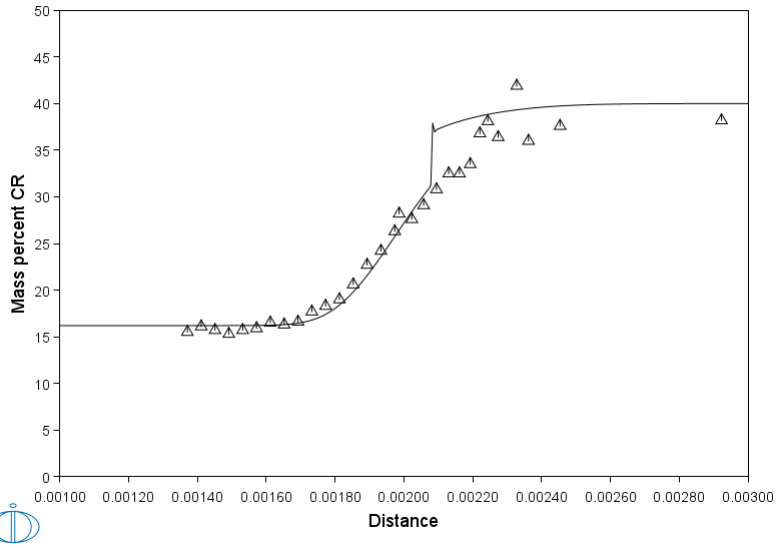

```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1: @@
POST-1: @@ LET US NOW PLOT HOW THE AVERAGE CR-CONCENTRATION VARIES WITH DISTANCE
POST-1: @@
POST-1: s-d-a y w-p cr
POST-1: s-p-c time last
POST-1: set-tit Figure D2.2
POST-1: plot
```

Figure D2.2



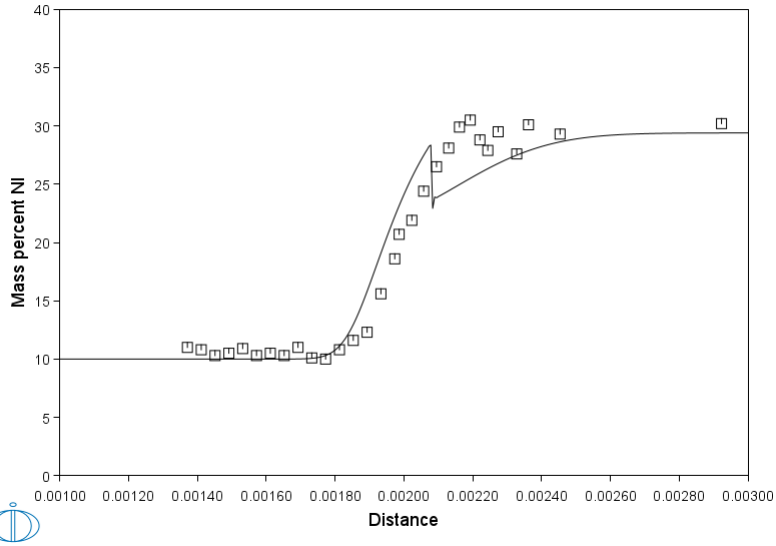

```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1: @@
POST-1: @@ WE SELECT A BETTER SCALING AND APPEND EXPERIMENTAL DATA
POST-1: @@
POST-1:
POST-1: app y exd2.exp
PROLOGUE NUMBER: /0/: 1
DATASET NUMBER(s): /-1/: 4
POST-1:
POST-1: s-s-s y n 0 50
POST-1: s-s-s x n 10e-4 30e-4
POST-1:
POST-1: set-tit Figure D2.3
POST-1: plot
```

Figure D2.3



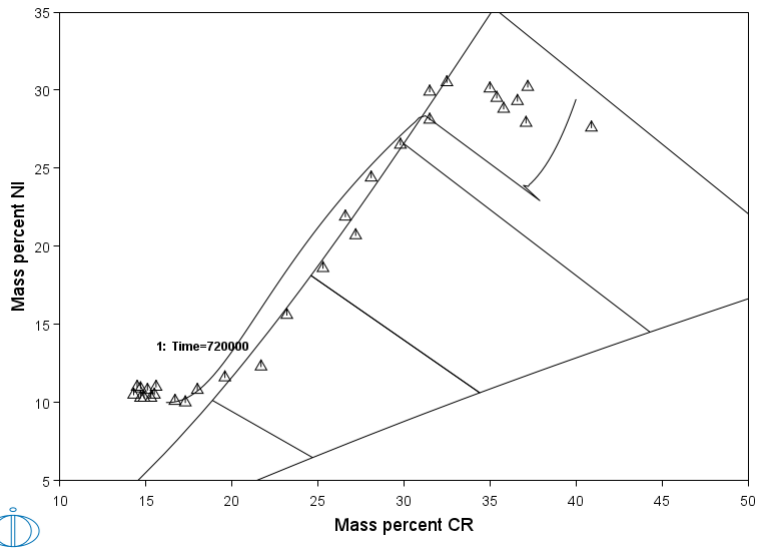

```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1: @@
POST-1: @@ NOW WE DO THE SAME FOR NICKEL
POST-1: @@
POST-1:
POST-1: s-d-a y w-p ni
POST-1:
POST-1: app y exd2.exp
PROLOGUE NUMBER: /1/: 1
DATASET NUMBER(s): /-1/: 5
POST-1:
POST-1: s-s-s x n 10e-4 30e-4
POST-1: s-s-s y n 0 40
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

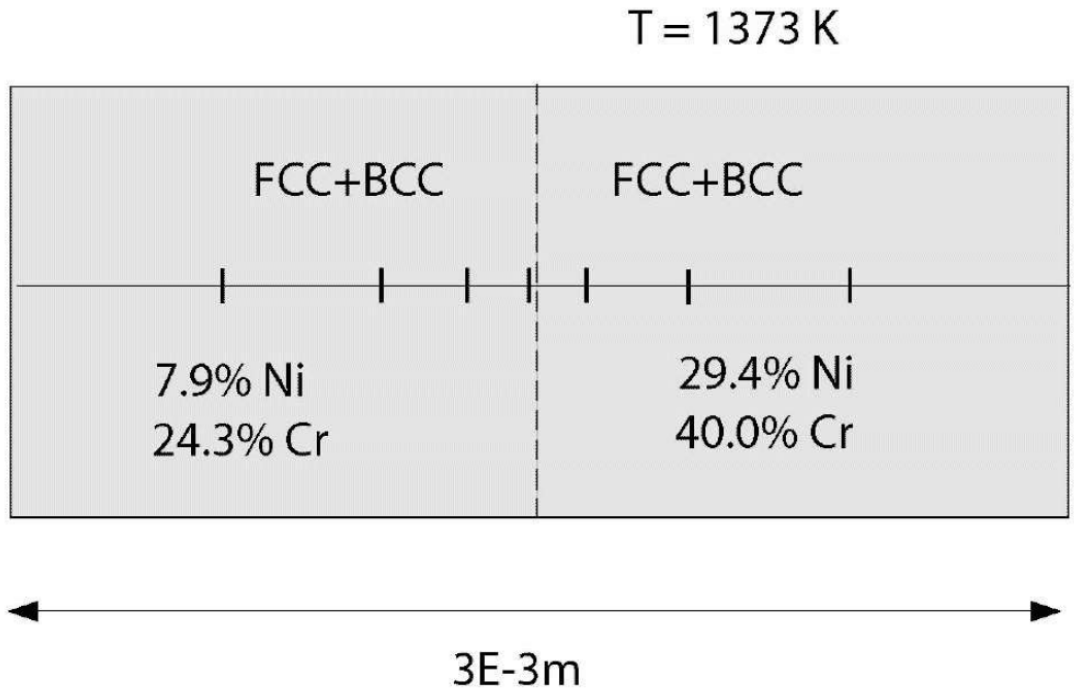



```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1: set-interactive
 --OK---
POST-1:
```

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: unknown compiler
 License library version: 9.7.0.0036
 Linked: Fri Oct 18 11:32:56 2024


SYS:SYS:MACRO exd3\setup.DCM
SYS: ï»¿@@
 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. EngstrÃ¶m, Acta. Mater. v.54 (2006), pp. 2431-2439.
SYS: @@ Experimental data from A. EngstrÃ¶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: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exd3_setup.DCM
SYS:
SYS:
SYS: go da
15:19:43,047 [Thread-0] INFO  LicenseManager: Initializing user: jenkins.integrationtest@thermocalc.se
15:19:43,061 [Thread-0] INFO  LicenseController: Running License Spring in DEV environment.
15:19:44,146 [Thread-0] INFO  LicenseManager: There is an activated standalone license for jenkins.integrationtest@thermocalc.se for TC-
Application
 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 v5.0

 VA                       /-  DEFINED
TDB_FEDEMO: def-sys fe cr ni
 FE                       CR                       NI
   DEFINED
TDB_FEDEMO: rej-ph *
 BCC_A2                   CBCC_A12                 CHI_A12
 CUB_A13                  FCC_A1                   GAS:G
 HCP_A3                   LAVES_PHASE_C14          LIQUID:L
 SIGMA  REJECTED
TDB_FEDEMO: rest-ph bcc,fcc
 BCC_A2                   FCC_A1  RESTORED
TDB_FEDEMO: get
15:19:45,197 [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 v4.0

 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
15:19:45,725 [Thread-0] INFO  StandaloneLicenseController: Checking out license for: Diffusion (DICTRA)
 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 /LINEAR/: 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 /LINEAR/: 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> s-s-c
NS01A PRINT CONTROL : /0/: 0
FLUX CORRECTION FACTOR : /1/: 1
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/: 2
CHECK INTERFACE POSITION /AUTO/: n
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/: act
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/: y
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/: 99
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -> 1): /AUTO/: .5
MAX TIMESTEP CHANGE PER TIMESTEP : /2/: 2
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/: n
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/: y
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/:
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 exd3\run.DCM 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: 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=   15.000000     dt=   16.000000
Starting time-step t0=   31.000000     dt=   32.000000
Starting time-step t0=   63.000000     dt=   64.000000
Starting time-step t0=   127.00000     dt=   128.00000
Starting time-step t0=   255.00000     dt=   256.00000
Starting time-step t0=   511.00000     dt=   256.00000
Starting time-step t0=   767.00000     dt=   256.00000
Starting time-step t0=   1023.0000     dt=   512.00000
Starting time-step t0=   1535.0000     dt=   512.00000
Starting time-step t0=   2047.0000     dt=   1024.0000
Starting time-step t0=   3071.0000     dt=   1024.0000
Starting time-step t0=   4095.0000     dt=   2048.0000
Starting time-step t0=   6143.0000     dt=   2048.0000
Starting time-step t0=   8191.0000     dt=   4096.0000
Starting time-step t0=   12287.000     dt=   4096.0000
Starting time-step t0=   16383.000     dt=   8192.0000
Starting time-step t0=   24575.000     dt=   8192.0000
Starting time-step t0=   32767.000     dt=   8192.0000
Starting time-step t0=   40959.000     dt=   8192.0000
Starting time-step t0=   49151.000     dt=   8192.0000
Starting time-step t0=   57343.000     dt=   8192.0000
Starting time-step t0=   65535.000     dt=   8192.0000
Starting time-step t0=   73727.000     dt=   16384.000
Starting time-step t0=   90111.000     dt=   32768.000
Starting time-step t0=   122879.00     dt=   32768.000
Starting time-step t0=   155647.00     dt=   32768.000
Starting time-step t0=   188415.00     dt=   32768.000
Starting time-step t0=   221183.00     dt=   32768.000
Starting time-step t0=   253951.00     dt=   32768.000
Starting time-step t0=   286719.00     dt=   32768.000
Starting time-step t0=   319487.00     dt=   32768.000
Starting time-step t0=   352255.00     dt=   7745.0000
 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    511.00000
 DELETING TIME-RECORD FOR TIME    1023.0000
 DELETING TIME-RECORD FOR TIME    1535.0000
 DELETING TIME-RECORD FOR TIME    2047.0000
 DELETING TIME-RECORD FOR TIME    3071.0000
 DELETING TIME-RECORD FOR TIME    4095.0000
 DELETING TIME-RECORD FOR TIME    6143.0000
 DELETING TIME-RECORD FOR TIME    8191.0000
 DELETING TIME-RECORD FOR TIME    12287.000
 DELETING TIME-RECORD FOR TIME    16383.000
 DELETING TIME-RECORD FOR TIME    24575.000
 DELETING TIME-RECORD FOR TIME    32767.000
 DELETING TIME-RECORD FOR TIME    40959.000
 DELETING TIME-RECORD FOR TIME    49151.000
 DELETING TIME-RECORD FOR TIME    57343.000
 DELETING TIME-RECORD FOR TIME    65535.000
 DELETING TIME-RECORD FOR TIME    73727.000
 DELETING TIME-RECORD FOR TIME    90111.000
 DELETING TIME-RECORD FOR TIME    122879.00
 DELETING TIME-RECORD FOR TIME    155647.00
 DELETING TIME-RECORD FOR TIME    188415.00
 DELETING TIME-RECORD FOR TIME    221183.00
 DELETING TIME-RECORD FOR TIME    253951.00
 DELETING TIME-RECORD FOR TIME    286719.00
 DELETING TIME-RECORD FOR TIME    319487.00

 KEEPING TIME-RECORD FOR TIME    352255.00
 AND FOR TIME                    360000.00
 WORKSPACE RECLAIMED
 -------------------------------------------------
 INTERPOLATION SCHEME USED THIS FRACTION OF
 THE ALLOCATED MEMORY:   2.363429568829154E-002
 EFFICIENCY FACTOR:    6.52636977519446
 -------------------------------------------------
 DEALLOCATING
 -------------------------------------------------

 TIMESTEP AT     360000.000     SELECTED

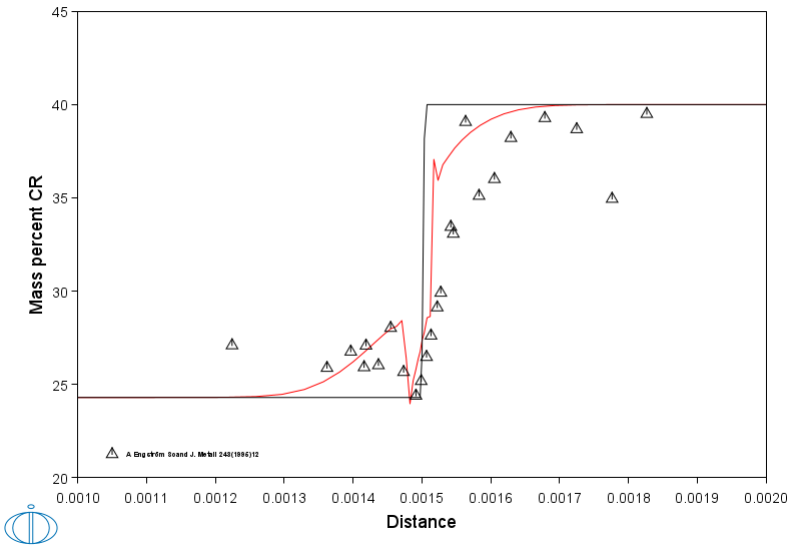
DIC>
DIC>
DIC> set-inter
 --OK---
DIC>
```

exd3-plot

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exd3\plot.DCM 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>
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

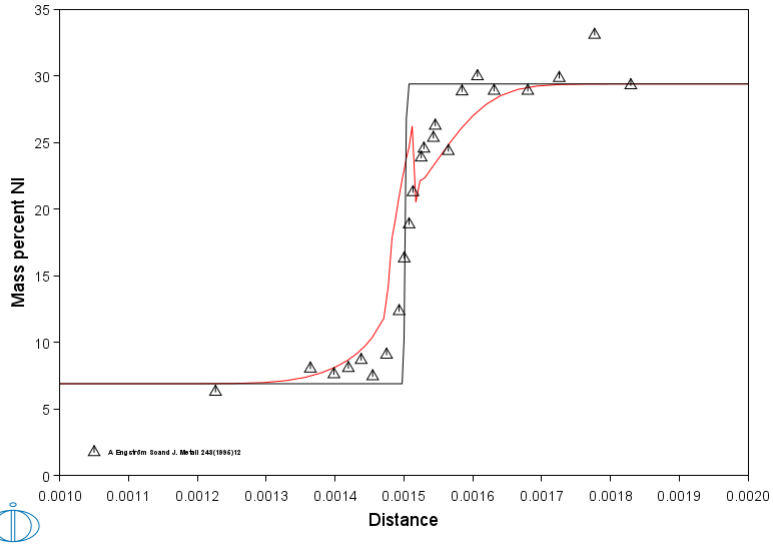
  INFO: Distance is set as independent variable
POST-1: s-d-a y w-p Cr
POST-1: s-p-c time 0 360000
POST-1: set-tit Figure D3.1
POST-1:
POST-1: app yes k5k7cr.exp 0; 1
POST-1:
POST-1: s-s-s x n 1e-3 2e-3
POST-1:
POST-1: s-s-s y n 20 45
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 3
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

Figure D3.1



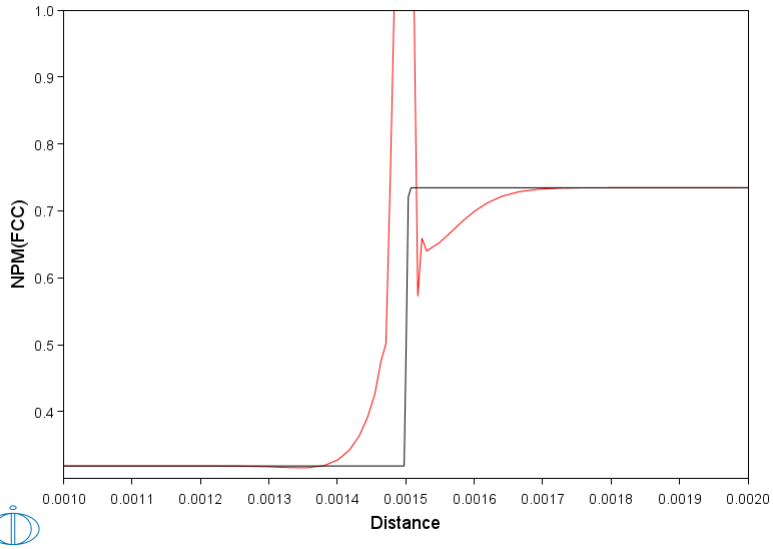

```
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1: s-d-a y w-p Ni
POST-1: set-tit Figure D3.2
POST-1:
POST-1: app yes k5k7ni.exp 0; 1
POST-1:
POST-1: s-s-s y n 0 35
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 3
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

Figure D3.2



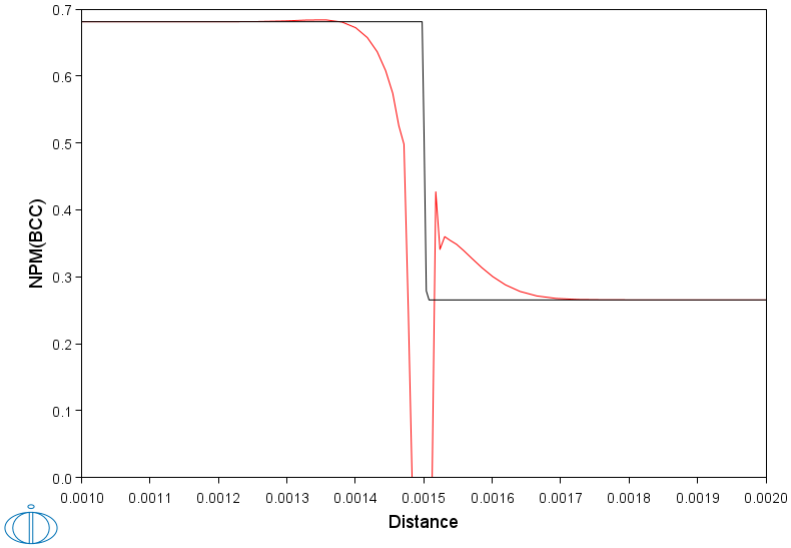

```
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1: @@
POST-1: @@ Then study the amount of FCC and BCC
POST-1: @@
POST-1: app no
POST-1: s-d-a y npm(fcc)
POST-1: set-tit Figure D3.3
POST-1:
POST-1: SET_EXP_FILE_FORMAT 3
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

Figure D3.3



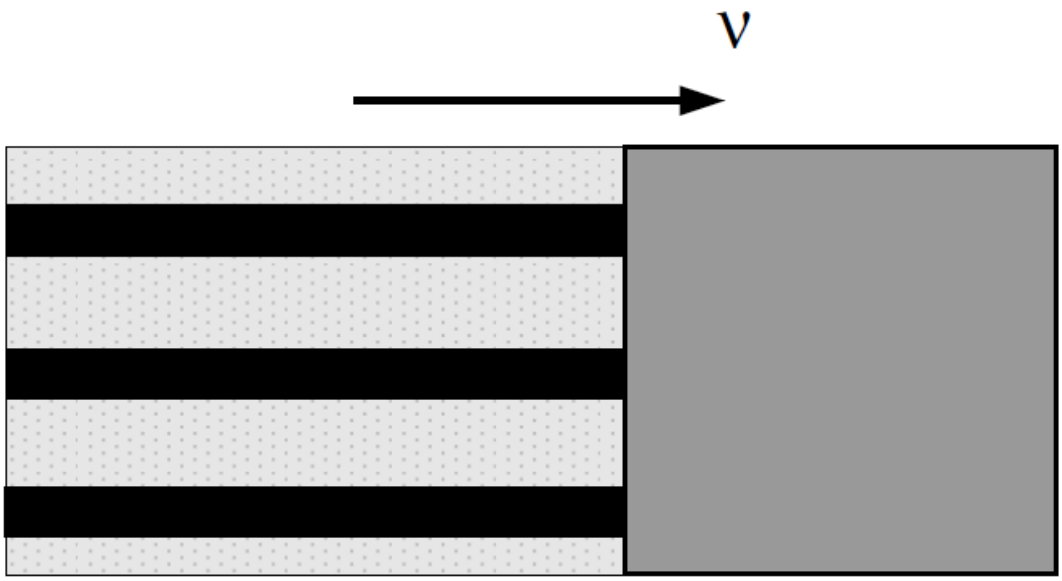

```
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1: s-d-a y npm(bcc)
POST-1: set-tit Figure D3.4
POST-1:
POST-1: SET_EXP_FILE_FORMAT 3
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

Figure D3.4




```
POST-1:
POST-1:
POST-1: set-interactive
 --OK---
POST-1:
```

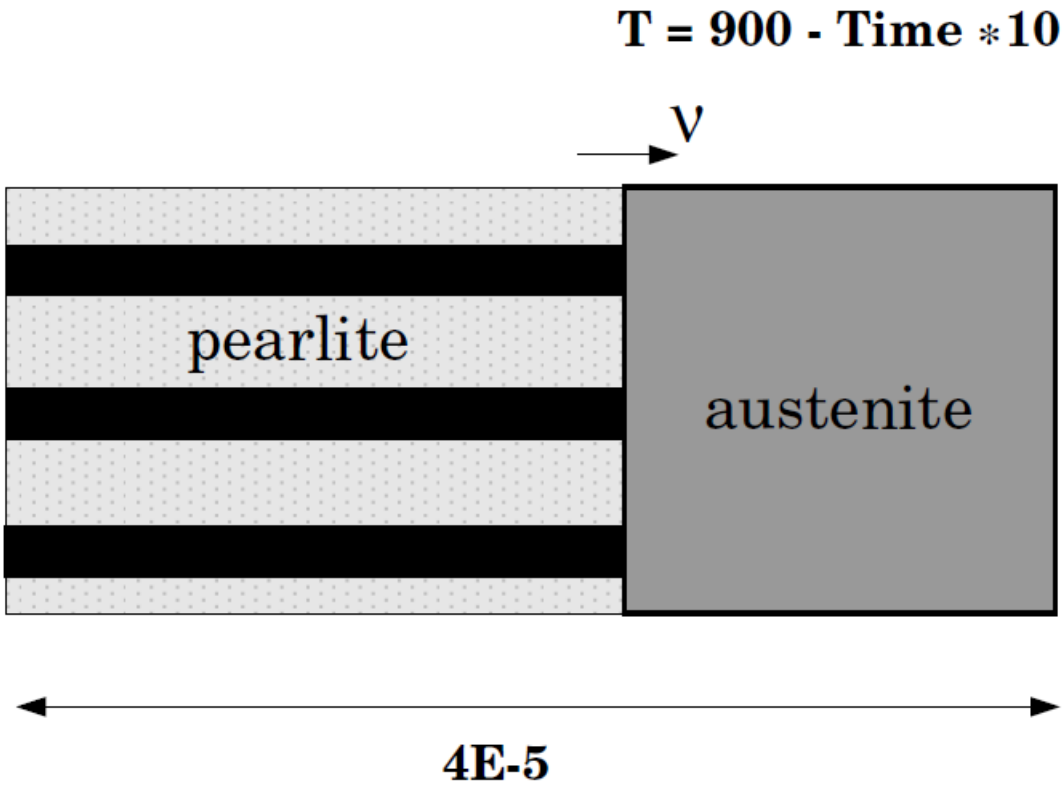
Cooperative Growth



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.



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: unknown compiler
 License library version: 9.7.0.0036
 Linked: Fri Oct 18 11:32:56 2024


SYS:SYS:MACRO exe1\setup.DCM
SYS: ï»¿@@
 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: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exe1_setup.DCM
SYS:
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASE
SYS: @@
SYS: go da
15:22:49,736 [Thread-0] INFO  LicenseManager: Initializing user: jenkins.integrationtest@thermocalc.se
15:22:49,748 [Thread-0] INFO  LicenseController: Running License Spring in DEV environment.
15:22:50,862 [Thread-0] INFO  LicenseManager: There is an activated standalone license for jenkins.integrationtest@thermocalc.se for TC-
Application
 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 v5.0

 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
 BCC_A2                    CBCC_A12                  CEMENTITE
 CUB_A13                   DIAMOND_FCC_A4            FCC_A1
 GAS:G                     GRAPHITE                  HCP_A3
 KSI_CARBIDE               LAVES_PHASE_C14           LIQUID:L
 M23C6                     M5C2                      M7C3
   REJECTED
TDB_FEDEMO: rest-ph fcc,bcc,cem
 FCC_A1                    BCC_A2                    CEMENTITE
   RESTORED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ GET THE THERMODYNAMIC DATA
TDB_FEDEMO: @@
TDB_FEDEMO: get
15:22:51,941 [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 mobfe4
 Current database: Steels/Fe-Alloys Mobility  v4.0

 VA  DEFINED
 B2_BCC  REJECTED
APP: def-sys fe c mn
 FE                        C                         MN
   DEFINED
APP: rej-ph /all
 BCC_A2                    CEMENTITE                 FCC_A1
 FE4N_LP1                  HCP_A3                    LIQUID:L
   REJECTED
APP: rest-ph bcc,fcc,cem
 BCC_A2                    FCC_A1                    CEMENTITE
   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
15:22:52,738 [Thread-0] INFO  StandaloneLicenseController: Checking out license for: Diffusion (DICTRA)
 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 exe1 Y
DIC>
DIC> set-inter
 --OK---
DIC>
```

exe1-run

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exe1\run.DCM 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
 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 = .00929232973121271
 TOTAL SIZE OF SYSTEM:  2.68092626329E-13 [m^3]
  10  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUSTENITE

  CPU time used in timestep                    2  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 = .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 =  0.13027344E-02 DT =  0.12026344E-02 SUM OF SQUARES =   0.0000000
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.77986231E-05 AND   0.77986231E-05
 POSITION OF INTERFACE PEARLITE / AUSTENITE IS   0.10659245E-07
 U-FRACTION IN SYSTEM:  C = .0233843320030518  FE = .990707670399294
                        MN = .0092923297312127
 TOTAL SIZE OF SYSTEM:  2.68092626329E-13 [m^3]
  CPU time used in timestep                    1  seconds
  2 GRIDPOINT(S) REMOVED FROM CELL#  1 REGION #  1
 TIME =  0.37080032E-02 DT =  0.24052688E-02 SUM OF SQUARES =   0.0000000
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.78044143E-05 AND   0.78044143E-05
 POSITION OF INTERFACE PEARLITE / AUSTENITE IS   0.29430959E-07
 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
  1 GRIDPOINT(S) REMOVED FROM CELL#  1 REGION #  1
 TIME =  0.85185408E-02 DT =  0.48105376E-02 SUM OF SQUARES =   0.0000000
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.78160014E-05 AND   0.78160014E-05
 POSITION OF INTERFACE PEARLITE / AUSTENITE IS   0.67030128E-07
 U-FRACTION IN SYSTEM:  C = .0233843320030517  FE = .990707670399295
                        MN = .00929232973121269
 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 =  0.18139616E-01 DT =  0.96210753E-02 SUM OF SQUARES =   0.0000000
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.78391943E-05 AND   0.78391943E-05
 POSITION OF INTERFACE PEARLITE / AUSTENITE IS   0.14245161E-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                    0  seconds
 TIME =  0.37381767E-01 DT =  0.19242151E-01 SUM OF SQUARES =   0.0000000
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.78856550E-05 AND   0.78856550E-05
 POSITION OF INTERFACE PEARLITE / AUSTENITE IS   0.29418857E-06
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399294
                        MN = .00929232973121267
 TOTAL SIZE OF SYSTEM:  2.68092626329E-13 [m^3]
  CPU time used in timestep                    1  seconds
 TIME =  0.75866068E-01 DT =  0.38484301E-01 SUM OF SQUARES =   0.0000000
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.79788730E-05 AND   0.79788730E-05
 POSITION OF INTERFACE PEARLITE / AUSTENITE IS   0.60124992E-06
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399294
                        MN = .00929232973121267
 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 =  0.15283467     DT =  0.76968602E-01 SUM OF SQUARES =   0.0000000
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.81664786E-05 AND   0.81664786E-05
 POSITION OF INTERFACE PEARLITE / AUSTENITE IS   0.12298124E-05
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399295
                        MN = .00929232973121266
 TOTAL SIZE OF SYSTEM:  2.68092626329E-13 [m^3]
  CPU time used in timestep                    0  seconds
 TIME =  0.25283467     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.84124940E-05 AND   0.84124940E-05
 POSITION OF INTERFACE PEARLITE / AUSTENITE IS   0.20710618E-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
  1 GRIDPOINT(S) REMOVED FROM CELL#  1 REGION #  1
 TIME =  0.35283467     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.86609946E-05 AND   0.86609946E-05
 POSITION OF INTERFACE PEARLITE / AUSTENITE IS   0.29371612E-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


output ignored...



... output resumed

 WORKSPACE RECLAIMED
  INFO: CELL   1 REGION AUSTENITE   DELETED
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399324
                        MN = .00929232973118255
 TOTAL SIZE OF SYSTEM:  2.68087982114E-13 [m^3]
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399324
                        MN = .00929232973118255
 TOTAL SIZE OF SYSTEM:  2.68087982114E-13 [m^3]
 TIME =   3.2743779     DT =  0.10000000E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399324
                        MN = .00929232973118255
 TOTAL SIZE OF SYSTEM:  2.68087982114E-13 [m^3]
  CPU time used in timestep                    0  seconds
 TIME =   3.2843779     DT =  0.10000000E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399324
                        MN = .00929232973118255
 TOTAL SIZE OF SYSTEM:  2.68087982114E-13 [m^3]
  CPU time used in timestep                    0  seconds
 TIME =   3.3843779     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399324
                        MN = .00929232973118255
 TOTAL SIZE OF SYSTEM:  2.68087982114E-13 [m^3]
  CPU time used in timestep                    0  seconds
 TIME =   3.4843779     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399324
                        MN = .00929232973118255
 TOTAL SIZE OF SYSTEM:  2.68087982114E-13 [m^3]
  CPU time used in timestep                    0  seconds
 TIME =   3.5843779     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399324
                        MN = .00929232973118255
 TOTAL SIZE OF SYSTEM:  2.68087982114E-13 [m^3]
  CPU time used in timestep                    0  seconds
 TIME =   3.6843779     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399324
                        MN = .00929232973118255
 TOTAL SIZE OF SYSTEM:  2.68087982114E-13 [m^3]
  CPU time used in timestep                    0  seconds
 TIME =   3.7843779     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399324
                        MN = .00929232973118255
 TOTAL SIZE OF SYSTEM:  2.68087982114E-13 [m^3]
  CPU time used in timestep                    0  seconds
 TIME =   3.8843779     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399324
                        MN = .00929232973118255
 TOTAL SIZE OF SYSTEM:  2.68087982114E-13 [m^3]
  CPU time used in timestep                    0  seconds
 TIME =   3.9843779     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399324
                        MN = .00929232973118255
 TOTAL SIZE OF SYSTEM:  2.68087982114E-13 [m^3]
  CPU time used in timestep                    0  seconds
 TIME =   4.0843779     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399324
                        MN = .00929232973118255
 TOTAL SIZE OF SYSTEM:  2.68087982114E-13 [m^3]
  CPU time used in timestep                    0  seconds
 TIME =   4.1843779     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399324
                        MN = .00929232973118255
 TOTAL SIZE OF SYSTEM:  2.68087982114E-13 [m^3]
  CPU time used in timestep                    0  seconds
 TIME =   4.2843779     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399324
                        MN = .00929232973118255
 TOTAL SIZE OF SYSTEM:  2.68087982114E-13 [m^3]
  CPU time used in timestep                    0  seconds
 TIME =   4.3843779     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399324
                        MN = .00929232973118255
 TOTAL SIZE OF SYSTEM:  2.68087982114E-13 [m^3]
  CPU time used in timestep                    0  seconds
 TIME =   4.4843779     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399324
                        MN = .00929232973118255
 TOTAL SIZE OF SYSTEM:  2.68087982114E-13 [m^3]
  CPU time used in timestep                    0  seconds
 TIME =   4.5843779     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399324
                        MN = .00929232973118255
 TOTAL SIZE OF SYSTEM:  2.68087982114E-13 [m^3]
  CPU time used in timestep                    0  seconds
 TIME =   4.6843779     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399324
                        MN = .00929232973118255
 TOTAL SIZE OF SYSTEM:  2.68087982114E-13 [m^3]
  CPU time used in timestep                    0  seconds
 TIME =   4.7843779     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399324
                        MN = .00929232973118255
 TOTAL SIZE OF SYSTEM:  2.68087982114E-13 [m^3]
  CPU time used in timestep                    0  seconds
 TIME =   4.8843779     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399324
                        MN = .00929232973118255
 TOTAL SIZE OF SYSTEM:  2.68087982114E-13 [m^3]
```

```
 CPU time used in timestep                    0  seconds
TIME =   4.9843779     DT =  0.10000000     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399324
                       MN = .00929232973118255
TOTAL SIZE OF SYSTEM:  2.68087982114E-13 [m^3]
 CPU time used in timestep                    0  seconds
TIME =   5.0000000     DT =  0.15622127E-01 SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399324
                       MN = .00929232973118255
TOTAL SIZE OF SYSTEM:  2.68087982114E-13 [m^3]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME    3.2528347
DELETING TIME-RECORD FOR TIME    3.2743679
DELETING TIME-RECORD FOR TIME    3.2743779
DELETING TIME-RECORD FOR TIME    3.2843779
DELETING TIME-RECORD FOR TIME    3.3843779
DELETING TIME-RECORD FOR TIME    3.4843779
DELETING TIME-RECORD FOR TIME    3.5843779
DELETING TIME-RECORD FOR TIME    3.6843779
DELETING TIME-RECORD FOR TIME    3.7843779
DELETING TIME-RECORD FOR TIME    3.8843779
DELETING TIME-RECORD FOR TIME    3.9843779
DELETING TIME-RECORD FOR TIME    4.0843779
DELETING TIME-RECORD FOR TIME    4.1843779
DELETING TIME-RECORD FOR TIME    4.2843779
DELETING TIME-RECORD FOR TIME    4.3843779
DELETING TIME-RECORD FOR TIME    4.4843779
DELETING TIME-RECORD FOR TIME    4.5843779
DELETING TIME-RECORD FOR TIME    4.6843779
DELETING TIME-RECORD FOR TIME    4.7843779
DELETING TIME-RECORD FOR TIME    4.8843779

KEEPING TIME-RECORD FOR TIME    4.9843779
AND FOR TIME                    5.0000000
WORKSPACE RECLAIMED

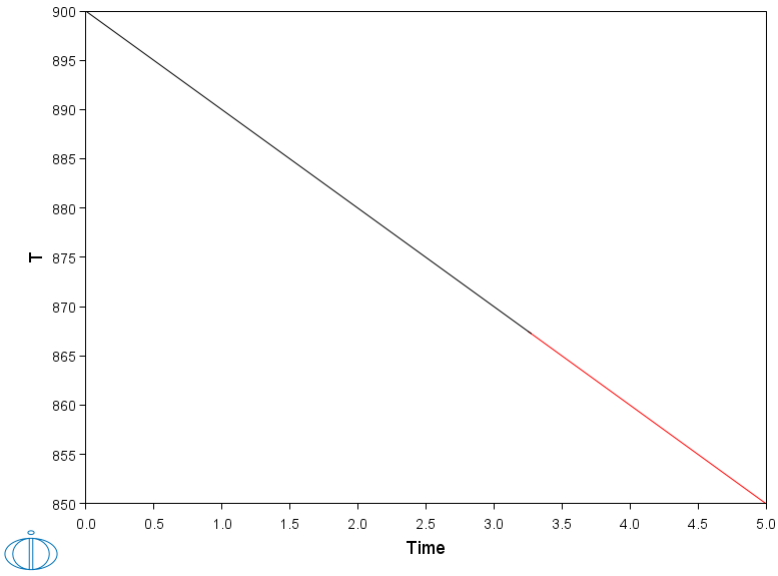
TIMESTEP AT     5.00000000     SELECTED

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

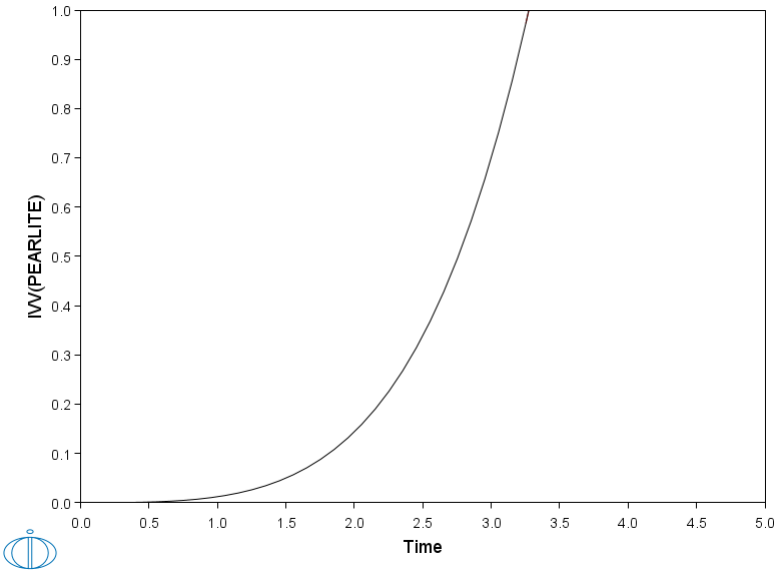
exe1-plot

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exe1\plot.DCM 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

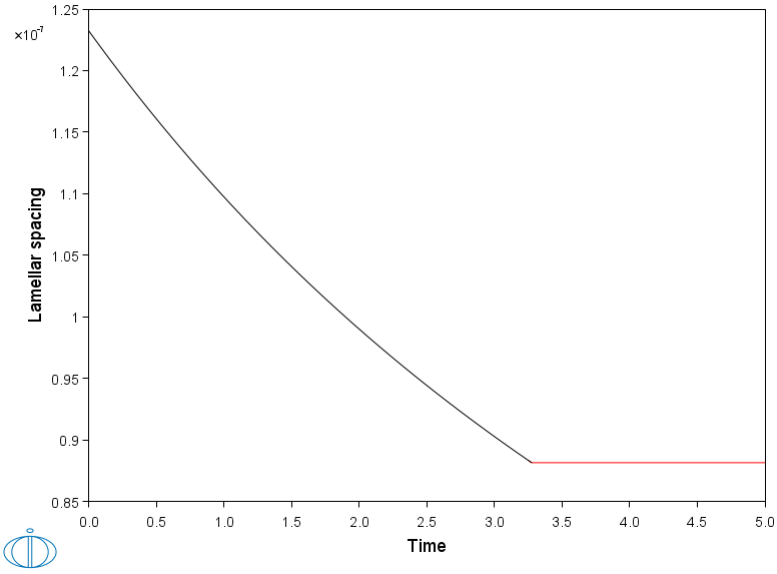
  INFO: Time is set as independent variable
POST-1: s-d-a y t
POST-1: s-p-c interface first
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 3
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples/unite/distribution\macroResult.exp Y
ORKING ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```



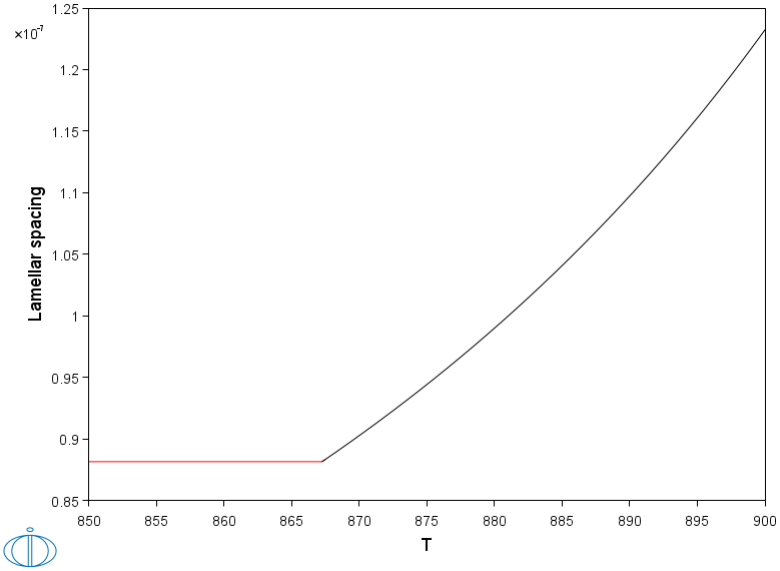

```
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ NOW PLOT THE FRACTION OF PEARLITE VS. TIME
POST-1: @@
POST-1: s-d-a y ivv(pearlite)
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 3
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples/unite/distribution\macroResult.exp Y
ORKING ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```



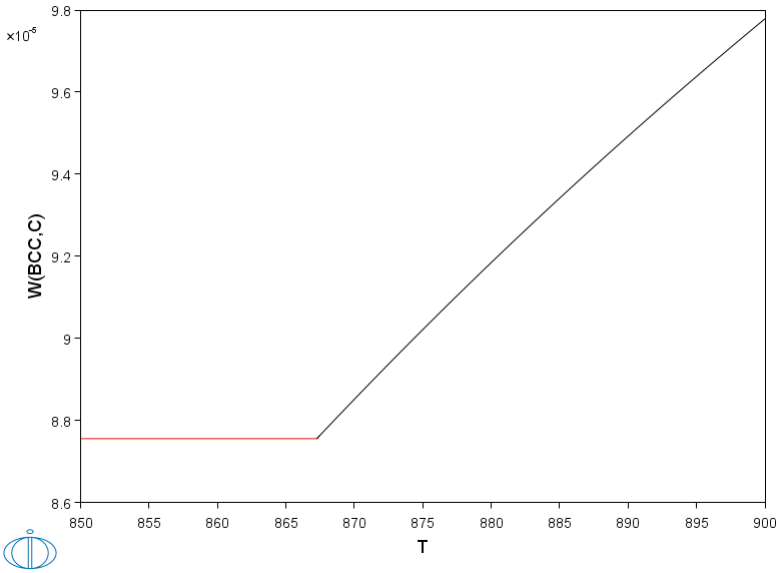

```
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ PLOT THE LAMELLAR SPACING AS A FUNCTION OF TIME
POST-1: @@
POST-1: s-d-a
AXIS (X, Y OR Z) : y
VARIABLE : lamellar-sp
IN REGION: /*/: pearlite
POST-1:
POST-1: s-p-c
CONDITION /INTEGRAL/: interface
INTERFACE : pearlite
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
ORKING ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```



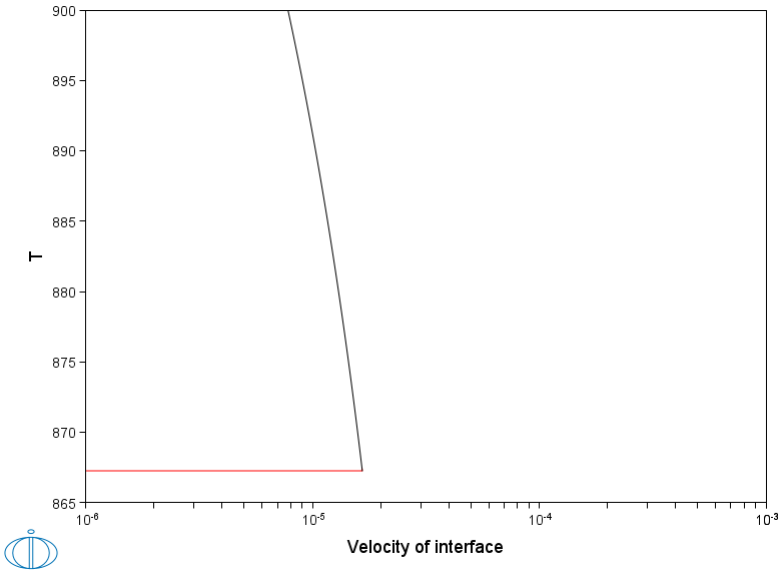

```
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ LET'S LOOK AT THE LAMELLAR SPACING VS. TEMPERATURE INSTEAD
POST-1: @@
POST-1: s-d-a x t
POST-1:
POST-1: s-p-c interface pearlite upper
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 3
POST-1: MAKE c:\jenkins\workspace\dev_pipeline\generate_dictra_console_examples/unite/distribution\macroResult.exp Y
ORKING ...          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
ORKING ... OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot

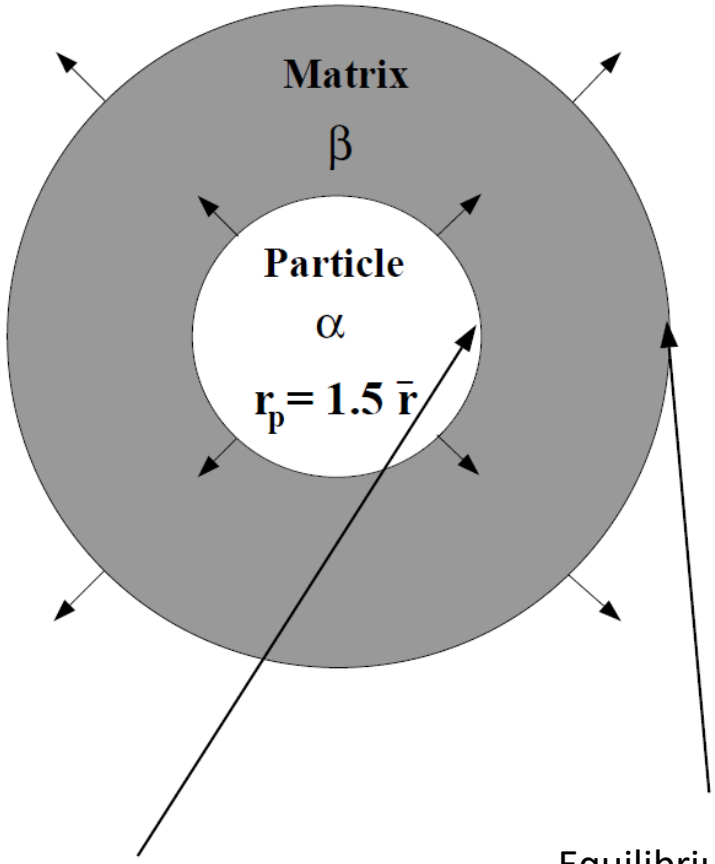


POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ FINALLY, LET'S LOOK AT THE VELOCITY OF THE INTERFACE VS. TEMP
POST-1: @@
POST-1: s-d-a y t
POST-1: s-d-a x velocity
INTERFACE : pearlite
UPPER OR LOWER INTERFACE OF REGION PEARLITE#1 /LOWER/: upper
POST-1: set-ax-ty x 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
ORKING ... 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 α and β in local equilibrium.

$\frac{2\sigma V_m}{r}$ Interfacial energy contribution for α phase

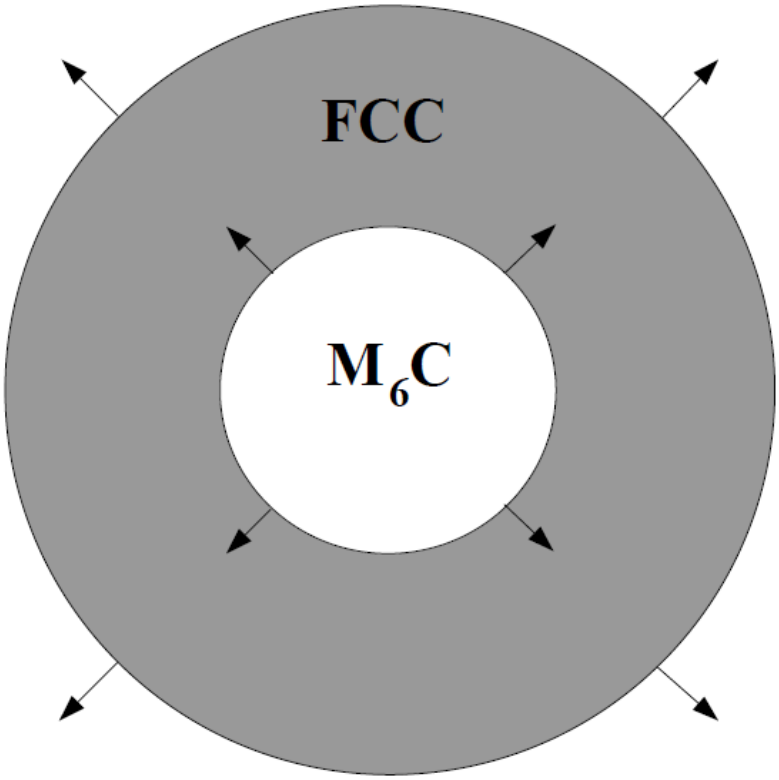
Equilibrium as defined by the average composition in the system.

$\frac{2\sigma V_m}{r_p}$ Interfacial energy contribution for α phase

Example exf1

Coarsening of an M_6C precipitate in an Fe-Mo-C alloy

This example calculates the Ostwald-ripening of a spherical M6C carbide in an austenite matrix.



T = 1173K **r_p = 0.228 μm**

exf1-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: unknown compiler
 License library version: 9.7.0.0036
 Linked: Fri Oct 18 11:32:56 2024


SYS:SYS:MACRO exf1\setup.DCM
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: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASES
SYS: @@
SYS: go da
15:25:51,107 [Thread-0] INFO  LicenseManager: Initializing user: jenkins.integrationtest@thermocalc.se
15:25:51,122 [Thread-0] INFO  LicenseController: Running License Spring in DEV environment.
15:25:52,170 [Thread-0] INFO  LicenseManager: There is an activated standalone license for jenkins.integrationtest@thermocalc.se for TC-
Application
 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
15:25:53,618 [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 v5.0
 MOB2    =  Alloys Mobility  v2.7
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBFE7  =  Steels/Fe-Alloys Mobility  v7.1
 MFEDEMO =  Fe-Alloys Mobility demo database v4.0
 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
15:25:55,591 [Thread-0] INFO  StandaloneLicenseController: Checking out license for: Diffusion (DICTRA)
 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 GEOMTRICAL 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 CHOOSEN TO MAINTAIN THE AVERAGE COMPOSITION.
DIC> @@
DIC> enter-grid
REGION NAME : /PART/: part
WIDTH OF REGION /1/: 0.228E-6
TYPE /LINEAR/: AUTO
DIC>
DIC> enter-grid
REGION NAME : /AUS/: aus
WIDTH OF REGION /1/: 4.53147041E-7
TYPE /LINEAR/: 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 SUBSTITIONAL ATOM.
DIC> @@
DIC> @@ THE SURFACE TENSION IS 0.7, THE MOLAR VOLUME IS 0.71 AND THE
DIC> @@ TRANSFORMATION TO MOLAR VOLUME PER SUBSTITIONAL 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 exf1 Y
DIC>
DIC> set-inter
 --OK---
DIC>
```

exf1-run

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exf1\run.DCM DIC> @@ exf1_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 exf1
 OK
DIC> sim
 Region: PART
 geometric   0.719099     dense at   0.228000E-06   99 points
 Region: AUS

 geometric    1.05435     dense at    0.00000       76 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 = .0190652843033664  FE = .970761291162784
                        MO = .0292387089677229
 TOTAL SIZE OF SYSTEM:  1.32376603026E-18 [m^3]
 U-FRACTION IN SYSTEM:  C = .0190652843033664  FE = .970761291162784
                        MO = .0292387089677229
 TOTAL SIZE OF SYSTEM:  1.32376603026E-18 [m^3]
 0.610226192272014        0.610394270619902        0.610226132878211        2.564838682333877E-002        2.1899395245898 56E-
003        1.207017414854853E-004        1.023120461010883E-003        1.218178721768246E-004        2.517633807956219E-
007        9.719018163791694E-010        1.143192107369703E-009        4.788525779255918E-009        8.208470533441581E-
010        7.852807426863805E-010        7.164147913924398E-010        3.414650428994940E-009        5.878095774070730E-
010        3.676297630615314E-010        7.952758759922585E-011        3.687325852901084E-014        3.588852654267949E-
019       TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =  0.33271373E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.33648562E-05 AND  -0.33648562E-05
 POSITION OF INTERFACE PART / AUS IS   0.22799966E-06
 U-FRACTION IN SYSTEM:  C = .0190658079671791  FE = .970759854855068
                        MO = .0292401452754388
 TOTAL SIZE OF SYSTEM:  1.32376016937E-18 [m^3]
  12  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: PART

  CPU time used in timestep                    2  seconds
 2.502011428410655E-005        2.502542753393348E-005        2.501395573147565E-005        1.071851945979826E-006        1.565931414482499E-
007        3.589706400460076E-012        2.034526710974865E-017       SWITCHING ACTIVITIES FOR INTERFACE #2, CELL #1
 FROM: C  TO: MO
 TIME =  0.11986832E-05 DT =  0.10986832E-05 SUM OF SQUARES =  0.20314210E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.53640186E-08 AND  -0.53640186E-08
 POSITION OF INTERFACE PART / AUS IS   0.22799966E-06
 U-FRACTION IN SYSTEM:  C = .019066137551205  FE = .970759852766409
                        MO = .0292401473640975
 TOTAL SIZE OF SYSTEM:  1.32376006672E-18 [m^3]
  CPU time used in timestep                    1  seconds
 4.168511413044171E-008        4.169572472887800E-008        4.134060969262297E-008        1.321582351576341E-009        1.250003026153813E-
009        1.112310125600152E-009        8.613791096708145E-010        8.615258426197119E-010        4.552183932425979E-
010        2.808156382933142E-011        7.761149409047003E-017       TIME =  0.33960497E-05 DT =  0.21973664E-
05 SUM OF SQUARES =  0.72436618E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.79710063E-09 AND  -0.79710063E-09
 POSITION OF INTERFACE PART / AUS IS   0.22799966E-06
 U-FRACTION IN SYSTEM:  C = .0190665444592517  FE = .970759852534804
                        MO = .0292401475957033
 TOTAL SIZE OF SYSTEM:  1.32376003621E-18 [m^3]
  CPU time used in timestep                    0  seconds
 8.617044278903503E-010        8.618851750855182E-010        8.798975513258887E-010        7.986939323110455E-010        7.971970954187355E-
010        7.942100180876864E-010        7.882168705758153E-010        7.892200457706786E-010        7.763334285740979E-
010        7.528033379241208E-010        7.068617315251412E-010        7.082747798572400E-010        6.192881314034981E-
010        4.615323619756609E-010        2.154560731003840E-010        2.165308435278966E-010        1.142576288744393E-
012        5.402338989545008E-023       TIME =  0.77907826E-05 DT =  0.43947329E-05 SUM OF SQUARES =  0.53260910E-22
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.16705040E-09 AND  -0.16705040E-09
 POSITION OF INTERFACE PART / AUS IS   0.22799966E-06
 U-FRACTION IN SYSTEM:  C = .0190670799729191  FE = .970759852768178
                        MO = .0292401473623295
 TOTAL SIZE OF SYSTEM:  1.32376002342E-18 [m^3]
  CPU time used in timestep                    1  seconds
 4.352313273852556E-011        4.353030179273932E-011

output ignored...



... output resumed

 2.055568706087755E-011        2.415633539231364E-011        8.276071234257102E-013        6.399087123628197E-014        6.793348128548265E-
023       TIME =   651001.87     DT =   100000.00     SUM OF SQUARES =  0.59772063E-22
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.22741005E-13 AND   0.22741005E-13
 POSITION OF INTERFACE PART / AUS IS   0.24360160E-06
 U-FRACTION IN SYSTEM:  C = .0195560141241856  FE = .970692207011243
                        MO = .0293077931192632
 TOTAL SIZE OF SYSTEM:  1.6145336252E-18 [m^3]
  18  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: PART
  17  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUS

  CPU time used in timestep                    0  seconds
 9.300606502034461E-012        9.611212424722388E-012        1.206999009868420E-011        1.534911110385506E-012        6.665993764812200E-
013        6.603529371604751E-022       TIME =   751001.87     DT =   100000.00     SUM OF SQUARES =  0.36010934E-21
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.22321276E-13 AND   0.22321276E-13
 POSITION OF INTERFACE PART / AUS IS   0.24583373E-06
 U-FRACTION IN SYSTEM:  C = .0195585249548054  FE = .970693993165916
                        MO = .0293060006964591
 TOTAL SIZE OF SYSTEM:  1.65932357781E-18 [m^3]
  28  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: PART
  28  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUS

  CPU time used in timestep                    1  seconds
 5.048861318933851E-012        5.105914105529700E-012        6.732216105761729E-012        2.393338756081908E-012        1.709134423325863E-
012        6.058104325457034E-013        3.026363883286354E-
022       TIME =   851001.87     DT =   100000.00     SUM OF SQUARES =  0.13688634E-23
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.21920390E-13 AND   0.21920390E-13
 POSITION OF INTERFACE PART / AUS IS   0.24802577E-06
 U-FRACTION IN SYSTEM:  C = .0195609607450678  FE = .970695754580921
                        MO = .0293042455495858
```

```
 TOTAL SIZE OF SYSTEM:  1.70410788906E-18 [m^3]
  25  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: PART
  26  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUS

  CPU time used in timestep                    0  seconds
 3.957557668768415E-012        3.814628526865988E-012        4.790207553171515E-012        3.345448982654202E-012        2.947447994739933E-
012        2.161112271217530E-012        8.448860052476941E-013        5.271705057892456E-
019       TIME =    951001.87     DT =    100000.00     SUM OF SQUARES =  0.22641349E-20
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.21537016E-13 AND   0.21537016E-13
 POSITION OF INTERFACE PART / AUS IS   0.25017947E-06
 U-FRACTION IN SYSTEM:  C = .0195633282771205  FE = .970697476918075
                        MO = .0293025232124324
 TOTAL SIZE OF SYSTEM:  1.7488867212E-18 [m^3]
  13  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: PART
  12  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUS

  CPU time used in timestep                    0  seconds
 1.766659302680313E-010        1.740026564922209E-010        1.660414132278637E-010        2.449667661230245E-011        9.885666630790687E-
012        3.959862424980931E-020       TIME =   1000000.0     DT =   48998.127     SUM OF SQUARES =  0.39222756E-19
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.21268367E-13 AND   0.21268367E-13
 POSITION OF INTERFACE PART / AUS IS   0.25122158E-06
 U-FRACTION IN SYSTEM:  C = .0195658210705057  FE = .970698666251374
                        MO = .0293013338791329
 TOTAL SIZE OF SYSTEM:  1.77083258443E-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   0.11986832E-05
 DELETING TIME-RECORD FOR TIME   0.33960497E-05
 DELETING TIME-RECORD FOR TIME   0.77907826E-05
 DELETING TIME-RECORD FOR TIME   0.16580248E-04
 DELETING TIME-RECORD FOR TIME   0.34159180E-04
 DELETING TIME-RECORD FOR TIME   0.69317043E-04
 DELETING TIME-RECORD FOR TIME   0.13963277E-03
 DELETING TIME-RECORD FOR TIME   0.28026422E-03
 DELETING TIME-RECORD FOR TIME   0.56152713E-03
 DELETING TIME-RECORD FOR TIME   0.11240529E-02
 DELETING TIME-RECORD FOR TIME   0.22491046E-02
 DELETING TIME-RECORD FOR TIME   0.44992078E-02
 DELETING TIME-RECORD FOR TIME   0.89994143E-02
 DELETING TIME-RECORD FOR TIME   0.17999827E-01
 DELETING TIME-RECORD FOR TIME   0.36000653E-01
 DELETING TIME-RECORD FOR TIME   0.72002305E-01
 DELETING TIME-RECORD FOR TIME   0.14400561
 DELETING TIME-RECORD FOR TIME   0.28801222
 DELETING TIME-RECORD FOR TIME   0.57602543
 DELETING TIME-RECORD FOR TIME    1.1520519
 DELETING TIME-RECORD FOR TIME    2.3041047
 DELETING TIME-RECORD FOR TIME    4.6082104
 DELETING TIME-RECORD FOR TIME    9.2164219
 DELETING TIME-RECORD FOR TIME    18.432845
 DELETING TIME-RECORD FOR TIME    36.865691
 DELETING TIME-RECORD FOR TIME    73.731382
 DELETING TIME-RECORD FOR TIME    147.46277
 DELETING TIME-RECORD FOR TIME    294.92553
 DELETING TIME-RECORD FOR TIME    589.85106
 DELETING TIME-RECORD FOR TIME    1179.7021
 DELETING TIME-RECORD FOR TIME    2359.4043
 DELETING TIME-RECORD FOR TIME    4718.8085
 DELETING TIME-RECORD FOR TIME    9437.6170
 DELETING TIME-RECORD FOR TIME    18875.234
 DELETING TIME-RECORD FOR TIME    37750.468
 DELETING TIME-RECORD FOR TIME    75500.936
 DELETING TIME-RECORD FOR TIME    151001.87
 DELETING TIME-RECORD FOR TIME    251001.87
 DELETING TIME-RECORD FOR TIME    351001.87
 DELETING TIME-RECORD FOR TIME    451001.87
 DELETING TIME-RECORD FOR TIME    551001.87
 DELETING TIME-RECORD FOR TIME    651001.87
 DELETING TIME-RECORD FOR TIME    751001.87
 DELETING TIME-RECORD FOR TIME    851001.87

 KEEPING TIME-RECORD FOR TIME    951001.87
 AND FOR TIME                    1000000.0
 WORKSPACE RECLAIMED

 TIMESTEP AT     1000000.00     SELECTED

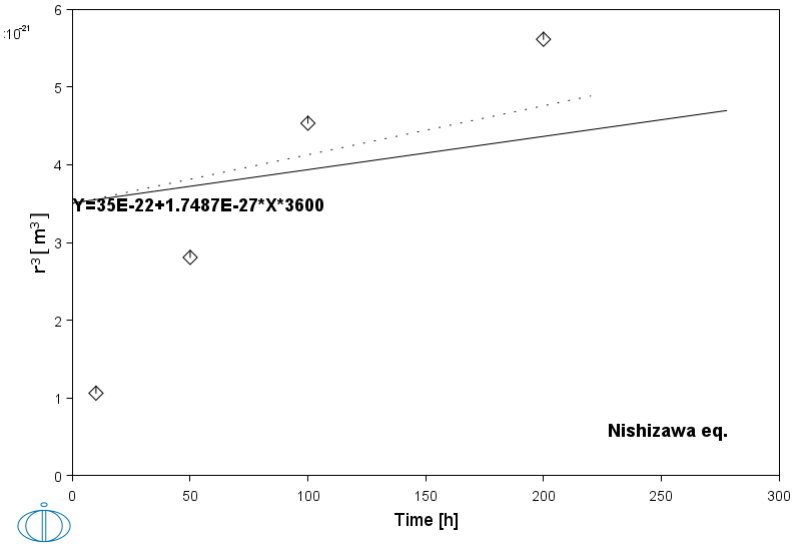
DIC>
DIC>
DIC> set-inter
 --OK---
DIC>
```

exf1-plot

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exf1\plot.DCM DIC> @@ exf1_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE f1
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+06
*** ENTERING M6C AS A DIFFUSION NONE PHASE
DIC> read exf1
 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 exf1
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

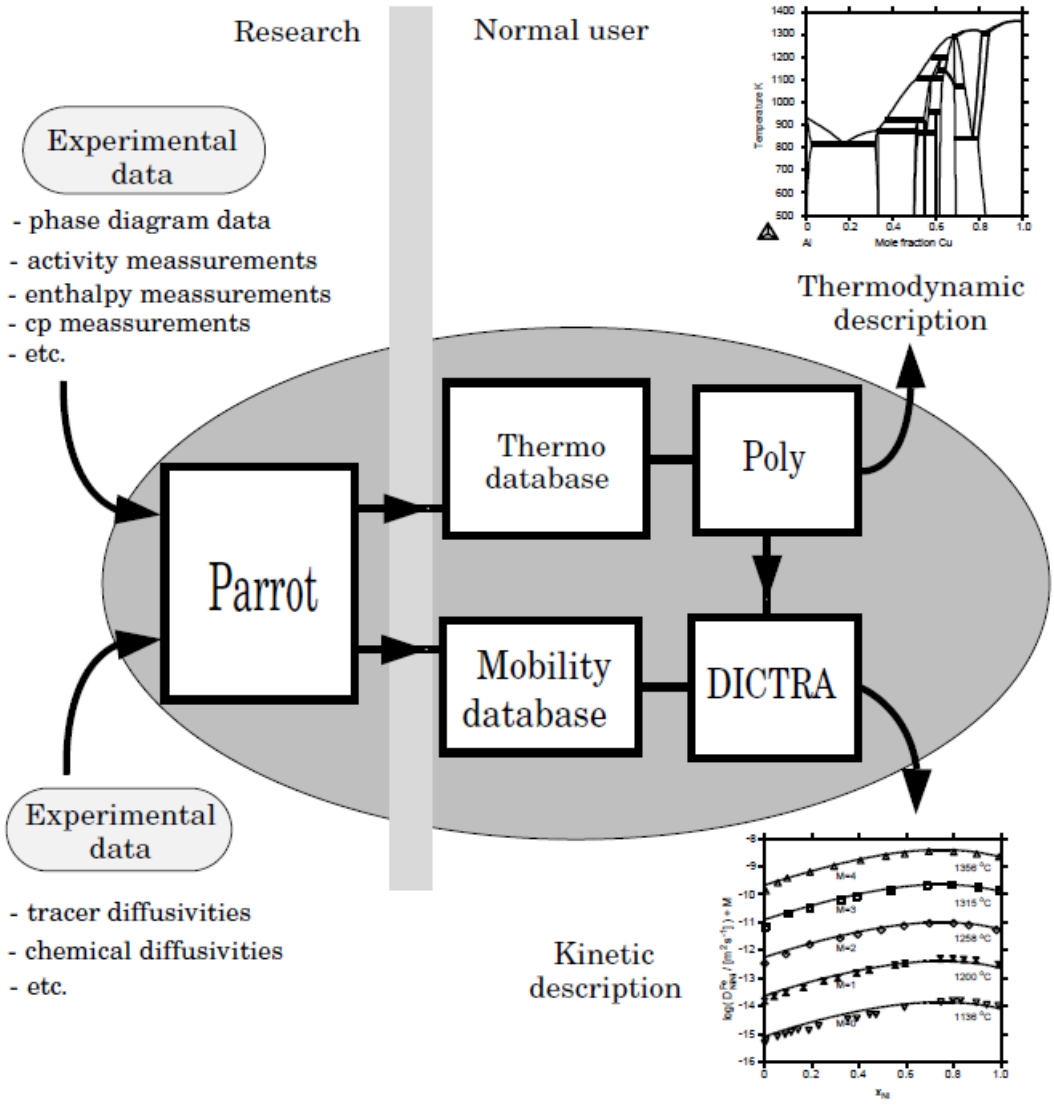
          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

Figure f1.1




```
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1: @@
POST-1: @@ THE DIFFENCE 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:
```

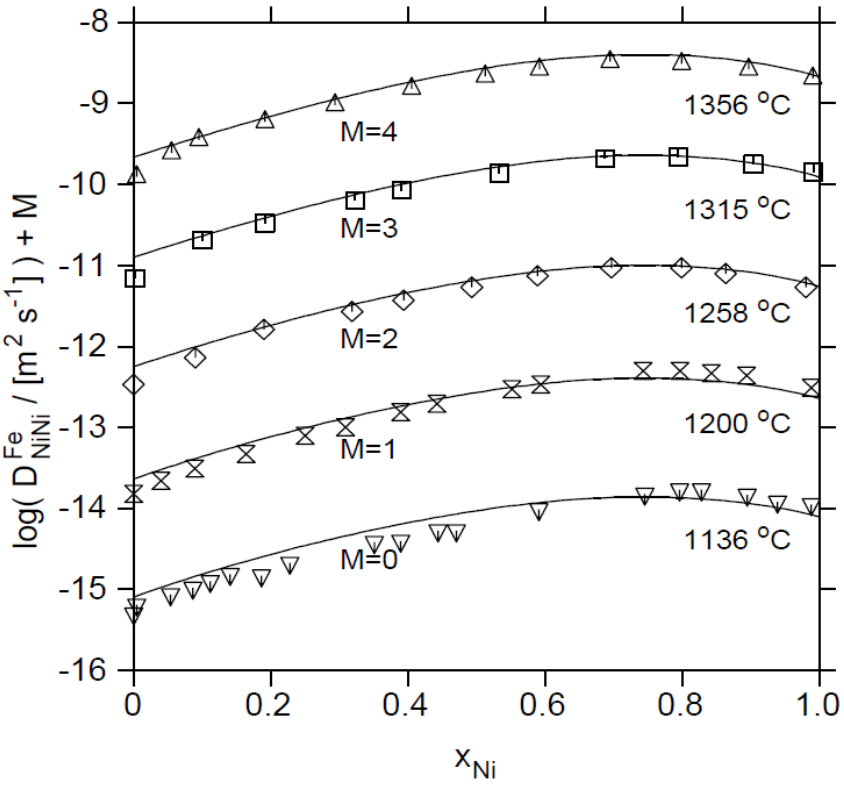
Kinetic Data



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: unknown compiler
 License library version: 9.7.0.0036
 Linked: Fri Oct 18 11:32:56 2024


SYS:SYS:MACRO exg1\setup.DCM
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: ----------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exg1_setup.DCM
SYS:
SYS: @@
SYS: @@ START BY GOING TO THE DATABASE MODULE
SYS: @@
SYS: go da
15:29:07,673 [Thread-0] INFO  LicenseManager: Initializing user: jenkins.integrationtest@thermocalc.se
15:29:07,688 [Thread-0] INFO  LicenseController: Running License Spring in DEV environment.
15:29:08,766 [Thread-0] INFO  LicenseManager: There is an activated standalone license for jenkins.integrationtest@thermocalc.se for TC-
Application
 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 v5.0

 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
 BCC_A2                   CBCC_A12                 CUB_A13
 FCC_A1                   GAS:G                    HCP_A3
 LAVES_PHASE_C14          LIQUID:L  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
15:29:09,858 [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 v5.0
 MOB2    =  Alloys Mobility  v2.7
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBFE7  =  Steels/Fe-Alloys Mobility  v7.1
 MFEDEMO =  Fe-Alloys Mobility demo database v4.0
 USER    =  User defined Database

DATABASE NAME /FEDEMO/: mfedemo
 Current database: Fe-Alloys Mobility demo database v4.0

 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: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP
APP: @@
APP: go d-m
15:29:10,368 [Thread-0] INFO  StandaloneLicenseController: Checking out license for: Diffusion (DICTRA)
 NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ CHECK THE DIFFUSIVITES
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 ( dlpbmx0ez or * ) /D/: dl

  Dkj (reduced n=FE)
  k / j NI
  NI   +4.86136E-15
   L0kj = Uk*Mvak IF (kES) ELSE Uk*Yva*Mvak
  k / j   FE             NI
  FE    +1.00113E-19
  NI                  +1.00113E-19

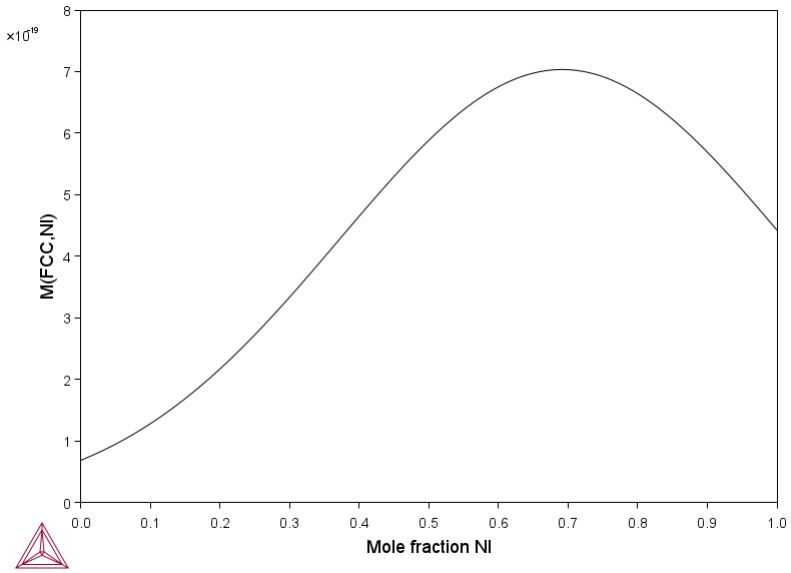

  Volume =   1.000000000000000E-005

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
15:29:10,640 [Thread-0] INFO  StandaloneLicenseController: Checking out license for: Thermo-Calc
15:29:10,831 [Thread-0] INFO  StandaloneLicenseController: Releasing license for: Diffusion (DICTRA)
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             1 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     1  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

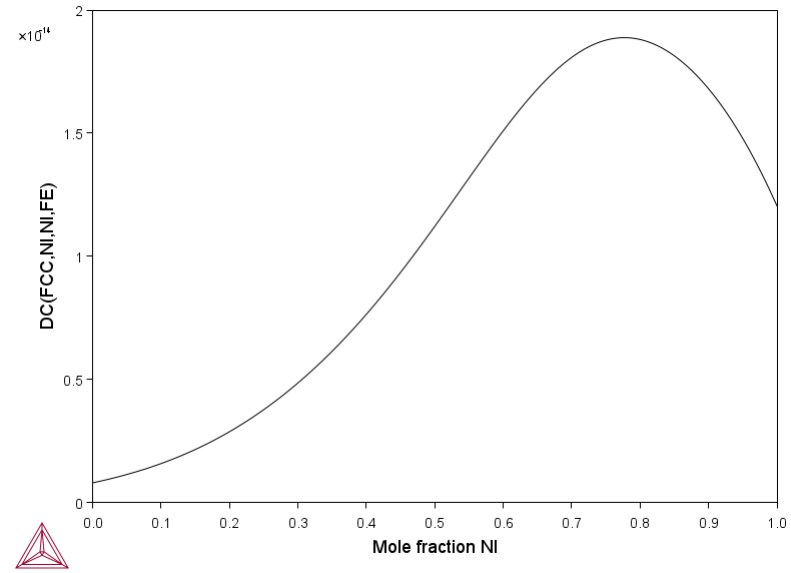
 Phase Region from   0.300000     for:
     FCC_A1
 Global test at  3.08000E-01 .... OK
 Global test at  3.18000E-01 .... OK
 Global test at  3.28000E-01 .... OK
 Global test at  3.38000E-01 .... OK
 Global test at  3.48000E-01 .... OK
 Global test at  3.58000E-01 .... OK
 Global test at  3.68000E-01 .... 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

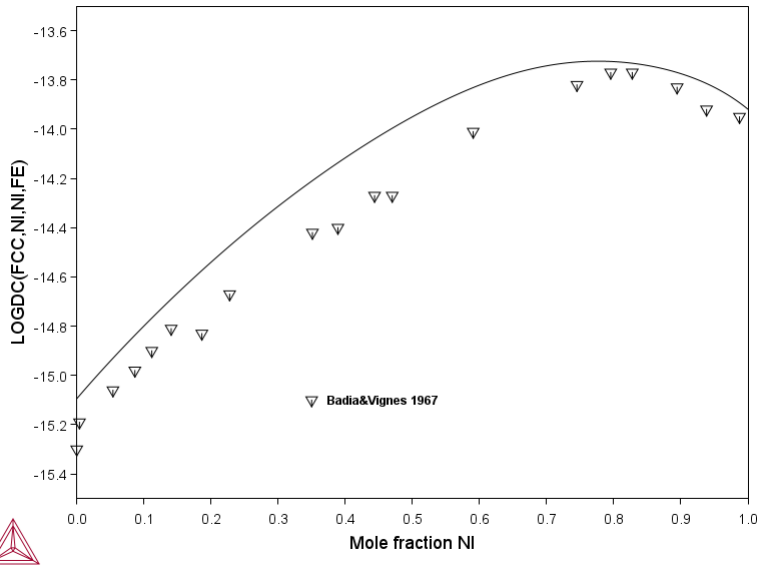
 Phase Region from   0.300000     for:
     FCC_A1
 Global test at  2.92000E-01 .... OK
 Global test at  2.82000E-01 .... OK
 Global test at  2.72000E-01 .... OK
 Global test at  2.62000E-01 .... OK
 Global test at  2.52000E-01 .... OK
 Global test at  2.42000E-01 .... OK
 Global test at  2.32000E-01 .... 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   0.100000E-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
```

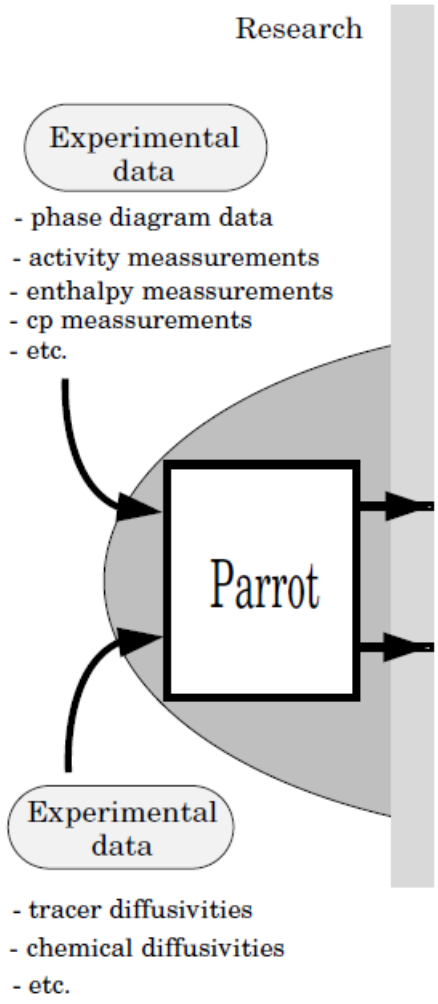



```
POST:
POST:
POST:@?<Hit_return_to_continue>
POST:
POST: set-inter
POST:
```

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: unknown compiler
 License library version: 9.7.0.0036
 Linked: Fri Oct 18 11:32:56 2024


SYS:SYS:MACRO exg2\setup.DCM
SYS: ï»¿@@
 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. EngstrÃ¶m and J. Ã…gren: ("Assessment of Diffusional
SYS: @@ Mobilities in Face-Centered Cubic Ni-Cr-Al Alloys" in
SYS: @@ Z. Metallkunde, Feb. 1996).
SYS: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
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
15:30:10,584 [Thread-0] INFO  LicenseManager: Initializing user: jenkins.integrationtest@thermocalc.se
15:30:10,597 [Thread-0] INFO  LicenseController: Running License Spring in DEV environment.
15:30:11,694 [Thread-0] INFO  LicenseManager: There is an activated standalone license for jenkins.integrationtest@thermocalc.se for TC-
Application
 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 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_a1
 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_a1
 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
15:30:12,666 [Thread-0] INFO  StandaloneLicenseController: Checking out license for: Diffusion (DICTRA)
```

```
 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_A1&AL,AL:VA) 298.15 -142000+R*T*LN(1.71E-4); 6000 N
 MQ(FCC_A1&AL#1,AL:VA;0)
DIC>
DIC> @@ MOBILITY OF Al IN Ni
DIC> ENTER-MOB-DATA
PARAMETER: MQ(FCC_A1&AL,NI:VA) 298.15 -284000+R*T*LN(7.5E-4); 6000 N
 MQ(FCC_A1&AL#1,NI:VA;0)
DIC>
DIC> @@ MOBILITY OF Al INTERACTION BETWEEN Al AND Ni
DIC> ENTER-MOB-DATA
PARAMETER: MQ(FCC_A1&AL,AL,NI:VA;0) 298.15 V1+V2*T; 6000 N
 MQ(FCC_A1&AL#1,AL,NI:VA;0)
DIC>
DIC> @@ MOBILITY OF Ni IN Al
DIC> ENTER-MOB-DATA
PARAMETER: MQ(FCC_A1&NI,AL:VA) 298.15 -145900+R*T*LN(4.4E-4); 6000 N
 MQ(FCC_A1&NI#1,AL:VA;0)
DIC>
DIC> @@ MOBILITY OF Ni IN Ni
DIC> ENTER-MOB-DATA
PARAMETER: MQ(FCC_A1&NI,NI:VA) 298.15 -287000-69.8*T; 6000 N
 MQ(FCC_A1&NI#1,NI:VA;0)
DIC>
DIC> @@ MOBILITY OF Ni INTERACTION BETWEEN Ni AND Al
DIC> ENTER-MOB-DATA
PARAMETER: MQ(FCC_A1&NI,NI,AL:VA;0) 298.15 V3+V4*T; 6000 N
 MQ(FCC_A1&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 exg2\run.DCM 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
```

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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:
```
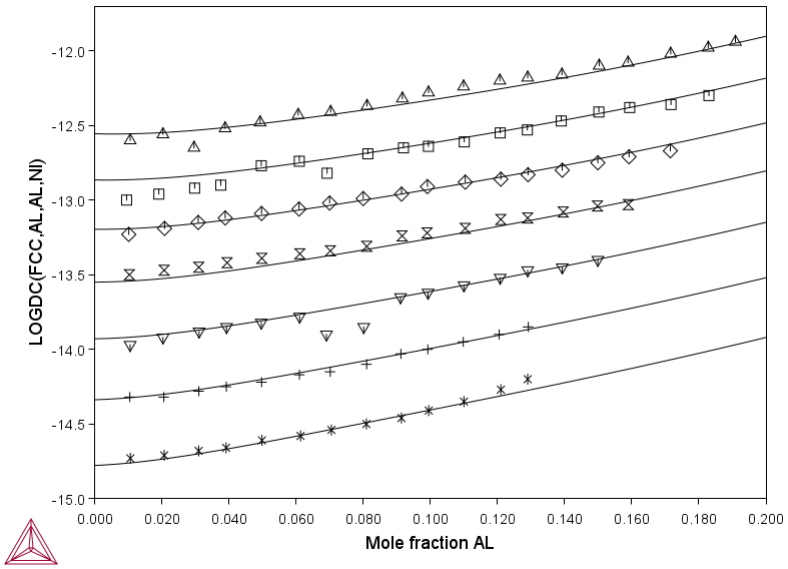

exg2-plot

```
PARROT:About
 NO SUCH COMMAND, USE HELP
PARROT:PARROT:MACRO exg2\plot.DCM
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
15:32:03,402 [Thread-0] INFO  StandaloneLicenseController: Checking out license for: Thermo-Calc
15:32:03,622 [Thread-0] INFO  StandaloneLicenseController: Releasing license for: Diffusion (DICTRA)
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 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  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 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  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 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  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 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  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 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  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
```

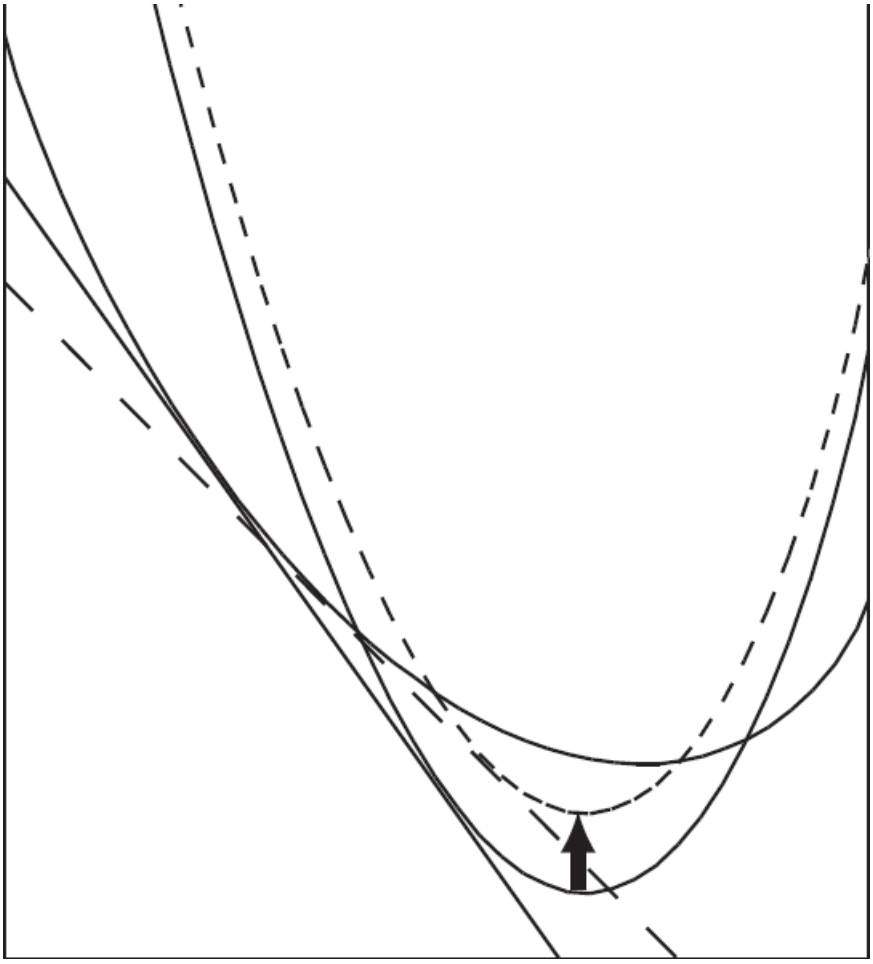
```
 Phase Region from   0.100000     for:
     FCC_A1
 Global test at  9.20000E-02 .... OK
 Global test at  8.20000E-02 .... OK
 Global test at  7.20000E-02 .... OK
 Global test at  6.20000E-02 .... OK
 Global test at  5.20000E-02 .... OK
 Global test at  4.20000E-02 .... OK
 Global test at  3.20000E-02 .... 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=1323,x(al)=.1
POLY: c-e,,,,,,,
 Using global minimization procedure
Calculated           209 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  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=1273,x(al)=.1
POLY: c-e,,,,,,,
 Using global minimization procedure
Calculated           209 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  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: @@
POLY: @@ ENTER THE POST MODULE, PLOT THE DIFFUSIVITY ON THE Y-AXIS
POLY: @@ AND MOLE-FRACTION Al 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:
```

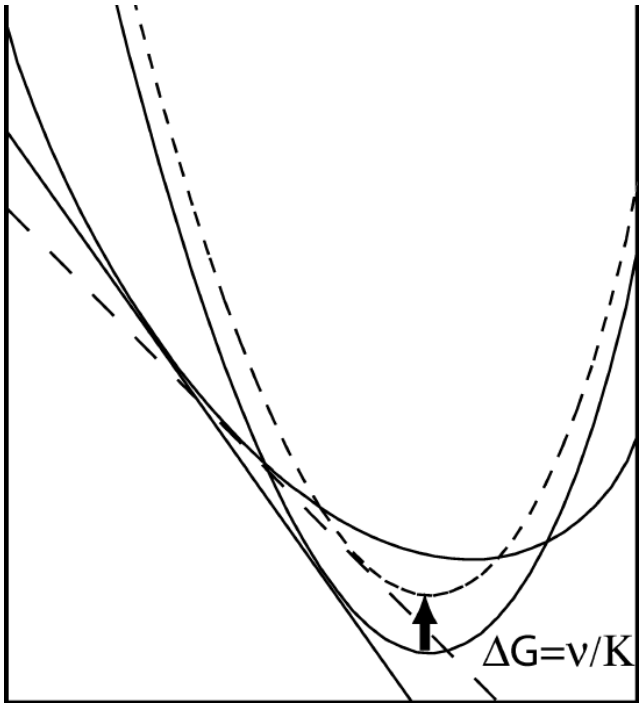
Deviation From Local Equilibrium



Example exh1

σ/γ diffusion couple with limited interface mobility

This example calculates the growth of ferrite (α) into austenite (γ) 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: unknown compiler
 License library version: 9.7.0.0036
 Linked: Fri Oct 18 11:32:56 2024


SYS:SYS:MACRO exh1\setup.DCM
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: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASE
SYS: @@
SYS: go da
15:33:05,524 [Thread-0] INFO  LicenseManager: Initializing user: jenkins.integrationtest@thermocalc.se
15:33:05,537 [Thread-0] INFO  LicenseController: Running License Spring in DEV environment.
15:33:06,692 [Thread-0] INFO  LicenseManager: There is an activated standalone license for jenkins.integrationtest@thermocalc.se for TC-
Application
 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 v5.0

 VA                       /-  DEFINED
TDB_FEDEMO: def-sys fe c
 FE                       C  DEFINED
TDB_FEDEMO: rej ph * all
 BCC_A2                   CBCC_A12                 CEMENTITE
 CUB_A13                  DIAMOND_FCC_A4           FCC_A1
 GAS:G                    GRAPHITE                 HCP_A3
 KSI_CARBIDE              LAVES_PHASE_C14          LIQUID:L
 M23C6                    M5C2                     M7C3
   REJECTED
TDB_FEDEMO: res ph bcc fcc
 BCC_A2                   FCC_A1  RESTORED
TDB_FEDEMO: get
15:33:07,784 [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 v4.0

 VA  DEFINED
APP: def-sys fe c
 FE                       C  DEFINED
APP: rej ph * all
 BCC_A2                   FCC_A1                   CEMENTITE
 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
15:33:08,304 [Thread-0] INFO  StandaloneLicenseController: Checking out license for: Diffusion (DICTRA)
 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 /LINEAR/: AUTO
DIC>
DIC> enter-grid austenite
WIDTH OF REGION /1/: 0.999e-6
TYPE /LINEAR/: 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> @@
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 exh1 y
DIC>
DIC> set-inter
 --OK---
DIC>
```

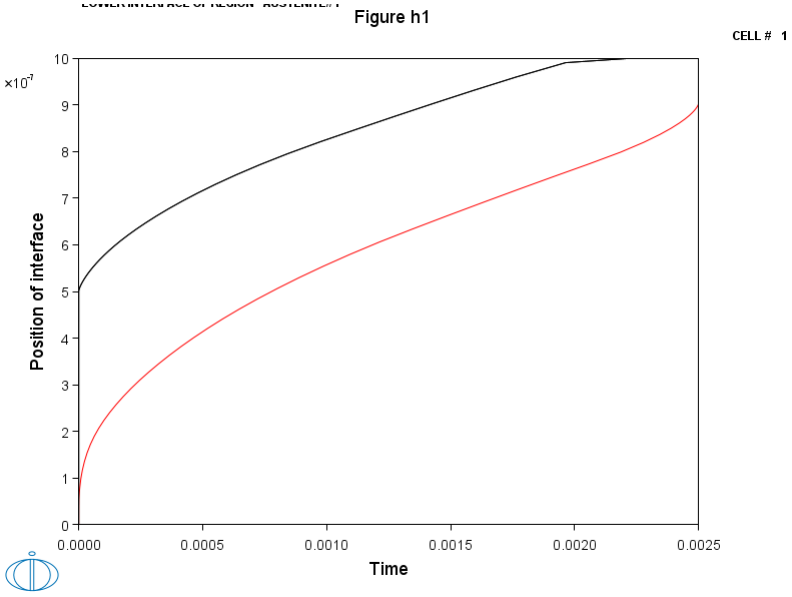
exh1-run

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exh1\run.DCM 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
 Region: FERRITE
 geometric   0.956340     dense at   0.100000E-08   76 points
 Region: AUSTENITE

 geometric    1.15218     dense at    0.00000       88 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]
 7.938044190665376E-005        7.937710023253734E-005        6.82207097429483       7.884164585500397E-005        7.857293587000751E-
005        7.843875288771839E-005        7.837170439911923E-005        7.830468457890465E-005        7.822878117532253E-
005        7.807708478532028E-005        7.777413367394015E-005        7.716999812574442E-005        7.596879372760469E-
005        7.359465172472982E-005        6.895943489316783E-005        6.014126992561462E-005        4.431401477294380E-
005        1.989580359734839E-005         6.18384998131949       1.982569952307290E-005       1.979069388320350E-
005        1.977320266257898E-005        1.976445995211993E-005        1.975571917484897E-005        1.974655887752673E-005


     ERROR RETURN FROM NS01A BECAUSE THERE HAVE BEEN   25 CALLS OF CALFUN
  RESCALING
 2.088978290317390E-005        2.088410267821287E-005        6.82207078779667       2.081686503051677E-005        2.078045390149663E-
005        2.076226028881366E-005        2.075316647041682E-005        2.074407464401544E-005        2.073455451312070E-
005        2.071552080644188E-005        2.067747961372094E-005        2.060150211069647E-005        2.044996663431713E-
005        2.014857380023687E-005        1.955250060679010E-005        1.838720411877430E-005        1.616401073813665E-
005        1.214722235854371E-005        5.832039126026385E-006         4.42855169664992       5.820193815275725E-
006        5.814275675509861E-006        5.811279136473229E-006        5.808283369803743E-006        5.805288375497124E-006


     ERROR RETURN FROM NS01A BECAUSE THERE HAVE BEEN   25 CALLS OF CALFUN
 *** ERROR  1890 IN DCNS01: ERROR RETURN FROM NS01A
 5.805288375497124E-006        5.805287774082395E-006        5.805288375497124E-006         6.82200513010403       5.805288375497124E-
006        5.794592709589948E-006        5.794592108571284E-006        5.794592709589948E-006        5.789248574843406E-
006        5.789248574843406E-006        5.778567701841365E-006        5.778567701841365E-006        5.757235541621946E-
006        5.757235541621946E-006        5.714689564445564E-006        5.714689564445564E-006

output ignored...



... output resumed

 4.221403196081389E-012        3.949198343686763E-016        3.600336222485029E-022       TIME =  0.24982362E-02 DT =  0.12087202E-
05 SUM OF SQUARES =  0.36003362E-21
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.11004268E-02 AND   0.11004268E-02
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.90001287E-06
 U-FRACTION IN SYSTEM:  C = 8.95344150093146E-04  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-06 [m]
  CPU time used in timestep                  0  seconds
 9.819180203648575E-008        9.805770501062171E-008        4.935575299284409E-010        3.190956539249883E-012        1.245284115630167E-
016        3.221603607850745E-023       TIME =  0.24990357E-02 DT =  0.79950704E-06 SUM OF SQUARES =  0.32216036E-22
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.12494049E-02 AND   0.12494049E-02
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.90101177E-06
 U-FRACTION IN SYSTEM:  C = 8.95426596939559E-04  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-06 [m]
  CPU time used in timestep                  0  seconds
 2.388662583620537E-007        2.385993102819282E-007        9.036134617005146E-010        4.388876753787587E-012        1.082711783534734E-
016        1.322963966343475E-023       TIME =  0.24995089E-02 DT =  0.47320711E-06 SUM OF SQUARES =  0.13229640E-22
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.14589155E-02 AND   0.14589155E-02
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.90170214E-06
 U-FRACTION IN SYSTEM:  C = 8.95495122177643E-04  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-06 [m]
  CPU time used in timestep                  0  seconds
 3.220677150312275E-007        3.216764126431214E-007        6.277603042024019E-010        1.477813312473914E-012        8.287632968623834E-
018       TIME =  0.24997856E-02 DT =  0.27671917E-06 SUM OF SQUARES =  0.82876330E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.16764408E-02 AND   0.16764408E-02
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.90216605E-06
 U-FRACTION IN SYSTEM:  C = 8.95588693064985E-04  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-06 [m]
  CPU time used in timestep                  0  seconds
 4.803629481965689E-007        4.797731470253179E-007        4.428533477271799E-010        4.629023328487597E-013        5.097634227005877E-
019       TIME =  0.24999387E-02 DT =  0.15304466E-06 SUM OF SQUARES =  0.50976342E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.19191007E-02 AND   0.19191007E-02
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.90245976E-06
 U-FRACTION IN SYSTEM:  C = 8.95689785742319E-04  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-06 [m]
  CPU time used in timestep                  1  seconds
 1.494146210671713E-006        1.492827264009228E-006        8.072576087545080E-010        4.724474132079392E-013        1.673918727983957E-
019       TIME =  0.25000000E-02 DT =  0.61325012E-07 SUM OF SQUARES =  0.16739187E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.23171219E-02 AND   0.23171219E-02
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.90260185E-06
 U-FRACTION IN SYSTEM:  C = 8.95818151685823E-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   0.13445126E-05
 DELETING TIME-RECORD FOR TIME   0.23899618E-05
 DELETING TIME-RECORD FOR TIME   0.44808600E-05
 DELETING TIME-RECORD FOR TIME   0.85492458E-05
 DELETING TIME-RECORD FOR TIME   0.14727284E-04
 DELETING TIME-RECORD FOR TIME   0.23147820E-04
 DELETING TIME-RECORD FOR TIME   0.33914169E-04
 DELETING TIME-RECORD FOR TIME   0.47103506E-04
 DELETING TIME-RECORD FOR TIME   0.62772814E-04
 DELETING TIME-RECORD FOR TIME   0.80964909E-04
 DELETING TIME-RECORD FOR TIME   0.10171456E-03
 DELETING TIME-RECORD FOR TIME   0.12505328E-03
 DELETING TIME-RECORD FOR TIME   0.15101085E-03
 DELETING TIME-RECORD FOR TIME   0.17963122E-03
 DELETING TIME-RECORD FOR TIME   0.21098410E-03
 DELETING TIME-RECORD FOR TIME   0.24517078E-03
 DELETING TIME-RECORD FOR TIME   0.28232888E-03
 DELETING TIME-RECORD FOR TIME   0.32259549E-03
 DELETING TIME-RECORD FOR TIME   0.36612394E-03
 DELETING TIME-RECORD FOR TIME   0.41324568E-03
 DELETING TIME-RECORD FOR TIME   0.46436785E-03
 DELETING TIME-RECORD FOR TIME   0.51988765E-03
 DELETING TIME-RECORD FOR TIME   0.58039472E-03
 DELETING TIME-RECORD FOR TIME   0.64682298E-03
 DELETING TIME-RECORD FOR TIME   0.71999684E-03
 DELETING TIME-RECORD FOR TIME   0.80052972E-03
 DELETING TIME-RECORD FOR TIME   0.88885857E-03
 DELETING TIME-RECORD FOR TIME   0.98610271E-03
 DELETING TIME-RECORD FOR TIME   0.10932973E-02
 DELETING TIME-RECORD FOR TIME   0.12125955E-02
 DELETING TIME-RECORD FOR TIME   0.13461997E-02
 DELETING TIME-RECORD FOR TIME   0.14863550E-02
 DELETING TIME-RECORD FOR TIME   0.16275333E-02
 DELETING TIME-RECORD FOR TIME   0.17697526E-02
 DELETING TIME-RECORD FOR TIME   0.19131766E-02
 DELETING TIME-RECORD FOR TIME   0.20576933E-02
 DELETING TIME-RECORD FOR TIME   0.21862891E-02
 DELETING TIME-RECORD FOR TIME   0.22778111E-02
 DELETING TIME-RECORD FOR TIME   0.23431198E-02
 DELETING TIME-RECORD FOR TIME   0.23895484E-02
 DELETING TIME-RECORD FOR TIME   0.24227176E-02
 DELETING TIME-RECORD FOR TIME   0.24463076E-02
 DELETING TIME-RECORD FOR TIME   0.24629439E-02
 DELETING TIME-RECORD FOR TIME   0.24746306E-02
 DELETING TIME-RECORD FOR TIME   0.24828278E-02
 DELETING TIME-RECORD FOR TIME   0.24885597E-02
 DELETING TIME-RECORD FOR TIME   0.24925298E-02
 DELETING TIME-RECORD FOR TIME   0.24952173E-02
 DELETING TIME-RECORD FOR TIME   0.24970275E-02
 DELETING TIME-RECORD FOR TIME   0.24982362E-02
 DELETING TIME-RECORD FOR TIME   0.24990357E-02
 DELETING TIME-RECORD FOR TIME   0.24995089E-02
 DELETING TIME-RECORD FOR TIME   0.24997856E-02

 KEEPING TIME-RECORD FOR TIME   0.24999387E-02
 AND FOR TIME                   0.25000000E-02
 WORKSPACE RECLAIMED

 TIMESTEP AT    0.250000000E-02 SELECTED

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

exh1-plot

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exh1\plot.DCM 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
ORKING ...           OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

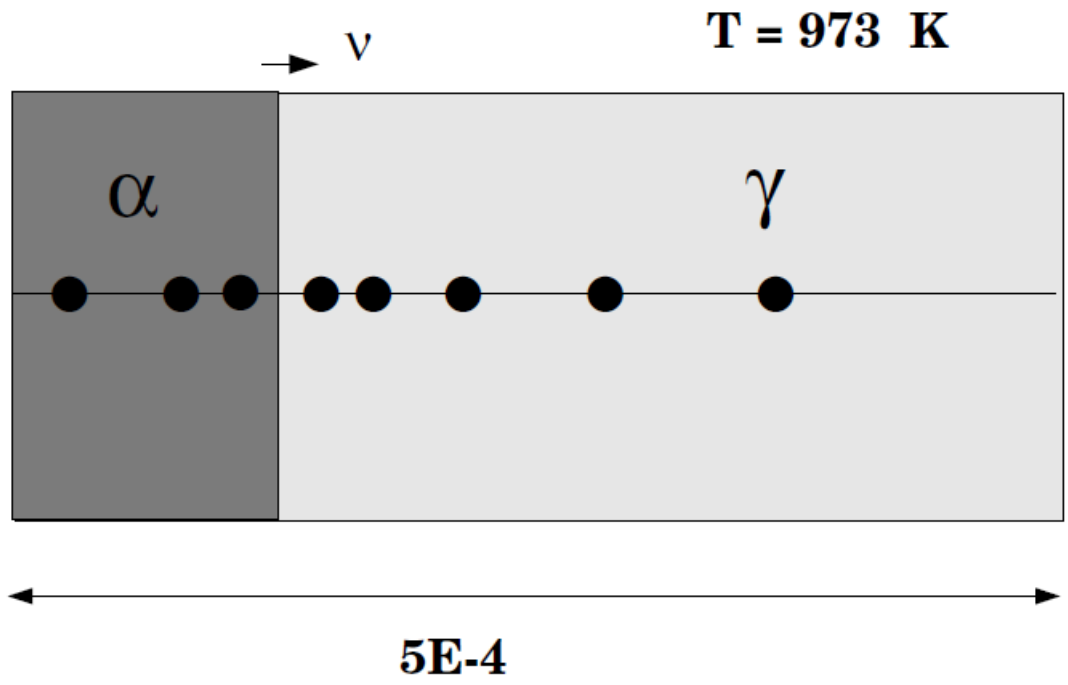



```
POST-1:
POST-1:
POST-1: set-inter
 --OK---
POST-1:
```

Example exh2

σ/γ para-equilibrium in an Fe-Ni-C alloy

This example calculates the growth of ferrite (α) into austenite (γ) 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: unknown compiler
 License library version: 9.7.0.0036
 Linked: Fri Oct 18 11:32:56 2024


SYS:SYS:MACRO exh2\setup.DCM
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: ----------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASE
SYS: @@
SYS: go da
15:36:24,130 [Thread-0] INFO  LicenseManager: Initializing user: jenkins.integrationtest@thermocalc.se
15:36:24,145 [Thread-0] INFO  LicenseController: Running License Spring in DEV environment.
15:36:25,285 [Thread-0] INFO  LicenseManager: There is an activated standalone license for jenkins.integrationtest@thermocalc.se for TC-
Application
 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 v5.0

 VA                       /-  DEFINED
TDB_FEDEMO: def-sys fe ni c
 FE                       NI                       C
   DEFINED
TDB_FEDEMO: rej ph * all
 BCC_A2                   CBCC_A12                 CEMENTITE
 CUB_A13                  DIAMOND_FCC_A4           FCC_A1
 GAS:G                    GRAPHITE                 HCP_A3
 KSI_CARBIDE              LAVES_PHASE_C14          LIQUID:L
 M23C6                    M5C2                     M7C3
   REJECTED
TDB_FEDEMO: res ph bcc fcc
 BCC_A2                   FCC_A1  RESTORED
TDB_FEDEMO: get
15:36:26,361 [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 v4.0

 VA  DEFINED
APP: def-sys fe ni c
 FE                       NI                       C
   DEFINED
APP: rej ph * all
 BCC_A2                   FCC_A1                   CEMENTITE
 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
15:36:26,999 [Thread-0] INFO  StandaloneLicenseController: Checking out license for: Diffusion (DICTRA)
 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 /LINEAR/: AUTO
DIC>
DIC> enter-grid austenite
WIDTH OF REGION /1/: 50e-6
TYPE /LINEAR/: 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> @@
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

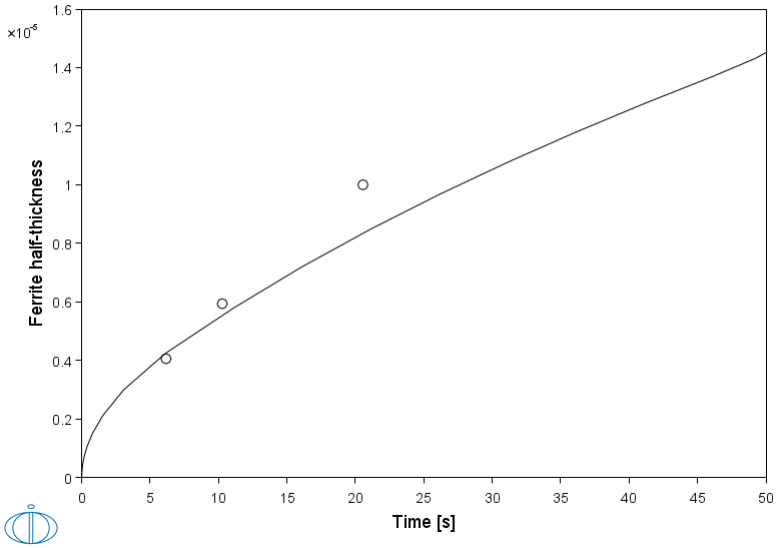
```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exh2\run.DCM DIC>
DIC>
DIC>
DIC> @@
DIC> @@ FILE TO RUN EXAMPLE exh2
DIC> @@
DIC>
DIC> @@
DIC> @@ READ THE SETUP FROM FILE
DIC> @@
DIC>
DIC> go d-m
 TIME STEP AT TIME  0.00000E+00
DIC>
DIC> read exh2
 OK
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-sim-time 50,,,,,,,,,

DIC>
DIC>
DIC>
DIC> @@
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
 Region: FERRITE
 geometric   0.956338     dense at   0.100000E-08   76 points
 Region: AUSTENITE
 geometric    1.25912     dense at    0.00000       94 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
USE NEW SCHEME /YES/:
  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]
  2232.10931178155         2232.10931178547         2228.18551728005         2.32383489339861        1.946749851382089E-
003        8.415416277377267E-003        6.710264020635073E-006        1.891337182609781E-003        4.398065287394721E-
006        1.657225510608593E-006        1.065019577740872E-014       TIME =  0.10000000E-06 DT =  0.10000000E-
06 SUM OF SQUARES =  0.25940384E-20
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.69881845E-01 AND   0.69881845E-01
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.79881845E-08
 U-FRACTION IN SYSTEM:  C = .00412291487299393  FE = .980742621143594
                        NI = .0192573788564064
 TOTAL SIZE OF SYSTEM:  5.0001E-05 [m]
  39  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: FERRITE
  4  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUSTENITE

  CPU time used in timestep                    3  seconds
  2189.02036583756         2189.02036583977         2185.12780796211         2.22490782887878        1.820835197641041E-
003        7.877350106897017E-003        3.917525998538681E-006        1.895308042543652E-003        2.542966429567954E-006

output ignored...



... output resumed

  1192.63240780067         1192.63240780318         1189.62544963766        0.586696675278459        2.470347775651576E-
004        1.644178107861449E-006        7.371594133648919E-010        2.065832855473172E-003        5.084320285003332E-
019       TIME =   36.119232     DT =   5.0000000     SUM OF SQUARES =  0.50843153E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.20650414E-06 AND   0.20650414E-06
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.11799654E-04
 U-FRACTION IN SYSTEM:  C = .00412986835226155  FE = .980742621143593
                        NI = .0192573788564066
 TOTAL SIZE OF SYSTEM:  5.0001E-05 [m]
  21  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: FERRITE

  CPU time used in timestep                    1  seconds
  1169.39662381185         1169.39662381330         1166.41547102204        0.562252758083153        2.317821886822820E-
004        1.516388173134960E-006        6.707143176389857E-010        2.068897440626551E-003        4.677742097626163E-
019       TIME =   41.119232     DT =   5.0000000     SUM OF SQUARES =  0.46777395E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.19501454E-06 AND   0.19501454E-06
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.12774727E-04
 U-FRACTION IN SYSTEM:  C = .00413078918298148  FE = .980742621143593
                        NI = .0192573788564067
 TOTAL SIZE OF SYSTEM:  5.0001E-05 [m]
  9  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: FERRITE

  CPU time used in timestep                    1  seconds
  1146.60821641460         1146.60821641600         1143.65269452660        0.538840285898953        2.174786977267588E-
004        1.373695766330672E-006        5.890094541072740E-010        2.071889866172714E-003        4.288105449062012E-
019       TIME =   46.119232     DT =   5.0000000     SUM OF SQUARES =  0.42881043E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.18506009E-06 AND   0.18506009E-06
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.13700027E-04
 U-FRACTION IN SYSTEM:  C = .00413171959601196  FE = .980742621143593
```

```
                      NI = .0192573788564067
 TOTAL SIZE OF SYSTEM:  5.0001E-05 [m]
  9  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: FERRITE

  CPU time used in timestep                    1  seconds
  1124.25873698305         1124.25873698208         1121.32867166880        0.516415116325854        2.040652216253534E-
004        1.016971856171830E-005        4.143310090003984E-009        2.110304149454083E-012        2.062994805027931E-
003        4.764560328683764E-022       TIME =   49.232182     DT =   3.1129497     SUM OF SQUARES =  0.47645603E-21
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.19806331E-06 AND   0.19806331E-06
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.14316588E-04
 U-FRACTION IN SYSTEM:  C = .00413221468491343  FE = .980742621143594
                      NI = .0192573788564067
 TOTAL SIZE OF SYSTEM:  5.0001E-05 [m]
  7  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: FERRITE

  CPU time used in timestep                    1  seconds
  1102.33989435972         1102.33989435877         1099.43511145260        0.494935050523980        1.915024201253597E-
004        8.105439920479784E-004        2.796019951742093E-008        2.063250659310692E-003        2.352205678993389E-
009        4.115667427979870E-016       TIME =   50.000000     DT =  0.76781835     SUM OF SQUARES =  0.17870331E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.25570510E-06 AND   0.25570510E-06
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.14512923E-04
 U-FRACTION IN SYSTEM:  C = .00413346041156177  FE = .980742621143593
                      NI = .0192573788564067
 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   0.40000000E-06
 DELETING TIME-RECORD FOR TIME   0.80000000E-06
 DELETING TIME-RECORD FOR TIME   0.16000000E-05
 DELETING TIME-RECORD FOR TIME   0.32000000E-05
 DELETING TIME-RECORD FOR TIME   0.64000000E-05
 DELETING TIME-RECORD FOR TIME   0.12800000E-04
 DELETING TIME-RECORD FOR TIME   0.25600000E-04
 DELETING TIME-RECORD FOR TIME   0.51200000E-04
 DELETING TIME-RECORD FOR TIME   0.10240000E-03
 DELETING TIME-RECORD FOR TIME   0.20480000E-03
 DELETING TIME-RECORD FOR TIME   0.40960000E-03
 DELETING TIME-RECORD FOR TIME   0.81920000E-03
 DELETING TIME-RECORD FOR TIME   0.16230121E-02
 DELETING TIME-RECORD FOR TIME   0.31209881E-02
 DELETING TIME-RECORD FOR TIME   0.61169400E-02
 DELETING TIME-RECORD FOR TIME   0.12108844E-01
 DELETING TIME-RECORD FOR TIME   0.24092651E-01
 DELETING TIME-RECORD FOR TIME   0.48060266E-01
 DELETING TIME-RECORD FOR TIME   0.95864768E-01
 DELETING TIME-RECORD FOR TIME   0.19147377
 DELETING TIME-RECORD FOR TIME   0.38269178
 DELETING TIME-RECORD FOR TIME   0.76512779
 DELETING TIME-RECORD FOR TIME    1.5299998
 DELETING TIME-RECORD FOR TIME    3.0597439
 DELETING TIME-RECORD FOR TIME    6.1192320
 DELETING TIME-RECORD FOR TIME    11.119232
 DELETING TIME-RECORD FOR TIME    16.119232
 DELETING TIME-RECORD FOR TIME    21.119232
 DELETING TIME-RECORD FOR TIME    26.119232
 DELETING TIME-RECORD FOR TIME    31.119232
 DELETING TIME-RECORD FOR TIME    36.119232
 DELETING TIME-RECORD FOR TIME    41.119232
 DELETING TIME-RECORD FOR TIME    46.119232

 KEEPING TIME-RECORD FOR TIME    49.232182
 AND FOR TIME                    50.000000
 WORKSPACE RECLAIMED

 TIMESTEP AT     50.0000000     SELECTED

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

exh2-plot

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exh2\plot.DCM 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



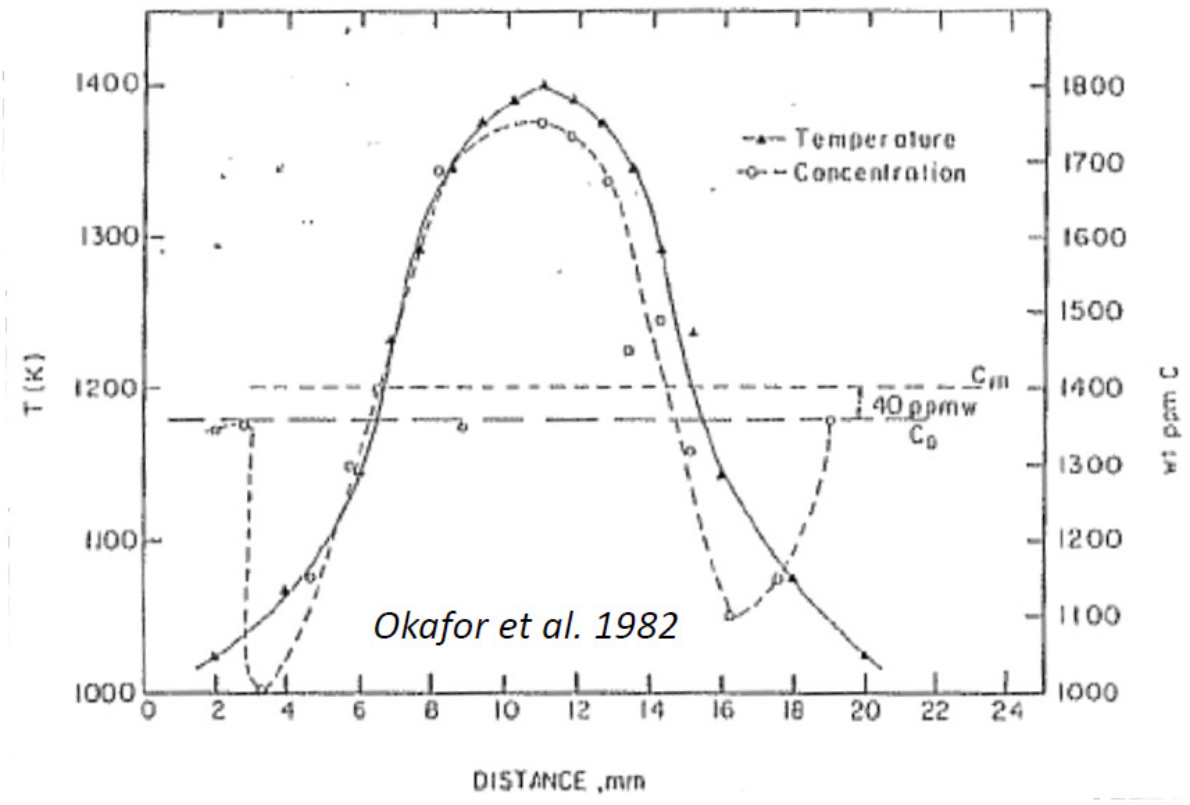

```
POST-1:
POST-1:
POST-1:
POST-1: set-inter
 --OK---
POST-1:
```

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: unknown compiler
 License library version: 9.7.0.0036
 Linked: Fri Oct 18 11:32:56 2024


SYS:SYS:MACRO exh3\setup.DCM
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: ----------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: go da
15:39:50,841 [Thread-0] INFO  LicenseManager: Initializing user: jenkins.integrationtest@thermocalc.se
15:39:50,854 [Thread-0] INFO  LicenseController: Running License Spring in DEV environment.
15:39:51,900 [Thread-0] INFO  LicenseManager: There is an activated standalone license for jenkins.integrationtest@thermocalc.se for TC-
Application
 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 v5.0

 VA                       /-  DEFINED
TDB_FEDEMO: def-sys fe ni c
 FE                       NI                       C
   DEFINED
TDB_FEDEMO: rej ph * all
 BCC_A2                   CBCC_A12                 CEMENTITE
 CUB_A13                  DIAMOND_FCC_A4           FCC_A1
 GAS:G                    GRAPHITE                 HCP_A3
 KSI_CARBIDE              LAVES_PHASE_C14          LIQUID:L
 M23C6                    M5C2                     M7C3
   REJECTED
TDB_FEDEMO: res ph fcc graph
 FCC_A1                   GRAPHITE  RESTORED
TDB_FEDEMO: get
15:39:52,967 [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: app mfedemo
 Current database: Fe-Alloys Mobility demo database v4.0

 VA  DEFINED
APP: def-sys fe ni c
 FE                       NI                       C
   DEFINED
APP: rej ph * all
 BCC_A2                   FCC_A1                   CEMENTITE
 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: go d-m
15:39:53,492 [Thread-0] INFO  StandaloneLicenseController: Checking out license for: Diffusion (DICTRA)
 NO TIME STEP DEFINED
 *** ENTERING GRAPHITE 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 /0/: -42000
DIC>
DIC>
DIC> save exh3 y
DIC>
DIC> set-inter
 --OK---
DIC>
```

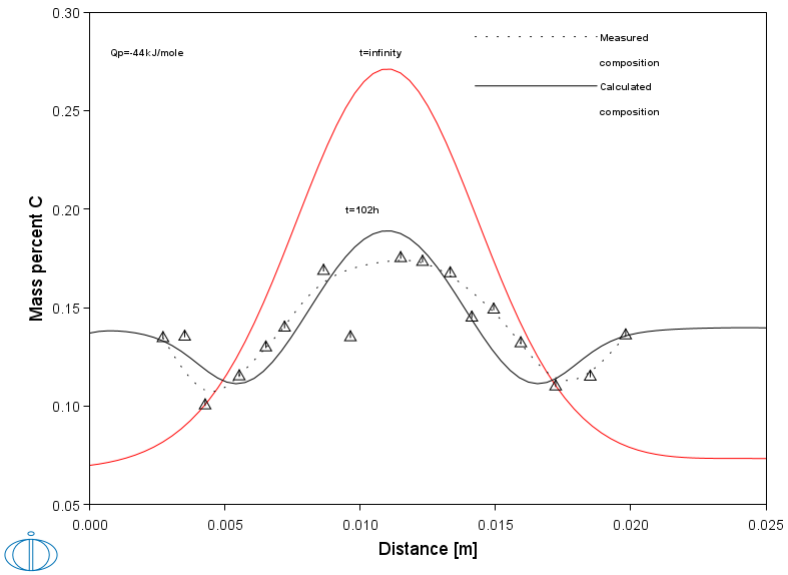
exh3-run

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exh3\run.DCM DIC>
DIC> go d-m
 TIME STEP AT TIME  0.00000E+00
*** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
DIC>
DIC> read exh3
 OK
DIC>
DIC> sim
 Region: AUS
 linear    75 points
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
 U-FRACTION IN SYSTEM:  C = .00662305741857947  FE = .68534915460493
                        NI = .31465084539507
 TOTAL SIZE OF SYSTEM:  .025 [m]
 U-FRACTION IN SYSTEM:  C = .00662305741857947  FE = .68534915460493
                        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 = .68534915460493
                                                                        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 = .68534915460493

                        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 = .00662305741857945  FE = .685349154604931
                        NI = .31465084539507
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    1  seconds
 TIME =   713.62003     DT =   713.21993     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741857946  FE = .685349154604931
                        NI = .314650845395069
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    0  seconds
 TIME =   2140.0599     DT =   1426.4399     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741857945  FE = .68534915460493
                        NI = .314650845395069
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    1  seconds
 TIME =   4992.9396     DT =   2852.8797     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741857944  FE = .68534915460493
                        NI = .314650845395069
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    0  seconds
 TIME =   10698.699     DT =   5705.7594     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741857931  FE = .685349154604931
                        NI = .314650845395069
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    0  seconds
 TIME =   22110.218     DT =   11411.519     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741857815  FE = .685349154604931
                        NI = .314650845395069
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    1  seconds
 TIME =   95928.651     DT =   73818.433     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741845141  FE = .685349154604931
                        NI = .314650845395069
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    0  seconds
 TIME =   243565.52     DT =   147636.87     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741806347  FE = .685349154604931
                        NI = .314650845395069
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    0  seconds
 TIME =   538839.25     DT =   295273.73     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741806284  FE = .685349154604931
                        NI = .314650845395069
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    0  seconds
 TIME =   1129386.7     DT =   590547.46     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741806167  FE = .685349154604931
                        NI = .314650845395069
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    0  seconds
 TIME =   2310481.6     DT =   1181094.9     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741806245  FE = .685349154604931
                        NI = .314650845395069
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    1  seconds
 TIME =   4672671.5     DT =   2362189.9     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0066230574179999  FE = .685349154604931
                        NI = .314650845395069
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    0  seconds
 TIME =   9397051.2     DT =   4724379.7     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741801717  FE = .68534915460493
                        NI = .314650845395069
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    0  seconds
 TIME =   13622714.     DT =   4225662.5     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741802533  FE = .685349154604931
                        NI = .314650845395069
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    1  seconds
 TIME =   17553927.     DT =   3931213.3     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741803165  FE = .685349154604931
                        NI = .314650845395069
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    0  seconds
 TIME =   21379744.     DT =   3825816.5     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741803515  FE = .685349154604931
                        NI = .314650845395069
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    0  seconds
 TIME =   25162824.     DT =   3783080.8     SUM OF SQUARES =   0.0000000
```

```
 U-FRACTION IN SYSTEM:  C = .00662305741803803  FE = .685349154604931
                        NI = .314650845395069
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    0  seconds
 TIME =   28928550.     DT =   3765726.0     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741803984  FE = .685349154604931
                        NI = .314650845395069
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    1  seconds
 TIME =   32687844.     DT =   3759294.0     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741772484  FE = .685349154604931
                        NI = .314650845395069
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    0  seconds
 TIME =   36445450.     DT =   3757605.3     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741750546  FE = .685349154604931
                        NI = .314650845395069
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    0  seconds
 TIME =   40203391.     DT =   3757941.0     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741693398  FE = .685349154604931
                        NI = .314650845395069
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    0  seconds
 TIME =   43877566.     DT =   3674174.8     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741647826  FE = .685349154604931
                        NI = .314650845395069
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    0  seconds
 TIME =   46159380.     DT =   2281815.0     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741628053  FE = .685349154604931
                        NI = .314650845395069
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    1  seconds
 TIME =   47751923.     DT =   1592542.4     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0066230574161792  FE = .68534915460493
                        NI = .314650845395069
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    0  seconds
 TIME =   49034799.     DT =   1282876.2     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741611517  FE = .685349154604931
                        NI = .314650845395069
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    0  seconds
 TIME =   49764724.     DT =   729925.30     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741609296  FE = .685349154604931
                        NI = .314650845395069
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    0  seconds
 TIME =   50000000.     DT =   235275.68     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741609156  FE = .685349154604931
                        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   0.10000000E-06
 DELETING TIME-RECORD FOR TIME   0.10010000E-03
 DELETING TIME-RECORD FOR TIME   0.40010010
 DELETING TIME-RECORD FOR TIME    713.62003
 DELETING TIME-RECORD FOR TIME    2140.0599
 DELETING TIME-RECORD FOR TIME    4992.9396
 DELETING TIME-RECORD FOR TIME    10698.699
 DELETING TIME-RECORD FOR TIME    22110.218
 DELETING TIME-RECORD FOR TIME    95928.651
 DELETING TIME-RECORD FOR TIME    243565.52
 DELETING TIME-RECORD FOR TIME    538839.25
 DELETING TIME-RECORD FOR TIME    1129386.7
 DELETING TIME-RECORD FOR TIME    2310481.6
 DELETING TIME-RECORD FOR TIME    4672671.5
 DELETING TIME-RECORD FOR TIME    9397051.2
 DELETING TIME-RECORD FOR TIME    13622714.
 DELETING TIME-RECORD FOR TIME    17553927.
 DELETING TIME-RECORD FOR TIME    21379744.
 DELETING TIME-RECORD FOR TIME    25162824.
 DELETING TIME-RECORD FOR TIME    28928550.
 DELETING TIME-RECORD FOR TIME    32687844.
 DELETING TIME-RECORD FOR TIME    36445450.
 DELETING TIME-RECORD FOR TIME    40203391.
 DELETING TIME-RECORD FOR TIME    43877566.
 DELETING TIME-RECORD FOR TIME    46159380.
 DELETING TIME-RECORD FOR TIME    47751923.
 DELETING TIME-RECORD FOR TIME    49034799.

 KEEPING TIME-RECORD FOR TIME    49764724.
 AND FOR TIME                    50000000.
 WORKSPACE RECLAIMED

 TIMESTEP AT     50000000.0     SELECTED

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

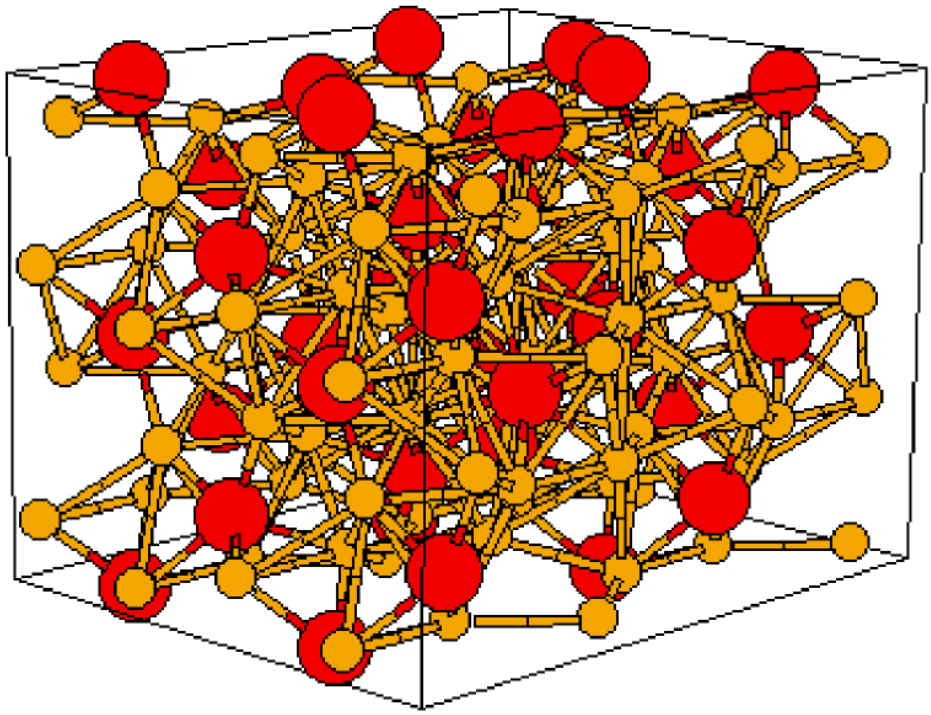
exh3-plot

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exh3\plot.DCM DIC> go d-m
 TIME STEP AT TIME  5.00000E+07
*** ENTERING GRAPHITE 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:
```

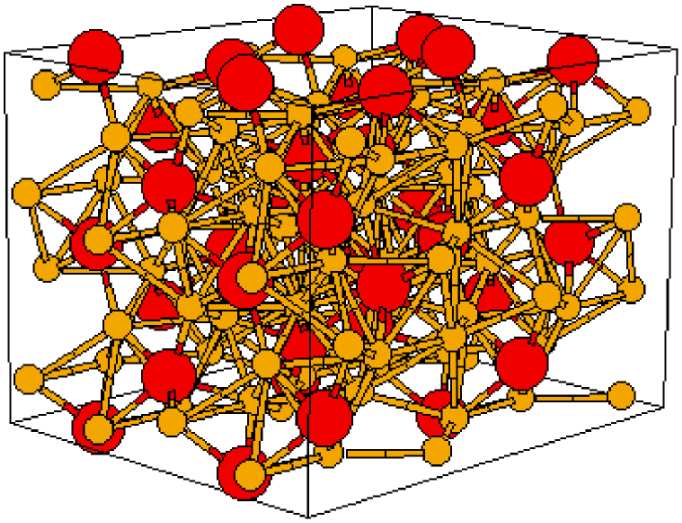
Diffusion in Complex Phases



Example exi1

Diffusion in system with B2 ordering

Diffusion in 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.



exi1-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: unknown compiler
 License library version: 9.7.0.0036
 Linked: Fri Oct 18 11:32:56 2024


SYS:SYS:MACRO exi1\setup.DCM
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: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exi1_setup.DCM
SYS:
SYS:
SYS: go da
15:42:52,848 [Thread-0] INFO  LicenseManager: Initializing user: jenkins.integrationtest@thermocalc.se
15:42:52,861 [Thread-0] INFO  LicenseController: Running License Spring in DEV environment.
15:42:53,947 [Thread-0] INFO  LicenseManager: There is an activated standalone license for jenkins.integrationtest@thermocalc.se for TC-
Application
 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
15:42:54,892 [Thread-0] INFO  TDBFileParser: USER_1695849785_19, number of lines read: 609
15:42:55,335 [Thread-0] INFO  DatabaseUtils: Parsing of USER_1695849785_19 completed in 520 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
15:42:55,510 [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
15:42:55,953 [Thread-0] INFO  StandaloneLicenseController: Checking out license for: Diffusion (DICTRA)
 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 /LINEAR/: 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 /LINEAR/: function
Function F(X)= 0.4295-0.0105*erf((x-1e-3)/3e-6);
15:42:56,359 [Thread-0] INFO  Database: Preparing system for use: USER_1695849785_19
15:42:57,422 [Thread-0] INFO  Phase: Preparing phase for use: B2_ORD
15:42:57,889 [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> save exi1 yes
DIC>
DIC> set-inter
 --OK---
DIC>
```

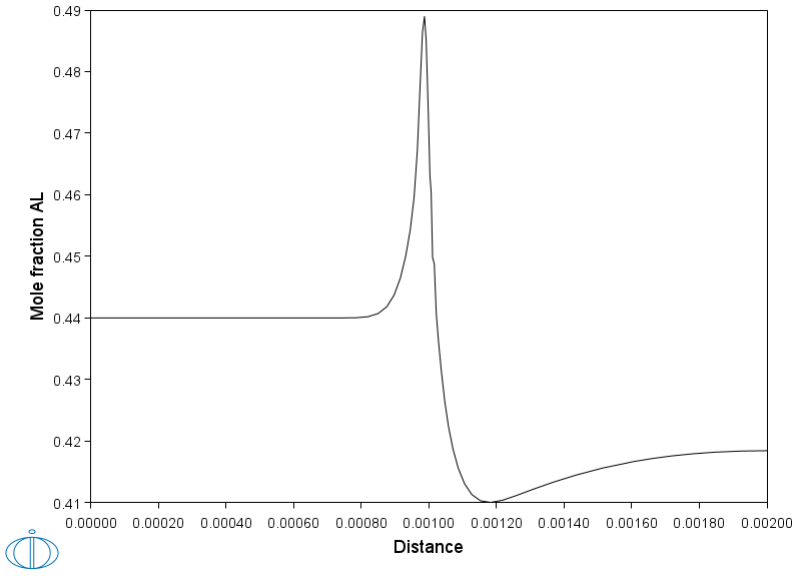
exi1-run

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exi1\run.DCM DIC>
DIC>
DIC> @@ exi1_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 exi1
 OK
DIC>
DIC> @@
DIC> @@ START THE SIMULATION
DIC> @@
DIC> sim
 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                    4  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 =  0.40000000     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 = .429499345639248  FE = .290517917020327
                        NI = .279982737340426
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    2  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                    0  seconds
 TIME =   7690.7270     DT =   4101.5077     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  AL = .429499345639227  FE = .290517917020346
                        NI = .279982737340427
 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 = .279982737340425
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    1  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 = .429499345639089  FE = .290517917020497
                        NI = .279982737340415
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    1  seconds
 TIME =   134231.83     DT =   34560.000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  AL = .429499345639132  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                    1  seconds
 TIME =   203351.83     DT =   34560.000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  AL = .429499345639157  FE = .290517917020456
                        NI = .279982737340387
 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 = .429499345639152  FE = .290517917020425
                        NI = .279982737340423
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    1  seconds
```

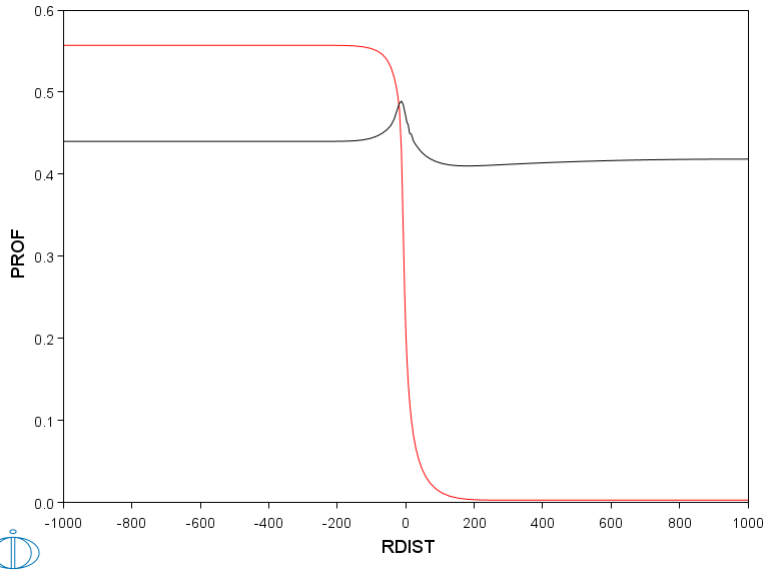
```
 TIME =   307031.83     DT =   34560.000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  AL = .42949934563916  FE = .290517917020412
                        NI = .279982737340428
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    1  seconds
 TIME =   341591.83     DT =   34560.000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  AL = .429499345639173  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 = .429499345639173  FE = .290517917020401
                        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>
```

exi1-plot

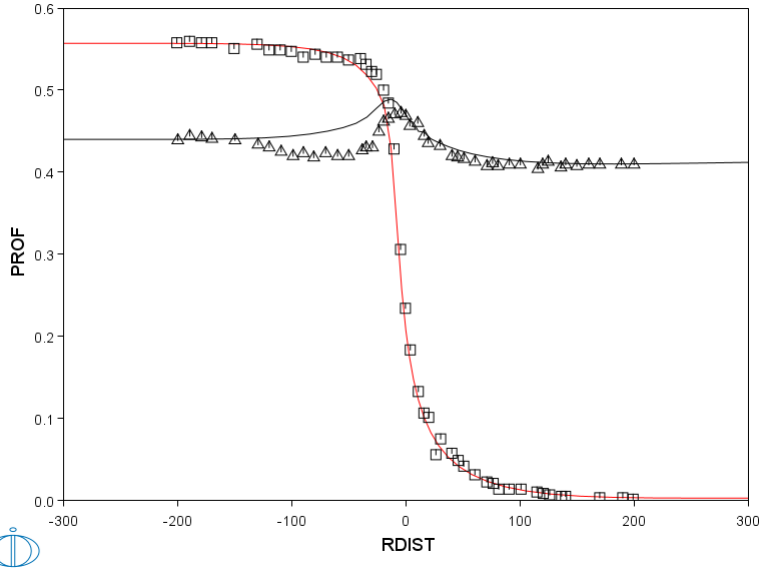
```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exi1\plot.DCM DIC>
DIC> @@ exi1_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE i1
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  3.45600E+05
DIC> read exi1
 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 exi1.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: unknown compiler
 License library version: 9.7.0.0036
 Linked: Fri Oct 18 11:32:56 2024


SYS:SYS:MACRO exi2\setup.DCM
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: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASES
SYS: @@
SYS: go da
15:46:10,250 [Thread-0] INFO  LicenseManager: Initializing user: jenkins.integrationtest@thermocalc.se
15:46:10,262 [Thread-0] INFO  LicenseController: Running License Spring in DEV environment.
15:46:11,356 [Thread-0] INFO  LicenseManager: There is an activated standalone license for jenkins.integrationtest@thermocalc.se for TC-
Application
 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 v5.0

 VA                        /-  DEFINED
TDB_FEDEMO: def-sys fe c
 FE                        C  DEFINED
TDB_FEDEMO: rej ph * all
 BCC_A2                    CBCC_A12                  CEMENTITE
 CUB_A13                   DIAMOND_FCC_A4            FCC_A1
 GAS:G                     GRAPHITE                  HCP_A3
 KSI_CARBIDE               LAVES_PHASE_C14           LIQUID:L
 M23C6                     M5C2                      M7C3
   REJECTED
TDB_FEDEMO: res ph bcc fcc cementite grap
 BCC_A2                    FCC_A1                    CEMENTITE
 GRAPHITE  RESTORED
TDB_FEDEMO: get
15:46:12,444 [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 v4.0

 VA  DEFINED
APP: def-sys fe c
 FE                        C  DEFINED
APP: rej ph * all
 BCC_A2                    FCC_A1                    CEMENTITE
 LIQUID:L  REJECTED
APP: res ph fcc bcc cementite
 FCC_A1                    BCC_A2                    CEMENTITE
   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
15:46:12,977 [Thread-0] INFO  StandaloneLicenseController: Checking out license for: Diffusion (DICTRA)
 NO TIME STEP DEFINED
 *** ENTERING GRAPHITE 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> @@
DIC> @@ ENTER A SIZE FOR THE FERRITE
DIC> @@
DIC> enter-grid
REGION NAME : /FER/: fer
WIDTH OF REGION /1/: 3.3E-6
TYPE /LINEAR/: 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 /LINEAR/: AUTO
DIC>
DIC>
DIC> @@
DIC> @@ ENTER PHASES INTO THE REGIONS
DIC> @@
DIC> enter-phase act carb  matrix   cementite
  COMPOSITION RECORD FOR STOICHIOMETRIC PHASE CEMENTITE 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/: 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> @@
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>
```

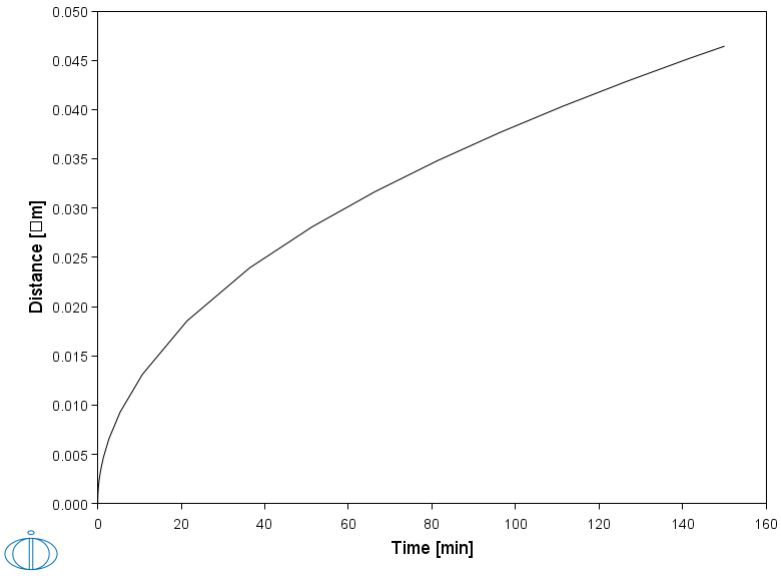
exi2-run

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exi2\run.DCM 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 AS A DIFFUSION NONE PHASE
DIC> read exi2
 OK
DIC>
DIC> @@
DIC> @@ START THE SIMULATION
DIC> @@
DIC> sim

 Region: FER
 geometric   0.845149     dense at   0.330000E-05   91 points
 Region: CARB
 geometric    1.04576     dense at    0.00000       44 points
 geometric   0.956243     dense at   0.100000E-11   45 points
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
  Trying old scheme                   3
 U-FRACTION IN SYSTEM:  C = 4.65980057843839E-05  FE = 1
 TOTAL SIZE OF SYSTEM:  3.300001E-06 [m]
 U-FRACTION IN SYSTEM:  C = 4.65980057843839E-05  FE = 1
 TOTAL SIZE OF SYSTEM:  3.300001E-06 [m]
 0.111094081648858        0.111116301566354        6.897809989216735E-023       TIME =  0.10000000E-06 DT =  0.10000000E-
06 SUM OF SQUARES =  0.68978100E-22
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.43989679E-06 AND  -0.43989679E-06
 POSITION OF INTERFACE FER / CARB IS   0.33000000E-05
 U-FRACTION IN SYSTEM:  C = 4.65976353525672E-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
 9.513206249531729E-007        9.516009355993388E-007        2.279391883026148E-022       TIME =  0.12952912E-05 DT =  0.11952912E-
05 SUM OF SQUARES =  0.22793919E-21
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.13846392E-06 AND  -0.13846392E-06
 POSITION OF INTERFACE FER / CARB IS   0.32999998E-05
 U-FRACTION IN SYSTEM:  C = 4.66104732978308E-05  FE = 1
 TOTAL SIZE OF SYSTEM:  3.300001E-06 [m]
  14  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: CARB

  CPU time used in timestep                   0  seconds
 6.683660105914452E-007        6.691057105208005E-007        1.259487203711079E-023       TIME =  0.36858737E-05 DT =  0.23905825E-
05 SUM OF SQUARES =  0.12594872E-22
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.11116611E-06 AND  -0.11116611E-06
 POSITION OF INTERFACE FER / CARB IS   0.32999995E-05
 U-FRACTION IN SYSTEM:  C = 4.66326359222793E-05  FE = 1
 TOTAL SIZE OF SYSTEM:  3.300001E-06 [m]
  22  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: CARB

  CPU time used in timestep                   0  seconds
 4.797245049843012E-007        4.802276308804607E-007        3.364540615483628E-024       TIME =  0.84670387E-05 DT =  0.47811650E-
05 SUM OF SQUARES =  0.33645406E-23
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.88162211E-07 AND  -0.88162211E-07
 POSITION OF INTERFACE FER / CARB IS   0.32999991E-05
 U-FRACTION IN SYSTEM:  C = 4.66689763610185E-05  FE = 1
 TOTAL SIZE OF SYSTEM:  3.300001E-06 [m]
  14  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: CARB

  CPU time used in timestep                   0  seconds
 4.001121279918420E-007        4.004765196988336E-007        3.349015457272102E-025       TIME =  0.18029369E-04 DT =  0.95623300E-
05 SUM OF SQUARES =  0.33490155E-24
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.67420959E-07 AND  -0.67420959E-07
 POSITION OF INTERFACE FER / CARB IS   0.32999985E-05
 U-FRACTION IN SYSTEM:  C = 4.67255053040509E-05  FE = 1
 TOTAL SIZE OF SYSTEM:  3.300001E-06 [m]
  52  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: CARB

  CPU time used in timestep                   0  seconds
 2.908494098464700E-007        2.910869927528465E-007        1.219959590728402E-025       TIME =  0.37154029E-04 DT =  0.19124660E-
04 SUM OF SQUARES =  0.12199596E-24
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.49892013E-07 AND  -0.49892013E-07
 POSITION OF INTERFACE FER / CARB IS   0.32999975E-05
 U-FRACTION IN SYSTEM:  C = 4.68098833784781E-05  FE = 1
 TOTAL SIZE OF SYSTEM:  3.300001E-06 [m]
  20  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: CARB

  CPU time used in timestep                   0  seconds
 1.811837247874280E-007        1.813224872769976E-007        4.879938337392062E-025       TIME =  0.75403349E-04 DT =  0.38249320E-
04 SUM OF SQUARES =  0.48799383E-24
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.36123396E-07 AND  -0.36123396E-07
 POSITION OF INTERFACE FER / CARB IS   0.32999961E-05
 U-FRACTION IN SYSTEM:  C = 4.6932575789548E-05  FE = 1
 TOTAL SIZE OF SYSTEM:  3.300001E-06 [m]
  42  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: CARB

  CPU time used in timestep                   1  seconds


output ignored...


... output resumed


 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.46380048E-11 AND  -0.46380048E-11
 POSITION OF INTERFACE FER / CARB IS   0.32718906E-05
 U-FRACTION IN SYSTEM:  C = .00286490957242564  FE = 1
 TOTAL SIZE OF SYSTEM:  3.300001E-06 [m]
  55  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: CARB
```

```
  CPU time used in timestep                    0  seconds
 3.9455949357163 30E-008        3.9516157378778 46E-008        5.252285600844118E-
028       TIME =   3983.4342     DT =   900.00000     SUM OF SQUARES =  0.52522856E-27
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.39492931E-11 AND  -0.39492931E-11
 POSITION OF INTERFACE FER / CARB IS   0.32683362E-05
 U-FRACTION IN SYSTEM:  C = .00322390842746482  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
 1.4745494647529 33E-008        1.4776840565500 07E-008        5.245966115002233E-
029       TIME =   4883.4342     DT =   900.00000     SUM OF SQUARES =  0.52459661E-28
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.35059861E-11 AND  -0.35059861E-11
 POSITION OF INTERFACE FER / CARB IS   0.32651808E-05
 U-FRACTION IN SYSTEM:  C = .00354260976298867  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
 6.8102067120653 50E-009        6.8291211264602 09E-009        4.385861769754155E-
030       TIME =   5783.4342     DT =   900.00000     SUM OF SQUARES =  0.43858618E-29
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.31882754E-11 AND  -0.31882754E-11
 POSITION OF INTERFACE FER / CARB IS   0.32623114E-05
 U-FRACTION IN SYSTEM:  C = .00383243054008672  FE = 1
 TOTAL SIZE OF SYSTEM:  3.300001E-06 [m]
  19  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: CARB

  CPU time used in timestep                    0  seconds
 3.5583472392299 20E-009        3.5707826533210 02E-009        4.636380116535863E-
030       TIME =   6683.4342     DT =   900.00000     SUM OF SQUARES =  0.46363801E-29
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.29455404E-11 AND  -0.29455404E-11
 POSITION OF INTERFACE FER / CARB IS   0.32596604E-05
 U-FRACTION IN SYSTEM:  C = .00410018621140539  FE = 1
 TOTAL SIZE OF SYSTEM:  3.300001E-06 [m]
  6  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: CARB

  CPU time used in timestep                    0  seconds
 2.0143705117851 82E-007        2.0230162332905 08E-007        2.641945257800785E-
029       TIME =   7583.4342     DT =   900.00000     SUM OF SQUARES =  0.26419453E-28
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.27519740E-11 AND  -0.27519740E-11
 POSITION OF INTERFACE FER / CARB IS   0.32571836E-05
 U-FRACTION IN SYSTEM:  C = .0043503462990152  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
 1.2050323985039 65E-007        1.2112813471469 28E-007        1.073802541419657E-
029       TIME =   8483.4342     DT =   900.00000     SUM OF SQUARES =  0.10738025E-28
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.25927857E-11 AND  -0.25927857E-11
 POSITION OF INTERFACE FER / CARB IS   0.32548501E-05
 U-FRACTION IN SYSTEM:  C = .00458603584893226  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
 7.4965291437768 56E-008        7.5429773810748 34E-008        1.516677354368793E-
029       TIME =   9000.0000     DT =   516.56580     SUM OF SQUARES =  0.15166774E-28
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.24587843E-11 AND  -0.24587843E-11
 POSITION OF INTERFACE FER / CARB IS   0.32535800E-05
 U-FRACTION IN SYSTEM:  C = .00471432126027761  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   0.12952912E-05
 DELETING TIME-RECORD FOR TIME   0.36858737E-05
 DELETING TIME-RECORD FOR TIME   0.84670387E-05
 DELETING TIME-RECORD FOR TIME   0.18029369E-04
 DELETING TIME-RECORD FOR TIME   0.37154029E-04
 DELETING TIME-RECORD FOR TIME   0.75403349E-04
 DELETING TIME-RECORD FOR TIME   0.15190199E-03
 DELETING TIME-RECORD FOR TIME   0.30489927E-03
 DELETING TIME-RECORD FOR TIME   0.61089383E-03
 DELETING TIME-RECORD FOR TIME   0.12228829E-02
 DELETING TIME-RECORD FOR TIME   0.24468612E-02
 DELETING TIME-RECORD FOR TIME   0.48948177E-02
 DELETING TIME-RECORD FOR TIME   0.97907306E-02
 DELETING TIME-RECORD FOR TIME   0.19582557E-01
 DELETING TIME-RECORD FOR TIME   0.39166208E-01
 DELETING TIME-RECORD FOR TIME   0.78333512E-01
 DELETING TIME-RECORD FOR TIME   0.15666812
 DELETING TIME-RECORD FOR TIME   0.31333733
 DELETING TIME-RECORD FOR TIME   0.62667576
 DELETING TIME-RECORD FOR TIME    1.2533526
 DELETING TIME-RECORD FOR TIME    2.5067063
 DELETING TIME-RECORD FOR TIME    5.0134138
 DELETING TIME-RECORD FOR TIME    10.026829
 DELETING TIME-RECORD FOR TIME    20.053658
 DELETING TIME-RECORD FOR TIME    40.107318
 DELETING TIME-RECORD FOR TIME    80.214637
 DELETING TIME-RECORD FOR TIME    160.42927
 DELETING TIME-RECORD FOR TIME    320.85855
 DELETING TIME-RECORD FOR TIME    641.71710
 DELETING TIME-RECORD FOR TIME    1283.4342
 DELETING TIME-RECORD FOR TIME    2183.4342
 DELETING TIME-RECORD FOR TIME    3083.4342
 DELETING TIME-RECORD FOR TIME    3983.4342
 DELETING TIME-RECORD FOR TIME    4883.4342
 DELETING TIME-RECORD FOR TIME    5783.4342
 DELETING TIME-RECORD FOR TIME    6683.4342
 DELETING TIME-RECORD FOR TIME    7583.4342

 KEEPING TIME-RECORD FOR TIME    8483.4342
 AND FOR TIME                    9000.0000
 WORKSPACE RECLAIMED

 TIMESTEP AT     9000.00000     SELECTED

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

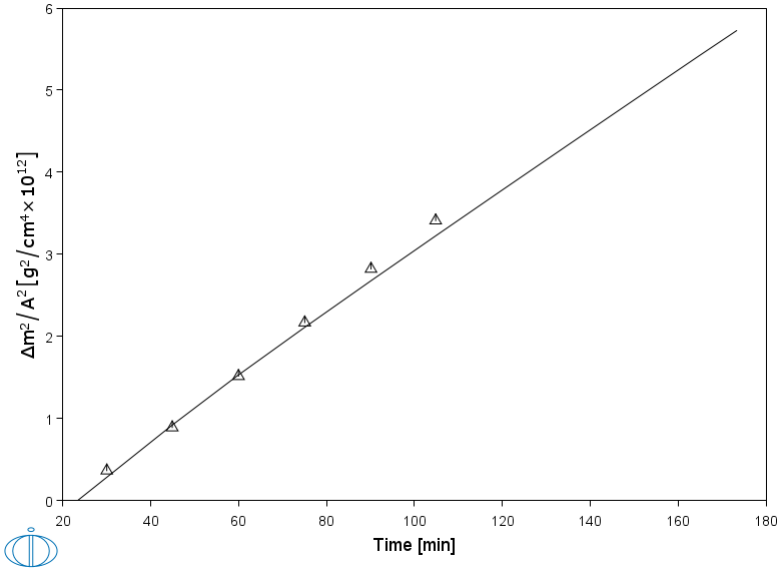
exi2-plot

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exi2\plot.DCM 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 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 [ï¿½m]
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
```

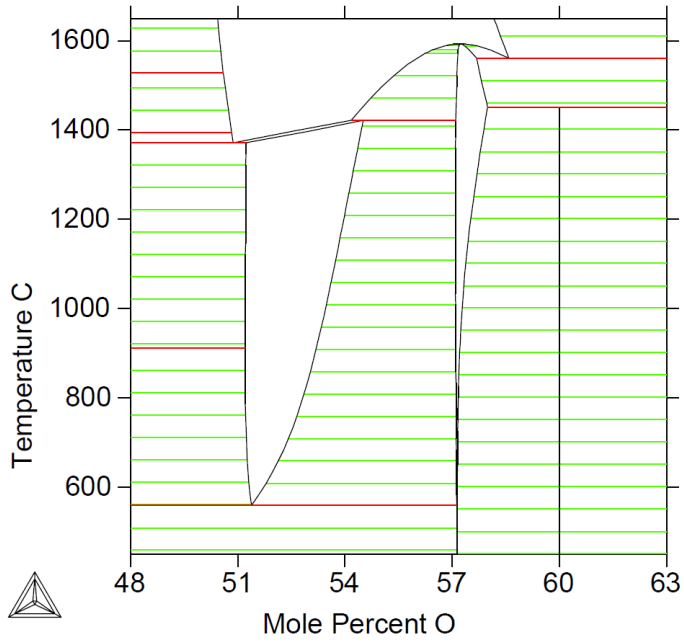



```
POST-1:
POST-1:
POST-1: set-inter
 --OK---
POST-1:
```

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: unknown compiler
 License library version: 9.7.0.0036
 Linked: Fri Oct 18 11:32:56 2024


SYS:SYS:MACRO exi3a\setup.DCM
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: ----------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exi3_setup.DCM
SYS:
SYS: @@
SYS: @@ START BY GOING TO THE DATABASE MODULE
SYS: @@
SYS: go da
15:49:07,890 [Thread-0] INFO  LicenseManager: Initializing user: jenkins.integrationtest@thermocalc.se
15:49:07,903 [Thread-0] INFO  LicenseController: Running License Spring in DEV environment.
15:49:09,012 [Thread-0] INFO  LicenseManager: There is an activated standalone license for jenkins.integrationtest@thermocalc.se for TC-
Application
 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
15:49:09,982 [Thread-0] INFO  TDBFileParser: USER_190315336_19, number of lines read: 217
15:49:10,265 [Thread-0] INFO  DatabaseUtils: Parsing of USER_190315336_19 completed in 374 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
15:49:10,385 [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
15:49:10,697 [Thread-0] INFO  TDBFileParser: USER_1269960560_19, number of lines read: 129
15:49:10,757 [Thread-0] INFO  DatabaseUtils: Parsing of USER_1269960560_19 completed in 63 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
15:49:10,795 [Thread-0] INFO  StandaloneLicenseController: Checking out license for: Diffusion (DICTRA)
 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 EXTERNALY. 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 /0/: 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> s-s-c 0 1 1 YES POT YES YES 1 2,,,,,,,,,
 RELEASING OLD STARTING VALUES
DIC>
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>
```

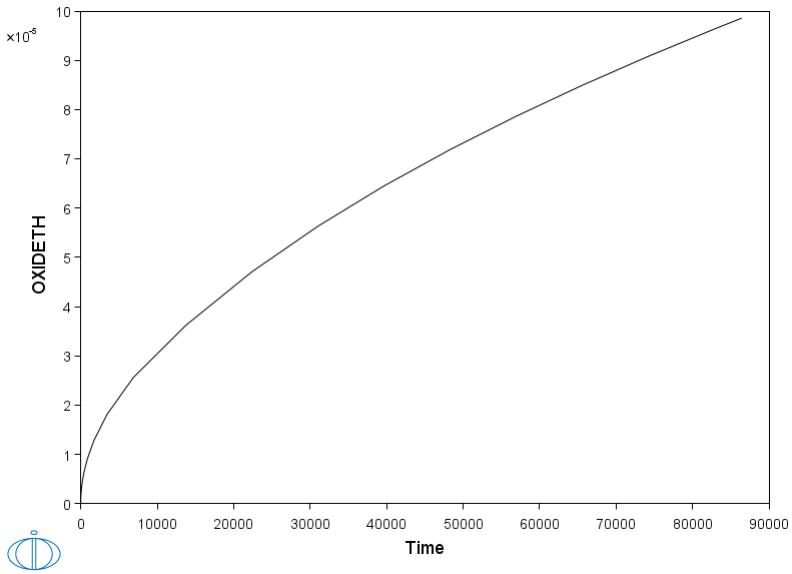
exi3a-run

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exi3a\run.DCM 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

 Region: FER
 geometric   0.772465     dense at   0.499999E-02   97 points
 Region: SP
 geometric    1.04572     dense at    0.00000       44 points
 geometric   0.956275     dense at   0.100000E-09   45 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]
 0.350071488936801        0.350070712673700        0.350070886569849        4.652132339660341E-002        2.191687616260677E-
023       TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =  0.35454565E-25
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.39813205E-03 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49999900E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.67213742E-03 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.49999901E-02
 U-FRACTION IN SYSTEM:  FE = 0.99999998953623  O = 3.44452798024126E-08
 TOTAL SIZE OF SYSTEM:  .0049999901274 [m]
  7  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: FER
  9  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    4  seconds
 1.524282901461111E-005        1.524471433476572E-005        1.524555424479982E-005        2.228437187158867E-007        3.957755360015191E-
029       TIME =  0.30000000E-06 DT =  0.20000000E-06 SUM OF SQUARES =  0.39570906E-28
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.14858615E-03 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49999899E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.20394305E-03 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.49999901E-02
 U-FRACTION IN SYSTEM:  FE = 0.99999998712736  O = 4.26040716676657E-08
 TOTAL SIZE OF SYSTEM:  .00499999013847 [m]
  22  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    0  seconds
 1.442476760835493E-008        1.441402193642448E-008        1.439397915124679E-008        3.334698651738925E-011        2.917576978740918E-
033       TIME =  0.70000000E-06 DT =  0.40000000E-06 SUM OF SQUARES =  0.29152730E-32
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.14931148E-03 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49999899E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.21680740E-03 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.49999902E-02
 U-FRACTION IN SYSTEM:  FE = 0.99999998165912  O = 5.99515431755429E-08
 TOTAL SIZE OF SYSTEM:  .00499999016547 [m]
  4  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    1  seconds
 5.641131931926223E-007        5.642680406502237E-007        5.642660057087331E-007        2.463317753593780E-010        2.233168902861657E-
033       TIME =  0.15000000E-05 DT =  0.80000000E-06 SUM OF SQUARES =  0.21132567E-32
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.93420491E-04 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49999898E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.13342396E-03 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.49999902E-02
 U-FRACTION IN SYSTEM:  FE = 0.99999997505757  O = 8.13036901276143E-08
 TOTAL SIZE OF SYSTEM:  .00499999019747 [m]
  31  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    0  seconds
 8.108291677577342E-006        8.112094941000955E-006        8.111728708044934E-006        1.124896677017162E-008        8.352592659202846E-
032       TIME =  0.31000000E-05 DT =  0.16000000E-05 SUM OF SQUARES =  0.65914952E-31
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.70785621E-04 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49999897E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.10186785E-03 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.49999902E-02
 U-FRACTION IN SYSTEM:  FE = 0.99999996488305  O = 1.13906559479276E-07
 TOTAL SIZE OF SYSTEM:  .0049999902472 [m]
  34  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    0  seconds
 8.117404326365275E-006        8.120228995065965E-006        8.120089100807907E-006        7.212736035075093E-009        1.747931887808322E-
032       TIME =  0.63000000E-05 DT =  0.32000000E-05 SUM OF SQUARES =  0.15817452E-31

output ignored...



... output resumed

 POSITION OF INTERFACE FER / SP IS   0.49497261E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.85406491E-09 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.50216008E-02
 U-FRACTION IN SYSTEM:  FE = .995601410481655  O = .0143132757010586
 TOTAL SIZE OF SYSTEM:  .00502160079 [m]
  20  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    0  seconds
 2.791714535239042E-007        2.796216853410687E-007        2.795815212609476E-007        3.797570045281066E-010        2.735422374137496E-
033       TIME =   56943.895     DT =   8640.0000     SUM OF SQUARES =  0.27083390E-32
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.54740664E-09 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49449965E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.78317055E-09 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.50236378E-02
```

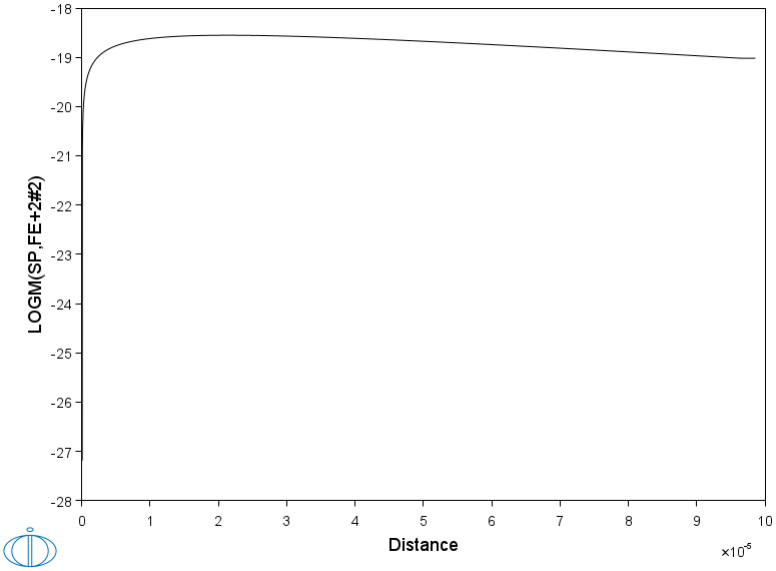
```
 U-FRACTION IN SYSTEM:  FE = .995194700022924  O = .0156544226659285
 TOTAL SIZE OF SYSTEM:  .00502363779015 [m]
  8  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    1  seconds
 1.595441147549657E-007        1.598553198831170E-007        1.598289742704802E-007        2.017857732644064E-010        8.726870060504662E-
035       TIME =   65583.895     DT =   8640.0000     SUM OF SQUARES =  0.75231638E-34
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.50747982E-09 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49406119E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.72674788E-09 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.50255323E-02
 U-FRACTION IN SYSTEM:  FE = .99481722394009  O = .0168979613905518
 TOTAL SIZE OF SYSTEM:  .00502553226622 [m]
  9  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    0  seconds
 9.548753454220980E-008        9.571036752768618E-008        9.569248341548456E-008        1.144366119908907E-010        7.500594353726852E-
034       TIME =   74223.895     DT =   8640.0000     SUM OF SQUARES =  0.72297605E-33
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.47495217E-09 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49365083E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.68061685E-09 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.50273092E-02
 U-FRACTION IN SYSTEM:  FE = .994463750183448  O = .0180617056273036
 TOTAL SIZE OF SYSTEM:  .00502730920905 [m]
  10  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    1  seconds
 5.962842883630616E-008        5.979318568000544E-008        5.978021734461116E-008        6.878306038221867E-011        1.668637740879254E-
033       TIME =   82863.895     DT =   8640.0000     SUM OF SQUARES =  0.16618669E-32
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.44777785E-09 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49326395E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.64202307E-09 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.50289875E-02
 U-FRACTION IN SYSTEM:  FE = .994130362421338  O = .0191586990305838
 TOTAL SIZE OF SYSTEM:  .00502898748776 [m]
  8  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    0  seconds
 9.164574858514905E-009        9.110538099145216E-009        9.226811522920826E-009        1.012262672520405E-011        3.987276837989199E-
035       TIME =   86400.000     DT =   3536.1047     SUM OF SQUARES =  0.36863503E-34
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.44500126E-09 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49310659E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.61834090E-09 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.50296004E-02
 U-FRACTION IN SYSTEM:  FE = .994008768142203  O = .0195910941308667
 TOTAL SIZE OF SYSTEM:  .00502960043487 [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

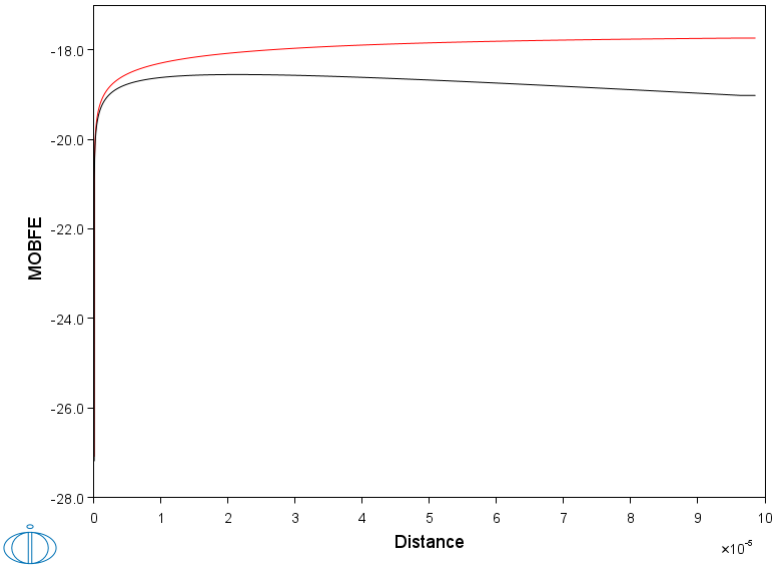
```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exi3a\plot.DCM DIC>
DIC> @@ exi3_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE i3
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  8.64000E+04
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
```



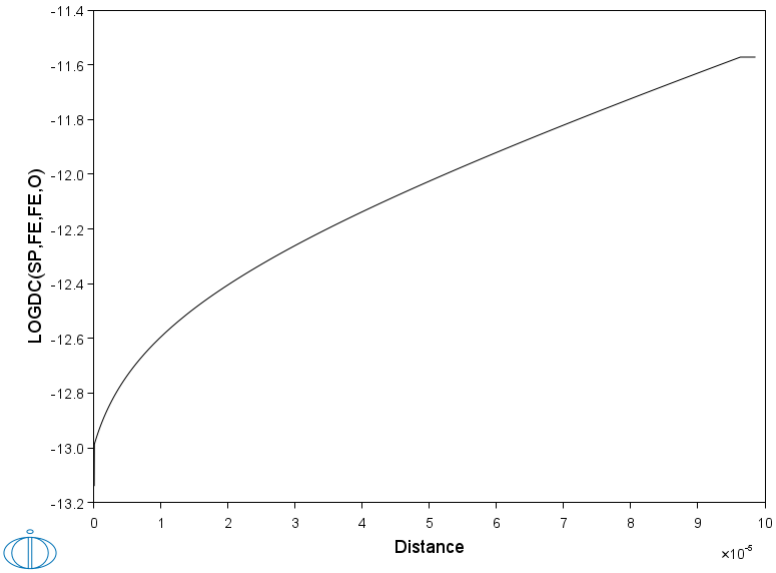

```
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: @@
POST-1: @@ NOW PLOT THE MOBILITY IN A SPINEL FOR Fe+2 ON THE SECOND SUBLATTICE
POST-1: @@
POST-1: s-d-a y logm(sp,fe+2#2)
POST-1:
POST-1: @@
POST-1: @@ LIMIT THE PLOT TO THE SPINEL PHASE
POST-1: @@
POST-1: s-d-a x dis local sp
  INFO: Distance 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
```

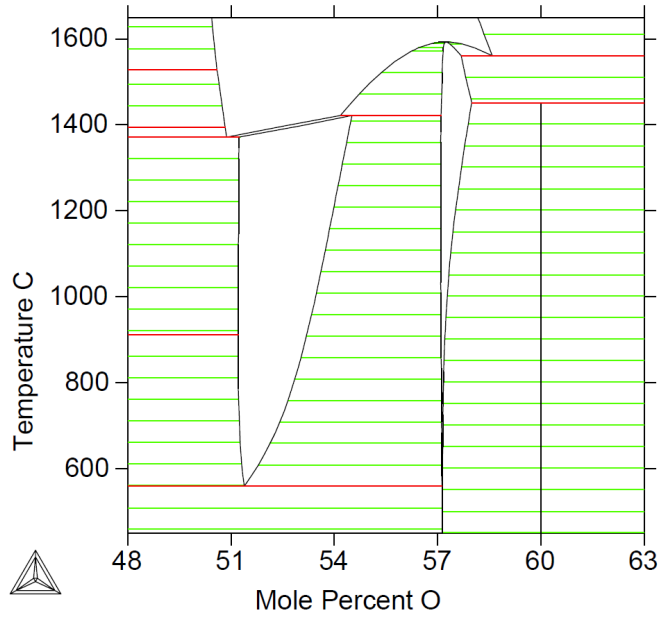


POST-1:
POST-1:
POST-1: set-inter
--OK---
POST-1:

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: unknown compiler
 License library version: 9.7.0.0036
 Linked: Fri Oct 18 11:32:56 2024


SYS:SYS:MACRO exi3b\setup.DCM
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: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exi3_setup.DCM
SYS:
SYS: @@
SYS: @@ START BY GOING TO THE DATABASE MODULE
SYS: @@
SYS: go da
15:52:29,046 [Thread-0] INFO  LicenseManager: Initializing user: jenkins.integrationtest@thermocalc.se
15:52:29,057 [Thread-0] INFO  LicenseController: Running License Spring in DEV environment.
15:52:30,193 [Thread-0] INFO  LicenseManager: There is an activated standalone license for jenkins.integrationtest@thermocalc.se for TC-
Application
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
15:52:31,156 [Thread-0] INFO  TDBFileParser: USER_1997769799_19, number of lines read: 217
15:52:31,431 [Thread-0] INFO  DatabaseUtils: Parsing of USER_1997769799_19 completed in 355 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
15:52:31,551 [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
15:52:31,922 [Thread-0] INFO  TDBFileParser: USER_1399043279_19, number of lines read: 128
15:52:31,988 [Thread-0] INFO  DatabaseUtils: Parsing of USER_1399043279_19 completed in 68 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
15:52:32,026 [Thread-0] INFO  StandaloneLicenseController: Checking out license for: Diffusion (DICTRA)
 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 EXTERNALY. 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 /0/: 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> s-s-c 0 1 1 YES POT YES YES 1 2,,,,,,,,,
 RELEASING OLD STARTING VALUES
DIC>
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>
```

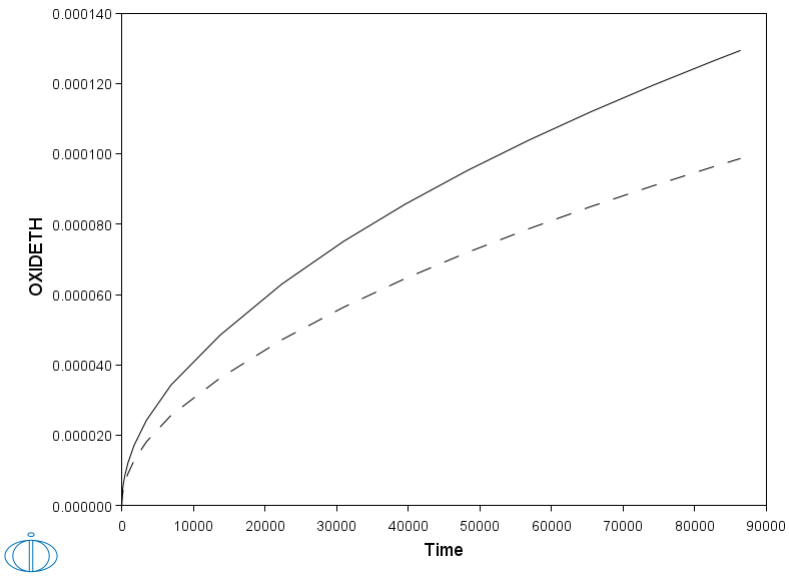
exi3b-run

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO exi3b\run.DCM 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

 Region: FER
 geometric   0.772465     dense at   0.499999E-02   97 points
 Region: SP
 geometric    1.04572     dense at    0.00000       44 points
 geometric   0.956275     dense at   0.100000E-09   45 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]
 3.603197580455816E-002        3.603197282534953E-002        3.603172054997469E-002        2.122437603184462E-004        8.103761824275473E-
027       TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =  0.61846695E-27
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.15896093E-03 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49999900E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.29058276E-03 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.49999901E-02
 U-FRACTION IN SYSTEM:  FE = 0.99999999238031  O = 2.68141716438222E-08
 TOTAL SIZE OF SYSTEM:  .00499999011316 [m]
  7  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: FER
  4  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    0  seconds
 8.109105568551964E-006        8.108439526402522E-006        8.108383006023899E-006        3.430958284997536E-007        1.112500078759461E-
030       TIME =  0.30000000E-06 DT =  0.20000000E-06 SUM OF SQUARES =  0.11005563E-29
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.36956368E-03 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49999899E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.56369669E-03 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.49999902E-02
 U-FRACTION IN SYSTEM:  FE = 0.99999998474497  O = 4.93631370297068E-08
 TOTAL SIZE OF SYSTEM:  .00499999015199 [m]
  43  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    1  seconds
 7.722362235177165E-006        7.723696951549050E-006        7.723912509644285E-006        6.052262356449636E-009        9.934949114731744E-
033       TIME =  0.70000000E-06 DT =  0.40000000E-06 SUM OF SQUARES =  0.96488808E-32
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.17792518E-03 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49999898E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.24397273E-03 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.49999902E-02
 U-FRACTION IN SYSTEM:  FE = 0.99999997895004  O = 6.88838385478754E-08
 TOTAL SIZE OF SYSTEM:  .00499999017841 [m]
  10  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    1  seconds
 1.354675784993464E-007        1.355736620725613E-007        1.355344692272980E-007        6.721754149868455E-010        5.699746412221914E-
032       TIME =  0.15000000E-05 DT =  0.80000000E-06 SUM OF SQUARES =  0.56997417E-31
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.14395572E-03 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49999897E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.20835239E-03 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.49999902E-02
 U-FRACTION IN SYSTEM:  FE = 0.99999996844848  O = 1.02224557591543E-07
 TOTAL SIZE OF SYSTEM:  .00499999022993 [m]
  15  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    2  seconds
 4.455333975350134E-007        4.456661481604863E-007        4.456638384074687E-007        2.596913177917200E-010        2.136919425416328E-
032       TIME =  0.31000000E-05 DT =  0.16000000E-05 SUM OF SQUARES =  0.21328275E-31
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.94034526E-04 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49999896E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.13397313E-03 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.49999903E-02
 U-FRACTION IN SYSTEM:  FE = 0.99999995520645  O = 1.45101135885996E-07
 TOTAL SIZE OF SYSTEM:  .00499999029383 [m]
  29  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    1  seconds
 1.104878748072100E-005        1.105325230102506E-005        1.105281997492597E-005        1.738963857726395E-008        1.193963718062407E-
030       TIME =  0.63000000E-05 DT =  0.32000000E-05 SUM OF SQUARES =  0.11698587E-29

output ignored...



... output resumed

 POSITION OF INTERFACE FER / SP IS   0.49333469E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.11009832E-08 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.50286092E-02
 U-FRACTION IN SYSTEM:  FE = .99418084415605  O = .0189442392521356
 TOTAL SIZE OF SYSTEM:  .00502860924776 [m]
  21  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    2  seconds
 5.273133320950391E-007        5.281062365100956E-007        5.280443729228357E-007        7.076362320696338E-010        3.912045199536573E-
034       TIME =   56943.895     DT =   8640.0000     SUM OF SQUARES =  0.27083390E-34
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.70247284E-09 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49272776E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.10045406E-08 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.50312191E-02
```

```
 U-FRACTION IN SYSTEM:  FE = .9936613170053 64  O = .0206594871616782
 TOTAL SIZE OF SYSTEM:  .00503121911346 [m]
  9  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    1  seconds
 2.946692819116459E-007        2.952132903578597E-007        2.951644928839408E-007        3.823713469258932E-010        1.313544407382857E-
032       TIME =   65583.895     DT =   8640.0000     SUM OF SQUARES =  0.13108361E-31
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.64894662E-09 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49216707E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.92920436E-09 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.50336405E-02
 U-FRACTION IN SYSTEM:  FE = .993180429046611  O = .0222444829908245
 TOTAL SIZE OF SYSTEM:  .00503364054032 [m]
  8  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    1  seconds
 1.646046703289139E-007        1.649792727269746E-007        1.649482143521673E-007        1.988142581530953E-010        2.037272769297123E-
033       TIME =   74223.895     DT =   8640.0000     SUM OF SQUARES =  0.20342635E-32
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.60654812E-09 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49164301E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.86919602E-09 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.50359098E-02
 U-FRACTION IN SYSTEM:  FE = .992730593064681  O = .0237257195654118
 TOTAL SIZE OF SYSTEM:  .00503590981822 [m]
  11  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    1  seconds
 1.056449587111593E-007        1.059236432946871E-007        1.059043396681829E-007        1.220611552948889E-010        6.394689268473244E-
035       TIME =   82863.895     DT =   8640.0000     SUM OF SQUARES =  0.36863503E-34
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.57100504E-09 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49114966E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.81838275E-09 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.50380472E-02
 U-FRACTION IN SYSTEM:  FE = .992307543196515  O = .0251191396439801
 TOTAL SIZE OF SYSTEM:  .00503804716161 [m]
  7  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    1  seconds
 1.518638876387760E-008        1.512792765316855E-008        1.530728569580852E-008        1.085094308293444E-011        5.189478420462169E-
033       TIME =   86400.000     DT =   3536.1047     SUM OF SQUARES =  0.51827076E-32
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.56483653E-09 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49094993E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.78548531E-09 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.50388274E-02
 U-FRACTION IN SYSTEM:  FE = .992153350206985  O = .025666481081554
 TOTAL SIZE OF SYSTEM:  .00503882739878 [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 exi3b\plot.DCM 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: @@
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:
```