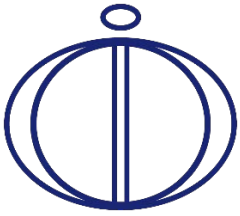
Diffusion Module (DICTRA) Example Macros

Thermo-Calc Version 2018a



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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

Moving boundary problem. 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.

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

Moving boundary problem. Moving boundary problem with multiple phases on each side 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.

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 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.

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. Höglund, B. Jönsson and J. Ågren: Metall.Trans.A, v. 22A (1991), pp. 1745-1752.

exd1a

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

exd1b

Diffusion in dispersed systems. Carburization of Ni-25%Cr alloy: Homogenization model This example is about carburization of a Ni-25Cr alloy. In this case the M3C2 and M7C3 carbides are entered as spheroid phases in a FCC matrix. This case is from A. Engström, L. Höglund and J. Ågren: Metall.Trans. A, v.25A (1994), pp. 1127-1134. This simulation can be run with the DISPERSED SYSTEM MODEL or HOMOGENIZATION MODEL. The default HOMOGENIZATION MODEL is used and then ENTER_HOMOGENIZATION_FUNCTION should be used instead of ENTER_LABYRINTH_FUNCTION.

exd2a

Diffusion in dispersed systems. Diffusion couple of Fe-Cr-Ni alloys: Dispersed system model This example calculates the interdiffusion in a diffusion couple between a two-phase (FCC+BCC) and a single-phase (FCC) Fe-Ni-Cr alloy. This case is from A. Engström: Scand. J. Met., v. 24, 1995, pp.12-20. This simulation can be run with either the DISPERSED SYSTEM MODEL or the HOMOGENIZATION MODEL. In this example the DISPERSED SYSTEM MODEL is used, which requires that the default HOMOGENIZATION MODEL is disabled. With the DISPERSED SYSTEM MODEL the command ENTER_LABYRINTH_FUNCTION is used to take into account the impeding effect of dispersed phases on long-range diffusion. For the HOMOGENIZATION MODEL the command ENTER_HOMOGENIZATION_FUNCTION should be used.

exd2b

Diffusion in dispersed systems. Diffusion couple of Fe-Cr-Ni alloys: Homogenization model This example calculates the interdiffusion in a diffusion couple between a two-phase (FCC+BCC) and a single-phase (FCC) Fe-Ni-Cr alloy. This case is from A. Engström: Scand. J. Met., v. 24, 1995, pp.12-20. This simulation can be run with either the DISPERSED SYSTEM MODEL or the HOMOGENIZATION MODEL. Here the default HOMOGENIZATION MODEL is used and then ENTER_HOMOGENIZATION_FUNCTION should be used instead of ENTER_LABYRINTH_FUNCTION.

exd3

Diffusion in dispersed systems. Diffusion couple of Fe-Cr-Ni alloys: Homogenization model This example uses the homogenization model. It is taken from H. Larsson and A. Engström, Acta. Mater. v.54 (2006), pp. 2431-2439. Experimental data from A. Engström, Scand J Metall, v.243 (1995), p.12. The homogenization model can be used for multiphase simulations like the dispersed system model, but unlike the dispersed system model there is no need to have a single continuous matrix phase and, furthermore, there is no need to limit the size of time-steps. The set-up is performed in the same manner as for the dispersed system model, which means that a certain phase is entered as the matrix phase and the other phases are entered as spheroidal, but the choice of matrix phase will not affect the simulation.

exe1

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

exf1

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

exg1

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

exg2

Kinetic data example. Optimization of mobilities in Ni-Al fcc alloys A file for reading thermodynamic data and setting up the kinetic parameters that are needed for an optimization of the FCC phase in the binary Ni-Al system. See also A. Engström and J. Ågren: ("Assessment of Diffusional Mobilities in Face-Centered Cubic Ni-Cr-Al Alloys" in Z. Metallkunde, Feb. 1996).

exh1

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

exh2

Deviation from local equilibrium. Ferrite/austenite para-equilibrium in an Fe-Ni-C alloy This example calculates the growth of ferrite into austenite in an Fe-2.02%Ni-0.0885%C alloy using the para-equilibrium model. The results are compared with experimental information from Hutchinson, C. R., A. Fuchsmann, and Yves Brechet. "The diffusional formation of ferrite from austenite in Fe-C-Ni alloys." Metall. Mat. Trans. A 35.4 (2004): 1211-1221.

exh3

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

exi1

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

exi2

Diffusion in complex phases. Diffusion of carbon in cementite This example demonstrates the use of the model for calculation of diffusion through a stoichiometric phase. The flux of a component in the stoichiometric phase is assumed to be proportional to the difference in chemical potential at each side of the stoichiometric phase multiplied with the mobility for the component in the phase. The mobility is assessed from experimental information and is basically the tracer diffusivity for the component.

exi3a

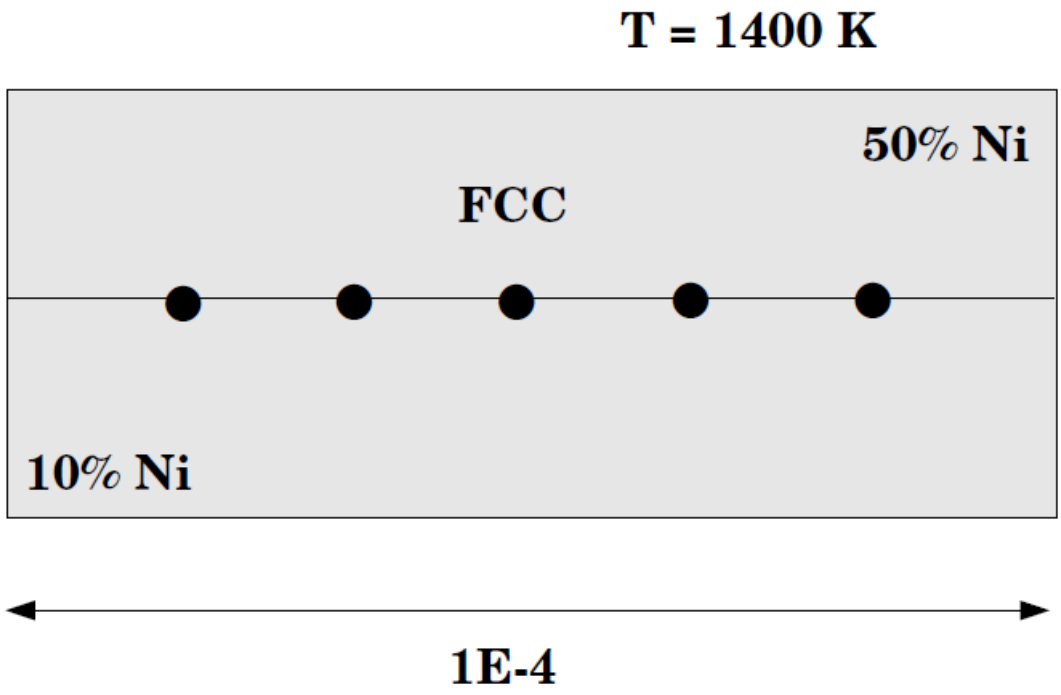
Diffusion in complex phases. Diffusion in iron oxide (FeO) This example shows the oxidation of an iron sample and the consequent growth of an oxide layer.

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.



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.

Results

exa1-setup

```
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 Software  (build 12987) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri Feb 16 15:22:08 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

 VA                       /-  DEFINED
 L12_FCC                  B2_BCC                   DICTRA_FCC_A1
   REJECTED
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ USE THERMODYNAMIC DATABASE TO RETRIEVE DATA
TDB_TCFE9: @@
TDB_TCFE9: switch_database
 Use one of these databases

 TCFE9   =  Steels/Fe-Alloys  v9.0
 TCFE10  =  Steels/Fe-Alloys  v10.0 SNAPSHOT
 TCFE8   =  Steels/Fe-Alloys  v8.1
 FROST1  =  FROST database v1.0
 TCFE7   =  Steels/Fe-Alloys  v7.0
 TCFE6   =  Steels/Fe-Alloys  v6.2
 TCFE5   =  Steels/Fe-Alloys  v5.0
 TCFE4   =  Steels/Fe-Alloys  v4.1
 TCFE3   =  Steels/Fe-Alloys  v3.1
 TCFE2   =  Steels/Fe-Alloys  v2.1
 TCFE1   =  Steels/Fe-Alloys  v1.0
 TCNI9   =  Ni-Alloys  v9.0 SNAPSHOT
 NI25    =  NI25 database
 TCNI8   =  Ni-Alloys  v8.1
 TCNI7   =  Ni-Alloys  v7.1
 TCNI6   =  Ni-Alloys  v6.0
 TCNI5   =  Ni-Alloys  v5.1
 TCNI4   =  Ni-Alloys  v4.0
 TCNI1   =  Ni-Alloys  v1.3
 TCAL5   =  Al-Alloys  v5.0
 TCAL4   =  Al-Alloys  v4.0
 TCAL3   =  Al-Alloys  v3.0
 TCAL2   =  Al-Alloys  v2.1
 TCAL1   =  Al-Alloys  v1.2
 TCMG4   =  Mg-Alloys  v4.0
 TCMG3   =  Mg-Alloys  v3.0
 TCMG2   =  Mg-Alloys  v2.0
 TCMG1   =  Mg-Alloys  v1.1
 TCTI1   =  Ti-Alloys  v1.0
 TCCU2   =  Cu-Alloys  v2.0
 TCCU1   =  Cu-Alloys  v1.0
 TCCC1   =  Cemented carbide  v1.0
 TCHEA2  =  High Entropy Alloy  v2.1
 TCHEA1  =  High Entropy Alloy  v1.0
 SSOL6   =  SGTE Alloy Solutions Database v6.0
 SSOL5   =  SGTE Alloy Solutions Database v5.0
 SSOL4   =  SGTE Alloy Solutions Database v4.9g
 SSOL2   =  SGTE Alloy Solutions Database v2.1
 SSUB6   =  SGTE Substances Database v6.0
 SSUB5   =  SGTE Substances Database v5.2
 SSUB4   =  SGTE Substances Database v4.1
 SSUB3   =  SGTE Substances Database v3.3
 SSUB2   =  SGTE Substances Database v2.2
 SNOB3   =  SGTE Noble Metal Alloys Database v3.1
 STBC2   =  SGTE Thermal Barrier Coating TDB v2.2
 STBC1   =  SGTE Thermal Barrier Coating TDB v1.1
 SALT1   =  SGTE Molten Salts Database v1.2
 SEMC2   =  TC Semi-Conductors  v2.1
 SLAG4   =  Fe-containing Slag  v4.1
 SLAG3   =  Fe-containing Slag  v3.2
 SLAG2   =  Fe-containing Slag  v2.2
 SLAG1   =  Fe-containing Slag  v1.2
 TCOX7   =  Metal Oxide Solutions  v7.0
 TCOX6   =  Metal Oxide Solutions  v6.0
 TCOX5   =  Metal Oxide Solutions  v5.1
 TCOX4   =  Metal Oxide Solutions  v4.1
 ION3    =  Ionic Solutions  v3.0
 ION2    =  Ionic Solutions  v2.6
 ION1    =  Ionic Solutions  v1.5
 NOX2    =  NPL Oxide Solutions Database v2.1
 TCNOBL1 =  Noble Metals Alloys v1.0
 TCSLD3  =  Solder Alloys  v3.2
 TCSLD2  =  Solder Alloys  v2.0
 TCSI1   =  Ultrapure Silicon  v1.2
```

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 TCMP2   =  Materials Processing  v2.5
 TCES1   =  Combustion/Sintering  v1.1
 TCSC1   =  Super Conductor  v1.0
 TCFC1   =  SOFC Database v1.0
 NUMT2   =  Nuclear Materials  v2.1
 NUOX4   =  Nuclear Oxides  v4.2
 NUCL15  =  IRSN NUCLEA-15_4
 NUCL10  =  ThermoData NUCLEA Alloys-oxides TDB v10.2
 MEPH15  =  IRSN Mephista-15_1
 MEPH11  =  ThermoData MEPHISTA Nuclear Fuels TDB v11.2
 TCAQ3   =  Aqueous Solution  v3.0
 TCAQ2   =  Aqueous Solution  v2.6
 AQS2    =  TGG Aqueous Solution Database v2.6
 GCE2    =  TGG Geochemical/Environmental TDB v2.3
 FEDEMO  =  Iron Demo Database v2.0
 ALDEMO  =  Aluminum Demo Database v2.0
 NIDEMO  =  Nickel Demo Database v1.0
 CUDEMO  =  Copper Demo Database v1.0
 SLDEMO  =  Solder Demo Database v1.0
 OXDEMO  =  Oxide Demo Database v1.0
 SUBDEMO =  Substance Demo Database v1.0
 PTERN   =  Public Ternary Alloys TDB v1.3
 PAQ2    =  Public Aqueous Soln (SIT) TDB v2.4
 PG35    =  G35 Binary Semi-Conductors TDB v1.2
 PURE5   =  SGTE Unary (Pure Elements) TDB v5.1
 MOB2    =  Alloys Mobility  v2.7
 MOB1    =  Alloys Mobility  v1.3
 MOBFE1  =  Steels/Fe-Alloys Mobility  v1.0
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBNI4  =  Ni-Alloys Mobility  v4.0
 MOBNI3  =  Ni-Alloys Mobility  v3.1
 MOBNI2  =  Ni-Alloys Mobility  v2.4
 MOBNI1  =  Ni-Alloys Mobility  v1.0
 MOBAL3  =  Al-Alloys Mobility  v3.0
 MOBAL2  =  Al-Alloys Mobility  v2.0
 MOBAL1  =  Al-Alloys Mobility  v1.0
 MOBCU1  =  Cu-Alloys Mobility  v1.0
 MOBCU2  =  Cu-Alloys Mobility  v2.0
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBSLD1 =  Solder-Alloys Mobility  v1.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0 SNAPSHOT
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v1.0
 MFEDEMO =  Fe-Alloys Mobility demo database v2.0
 MNIDEMO =  Ni-Alloys Mobility demo database v1.0
 MCUDEMO =  Cu-Alloys Mobility demo database v1.0
 USER    =  User defined Database

DATABASE NAME /TCFE9/: fedemo
 Current database: Iron Demo Database v2.0

 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: *
 LIQUID:L                 BCC_A2                   FCC_A1
 HCP_A3                   LAVES_PHASE_C14  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
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'X.-G. Lu, M. Selleby, B. Sundman, CALPHAD, 29 (2005) 49-55; Fe P-T diagram'
  'A. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); FE-NI'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
 -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

 TCFE9   =  Steels/Fe-Alloys  v9.0
 TCFE10  =  Steels/Fe-Alloys  v10.0 SNAPSHOT
 TCFE8   =  Steels/Fe-Alloys  v8.1
 FROST1  =  FROST database v1.0
 TCFE7   =  Steels/Fe-Alloys  v7.0
 TCFE6   =  Steels/Fe-Alloys  v6.2
```

```
 TCFE5   =  Steels/Fe-Alloys  v5.0
 TCFE4   =  Steels/Fe-Alloys  v4.1
 TCFE3   =  Steels/Fe-Alloys  v3.1
 TCFE2   =  Steels/Fe-Alloys  v2.1
 TCFE1   =  Steels/Fe-Alloys  v1.0
 TCNI9   =  Ni-Alloys  v9.0 SNAPSHOT
 NI25    =  NI25 database
 TCNI8   =  Ni-Alloys  v8.1
 TCNI7   =  Ni-Alloys  v7.1
 TCNI6   =  Ni-Alloys  v6.0
 TCNI5   =  Ni-Alloys  v5.1
 TCNI4   =  Ni-Alloys  v4.0
 TCNI1   =  Ni-Alloys  v1.3
 TCAL5   =  Al-Alloys  v5.0
 TCAL4   =  Al-Alloys  v4.0
 TCAL3   =  Al-Alloys  v3.0
 TCAL2   =  Al-Alloys  v2.1
 TCAL1   =  Al-Alloys  v1.2
 TCMG4   =  Mg-Alloys  v4.0
 TCMG3   =  Mg-Alloys  v3.0
 TCMG2   =  Mg-Alloys  v2.0
 TCMG1   =  Mg-Alloys  v1.1
 TCTI1   =  Ti-Alloys  v1.0
 TCCU2   =  Cu-Alloys  v2.0
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 TCCC1   =  Cemented carbide  v1.0
 TCHEA2  =  High Entropy Alloy  v2.1
 TCHEA1  =  High Entropy Alloy  v1.0
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 SSUB5   =  SGTE Substances Database v5.2
 SSUB4   =  SGTE Substances Database v4.1
 SSUB3   =  SGTE Substances Database v3.3
 SSUB2   =  SGTE Substances Database v2.2
 SNOB3   =  SGTE Noble Metal Alloys Database v3.1
 STBC2   =  SGTE Thermal Barrier Coating TDB v2.2
 STBC1   =  SGTE Thermal Barrier Coating TDB v1.1
 SALT1   =  SGTE Molten Salts Database v1.2
 SEMC2   =  TC Semi-Conductors  v2.1
 SLAG4   =  Fe-containing Slag  v4.1
 SLAG3   =  Fe-containing Slag  v3.2
 SLAG2   =  Fe-containing Slag  v2.2
 SLAG1   =  Fe-containing Slag  v1.2
 TCOX7   =  Metal Oxide Solutions  v7.0
 TCOX6   =  Metal Oxide Solutions  v6.0
 TCOX5   =  Metal Oxide Solutions  v5.1
 TCOX4   =  Metal Oxide Solutions  v4.1
 ION3    =  Ionic Solutions  v3.0
 ION2    =  Ionic Solutions  v2.6
 ION1    =  Ionic Solutions  v1.5
 NOX2    =  NPL Oxide Solutions Database v2.1
 TCNOBL1 =  Noble Metals Alloys v1.0
 TCSLD3  =  Solder Alloys  v3.2
 TCSLD2  =  Solder Alloys  v2.0
 TCSI1   =  Ultrapure Silicon  v1.2
 TCMP2   =  Materials Processing  v2.5
 TCES1   =  Combustion/Sintering  v1.1
 TCSC1   =  Super Conductor  v1.0
 TCFC1   =  SOFC Database v1.0
 NUMT2   =  Nuclear Materials  v2.1
 NUOX4   =  Nuclear Oxides  v4.2
 NUCL15  =  IRSN NUCLEA-15_4
 NUCL10  =  ThermoData NUCLEA Alloys-oxides TDB v10.2
 MEPH15  =  IRSN Mephista-15_1
 MEPH11  =  ThermoData MEPHISTA Nuclear Fuels TDB v11.2
 TCAQ3   =  Aqueous Solution  v3.0
 TCAQ2   =  Aqueous Solution  v2.6
 AQS2    =  TGG Aqueous Solution Database v2.6
 GCE2    =  TGG Geochemical/Environmental TDB v2.3
 FEDEMO  =  Iron Demo Database v2.0
 ALDEMO  =  Aluminum Demo Database v2.0
 NIDEMO  =  Nickel Demo Database v1.0
 CUDEMO  =  Copper Demo Database v1.0
 SLDEMO  =  Solder Demo Database v1.0
 OXDEMO  =  Oxide Demo Database v1.0
 SUBDEMO =  Substance Demo Database v1.0
 PTERN   =  Public Ternary Alloys TDB v1.3
 PAQ2    =  Public Aqueous Soln (SIT) TDB v2.4
 PG35    =  G35 Binary Semi-Conductors TDB v1.2
 PURE5   =  SGTE Unary (Pure Elements) TDB v5.1
 MOB2    =  Alloys Mobility  v2.7
 MOB1    =  Alloys Mobility  v1.3
 MOBFE1  =  Steels/Fe-Alloys Mobility  v1.0
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBNI4  =  Ni-Alloys Mobility  v4.0
 MOBNI3  =  Ni-Alloys Mobility  v3.1
 MOBNI2  =  Ni-Alloys Mobility  v2.4
 MOBNI1  =  Ni-Alloys Mobility  v1.0
 MOBAL3  =  Al-Alloys Mobility  v3.0
 MOBAL2  =  Al-Alloys Mobility  v2.0
 MOBAL1  =  Al-Alloys Mobility  v1.0
 MOBCU1  =  Cu-Alloys Mobility  v1.0
 MOBCU2  =  Cu-Alloys Mobility  v2.0
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBSLD1 =  Solder-Alloys Mobility  v1.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0 SNAPSHOT
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v1.0
 MFEDEMO =  Fe-Alloys Mobility demo database v2.0
 MNIDEMO =  Ni-Alloys Mobility demo database v1.0
 MCUDEMO =  Cu-Alloys Mobility demo database v1.0
 USER    =  User defined Database

DATABASE NAME /FEDEMO/: mfedemo
 Current database: Fe-Alloys Mobility demo database v2.0

 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  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 ....

 List of references for assessed data

  'This parameter has not been assessed'
  'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
      -Ni'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Ni self-diffusion'
 -OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP
APP: @@
APP: goto_module
MODULE NAME: dictra_monitor
 NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set_condition

GLOBAL OR BOUNDARY CONDITION /GLOBAL/: global
VARIABLE : T
LOW TIME LIMIT /0/: 0
T(TIME,X)= 1400;
HIGH TIME LIMIT /*/: *
ANY MORE RANGES /N/: N
DIC>
DIC> @@
DIC> @@ START BY ENTERING A REGION
DIC> @@
DIC> enter_region
REGION NAME : austenite
DIC>
DIC> @@
DIC> @@ ENTER A GRID INTO THE REGION
DIC> @@
DIC> @@ FOR SIMPLICITY, AN EQUIDISTANT GRID IS USED
DIC> @@
DIC> enter_grid_coordinates
REGION NAME : /AUSTENITE/: austenite
WIDTH OF REGION /1/: 1e-4
TYPE /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>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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 grid   75
 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 =   241.69569     DT =   241.29559     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 =   724.28686     DT =   482.59117     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 =   1689.4692     DT =   965.18235     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 =   3619.8339     DT =   1930.3647     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 =   7480.5633     DT =   3860.7294     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 =   15202.022     DT =   7721.4588     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 =   30644.940     DT =   15442.918     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 =   61530.775     DT =   30885.835     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 =   123302.44     DT =   61771.670     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 =   223302.44     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 =   323302.44     DT =   100000.00     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .709680136600386  NI = .290319863399613
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   423302.44     DT =   100000.00     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .709680136600386  NI = .290319863399614
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   523302.44     DT =   100000.00     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .709680136600386  NI = .290319863399614
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   623302.44     DT =   100000.00     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .709680136600386  NI = .290319863399614
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   723302.44     DT =   100000.00     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .709680136600386  NI = .290319863399614
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   823302.44     DT =   100000.00     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .709680136600386  NI = .290319863399614
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   923302.44     DT =   100000.00     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .709680136600386  NI = .290319863399615
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    1 seconds
 TIME =   1000000.0     DT =   76697.555     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    241.69569
 DELETING TIME-RECORD FOR TIME    724.28686
 DELETING TIME-RECORD FOR TIME    1689.4692
 DELETING TIME-RECORD FOR TIME    3619.8339
 DELETING TIME-RECORD FOR TIME    7480.5633
 DELETING TIME-RECORD FOR TIME    15202.022
 DELETING TIME-RECORD FOR TIME    30644.940
 DELETING TIME-RECORD FOR TIME    61530.775
 DELETING TIME-RECORD FOR TIME    123302.44
 DELETING TIME-RECORD FOR TIME    223302.44
 DELETING TIME-RECORD FOR TIME    323302.44
 DELETING TIME-RECORD FOR TIME    423302.44
 DELETING TIME-RECORD FOR TIME    523302.44
 DELETING TIME-RECORD FOR TIME    623302.44
 DELETING TIME-RECORD FOR TIME    723302.44
 DELETING TIME-RECORD FOR TIME    823302.44

 KEEPING TIME-RECORD FOR TIME    923302.44
 AND FOR TIME                    1000000.0
 WORKSPACE RECLAIMED

 TIMESTEP AT     1000000.00     SELECTED

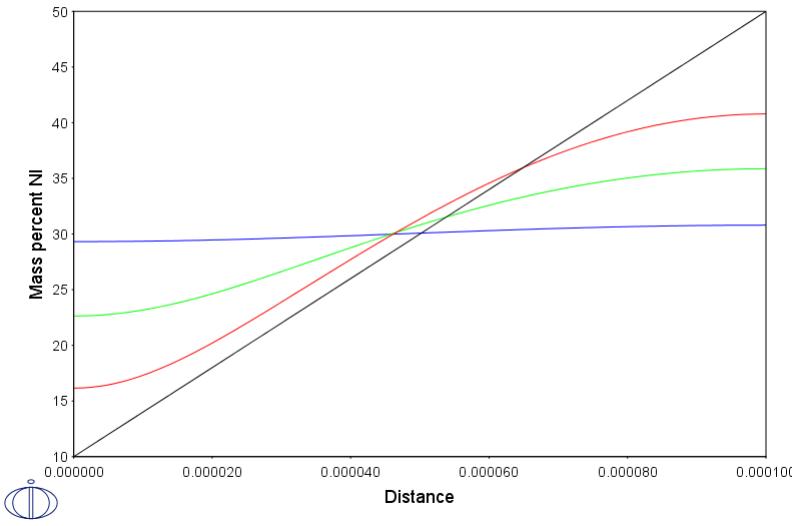
DIC>
DIC> @@
DIC> @@ THE SIMULATION IS FINISHED
DIC> @@
DIC>
DIC> set_interactive
 --OK---
DIC>
```

exa1-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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: plot_diagram
   2018.02.18.18.26.44
   Time = 0,100000,300000,1000000
   CELL #1
```

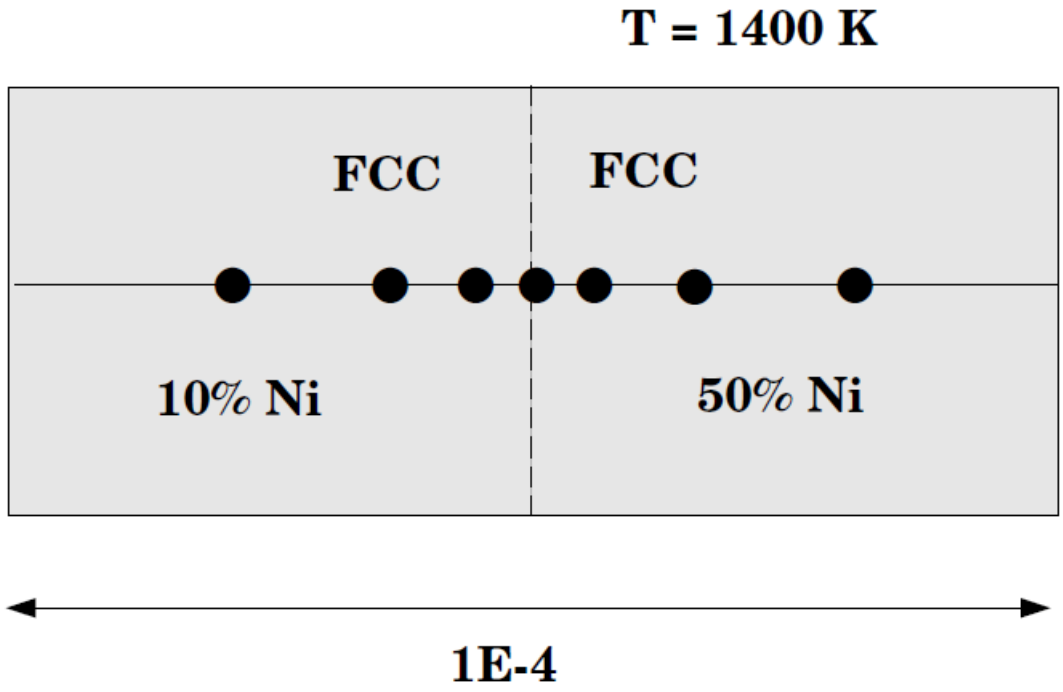



```
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: set_interactive
 --OK---
POST-1:
```

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

```
About simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 12987) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri Feb 16 15:22:08 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa2a\setup.DCM" @@
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
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

 VA                     /-  DEFINED
 L12_FCC                B2_BCC                  DICTRA_FCC_A1
   REJECTED
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA
TDB_TCFE9: @@
TDB_TCFE9: sw FEDEMO
   ... the command in full is SWITCH_DATABASE
 Current database: Iron Demo Database v2.0

 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
 LIQUID:L               BCC_A2                  FCC_A1
 HCP_A3                 LAVES_PHASE_C14  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
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'X.-G. Lu, M. Selleby, B. Sundman, CALPHAD, 29 (2005) 49-55; Fe P-T diagram'
  'A. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); FE-NI'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
 -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

 TCFE9   =  Steels/Fe-Alloys  v9.0
 TCFE10  =  Steels/Fe-Alloys  v10.0 SNAPSHOT
 TCFE8   =  Steels/Fe-Alloys  v8.1
 FROST1  =  FROST database v1.0
 TCFE7   =  Steels/Fe-Alloys  v7.0
 TCFE6   =  Steels/Fe-Alloys  v6.2
 TCFE5   =  Steels/Fe-Alloys  v5.0
 TCFE4   =  Steels/Fe-Alloys  v4.1
 TCFE3   =  Steels/Fe-Alloys  v3.1
```

```
 TCFE2   =  Steels/Fe-Alloys  v2.1
 TCFE1   =  Steels/Fe-Alloys  v1.0
 TCNI9   =  Ni-Alloys  v9.0 SNAPSHOT
 NI25    =  NI25 database
 TCNI8   =  Ni-Alloys  v8.1
 TCNI7   =  Ni-Alloys  v7.1
 TCNI6   =  Ni-Alloys  v6.0
 TCNI5   =  Ni-Alloys  v5.1
 TCNI4   =  Ni-Alloys  v4.0
 TCNI1   =  Ni-Alloys  v1.3
 TCAL5   =  Al-Alloys  v5.0
 TCAL4   =  Al-Alloys  v4.0
 TCAL3   =  Al-Alloys  v3.0
 TCAL2   =  Al-Alloys  v2.1
 TCAL1   =  Al-Alloys  v1.2
 TCMG4   =  Mg-Alloys  v4.0
 TCMG3   =  Mg-Alloys  v3.0
 TCMG2   =  Mg-Alloys  v2.0
 TCMG1   =  Mg-Alloys  v1.1
 TCTI1   =  Ti-Alloys  v1.0
 TCCU2   =  Cu-Alloys  v2.0
 TCCU1   =  Cu-Alloys  v1.0
 TCCC1   =  Cemented carbide  v1.0
 TCHEA2  =  High Entropy Alloy  v2.1
 TCHEA1  =  High Entropy Alloy  v1.0
 SSOL6   =  SGTE Alloy Solutions Database v6.0
 SSOL5   =  SGTE Alloy Solutions Database v5.0
 SSOL4   =  SGTE Alloy Solutions Database v4.9g
 SSOL2   =  SGTE Alloy Solutions Database v2.1
 SSUB6   =  SGTE Substances Database v6.0
 SSUB5   =  SGTE Substances Database v5.2
 SSUB4   =  SGTE Substances Database v4.1
 SSUB3   =  SGTE Substances Database v3.3
 SSUB2   =  SGTE Substances Database v2.2
 SNOB3   =  SGTE Noble Metal Alloys Database v3.1
 STBC2   =  SGTE Thermal Barrier Coating TDB v2.2
 STBC1   =  SGTE Thermal Barrier Coating TDB v1.1
 SALT1   =  SGTE Molten Salts Database v1.2
 SEMC2   =  TC Semi-Conductors  v2.1
 SLAG4   =  Fe-containing Slag  v4.1
 SLAG3   =  Fe-containing Slag  v3.2
 SLAG2   =  Fe-containing Slag  v2.2
 SLAG1   =  Fe-containing Slag  v1.2
 TCOX7   =  Metal Oxide Solutions  v7.0
 TCOX6   =  Metal Oxide Solutions  v6.0
 TCOX5   =  Metal Oxide Solutions  v5.1
 TCOX4   =  Metal Oxide Solutions  v4.1
 ION3    =  Ionic Solutions  v3.0
 ION2    =  Ionic Solutions  v2.6
 ION1    =  Ionic Solutions  v1.5
 NOX2    =  NPL Oxide Solutions Database v2.1
 TCNOBL1 =  Noble Metals Alloys v1.0
 TCSLD3  =  Solder Alloys  v3.2
 TCSLD2  =  Solder Alloys  v2.0
 TCSI1   =  Ultrapure Silicon  v1.2
 TCMP2   =  Materials Processing  v2.5
 TCES1   =  Combustion/Sintering  v1.1
 TCSC1   =  Super Conductor  v1.0
 TCFC1   =  SOFC Database v1.0
 NUMT2   =  Nuclear Materials  v2.1
 NUOX4   =  Nuclear Oxides  v4.2
 NUCL15  =  IRSN NUCLEA-15_4
 NUCL10  =  ThermoData NUCLEA Alloys-oxides TDB v10.2
 MEPH15  =  IRSN Mephista-15_1
 MEPH11  =  ThermoData MEPHISTA Nuclear Fuels TDB v11.2
 TCAQ3   =  Aqueous Solution  v3.0
 TCAQ2   =  Aqueous Solution  v2.6
 AQS2    =  TGG Aqueous Solution Database v2.6
 GCE2    =  TGG Geochemical/Environmental TDB v2.3
 FEDEMO  =  Iron Demo Database v2.0
 ALDEMO  =  Aluminum Demo Database v2.0
 NIDEMO  =  Nickel Demo Database v1.0
 CUDEMO  =  Copper Demo Database v1.0
 SLDEMO  =  Solder Demo Database v1.0
 OXDEMO  =  Oxide Demo Database v1.0
 SUBDEMO =  Substance Demo Database v1.0
 PTERN   =  Public Ternary Alloys TDB v1.3
 PAQ2    =  Public Aqueous Soln (SIT) TDB v2.4
 PG35    =  G35 Binary Semi-Conductors TDB v1.2
 PURE5   =  SGTE Unary (Pure Elements) TDB v5.1
 MOB2    =  Alloys Mobility  v2.7
 MOB1    =  Alloys Mobility  v1.3
 MOBFE1  =  Steels/Fe-Alloys Mobility  v1.0
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBNI4  =  Ni-Alloys Mobility  v4.0
 MOBNI3  =  Ni-Alloys Mobility  v3.1
 MOBNI2  =  Ni-Alloys Mobility  v2.4
 MOBNI1  =  Ni-Alloys Mobility  v1.0
 MOBAL3  =  Al-Alloys Mobility  v3.0
 MOBAL2  =  Al-Alloys Mobility  v2.0
 MOBAL1  =  Al-Alloys Mobility  v1.0
 MOBCU1  =  Cu-Alloys Mobility  v1.0
 MOBCU2  =  Cu-Alloys Mobility  v2.0
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBSLD1 =  Solder-Alloys Mobility  v1.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0 SNAPSHOT
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v1.0
 MFEDEMO =  Fe-Alloys Mobility demo database v2.0
 MNIDEMO =  Ni-Alloys Mobility demo database v1.0
 MCUDEMO =  Cu-Alloys Mobility demo database v1.0
 USER    =  User defined Database

DATABASE NAME /FEDEMO/: mfedemo
 Current database: Fe-Alloys Mobility demo database v2.0

 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  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 ....

 List of references for assessed data

  'This parameter has not been assessed'
  'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
      -Ni'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Ni self-diffusion'
 -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
 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
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   ... 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> @@ 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>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa2a\run.DCM"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
   ... 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 =   10.408313     DT =   10.008213     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 =   30.424739     DT =   20.016426     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 =   70.457590     DT =   40.032851     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 =   150.52329     DT =   80.065703     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 =   310.65470     DT =   160.13141     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 =   630.91751     DT =   320.26281     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 =   1271.4431     DT =   640.52562     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 =   2552.4944     DT =   1281.0512     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 =   5114.5969     DT =   2562.1025     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 =   10238.802     DT =   5124.2050     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 =   20487.212     DT =   10248.410     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 =   40984.032     DT =   20496.820     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 =   81977.671     DT =   40993.640     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 =   163964.95     DT =   81987.280     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 =   263964.95     DT =   100000.00     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .70888824540617  NI = .29111175459383
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   363964.95     DT =   100000.00     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .708888245406171  NI = .291111754593829
```

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 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   463964.95     DT =   100000.00     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .70888824540617  NI = .29111175459383
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   563964.95     DT =   100000.00     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .708888245406168  NI = .291111754593831
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   663964.95     DT =   100000.00     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .70888824540617  NI = .29111175459383
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   763964.95     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 =   863964.95     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                    1 seconds
 TIME =   963964.95     DT =   100000.00     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .708888245406171  NI = .291111754593829
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   1000000.0     DT =   36035.049     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .708888245406172  NI = .291111754593829
 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    10.408313
 DELETING TIME-RECORD FOR TIME    30.424739
 DELETING TIME-RECORD FOR TIME    70.457590
 DELETING TIME-RECORD FOR TIME    150.52329
 DELETING TIME-RECORD FOR TIME    310.65470
 DELETING TIME-RECORD FOR TIME    630.91751
 DELETING TIME-RECORD FOR TIME    1271.4431
 DELETING TIME-RECORD FOR TIME    2552.4944
 DELETING TIME-RECORD FOR TIME    5114.5969
 DELETING TIME-RECORD FOR TIME    10238.802
 DELETING TIME-RECORD FOR TIME    20487.212
 DELETING TIME-RECORD FOR TIME    40984.032
 DELETING TIME-RECORD FOR TIME    81977.671
 DELETING TIME-RECORD FOR TIME    163964.95
 DELETING TIME-RECORD FOR TIME    263964.95
 DELETING TIME-RECORD FOR TIME    363964.95
 DELETING TIME-RECORD FOR TIME    463964.95
 DELETING TIME-RECORD FOR TIME    563964.95
 DELETING TIME-RECORD FOR TIME    663964.95
 DELETING TIME-RECORD FOR TIME    763964.95
 DELETING TIME-RECORD FOR TIME    863964.95

 KEEPING TIME-RECORD FOR TIME    963964.95
 AND FOR TIME                    1000000.0
 WORKSPACE RECLAIMED

 TIMESTEP AT     1000000.00     SELECTED

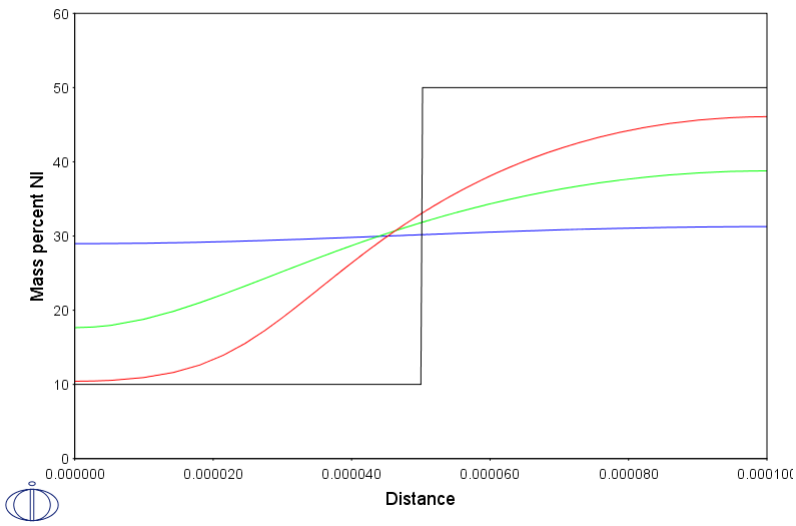
DIC>
DIC> @@
DIC> @@ THE SIMULATION IS FINISHED
DIC> @@
DIC>
DIC> set-inter
   ... the command in full is SET_INTERACTIVE
 --OK---
DIC>
```

exa2a-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa2a\plot.DCM"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: plot
   ... the command in full is PLOT_DIAGRAM
   2018.02.18.18.29.45
   Time = 0,100000,300000,1000000
   CELL #1
```



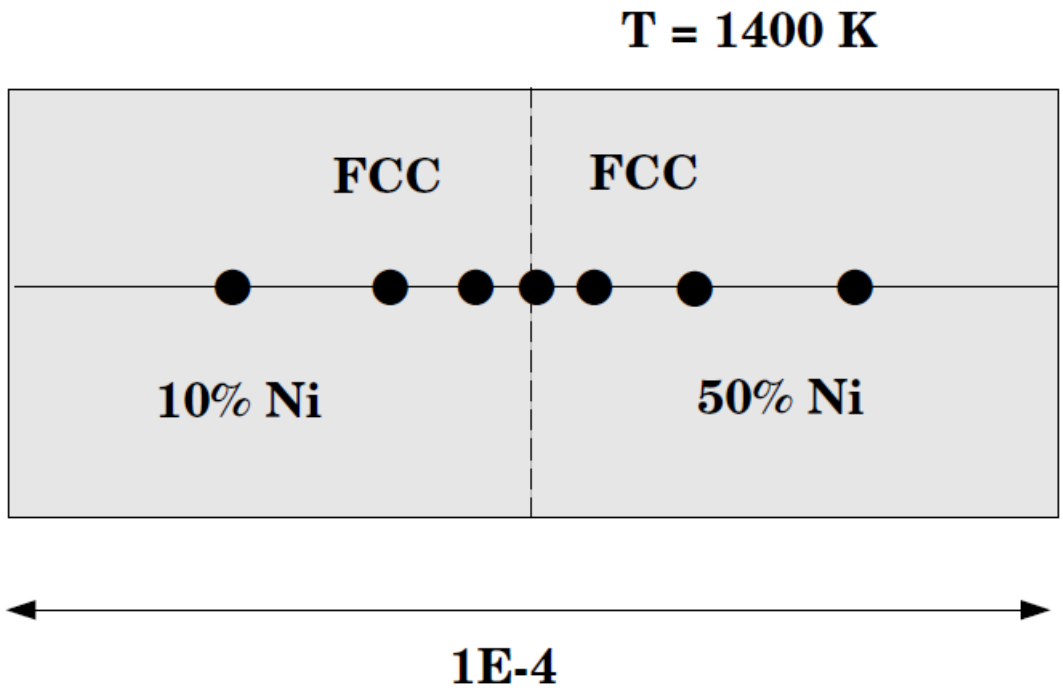

```
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
```

```
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

```
About
 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 12987) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri Feb 16 15:22:08 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa2b\setup.DCM" @@
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
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

 VA                     /-  DEFINED
 L12_FCC                B2_BCC                 DICTRA_FCC_A1
   REJECTED
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ USE THE TCFE DATABASE FOR THERMODYNAMIC DATA
TDB_TCFE9: @@
TDB_TCFE9: sw tcfe7
   ... the command in full is SWITCH_DATABASE
 Current database: Steels/Fe-Alloys  v7.0

 VA  DEFINED
 L12_FCC                B2_BCC                 B2_VACANCY
 HIGH_SIGMA             DICTRA_FCC_A1  REJECTED
TDB_TCFE7:
TDB_TCFE7: @@
TDB_TCFE7: @@ DEFINE THE SYSTEM TO WORK WITH
TDB_TCFE7: @@
TDB_TCFE7: def-system fe ni
   ... the command in full is DEFINE_SYSTEM
 FE                     NI  DEFINED
TDB_TCFE7:
TDB_TCFE7: @@
TDB_TCFE7: @@ EXCLUDE THE THERMODYNAMIC DATA FOR THE PHASES THAT ARE NOT NEEDED
TDB_TCFE7: @@
TDB_TCFE7: rej ph * all
   ... the command in full is REJECT
 LIQUID:L               BCC_A2                 FCC_A1
 HCP_A3                 A1_KAPPA               KAPPA
 LAVES_PHASE_C14        NBNI3                  NI3TI
   REJECTED
TDB_TCFE7: res ph fcc
   ... the command in full is RESTORE
 FCC_A1  RESTORED
TDB_TCFE7:
TDB_TCFE7: @@
TDB_TCFE7: @@ RETRIEVE DATA FROM THE DATABASE FILE
TDB_TCFE7: @@
TDB_TCFE7: get
   ... the command in full is GET_DATA
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'
  'A. Dinsdale, T. Chart, MTDS NPL, unpublished work (1986); FE-NI'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
      Molar volumes'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
 -OK-
TDB_TCFE7:
TDB_TCFE7: @@
TDB_TCFE7: @@ MOBILITY/DIFFUSIVITY DATA ARE STORED IN A SEPARATE DATABASE FILE.
TDB_TCFE7: @@ SWITCH TO THE MOBILITY DATABASE TO RETRIEVE DATA.
TDB_TCFE7: @@
TDB_TCFE7: app
   ... the command in full is APPEND_DATABASE
 Use one of these databases

 TCFE9   =  Steels/Fe-Alloys  v9.0
 TCFE10  =  Steels/Fe-Alloys  v10.0 SNAPSHOT
 TCFE8   =  Steels/Fe-Alloys  v8.1
 FROST1  =  FROST database v1.0
 TCFE7   =  Steels/Fe-Alloys  v7.0
 TCFE6   =  Steels/Fe-Alloys  v6.2
 TCFE5   =  Steels/Fe-Alloys  v5.0
 TCFE4   =  Steels/Fe-Alloys  v4.1
 TCFE3   =  Steels/Fe-Alloys  v3.1
 TCFE2   =  Steels/Fe-Alloys  v2.1
 TCFE1   =  Steels/Fe-Alloys  v1.0
 TCNI9   =  Ni-Alloys  v9.0 SNAPSHOT
```

```
 NI25    =  NI25 database
 TCNI8   =  Ni-Alloys  v8.1
 TCNI7   =  Ni-Alloys  v7.1
 TCNI6   =  Ni-Alloys  v6.0
 TCNI5   =  Ni-Alloys  v5.1
 TCNI4   =  Ni-Alloys  v4.0
 TCNI1   =  Ni-Alloys  v1.3
 TCAL5   =  Al-Alloys  v5.0
 TCAL4   =  Al-Alloys  v4.0
 TCAL3   =  Al-Alloys  v3.0
 TCAL2   =  Al-Alloys  v2.1
 TCAL1   =  Al-Alloys  v1.2
 TCMG4   =  Mg-Alloys  v4.0
 TCMG3   =  Mg-Alloys  v3.0
 TCMG2   =  Mg-Alloys  v2.0
 TCMG1   =  Mg-Alloys  v1.1
 TCTI1   =  Ti-Alloys  v1.0
 TCCU2   =  Cu-Alloys  v2.0
 TCCU1   =  Cu-Alloys  v1.0
 TCCC1   =  Cemented carbide  v1.0
 TCHEA2  =  High Entropy Alloy  v2.1
 TCHEA1  =  High Entropy Alloy  v1.0
 SSOL6   =  SGTE Alloy Solutions Database v6.0
 SSOL5   =  SGTE Alloy Solutions Database v5.0
 SSOL4   =  SGTE Alloy Solutions Database v4.9g
 SSOL2   =  SGTE Alloy Solutions Database v2.1
 SSUB6   =  SGTE Substances Database v6.0
 SSUB5   =  SGTE Substances Database v5.2
 SSUB4   =  SGTE Substances Database v4.1
 SSUB3   =  SGTE Substances Database v3.3
 SSUB2   =  SGTE Substances Database v2.2
 SNOB3   =  SGTE Noble Metal Alloys Database v3.1
 STBC2   =  SGTE Thermal Barrier Coating TDB v2.2
 STBC1   =  SGTE Thermal Barrier Coating TDB v1.1
 SALT1   =  SGTE Molten Salts Database v1.2
 SEMC2   =  TC Semi-Conductors  v2.1
 SLAG4   =  Fe-containing Slag  v4.1
 SLAG3   =  Fe-containing Slag  v3.2
 SLAG2   =  Fe-containing Slag  v2.2
 SLAG1   =  Fe-containing Slag  v1.2
 TCOX7   =  Metal Oxide Solutions  v7.0
 TCOX6   =  Metal Oxide Solutions  v6.0
 TCOX5   =  Metal Oxide Solutions  v5.1
 TCOX4   =  Metal Oxide Solutions  v4.1
 ION3    =  Ionic Solutions  v3.0
 ION2    =  Ionic Solutions  v2.6
 ION1    =  Ionic Solutions  v1.5
 NOX2    =  NPL Oxide Solutions Database v2.1
 TCNOBL1 =  Noble Metals Alloys v1.0
 TCSLD3  =  Solder Alloys  v3.2
 TCSLD2  =  Solder Alloys  v2.0
 TCSI1   =  Ultrapure Silicon  v1.2
 TCMP2   =  Materials Processing  v2.5
 TCES1   =  Combustion/Sintering  v1.1
 TCSC1   =  Super Conductor  v1.0
 TCFC1   =  SOFC Database v1.0
 NUMT2   =  Nuclear Materials  v2.1
 NUOX4   =  Nuclear Oxides  v4.2
 NUCL15  =  IRSN NUCLEA-15_4
 NUCL10  =  ThermoData NUCLEA Alloys-oxides TDB v10.2
 MEPH15  =  IRSN Mephista-15_1
 MEPH11  =  ThermoData MEPHISTA Nuclear Fuels TDB v11.2
 TCAQ3   =  Aqueous Solution  v3.0
 TCAQ2   =  Aqueous Solution  v2.6
 AQS2    =  TGG Aqueous Solution Database v2.6
 GCE2    =  TGG Geochemical/Environmental TDB v2.3
 FEDEMO  =  Iron Demo Database v2.0
 ALDEMO  =  Aluminum Demo Database v2.0
 NIDEMO  =  Nickel Demo Database v1.0
 CUDEMO  =  Copper Demo Database v1.0
 SLDEMO  =  Solder Demo Database v1.0
 OXDEMO  =  Oxide Demo Database v1.0
 SUBDEMO =  Substance Demo Database v1.0
 PTERN   =  Public Ternary Alloys TDB v1.3
 PAQ2    =  Public Aqueous Soln (SIT) TDB v2.4
 PG35    =  G35 Binary Semi-Conductors TDB v1.2
 PURE5   =  SGTE Unary (Pure Elements) TDB v5.1
 MOB2    =  Alloys Mobility  v2.7
 MOB1    =  Alloys Mobility  v1.3
 MOBFE1  =  Steels/Fe-Alloys Mobility  v1.0
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBNI4  =  Ni-Alloys Mobility  v4.0
 MOBNI3  =  Ni-Alloys Mobility  v3.1
 MOBNI2  =  Ni-Alloys Mobility  v2.4
 MOBNI1  =  Ni-Alloys Mobility  v1.0
 MOBAL3  =  Al-Alloys Mobility  v3.0
 MOBAL2  =  Al-Alloys Mobility  v2.0
 MOBAL1  =  Al-Alloys Mobility  v1.0
 MOBCU1  =  Cu-Alloys Mobility  v1.0
 MOBCU2  =  Cu-Alloys Mobility  v2.0
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBSLD1 =  Solder-Alloys Mobility  v1.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0 SNAPSHOT
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v1.0
 MFEDEMO =  Fe-Alloys Mobility demo database v2.0
 MNIDEMO =  Ni-Alloys Mobility demo database v1.0
 MCUDEMO =  Cu-Alloys Mobility demo database v1.0
 USER    =  User defined Database

DATABASE NAME /TCFE7/: mobfe2
 Current database: Steels/Fe-Alloys Mobility  v2.0
   TCS Steel Mobility Database Version 2.0 from 2011-12-09.

 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                HCP_A3
 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 ....

 List of references for assessed data

  'This parameter has not been assessed'
  'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
      -Ni'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Ni self-diffusion'
 -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
 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
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   ... 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 /NO/:
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 (0 -> 0.5 -> 1): /.5/: 1.0
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /NO/: @@
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>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa2b\run.DCM"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 = .70888824540617  NI = .29111175459383
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 U-FRACTION IN SYSTEM:  FE = .70888824540617  NI = .29111175459383
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  2  GRIDPOINT(S) ADDED   TO   CELL #1   REGION: AUSTENITE
 TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .708888245406169  NI = .29111175459383
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.10010000E-03 DT =  0.10000000E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .70888824540617  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 =   10.403455     DT =   10.003355     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 =   30.410165     DT =   20.006710     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 =   70.423585     DT =   40.013420     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 =   150.45043     DT =   80.026840     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 =   310.50411     DT =   160.05368     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 =   630.61147     DT =   320.10736     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 =   1270.8262     DT =   640.21472     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 =   2551.2556     DT =   1280.4294     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 =   5112.1145     DT =   2560.8589     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 =   10233.832     DT =   5121.7178     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 =   20477.268     DT =   10243.436     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 =   40964.139     DT =   20486.871     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 =   81937.881     DT =   40973.742     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 =   163885.37     DT =   81947.484     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .708888245406167  NI = .291111754593833
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   263885.37     DT =   100000.00     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .708888245406165  NI = .291111754593835
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   363885.37     DT =   100000.00     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .708888245406164  NI = .291111754593836
```

```
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   463885.37     DT =   100000.00     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .708888245406165  NI = .291111754593835
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   563885.37     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 =   663885.37     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 =   763885.37     DT =   100000.00     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .708888245406157  NI = .291111754593843
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   863885.37     DT =   100000.00     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .708888245406157  NI = .291111754593843
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   963885.37     DT =   100000.00     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .708888245406154  NI = .291111754593846
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   1000000.0     DT =   36114.635     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .708888245406156  NI = .291111754593844
 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    10.403455
 DELETING TIME-RECORD FOR TIME    30.410165
 DELETING TIME-RECORD FOR TIME    70.423585
 DELETING TIME-RECORD FOR TIME    150.45043
 DELETING TIME-RECORD FOR TIME    310.50411
 DELETING TIME-RECORD FOR TIME    630.61147
 DELETING TIME-RECORD FOR TIME    1270.8262
 DELETING TIME-RECORD FOR TIME    2551.2556
 DELETING TIME-RECORD FOR TIME    5112.1145
 DELETING TIME-RECORD FOR TIME    10233.832
 DELETING TIME-RECORD FOR TIME    20477.268
 DELETING TIME-RECORD FOR TIME    40964.139
 DELETING TIME-RECORD FOR TIME    81937.881
 DELETING TIME-RECORD FOR TIME    163885.37
 DELETING TIME-RECORD FOR TIME    263885.37
 DELETING TIME-RECORD FOR TIME    363885.37
 DELETING TIME-RECORD FOR TIME    463885.37
 DELETING TIME-RECORD FOR TIME    563885.37
 DELETING TIME-RECORD FOR TIME    663885.37
 DELETING TIME-RECORD FOR TIME    763885.37
 DELETING TIME-RECORD FOR TIME    863885.37

 KEEPING TIME-RECORD FOR TIME    963885.37
 AND FOR TIME                    1000000.0
 WORKSPACE RECLAIMED

 TIMESTEP AT     1000000.00     SELECTED

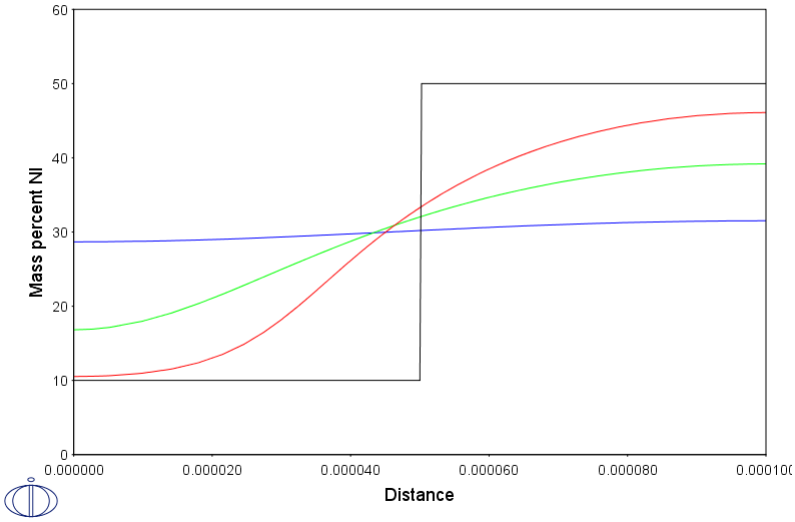
DIC>
DIC> @@
DIC> @@ THE SIMULATION IS FINISHED
DIC> @@
DIC>
DIC> set-inter
   ... the command in full is SET_INTERACTIVE
 --OK---
DIC>
```

exa2b-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa2b\plot.DCM"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: plot
   ... the command in full is PLOT_DIAGRAM
   2018.02.18.18.32.49
   Time = 0,100000,300000,1000000
   CELL #1
```




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

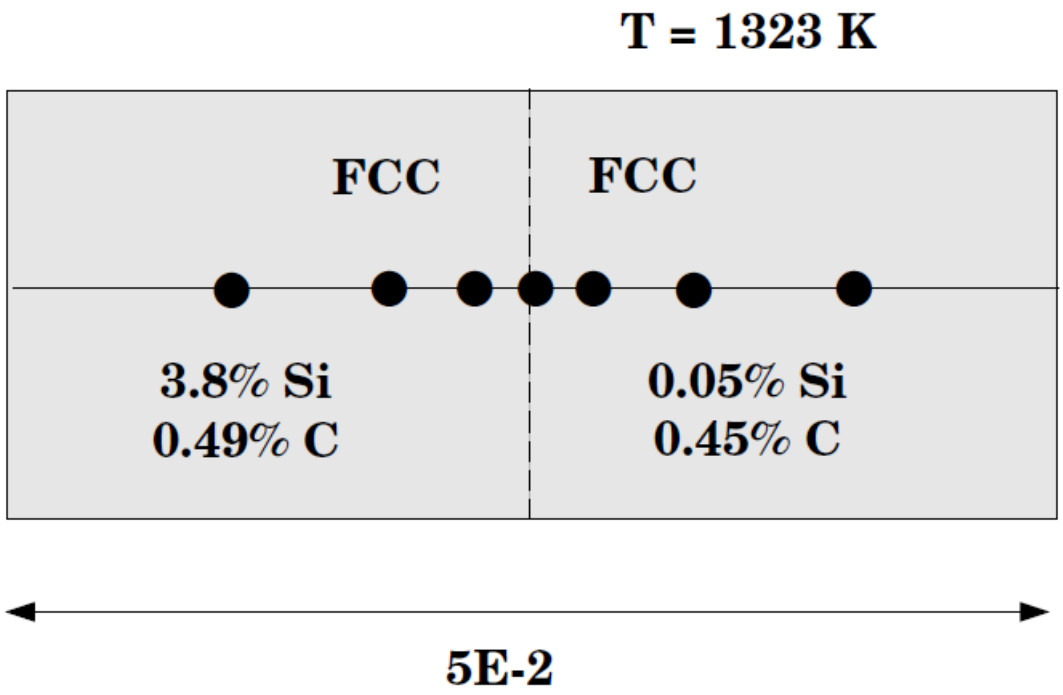
```
POST-1: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
 --OK---
POST-1:
```

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

```
AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa3\setup.DCM" @@
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
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

 VA                     /-  DEFINED
 L12_FCC                B2_BCC                 DICTRA_FCC_A1
   REJECTED
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ USE A TCFE DATABASE FOR THE THERMODYNAMIC DATA
TDB_TCFE9: @@
TDB_TCFE9: sw tcfe7
 Current database: Steels/Fe-Alloys  v7.0

 VA  DEFINED
 L12_FCC                B2_BCC                 B2_VACANCY
 HIGH_SIGMA             DICTRA_FCC_A1  REJECTED
TDB_TCFE7: def-sys fe si c
 FE                     SI                     C
   DEFINED
TDB_TCFE7: rej ph * all
 GAS:G                  LIQUID:L               BCC_A2
 FCC_A1                 HCP_A3                 DIAMOND_FCC_A4
 GRAPHITE               CEMENTITE              M23C6
 M7C3                   M5C2                   KSI_CARBIDE
 A1_KAPPA               KAPPA                  FE4N_LP1
 FECN_CHI               LAVES_PHASE_C14        M3SI
 CR3SI                  FE2SI                  MSI
 M5SI3                  AL4C3                  FE8SI2C
 SIC  REJECTED
TDB_TCFE7: res ph fcc
 FCC_A1  RESTORED
TDB_TCFE7: get
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'
  'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C
      -FE'
  'J. Lacaze and B. Sundman, Metall. Mater. Trans. A, 22A (1991), 2211-2223;
      Fe-Si and Fe-Si-C'
  'J. Miettinen and B. Hallstedt, Calphad, 22 (1998), 231-256; Fe-Si and Fe
      -Si-C'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
      Molar volumes'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
 -OK-
TDB_TCFE7:
TDB_TCFE7: @@
TDB_TCFE7: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE MOBILITY DATA
TDB_TCFE7: @@
TDB_TCFE7: app mobfe2
 Current database: Steels/Fe-Alloys Mobility  v2.0
   TCS Steel Mobility Database Version 2.0 from 2011-12-09.

 VA  DEFINED
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 ....

 List of references for assessed data

  'This parameter has not been assessed'
  'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'
  'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
      -Ni'
```

```
  'D. Bergner et al., Defect and Diffusion Forum 66-69(1989)409. Impurity
      diffusion of Si in fcc Fe.'
 -OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR
APP: @@
APP: go d-m
 NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@  ENTER GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 1323; * N

DIC>
DIC> @@
DIC> @@ ENTER THE REGION austenite
DIC> @@
DIC> enter-region
REGION NAME : austenite
DIC>
DIC> @@
DIC> @@ ENTER THE GRID
DIC> @@ NOTE THAT GRID POINT DISTANCES ARE SMALLEST AROUND THE MIDDLE
DIC> @@
DIC> enter-grid
REGION NAME : /AUSTENITE/: austenite
WIDTH OF REGION /1/: 50E-3
TYPE /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>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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
 double geometric
 coarse at outer boundaries dense at  0.25047E-01
lower part  0.80000       22
upper part   1.2500       22
 U-FRACTION IN SYSTEM:  C = .0215351122808224  FE = .96291921367461
                        SI = .0370807863253901
 TOTAL SIZE OF SYSTEM:  .05 [m]
 U-FRACTION IN SYSTEM:  C = .0215351122808224  FE = .96291921367461
                        SI = .0370807863253901
 TOTAL SIZE OF SYSTEM:  .05 [m]
 TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351122808224  FE = .96291921367461
                        SI = .0370807863253901
 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 = .0215351122808224  FE = .96291921367461
                        SI = .0370807863253901
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.40010010     DT =  0.40000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351122808224  FE = .96291921367461
                        SI = .0370807863253901
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    0 seconds
 TIME =   21.165600     DT =   20.765500     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351122808224  FE = .96291921367461
                        SI = .0370807863253901
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    0 seconds
 TIME =   62.696601     DT =   41.531000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351122808224  FE = .96291921367461
                        SI = .0370807863253901
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    0 seconds
 TIME =   145.75860     DT =   83.062001     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351122808224  FE = .96291921367461
                        SI = .0370807863253901
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    0 seconds
 TIME =   311.88260     DT =   166.12400     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351122808223  FE = .96291921367461
                        SI = .0370807863253901
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    0 seconds
 TIME =   644.13060     DT =   332.24800     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351122808223  FE = .96291921367461
                        SI = .0370807863253901
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    0 seconds
 TIME =   1308.6266     DT =   664.49600     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351122808225  FE = .96291921367461
                        SI = .0370807863253901
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    0 seconds
 TIME =   2637.6186     DT =   1328.9920     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .021535112280823  FE = .96291921367461
                        SI = .0370807863253901
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    1 seconds
 TIME =   5295.6026     DT =   2657.9840     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351122808237  FE = .96291921367461
                        SI = .0370807863253901
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    0 seconds
 TIME =   10611.571     DT =   5315.9680     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351122808241  FE = .96291921367461
                        SI = .0370807863253901
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    0 seconds
 TIME =   21243.507     DT =   10631.936     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351122808231  FE = .96291921367461
                        SI = .0370807863253901
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    0 seconds
 TIME =   42507.379     DT =   21263.872     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .021535112280823  FE = .96291921367461
                        SI = .03708078632539
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    0 seconds
 TIME =   85035.123     DT =   42527.744     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351122808147  FE = .96291921367461
                        SI = .03708078632539
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    0 seconds
 TIME =   170090.61     DT =   85055.489     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351122808122  FE = .96291921367461
                        SI = .03708078632539
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    0 seconds
 TIME =   340201.59     DT =   170110.98     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351122808354  FE = .96291921367461
                        SI = .03708078632539
 TOTAL SIZE OF SYSTEM:  .05 [m]
```

```
 CPU time used in timestep                    0 seconds
TIME =   680423.54     DT =   340221.95     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .021535112280 95  FE = .96291921367461
                       SI = .03708078632539
TOTAL SIZE OF SYSTEM:  .05 [m]
 CPU time used in timestep                    0 seconds
TIME =   1360867.5     DT =   680443.91     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0215351122812752  FE = .96291921367461
                       SI = .03708078632539
TOTAL SIZE OF SYSTEM:  .05 [m]
 CPU time used in timestep                    1 seconds
TIME =   2721755.3     DT =   1360887.8     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0215351122812751  FE = .96291921367461
                       SI = .03708078632539
TOTAL SIZE OF SYSTEM:  .05 [m]
 CPU time used in timestep                    0 seconds
TIME =   5443530.9     DT =   2721775.6     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0215351122811045  FE = .96291921367461
                       SI = .03708078632539
TOTAL SIZE OF SYSTEM:  .05 [m]
 CPU time used in timestep                    0 seconds
TIME =   10887082.     DT =   5443551.3     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0215351122807841  FE = .96291921367461
                       SI = .03708078632539
TOTAL SIZE OF SYSTEM:  .05 [m]
 CPU time used in timestep                    0 seconds
TIME =   21774185.     DT =   10887103.     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0215351122805241  FE = .96291921367461
                       SI = .03708078632539
TOTAL SIZE OF SYSTEM:  .05 [m]
 CPU time used in timestep                    0 seconds
TIME =   43548390.     DT =   21774205.     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0215351122804155  FE = .96291921367461
                       SI = .03708078632539
TOTAL SIZE OF SYSTEM:  .05 [m]
 CPU time used in timestep                    0 seconds
TIME =   87096800.     DT =   43548410.     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0215351122803582  FE = .96291921367461
                       SI = .03708078632539
TOTAL SIZE OF SYSTEM:  .05 [m]
 CPU time used in timestep                    0 seconds
TIME =  0.17419362E+09 DT =   87096820.     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0215351122803557  FE = .96291921367461
                       SI = .03708078632539
TOTAL SIZE OF SYSTEM:  .05 [m]
 CPU time used in timestep                    0 seconds
TIME =  0.34838726E+09 DT =  0.17419364E+09 SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0215351122804245  FE = .96291921367461
                       SI = .03708078632539
TOTAL SIZE OF SYSTEM:  .05 [m]
 CPU time used in timestep                    1 seconds
TIME =  0.69677454E+09 DT =  0.34838728E+09 SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0215351122805529  FE = .96291921367461
                       SI = .03708078632539
TOTAL SIZE OF SYSTEM:  .05 [m]
 CPU time used in timestep                    0 seconds
TIME =  0.13935491E+10 DT =  0.69677456E+09 SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0215351122807361  FE = .96291921367461
                       SI = .0370807863253899
TOTAL SIZE OF SYSTEM:  .05 [m]
 CPU time used in timestep                    0 seconds
TIME =  0.23935491E+10 DT =  0.10000000E+10 SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .021535112280747  FE = .96291921367461
                       SI = .03708078632539
TOTAL SIZE OF SYSTEM:  .05 [m]
 CPU time used in timestep                    0 seconds
TIME =  0.33935491E+10 DT =  0.10000000E+10 SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0215351122809185  FE = .96291921367461
                       SI = .03708078632539
TOTAL SIZE OF SYSTEM:  .05 [m]
 CPU time used in timestep                    0 seconds
TIME =  0.43935491E+10 DT =  0.10000000E+10 SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0215351122812697  FE = .96291921367461
                       SI = .03708078632539
TOTAL SIZE OF SYSTEM:  .05 [m]
 CPU time used in timestep                    0 seconds
TIME =  0.53935491E+10 DT =  0.10000000E+10 SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0215351122817882  FE = .96291921367461
                       SI = .0370807863253899
TOTAL SIZE OF SYSTEM:  .05 [m]
 CPU time used in timestep                    0 seconds
TIME =  0.63935491E+10 DT =  0.10000000E+10 SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0215351122822708  FE = .96291921367461
                       SI = .03708078632539
TOTAL SIZE OF SYSTEM:  .05 [m]
 CPU time used in timestep                    0 seconds
TIME =  0.73935491E+10 DT =  0.10000000E+10 SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0215351122827224  FE = .96291921367461
                       SI = .03708078632539
TOTAL SIZE OF SYSTEM:  .05 [m]
 CPU time used in timestep                    1 seconds
TIME =  0.83935491E+10 DT =  0.10000000E+10 SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0215351122831034  FE = .96291921367461
                       SI = .03708078632539
TOTAL SIZE OF SYSTEM:  .05 [m]
 CPU time used in timestep                    0 seconds
TIME =  0.93935491E+10 DT =  0.10000000E+10 SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0215351122832345  FE = .96291921367461
                       SI = .03708078632539
TOTAL SIZE OF SYSTEM:  .05 [m]
 CPU time used in timestep                    0 seconds
TIME =  0.10000000E+11 DT =  0.60645090E+09 SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0215351122834003  FE = .96291921367461
                       SI = .03708078632539
TOTAL SIZE OF SYSTEM:  .05 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME    0.0000000
DELETING TIME-RECORD FOR TIME   0.10000000E-06
DELETING TIME-RECORD FOR TIME   0.10010000E-03
DELETING TIME-RECORD FOR TIME   0.40010010
DELETING TIME-RECORD FOR TIME    21.165600
DELETING TIME-RECORD FOR TIME    62.696601
DELETING TIME-RECORD FOR TIME    145.75860
DELETING TIME-RECORD FOR TIME    311.88260
```

```
 DELETING TIME-RECORD FOR TIME    644.13060
 DELETING TIME-RECORD FOR TIME    1308.6266
 DELETING TIME-RECORD FOR TIME    2637.6186
 DELETING TIME-RECORD FOR TIME    5295.6026
 DELETING TIME-RECORD FOR TIME    10611.571
 DELETING TIME-RECORD FOR TIME    21243.507
 DELETING TIME-RECORD FOR TIME    42507.379
 DELETING TIME-RECORD FOR TIME    85035.123
 DELETING TIME-RECORD FOR TIME    170090.61
 DELETING TIME-RECORD FOR TIME    340201.59
 DELETING TIME-RECORD FOR TIME    680423.54
 DELETING TIME-RECORD FOR TIME    1360867.5
 DELETING TIME-RECORD FOR TIME    2721755.3
 DELETING TIME-RECORD FOR TIME    5443530.9
 DELETING TIME-RECORD FOR TIME    10887082.
 DELETING TIME-RECORD FOR TIME    21774185.
 DELETING TIME-RECORD FOR TIME    43548390.
 DELETING TIME-RECORD FOR TIME    87096800.
 DELETING TIME-RECORD FOR TIME   0.17419362E+09
 DELETING TIME-RECORD FOR TIME   0.34838726E+09
 DELETING TIME-RECORD FOR TIME   0.69677454E+09
 DELETING TIME-RECORD FOR TIME   0.13935491E+10
 DELETING TIME-RECORD FOR TIME   0.23935491E+10
 DELETING TIME-RECORD FOR TIME   0.33935491E+10
 DELETING TIME-RECORD FOR TIME   0.43935491E+10
 DELETING TIME-RECORD FOR TIME   0.53935491E+10
 DELETING TIME-RECORD FOR TIME   0.63935491E+10
 DELETING TIME-RECORD FOR TIME   0.73935491E+10
 DELETING TIME-RECORD FOR TIME   0.83935491E+10

 KEEPING TIME-RECORD FOR TIME   0.93935491E+10
 AND FOR TIME                   0.10000000E+11
 WORKSPACE RECLAIMED

 TIMESTEP AT    0.100000000E+11 SELECTED

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

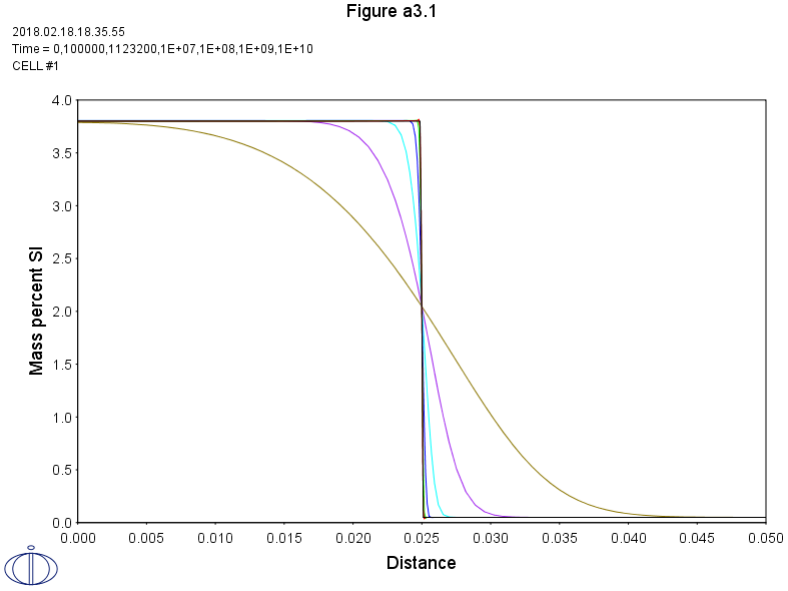
exa3-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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: plot
```

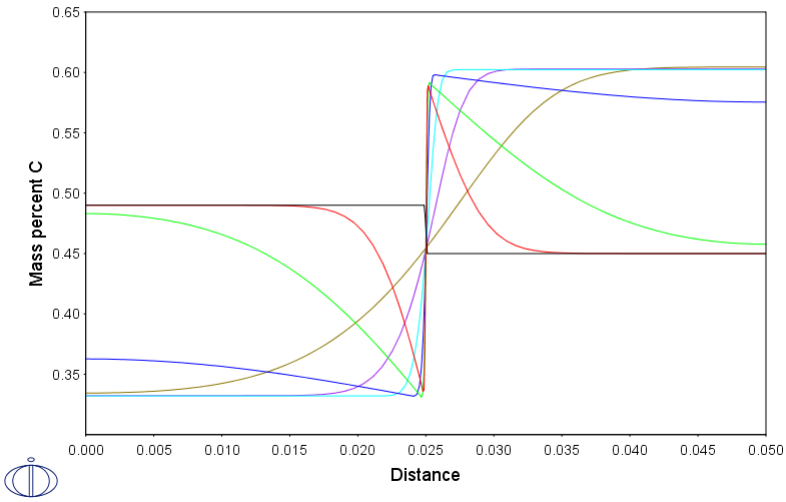
Figure a3.1




```
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: plot
```

Figure a3.2

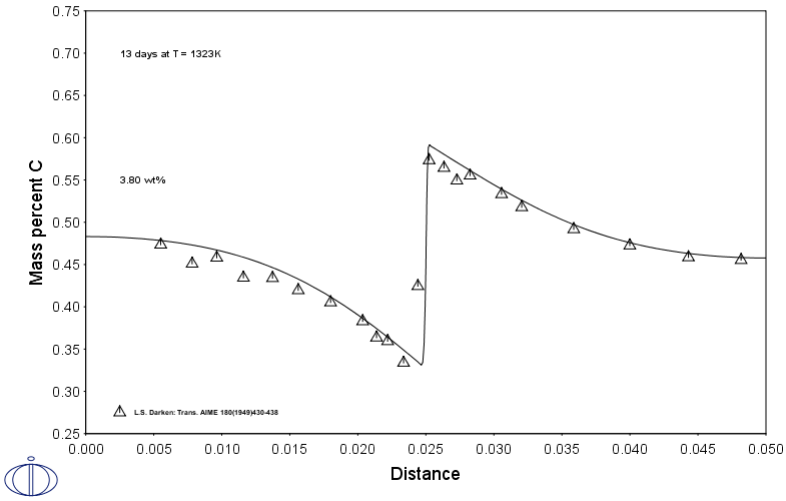
2018.02.18.18.35.55
Time = 0,100000,1123200,1E+07,1E+08,1E+09,1E+10
CELL #1



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: plot

Figure a3.3

2018.02.18.18.35.56
Time = 1123200
CELL #1

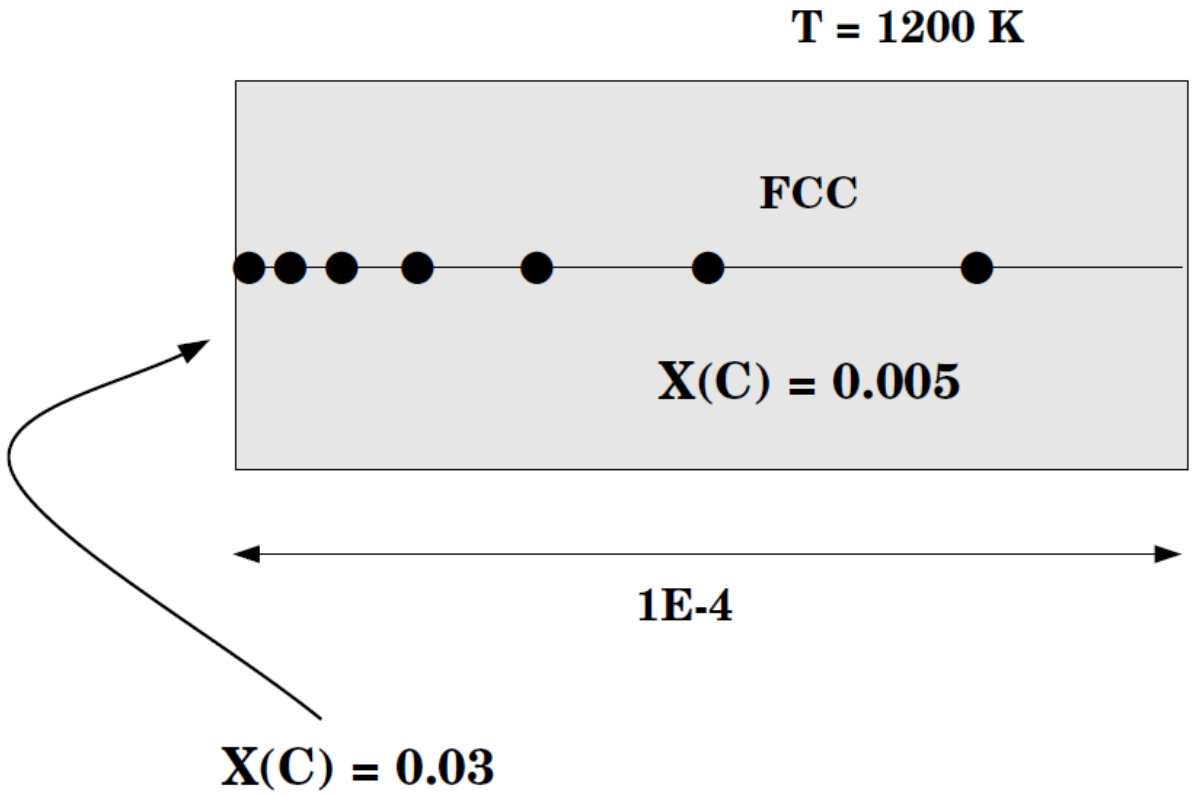


POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1: set-inter
 --OK---
POST-1:

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

```
About Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 12987) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri Feb 16 15:22:08 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa4\setup.DCM" @@
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
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

 VA                     /-  DEFINED
 L12_FCC                B2_BCC                 DICTRA_FCC_A1
   REJECTED
TDB_TCFE9: sw FEDEMO
 Current database: Iron Demo Database v2.0

 VA                     /-  DEFINED
TDB_FEDEMO: def-system fe,c
 FE                     C  DEFINED
TDB_FEDEMO: rej-ph *
 GAS:G                  LIQUID:L               BCC_A2
 CEMENTITE              DIAMOND_FCC_A4         FCC_A1
 GRAPHITE               HCP_A3                 KSI_CARBIDE
 LAVES_PHASE_C14        M23C6                  M5C2
 M7C3  REJECTED
TDB_FEDEMO: rest-ph fcc
 FCC_A1  RESTORED
TDB_FEDEMO: get
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'X.-G. Lu, M. Selleby, B. Sundman, CALPHAD, 29 (2005) 49-55; Fe P-T diagram'
  'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
 -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
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
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....
 -OK-
TDB_APP:
TDB_APP: @@
TDB_APP: @@ GO TO THE DICTRA MODULE AND SET UP THE SYSTEM
TDB_APP: @@
TDB_APP: go d-m
 NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@  ENTER GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 1200; * N

DIC>
DIC> @@
DIC> @@ ENTER THE REGION steel
DIC> @@
DIC> enter-region
REGION NAME : steel
DIC>
DIC> @@
DIC> @@ ENTER THE GRID
DIC> @@ CARBON ENTERS THE SYSTEM FROM THE LOWER BOUNDARY AND CONSEQUENTLY
DIC> @@ MORE POINTS ARE REQUIRED AT THAT BOUNDARY. THIS IS WHY A GEOMETRIC
DIC> @@ GRID IS USED.
DIC> @@
DIC> enter-grid
REGION NAME : /STEEL/: steel
```

```
WIDTH OF REGION /1/: 1E-4
TYPE /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
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>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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
 single geometric dense at   0.0000
  1.1388       96
 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 = .00502599895421297  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.26001020E-05 DT =  0.25001020E-05 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00502674234772398  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.76003060E-05 DT =  0.50002040E-05 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00502762855271361  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.17600714E-04 DT =  0.10000408E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00502880490898696  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.37601530E-04 DT =  0.20000816E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00503042289514107  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.77603162E-04 DT =  0.40001632E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00503268130112881  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.15760643E-03 DT =  0.80003264E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00503585491527872  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.31761295E-03 DT =  0.16000653E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00504032903043467  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.63762601E-03 DT =  0.32001306E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00504664654067874  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.12776521E-02 DT =  0.64002611E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00505557392100181  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.25577043E-02 DT =  0.12800522E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00506819425567398  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.51178088E-02 DT =  0.25601044E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00508603865206295  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.10238018E-01 DT =  0.51202089E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00511127199989312  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.20478435E-01 DT =  0.10240418E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0051469556180961  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.40959271E-01 DT =  0.20480836E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00519741865567009  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.81920942E-01 DT =  0.40961671E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00526878330573381  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.16384428     DT =  0.81923342E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00536970755217346  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.32769097     DT =  0.16384668     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00551243555924854  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.65538434     DT =  0.32769337     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00571428313781583  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   1.3107711     DT =  0.65538674     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00599973850521004  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   2.6215446     DT =   1.3107735     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00640343298842195  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   5.2430915     DT =   2.6215470     SUM OF SQUARES =   0.0000000
```

```
 U-FRACTION IN SYSTEM:  C = .00697433052866846  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   10.486185     DT =   5.2430939     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00778159421638381  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   20.486185     DT =   10.000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00887736257293559  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   30.486185     DT =   10.000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00972196664325365  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   40.486185     DT =   10.000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0104363519865359  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   50.486185     DT =   10.000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0110669328932657  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   60.486185     DT =   10.000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0116377078880251  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   70.486185     DT =   10.000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0121630223717782  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   80.486185     DT =   10.000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0126522650845277  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   90.486185     DT =   10.000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0131119785059757  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   100.00000     DT =   9.5138146     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .013526298212787  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   0.26001020E-05
 DELETING TIME-RECORD FOR TIME   0.76003060E-05
 DELETING TIME-RECORD FOR TIME   0.17600714E-04
 DELETING TIME-RECORD FOR TIME   0.37601530E-04
 DELETING TIME-RECORD FOR TIME   0.77603162E-04
 DELETING TIME-RECORD FOR TIME   0.15760643E-03
 DELETING TIME-RECORD FOR TIME   0.31761295E-03
 DELETING TIME-RECORD FOR TIME   0.63762601E-03
 DELETING TIME-RECORD FOR TIME   0.12776521E-02
 DELETING TIME-RECORD FOR TIME   0.25577043E-02
 DELETING TIME-RECORD FOR TIME   0.51178088E-02
 DELETING TIME-RECORD FOR TIME   0.10238018E-01
 DELETING TIME-RECORD FOR TIME   0.20478435E-01
 DELETING TIME-RECORD FOR TIME   0.40959271E-01
 DELETING TIME-RECORD FOR TIME   0.81920942E-01
 DELETING TIME-RECORD FOR TIME   0.16384428
 DELETING TIME-RECORD FOR TIME   0.32769097
 DELETING TIME-RECORD FOR TIME   0.65538434
 DELETING TIME-RECORD FOR TIME    1.3107711
 DELETING TIME-RECORD FOR TIME    2.6215446
 DELETING TIME-RECORD FOR TIME    5.2430915
 DELETING TIME-RECORD FOR TIME    10.486185
 DELETING TIME-RECORD FOR TIME    20.486185
 DELETING TIME-RECORD FOR TIME    30.486185
 DELETING TIME-RECORD FOR TIME    40.486185
 DELETING TIME-RECORD FOR TIME    50.486185
 DELETING TIME-RECORD FOR TIME    60.486185
 DELETING TIME-RECORD FOR TIME    70.486185
 DELETING TIME-RECORD FOR TIME    80.486185

 KEEPING TIME-RECORD FOR TIME    90.486185
 AND FOR TIME                    100.00000
 WORKSPACE RECLAIMED

 TIMESTEP AT     100.000000     SELECTED

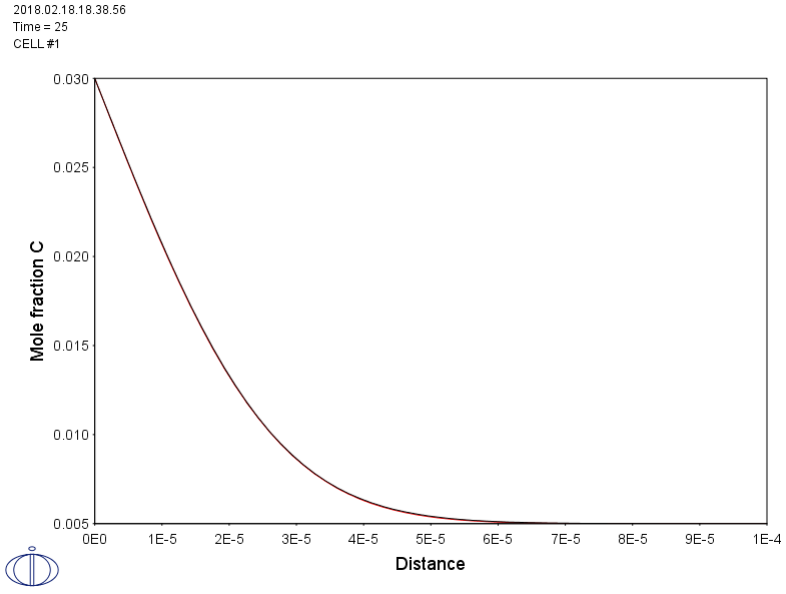
DIC>
DIC> @@
DIC> @@ THE SIMULATION IS FINISHED
DIC> @@
DIC>
DIC> set-inter
 --OK---
DIC>
```

exa4-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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

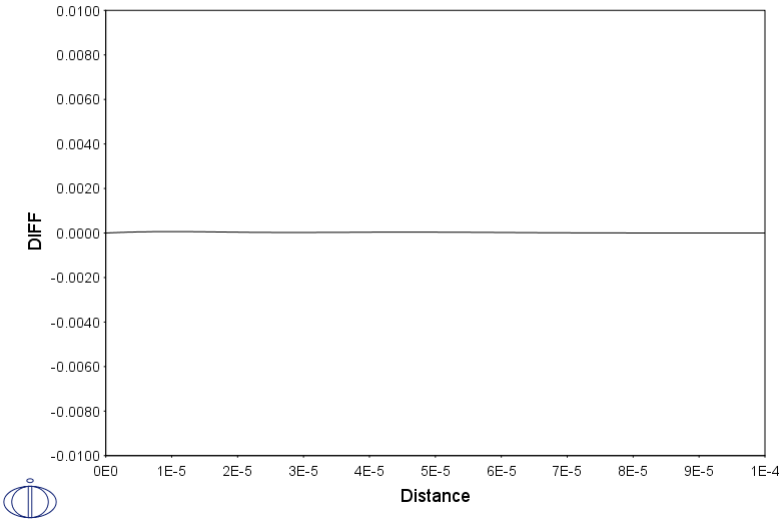
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson

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: 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: plot
```

2018.02.18.18.38.56
Time = 25
CELL #1

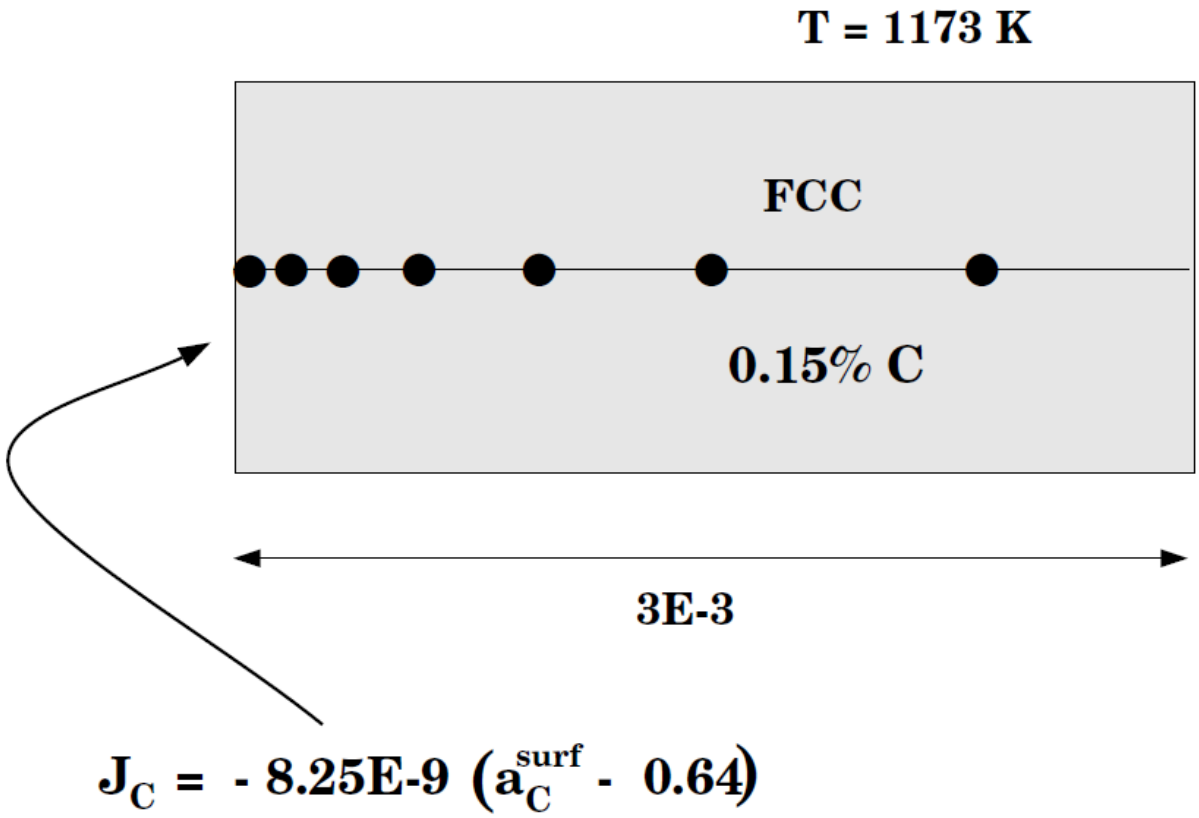


POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: set-interactive
--OK---
POST-1:

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

About Linked: Fri Feb 16 15:22:08 2018

```
SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa5\setup.DCM"SYS: ?@@
 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
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

 VA                        /-  DEFINED
 L12_FCC                   B2_BCC                    DICTRA_FCC_A1
   REJECTED
TDB_TCFE9: sw FEDEMO
 Current database: Iron Demo Database v2.0

 VA                        /-  DEFINED
TDB_FEDEMO: def-sys fe,c
 FE                        C  DEFINED
TDB_FEDEMO: rej-ph *
 GAS:G                     LIQUID:L                  BCC_A2
 CEMENTITE                 DIAMOND_FCC_A4            FCC_A1
 GRAPHITE                  HCP_A3                    KSI_CARBIDE
 LAVES_PHASE_C14           M23C6                     M5C2
 M7C3  REJECTED
TDB_FEDEMO: rest-ph fcc graphite
 FCC_A1                    GRAPHITE  RESTORED
TDB_FEDEMO: get
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'X.-G. Lu, M. Selleby, B. Sundman, CALPHAD, 29 (2005) 49-55; Fe P-T diagram'
  'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
  'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121 -127; Molar
      volumes'
 -OK-
TDB_FEDEMO:@?
TDB_FEDEMO: append
 Use one of these databases

 TCFE9   =  Steels/Fe-Alloys  v9.0
 TCFE10  =  Steels/Fe-Alloys  v10.0 SNAPSHOT
 TCFE8   =  Steels/Fe-Alloys  v8.1
 FROST1  =  FROST database v1.0
 TCFE7   =  Steels/Fe-Alloys  v7.0
 TCFE6   =  Steels/Fe-Alloys  v6.2
 TCFE5   =  Steels/Fe-Alloys  v5.0
 TCFE4   =  Steels/Fe-Alloys  v4.1
 TCFE3   =  Steels/Fe-Alloys  v3.1
 TCFE2   =  Steels/Fe-Alloys  v2.1
 TCFE1   =  Steels/Fe-Alloys  v1.0
 TCNI9   =  Ni-Alloys  v9.0 SNAPSHOT
 NI25    =  NI25 database
 TCNI8   =  Ni-Alloys  v8.1
 TCNI7   =  Ni-Alloys  v7.1
 TCNI6   =  Ni-Alloys  v6.0
 TCNI5   =  Ni-Alloys  v5.1
 TCNI4   =  Ni-Alloys  v4.0
 TCNI1   =  Ni-Alloys  v1.3
 TCAL5   =  Al-Alloys  v5.0
 TCAL4   =  Al-Alloys  v4.0
 TCAL3   =  Al-Alloys  v3.0
 TCAL2   =  Al-Alloys  v2.1
 TCAL1   =  Al-Alloys  v1.2
 TCMG4   =  Mg-Alloys  v4.0
 TCMG3   =  Mg-Alloys  v3.0
 TCMG2   =  Mg-Alloys  v2.0
 TCMG1   =  Mg-Alloys  v1.1
 TCTI1   =  Ti-Alloys  v1.0
 TCCU2   =  Cu-Alloys  v2.0
 TCCU1   =  Cu-Alloys  v1.0
 TCCC1   =  Cemented carbide  v1.0
 TCHEA2  =  High Entropy Alloy  v2.1
 TCHEA1  =  High Entropy Alloy  v1.0
 SSOL6   =  SGTE Alloy Solutions Database v6.0
 SSOL5   =  SGTE Alloy Solutions Database v5.0
 SSOL4   =  SGTE Alloy Solutions Database v4.9g
 SSOL2   =  SGTE Alloy Solutions Database v2.1
 SSUB6   =  SGTE Substances Database v6.0
 SSUB5   =  SGTE Substances Database v5.2
 SSUB4   =  SGTE Substances Database v4.1
 SSUB3   =  SGTE Substances Database v3.3
 SSUB2   =  SGTE Substances Database v2.2
 SNOB3   =  SGTE Noble Metal Alloys Database v3.1
 STBC2   =  SGTE Thermal Barrier Coating TDB v2.2
 STBC1   =  SGTE Thermal Barrier Coating TDB v1.1
 SALT1   =  SGTE Molten Salts Database v1.2
 SEMC2   =  TC Semi-Conductors  v2.1
```

```
 SLAG4   =  Fe-containing Slag  v4.1
 SLAG3   =  Fe-containing Slag  v3.2
 SLAG2   =  Fe-containing Slag  v2.2
 SLAG1   =  Fe-containing Slag  v1.2
 TCOX7   =  Metal Oxide Solutions  v7.0
 TCOX6   =  Metal Oxide Solutions  v6.0
 TCOX5   =  Metal Oxide Solutions  v5.1
 TCOX4   =  Metal Oxide Solutions  v4.1
 ION3    =  Ionic Solutions  v3.0
 ION2    =  Ionic Solutions  v2.6
 ION1    =  Ionic Solutions  v1.5
 NOX2    =  NPL Oxide Solutions Database v2.1
 TCNOBL1 =  Noble Metals Alloys v1.0
 TCSLD3  =  Solder Alloys  v3.2
 TCSLD2  =  Solder Alloys  v2.0
 TCSI1   =  Ultrapure Silicon  v1.2
 TCMP2   =  Materials Processing  v2.5
 TCES1   =  Combustion/Sintering  v1.1
 TCSC1   =  Super Conductor  v1.0
 TCFC1   =  SOFC Database v1.0
 NUMT2   =  Nuclear Materials  v2.1
 NUOX4   =  Nuclear Oxides  v4.2
 NUCL15  =  IRSN NUCLEA-15_4
 NUCL10  =  ThermoData NUCLEA Alloys-oxides TDB v10.2
 MEPH15  =  IRSN Mephista-15_1
 MEPH11  =  ThermoData MEPHISTA Nuclear Fuels TDB v11.2
 TCAQ3   =  Aqueous Solution  v3.0
 TCAQ2   =  Aqueous Solution  v2.6
 AQS2    =  TGG Aqueous Solution Database v2.6
 GCE2    =  TGG Geochemical/Environmental TDB v2.3
 FEDEMO  =  Iron Demo Database v2.0
 ALDEMO  =  Aluminum Demo Database v2.0
 NIDEMO  =  Nickel Demo Database v1.0
 CUDEMO  =  Copper Demo Database v1.0
 SLDEMO  =  Solder Demo Database v1.0
 OXDEMO  =  Oxide Demo Database v1.0
 SUBDEMO =  Substance Demo Database v1.0
 PTERN   =  Public Ternary Alloys TDB v1.3
 PAQ2    =  Public Aqueous Soln (SIT) TDB v2.4
 PG35    =  G35 Binary Semi-Conductors TDB v1.2
 PURE5   =  SGTE Unary (Pure Elements) TDB v5.1
 MOB2    =  Alloys Mobility  v2.7
 MOB1    =  Alloys Mobility  v1.3
 MOBFE1  =  Steels/Fe-Alloys Mobility  v1.0
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBNI4  =  Ni-Alloys Mobility  v4.0
 MOBNI3  =  Ni-Alloys Mobility  v3.1
 MOBNI2  =  Ni-Alloys Mobility  v2.4
 MOBNI1  =  Ni-Alloys Mobility  v1.0
 MOBAL3  =  Al-Alloys Mobility  v3.0
 MOBAL2  =  Al-Alloys Mobility  v2.0
 MOBAL1  =  Al-Alloys Mobility  v1.0
 MOBCU1  =  Cu-Alloys Mobility  v1.0
 MOBCU2  =  Cu-Alloys Mobility  v2.0
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBSLD1 =  Solder-Alloys Mobility  v1.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0 SNAPSHOT
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v1.0
 MFEDEMO =  Fe-Alloys Mobility demo database v2.0
 MNIDEMO =  Ni-Alloys Mobility demo database v1.0
 MCUDEMO =  Cu-Alloys Mobility demo database v1.0
 USER    =  User defined Database

DATABASE NAME /FEDEMO/: mfedemo
 Current database: Fe-Alloys Mobility demo database v2.0

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

 List of references for assessed data

  'This parameter has not been assessed'
  'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'
  'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
      -Ni'
 -OK-
APP:@?
APP: @@
APP: @@ GO TO THE DICTRA MONITOR TO SET UP THE INITIAL STATE OF THE SPECIMEN
APP: @@
APP: go d-m
 NO TIME STEP DEFINED
 *** ENTERING GRAPHITE 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 Ågren (J. Heat Treating, v6, no 1, 1988 pp. 9-19)
DIC> @@ we calculate the mass-transfer coefficient for carbon, f in
DIC> @@ eq. 1 above by means of eq. 3, 4 and 12 in Sproge and Ågren's paper.
DIC> @@
DIC> @@
DIC> @@          A *  K *  P  *  sqrt( P   )
DIC> @@               I    CO          H
DIC> @@                                2
DIC> @@   f  =  ----------------------------  / gamma        (2)
DIC> @@          a  +  B * K * P  * sqrt( P  )
DIC> @@           C         I   CO         H
DIC> @@                                   2
DIC> @@
DIC> @@ K  is the equilibrium constant for reaction (I)
DIC> @@  I
DIC> @@
DIC> @@ A and B are constants defined in Sproge and Ågren's paper. gamma
DIC> @@ is the activity coefficient for carbon in the steel.
DIC> @@
DIC> @@ Assume a constant value for  P  *  sqrt( P   ) = 0.14
DIC> @@                                            CO          H
DIC> @@                                                         2
DIC> @@ The carbon activity in the gas is controlled by the partial
DIC> @@ pressure of water as can be understood from reaction (I).
DIC> @@
DIC> @@ Assume that the carbon activity, a of the gas is 0.64
DIC> @@                                                  C
DIC> @@ which corresponds to a carburizing "carbon potential" of 0.85 wt%.
DIC> @@
DIC> @@ In this way we may calculate f to 8.25E-9 mol/s.
DIC> @@
DIC>
DIC> set-cond

GLOBAL OR BOUNDARY CONDITION /GLOBAL/: bound
BOUNDARY /LOWER/: lower
CONDITION TYPE /CLOSED_SYSTEM/: activity_flux_function
 ENTER THE EXPRESSION AS:
                                  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>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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
 single geometric dense at   0.0000
  1.2176      101
 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                    0 seconds
 TIME =  0.24659766E-05 DT =  0.23659766E-05 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698495916758908  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.71979297E-05 DT =  0.47319532E-05 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698495917479989  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.16661836E-04 DT =  0.94639063E-05 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698495918922068  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.35589649E-04 DT =  0.18927813E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698495921806013  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.73445274E-04 DT =  0.37855625E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698495927573319  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.14915652E-03 DT =  0.75711250E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698495939106306  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.30057903E-03 DT =  0.15142250E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698495962167 72  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.60342403E-03 DT =  0.30284500E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698496008277711  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.12091140E-02 DT =  0.60569000E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698496100461467  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.24204940E-02 DT =  0.12113800E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698496284726693  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.48432541E-02 DT =  0.24227600E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698496652968263  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.96887741E-02 DT =  0.48455200E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698497388635673  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.19379814E-01 DT =  0.96910401E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698498857668281  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.38761894E-01 DT =  0.19382080E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698501789240894  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.77526054E-01 DT =  0.38764160E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698507634097207  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.15505437     DT =  0.77528320E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698519272377669  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.31011102     DT =  0.15505664     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698542404641377  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.62022430     DT =  0.31011328     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698588265674896  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   1.2404509     DT =  0.62022656     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698678864751836  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1 seconds
 TIME =   2.4809040     DT =   1.2404531     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698856957978377  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
```

```
TIME =   4.9618102     DT =   2.4809063     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0069920463860113  FE = 1
TOTAL SIZE OF SYSTEM:  .003 [m]
 CPU time used in timestep                    0 seconds
TIME =   9.9236228     DT =   4.9618125     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00699876996632461  FE = 1
TOTAL SIZE OF SYSTEM:  .003 [m]
 CPU time used in timestep                    0 seconds
TIME =   19.847248     DT =   9.9236250     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0070116060159071  FE = 1
TOTAL SIZE OF SYSTEM:  .003 [m]
 CPU time used in timestep                    0 seconds
TIME =   39.694498     DT =   19.847250     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00703569376361486  FE = 1
TOTAL SIZE OF SYSTEM:  .003 [m]
 CPU time used in timestep                    0 seconds
TIME =   79.388998     DT =   39.694500     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00707989462116314  FE = 1
TOTAL SIZE OF SYSTEM:  .003 [m]
 CPU time used in timestep                    0 seconds
TIME =   158.77800     DT =   79.389000     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00715874757109928  FE = 1
TOTAL SIZE OF SYSTEM:  .003 [m]
 CPU time used in timestep                    0 seconds
TIME =   317.55600     DT =   158.77800     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00729474138750415  FE = 1
TOTAL SIZE OF SYSTEM:  .003 [m]
 CPU time used in timestep                    0 seconds
TIME =   635.11200     DT =   317.55600     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00752054375503615  FE = 1
TOTAL SIZE OF SYSTEM:  .003 [m]
 CPU time used in timestep                    0 seconds
TIME =   1270.2240     DT =   635.11200     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00788106518443645  FE = 1
TOTAL SIZE OF SYSTEM:  .003 [m]
 CPU time used in timestep                    0 seconds
TIME =   2540.4480     DT =   1270.2240     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00843611780537184  FE = 1
TOTAL SIZE OF SYSTEM:  .003 [m]
 CPU time used in timestep                    0 seconds
TIME =   4340.4480     DT =   1800.0000     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .009047102269993  FE = 1
TOTAL SIZE OF SYSTEM:  .003 [m]
 CPU time used in timestep                    0 seconds
TIME =   6140.4480     DT =   1800.0000     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00955134567260647  FE = 1
TOTAL SIZE OF SYSTEM:  .003 [m]
 CPU time used in timestep                    0 seconds
TIME =   7940.4480     DT =   1800.0000     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00999113675765163  FE = 1
TOTAL SIZE OF SYSTEM:  .003 [m]
 CPU time used in timestep                    1 seconds
TIME =   9740.4480     DT =   1800.0000     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0103863764716823  FE = 1
TOTAL SIZE OF SYSTEM:  .003 [m]
 CPU time used in timestep                    0 seconds
TIME =   11540.448     DT =   1800.0000     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0107484090267409  FE = 1
TOTAL SIZE OF SYSTEM:  .003 [m]
 CPU time used in timestep                    0 seconds
TIME =   13340.448     DT =   1800.0000     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0110844421240477  FE = 1
TOTAL SIZE OF SYSTEM:  .003 [m]
 CPU time used in timestep                    0 seconds
TIME =   15140.448     DT =   1800.0000     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0113993948509805  FE = 1
TOTAL SIZE OF SYSTEM:  .003 [m]
 CPU time used in timestep                    0 seconds
TIME =   16940.448     DT =   1800.0000     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0116968050295665  FE = 1
TOTAL SIZE OF SYSTEM:  .003 [m]
 CPU time used in timestep                    0 seconds
TIME =   18000.000     DT =   1059.5520     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0118647499013449  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   0.24659766E-05
DELETING TIME-RECORD FOR TIME   0.71979297E-05
DELETING TIME-RECORD FOR TIME   0.16661836E-04
DELETING TIME-RECORD FOR TIME   0.35589649E-04
DELETING TIME-RECORD FOR TIME   0.73445274E-04
DELETING TIME-RECORD FOR TIME   0.14915652E-03
DELETING TIME-RECORD FOR TIME   0.30057903E-03
DELETING TIME-RECORD FOR TIME   0.60342403E-03
DELETING TIME-RECORD FOR TIME   0.12091140E-02
DELETING TIME-RECORD FOR TIME   0.24204940E-02
DELETING TIME-RECORD FOR TIME   0.48432541E-02
DELETING TIME-RECORD FOR TIME   0.96887741E-02
DELETING TIME-RECORD FOR TIME   0.19379814E-01
DELETING TIME-RECORD FOR TIME   0.38761894E-01
DELETING TIME-RECORD FOR TIME   0.77526054E-01
DELETING TIME-RECORD FOR TIME   0.15505437
DELETING TIME-RECORD FOR TIME   0.31011102
DELETING TIME-RECORD FOR TIME   0.62022430
DELETING TIME-RECORD FOR TIME    1.2404509
DELETING TIME-RECORD FOR TIME    2.4809040
DELETING TIME-RECORD FOR TIME    4.9618102
DELETING TIME-RECORD FOR TIME    9.9236228
DELETING TIME-RECORD FOR TIME    19.847248
DELETING TIME-RECORD FOR TIME    39.694498
DELETING TIME-RECORD FOR TIME    79.388998
DELETING TIME-RECORD FOR TIME    158.77800
DELETING TIME-RECORD FOR TIME    317.55600
DELETING TIME-RECORD FOR TIME    635.11200
DELETING TIME-RECORD FOR TIME    1270.2240
DELETING TIME-RECORD FOR TIME    2540.4480
DELETING TIME-RECORD FOR TIME    4340.4480
DELETING TIME-RECORD FOR TIME    6140.4480
DELETING TIME-RECORD FOR TIME    7940.4480
DELETING TIME-RECORD FOR TIME    9740.4480
DELETING TIME-RECORD FOR TIME    11540.448
DELETING TIME-RECORD FOR TIME    13340.448
```

```
 DELETING TIME-RECORD FOR TIME    15140.448

 KEEPING TIME-RECORD FOR TIME    16940.448
 AND FOR TIME                    18000.000
 WORKSPACE RECLAIMED

 TIMESTEP AT     18000.0000     SELECTED

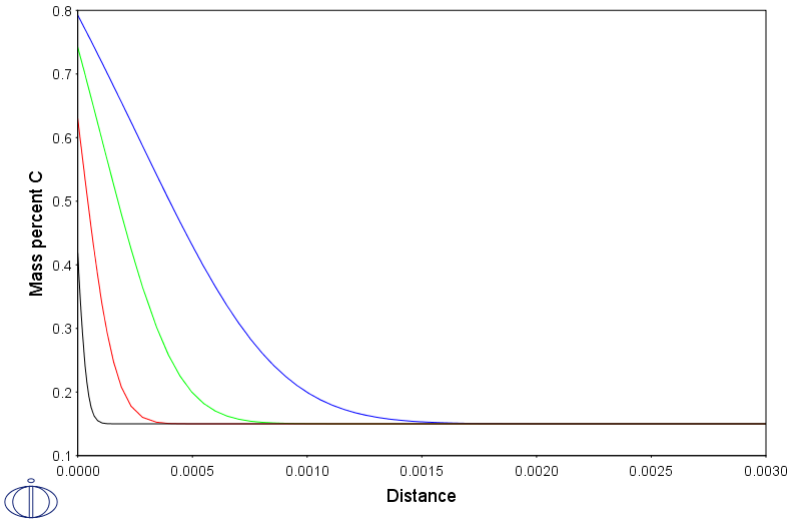
DIC>
DIC> set-inter
 --OK---
DIC>
```

exa5-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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

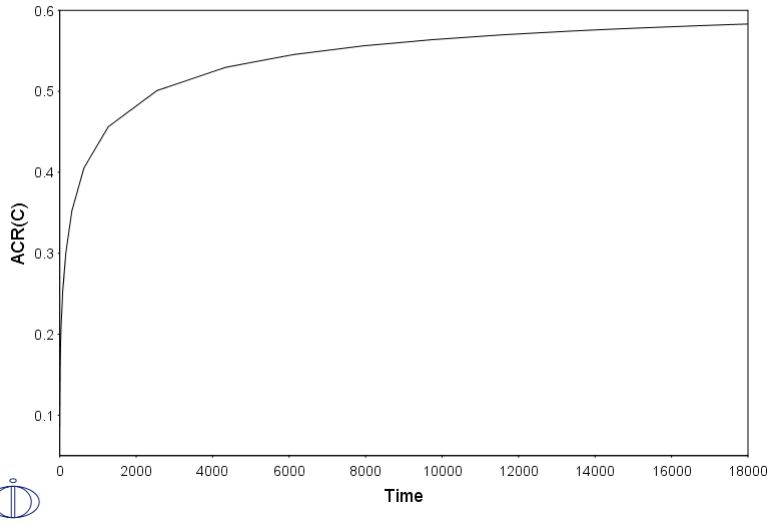
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson

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: plot
   2018.02.18.18.41.57
   Time = 100,1000,5000,18000
   CELL #1
```



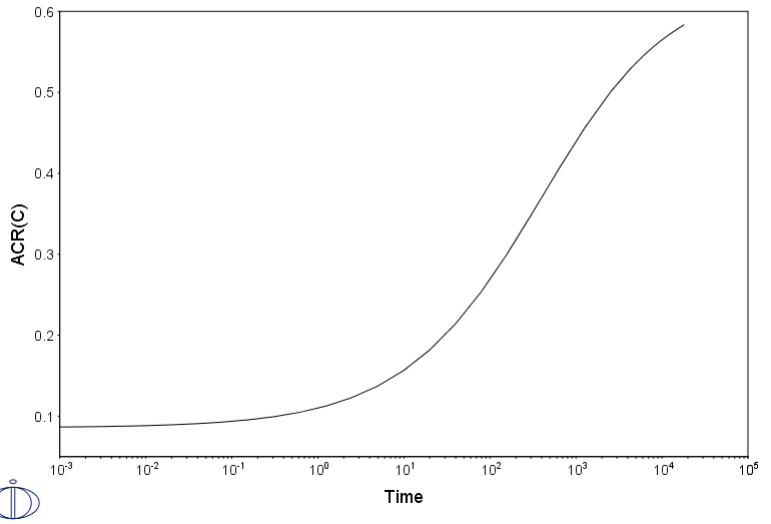

```
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: @@
POST-1: @@ PLOT THE VARIATION OF THE C ACTIVITY AT THE SURFACE
POST-1: @@
POST-1: s-d-a y acr(c)
POST-1:
POST-1: s-d-a x time
  INFO: Time is set as independent variable
POST-1:
POST-1: s-p-c
CONDITION /TIME/: interface
INTERFACE : first
POST-1:
POST-1: plot
```

2018.02.18.18.41.58
"FIRST" INTERFACE OF SYSTEM
CELL #1



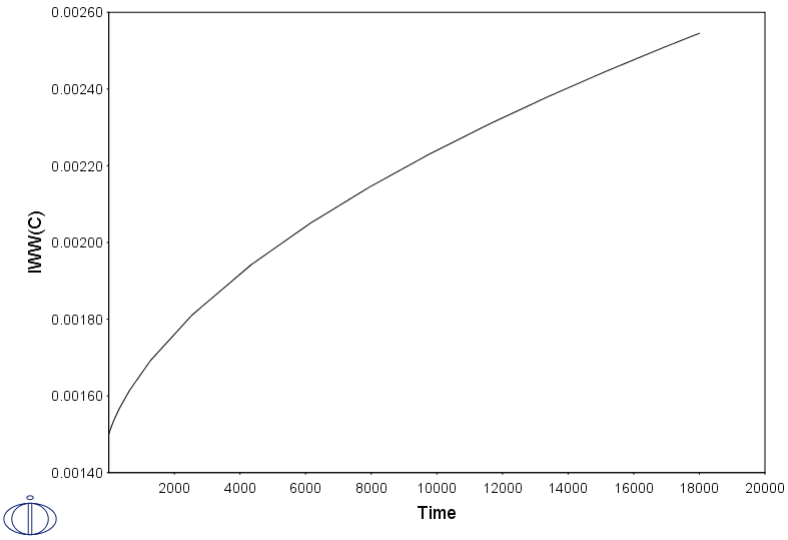
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: @@
POST-1: @@ USE A LOGARITHMIC SCALE ON THE X-AXIS
POST-1: @@
POST-1: set-axis-type
AXIS (X, Y OR Z) : x
AXIS TYPE /LINEAR/: logarithmic
POST-1:
POST-1: s-s-s x n 0.001 2e4
POST-1:
POST-1: plot

2018.02.18.18.41.58
"FIRST" INTERFACE OF SYSTEM
CELL #1



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: plot

2018.02.18.18.41.59
CELL #1

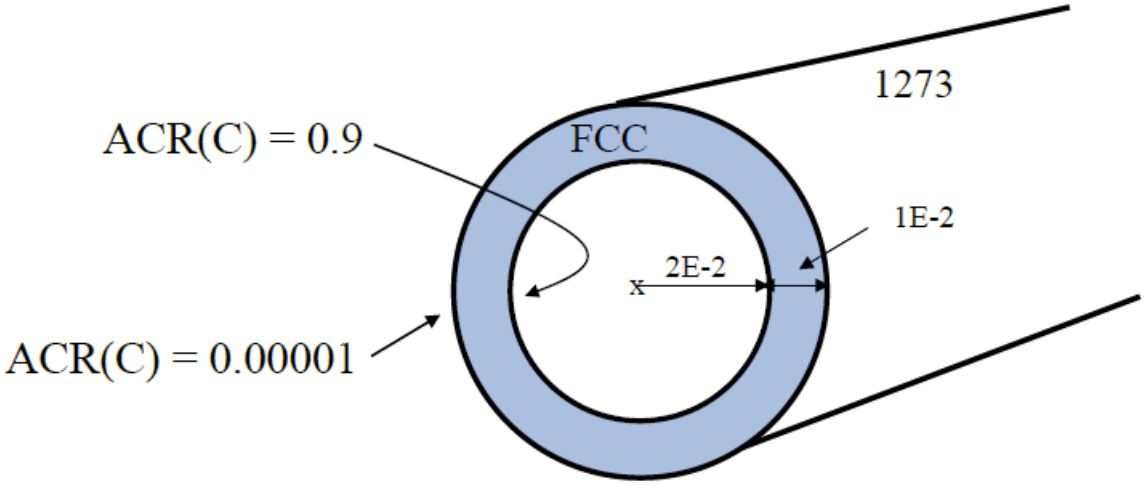


POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1:
POST-1: set-inter
--OK---
POST-1:

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

```
About Stockholm, Sweden

 Software  (build 12987) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri Feb 16 15:22:08 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

 VA                     /-  DEFINED
 L12_FCC                B2_BCC                 DICTRA_FCC_A1
   REJECTED
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ USE THE TCFE DATABASE FOR THERMODYNAMIC DATA
TDB_TCFE9: @@
TDB_TCFE9: sw tcfe7
 Current database: Steels/Fe-Alloys  v7.0

 VA  DEFINED
 L12_FCC                B2_BCC                 B2_VACANCY
 HIGH_SIGMA             DICTRA_FCC_A1  REJECTED
TDB_TCFE7: def-sys fe si mn c
 FE                     SI                     MN
 C  DEFINED
TDB_TCFE7: rej ph * all
 GAS:G                  LIQUID:L               BCC_A2
 FCC_A1                 HCP_A3                 DIAMOND_FCC_A4
 GRAPHITE               CEMENTITE              M23C6
 M7C3                   M5C2                   KSI_CARBIDE
 A1_KAPPA               KAPPA                  FE4N_LP1
 FECN_CHI               LAVES_PHASE_C14        M3SI
 G_PHASE                CR3SI                  FE2SI
 MSI                    M5SI3                  AL4C3
 FE8SI2C                SIC  REJECTED
TDB_TCFE7: res ph fcc,grap
 FCC_A1                 GRAPHITE  RESTORED
TDB_TCFE7: get
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'
  'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C
      -FE'
  'W. Huang, Metall. Trans. A, 21A (1990), 2115-2123; TRITA-MAC 411 (Rev
      1989); C-FE-MN'
  'J. Lacaze and B. Sundman, Metall. Mater. Trans. A, 22A (1991), 2211-2223;
      Fe-Si and Fe-Si-C'
  'W. Huang, Calphad, 13 (1989), 243-252; TRITA-MAC 388 (rev 1989); FE-MN'
  'J.E. Tibballs, SI Norway (1991) Rep. 890221-5; Mn-Si'
  'J. Miettinen and B. Hallstedt, Calphad, 22 (1998), 231-256; Fe-Si and Fe
      -Si-C'
  'A. Forsberg and J. Agren, J. Phase Equil., 14 (1993), 354-363; Fe-Mn-Si'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
      Molar volumes'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'B. Uhrenius (1993-1994), International journal of refractory metals and
      hard mater, Vol. 12, pp. 121-127; Molar volumes'
 -OK-
TDB_TCFE7:
TDB_TCFE7: @@
TDB_TCFE7: @@ SWITCH TO A MOBILITY DATABASE TO RETRIVE KINETIC DATA
TDB_TCFE7: @@
TDB_TCFE7: app
 Use one of these databases

 TCFE9   =  Steels/Fe-Alloys  v9.0
 TCFE10  =  Steels/Fe-Alloys  v10.0 SNAPSHOT
 TCFE8   =  Steels/Fe-Alloys  v8.1
 FROST1  =  FROST database v1.0
 TCFE7   =  Steels/Fe-Alloys  v7.0
 TCFE6   =  Steels/Fe-Alloys  v6.2
 TCFE5   =  Steels/Fe-Alloys  v5.0
 TCFE4   =  Steels/Fe-Alloys  v4.1
 TCFE3   =  Steels/Fe-Alloys  v3.1
 TCFE2   =  Steels/Fe-Alloys  v2.1
 TCFE1   =  Steels/Fe-Alloys  v1.0
 TCNI9   =  Ni-Alloys  v9.0 SNAPSHOT
 NI25    =  NI25 database
 TCNI8   =  Ni-Alloys  v8.1
 TCNI7   =  Ni-Alloys  v7.1
 TCNI6   =  Ni-Alloys  v6.0
 TCNI5   =  Ni-Alloys  v5.1
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 TCNI4   =  Ni-Alloys  v4.0
 TCNI1   =  Ni-Alloys  v1.3
 TCAL5   =  Al-Alloys  v5.0
 TCAL4   =  Al-Alloys  v4.0
 TCAL3   =  Al-Alloys  v3.0
 TCAL2   =  Al-Alloys  v2.1
 TCAL1   =  Al-Alloys  v1.2
 TCMG4   =  Mg-Alloys  v4.0
 TCMG3   =  Mg-Alloys  v3.0
 TCMG2   =  Mg-Alloys  v2.0
 TCMG1   =  Mg-Alloys  v1.1
 TCTI1   =  Ti-Alloys  v1.0
 TCCU2   =  Cu-Alloys  v2.0
 TCCU1   =  Cu-Alloys  v1.0
 TCCC1   =  Cemented carbide  v1.0
 TCHEA2  =  High Entropy Alloy  v2.1
 TCHEA1  =  High Entropy Alloy  v1.0
 SSOL6   =  SGTE Alloy Solutions Database v6.0
 SSOL5   =  SGTE Alloy Solutions Database v5.0
 SSOL4   =  SGTE Alloy Solutions Database v4.9g
 SSOL2   =  SGTE Alloy Solutions Database v2.1
 SSUB6   =  SGTE Substances Database v6.0
 SSUB5   =  SGTE Substances Database v5.2
 SSUB4   =  SGTE Substances Database v4.1
 SSUB3   =  SGTE Substances Database v3.3
 SSUB2   =  SGTE Substances Database v2.2
 SNOB3   =  SGTE Noble Metal Alloys Database v3.1
 STBC2   =  SGTE Thermal Barrier Coating TDB v2.2
 STBC1   =  SGTE Thermal Barrier Coating TDB v1.1
 SALT1   =  SGTE Molten Salts Database v1.2
 SEMC2   =  TC Semi-Conductors  v2.1
 SLAG4   =  Fe-containing Slag  v4.1
 SLAG3   =  Fe-containing Slag  v3.2
 SLAG2   =  Fe-containing Slag  v2.2
 SLAG1   =  Fe-containing Slag  v1.2
 TCOX7   =  Metal Oxide Solutions  v7.0
 TCOX6   =  Metal Oxide Solutions  v6.0
 TCOX5   =  Metal Oxide Solutions  v5.1
 TCOX4   =  Metal Oxide Solutions  v4.1
 ION3    =  Ionic Solutions  v3.0
 ION2    =  Ionic Solutions  v2.6
 ION1    =  Ionic Solutions  v1.5
 NOX2    =  NPL Oxide Solutions Database v2.1
 TCNOBL1 =  Noble Metals Alloys v1.0
 TCSLD3  =  Solder Alloys  v3.2
 TCSLD2  =  Solder Alloys  v2.0
 TCSI1   =  Ultrapure Silicon  v1.2
 TCMP2   =  Materials Processing  v2.5
 TCES1   =  Combustion/Sintering  v1.1
 TCSC1   =  Super Conductor  v1.0
 TCFC1   =  SOFC Database v1.0
 NUMT2   =  Nuclear Materials  v2.1
 NUOX4   =  Nuclear Oxides  v4.2
 NUCL15  =  IRSN NUCLEA-15_4
 NUCL10  =  ThermoData NUCLEA Alloys-oxides TDB v10.2
 MEPH15  =  IRSN Mephista-15_1
 MEPH11  =  ThermoData MEPHISTA Nuclear Fuels TDB v11.2
 TCAQ3   =  Aqueous Solution  v3.0
 TCAQ2   =  Aqueous Solution  v2.6
 AQS2    =  TGG Aqueous Solution Database v2.6
 GCE2    =  TGG Geochemical/Environmental TDB v2.3
 FEDEMO  =  Iron Demo Database v2.0
 ALDEMO  =  Aluminum Demo Database v2.0
 NIDEMO  =  Nickel Demo Database v1.0
 CUDEMO  =  Copper Demo Database v1.0
 SLDEMO  =  Solder Demo Database v1.0
 OXDEMO  =  Oxide Demo Database v1.0
 SUBDEMO =  Substance Demo Database v1.0
 PTERN   =  Public Ternary Alloys TDB v1.3
 PAQ2    =  Public Aqueous Soln (SIT) TDB v2.4
 PG35    =  G35 Binary Semi-Conductors TDB v1.2
 PURE5   =  SGTE Unary (Pure Elements) TDB v5.1
 MOB2    =  Alloys Mobility  v2.7
 MOB1    =  Alloys Mobility  v1.3
 MOBFE1  =  Steels/Fe-Alloys Mobility  v1.0
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBNI4  =  Ni-Alloys Mobility  v4.0
 MOBNI3  =  Ni-Alloys Mobility  v3.1
 MOBNI2  =  Ni-Alloys Mobility  v2.4
 MOBNI1  =  Ni-Alloys Mobility  v1.0
 MOBAL3  =  Al-Alloys Mobility  v3.0
 MOBAL2  =  Al-Alloys Mobility  v2.0
 MOBAL1  =  Al-Alloys Mobility  v1.0
 MOBCU1  =  Cu-Alloys Mobility  v1.0
 MOBCU2  =  Cu-Alloys Mobility  v2.0
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBSLD1 =  Solder-Alloys Mobility  v1.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0 SNAPSHOT
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v1.0
 MFEDEMO =  Fe-Alloys Mobility demo database v2.0
 MNIDEMO =  Ni-Alloys Mobility demo database v1.0
 MCUDEMO =  Cu-Alloys Mobility demo database v1.0
 USER    =  User defined Database

DATABASE NAME /TCFE7/: mobfe2
 Current database: Steels/Fe-Alloys Mobility  v2.0
   TCS Steel Mobility Database Version 2.0 from 2011-12-09.

 VA  DEFINED
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 ....

 List of references for assessed data

  'This parameter has not been assessed'
  'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'
  'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
      -Ni'
  'Bae et al.: Z. Metallkunde 91(2000)672-674; fcc Fe-Mn
       Mn-Ni'
  'D. Bergner et al., Defect and Diffusion Forum 66-69(1989)409. Impurity
      diffusion of Si in fcc Fe.'
 -OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE PROBLEM IS SET UP
APP: @@
APP: go d-m
 NO TIME STEP DEFINED
 *** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
DIC>
DIC> @@
DIC> @@ ENTER GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 1273; * N

DIC>
DIC> @@
DIC> @@ SET THE REFERENCE STATE FOR CARBON
DIC> @@
DIC> set-ref C grap * 101325
DIC>
DIC> @@
DIC> @@ ENTER A REGION
DIC> @@
DIC> enter-region aus
DIC>
DIC> @@
DIC> @@ ENTER A DOUBLE GEOMETRIC GRID INTO THE REGION
DIC> @@
DIC> enter-grid
REGION NAME : /AUS/: aus
WIDTH OF REGION /1/: 1e-2
TYPE /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>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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
 double geometric
 dense at outer boundaries, coarse at  0.50000E-02
lower part   1.2500       22
upper part  0.80000       22
 U-FRACTION IN SYSTEM:  C = .00115488575879621  FE = .490055682684517
                        MN = .00302988813183617  SI = .00691442924890045
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
 U-FRACTION IN SYSTEM:  C = .00115488575879621  FE = .490055682684517
                        MN = .00302988813183617  SI = .00691442924890045
 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 = .001168232207708  FE = .490055682684517
                        MN = .00302988813183617  SI = .00691442924890045
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0 seconds
 TIME =  0.10010000E-03 DT =  0.10000000E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00116829562757795  FE = .490055682684517
                        MN = .00302988813183617  SI = .00691442924890045
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0 seconds
 TIME =   3.0557506     DT =   3.0556505     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00118960627023709  FE = .490055682684521
                        MN = .00302988813183657  SI = .00691442924889595
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0 seconds
 TIME =   9.1670515     DT =   6.1113009     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00121114065253319  FE = .490055682684524
                        MN = .00302988813183688  SI = .00691442924889252
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0 seconds
 TIME =   21.389653     DT =   12.222602     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00123894224179207  FE = .490055682684528
                        MN = .00302988813183725  SI = .00691442924888855
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    1 seconds
 TIME =   45.834857     DT =   24.445204     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00127675531962732  FE = .490055682684532
                        MN = .00302988813183768  SI = .00691442924888393
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0 seconds
 TIME =   94.725265     DT =   48.890408     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00132929244094337  FE = .490055682684536
                        MN = .00302988813183816  SI = .0069144292488789
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0 seconds
 TIME =   192.50608     DT =   97.780815     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00140301692405163  FE = .490055682684541
                        MN = .00302988813183861  SI = .00691442924887446
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0 seconds
 TIME =   388.06771     DT =   195.56163     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00150699028673373  FE = .490055682684541
                        MN = .0030298881318388  SI = .00691442924887331
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0 seconds
 TIME =   779.19097     DT =   391.12326     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00165403563506009  FE = .490055682684533
                        MN = .00302988813183819  SI = .00691442924888217
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    1 seconds
 TIME =   1561.4375     DT =   782.24652     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00186239344623103  FE = .49005568268452
                        MN = .00302988813183713  SI = .00691442924889648
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0 seconds
 TIME =   3125.9305     DT =   1564.4930     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00215807121249969  FE = .490055682684546
                        MN = .00302988813183974  SI = .00691442924886796
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0 seconds
 TIME =   6254.9166     DT =   3128.9861     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00257823536978672  FE = .490055682684616
                        MN = .00302988813184698  SI = .00691442924879113
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0 seconds
 TIME =   12512.889     DT =   6257.9722     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00317699718807945  FE = .490055682684705
                        MN = .0030298881318573  SI = .00691442924869157
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0 seconds
 TIME =   25028.833     DT =   12515.944     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00403336961093126  FE = .490055682684793
                        MN = .00302988813186931  SI = .00691442924859118
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    1 seconds
 TIME =   50060.722     DT =   25031.889     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00526363637174368  FE = .490055682684873
                        MN = .00302988813188164  SI = .00691442924849893
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0 seconds
```

```
 TIME =   100124.50     DT =   50063.777     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00704133724521602  FE = .490055682684964
                        MN = .0030298881318934  SI = .00691442924839638
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    1 seconds
 TIME =   200252.05     DT =   100127.55     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00961836049920387  FE = .490055682685094
                        MN = .00302988813190605  SI = .00691442924825385
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0 seconds
 TIME =   400507.16     DT =   200255.11     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0130439049348442  FE = .490055682685357
                        MN = .00302988813193134  SI = .00691442924796516
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0 seconds
 TIME =   801017.38     DT =   400510.22     SUM OF SQUARES =   0.0000000


output ignored...



... output resumed

  CPU time used in timestep                    1 seconds
 TIME =   1602037.8     DT =   801020.44     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165218937291276  FE = .490055682687136
                        MN = .00302988813210615  SI = .00691442924601151
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0 seconds
 TIME =   3070759.8     DT =   1468722.0     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165306302137249  FE = .490055682689487
                        MN = .00302988813231524  SI = .00691442924345072
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0 seconds
 TIME =   5520081.8     DT =   2449321.9     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165307407276147  FE = .490055682694412
                        MN = .00302988813270145  SI = .0069144292384322
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    1 seconds
 TIME =   9712140.3     DT =   4192058.5     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165306049407457  FE = .490055682702373
                        MN = .00302988813346508  SI = .00691442922805808
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0 seconds
 TIME =   17804358.     DT =   8092217.5     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165302884173806  FE = .490055682726962
                        MN = .00302988813524102  SI = .00691442920305048
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    1 seconds
 TIME =   33988793.     DT =   16184435.     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165299095291916  FE = .490055682786251
                        MN = .00302988813967787  SI = .00691442913932503
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0 seconds
 TIME =   66357663.     DT =   32368870.     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165296370794655  FE = .490055682925557
                        MN = .00302988815056947  SI = .00691442898912743
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0 seconds
 TIME =  0.13109540E+09 DT =   64737740.     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165297311657981  FE = .490055683202508
                        MN = .00302988817529088  SI = .0069144286874545
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    1 seconds
 TIME =  0.23051887E+09 DT =   99423470.     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165316513851906  FE = .490055683573445
                        MN = .00302988822136918  SI = .00691442827811698
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0 seconds
 TIME =  0.33003492E+09 DT =   99516053.     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165355763010635  FE = .490055683890079
                        MN = .00302988824987424  SI = .0069144279245888
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    1 seconds
 TIME =  0.42961658E+09 DT =   99581650.     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165388724264922  FE = .490055684170609
                        MN = .00302988828351862  SI = .00691442761112566
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0 seconds
 TIME =  0.52925282E+09 DT =   99636240.     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165418605270749  FE = .490055684422996
                        MN = .00302988831490655  SI = .00691442732735122
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0 seconds
 TIME =  0.62893535E+09 DT =   99682537.     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165446599910542  FE = .490055684654308
                        MN = .00302988834435435  SI = .00691442706659145
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    1 seconds
 TIME =  0.72865867E+09 DT =   99723322.     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165473274287305  FE = .490055684868825
                        MN = .00302988837213727  SI = .00691442682429134
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0 seconds
 TIME =  0.82841842E+09 DT =   99759750.     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165498943962927  FE = .490055685069575
                        MN = .00302988839848144  SI = .00691442659719764
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    1 seconds
 TIME =  0.92821105E+09 DT =   99792624.     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165523804304784  FE = .490055685258784
                        MN = .00302988842357088  SI = .00691442638289816
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0 seconds
 TIME =  0.98981461E+09 DT =   61603559.     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165550594430682  FE = .490055685370543
                        MN = .00302988843849379  SI = .0069144262562169
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    1 seconds
 TIME =  0.10000000E+10 DT =   10185394.     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165567958948894  FE = .490055685388685
                        MN = .00302988844092304  SI = .00691442623564514
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
 MUST SAVE WORKSPACE ON FILE
 WORKSPACE SAVED ON FILE
```

```
 RECLAIMING WORKSPACE
 DELETING TIME-RECORD FOR TIME    0.0000000
 DELETING TIME-RECORD FOR TIME   0.10000000E-06
 DELETING TIME-RECORD FOR TIME   0.10010000E-03
 DELETING TIME-RECORD FOR TIME    3.0557506
 DELETING TIME-RECORD FOR TIME    9.1670515
 DELETING TIME-RECORD FOR TIME    21.389653
 DELETING TIME-RECORD FOR TIME    45.834857
 DELETING TIME-RECORD FOR TIME    94.725265
 DELETING TIME-RECORD FOR TIME    192.50608
 DELETING TIME-RECORD FOR TIME    388.06771
 DELETING TIME-RECORD FOR TIME    779.19097
 DELETING TIME-RECORD FOR TIME    1561.4375
 DELETING TIME-RECORD FOR TIME    3125.9305
 DELETING TIME-RECORD FOR TIME    6254.9166
 DELETING TIME-RECORD FOR TIME    12512.889
 DELETING TIME-RECORD FOR TIME    25028.833
 DELETING TIME-RECORD FOR TIME    50060.722
 DELETING TIME-RECORD FOR TIME    100124.50
 DELETING TIME-RECORD FOR TIME    200252.05
 DELETING TIME-RECORD FOR TIME    400507.16
 DELETING TIME-RECORD FOR TIME    801017.38
 DELETING TIME-RECORD FOR TIME    1602037.8
 DELETING TIME-RECORD FOR TIME    3070759.8
 DELETING TIME-RECORD FOR TIME    5520081.8
 DELETING TIME-RECORD FOR TIME    9712140.3
 DELETING TIME-RECORD FOR TIME    17804358.
 DELETING TIME-RECORD FOR TIME    33988793.
 DELETING TIME-RECORD FOR TIME    66357663.
 DELETING TIME-RECORD FOR TIME   0.13109540E+09
 DELETING TIME-RECORD FOR TIME   0.23051887E+09
 DELETING TIME-RECORD FOR TIME   0.33003492E+09
 DELETING TIME-RECORD FOR TIME   0.42961658E+09
 DELETING TIME-RECORD FOR TIME   0.52925282E+09
 DELETING TIME-RECORD FOR TIME   0.62893535E+09
 DELETING TIME-RECORD FOR TIME   0.72865867E+09
 DELETING TIME-RECORD FOR TIME   0.82841842E+09
 DELETING TIME-RECORD FOR TIME   0.92821105E+09

 KEEPING TIME-RECORD FOR TIME   0.98981461E+09
 AND FOR TIME                   0.10000000E+10
 WORKSPACE RECLAIMED

 TIMESTEP AT    0.100000000E+10 SELECTED

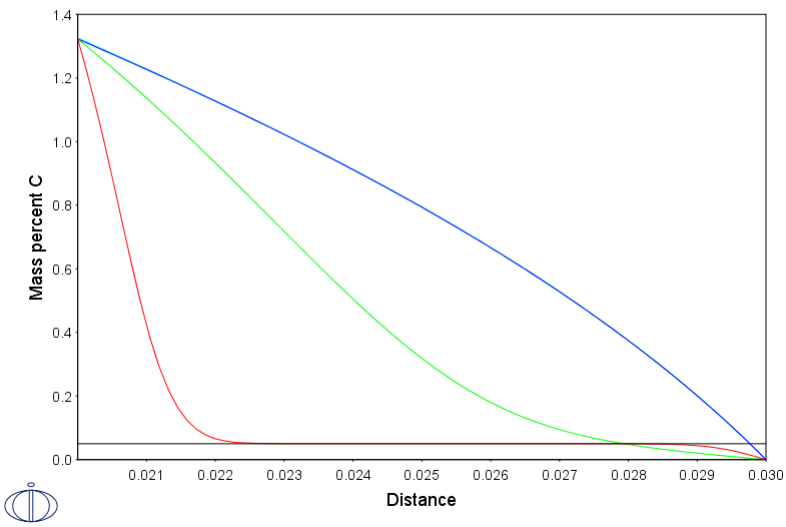
DIC>
DIC> @@
DIC> @@ THE SIMULATION IS FINISHED
DIC> @@
DIC>
DIC> set-inter
 --OK---
DIC>
```

exa6-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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

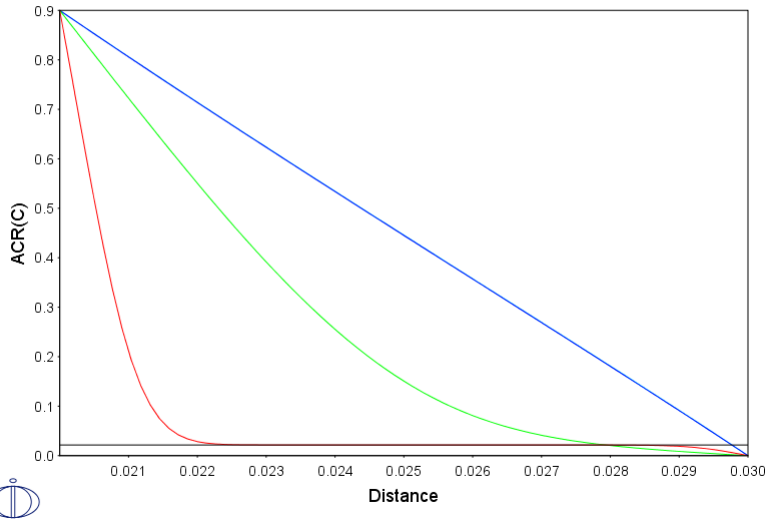
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson

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: plot
```



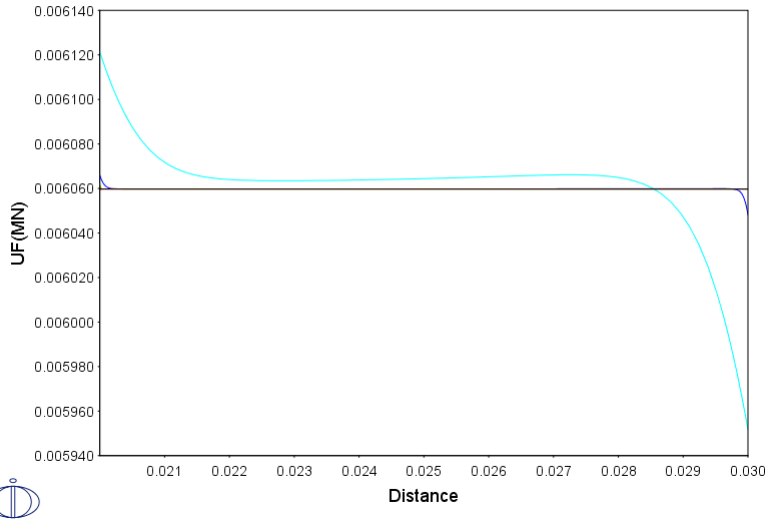

```
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ PLOT THE ACTIVITY OF C
POST-1: @@
POST-1:
POST-1: s-d-a y acr(c)
POST-1:
POST-1: plot
```

2018.02.18.18.45.15
Time = 0,10000,200000,1E+07,1E+09
CELL #1



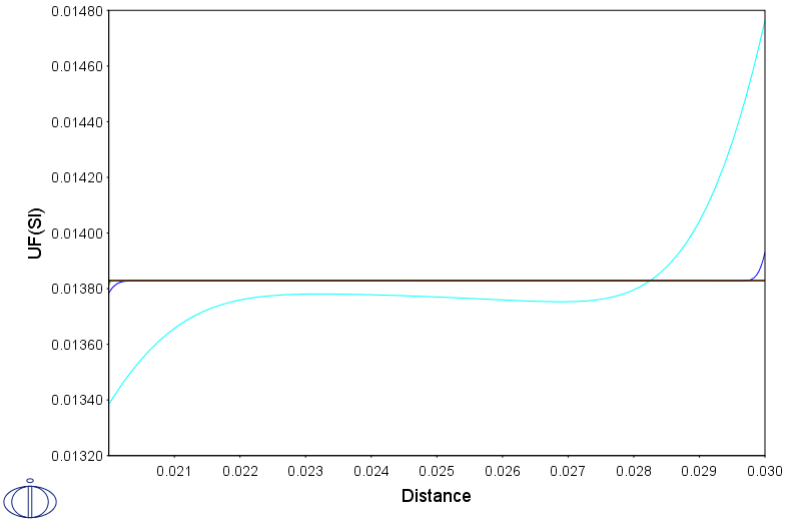
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ LET US LOOK AT THE MN AND SI PROFILES
POST-1: @@
POST-1: @@ WE PLOT THE U-FRACTION OF MN AND SI WHICH WILL BE INDEPENDENT
POST-1: @@ OF THE C-CONCENTRATION.
POST-1: @@
POST-1: s-d-a y u-f mn
POST-1:
POST-1: plot

2018.02.18.18.45.16
Time = 0,10000,200000,1E+07,1E+09
CELL #1



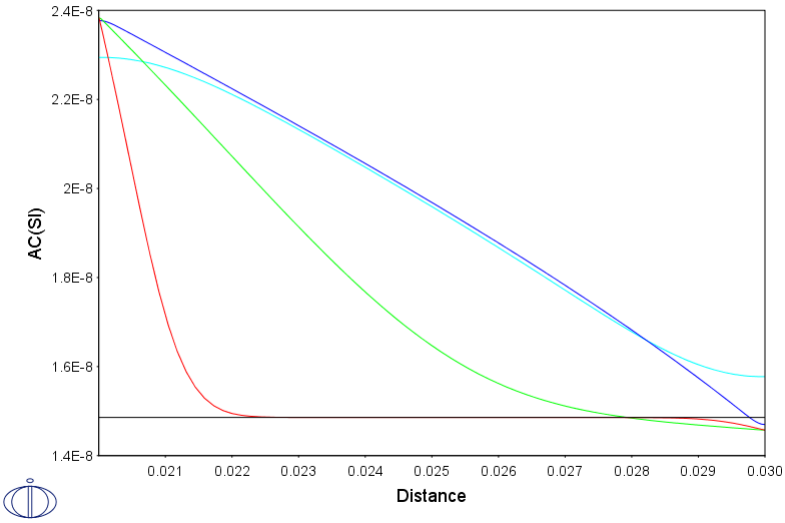
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: s-d-a y u-f si
POST-1:
POST-1: plot

2018.02.18.18.45.17
Time = 0,10000,200000,1E+07,1E+09
CELL #1



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: plot

2018.02.18.18.45.18
Time = 0,10000,200000,1E+07,1E+09
CELL #1



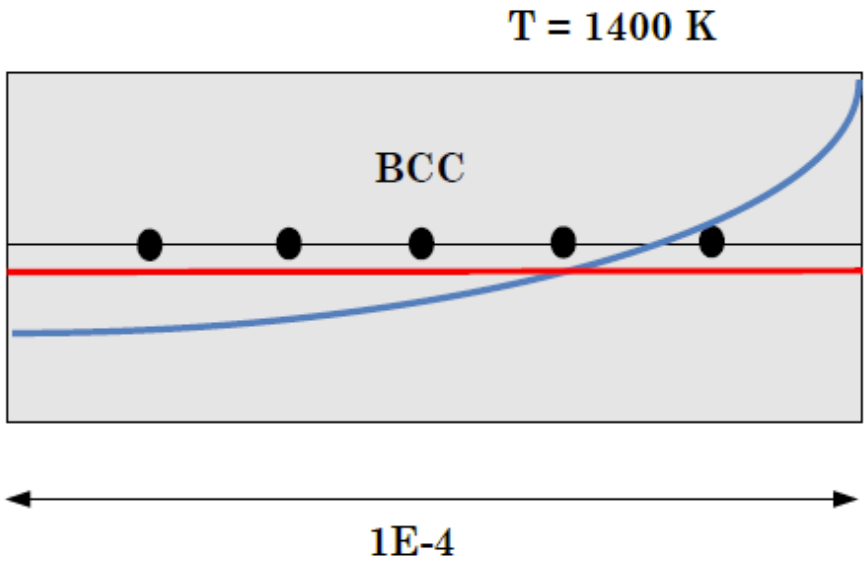
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: set-inter
--OK---
POST-1:

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

```
About Stockholm, Sweden

 Software  (build 12987) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri Feb 16 15:22:08 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa7\setup.DCM" @@ 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
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

 VA                     /-  DEFINED
 L12_FCC                B2_BCC                 DICTRA_FCC_A1
   REJECTED
TDB_TCFE9: sw FEDEMO
 Current database: Iron Demo Database v2.0

 VA                     /-  DEFINED
TDB_FEDEMO: def-sys fe cr ni mn
 FE                     CR                     NI
 MN  DEFINED
TDB_FEDEMO: rej ph *
 LIQUID:L               BCC_A2                 CHI_A12
 DIAMOND_FCC_A4         FCC_A1                 HCP_A3
 LAVES_PHASE_C14        SIGMA  REJECTED
TDB_FEDEMO: rest ph bcc
 BCC_A2  RESTORED
TDB_FEDEMO: get
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'X.-G. Lu, M. Selleby, B. Sundman, CALPHAD, 29 (2005) 49-55; Fe P-T diagram'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270
      (1986); CR-FE'
  'B.-J. Lee, Metall. Trans. A, 24A (1993) 1919-1933; Cr-Mn, Fe-Cr -Mn'
  'B.-J. Lee, CALPHAD, 17 (1993) 251-268; revision of Fe-Cr and Fe -Ni liquid'
  'B.-J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
  'A. Dinsdale and T. Chart, MTDS NPL, Unpublished work (1986); CR -NI'
  'W. Huang, CALPHAD, 13 (1989) 243-252; TRITA-MAC 388 (rev 1989); FE-MN'
  'L. Zhang, Y. Du, H. Xu, S. Liu, Y. Liu, F. Zheng, et al., Int. J. Mater.
      Res. 100 (2009) 160-175; Fe-Mn-Ni'
  'A. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); FE-NI'
  'S. Liu, Unpublished work (2010); Mn-Ni'
 -OK-
TDB_FEDEMO:
TDB_FEDEMO: app MFEDEMO
 Current database: Fe-Alloys Mobility demo database v2.0

 VA  DEFINED
APP: def-sys fe cr ni mn
 FE                     CR                     NI
 MN  DEFINED
APP: rej ph *
 BCC_A2                 FCC_A1  REJECTED
APP: rest ph bcc
 BCC_A2  RESTORED
APP: get
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'This parameter has not been assessed'
  'B. Jonsson: ISIJ International, 35(1995)1415-1421; Cr, Fe and Ni
      diffusion bcc Cr-Fe-Ni'
  'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
      in bcc Fe'
  'Assessed from data presented in Landholt-Bornstein, Vol. 26, ed. H.
      Mehrer, springer (1990); Impurity diff of Mn in bcc Fe.'
 -OK-
APP:
APP: go dict-mon
 NO TIME STEP DEFINED
DIC>
DIC>
DIC> @@ THE INPUT_SCHEIL_PROFILE COMMAND PERFORMS MOST OF THE SET UP
DIC> input_scheil_profile
 INFO: SCHEIL_REGION CREATED
FILE NAME /XF.TXT/: segregation_profile.TXT
ENTER WIDTH OF REGION /1/: 100e-6
 INFO: LINEAR GRID IN SCHEIL_REGION ENTERED WITH 100 GRID POINTS
 ENTER MAIN SOLID SOLUTION PHASE
PHASE NAME: bcc#1
 INFO: 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>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa7\run.DCM"DIC> go dict-mon
 TIME STEP AT TIME  0.00000E+00
DIC>
DIC> read exa7
 OK
DIC>
DIC> sim
 U-FRACTION IN SYSTEM:  CR = .180420497424242  FE = .796498787878788
                        MN = .00999016878282829  NI = .0130905459141414
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 U-FRACTION IN SYSTEM:  CR = .180420497424242  FE = .796498787878788
                        MN = .00999016878282829  NI = .0130905459141414
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .180420497424242  FE = .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 = .180420497424243  FE = .796498787878788
                        MN = .00999016878282829  NI = .0130905459141415
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.41908397     DT =  0.41898387     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .180420497424242  FE = .796498787878788
                        MN = .0099901687828279  NI = .0130905459141419
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   1.2570517     DT =  0.83796774     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .180420497424242  FE = .796498787878788
                        MN = .0099901687828279  NI = .0130905459141418
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   2.9329872     DT =   1.6759355     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .180420497424243  FE = .796498787878789
                        MN = .00999016878282889  NI = .0130905459141397
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    1 seconds
 TIME =   6.2848581     DT =   3.3518710     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .180420497424257  FE = .796498787878809
                        MN = .00999016878284567  NI = .0130905459140889
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   12.988600     DT =   6.7037419     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .180420497424302  FE = .796498787878888
                        MN = .0099901687828762  NI = .0130905459139341
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   26.396084     DT =   13.407484     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .180420497424318  FE = .796498787878861
                        MN = .0099901687829013  NI = .0130905459139194
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   53.211052     DT =   26.814968     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .180420497424435  FE = .796498787878771
                        MN = .00999016878299364  NI = .0130905459138002
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   106.84099     DT =   53.629935     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .180420497424575  FE = .796498787878385
                        MN = .00999016878336974  NI = .0130905459136702
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    1 seconds
 TIME =   214.10086     DT =   107.25987     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .180420497424432  FE = .796498787878199
                        MN = .00999016878339541  NI = .0130905459139735
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   428.62060     DT =   214.51974     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .18042049742409  FE = .796498787877756
                        MN = .00999016878350895  NI = .0130905459146442
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   788.62060     DT =   360.00000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .180420497424077  FE = .796498787877899
                        MN = .00999016878346233  NI = .0130905459145616
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   1148.6206     DT =   360.00000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .180420497423613  FE = .796498787877388
                        MN = .00999016878332526  NI = .0130905459156739
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    1 seconds
 TIME =   1508.6206     DT =   360.00000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .180420497423265  FE = .796498787877026
                        MN = .0099901687831702  NI = .0130905459165386
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   1868.6206     DT =   360.00000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .180420497422966  FE = .796498787875233
                        MN = .00999016878344972  NI = .0130905459183517
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   2228.6206     DT =   360.00000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .180420497422686  FE = .79649878787269
                        MN = .00999016878399045  NI = .0130905459206335
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   2588.6206     DT =   360.00000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .180420497422472  FE = .796498787870928
                        MN = .00999016878437055  NI = .0130905459222304
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   2948.6206     DT =   360.00000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .180420497422317  FE = .796498787869701
                        MN = .00999016878464137  NI = .0130905459233406
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3308.6206     DT =   360.00000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .180420497422203  FE = .796498787868854
                        MN = .00999016878483073  NI = .0130905459241122
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
```

```
 CPU time used in timestep                    1 seconds
TIME =   3600.0000     DT =   291.37940     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  CR = .180420497422138  FE = .796498787868426
                       MN = .00999016878491876  NI = .0130905459245169
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   0.41908397
DELETING TIME-RECORD FOR TIME    1.2570517
DELETING TIME-RECORD FOR TIME    2.9329872
DELETING TIME-RECORD FOR TIME    6.2848581
DELETING TIME-RECORD FOR TIME    12.988600
DELETING TIME-RECORD FOR TIME    26.396084
DELETING TIME-RECORD FOR TIME    53.211052
DELETING TIME-RECORD FOR TIME    106.84099
DELETING TIME-RECORD FOR TIME    214.10086
DELETING TIME-RECORD FOR TIME    428.62060
DELETING TIME-RECORD FOR TIME    788.62060
DELETING TIME-RECORD FOR TIME    1148.6206
DELETING TIME-RECORD FOR TIME    1508.6206
DELETING TIME-RECORD FOR TIME    1868.6206
DELETING TIME-RECORD FOR TIME    2228.6206
DELETING TIME-RECORD FOR TIME    2588.6206
DELETING TIME-RECORD FOR TIME    2948.6206

KEEPING TIME-RECORD FOR TIME    3308.6206
AND FOR TIME                    3600.0000
WORKSPACE RECLAIMED

TIMESTEP AT     3600.00000     SELECTED

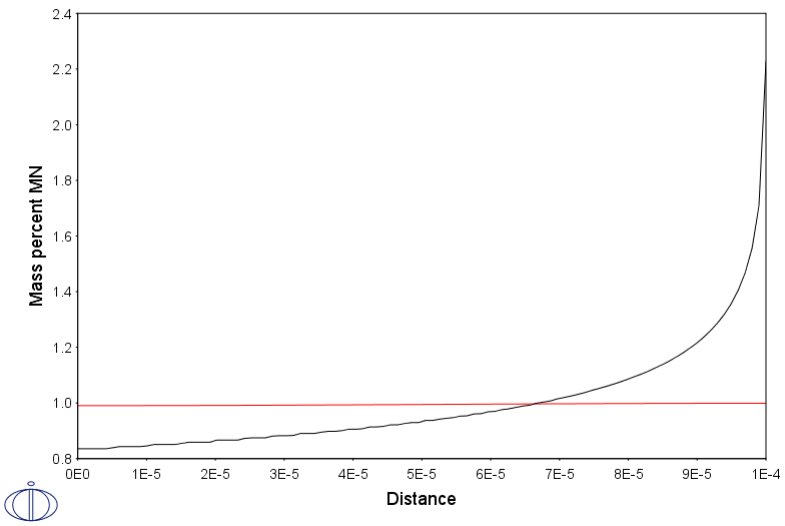
DIC>
DIC> set-inter
 --OK---
DIC>
```

exa7-plot

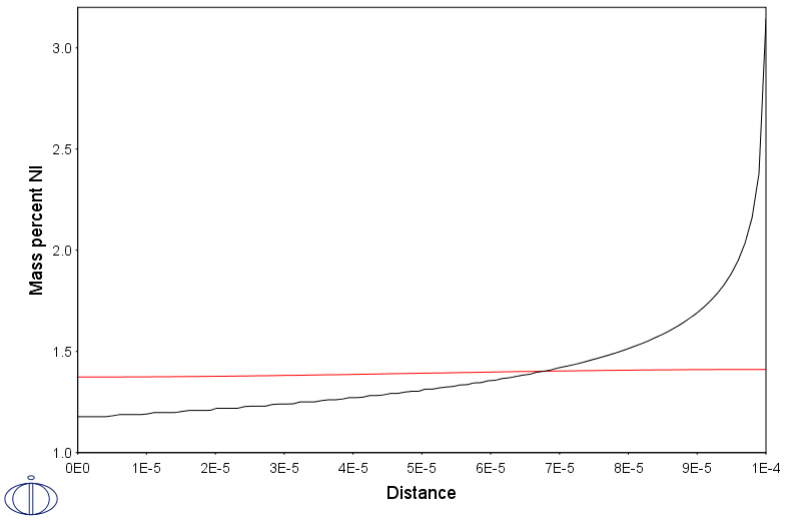
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa7\plot.DCM"DIC> go dict-mon
 TIME STEP AT TIME  3.60000E+03
DIC>
DIC> read exa7
 OK
DIC>
DIC> post

  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: plot
   2018.02.18.18.48.22
   Time = 0,3600
   CELL #1
```

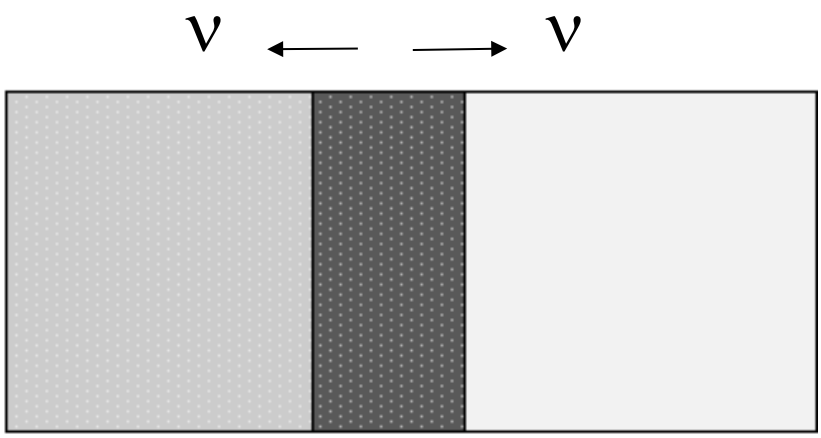



```
POST-1:
POST-1: @@ Hit enter for the next plot
POST-1:@?
POST-1:
POST-1: s-d-a y w-p ni
POST-1: plot
   2018.02.18.18.48.22
   Time = 0,3600
   CELL #1
```




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

Moving Boundary Problems

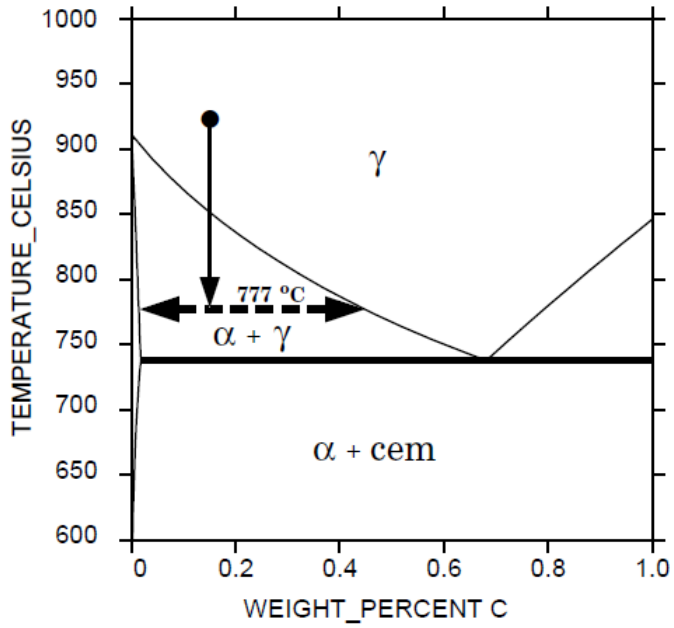


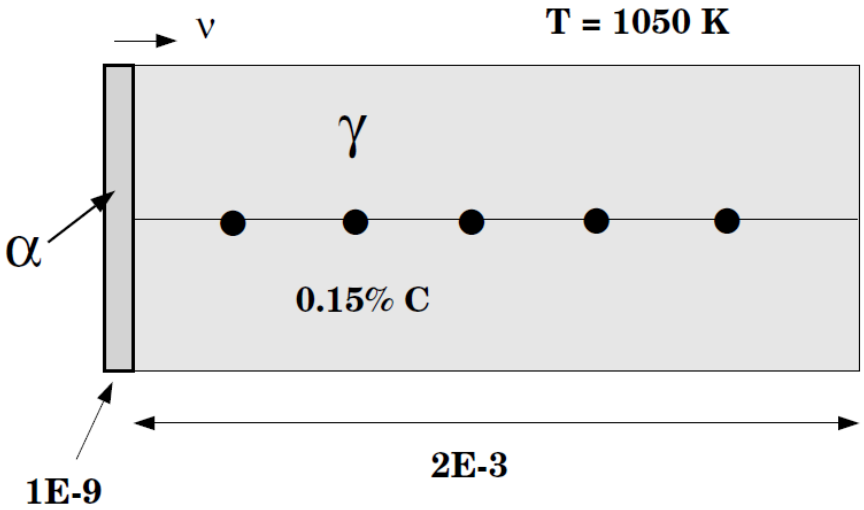
Example exb1a

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

```
About Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri Feb 16 15:22:08 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb1a\setup.DCM" @@
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
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

 VA                     /-  DEFINED
 L12_FCC                B2_BCC                  DICTRA_FCC_A1
   REJECTED
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE THE DATA
TDB_TCFE9: @@
TDB_TCFE9: sw FEDEMO
 Current database: Iron Demo Database v2.0

 VA                     /-  DEFINED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ DEFINE THE SYSTEM TO WORK WITH
TDB_FEDEMO: @@
TDB_FEDEMO: def-sys fe c
 FE                     C  DEFINED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ EXCLUDE THE THERMODYNAMIC DATA FOR THE PHASES THAT ARE NOT NEEDED
TDB_FEDEMO: @@
TDB_FEDEMO: rej ph * all
 GAS:G                  LIQUID:L                BCC_A2
 CEMENTITE              DIAMOND_FCC_A4          FCC_A1
 GRAPHITE               HCP_A3                  KSI_CARBIDE
 LAVES_PHASE_C14        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
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'P. Franke, Estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
  'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'X.-G. Lu, M. Selleby, B. Sundman, CALPHAD, 29 (2005) 49-55; Fe P-T diagram'
  'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
 -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

 TCFE9   =  Steels/Fe-Alloys  v9.0
 TCFE10  =  Steels/Fe-Alloys  v10.0 SNAPSHOT
 TCFE8   =  Steels/Fe-Alloys  v8.1
 FROST1  =  FROST database v1.0
 TCFE7   =  Steels/Fe-Alloys  v7.0
 TCFE6   =  Steels/Fe-Alloys  v6.2
 TCFE5   =  Steels/Fe-Alloys  v5.0
 TCFE4   =  Steels/Fe-Alloys  v4.1
 TCFE3   =  Steels/Fe-Alloys  v3.1
 TCFE2   =  Steels/Fe-Alloys  v2.1
 TCFE1   =  Steels/Fe-Alloys  v1.0
 TCNI9   =  Ni-Alloys  v9.0 SNAPSHOT
 NI25    =  NI25 database
 TCNI8   =  Ni-Alloys  v8.1
 TCNI7   =  Ni-Alloys  v7.1
 TCNI6   =  Ni-Alloys  v6.0
 TCNI5   =  Ni-Alloys  v5.1
 TCNI4   =  Ni-Alloys  v4.0
 TCNI1   =  Ni-Alloys  v1.3
 TCAL5   =  Al-Alloys  v5.0
```

```
 TCAL4   =  Al-Alloys  v4.0
 TCAL3   =  Al-Alloys  v3.0
 TCAL2   =  Al-Alloys  v2.1
 TCAL1   =  Al-Alloys  v1.2
 TCMG4   =  Mg-Alloys  v4.0
 TCMG3   =  Mg-Alloys  v3.0
 TCMG2   =  Mg-Alloys  v2.0
 TCMG1   =  Mg-Alloys  v1.1
 TCTI1   =  Ti-Alloys  v1.0
 TCCU2   =  Cu-Alloys  v2.0
 TCCU1   =  Cu-Alloys  v1.0
 TCCC1   =  Cemented carbide  v1.0
 TCHEA2  =  High Entropy Alloy  v2.1
 TCHEA1  =  High Entropy Alloy  v1.0
 SSOL6   =  SGTE Alloy Solutions Database v6.0
 SSOL5   =  SGTE Alloy Solutions Database v5.0
 SSOL4   =  SGTE Alloy Solutions Database v4.9g
 SSOL2   =  SGTE Alloy Solutions Database v2.1
 SSUB6   =  SGTE Substances Database v6.0
 SSUB5   =  SGTE Substances Database v5.2
 SSUB4   =  SGTE Substances Database v4.1
 SSUB3   =  SGTE Substances Database v3.3
 SSUB2   =  SGTE Substances Database v2.2
 SNOB3   =  SGTE Noble Metal Alloys Database v3.1
 STBC2   =  SGTE Thermal Barrier Coating TDB v2.2
 STBC1   =  SGTE Thermal Barrier Coating TDB v1.1
 SALT1   =  SGTE Molten Salts Database v1.2
 SEMC2   =  TC Semi-Conductors  v2.1
 SLAG4   =  Fe-containing Slag  v4.1
 SLAG3   =  Fe-containing Slag  v3.2
 SLAG2   =  Fe-containing Slag  v2.2
 SLAG1   =  Fe-containing Slag  v1.2
 TCOX7   =  Metal Oxide Solutions  v7.0
 TCOX6   =  Metal Oxide Solutions  v6.0
 TCOX5   =  Metal Oxide Solutions  v5.1
 TCOX4   =  Metal Oxide Solutions  v4.1
 ION3    =  Ionic Solutions  v3.0
 ION2    =  Ionic Solutions  v2.6
 ION1    =  Ionic Solutions  v1.5
 NOX2    =  NPL Oxide Solutions Database v2.1
 TCNOBL1 =  Noble Metals Alloys v1.0
 TCSLD3  =  Solder Alloys  v3.2
 TCSLD2  =  Solder Alloys  v2.0
 TCSI1   =  Ultrapure Silicon  v1.2
 TCMP2   =  Materials Processing  v2.5
 TCES1   =  Combustion/Sintering  v1.1
 TCSC1   =  Super Conductor  v1.0
 TCFC1   =  SOFC Database v1.0
 NUMT2   =  Nuclear Materials  v2.1
 NUOX4   =  Nuclear Oxides  v4.2
 NUCL15  =  IRSN NUCLEA-15_4
 NUCL10  =  ThermoData NUCLEA Alloys-oxides TDB v10.2
 MEPH15  =  IRSN Mephista-15_1
 MEPH11  =  ThermoData MEPHISTA Nuclear Fuels TDB v11.2
 TCAQ3   =  Aqueous Solution  v3.0
 TCAQ2   =  Aqueous Solution  v2.6
 AQS2    =  TGG Aqueous Solution Database v2.6
 GCE2    =  TGG Geochemical/Environmental TDB v2.3
 FEDEMO  =  Iron Demo Database v2.0
 ALDEMO  =  Aluminum Demo Database v2.0
 NIDEMO  =  Nickel Demo Database v1.0
 CUDEMO  =  Copper Demo Database v1.0
 SLDEMO  =  Solder Demo Database v1.0
 OXDEMO  =  Oxide Demo Database v1.0
 SUBDEMO =  Substance Demo Database v1.0
 PTERN   =  Public Ternary Alloys TDB v1.3
 PAQ2    =  Public Aqueous Soln (SIT) TDB v2.4
 PG35    =  G35 Binary Semi-Conductors TDB v1.2
 PURE5   =  SGTE Unary (Pure Elements) TDB v5.1
 MOB2    =  Alloys Mobility  v2.7
 MOB1    =  Alloys Mobility  v1.3
 MOBFE1  =  Steels/Fe-Alloys Mobility  v1.0
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBNI4  =  Ni-Alloys Mobility  v4.0
 MOBNI3  =  Ni-Alloys Mobility  v3.1
 MOBNI2  =  Ni-Alloys Mobility  v2.4
 MOBNI1  =  Ni-Alloys Mobility  v1.0
 MOBAL3  =  Al-Alloys Mobility  v3.0
 MOBAL2  =  Al-Alloys Mobility  v2.0
 MOBAL1  =  Al-Alloys Mobility  v1.0
 MOBCU1  =  Cu-Alloys Mobility  v1.0
 MOBCU2  =  Cu-Alloys Mobility  v2.0
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBSLD1 =  Solder-Alloys Mobility  v1.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0 SNAPSHOT
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v1.0
 MFEDEMO =  Fe-Alloys Mobility demo database v2.0
 MNIDEMO =  Ni-Alloys Mobility demo database v1.0
 MCUDEMO =  Cu-Alloys Mobility demo database v1.0
 USER    =  User defined Database

DATABASE NAME /FEDEMO/: MFEDEMO
 Current database: Fe-Alloys Mobility demo database v2.0

 VA  DEFINED
APP: def-sys fe c
 FE                     C  DEFINED
APP: rej ph * all
 BCC_A2                 FCC_A1  REJECTED
APP: res ph fcc bcc
 FCC_A1                 BCC_A2  RESTORED
APP: get
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'This parameter has not been assessed'
  'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'
```

```
  'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
      -Ni'
  'B. Jonsson: Z. Metallkunde 85(1994)498-501; C and N diffusion in bcc Cr
      -Fe-Ni'
  'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
      in bcc Fe'
 -OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP
APP: @@
APP: go d-m
 NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER GLOBAL CONDITION T
DIC> @@
DIC> set-condition global T 0 1050; * N

DIC>
DIC> @@
DIC> @@ START BY ENTERING THE REGIONS ferrite AND austenite WHERE WE
DIC> @@ PUT THE BCC AND FCC PHASE, RESPECTIVELY. THE FERRITE REGION IS
DIC> @@ ASSUMED INITIALLY TO BE VERY THIN, 1E-9 METERS.
DIC> @@
DIC> enter-region
REGION NAME : ferrite
DIC>
DIC> enter-region
REGION NAME : austenite
ATTACH TO REGION NAMED /FERRITE/:
ATTACHED TO THE RIGHT OF FERRITE /YES/:
DIC>
DIC> @@
DIC> @@ ENTER GRIDS INTO THE REGIONS
DIC> @@
DIC> enter-grid
REGION NAME : /FERRITE/: ferrite
WIDTH OF REGION /1/: 1e-9
TYPE /LINEAR/: AUTO
DIC>
DIC> enter-grid austenite
WIDTH OF REGION /1/: 20e-4
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 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> @@ 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-5
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/: 1E-5
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 /NO/:
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 (0 -> 0.5 -> 1): /.5/: 1.0
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /NO/:
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>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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
 Region: FERRITE
 single geometric dense at  0.10000E-08
  1.0000       24
 Region: AUSTENITE
 single geometric dense at   0.0000
  1.1762       99
  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]
 3.981486698393685E-005        3.982285206222398E-005        1.590375607321276E-012        8.419473575737259E-020       TIME =  0.10000000E-
04 DT =  0.10000000E-04 SUM OF SQUARES =  0.84194736E-19
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.29175547E-02 AND   0.29175547E-02
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.30175547E-07
 U-FRACTION IN SYSTEM:  C = .00698495590212148  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]
  13  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUSTENITE

  CPU time used in timestep                    0 seconds
 3.499840002568411E-006        3.500511889993114E-006        1.189299434788915E-007        4.111401576598501E-008        2.962726993130442E-
009        2.530772144886703E-012        1.388227002542885E-016        6.426175603022755E-024       TIME =  0.30000000E-04 DT =  0.20000000E-
04 SUM OF SQUARES =  0.64261756E-23
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.11112117E-03 AND   0.11112117E-03
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.32397971E-07
 U-FRACTION IN SYSTEM:  C = .00698495800112181  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]
  CPU time used in timestep                    0 seconds
 8.791374354180113E-008        8.798286115257557E-008        8.687492419359386E-012        8.244289164138366E-016        9.083754645801766E-
024       TIME =  0.70000000E-04 DT =  0.40000000E-04 SUM OF SQUARES =  0.90837546E-23
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.81460777E-04 AND   0.81460777E-04
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.35656402E-07
 U-FRACTION IN SYSTEM:  C = .00698495800112175  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]
  CPU time used in timestep                    0 seconds
 3.282053171774396E-006        3.283518213767685E-006        3.522763709445169E-006        1.817577627940967E-007        4.865266735792592E-
008        3.905717951157300E-011        5.263894590768058E-015        6.022271074110701E-022       TIME =  0.15000000E-03 DT =  0.80000000E-
04 SUM OF SQUARES =  0.60222711E-21
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.58646939E-04 AND   0.58646939E-04
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.40348157E-07
 U-FRACTION IN SYSTEM:  C = .00698495794642446  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]
  CPU time used in timestep                    0 seconds
  2  GRIDPOINT(S) ADDED   TO   CELL #1   REGION: FERRITE
 4.713654697301727E-007        4.723390808321862E-007        4.586676313054539E-012        4.398744297142028E-017       TIME =  0.31000000E-
03 DT =  0.16000000E-03 SUM OF SQUARES =  0.43987443E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.51923334E-04 AND   0.51923334E-04
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.48655890E-07
 U-FRACTION IN SYSTEM:  C = .00698495386454096  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]
  CPU time used in timestep                    0 seconds
 4.378612634787046E-006        4.381488084408341E-006        1.153704644838280E-009        2.848483939962826E-013        1.742320575503163E-
020       TIME =  0.63000000E-03 DT =  0.32000000E-03 SUM OF SQUARES =  0.17423206E-19
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.35629005E-04 AND   0.35629005E-04
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.60057172E-07
 U-FRACTION IN SYSTEM:  C = .00698494858774125  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]
  CPU time used in timestep                    0 seconds
 2.098301745605616E-006        2.099772515393114E-006        6.174151486876837E-010        1.696054835699411E-013        1.283482922433271E-
020       TIME =  0.12700000E-02 DT =  0.64000000E-03 SUM OF SQUARES =  0.12834829E-19
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.25117149E-04 AND   0.25117149E-04
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.76132147E-07
 U-FRACTION IN SYSTEM:  C = .00698494270976061  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]


output ignored...



... output resumed

TIME =  0.57592186E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.18572590E-22
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.71320180E-17 AND  -0.71320180E-17
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.13795042E-02
 U-FRACTION IN SYSTEM:  C = .00698538137740139  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUSTENITE

  CPU time used in timestep                    1 seconds
 7.876430368074911E-006        7.877230502301119E-006        8.670326884772467E-
020       TIME =  0.67592186E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.86703269E-19
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.67714996E-17 AND   0.67714996E-17
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.13795049E-02
 U-FRACTION IN SYSTEM:  C = .00698537447225076  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: FERRITE

  CPU time used in timestep                    0 seconds
 1.197242411328478E-004        1.197253828931874E-004        2.219521099311381E-
025       TIME =  0.77592186E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.22195211E-24
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.47013865E-16 AND  -0.47013865E-16
```

```
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.13795002E-02
 U-FRACTION IN SYSTEM:  C = .00698542241404763  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUSTENITE

  CPU time used in timestep                    0 seconds
 2.955421017074509E-002        2.955388709148415E-002        2.998282669477928E-
017       TIME =  0.87592186E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.29982827E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.88900282E-15 AND  -0.88900282E-15
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.13794113E-02
 U-FRACTION IN SYSTEM:  C = .00698632896344563  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUSTENITE

  CPU time used in timestep                    0 seconds
 1.209637748021748E-005        1.209761347466415E-005        5.339093791545415E-
023       TIME =  0.97592186E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.53390938E-22
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.83410991E-15 AND   0.83410991E-15
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.13794947E-02
 U-FRACTION IN SYSTEM:  C = .00698547839039059  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]
  32  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: FERRITE

  CPU time used in timestep                    0 seconds
 3.580785187466553E-006        3.581416153708028E-006        4.119529880739355E-
020       TIME =  0.10000000E+10 DT =   24078140.     SUM OF SQUARES =  0.41195299E-19
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.11040702E-15 AND  -0.11040702E-15
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.13794921E-02
 U-FRACTION IN SYSTEM:  C = .00698550549904436  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-04
 DELETING TIME-RECORD FOR TIME   0.30000000E-04
 DELETING TIME-RECORD FOR TIME   0.70000000E-04
 DELETING TIME-RECORD FOR TIME   0.15000000E-03
 DELETING TIME-RECORD FOR TIME   0.31000000E-03
 DELETING TIME-RECORD FOR TIME   0.63000000E-03
 DELETING TIME-RECORD FOR TIME   0.12700000E-02
 DELETING TIME-RECORD FOR TIME   0.25500000E-02
 DELETING TIME-RECORD FOR TIME   0.51100000E-02
 DELETING TIME-RECORD FOR TIME   0.10230000E-01
 DELETING TIME-RECORD FOR TIME   0.20470000E-01
 DELETING TIME-RECORD FOR TIME   0.40950000E-01
 DELETING TIME-RECORD FOR TIME   0.81910000E-01
 DELETING TIME-RECORD FOR TIME   0.16383000
 DELETING TIME-RECORD FOR TIME   0.32767000
 DELETING TIME-RECORD FOR TIME   0.65535000
 DELETING TIME-RECORD FOR TIME    1.3107100
 DELETING TIME-RECORD FOR TIME    2.6214300
 DELETING TIME-RECORD FOR TIME    5.2428700
 DELETING TIME-RECORD FOR TIME    10.485750
 DELETING TIME-RECORD FOR TIME    20.971510
 DELETING TIME-RECORD FOR TIME    41.943030
 DELETING TIME-RECORD FOR TIME    83.886070
 DELETING TIME-RECORD FOR TIME    167.77215
 DELETING TIME-RECORD FOR TIME    335.54431
 DELETING TIME-RECORD FOR TIME    671.08863
 DELETING TIME-RECORD FOR TIME    1342.1773
 DELETING TIME-RECORD FOR TIME    2684.3546
 DELETING TIME-RECORD FOR TIME    5368.7091
 DELETING TIME-RECORD FOR TIME    10737.418
 DELETING TIME-RECORD FOR TIME    21474.836
 DELETING TIME-RECORD FOR TIME    42949.673
 DELETING TIME-RECORD FOR TIME    85899.346
 DELETING TIME-RECORD FOR TIME    171798.69
 DELETING TIME-RECORD FOR TIME    343597.38
 DELETING TIME-RECORD FOR TIME    687194.77
 DELETING TIME-RECORD FOR TIME    1374389.5
 DELETING TIME-RECORD FOR TIME    2748779.1
 DELETING TIME-RECORD FOR TIME    5497558.1
 DELETING TIME-RECORD FOR TIME    10995116.
 DELETING TIME-RECORD FOR TIME    21990233.
 DELETING TIME-RECORD FOR TIME    43980465.
 DELETING TIME-RECORD FOR TIME    87960930.
 DELETING TIME-RECORD FOR TIME   0.17592186E+09
 DELETING TIME-RECORD FOR TIME   0.27592186E+09
 DELETING TIME-RECORD FOR TIME   0.37592186E+09
 DELETING TIME-RECORD FOR TIME   0.47592186E+09
 DELETING TIME-RECORD FOR TIME   0.57592186E+09
 DELETING TIME-RECORD FOR TIME   0.67592186E+09
 DELETING TIME-RECORD FOR TIME   0.77592186E+09
 DELETING TIME-RECORD FOR TIME   0.87592186E+09

 KEEPING TIME-RECORD FOR TIME   0.97592186E+09
 AND FOR TIME                   0.10000000E+10
 WORKSPACE RECLAIMED

 TIMESTEP AT    0.100000000E+10 SELECTED

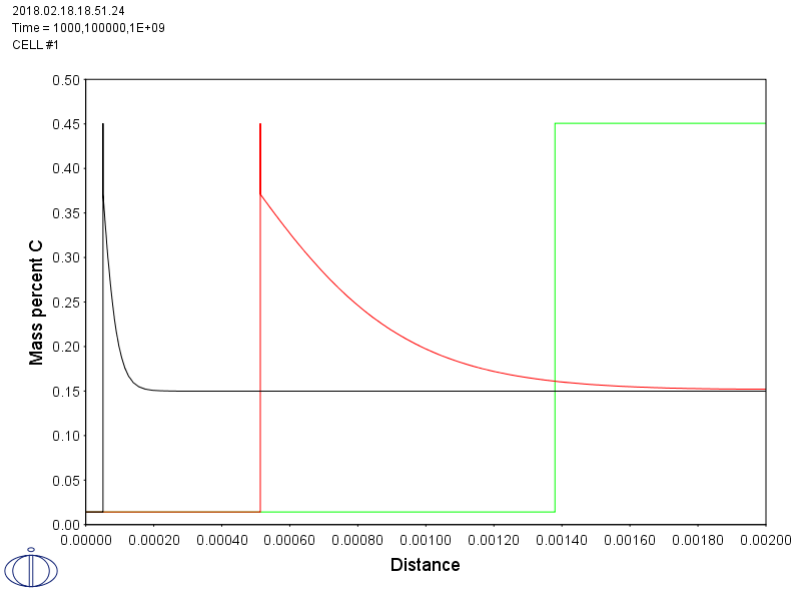
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ THE SIMULATION IS FINISHED
DIC> @@
DIC>
DIC> set-inter
 --OK---
DIC>
```

exb1a-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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

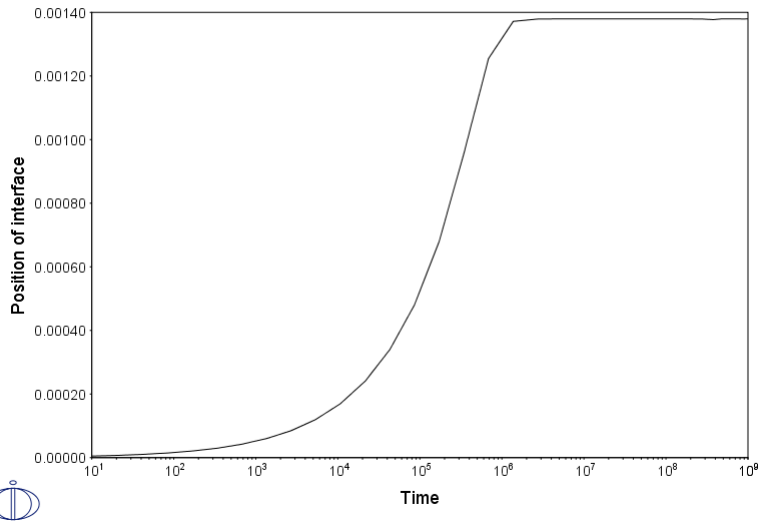
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson

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: plot
```



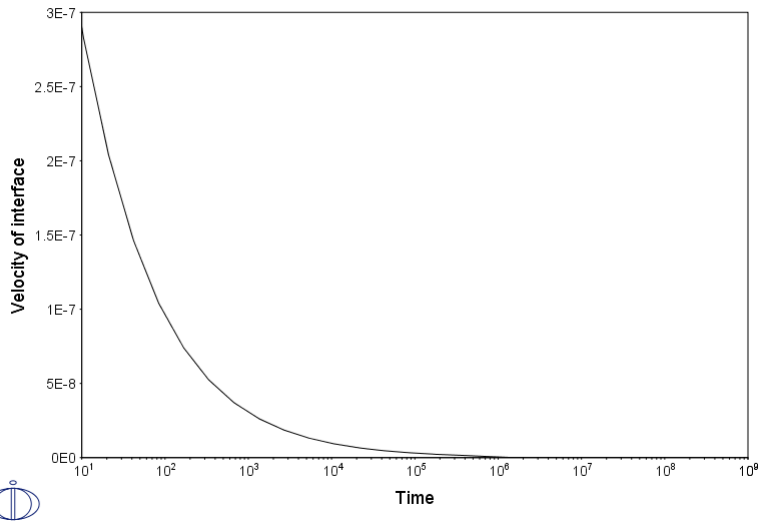

```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ PLOT THE POSITION OF THE BCC/FCC INTERPHASE
POST-1: @@
POST-1: s-d-a x time
  INFO: Time is set as independent variable
POST-1: s-d-a y
VARIABLE : pos
INTERFACE : aus
UPPER OR LOWER INTERFACE OF REGION AUSTENITE#1 /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: plot
```

2018.02.18.18.51.25
LOWER INTERFACE OF REGION "AUSTENITE#1"
CELL #1



POST-1:
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
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: plot

2018.02.18.18.51.25
LOWER INTERFACE OF REGION "AUSTENITE#1"
CELL #1

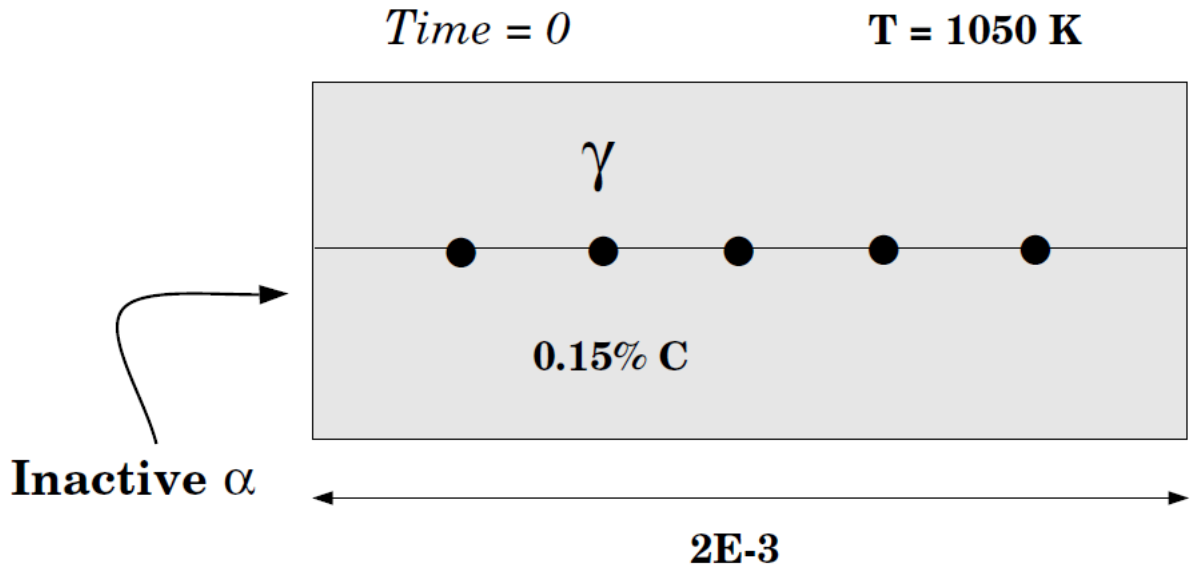


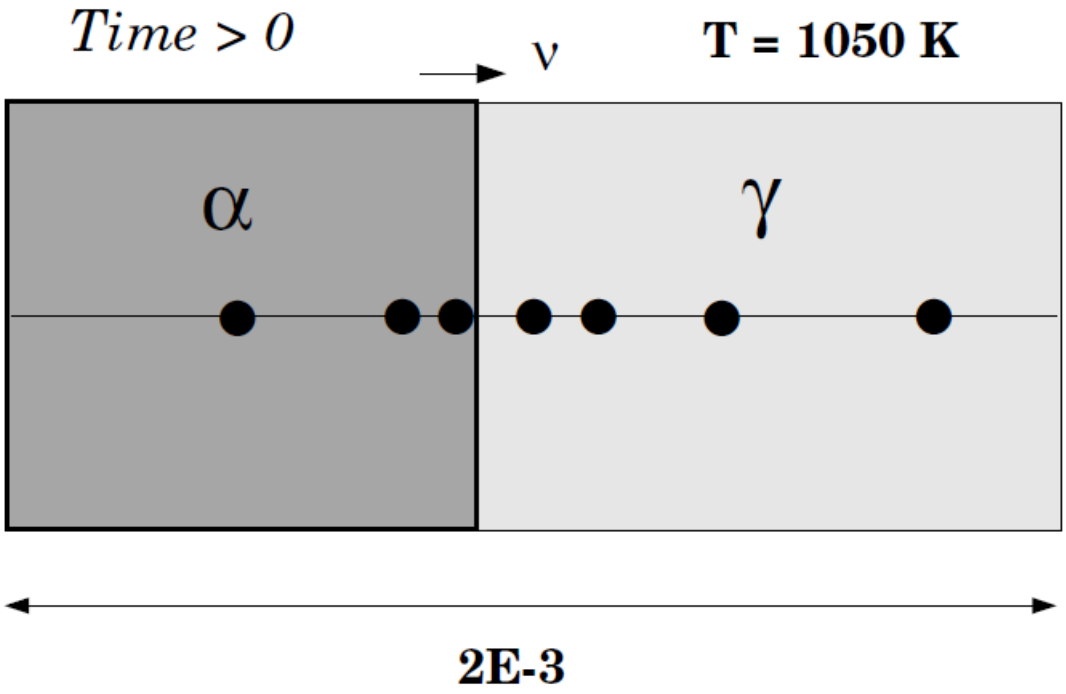
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: set-inter
--OK---
POST-1:

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

```
About Stockholm, Sweden

 Software  (build 12987) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri Feb 16 15:22:08 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb1b\setup.DCM" @@
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
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

 VA                     /-  DEFINED
 L12_FCC                B2_BCC                 DICTRA_FCC_A1
   REJECTED
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA
TDB_TCFE9: @@
TDB_TCFE9: sw FEDEMO
 Current database: Iron Demo Database v2.0

 VA                     /-  DEFINED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ DEFINE THE SYSTEM TO WORK WITH
TDB_FEDEMO: @@
TDB_FEDEMO: def-sys fe c
 FE                     C  DEFINED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ EXCLUDE THE THERMODYNAMIC DATA FOR THE PHASES THAT ARE NOT NEEDED
TDB_FEDEMO: @@
TDB_FEDEMO: rej ph * all
 GAS:G                  LIQUID:L               BCC_A2
 CEMENTITE              DIAMOND_FCC_A4         FCC_A1
 GRAPHITE               HCP_A3                 KSI_CARBIDE
 LAVES_PHASE_C14        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
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'P. Franke, Estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
  'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'X.-G. Lu, M. Selleby, B. Sundman, CALPHAD, 29 (2005) 49-55; Fe P-T diagram'
  'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
 -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

 TCFE9   =  Steels/Fe-Alloys  v9.0
 TCFE10  =  Steels/Fe-Alloys  v10.0 SNAPSHOT
 TCFE8   =  Steels/Fe-Alloys  v8.1
 FROST1  =  FROST database v1.0
 TCFE7   =  Steels/Fe-Alloys  v7.0
 TCFE6   =  Steels/Fe-Alloys  v6.2
 TCFE5   =  Steels/Fe-Alloys  v5.0
 TCFE4   =  Steels/Fe-Alloys  v4.1
 TCFE3   =  Steels/Fe-Alloys  v3.1
 TCFE2   =  Steels/Fe-Alloys  v2.1
 TCFE1   =  Steels/Fe-Alloys  v1.0
 TCNI9   =  Ni-Alloys  v9.0 SNAPSHOT
 NI25    =  NI25 database
 TCNI8   =  Ni-Alloys  v8.1
 TCNI7   =  Ni-Alloys  v7.1
 TCNI6   =  Ni-Alloys  v6.0
 TCNI5   =  Ni-Alloys  v5.1
 TCNI4   =  Ni-Alloys  v4.0
 TCNI1   =  Ni-Alloys  v1.3
 TCAL5   =  Al-Alloys  v5.0
 TCAL4   =  Al-Alloys  v4.0
 TCAL3   =  Al-Alloys  v3.0
 TCAL2   =  Al-Alloys  v2.1
 TCAL1   =  Al-Alloys  v1.2
 TCMG4   =  Mg-Alloys  v4.0
```

```
 TCMG3   =  Mg-Alloys  v3.0
 TCMG2   =  Mg-Alloys  v2.0
 TCMG1   =  Mg-Alloys  v1.1
 TCTI1   =  Ti-Alloys  v1.0
 TCCU2   =  Cu-Alloys  v2.0
 TCCU1   =  Cu-Alloys  v1.0
 TCCC1   =  Cemented carbide  v1.0
 TCHEA2  =  High Entropy Alloy  v2.1
 TCHEA1  =  High Entropy Alloy  v1.0
 SSOL6   =  SGTE Alloy Solutions Database v6.0
 SSOL5   =  SGTE Alloy Solutions Database v5.0
 SSOL4   =  SGTE Alloy Solutions Database v4.9g
 SSOL2   =  SGTE Alloy Solutions Database v2.1
 SSUB6   =  SGTE Substances Database v6.0
 SSUB5   =  SGTE Substances Database v5.2
 SSUB4   =  SGTE Substances Database v4.1
 SSUB3   =  SGTE Substances Database v3.3
 SSUB2   =  SGTE Substances Database v2.2
 SNOB3   =  SGTE Noble Metal Alloys Database v3.1
 STBC2   =  SGTE Thermal Barrier Coating TDB v2.2
 STBC1   =  SGTE Thermal Barrier Coating TDB v1.1
 SALT1   =  SGTE Molten Salts Database v1.2
 SEMC2   =  TC Semi-Conductors  v2.1
 SLAG4   =  Fe-containing Slag  v4.1
 SLAG3   =  Fe-containing Slag  v3.2
 SLAG2   =  Fe-containing Slag  v2.2
 SLAG1   =  Fe-containing Slag  v1.2
 TCOX7   =  Metal Oxide Solutions  v7.0
 TCOX6   =  Metal Oxide Solutions  v6.0
 TCOX5   =  Metal Oxide Solutions  v5.1
 TCOX4   =  Metal Oxide Solutions  v4.1
 ION3    =  Ionic Solutions  v3.0
 ION2    =  Ionic Solutions  v2.6
 ION1    =  Ionic Solutions  v1.5
 NOX2    =  NPL Oxide Solutions Database v2.1
 TCNOBL1 =  Noble Metals Alloys v1.0
 TCSLD3  =  Solder Alloys  v3.2
 TCSLD2  =  Solder Alloys  v2.0
 TCSI1   =  Ultrapure Silicon  v1.2
 TCMP2   =  Materials Processing  v2.5
 TCES1   =  Combustion/Sintering  v1.1
 TCSC1   =  Super Conductor  v1.0
 TCFC1   =  SOFC Database v1.0
 NUMT2   =  Nuclear Materials  v2.1
 NUOX4   =  Nuclear Oxides  v4.2
 NUCL15  =  IRSN NUCLEA-15_4
 NUCL10  =  ThermoData NUCLEA Alloys-oxides TDB v10.2
 MEPH15  =  IRSN Mephista-15_1
 MEPH11  =  ThermoData MEPHISTA Nuclear Fuels TDB v11.2
 TCAQ3   =  Aqueous Solution  v3.0
 TCAQ2   =  Aqueous Solution  v2.6
 AQS2    =  TGG Aqueous Solution Database v2.6
 GCE2    =  TGG Geochemical/Environmental TDB v2.3
 FEDEMO  =  Iron Demo Database v2.0
 ALDEMO  =  Aluminum Demo Database v2.0
 NIDEMO  =  Nickel Demo Database v1.0
 CUDEMO  =  Copper Demo Database v1.0
 SLDEMO  =  Solder Demo Database v1.0
 OXDEMO  =  Oxide Demo Database v1.0
 SUBDEMO =  Substance Demo Database v1.0
 PTERN   =  Public Ternary Alloys TDB v1.3
 PAQ2    =  Public Aqueous Soln (SIT) TDB v2.4
 PG35    =  G35 Binary Semi-Conductors TDB v1.2
 PURE5   =  SGTE Unary (Pure Elements) TDB v5.1
 MOB2    =  Alloys Mobility  v2.7
 MOB1    =  Alloys Mobility  v1.3
 MOBFE1  =  Steels/Fe-Alloys Mobility  v1.0
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBNI4  =  Ni-Alloys Mobility  v4.0
 MOBNI3  =  Ni-Alloys Mobility  v3.1
 MOBNI2  =  Ni-Alloys Mobility  v2.4
 MOBNI1  =  Ni-Alloys Mobility  v1.0
 MOBAL3  =  Al-Alloys Mobility  v3.0
 MOBAL2  =  Al-Alloys Mobility  v2.0
 MOBAL1  =  Al-Alloys Mobility  v1.0
 MOBCU1  =  Cu-Alloys Mobility  v1.0
 MOBCU2  =  Cu-Alloys Mobility  v2.0
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBSLD1 =  Solder-Alloys Mobility  v1.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0 SNAPSHOT
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v1.0
 MFEDEMO =  Fe-Alloys Mobility demo database v2.0
 MNIDEMO =  Ni-Alloys Mobility demo database v1.0
 MCUDEMO =  Cu-Alloys Mobility demo database v1.0
 USER    =  User defined Database

DATABASE NAME /FEDEMO/: MFEDEMO
 Current database: Fe-Alloys Mobility demo database v2.0

 VA  DEFINED
APP: def-sys fe c
 FE                     C  DEFINED
APP: rej ph * all
 BCC_A2                 FCC_A1  REJECTED
APP: res ph fcc bcc
 FCC_A1                 BCC_A2  RESTORED
APP: get
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'This parameter has not been assessed'
  'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'
  'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
      -Ni'
  'B. Jonsson: Z. Metallkunde 85(1994)498-501; C and N diffusion in bcc Cr
      -Fe-Ni'
  'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
```

```
     in bcc Fe'
 -OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP
APP: @@
APP: go d-m
 NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> 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/: AUTO
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> @@
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 /NO/:
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 (0 -> 0.5 -> 1): /.5/: 1.0
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /NO/:
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

 This file contains results from a previous SIMULATE_REACTION command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous simulation.

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

exb1b-run

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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
 Region: AUSTENITE
 single geometric dense at   0.0000
  1.2284      102
 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]
 INFO: PHASE BCC_A2 IS SCHEDULED TO APPEAR
   REGION STATUS CHANGE, ITERATING: TIME=  0.50000000E-07
   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
WIDTH OF NEW REGION R_BCC_A2 /1E-06/:
  Trying old scheme                  3
 START VALUE(S) FOR INTERFACE #2 R_BCC_A2/AUSTENITE, CELL #1
 ------------------------------------------------------------
VELOCITY /1/:
  25  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUSTENITE

  Trying old scheme                     3
 U-FRACTION IN SYSTEM:  C = .00698156310125389  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
 U-FRACTION IN SYSTEM:  C = .00698156310125389  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  1  GRIDPOINT(S) ADDED   TO   CELL #1   REGION: R_BCC_A2
 2.641796457611307E-003        2.641820164602526E-003        0.237813344814168        2.896595832939294E-003        2.863309992288289E-
003        2.465854448694629E-003        3.038053031129606E-003        2.558808985662677E-003        2.415833959662654E-
003        2.363564691276574E-003        3.038053031129606E-003        2.415833959662654E-003        2.496303854395677E-
003        2.376837933638304E-003        2.369135026131276E-003        2.366895703929962E-003        2.361896022229608E-
003        2.360225248520155E-003        2.369135026131276E-003        2.361896022229608E-003        2.359389073324242E-
003        2.358662147350008E-003        2.369135026131276E-003        2.359389073324242E-003        2.361278827669174E-
003        2.358761597295600E-003        2.358656989247688E-003        2.358709294258692E-003        2.358624351344181E-
003        2.358591712679603E-003        2.358824313562941E-003        2.358624351344181E-003        2.358620260492668E-
003        2.358624351344181E-003        2.358620260492668E-003        2.358624351344181E-003


     ERROR RETURN FROM NS01A BECAUSE    5 CALLS OF CALFUN FAILED TO IMPROVE THE RESIDUALS

 *** ERROR  1890 IN DCNS01
 *** ERROR RETURN FROM NS01A
 2.641796457611307E-003        2.641796461146320E-003        2.641796457611307E-003        0.237508579819625        2.641796457611307E-
003        2.896591057254211E-003        2.641796461146320E-003        2.641796457611307E-
003        0.237508579819625        2.641796457611307E-003        2.896591057254211E-003        2.641796457611307E-
003        3.038163915823555E-003        2.641796457611307E-003        2.775733791464641E-003        2.641796457611307E-
003        2.558805763209186E-003        2.558805763209186E-003        2.363552975725973E-003        2.363552975725973E-
003        5.738025859318450E-003        2.363552975725973E-003        2.558805763209186E-003        2.363552975816642E-
003        2.363552975725973E-003        3.038163915823555E-003        2.363552975725973E-003        2.415824599932537E-003

output ignored...



... output resumed

 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.16511845E-16 AND  -0.16511845E-16
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13796707E-02
 U-FRACTION IN SYSTEM:  C = .00698367673257223  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUSTENITE

  CPU time used in timestep                     0 seconds
 1.729079514080664E-003        1.729052068274378E-003        5.522801523349699E-
029       TIME =  0.60502330E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.55228015E-28
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.22006832E-15 AND  -0.22006832E-15
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13796487E-02
 U-FRACTION IN SYSTEM:  C = .00698390114458076  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUSTENITE

  CPU time used in timestep                     0 seconds
 9.469801368215668E-005        9.470657444388783E-005        6.819705971244688E-
029       TIME =  0.70502330E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.68197060E-28
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.26147970E-15 AND   0.26147970E-15
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13796749E-02
 U-FRACTION IN SYSTEM:  C = .00698363450382735  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  13  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_BCC_A2

  CPU time used in timestep                     0 seconds
 5.409203794879186E-005        5.409972561753078E-005        3.669117966294266E-
019       TIME =  0.80502330E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.36691180E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.10436852E-15 AND  -0.10436852E-15
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13796644E-02
 U-FRACTION IN SYSTEM:  C = .00698374093236642  FE = 1
```

```
 TOTAL SIZE OF SYSTEM:  .002 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUSTENITE

  CPU time used in timestep                    0 seconds
 9.704708018545921E-006        9.706007738984887E-006        4.992803409075867E-
022       TIME =  0.90502330E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.49928034E-21
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.50465843E-16 AND   0.50465843E-16
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13796695E-02
 U-FRACTION IN SYSTEM:  C = .00698368947043437  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  2  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_BCC_A2

  CPU time used in timestep                    0 seconds
 2.098982308023776E-007        2.099906631861657E-007        4.239461125711217E-
020       TIME =  0.10000000E+10 DT =   94976699.     SUM OF SQUARES =  0.42394611E-19
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.26992581E-16 AND   0.26992581E-16
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13796720E-02
 U-FRACTION IN SYSTEM:  C = .00698366332775786  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   0.60948835E-05
 DELETING TIME-RECORD FOR TIME   0.18034650E-04
 DELETING TIME-RECORD FOR TIME   0.41914184E-04
 DELETING TIME-RECORD FOR TIME   0.89673252E-04
 DELETING TIME-RECORD FOR TIME   0.18519139E-03
 DELETING TIME-RECORD FOR TIME   0.37622766E-03
 DELETING TIME-RECORD FOR TIME   0.75830020E-03
 DELETING TIME-RECORD FOR TIME   0.15224453E-02
 DELETING TIME-RECORD FOR TIME   0.30507355E-02
 DELETING TIME-RECORD FOR TIME   0.61073158E-02
 DELETING TIME-RECORD FOR TIME   0.12220476E-01
 DELETING TIME-RECORD FOR TIME   0.24446798E-01
 DELETING TIME-RECORD FOR TIME   0.48899441E-01
 DELETING TIME-RECORD FOR TIME   0.97804726E-01
 DELETING TIME-RECORD FOR TIME   0.19561530
 DELETING TIME-RECORD FOR TIME   0.39123644
 DELETING TIME-RECORD FOR TIME   0.78247872
 DELETING TIME-RECORD FOR TIME    1.5649633
 DELETING TIME-RECORD FOR TIME    3.1299324
 DELETING TIME-RECORD FOR TIME    6.2598707
 DELETING TIME-RECORD FOR TIME    12.519747
 DELETING TIME-RECORD FOR TIME    25.039500
 DELETING TIME-RECORD FOR TIME    50.079006
 DELETING TIME-RECORD FOR TIME    100.15802
 DELETING TIME-RECORD FOR TIME    200.31604
 DELETING TIME-RECORD FOR TIME    400.63209
 DELETING TIME-RECORD FOR TIME    801.26419
 DELETING TIME-RECORD FOR TIME    1602.5284
 DELETING TIME-RECORD FOR TIME    3205.0568
 DELETING TIME-RECORD FOR TIME    6410.1136
 DELETING TIME-RECORD FOR TIME    12820.227
 DELETING TIME-RECORD FOR TIME    25640.454
 DELETING TIME-RECORD FOR TIME    51280.909
 DELETING TIME-RECORD FOR TIME    102561.82
 DELETING TIME-RECORD FOR TIME    205123.63
 DELETING TIME-RECORD FOR TIME    410247.27
 DELETING TIME-RECORD FOR TIME    820494.54
 DELETING TIME-RECORD FOR TIME    1640989.1
 DELETING TIME-RECORD FOR TIME    3281978.2
 DELETING TIME-RECORD FOR TIME    6563956.3
 DELETING TIME-RECORD FOR TIME    13127913.
 DELETING TIME-RECORD FOR TIME    26255825.
 DELETING TIME-RECORD FOR TIME    52511650.
 DELETING TIME-RECORD FOR TIME   0.10502330E+09
 DELETING TIME-RECORD FOR TIME   0.20502330E+09
 DELETING TIME-RECORD FOR TIME   0.30502330E+09
 DELETING TIME-RECORD FOR TIME   0.40502330E+09
 DELETING TIME-RECORD FOR TIME   0.50502330E+09
 DELETING TIME-RECORD FOR TIME   0.60502330E+09
 DELETING TIME-RECORD FOR TIME   0.70502330E+09
 DELETING TIME-RECORD FOR TIME   0.80502330E+09

 KEEPING TIME-RECORD FOR TIME   0.90502330E+09
 AND FOR TIME                   0.10000000E+10
 WORKSPACE RECLAIMED

 TIMESTEP AT    0.100000000E+10 SELECTED

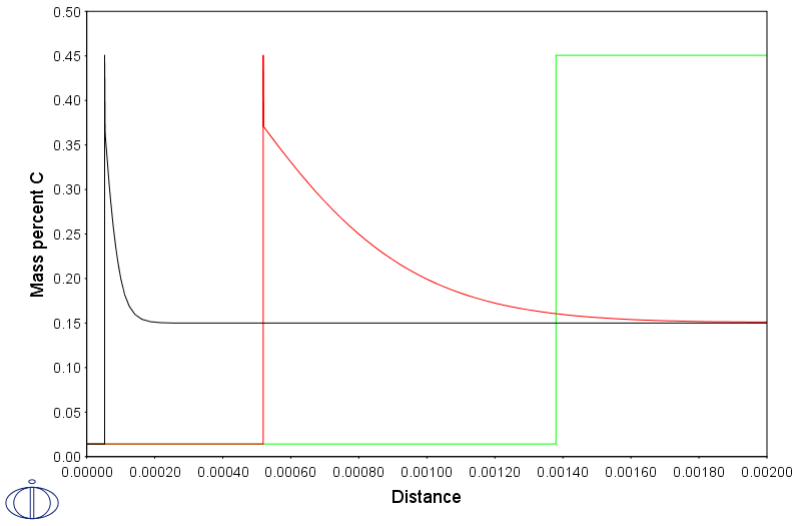
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ THE SIMULATION IS FINISHED
DIC> @@
DIC>
DIC> set-inter
 --OK---
DIC>
```

exb1b-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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

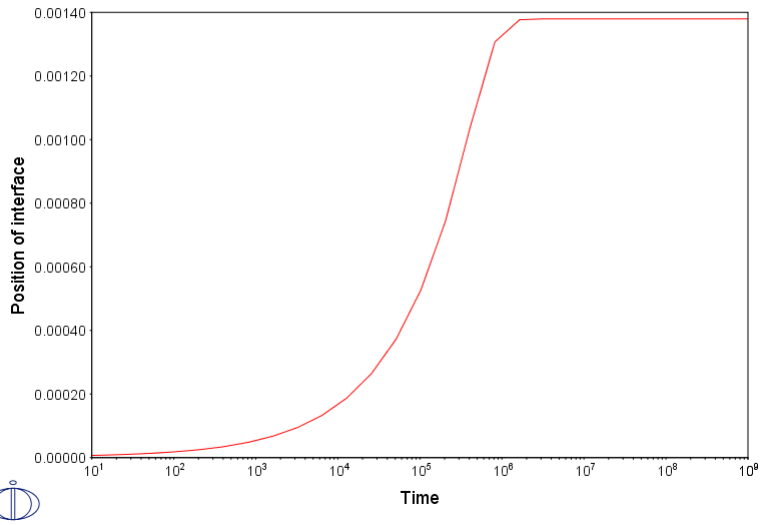
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson

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: plot
   2018.02.18.18.54.27
   Time = 1000,100000,1E+09
   CELL #1
```



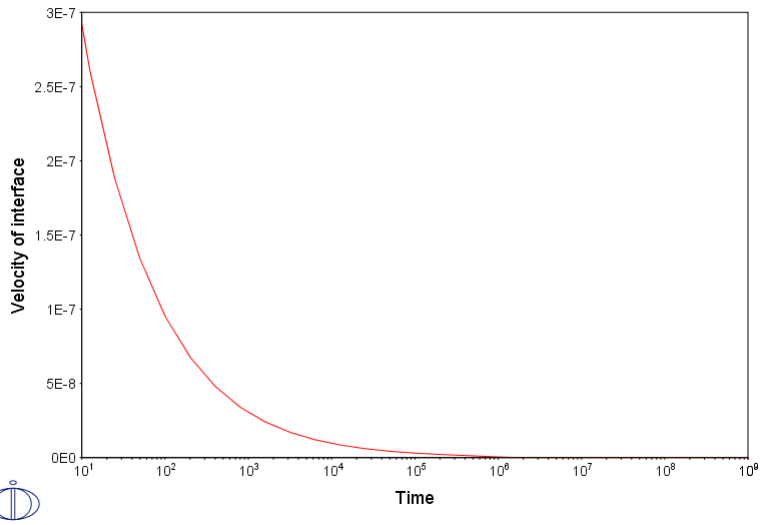

```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ PLOT THE POSITION OF THE BCC/FCC INTERPHASE
POST-1: @@
POST-1: s-d-a x time
  INFO: Time is set as independent variable
POST-1: s-d-a y
VARIABLE : pos
INTERFACE : aus
UPPER OR LOWER INTERFACE OF REGION AUSTENITE#1 /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: plot
```

2018.02.18.18.54.28
LOWER INTERFACE OF REGION "AUSTENITE#1"
CELL #1



POST-1:
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
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: plot

2018.02.18.18.54.28
LOWER INTERFACE OF REGION "AUSTENITE#1"
CELL #1

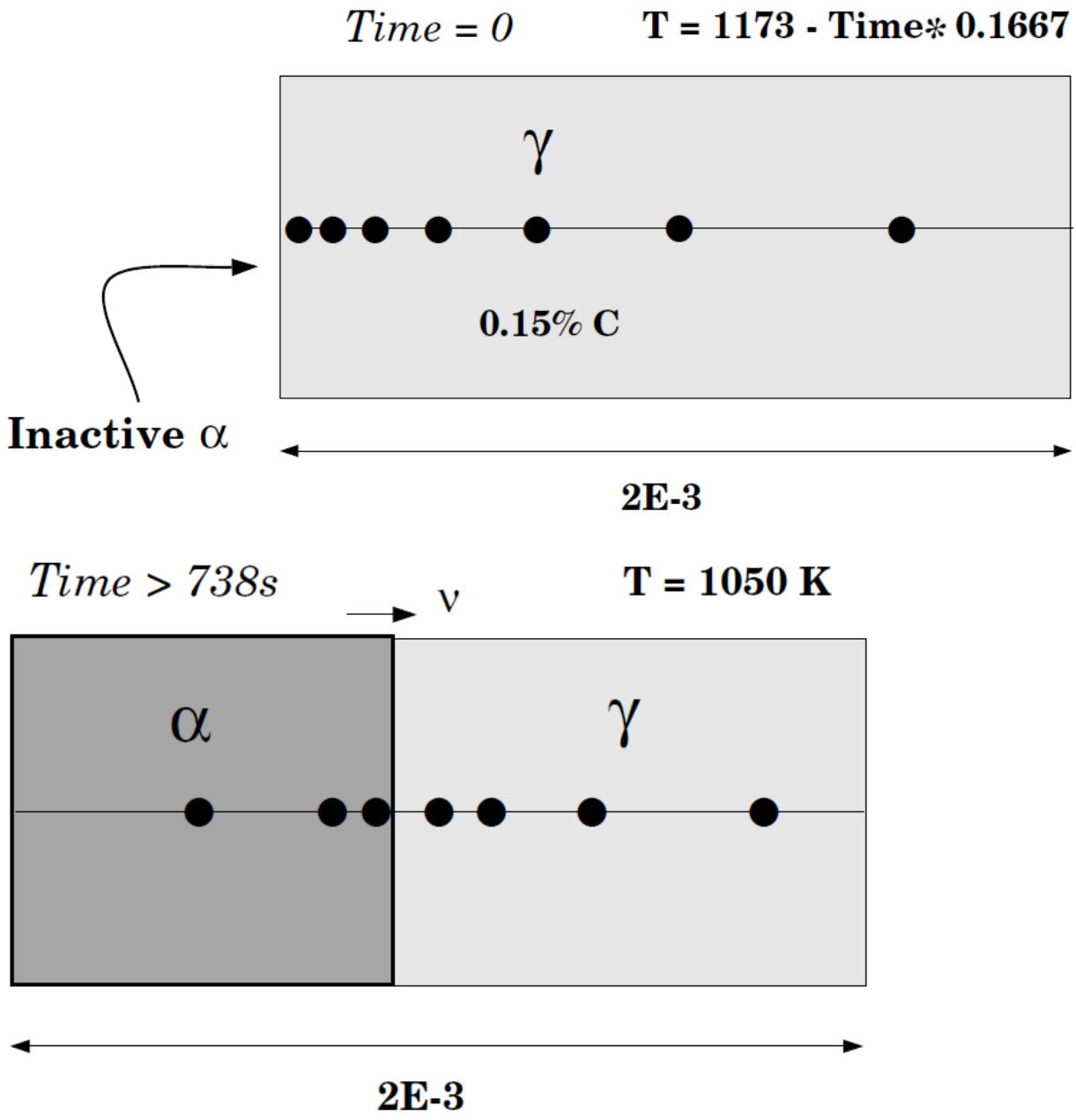


POST-1:
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: set-inter
--OK---
POST-1:

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

```
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 Stockholm, Sweden

 Software  (build 12987) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri Feb 16 15:22:08 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb1c\setup.DCM" @@
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
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

 VA                     /-  DEFINED
 L12_FCC                B2_BCC                 DICTRA_FCC_A1
   REJECTED
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA
TDB_TCFE9: @@
TDB_TCFE9: sw FEDEMO
 Current database: Iron Demo Database v2.0

 VA                     /-  DEFINED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ DEFINE THE SYSTEM TO WORK WITH
TDB_FEDEMO: @@
TDB_FEDEMO: def-sys fe c
 FE                     C  DEFINED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ EXCLUDE THE THERMODYNAMIC DATA FOR THE PHASES THAT ARE NOT NEEDED
TDB_FEDEMO: @@
TDB_FEDEMO: rej ph * all
 GAS:G                  LIQUID:L               BCC_A2
 CEMENTITE              DIAMOND_FCC_A4         FCC_A1
 GRAPHITE               HCP_A3                 KSI_CARBIDE
 LAVES_PHASE_C14        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
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'P. Franke, Estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
  'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'X.-G. Lu, M. Selleby, B. Sundman, CALPHAD, 29 (2005) 49-55; Fe P-T diagram'
  'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
 -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

 TCFE9   =  Steels/Fe-Alloys  v9.0
 TCFE10  =  Steels/Fe-Alloys  v10.0 SNAPSHOT
 TCFE8   =  Steels/Fe-Alloys  v8.1
 FROST1  =  FROST database v1.0
 TCFE7   =  Steels/Fe-Alloys  v7.0
 TCFE6   =  Steels/Fe-Alloys  v6.2
 TCFE5   =  Steels/Fe-Alloys  v5.0
 TCFE4   =  Steels/Fe-Alloys  v4.1
 TCFE3   =  Steels/Fe-Alloys  v3.1
 TCFE2   =  Steels/Fe-Alloys  v2.1
 TCFE1   =  Steels/Fe-Alloys  v1.0
 TCNI9   =  Ni-Alloys  v9.0 SNAPSHOT
 NI25    =  NI25 database
 TCNI8   =  Ni-Alloys  v8.1
 TCNI7   =  Ni-Alloys  v7.1
 TCNI6   =  Ni-Alloys  v6.0
 TCNI5   =  Ni-Alloys  v5.1
 TCNI4   =  Ni-Alloys  v4.0
 TCNI1   =  Ni-Alloys  v1.3
```

```
 TCAL5   =  Al-Alloys  v5.0
 TCAL4   =  Al-Alloys  v4.0
 TCAL3   =  Al-Alloys  v3.0
 TCAL2   =  Al-Alloys  v2.1
 TCAL1   =  Al-Alloys  v1.2
 TCMG4   =  Mg-Alloys  v4.0
 TCMG3   =  Mg-Alloys  v3.0
 TCMG2   =  Mg-Alloys  v2.0
 TCMG1   =  Mg-Alloys  v1.1
 TCTI1   =  Ti-Alloys  v1.0
 TCCU2   =  Cu-Alloys  v2.0
 TCCU1   =  Cu-Alloys  v1.0
 TCCC1   =  Cemented carbide  v1.0
 TCHEA2  =  High Entropy Alloy  v2.1
 TCHEA1  =  High Entropy Alloy  v1.0
 SSOL6   =  SGTE Alloy Solutions Database v6.0
 SSOL5   =  SGTE Alloy Solutions Database v5.0
 SSOL4   =  SGTE Alloy Solutions Database v4.9g
 SSOL2   =  SGTE Alloy Solutions Database v2.1
 SSUB6   =  SGTE Substances Database v6.0
 SSUB5   =  SGTE Substances Database v5.2
 SSUB4   =  SGTE Substances Database v4.1
 SSUB3   =  SGTE Substances Database v3.3
 SSUB2   =  SGTE Substances Database v2.2
 SNOB3   =  SGTE Noble Metal Alloys Database v3.1
 STBC2   =  SGTE Thermal Barrier Coating TDB v2.2
 STBC1   =  SGTE Thermal Barrier Coating TDB v1.1
 SALT1   =  SGTE Molten Salts Database v1.2
 SEMC2   =  TC Semi-Conductors  v2.1
 SLAG4   =  Fe-containing Slag  v4.1
 SLAG3   =  Fe-containing Slag  v3.2
 SLAG2   =  Fe-containing Slag  v2.2
 SLAG1   =  Fe-containing Slag  v1.2
 TCOX7   =  Metal Oxide Solutions  v7.0
 TCOX6   =  Metal Oxide Solutions  v6.0
 TCOX5   =  Metal Oxide Solutions  v5.1
 TCOX4   =  Metal Oxide Solutions  v4.1
 ION3    =  Ionic Solutions  v3.0
 ION2    =  Ionic Solutions  v2.6
 ION1    =  Ionic Solutions  v1.5
 NOX2    =  NPL Oxide Solutions Database v2.1
 TCNOBL1 =  Noble Metals Alloys v1.0
 TCSLD3  =  Solder Alloys  v3.2
 TCSLD2  =  Solder Alloys  v2.0
 TCSI1   =  Ultrapure Silicon  v1.2
 TCMP2   =  Materials Processing  v2.5
 TCES1   =  Combustion/Sintering  v1.1
 TCSC1   =  Super Conductor  v1.0
 TCFC1   =  SOFC Database v1.0
 NUMT2   =  Nuclear Materials  v2.1
 NUOX4   =  Nuclear Oxides  v4.2
 NUCL15  =  IRSN NUCLEA-15_4
 NUCL10  =  ThermoData NUCLEA Alloys-oxides TDB v10.2
 MEPH15  =  IRSN Mephista-15_1
 MEPH11  =  ThermoData MEPHISTA Nuclear Fuels TDB v11.2
 TCAQ3   =  Aqueous Solution  v3.0
 TCAQ2   =  Aqueous Solution  v2.6
 AQS2    =  TGG Aqueous Solution Database v2.6
 GCE2    =  TGG Geochemical/Environmental TDB v2.3
 FEDEMO  =  Iron Demo Database v2.0
 ALDEMO  =  Aluminum Demo Database v2.0
 NIDEMO  =  Nickel Demo Database v1.0
 CUDEMO  =  Copper Demo Database v1.0
 SLDEMO  =  Solder Demo Database v1.0
 OXDEMO  =  Oxide Demo Database v1.0
 SUBDEMO =  Substance Demo Database v1.0
 PTERN   =  Public Ternary Alloys TDB v1.3
 PAQ2    =  Public Aqueous Soln (SIT) TDB v2.4
 PG35    =  G35 Binary Semi-Conductors TDB v1.2
 PURE5   =  SGTE Unary (Pure Elements) TDB v5.1
 MOB2    =  Alloys Mobility  v2.7
 MOB1    =  Alloys Mobility  v1.3
 MOBFE1  =  Steels/Fe-Alloys Mobility  v1.0
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBNI4  =  Ni-Alloys Mobility  v4.0
 MOBNI3  =  Ni-Alloys Mobility  v3.1
 MOBNI2  =  Ni-Alloys Mobility  v2.4
 MOBNI1  =  Ni-Alloys Mobility  v1.0
 MOBAL3  =  Al-Alloys Mobility  v3.0
 MOBAL2  =  Al-Alloys Mobility  v2.0
 MOBAL1  =  Al-Alloys Mobility  v1.0
 MOBCU1  =  Cu-Alloys Mobility  v1.0
 MOBCU2  =  Cu-Alloys Mobility  v2.0
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBSLD1 =  Solder-Alloys Mobility  v1.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0 SNAPSHOT
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v1.0
 MFEDEMO =  Fe-Alloys Mobility demo database v2.0
 MNIDEMO =  Ni-Alloys Mobility demo database v1.0
 MCUDEMO =  Cu-Alloys Mobility demo database v1.0
 USER    =  User defined Database

DATABASE NAME /FEDEMO/: MFEDEMO
 Current database: Fe-Alloys Mobility demo database v2.0

 VA  DEFINED
APP: def-sys fe c
 FE                    C  DEFINED
APP: rej ph * all
 BCC_A2                FCC_A1  REJECTED
APP: res ph fcc bcc
 FCC_A1                BCC_A2  RESTORED
APP: get
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'This parameter has not been assessed'
```

```
  'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'
  'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
      -Ni'
  'B. Jonsson: Z. Metallkunde 85(1994)498-501; C and N diffusion in bcc Cr
      -Fe-Ni'
  'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
      in bcc Fe'
 -OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP
APP: @@
APP: go d-m
 NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER GLOBAL CONDITION T
DIC> @@
DIC> @@ 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 /NO/:
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 (0 -> 0.5 -> 1): /.5/: 1.0
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /NO/:
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>AboutDIC>DIC>MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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
 single geometric dense at   0.0000
  1.2084      101
 U-FRACTION IN SYSTEM:  C = .0069849591638311  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
 U-FRACTION IN SYSTEM:  C = .0069849591638311  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 = .0069849591638311  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.24660033E-05 DT =  0.23660033E-05 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 =  0.71980098E-05 DT =  0.47320065E-05 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 =  0.16662023E-04 DT =  0.94640131E-05 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 =  0.35590049E-04 DT =  0.18928026E-04 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 =  0.73446101E-04 DT =  0.37856052E-04 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 =  0.14915821E-03 DT =  0.75712105E-04 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 =  0.30058241E-03 DT =  0.15142421E-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 =  0.60343083E-03 DT =  0.30284842E-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 =  0.12091277E-02 DT =  0.60569684E-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 =  0.24205213E-02 DT =  0.12113937E-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 =  0.48433087E-02 DT =  0.24227873E-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 =  0.96888834E-02 DT =  0.48455747E-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 =  0.19380033E-01 DT =  0.96911494E-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 =  0.38762332E-01 DT =  0.19382299E-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 =  0.77526929E-01 DT =  0.38764598E-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 =  0.15505612     DT =  0.77529195E-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 =  0.31011451     DT =  0.15505839     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 =  0.62023129     DT =  0.31011678     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 =   1.2404649     DT =  0.62023356     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0069849591638311  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    0 seconds
 TIME =   2.4809320     DT =   1.2404671     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0069849591638311  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    0 seconds
 TIME =   4.9618662     DT =   2.4809342     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 =   9.9237347     DT =   4.9618685     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 =   19.847472     DT =   9.9237370     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0069849591638311  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    0 seconds
 TIME =   39.694946     DT =   19.847474     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0069849591638311  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    0 seconds
 TIME =   76.594946     DT =   36.900000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698495916383102  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    0 seconds
 TIME =   113.49495     DT =   36.900000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698495916383101  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]


output ignored...



... output resumed

 2.463921881023055E-005        2.464611889068162E-005        1.141415285565403E-
020       TIME =  0.43290424E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.11414153E-19
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.97384679E-17 AND  -0.97384679E-17
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13794958E-02
 U-FRACTION IN SYSTEM:  C = .0069854599126091  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUSTENITE

  CPU time used in timestep                    0 seconds
 4.949616379512275E-006        4.950482483474543E-006        1.854038485181288E-
029       TIME =  0.53290424E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.18540385E-28
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.13648563E-17 AND   0.13648563E-17
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13794960E-02
 U-FRACTION IN SYSTEM:  C = .00698545852081245  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_BCC_A2

  CPU time used in timestep                    0 seconds
 1.340510105722721E-003        1.340512103268622E-003        7.701100735462078E-
024       TIME =  0.63290424E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.77011007E-23
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.17818395E-15 AND  -0.17818395E-15
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13794782E-02
 U-FRACTION IN SYSTEM:  C = .00698564022173987  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUSTENITE

  CPU time used in timestep                    0 seconds
 2.723524390729022E-003        2.723561562249139E-003        1.918538267205872E-
019       TIME =  0.73290424E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.19185383E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.23842430E-14 AND   0.23842430E-14
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13797166E-02
 U-FRACTION IN SYSTEM:  C = .00698320891878288  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  31  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_BCC_A2

  CPU time used in timestep                    0 seconds
 7.962243396459047E-006        7.964932945973571E-006        6.487515206846051E-
022       TIME =  0.83290424E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.64875152E-21
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.95299444E-15 AND   0.95299444E-15
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13798119E-02
 U-FRACTION IN SYSTEM:  C = .00698223711426177  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  12  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_BCC_A2

  CPU time used in timestep                    0 seconds
 1.440034499273632E-005        1.440179063999719E-005        7.407006665689525E-
029       TIME =  0.93290424E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.74070067E-28
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.92672920E-15 AND  -0.92672920E-15
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13797192E-02
 U-FRACTION IN SYSTEM:  C = .00698318213512128  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    0 seconds
 3.754518665345077E-006        3.755236501551250E-006        2.175886568427993E-
023       TIME =  0.10000000E+10 DT =   67095763.     SUM OF SQUARES =  0.21758866E-22
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.41881901E-16 AND   0.41881901E-16
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13797220E-02
 U-FRACTION IN SYSTEM:  C = .00698315347948737  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    769.68667
 DELETING TIME-RECORD FOR TIME    833.06001
 DELETING TIME-RECORD FOR TIME    959.80670
 DELETING TIME-RECORD FOR TIME    1213.3001
 DELETING TIME-RECORD FOR TIME    1720.2868
 DELETING TIME-RECORD FOR TIME    2734.2603
 DELETING TIME-RECORD FOR TIME    4762.2072
 DELETING TIME-RECORD FOR TIME    8818.1011
 DELETING TIME-RECORD FOR TIME    16929.889
 DELETING TIME-RECORD FOR TIME    33153.464
 DELETING TIME-RECORD FOR TIME    65600.616
 DELETING TIME-RECORD FOR TIME    130494.92
 DELETING TIME-RECORD FOR TIME    260283.52
 DELETING TIME-RECORD FOR TIME    519860.73
 DELETING TIME-RECORD FOR TIME    1039015.1
 DELETING TIME-RECORD FOR TIME    2077324.0
 DELETING TIME-RECORD FOR TIME    4153941.7
 DELETING TIME-RECORD FOR TIME    8307177.0
 DELETING TIME-RECORD FOR TIME    16613648.
 DELETING TIME-RECORD FOR TIME    33226589.
 DELETING TIME-RECORD FOR TIME    66452472.
 DELETING TIME-RECORD FOR TIME   0.13290424E+09
 DELETING TIME-RECORD FOR TIME   0.23290424E+09
 DELETING TIME-RECORD FOR TIME   0.33290424E+09
 DELETING TIME-RECORD FOR TIME   0.43290424E+09
 DELETING TIME-RECORD FOR TIME   0.53290424E+09
 DELETING TIME-RECORD FOR TIME   0.63290424E+09
 DELETING TIME-RECORD FOR TIME   0.73290424E+09
```

```
 DELETING TIME-RECORD FOR TIME   0.83290424E+09

 KEEPING TIME-RECORD FOR TIME   0.93290424E+09
 AND FOR TIME                   0.10000000E+10
 WORKSPACE RECLAIMED

 TIMESTEP AT    0.100000000E+10 SELECTED

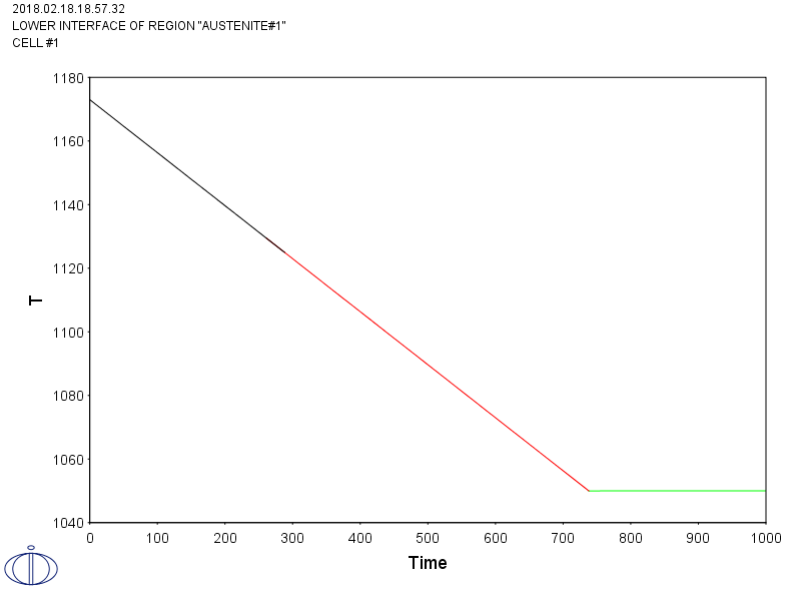
DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ THE SIMULATION IS FINISHED
DIC> @@
DIC>
DIC> set-inter
 --OK---
DIC>
```

exb1c-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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

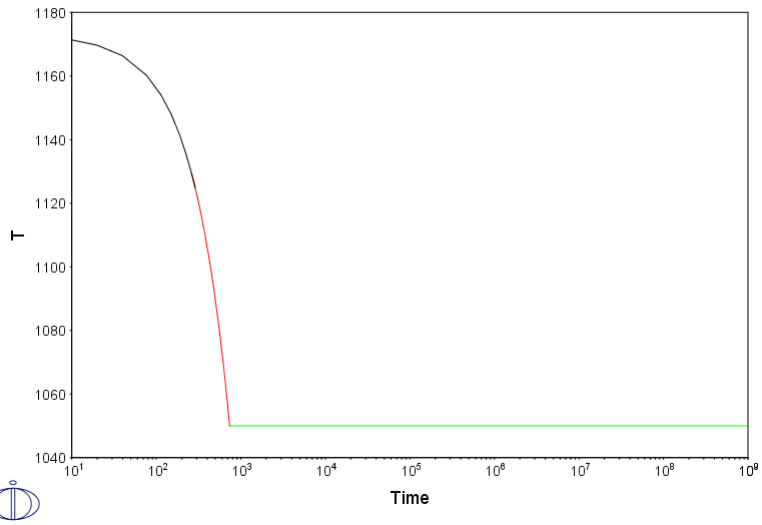
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson

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: plot
```



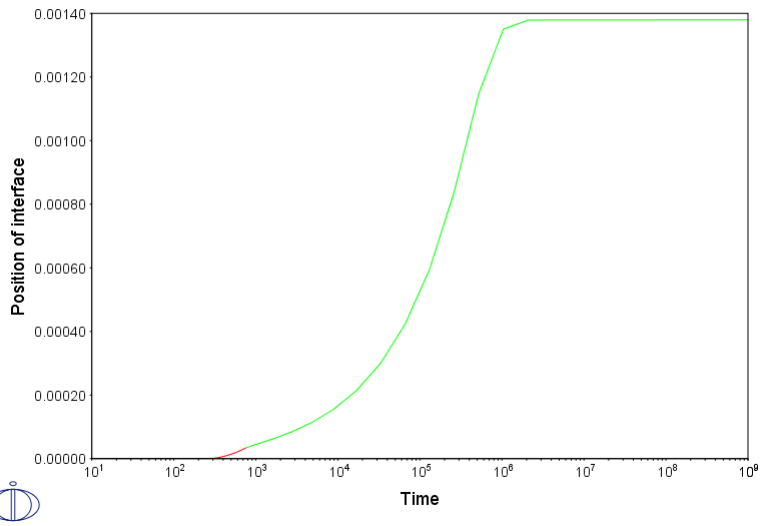

```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: @@
POST-1: @@ PLOT VS. LOG TIME
POST-1: @@
POST-1: set-axis-type x log
POST-1: s-s-s x n 10 1e9
POST-1:
POST-1: plot
```

2018.02.18.18.57.32
LOWER INTERFACE OF REGION "AUSTENITE#1"
CELL #1



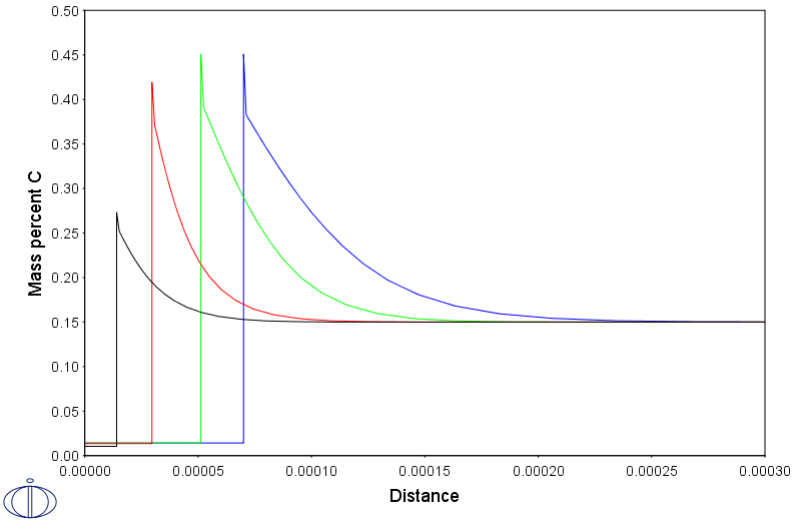

```
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: @@
POST-1: @@ PLOT THE POSITION OF THE BCC/FCC INTERPHASE
POST-1: @@
POST-1: s-d-a
AXIS (X, Y OR Z) : y
VARIABLE : position
INTERFACE : austenite
UPPER OR LOWER INTERFACE OF REGION AUSTENITE#1 /LOWER/: lower
POST-1:
POST-1: plot
```

2018.02.18.18.57.33
LOWER INTERFACE OF REGION "AUSTENITE#1"
CELL #1




```
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: plot
```

2018.02.18.18.57.33
Time = 500,700,1200,2000
CELL #1

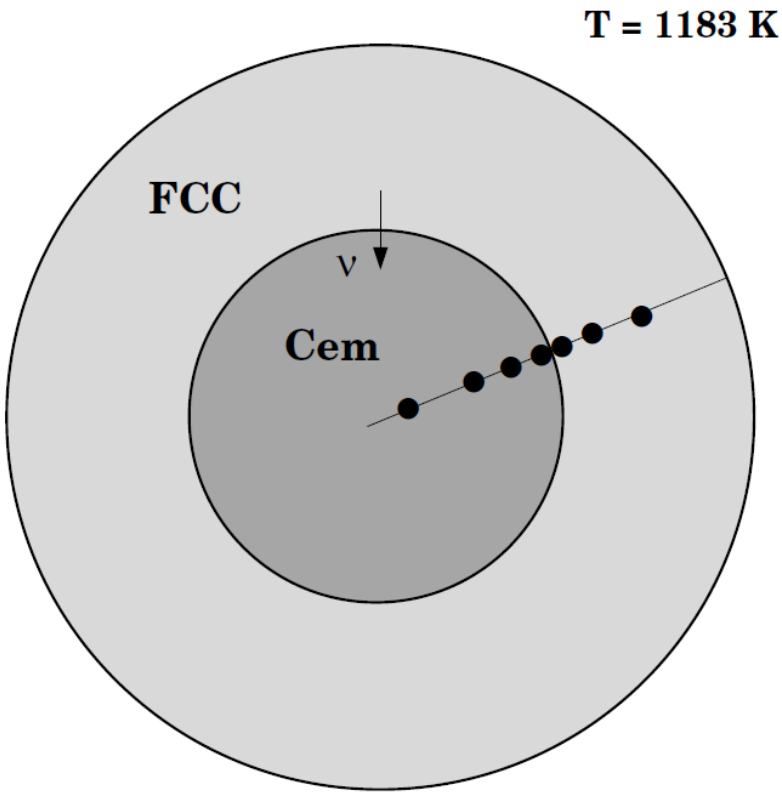


POST-1:
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1: set-inter
--OK---
POST-1:

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

```
About Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 12987) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri Feb 16 15:22:08 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb2\setup.DCM"SYS: ?@@
 NO SUCH COMMAND, USE HELP
SYS: @@ Moving boundary problem.
SYS: @@ Cementite dissolution in an Fe-Cr-C alloy
SYS: @@ This example calculates the dissolution of a spherical cementite
SYS: @@ particle in an austenite matrix.
SYS: @@ This case is from Z.-K. Liu, L. Höglund, B. Jönsson and J. Ågren:
SYS: @@ Metall. Trans.A, v.22A (1991), pp. 1745-1752.
SYS: ----------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS: @@
SYS: @@ In order to achieve the correct average composition in the calculation
SYS: @@ it is necessary to take into account that the calculation is set up
SYS: @@ using the volume fraction of the phases. To calculate the initial
SYS: @@ state at the heat treatment temperature we first need to determine
SYS: @@ the state at the normalizing temperature. To calculate the volume
SYS: @@ fraction of the phases we need to enter a number of functions
SYS: @@ that calculate these quantities. NOTE: The volume fractions are
SYS: @@ determined by assuming that only the substitutional components
SYS: @@ contribute to the volume of a system, whereas the interstitial
SYS: @@ components do not.
SYS: @@
SYS: @@ The total radius of the system can be calculated from the relation:
SYS: @@
SYS: @@    3
SYS: @@   R       V
SYS: @@    cem     cem    f
SYS: @@   ----  = ---- = V
SYS: @@    3              cem
SYS: @@   R       V
SYS: @@    tot     tot
SYS: @@
SYS: @@
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASES
SYS: @@
SYS: go da
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

 VA                       /-  DEFINED
 L12_FCC                  B2_BCC                   DICTRA_FCC_A1
   REJECTED
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE THE DATA
TDB_TCFE9: @@
TDB_TCFE9: sw FEDEMO
 Current database: Iron Demo Database v2.0

 VA                       /-  DEFINED
TDB_FEDEMO: def-sys fe cr c
 FE                       CR                       C
   DEFINED
TDB_FEDEMO: rej ph * all
 GAS:G                    LIQUID:L                 BCC_A2
 CEMENTITE                CHI_A12                  DIAMOND_FCC_A4
 FCC_A1                   GRAPHITE                 HCP_A3
 KSI_CARBIDE              LAVES_PHASE_C14          M23C6
 M3C2                     M5C2                     M7C3
 SIGMA  REJECTED
TDB_FEDEMO: res ph fcc bcc cem
 FCC_A1                   BCC_A2                   CEMENTITE
   RESTORED
TDB_FEDEMO: get
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'J-O. Andersson, CALPHAD, 11 (1987) 271-276; TRITA 0314; C-CR'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'P. Franke, Estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
  'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'X.-G. Lu, M. Selleby, B. Sundman, CALPHAD, 29 (2005) 49-55; Fe P-T diagram'
  'A.V. Khvan, B. Hallstedt, C. Broeckmann, CALPHAD, 46, 24 -33(2014); Cr-Fe
      -C'
  'J-O. Andersson, Metall. Trans. A, 19A (1988) 627-636 TRITA 0207 (1986); C
      -CR-FE'
  'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270
      (1986); CR-FE'
  'B.-J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
  'P. Villars and L.D. Calvert (1985). Pearson`s handbook of
      crystallographic data for intermetallic phases. Metals park, Ohio.
      American Society for Metals; Molar volumes'
  'B. Hallstedt, D. Djurovic, J. von Appen, R. Dronskowski, A. Dick, F.
      Koermann, T. Hickel, J. Neugebauer, CALPHAD, 34, 129 -33(2010); Fe-C'
  'J. Bratberg, Z. Metallkd., 96 (2005) 335-344; Fe-Cr-Mo-C'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, 2016; FCC Fe-Cr-C and C-Cr-Ni'
  'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
 -OK-
TDB_FEDEMO:
TDB_FEDEMO: @@
```

```
TDB_FEDEMO: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE THE MOBILITY DATA
TDB_FEDEMO: @@
TDB_FEDEMO: app mobfe2
 Current database: Steels/Fe-Alloys Mobility  v2.0
   TCS Steel Mobility Database Version 2.0 from 2011-12-09.

 VA  DEFINED
APP: def-sp fe cr c
 FE                     CR                     C
   DEFINED
APP: rej ph * all
 BCC_A2                 CEMENTITE              FCC_A1
 FE4N_LP1               HCP_A3                 LIQUID:L
   REJECTED
APP: res ph fcc cementite
 FCC_A1                 CEMENTITE  RESTORED
APP: get
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'This parameter has not been assessed'
  'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'
  'B. Jonsson: Z. Metallkunde 85(1994)502-509; C diffusion in fcc Cr-Fe-Ni'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Fe diffusion fcc Cr-Fe'
  'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
     -Ni'
  'This parameter has been estimated'
 -OK-
APP:
APP: @@
APP: @@ ENTER THE POLY-3 MONITOR
APP: @@
APP: go p-3

 POLY version  3.32
POLY_3:
POLY_3: @@
POLY_3: @@ SET THE CONDITIONS AT THE NORMALIZING TEMPERATURE
POLY_3: @@
POLY_3: set-cond T=1008,P=101325,N=1
POLY_3: set-cond X(CR)=0.0206,X(C)=0.0391
POLY_3:
POLY_3:
POLY_3: @@
POLY_3: @@ ENTER FUNCTIONS TO DETERMINE THE VOLUME-FRACTIONS
POLY_3: @@
POLY_3:
POLY_3: @@ Radius of the cementite particle
POLY_3: ent-symb var rcem=0.5255e-6;
POLY_3:
POLY_3: @@ total number of moles of substitutional components
POLY_3: ent-symb func nstot=n(fe)+n(cr);
POLY_3:
POLY_3: @@ number of moles of substitutional components in cementite
POLY_3: ent-symb func nscem=n(cem,fe)+n(cem,cr);
POLY_3:
POLY_3: @@ volume fraction (U-fraction) of cementite
POLY_3: ent-symb func vfcem=nscem/nstot;
POLY_3:
POLY_3: @@ total radius of the system
POLY_3: ent-symb func rtot=rcem/vfcem**(1/3);
POLY_3:
POLY_3: @@ radius of the surrounding austenite matrix
POLY_3: ent-symb func rmat=rtot-rcem;
POLY_3:
POLY_3:
POLY_3: @@
POLY_3: @@ COMPUTE THE EQUILIBRIUM
POLY_3: @@
POLY_3: compute-eq
 Using global minimization procedure
Calculated          4113 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_3:
POLY_3:
POLY_3: @@
POLY_3: @@ SHOW THE COMPUTED VALUES TO BE USED IN THE DICTRA CALCULATION
POLY_3: @@
POLY_3: show rmat
 RMAT=5.392487E-7
POLY_3: show w(cem,cr),w(bcc,cr),w(bcc,c)
 W(CEMENTITE,CR)=0.12581627
 W(BCC_A2,CR)=4.433258E-3
 W(BCC_A2,C)=1.510234E-4
POLY_3:
POLY_3: ent var wmatcr=w(bcc,cr);
POLY_3: ent var wmatc=w(bcc,c);
POLY_3: ent var wcemcr=w(cem,cr);
POLY_3:
POLY_3:
POLY_3: @@
POLY_3: @@ ENTER THE DICTRA MONITOR
POLY_3: @@
POLY_3: go d-m
 NO TIME STEP DEFINED
 *** ENTERING BCC_A2 AS A DIFFUSION NONE PHASE
DIC>
DIC> @@
DIC> @@ ENTER GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob t 0 1183; * n

DIC>
DIC> @@
DIC> @@ ENTER THE REGIONS carb AND aus
DIC> @@
```

```
DIC> enter-region
REGION NAME : carb
DIC>
DIC> enter-region
REGION NAME : aus
ATTACH TO REGION NAMED /CARB/:
ATTACHED TO THE RIGHT OF CARB /YES/:
DIC> @@
DIC> @@ ENTER GEOMTRICAL GRIDS INTO THE REGIONS
DIC> @@
DIC>
DIC> @@
DIC> @@ THE INITIAL SIZE OF THE CEMENTITE PARTICLE IS ASSUMED TO BE KNOWN
DIC> @@ (IN THIS CASE THE VALUE IS TAKEN FROM LIU ET AL. WHO ESTIMATED THE
DIC> @@ AVERAGE INITIAL DIAMETER OF THE PARTICLES TO 1.051E-6 METERS).
DIC> @@
DIC> enter-grid
REGION NAME : /CARB/: carb
WIDTH OF REGION /1/: rcem
TYPE /LINEAR/: AUTO
DIC>
DIC> @@
DIC> @@ THE SIZE OF THE FCC REGION CAN BE CALCULATED FROM A MASS BALANCE
DIC> @@ AFTER ESTIMATING THE INITIAL COMPOSITIONS IN THE TWO PHASES
DIC> @@
DIC> enter-grid
REGION NAME : /AUS/: aus
WIDTH OF REGION /1/: rmat
TYPE /LINEAR/: AUTO
DIC>
DIC> @@
DIC> @@ ENTER PHASES INTO REGIONS
DIC> @@
DIC> enter-phase act carb  matrix   cementite
DIC> enter-phase act aus   matrix   fcc#1
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITIONS IN THE PHASES
DIC> @@
DIC> enter-composition
REGION NAME : /CARB/: carb
PHASE NAME: /CEMENTITE/: cementite
COMPOSITION TYPE /MOLE_FRACTION/: weig-fraction
PROFILE FOR /CR/: cr lin wcemcr wcemcr
DIC>
DIC> enter-composition
REGION NAME : /AUS/: aus
PHASE NAME: /FCC_A1#1/: fcc#1
DEPENDENT COMPONENT ? /FE/: fe
COMPOSITION TYPE /MOLE_FRACTION/: weig-fraction
PROFILE FOR /C/: CR lin wmatcr wmatcr
PROFILE FOR /CR/: C  lin wmatc wmatc
DIC>
DIC> @@
DIC> @@ SET TO A SPHERICAL GEOMETRY
DIC> @@
DIC> enter-geo
GEOMETRICAL EXPONENT /0/: 2
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME AND OTHER SIMULATION PARAMETERS
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 10000
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /1000/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exb2 Y
DIC>
DIC> set-inter
 --OK---
DIC>
```

exb2-run

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb2\run.DCM"DIC>
DIC>
DIC> @@ exb2_run.DCM
DIC>
DIC> @@
DIC> @@ READ THE SET UP FROM FILE AND START THE SIMULATION
DIC> @@
DIC>
DIC> go d-m
 TIME STEP AT TIME  0.00000E+00
 *** ENTERING BCC_A2 AS A DIFFUSION NONE PHASE
DIC> read exb2
 OK
DIC> sim
 Region: CARB
 single geometric dense at  0.52550E-06
 0.85084       96
 Region: AUS
 single geometric dense at   0.0000
  1.0072       63
  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

 U-FRACTION IN SYSTEM:  C = .04069101884181 79  CR = .0214382349908299
                        FE = .978561765139677
 TOTAL SIZE OF SYSTEM:  5.0562665819E-18 [m^3]
 U-FRACTION IN SYSTEM:  C = .04069101884181 79  CR = .0214382349908299
                        FE = .978561765139677
 TOTAL SIZE OF SYSTEM:  5.0562665819E-18 [m^3]
 0.175650481269751        0.175691744058966        0.175650536404886        2.957532104484168E-003        7.754436530875758E-
005        5.789654735166348E-006        8.570960213922231E-007        3.747799259728377E-007        3.453263876444000E-
007        1.349945939910680E-007        1.350781757709255E-007        1.346762090320248E-007        1.361220011258119E-
007        1.343486474217425E-007        1.340758203772263E-007        1.335307568888863E-007        1.344901942324164E-
007        1.324431404508194E-007        1.302779893773460E-007        1.259883039615329E-007        1.269270720671105E-
007        1.175748901910759E-007        1.014429630745407E-007        7.217938870756822E-008        7.299666432258670E-
008        2.728114977158535E-008        7.241529806521035E-011        4.088996652349226E-014        7.514509141967509E-
019       TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =  0.75145091E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.39436719E-02 AND  -0.39436719E-02
 POSITION OF INTERFACE CARB / AUS IS   0.52510563E-06
 U-FRACTION IN SYSTEM:  C = .0407290154735827  CR = .0214383281160798
                        FE = .978561672014427
 TOTAL SIZE OF SYSTEM:  5.0562665819E-18 [m^3]
  15  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: CARB

  CPU time used in timestep                    1 seconds
 2.248317823774132E-005        2.248767785871598E-005        2.248316234366775E-005        1.887681598926652E-009        1.633889034216790E-
009        1.019554044105679E-009        6.882193013883610E-010        6.885272455086273E-010        2.216753491915168E-
010        6.151361467432378E-014        2.128398762358501E-017       TIME =  0.30000000E-06 DT =  0.20000000E-
06 SUM OF SQUARES =  0.21283988E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.22443467E-04 AND  -0.22443467E-04
 POSITION OF INTERFACE CARB / AUS IS   0.52510114E-06
 U-FRACTION IN SYSTEM:  C = .0407297653418501  CR = .0214383291133005
                        FE = .978561671017207
 TOTAL SIZE OF SYSTEM:  5.0562665819E-18 [m^3]
  CPU time used in timestep                    0 seconds
 6.026883998584040E-004        6.026580888942288E-004        6.026721103974375E-004        8.498819122335174E-005        3.515893844060556E-
005        2.728074750064295E-007        4.049324254833804E-010        6.350550454746669E-015        2.881437473850283E-
018       TIME =  0.70000000E-06 DT =  0.40000000E-06 SUM OF SQUARES =  0.28814375E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.46375369E-05 AND  -0.46375369E-05
 POSITION OF INTERFACE CARB / AUS IS   0.52509929E-06
 U-FRACTION IN SYSTEM:  C = .0407315536282503  CR = .0214383294271359
                        FE = .978561670703371
 TOTAL SIZE OF SYSTEM:  5.0562665819E-18 [m^3]
  CPU time used in timestep                    1 seconds
 2.365053298194977E-004        2.365033654325256E-004        2.364987107717018E-004        7.190732024202641E-005        1.444209573214119E-
007        4.667964222950008E-011        2.104118921106627E-014        2.043518107460929E-017       TIME =  0.15000000E-05 DT =  0.80000000E-
06 SUM OF SQUARES =  0.20435181E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.40628860E-05 AND  -0.40628860E-05
 POSITION OF INTERFACE CARB / AUS IS   0.52509604E-06
 U-FRACTION IN SYSTEM:  C = .0407314706589161  CR = .0214383297891356
                        FE = .978561670341372
 TOTAL SIZE OF SYSTEM:  5.0562665819E-18 [m^3]
  CPU time used in timestep                    0 seconds
 3.788612455941237E-005        3.788586871828255E-005        3.788453387382108E-005

output ignored...



... output resumed

 2.983577615403479E-009        6.454633484857469E-014        4.765435236071551E-
019       TIME =   8179.7139     DT =   1000.0000     SUM OF SQUARES =  0.47654352E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.10807344E-10 AND  -0.10807344E-10
 POSITION OF INTERFACE CARB / AUS IS   0.24757819E-06
 U-FRACTION IN SYSTEM:  C = .0407635155644673  CR = .0214383980828099
                        FE = .978561602047697
 TOTAL SIZE OF SYSTEM:  5.0562665819E-18 [m^3]
  CPU time used in timestep                    1 seconds
 9.541491481690836E-009        9.602297615637573E-009        9.559945434056129E-009        3.099188909764701E-009        1.052631177236939E-
009        7.570945912359031E-015        2.435855150451165E-
018       TIME =   9179.7139     DT =   1000.0000     SUM OF SQUARES =  0.24358552E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.10178497E-10 AND  -0.10178497E-10
 POSITION OF INTERFACE CARB / AUS IS   0.23739969E-06
 U-FRACTION IN SYSTEM:  C = .0407635351055688  CR = .0214383969215681
                        FE = .978561603208939
 TOTAL SIZE OF SYSTEM:  5.0562665819E-18 [m^3]
  CPU time used in timestep                    1 seconds
 1.943033399345351E-007        1.941096197641130E-007        1.939935593089594E-007        2.953461423144300E-008        3.247208203742438E-
009        3.923651150138315E-017       TIME =   10000.000     DT =   820.28605     SUM OF SQUARES =  0.39236512E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.96946211E-11 AND  -0.96946211E-11
 POSITION OF INTERFACE CARB / AUS IS   0.22944733E-06
 U-FRACTION IN SYSTEM:  C = .0407635386763659  CR = .0214383960997853
                        FE = .978561604030722
 TOTAL SIZE OF SYSTEM:  5.0562665819E-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   0.99418868E-04
 DELETING TIME-RECORD FOR TIME   0.17900397E-03
 DELETING TIME-RECORD FOR TIME   0.30071451E-03
 DELETING TIME-RECORD FOR TIME   0.47831845E-03
 DELETING TIME-RECORD FOR TIME   0.72934499E-03
 DELETING TIME-RECORD FOR TIME   0.10758345E-02
 DELETING TIME-RECORD FOR TIME   0.15428996E-02
 DELETING TIME-RECORD FOR TIME   0.21467218E-02
 DELETING TIME-RECORD FOR TIME   0.29017296E-02
 DELETING TIME-RECORD FOR TIME   0.38194698E-02
 DELETING TIME-RECORD FOR TIME   0.49085555E-02
 DELETING TIME-RECORD FOR TIME   0.61737650E-02
 DELETING TIME-RECORD FOR TIME   0.76141364E-02
 DELETING TIME-RECORD FOR TIME   0.92226414E-02
 DELETING TIME-RECORD FOR TIME   0.10986320E-01
 DELETING TIME-RECORD FOR TIME   0.12887767E-01
 DELETING TIME-RECORD FOR TIME   0.14913901E-01
 DELETING TIME-RECORD FOR TIME   0.17051564E-01
 DELETING TIME-RECORD FOR TIME   0.19291247E-01
 DELETING TIME-RECORD FOR TIME   0.21633944E-01
 DELETING TIME-RECORD FOR TIME   0.24076983E-01
 DELETING TIME-RECORD FOR TIME   0.26620133E-01
 DELETING TIME-RECORD FOR TIME   0.29265465E-01
 DELETING TIME-RECORD FOR TIME   0.32011145E-01
 DELETING TIME-RECORD FOR TIME   0.34863203E-01
 DELETING TIME-RECORD FOR TIME   0.37830557E-01
 DELETING TIME-RECORD FOR TIME   0.40922463E-01
 DELETING TIME-RECORD FOR TIME   0.44137344E-01
 DELETING TIME-RECORD FOR TIME   0.47481808E-01
 DELETING TIME-RECORD FOR TIME   0.50962589E-01
 DELETING TIME-RECORD FOR TIME   0.54594558E-01
 DELETING TIME-RECORD FOR TIME   0.58385150E-01
 DELETING TIME-RECORD FOR TIME   0.62359088E-01
 DELETING TIME-RECORD FOR TIME   0.66523452E-01
 DELETING TIME-RECORD FOR TIME   0.68804369E-01
 DELETING TIME-RECORD FOR TIME   0.71498821E-01
 DELETING TIME-RECORD FOR TIME   0.74614406E-01
 DELETING TIME-RECORD FOR TIME   0.78161085E-01
 DELETING TIME-RECORD FOR TIME   0.82117495E-01
 DELETING TIME-RECORD FOR TIME   0.86493409E-01
 DELETING TIME-RECORD FOR TIME   0.91279391E-01
 DELETING TIME-RECORD FOR TIME   0.96476033E-01
 DELETING TIME-RECORD FOR TIME   0.10206367
 DELETING TIME-RECORD FOR TIME   0.10805208
 DELETING TIME-RECORD FOR TIME   0.11445447
 DELETING TIME-RECORD FOR TIME   0.12133499
 DELETING TIME-RECORD FOR TIME   0.12873941
 DELETING TIME-RECORD FOR TIME   0.13675470
 DELETING TIME-RECORD FOR TIME   0.14544308
 DELETING TIME-RECORD FOR TIME   0.15495431
 DELETING TIME-RECORD FOR TIME   0.16561997
 DELETING TIME-RECORD FOR TIME   0.17787509
 DELETING TIME-RECORD FOR TIME   0.19240719
 DELETING TIME-RECORD FOR TIME   0.21036557
 DELETING TIME-RECORD FOR TIME   0.23443130
 DELETING TIME-RECORD FOR TIME   0.27070025
 DELETING TIME-RECORD FOR TIME   0.33547552
 DELETING TIME-RECORD FOR TIME   0.41276116
 DELETING TIME-RECORD FOR TIME   0.50861425
 DELETING TIME-RECORD FOR TIME   0.63495278
 DELETING TIME-RECORD FOR TIME   0.81541856
 DELETING TIME-RECORD FOR TIME   0.91426374
 DELETING TIME-RECORD FOR TIME    1.0967390
 DELETING TIME-RECORD FOR TIME    1.4417612
 DELETING TIME-RECORD FOR TIME    1.6307377
 DELETING TIME-RECORD FOR TIME    1.9963541
 DELETING TIME-RECORD FOR TIME    2.7114648
 DELETING TIME-RECORD FOR TIME    4.0769542
 DELETING TIME-RECORD FOR TIME    6.6739896
 DELETING TIME-RECORD FOR TIME    11.677852
 DELETING TIME-RECORD FOR TIME    21.553167
 DELETING TIME-RECORD FOR TIME    41.303796
 DELETING TIME-RECORD FOR TIME    80.805054
 DELETING TIME-RECORD FOR TIME    159.80757
 DELETING TIME-RECORD FOR TIME    317.81260
 DELETING TIME-RECORD FOR TIME    633.82267
 DELETING TIME-RECORD FOR TIME    1265.8428
 DELETING TIME-RECORD FOR TIME    2196.1016
 DELETING TIME-RECORD FOR TIME    3179.7139
 DELETING TIME-RECORD FOR TIME    4179.7139
 DELETING TIME-RECORD FOR TIME    5179.7139
 DELETING TIME-RECORD FOR TIME    6179.7139
 DELETING TIME-RECORD FOR TIME    7179.7139
 DELETING TIME-RECORD FOR TIME    8179.7139

 KEEPING TIME-RECORD FOR TIME    9179.7139
 AND FOR TIME                    10000.000
 WORKSPACE RECLAIMED

 TIMESTEP AT     10000.0000     SELECTED

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

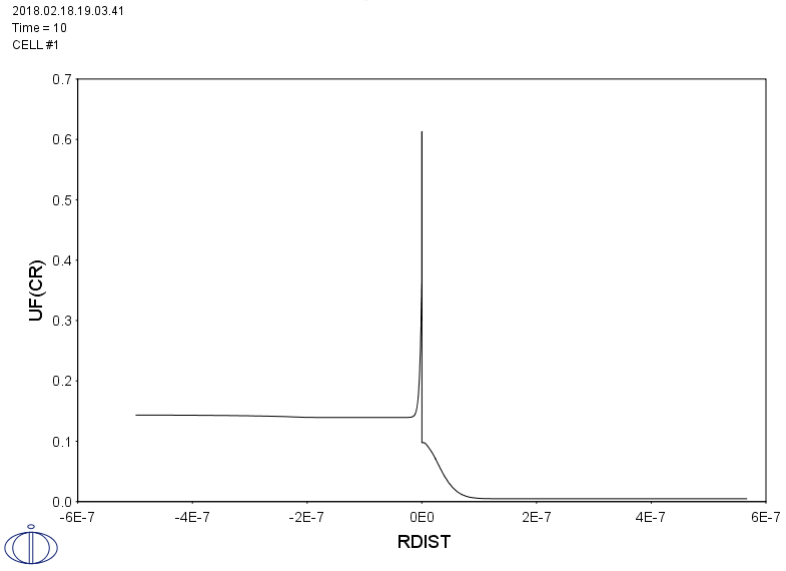
exb2-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb2\plot.DCM"DIC>
DIC>
DIC> @@ exb2_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE b2
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  1.00000E+04
 *** ENTERING BCC_A2 AS A DIFFUSION NONE PHASE
DIC> read exb2
 OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post

  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson

POST-1:
POST-1: @@
POST-1: @@ LET US PLOT CHROMIUM CONCENTRATION PROFILES
POST-1: @@ WE THEN SET THE DISTANCE AS X-AXIS (NOTE THAT DISTANCE IS AUTOMATICALLY
POST-1: @@ SET AS THE INDEPENDENT VARIABLE) AND U-FRACTION CARBON AS Y-AXIS
POST-1: @@ REMEMBER THAT THE PLOT CONDITION ALSO MUST BE SET.
POST-1: @@
POST-1: @@ NOTICE THAT ALL DISTANCES IN THE DATA FILE ARE GIVEN RELATIVE TO THE
POST-1: @@ CEM/FCC INTERFACE. FOR THIS REASON AN OFFSET MUST BE GIVEN TO THE
POST-1: @@ DATA ACCORDING TO THE ACTUAL PARTICLE RADIUS AT THE SPECIFIED TIME.
POST-1: @@
POST-1: enter-symb
Function or table /FUNCTION/: func
NAME: rdist
FUNCTION: gd-poi(carb,u);
POST-1:
POST-1: s-d-a x rdist
POST-1:
POST-1: s-i-v
VARIABLE /TIME/: dist
DISTANCE : /GLOBAL/: glo
POST-1:
POST-1: s-d-a y uf(cr)
POST-1:
POST-1: s-p-c time 10
POST-1:
POST-1: @@
POST-1: @@ SET THE TITLE ON THE PLOT
POST-1: @@
POST-1: set-title Figure b2.1
POST-1:
POST-1: plo
```

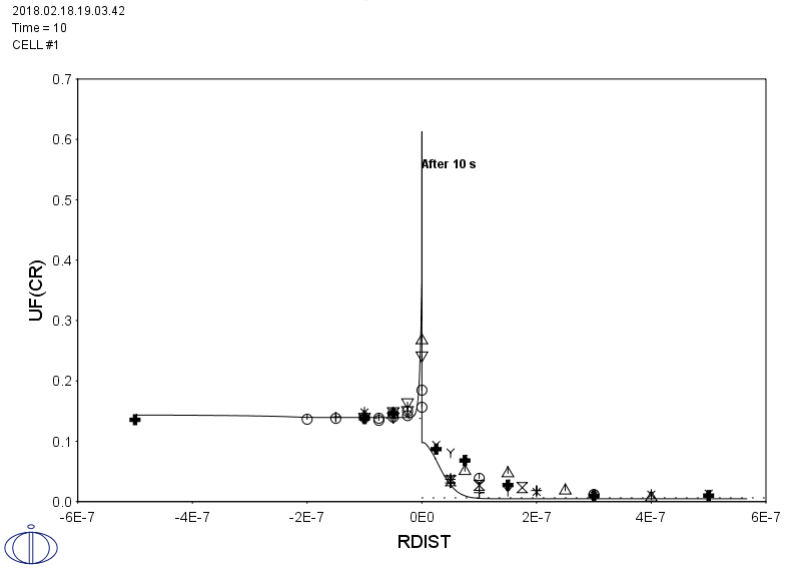
Figure b2.1




```
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
```

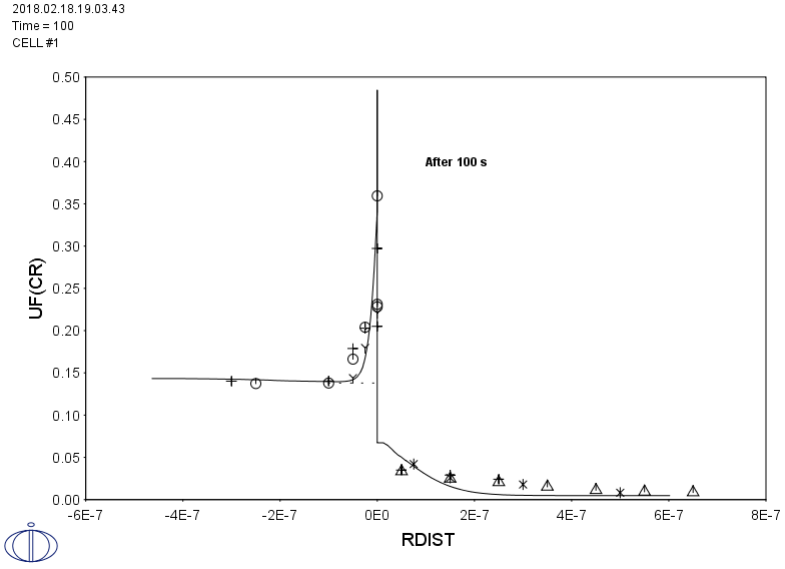
```
 DATASET 6 MEAN PARTICLE DIAMETER VS. TIME
POST-1:
POST-1: @@
POST-1: @@ SELECT THE PROPER DATASET
POST-1: @@
POST-1: app y exb2.exp
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 1
POST-1:
POST-1: set-title Figure b2.2
POST-1: plo
```

Figure b2.2



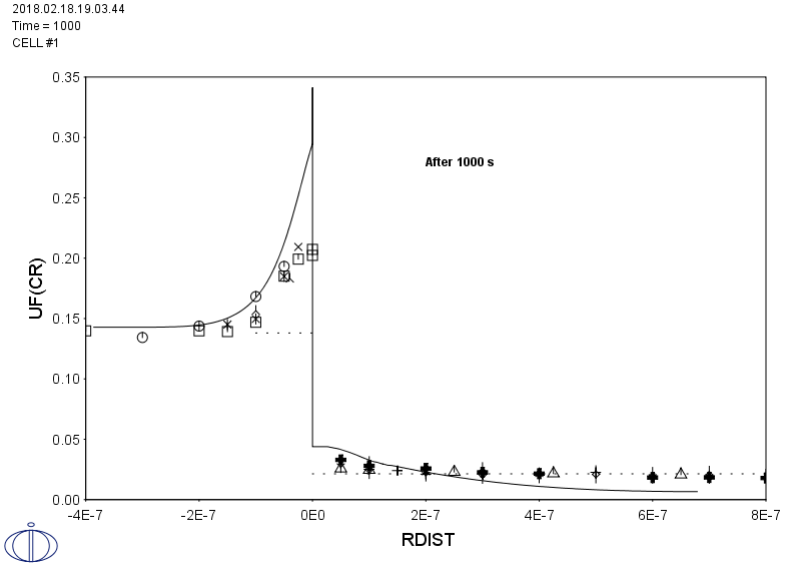

```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: @@
POST-1: @@ PLOT ALSO FOR 100, 1000 AND 10000 seconds
POST-1: @@
POST-1:
POST-1: s-p-c time 100
POST-1:
POST-1: app y exb2.exp
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 2
POST-1:
POST-1: set-title Figure b2.3
POST-1: plo
```

Figure b2.3



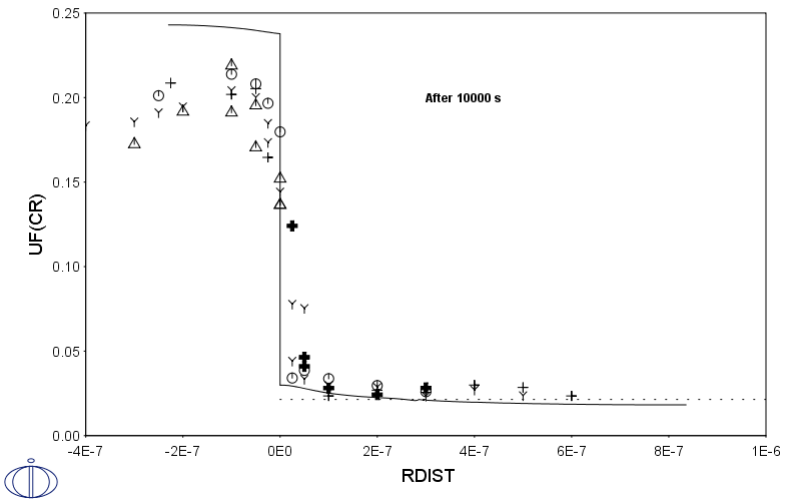

```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1:
POST-1: s-p-c time 1000
POST-1:
POST-1: app y exb2.exp
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 3
POST-1:
POST-1: set-title Figure b2.4
POST-1: plo
```

Figure b2.4



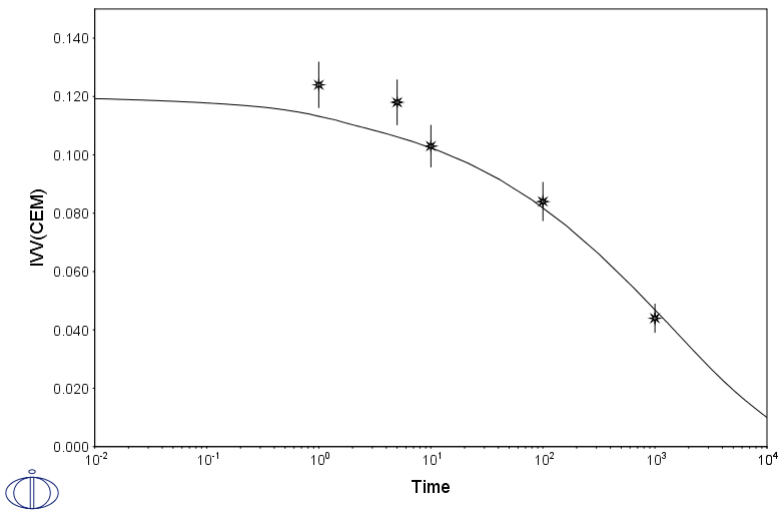

```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: s-p-c time 10000
POST-1:
POST-1: app y exb2.exp
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 4
POST-1:
POST-1: set-title Figure b2.5
POST-1: plo
```

Figure b2.5



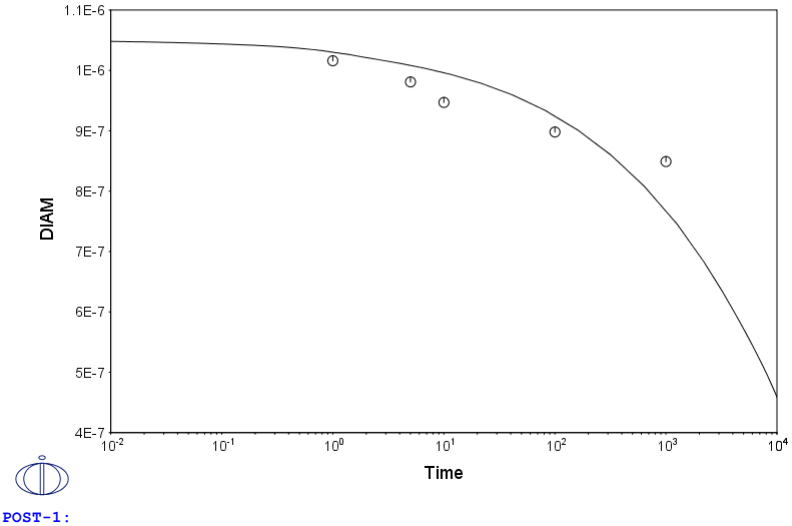

```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: @@
POST-1: @@ ALSO PLOT HOW THE VOLUME FRACTION OF CEMENTITE VARIES
POST-1: @@ WITH TIME
POST-1: @@
POST-1: s-d-a y ivv(cem)
POST-1: s-s-s y n 0 .15
POST-1:
POST-1: s-d-a x time
  INFO: Time is set as independent 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: plo
```

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: plo
```

Figure b2.7

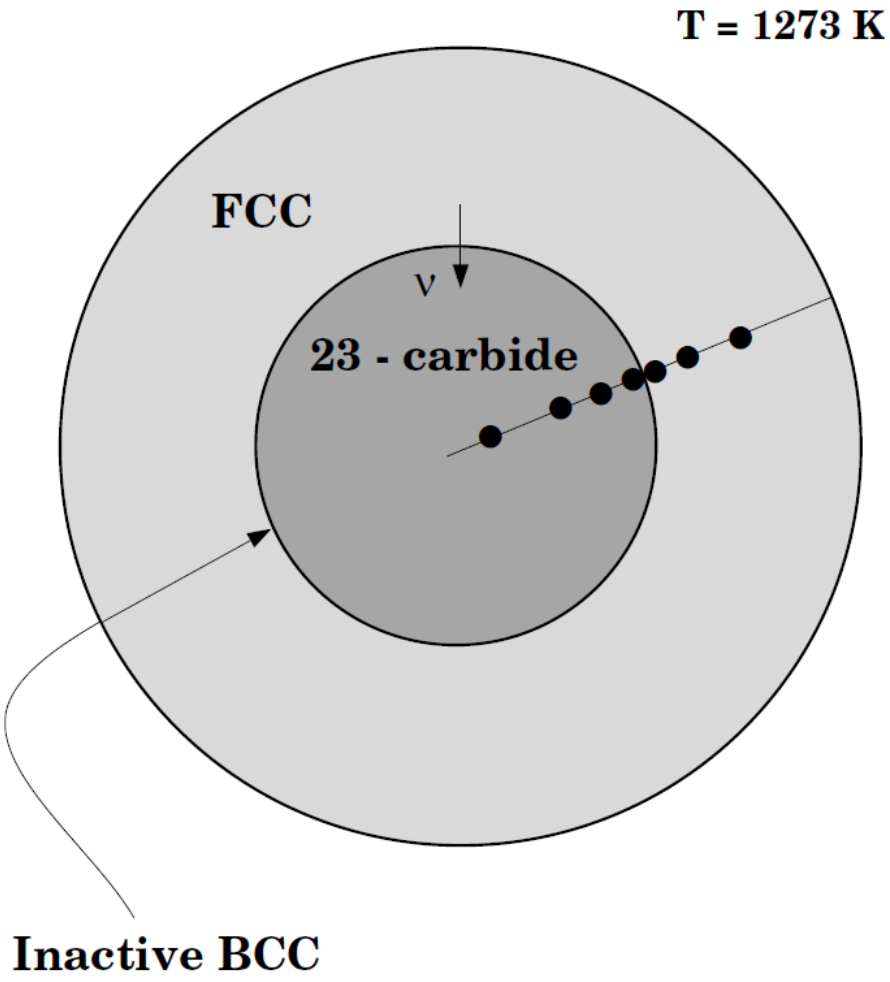



```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: set-inter
 --OK---
POST-1:
```

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

```
AboutSYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb3\setup.DCM"
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
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

 VA                     /-  DEFINED
 L12_FCC                B2_BCC                 DICTRA_FCC_A1
   REJECTED
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ USE A DATABASE FOR THERMODYNAMIC DATA
TDB_TCFE9: @@
TDB_TCFE9: sw fedemo
 Current database: Iron Demo Database v2.0

 VA                     /-  DEFINED
TDB_FEDEMO: def-sys fe c cr
 FE                     C                      CR
   DEFINED
TDB_FEDEMO: rej ph *
 GAS:G                  LIQUID:L               BCC_A2
 CEMENTITE              CHI_A12                DIAMOND_FCC_A4
 FCC_A1                 GRAPHITE               HCP_A3
 KSI_CARBIDE            LAVES_PHASE_C14        M23C6
 M3C2                   M5C2                   M7C3
 SIGMA  REJECTED
TDB_FEDEMO: res ph fcc bcc m23
 FCC_A1                 BCC_A2                 M23C6
   RESTORED
TDB_FEDEMO: get
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'J-O. Andersson, CALPHAD, 11 (1987) 271-276; TRITA 0314; C-CR'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'P. Franke, Estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
  'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'X.-G. Lu, M. Selleby, B. Sundman, CALPHAD, 29 (2005) 49-55; Fe P-T diagram'
  'A.V. Khvan, B. Hallstedt, C. Broeckmann, CALPHAD, 46, 24 -33(2014); Cr-Fe
      -C'
  'J-O. Andersson, Metall. Trans. A, 19A (1988) 627-636 TRITA 0207 (1986); C
      -CR-FE'
  'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270
      (1986); CR-FE'
  'J. Bratberg, Z. Metallkd., 96 (2005) 335-344; Fe-Cr-Mo-C'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, 2016; FCC Fe-Cr-C and C-Cr-Ni'
  'B.-J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
  'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
  'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, CALPHAD,
      submitted, 2011; Fe-Mn-C'
 -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 v2.0

 VA  DEFINED
APP: def-sys c cr fe
 C                      CR                     FE
   DEFINED
APP: rej ph *
 BCC_A2                 FCC_A1  REJECTED
APP: res ph fcc bcc
 FCC_A1                 BCC_A2  RESTORED
APP: get
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'This parameter has not been assessed'
  'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'
  'B. Jonsson: Z. Metallkunde 85(1994)502-509; C diffusion in fcc Cr-Fe-Ni'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Fe diffusion fcc Cr-Fe'
  'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
      -Ni'
  'B. Jonsson: Z. Metallkunde 85(1994)498-501; C and N diffusion in bcc Cr
      -Fe-Ni'
  'B. Jonsson: ISIJ International, 35(1995)1415-1421; Cr, Fe and Ni
      diffusion bcc Cr-Fe-Ni'
  'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
      in bcc Fe'
 -OK-
APP:
APP: @@
```

```
APP: @@ ENTER THE DICTRA MONITOR
APP: @@
APP: go d-m
 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>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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
 single geometric dense at  0.50000E-06
 0.83296       92
 Region: MATRIX
 single geometric dense at   0.0000
  1.0051       62
  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]
 0.565663007975143        0.565797019192577        0.565663812089356        1.015925208865390E-002        3.012654895008019E-
004        4.777345249237744E-005        2.965739032002669E-006        7.215362048263626E-007        8.262638023301182E-
007        4.246506051605422E-008        4.119324775682431E-008        3.974271203721860E-008        4.355497133554406E-
008        3.870625295026483E-008        3.673410108968729E-008        3.294771044059294E-008        3.668595704949160E-
008        2.600355360941065E-008        1.460917533598369E-008        1.658190571554172E-009        4.335933723645985E-
012        1.279149078571039E-015        2.899183529819540E-017       TIME =  0.10000000E-06 DT =  0.10000000E-
06 SUM OF SQUARES =  0.28991835E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.17310735E-02 AND  -0.17310735E-02
 POSITION OF INTERFACE CARBIDE / MATRIX IS   0.49982689E-06
 U-FRACTION IN SYSTEM:  C = .0278769048021911  CR = .149918499752463
                        FE = .850081500378044
 TOTAL SIZE OF SYSTEM:  4.93068569406E-18 [m^3]
  16  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: CARBIDE

  CPU time used in timestep                    1 seconds
 1.096405342623862E-004        1.096626445879963E-004        1.096405350851704E-004        5.301312531052159E-008        2.238795214918746E-
008        6.726062310361936E-011        8.232621485718108E-014        3.182662037225323E-019       TIME =  0.30000000E-06 DT =  0.20000000E-
06 SUM OF SQUARES =  0.31826620E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.29934902E-05 AND  -0.29934902E-05
 POSITION OF INTERFACE CARBIDE / MATRIX IS   0.49982629E-06
 U-FRACTION IN SYSTEM:  C = .0278774003819474  CR = .149918500361418
                        FE = .850081499769089
 TOTAL SIZE OF SYSTEM:  4.93068569406E-18 [m^3]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: MATRIX

  CPU time used in timestep                    1 seconds
 1.217834959639798E-004        1.217822143860332E-004        1.217736602728715E-004        6.952194334566076E-007        2.897690349262264E-
009        5.944810708355392E-012        3.496240359029881E-016        2.032256660449822E-022       TIME =  0.70000000E-06 DT =  0.40000000E-
06 SUM OF SQUARES =  0.20322567E-21
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.28086480E-05 AND  -0.28086480E-05
 POSITION OF INTERFACE CARBIDE / MATRIX IS   0.49982517E-06
 U-FRACTION IN SYSTEM:  C = .0278774419496498  CR = .149918501468152
                        FE = .850081498662355
 TOTAL SIZE OF SYSTEM:  4.93068569406E-18 [m^3]
  CPU time used in timestep                    0 seconds
 6.892011300109831E-006        6.891932131748709E-006        6.890942061713327E-006

output ignored...



... output resumed

 3.596091136776303E-008        8.216033691580668E-012        6.248152751737216E-
017       TIME =   5410.4257     DT =   800.00000     SUM OF SQUARES =  0.62481528E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.74030235E-12 AND  -0.74030235E-12
 POSITION OF INTERFACE CARBIDE / MATRIX IS   0.39236306E-06
 U-FRACTION IN SYSTEM:  C = .0277635741857872  CR = .149675658318268
                        FE = .850324341812239
 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
 7.397554469224484E-008        7.399690832891322E-008        7.390401694592549E-008        4.729538433889559E-008        3.738284861005563E-
008        1.904030934350095E-008        7.062238354706955E-010        1.249316828613806E-015        9.774450116579076E-
022       TIME =   6210.4257     DT =   800.00000     SUM OF SQUARES =  0.97744501E-21
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.30089948E-12 AND  -0.30089948E-12
 POSITION OF INTERFACE CARBIDE / MATRIX IS   0.39212234E-06
 U-FRACTION IN SYSTEM:  C = .0277635755152104  CR = .149675658812231
                        FE = .850324341318276
 TOTAL SIZE OF SYSTEM:  4.93068569406E-18 [m^3]
  CPU time used in timestep                    1 seconds
 2.558036433460315E-008        2.558546174339629E-008        2.553729557831349E-008        1.697014320315236E-008        1.554273078104043E-
008        1.249746186331826E-008        7.595600812641111E-009        7.591676980921429E-009        1.359289190143328E-
009        1.010790598659928E-015        6.469467549519251E-
020       TIME =   7010.4257     DT =   800.00000     SUM OF SQUARES =  0.64694675E-19
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.48195675E-13 AND  -0.48195675E-13
 POSITION OF INTERFACE CARBIDE / MATRIX IS   0.39208379E-06
```

```
 U-FRACTION IN SYSTEM:  C = .0277635745417878  CR = .149675659024147
                        FE = .85032434110636
 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
 8.755707216979695E-009        8.756183722699488E-009        8.729902660904552E-009        5.724347401567462E-009        5.650604863023250E-
009        5.461702834959989E-009        5.134317922419642E-009        5.136158545777380E-009        4.471776075599300E-
009        3.316831595143683E-009        1.518492536949695E-009        1.518354498850523E-009        4.843822582897689E-
012        1.867506911066414E-018       TIME =   7810.4257     DT =   800.00000     SUM OF SQUARES =  0.18675069E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.97015850E-13 AND   0.97015850E-13
 POSITION OF INTERFACE CARBIDE / MATRIX IS   0.39216140E-06
 U-FRACTION IN SYSTEM:  C = .0277635652652809  CR = .149675659039302
                        FE = .850324341091205
 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
 7.291179747246321E-008        7.290978922893142E-008        7.324387881826405E-008        2.924239425496701E-008        2.882473950708875E-
008        2.785550866674718E-008        2.609831532441511E-008        2.608909518860428E-008        2.264366027348484E-
008        1.655035603339147E-008        7.188348968447023E-009        3.836741804380008E-016        1.042063658795509E-
018       TIME =   8000.0000     DT =   189.57432     SUM OF SQUARES =  0.10420637E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.40784293E-12 AND   0.40784293E-12
 POSITION OF INTERFACE CARBIDE / MATRIX IS   0.39223872E-06
 U-FRACTION IN SYSTEM:  C = .0277635584898389  CR = .149675659044322
                        FE = .850324341086185
 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    45.271088
 DELETING TIME-RECORD FOR TIME    68.248413
 DELETING TIME-RECORD FOR TIME    68.248423
 DELETING TIME-RECORD FOR TIME    68.248443
 DELETING TIME-RECORD FOR TIME    68.248483
 DELETING TIME-RECORD FOR TIME    68.248563
 DELETING TIME-RECORD FOR TIME    68.248723
 DELETING TIME-RECORD FOR TIME    68.249043
 DELETING TIME-RECORD FOR TIME    68.249683
 DELETING TIME-RECORD FOR TIME    68.250963
 DELETING TIME-RECORD FOR TIME    68.253523
 DELETING TIME-RECORD FOR TIME    68.258643
 DELETING TIME-RECORD FOR TIME    68.268883
 DELETING TIME-RECORD FOR TIME    68.289363
 DELETING TIME-RECORD FOR TIME    68.330323
 DELETING TIME-RECORD FOR TIME    68.412243
 DELETING TIME-RECORD FOR TIME    68.576083
 DELETING TIME-RECORD FOR TIME    68.903763
 DELETING TIME-RECORD FOR TIME    69.559123
 DELETING TIME-RECORD FOR TIME    70.869843
 DELETING TIME-RECORD FOR TIME    73.491283
 DELETING TIME-RECORD FOR TIME    78.734163
 DELETING TIME-RECORD FOR TIME    89.219923
 DELETING TIME-RECORD FOR TIME    110.19144
 DELETING TIME-RECORD FOR TIME    152.13448
 DELETING TIME-RECORD FOR TIME    236.02056
 DELETING TIME-RECORD FOR TIME    403.79272
 DELETING TIME-RECORD FOR TIME    739.33704
 DELETING TIME-RECORD FOR TIME    1410.4257
 DELETING TIME-RECORD FOR TIME    2210.4257
 DELETING TIME-RECORD FOR TIME    3010.4257
 DELETING TIME-RECORD FOR TIME    3810.4257
 DELETING TIME-RECORD FOR TIME    4610.4257
 DELETING TIME-RECORD FOR TIME    5410.4257
 DELETING TIME-RECORD FOR TIME    6210.4257
 DELETING TIME-RECORD FOR TIME    7010.4257

 KEEPING TIME-RECORD FOR TIME    7810.4257
 AND FOR TIME                    8000.0000
 WORKSPACE RECLAIMED

 TIMESTEP AT     8000.00000     SELECTED

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

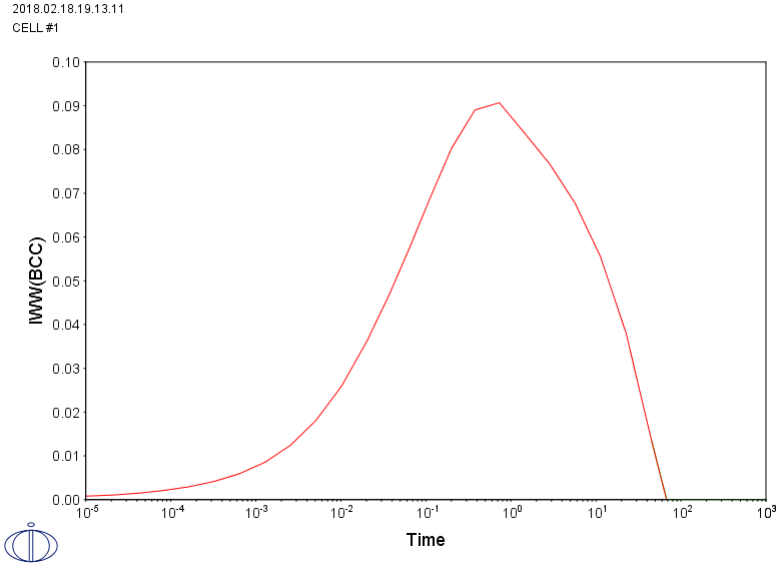
exb3-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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: plot
```

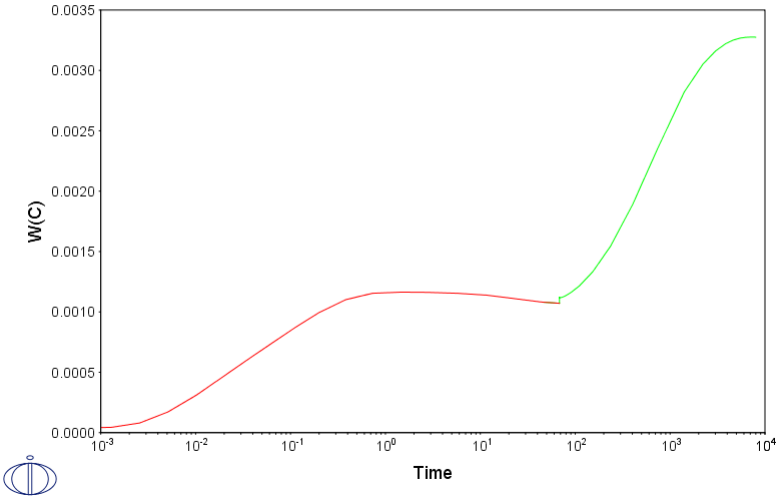
Figure b3.1




```
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: plot
```

Figure b3.2

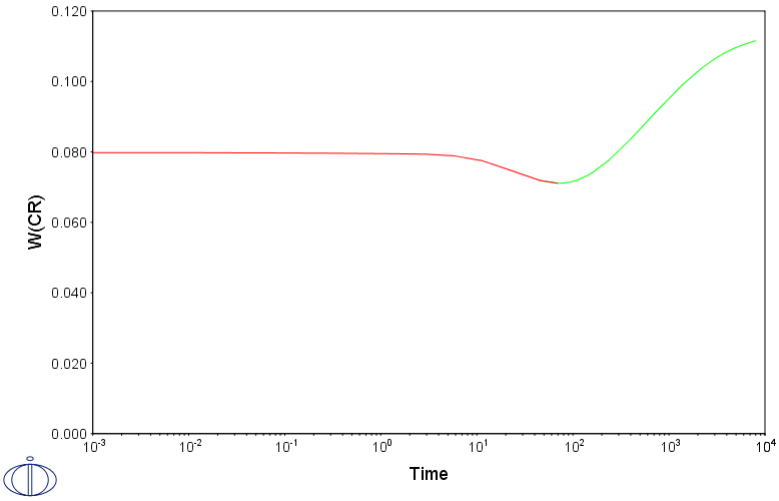
2018.02.18.19.13.12
UPPER INTERFACE OF REGION "LAST"
CELL #1




```
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: plot
```

Figure b3.3

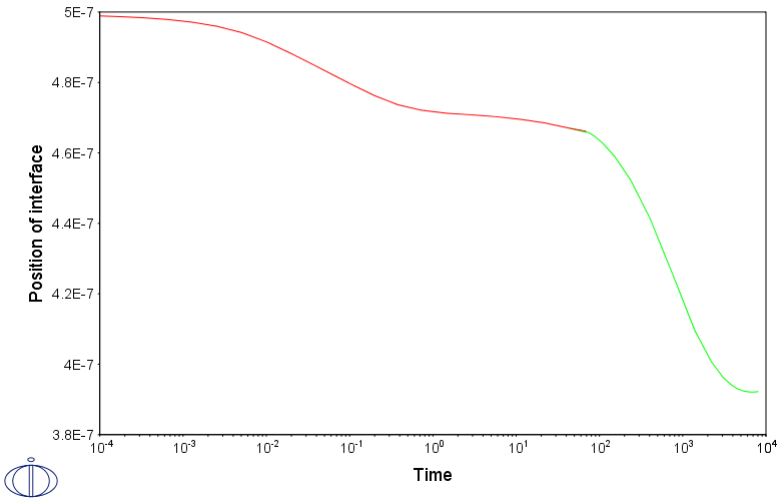
2018.02.18.19.13.13
UPPER INTERFACE OF REGION "LAST"
CELL #1




```
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: plot
```

Figure b3.4

2018.02.18.19.13.14
UPPER INTERFACE OF REGION "CARBIDE#1"
CELL #1

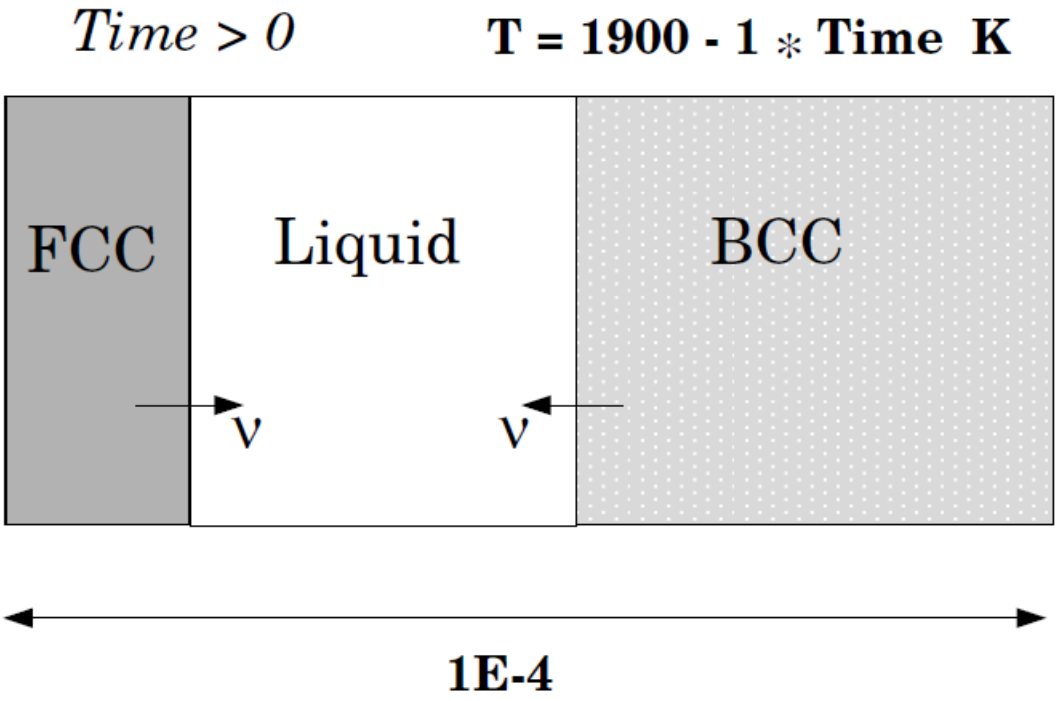



```
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1:
POST-1: set-inter
 --OK---
POST-1:
```

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

```
About Stockholm, Sweden

 Software  (build 12987) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri Feb 16 15:22:08 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb4a\setup.DCM" @@
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
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

 VA                     /-  DEFINED
 L12_FCC                B2_BCC                 DICTRA_FCC_A1
   REJECTED
TDB_TCFE9:
TDB_TCFE9: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA
TDB_TCFE9: sw fedemo
 Current database: Iron Demo Database v2.0

 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
 LIQUID:L               BCC_A2                 CHI_A12
 FCC_A1                 HCP_A3                 LAVES_PHASE_C14
 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
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'X.-G. Lu, M. Selleby, B. Sundman, CALPHAD, 29 (2005) 49-55; Fe P-T diagram'
  'J. Brillo and I. Egry, Int. J. Thermophysics, 24, 1155-1170'
  'B.-J. Lee, CALPHAD, 17 (1993) 251-268; revision of Fe-Cr and Fe -Ni liquid'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'B.-J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270
      (1986); CR-FE'
  'A. Dinsdale and T. Chart, MTDS NPL, Unpublished work (1986); CR -NI'
  'A. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); FE-NI'
 -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

 TCFE9    =  Steels/Fe-Alloys  v9.0
 TCFE10   =  Steels/Fe-Alloys  v10.0 SNAPSHOT
 TCFE8    =  Steels/Fe-Alloys  v8.1
 FROST1   =  FROST database v1.0
 TCFE7    =  Steels/Fe-Alloys  v7.0
 TCFE6    =  Steels/Fe-Alloys  v6.2
 TCFE5    =  Steels/Fe-Alloys  v5.0
 TCFE4    =  Steels/Fe-Alloys  v4.1
 TCFE3    =  Steels/Fe-Alloys  v3.1
 TCFE2    =  Steels/Fe-Alloys  v2.1
 TCFE1    =  Steels/Fe-Alloys  v1.0
 TCNI9    =  Ni-Alloys  v9.0 SNAPSHOT
 NI25     =  NI25 database
 TCNI8    =  Ni-Alloys  v8.1
 TCNI7    =  Ni-Alloys  v7.1
 TCNI6    =  Ni-Alloys  v6.0
 TCNI5    =  Ni-Alloys  v5.1
 TCNI4    =  Ni-Alloys  v4.0
 TCNI1    =  Ni-Alloys  v1.3
 TCAL5    =  Al-Alloys  v5.0
 TCAL4    =  Al-Alloys  v4.0
 TCAL3    =  Al-Alloys  v3.0
 TCAL2    =  Al-Alloys  v2.1
 TCAL1    =  Al-Alloys  v1.2
 TCMG4    =  Mg-Alloys  v4.0
```

```
 TCMG3   =  Mg-Alloys  v3.0
 TCMG2   =  Mg-Alloys  v2.0
 TCMG1   =  Mg-Alloys  v1.1
 TCTI1   =  Ti-Alloys  v1.0
 TCCU2   =  Cu-Alloys  v2.0
 TCCU1   =  Cu-Alloys  v1.0
 TCCC1   =  Cemented carbide  v1.0
 TCHEA2  =  High Entropy Alloy  v2.1
 TCHEA1  =  High Entropy Alloy  v1.0
 SSOL6   =  SGTE Alloy Solutions Database v6.0
 SSOL5   =  SGTE Alloy Solutions Database v5.0
 SSOL4   =  SGTE Alloy Solutions Database v4.9g
 SSOL2   =  SGTE Alloy Solutions Database v2.1
 SSUB6   =  SGTE Substances Database v6.0
 SSUB5   =  SGTE Substances Database v5.2
 SSUB4   =  SGTE Substances Database v4.1
 SSUB3   =  SGTE Substances Database v3.3
 SSUB2   =  SGTE Substances Database v2.2
 SNOB3   =  SGTE Noble Metal Alloys Database v3.1
 STBC2   =  SGTE Thermal Barrier Coating TDB v2.2
 STBC1   =  SGTE Thermal Barrier Coating TDB v1.1
 SALT1   =  SGTE Molten Salts Database v1.2
 SEMC2   =  TC Semi-Conductors  v2.1
 SLAG4   =  Fe-containing Slag  v4.1
 SLAG3   =  Fe-containing Slag  v3.2
 SLAG2   =  Fe-containing Slag  v2.2
 SLAG1   =  Fe-containing Slag  v1.2
 TCOX7   =  Metal Oxide Solutions  v7.0
 TCOX6   =  Metal Oxide Solutions  v6.0
 TCOX5   =  Metal Oxide Solutions  v5.1
 TCOX4   =  Metal Oxide Solutions  v4.1
 ION3    =  Ionic Solutions  v3.0
 ION2    =  Ionic Solutions  v2.6
 ION1    =  Ionic Solutions  v1.5
 NOX2    =  NPL Oxide Solutions Database v2.1
 TCNOBL1 =  Noble Metals Alloys v1.0
 TCSLD3  =  Solder Alloys  v3.2
 TCSLD2  =  Solder Alloys  v2.0
 TCSI1   =  Ultrapure Silicon  v1.2
 TCMP2   =  Materials Processing  v2.5
 TCES1   =  Combustion/Sintering  v1.1
 TCSC1   =  Super Conductor  v1.0
 TCFC1   =  SOFC Database v1.0
 NUMT2   =  Nuclear Materials  v2.1
 NUOX4   =  Nuclear Oxides  v4.2
 NUCL15  =  IRSN NUCLEA-15_4
 NUCL10  =  ThermoData NUCLEA Alloys-oxides TDB v10.2
 MEPH15  =  IRSN Mephista-15_1
 MEPH11  =  ThermoData MEPHISTA Nuclear Fuels TDB v11.2
 TCAQ3   =  Aqueous Solution  v3.0
 TCAQ2   =  Aqueous Solution  v2.6
 AQS2    =  TGG Aqueous Solution Database v2.6
 GCE2    =  TGG Geochemical/Environmental TDB v2.3
 FEDEMO  =  Iron Demo Database v2.0
 ALDEMO  =  Aluminum Demo Database v2.0
 NIDEMO  =  Nickel Demo Database v1.0
 CUDEMO  =  Copper Demo Database v1.0
 SLDEMO  =  Solder Demo Database v1.0
 OXDEMO  =  Oxide Demo Database v1.0
 SUBDEMO =  Substance Demo Database v1.0
 PTERN   =  Public Ternary Alloys TDB v1.3
 PAQ2    =  Public Aqueous Soln (SIT) TDB v2.4
 PG35    =  G35 Binary Semi-Conductors TDB v1.2
 PURE5   =  SGTE Unary (Pure Elements) TDB v5.1
 MOB2    =  Alloys Mobility  v2.7
 MOB1    =  Alloys Mobility  v1.3
 MOBFE1  =  Steels/Fe-Alloys Mobility  v1.0
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBNI4  =  Ni-Alloys Mobility  v4.0
 MOBNI3  =  Ni-Alloys Mobility  v3.1
 MOBNI2  =  Ni-Alloys Mobility  v2.4
 MOBNI1  =  Ni-Alloys Mobility  v1.0
 MOBAL3  =  Al-Alloys Mobility  v3.0
 MOBAL2  =  Al-Alloys Mobility  v2.0
 MOBAL1  =  Al-Alloys Mobility  v1.0
 MOBCU1  =  Cu-Alloys Mobility  v1.0
 MOBCU2  =  Cu-Alloys Mobility  v2.0
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBSLD1 =  Solder-Alloys Mobility  v1.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0 SNAPSHOT
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v1.0
 MFEDEMO =  Fe-Alloys Mobility demo database v2.0
 MNIDEMO =  Ni-Alloys Mobility demo database v1.0
 MCUDEMO =  Cu-Alloys Mobility demo database v1.0
 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
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 ....

 List of references for assessed data

  'This parameter has not been assessed'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Fe diffusion fcc Cr-Fe'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Ni diffusion fcc Cr-Ni'
```

```
  'B. Jonsson: Z. Metallkunde 86(1995)686-692; Cr, Fe and Ni diffusion fcc
      Cr-Fe-Ni'
  'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
      -Ni'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Ni self-diffusion'
  'B. Jonsson: ISIJ International, 35(1995)1415-1421; Cr, Fe and Ni
      diffusion bcc Cr-Fe-Ni'
  'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
      in bcc Fe'
 -OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP
APP: @@
APP: go d-m
 NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER GLOBAL CONDITION T
DIC> @@
DIC> @@ LOWER THE TEMPERATURE TO A RATE OF 1 K/s
DIC> @@
DIC> set-cond glob T 0 1900-1*TIME; * N

DIC>
DIC> @@
DIC> @@ ENTER A REGION CALLED smalta
DIC> @@
DIC> enter-region smalta
DIC>
DIC> @@
DIC> @@ ENTER A DOUBLE GEOMETRIC GRID INTO THE REGION
DIC> @@
DIC> enter-grid
REGION NAME : /SMALTA/: smalta
WIDTH OF REGION /1/: 1e-4
TYPE /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
 SETTING CHECK INTERFACE POSITION ON
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 /YES/: 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 (0 -> 0.5 -> 1): /.5/:
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /NO/:
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>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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
 double geometric
 dense at outer boundaries, coarse at  0.50000E-04
lower part   1.2500       22
upper part  0.80000       22
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882254
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882254
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882254
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.65057363E-05 DT =  0.64057363E-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 =  0.19317209E-04 DT =  0.12811473E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882254
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.44940154E-04 DT =  0.25622945E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882254
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.96186044E-04 DT =  0.51245890E-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 =  0.19867782E-03 DT =  0.10249178E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882254
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.40366139E-03 DT =  0.20498356E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882254
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.81362851E-03 DT =  0.40996712E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882254
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.16335628E-02 DT =  0.81993424E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882254
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.32734312E-02 DT =  0.16398685E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882254
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.65531682E-02 DT =  0.32797370E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882254
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.13112642E-01 DT =  0.65594740E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882254
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.26231590E-01 DT =  0.13118948E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.52469486E-01 DT =  0.26237896E-01 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 =  0.10494528     DT =  0.52475792E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.20989686     DT =  0.10495158     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992482  FE = .733068011219292
                        NI = .0754116207882253
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.41980003     DT =  0.20990317     SUM OF SQUARES =   0.0000000
```

```
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882252
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.83960636     DT =  0.41980633     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 =   1.6792190     DT =  0.83961267     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                        NI = .0754116207882252
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3.3584444     DT =   1.6792253     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992488  FE = .73306801121929


output ignored...



... output resumed

 5.514005299448755E-006        5.509376563838510E-006        7.547294441383454E-010        5.022583224199097E-014        5.481369063070259E-
019       TIME =   178.06453     DT =   1.3107200     SUM OF SQUARES =  0.54813691E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.60791645E-07 AND  -0.60791645E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.64305088E-05
 U-FRACTION IN SYSTEM:  CR = .191499811939236  FE = .733100727058195
                        NI = .0753994610025692
 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
 1.053156852724598E-005        1.053152073815954E-005        1.052555445432811E-005        4.057250259300867E-007        3.528412544722028E-
011        3.011930265008765E-016        4.421460299214064E-
021       TIME =   180.68597     DT =   2.6214400     SUM OF SQUARES =  0.44214603E-20
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.44074694E-07 AND  -0.44074694E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.63149697E-05
 U-FRACTION IN SYSTEM:  CR = .191499811958015  FE = .73310072702147
                        NI = .075399461020515
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  3  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_BCC_A2

  CPU time used in timestep                    3 seconds
 7.659975284018353E-006        7.660132765574592E-006        7.656721414781887E-006        1.049739953313493E-006        2.121510544843710E-
007        2.260034806150486E-012        4.796864873246992E-
017       TIME =   185.92885     DT =   5.2428800     SUM OF SQUARES =  0.47968649E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.16957857E-07 AND  -0.16957857E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.62260617E-05
 U-FRACTION IN SYSTEM:  CR = .191499811977765  FE = .733100726963597
                        NI = .0753994610586384
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  3  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_BCC_A2

  CPU time used in timestep                    2 seconds
 5.642974296566065E-006        5.643125095318699E-006        5.641517484928644E-006        2.458262515757805E-006        1.706103643042057E-
006        5.102549567539333E-007        4.488461283369183E-011        3.063522581558072E-015        6.513585356447460E-
019       TIME =   196.41461     DT =   10.485760     SUM OF SQUARES =  0.65135854E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.23346098E-07 AND   0.23346098E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.64708632E-05
 U-FRACTION IN SYSTEM:  CR = .191499811976631  FE = .733100726947108
                        NI = .0753994610762612
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  5  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_FCC_A1

  CPU time used in timestep                    2 seconds
 1.293494529309763E-005        1.293515101167310E-005        1.293008550633410E-005        2.658335068138821E-008        8.679707504660311E-
012        1.146811880809633E-016       TIME =   200.00000     DT =   3.5853947     SUM OF SQUARES =  0.11468119E-15
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.18287074E-07 AND   0.18287074E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.65364296E-05
 U-FRACTION IN SYSTEM:  CR = .191499811977615  FE = .733100726940699
                        NI = .0753994610816858
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 MUST SAVE WORKSPACE ON FILE
 WORKSPACE SAVED ON FILE
 RECLAIMING WORKSPACE
 DELETING TIME-RECORD FOR TIME    175.02035
 DELETING TIME-RECORD FOR TIME    175.44310
 DELETING TIME-RECORD FOR TIME    175.44311
 DELETING TIME-RECORD FOR TIME    175.44313
 DELETING TIME-RECORD FOR TIME    175.44317
 DELETING TIME-RECORD FOR TIME    175.44325
 DELETING TIME-RECORD FOR TIME    175.44341
 DELETING TIME-RECORD FOR TIME    175.44373
 DELETING TIME-RECORD FOR TIME    175.44437
 DELETING TIME-RECORD FOR TIME    175.44565
 DELETING TIME-RECORD FOR TIME    175.44821
 DELETING TIME-RECORD FOR TIME    175.45333
 DELETING TIME-RECORD FOR TIME    175.46357
 DELETING TIME-RECORD FOR TIME    175.48405
 DELETING TIME-RECORD FOR TIME    175.52501
 DELETING TIME-RECORD FOR TIME    175.60693
 DELETING TIME-RECORD FOR TIME    175.77077
 DELETING TIME-RECORD FOR TIME    176.09845
 DELETING TIME-RECORD FOR TIME    176.75381
 DELETING TIME-RECORD FOR TIME    178.06453
 DELETING TIME-RECORD FOR TIME    180.68597
 DELETING TIME-RECORD FOR TIME    185.92885

 KEEPING TIME-RECORD FOR TIME    196.41461
 AND FOR TIME                    200.00000
 WORKSPACE RECLAIMED

 TIMESTEP AT     200.000000     SELECTED

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

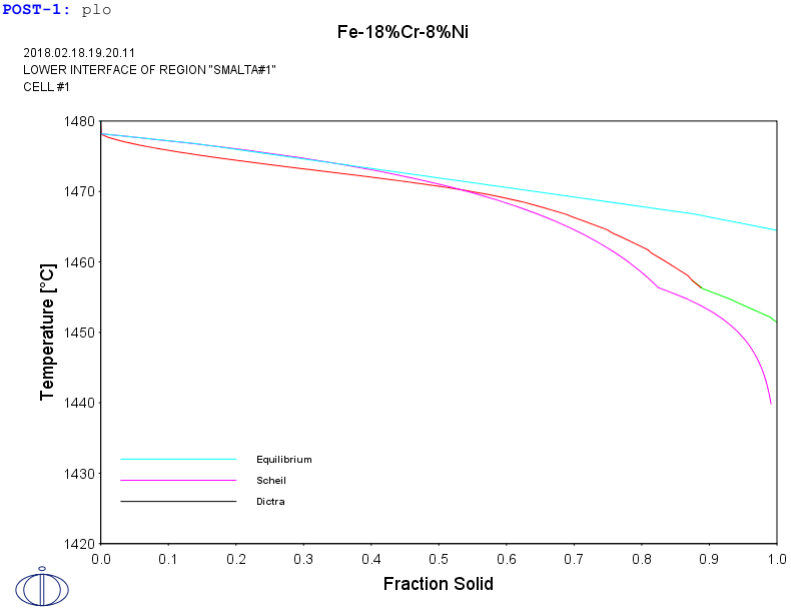
```
DIC>
DIC>
DIC> @@
DIC> @@ THE SIMULATION IS FINISHED
DIC> @@
DIC>
DIC> set-inter
 --OK---
DIC>
```

exb4a-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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: plo
```

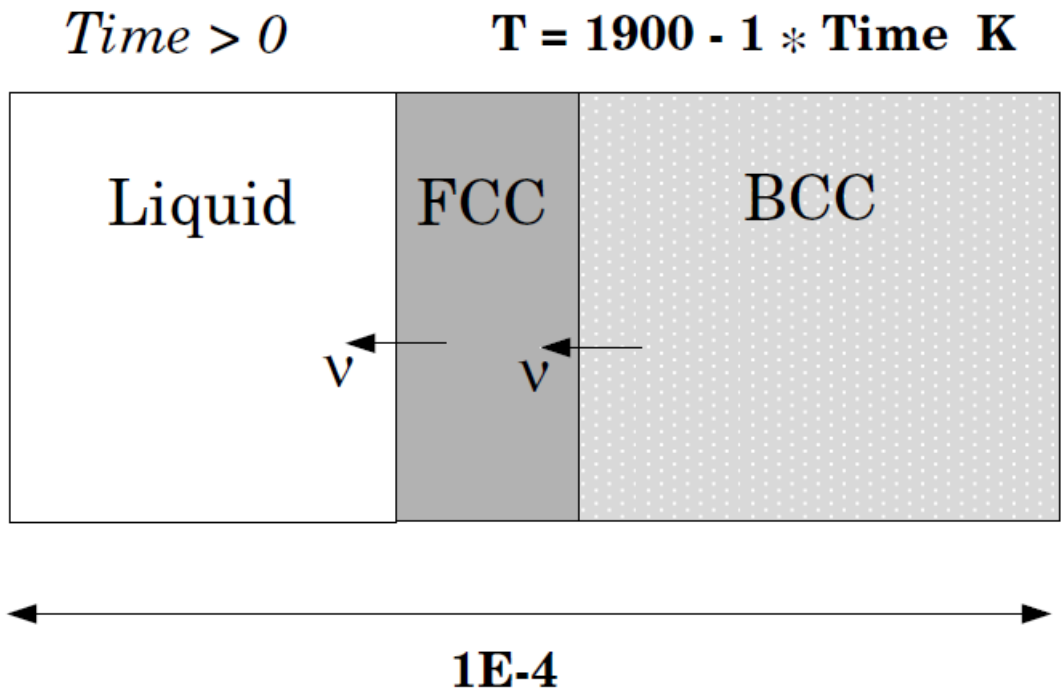



```
POST-1:
POST-1:
POST-1: set-inter
 --OK---
POST-1:
```

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

```
About Stockholm, Sweden

 Software  (build 12987) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri Feb 16 15:22:08 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb4b\setup.DCM" @@
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
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

 VA                     /-  DEFINED
 L12_FCC                B2_BCC                 DICTRA_FCC_A1
   REJECTED
TDB_TCFE9:
TDB_TCFE9: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA
TDB_TCFE9: sw fedemo
 Current database: Iron Demo Database v2.0

 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
 LIQUID:L               BCC_A2                 CHI_A12
 FCC_A1                 HCP_A3                 LAVES_PHASE_C14
 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
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'X.-G. Lu, M. Selleby, B. Sundman, CALPHAD, 29 (2005) 49-55; Fe P-T diagram'
  'J. Brillo and I. Egry, Int. J. Thermophysics, 24, 1155-1170'
  'B.-J. Lee, CALPHAD, 17 (1993) 251-268; revision of Fe-Cr and Fe -Ni liquid'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'B.-J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270
      (1986); CR-FE'
  'A. Dinsdale and T. Chart, MTDS NPL, Unpublished work (1986); CR -NI'
  'A. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); FE-NI'
 -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

 TCFE9   =  Steels/Fe-Alloys  v9.0
 TCFE10  =  Steels/Fe-Alloys  v10.0 SNAPSHOT
 TCFE8   =  Steels/Fe-Alloys  v8.1
 FROST1  =  FROST database v1.0
 TCFE7   =  Steels/Fe-Alloys  v7.0
 TCFE6   =  Steels/Fe-Alloys  v6.2
 TCFE5   =  Steels/Fe-Alloys  v5.0
 TCFE4   =  Steels/Fe-Alloys  v4.1
 TCFE3   =  Steels/Fe-Alloys  v3.1
 TCFE2   =  Steels/Fe-Alloys  v2.1
 TCFE1   =  Steels/Fe-Alloys  v1.0
 TCNI9   =  Ni-Alloys  v9.0 SNAPSHOT
 NI25    =  NI25 database
 TCNI8   =  Ni-Alloys  v8.1
 TCNI7   =  Ni-Alloys  v7.1
 TCNI6   =  Ni-Alloys  v6.0
 TCNI5   =  Ni-Alloys  v5.1
 TCNI4   =  Ni-Alloys  v4.0
 TCNI1   =  Ni-Alloys  v1.3
 TCAL5   =  Al-Alloys  v5.0
 TCAL4   =  Al-Alloys  v4.0
 TCAL3   =  Al-Alloys  v3.0
 TCAL2   =  Al-Alloys  v2.1
 TCAL1   =  Al-Alloys  v1.2
 TCMG4   =  Mg-Alloys  v4.0
 TCMG3   =  Mg-Alloys  v3.0
```

```
 TCMG2   =  Mg-Alloys  v2.0
 TCMG1   =  Mg-Alloys  v1.1
 TCTI1   =  Ti-Alloys  v1.0
 TCCU2   =  Cu-Alloys  v2.0
 TCCU1   =  Cu-Alloys  v1.0
 TCCC1   =  Cemented carbide  v1.0
 TCHEA2  =  High Entropy Alloy  v2.1
 TCHEA1  =  High Entropy Alloy  v1.0
 SSOL6   =  SGTE Alloy Solutions Database v6.0
 SSOL5   =  SGTE Alloy Solutions Database v5.0
 SSOL4   =  SGTE Alloy Solutions Database v4.9g
 SSOL2   =  SGTE Alloy Solutions Database v2.1
 SSUB6   =  SGTE Substances Database v6.0
 SSUB5   =  SGTE Substances Database v5.2
 SSUB4   =  SGTE Substances Database v4.1
 SSUB3   =  SGTE Substances Database v3.3
 SSUB2   =  SGTE Substances Database v2.2
 SNOB3   =  SGTE Noble Metal Alloys Database v3.1
 STBC2   =  SGTE Thermal Barrier Coating TDB v2.2
 STBC1   =  SGTE Thermal Barrier Coating TDB v1.1
 SALT1   =  SGTE Molten Salts Database v1.2
 SEMC2   =  TC Semi-Conductors  v2.1
 SLAG4   =  Fe-containing Slag  v4.1
 SLAG3   =  Fe-containing Slag  v3.2
 SLAG2   =  Fe-containing Slag  v2.2
 SLAG1   =  Fe-containing Slag  v1.2
 TCOX7   =  Metal Oxide Solutions  v7.0
 TCOX6   =  Metal Oxide Solutions  v6.0
 TCOX5   =  Metal Oxide Solutions  v5.1
 TCOX4   =  Metal Oxide Solutions  v4.1
 ION3    =  Ionic Solutions  v3.0
 ION2    =  Ionic Solutions  v2.6
 ION1    =  Ionic Solutions  v1.5
 NOX2    =  NPL Oxide Solutions Database v2.1
 TCNOBL1 =  Noble Metals Alloys v1.0
 TCSLD3  =  Solder Alloys  v3.2
 TCSLD2  =  Solder Alloys  v2.0
 TCSI1   =  Ultrapure Silicon  v1.2
 TCMP2   =  Materials Processing  v2.5
 TCES1   =  Combustion/Sintering  v1.1
 TCSC1   =  Super Conductor  v1.0
 TCFC1   =  SOFC Database v1.0
 NUMT2   =  Nuclear Materials  v2.1
 NUOX4   =  Nuclear Oxides  v4.2
 NUCL15  =  IRSN NUCLEA-15_4
 NUCL10  =  ThermoData NUCLEA Alloys-oxides TDB v10.2
 MEPH15  =  IRSN Mephista-15_1
 MEPH11  =  ThermoData MEPHISTA Nuclear Fuels TDB v11.2
 TCAQ3   =  Aqueous Solution  v3.0
 TCAQ2   =  Aqueous Solution  v2.6
 AQS2    =  TGG Aqueous Solution Database v2.6
 GCE2    =  TGG Geochemical/Environmental TDB v2.3
 FEDEMO  =  Iron Demo Database v2.0
 ALDEMO  =  Aluminum Demo Database v2.0
 NIDEMO  =  Nickel Demo Database v1.0
 CUDEMO  =  Copper Demo Database v1.0
 SLDEMO  =  Solder Demo Database v1.0
 OXDEMO  =  Oxide Demo Database v1.0
 SUBDEMO =  Substance Demo Database v1.0
 PTERN   =  Public Ternary Alloys TDB v1.3
 PAQ2    =  Public Aqueous Soln (SIT) TDB v2.4
 PG35    =  G35 Binary Semi-Conductors TDB v1.2
 PURE5   =  SGTE Unary (Pure Elements) TDB v5.1
 MOB2    =  Alloys Mobility  v2.7
 MOB1    =  Alloys Mobility  v1.3
 MOBFE1  =  Steels/Fe-Alloys Mobility  v1.0
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBNI4  =  Ni-Alloys Mobility  v4.0
 MOBNI3  =  Ni-Alloys Mobility  v3.1
 MOBNI2  =  Ni-Alloys Mobility  v2.4
 MOBNI1  =  Ni-Alloys Mobility  v1.0
 MOBAL3  =  Al-Alloys Mobility  v3.0
 MOBAL2  =  Al-Alloys Mobility  v2.0
 MOBAL1  =  Al-Alloys Mobility  v1.0
 MOBCU1  =  Cu-Alloys Mobility  v1.0
 MOBCU2  =  Cu-Alloys Mobility  v2.0
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBSLD1 =  Solder-Alloys Mobility  v1.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0 SNAPSHOT
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v1.0
 MFEDEMO =  Fe-Alloys Mobility demo database v2.0
 MNIDEMO =  Ni-Alloys Mobility demo database v1.0
 MCUDEMO =  Cu-Alloys Mobility demo database v1.0
 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
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 ....

 List of references for assessed data

  'This parameter has not been assessed'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Fe diffusion fcc Cr-Fe'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Ni diffusion fcc Cr-Ni'
  'B. Jonsson: Z. Metallkunde 86(1995)686-692; Cr, Fe and Ni diffusion fcc
```

```
     Cr-Fe-Ni'
  'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
     -Ni'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Ni self-diffusion'
  'B. Jonsson: ISIJ International, 35(1995)1415-1421; Cr, Fe and Ni
     diffusion bcc Cr-Fe-Ni'
  'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
     in bcc Fe'
 -OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP
APP: @@
APP: go d-m
 NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER GLOBAL CONDITION T
DIC> @@
DIC> @@ LOWER THE TEMPERATURE TO A RATE OF 1 K/s
DIC> @@
DIC> set-cond glob T 0 1900-1*TIME; * N

DIC>
DIC> @@
DIC> @@ ENTER A REGION CALLED smalta
DIC> @@
DIC> enter-region smalta
DIC>
DIC> @@
DIC> @@ ENTER A 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
 SETTING CHECK INTERFACE POSITION ON
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 /YES/: 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 (0 -> 0.5 -> 1): /.5/:
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /NO/:
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>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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
 single geometric dense at  0.10000E-03
 0.92197       87
 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                    0 seconds
 TIME =  0.26002472E-05 DT =  0.25002472E-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 =  0.76007416E-05 DT =  0.50004944E-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 =  0.17601730E-04 DT =  0.10000989E-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 =  0.37603708E-04 DT =  0.20001978E-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 =  0.77607664E-04 DT =  0.40003955E-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 =  0.15761557E-03 DT =  0.80007911E-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 =  0.31763140E-03 DT =  0.16001582E-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 =  0.63766304E-03 DT =  0.32003164E-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                    1 seconds
 TIME =  0.12777263E-02 DT =  0.64006329E-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 =  0.25578529E-02 DT =  0.12801266E-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 =  0.51181060E-02 DT =  0.25602531E-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 =  0.10238612E-01 DT =  0.51205063E-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 =  0.20479625E-01 DT =  0.10241013E-01 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 =  0.40961650E-01 DT =  0.20482025E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992482  FE = .733068011219292
                        NI = .0754116207882253
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.81925700E-01 DT =  0.40964050E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992482  FE = .733068011219293
                        NI = .0754116207882251
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.16385380     DT =  0.81928101E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992481  FE = .733068011219295
                        NI = .0754116207882247
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
```

```
  CPU time used in timestep                    0 seconds
 TIME =  0.32771000     DT =  0.16385620     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992479  FE = .733068011219297
                        NI = .0754116207882238
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.65542241     DT =  0.32771240     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992475  FE = .733068011219302
                        NI = .0754116207882237
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   1.3108472     DT =  0.65542481     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992468  FE = .733068011219311
                        NI = .0754116207882209
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   2.6216968     DT =   1.3108496     SUM OF SQUARES =   0.0000000


output ignored...



... output resumed

 U-FRACTION IN SYSTEM:  CR = .191136322974996  FE = .733496609453061
                        NI = .0753670675719435
 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
 2.214709804303921E-007        2.215385460401687E-007        2.216770448001629E-007        2.115098782968949E-007        2.063345872780767E-
007        1.959186123520306E-007        1.733831687151275E-007        1.337617917600389E-007        1.336968115761490E-
007        6.882058399204979E-008        3.227535265879277E-009        1.153683491730604E-015        6.122429151319604E-
022       TIME =   196.49628     DT =   1.3107200     SUM OF SQUARES =  0.61224292E-21
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.60932683E-08 AND  -0.60932683E-08
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.94742869E-05
 U-FRACTION IN SYSTEM:  CR = .191136322974779  FE = .733496609453115
                        NI = .0753670675721055
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_BCC_A2

  CPU time used in timestep                    4 seconds
 3.346201665019063E-007        3.346476252419448E-007        3.348322409195427E-007        3.159349562594239E-007        3.116731301524201E-
007        3.029835579558274E-007        2.854702000271923E-007        2.854481596102823E-007        2.523431439625368E-
007        1.918632389670062E-007        9.592618439312550E-008        9.594385624737205E-008        2.821071361742472E-
009        3.643190617473913E-016        1.567471384585235E-
024       TIME =   199.11772     DT =   2.6214400     SUM OF SQUARES =  0.15674714E-23
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.87055618E-08 AND   0.87055618E-08
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.94971080E-05
 U-FRACTION IN SYSTEM:  CR = .191136322982257  FE = .733496609451973
                        NI = .0753670675657698
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  27  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_FCC_A1

  CPU time used in timestep                    3 seconds
 9.465531871564794E-008        9.466870479524691E-008        9.512370642699078E-008        1.092917612720854E-009        9.467378338837387E-
010        6.854478379900974E-010        2.893322689718910E-010        1.625499958320008E-015        6.555656754706132E-
022       TIME =   200.00000     DT =  0.88228308     SUM OF SQUARES =  0.65556568E-21
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.36067992E-08 AND   0.36067992E-08
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.95002902E-05
 U-FRACTION IN SYSTEM:  CR = .191136322984313  FE = .733496609452615
                        NI = .0753670675630715
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 MUST SAVE WORKSPACE ON FILE
 WORKSPACE SAVED ON FILE
 RECLAIMING WORKSPACE
 DELETING TIME-RECORD FOR TIME    187.26882
 DELETING TIME-RECORD FOR TIME    193.87485
 DELETING TIME-RECORD FOR TIME    193.87486
 DELETING TIME-RECORD FOR TIME    193.87488
 DELETING TIME-RECORD FOR TIME    193.87492
 DELETING TIME-RECORD FOR TIME    193.87500
 DELETING TIME-RECORD FOR TIME    193.87516
 DELETING TIME-RECORD FOR TIME    193.87548
 DELETING TIME-RECORD FOR TIME    193.87612
 DELETING TIME-RECORD FOR TIME    193.87740
 DELETING TIME-RECORD FOR TIME    193.87996
 DELETING TIME-RECORD FOR TIME    193.88508
 DELETING TIME-RECORD FOR TIME    193.89532
 DELETING TIME-RECORD FOR TIME    193.91580
 DELETING TIME-RECORD FOR TIME    193.95676
 DELETING TIME-RECORD FOR TIME    194.03868
 DELETING TIME-RECORD FOR TIME    194.20252
 DELETING TIME-RECORD FOR TIME    194.53020
 DELETING TIME-RECORD FOR TIME    195.18556
 DELETING TIME-RECORD FOR TIME    196.49628

 KEEPING TIME-RECORD FOR TIME    199.11772
 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> @@ THE SIMULATION IS FINISHED
DIC> @@
```

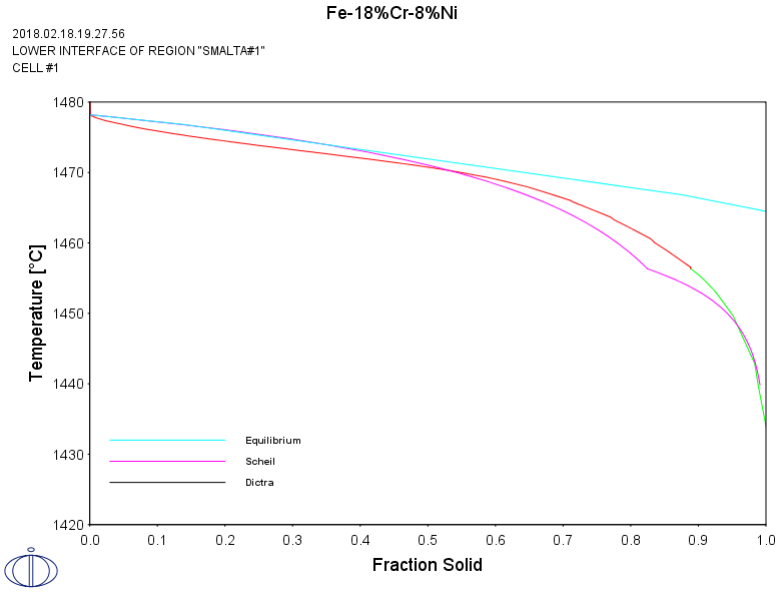
```
DIC>
DIC> set-inter
 --OK---
DIC>
```

exb4b-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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: plo
```

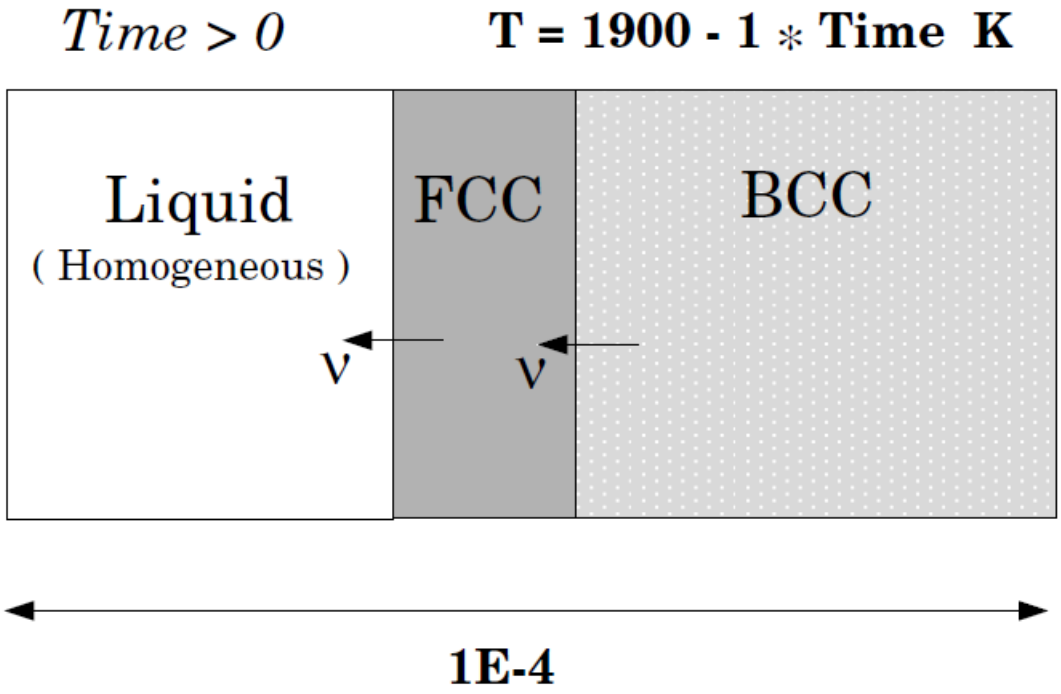



```
POST-1:
POST-1:
POST-1:
POST-1: set-inter
 --OK---
POST-1:
```

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

```
About
 Software  (build 12987) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri Feb 16 15:22:08 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb4c\setup.DCM" @@
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
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

 VA                     /-  DEFINED
 L12_FCC                B2_BCC                 DICTRA_FCC_A1
   REJECTED
TDB_TCFE9:
TDB_TCFE9: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA
TDB_TCFE9: sw fedemo
 Current database: Iron Demo Database v2.0

 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
 LIQUID:L               BCC_A2                 CHI_A12
 FCC_A1                 HCP_A3                 LAVES_PHASE_C14
 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
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'X.-G. Lu, M. Selleby, B. Sundman, CALPHAD, 29 (2005) 49-55; Fe P-T diagram'
  'J. Brillo and I. Egry, Int. J. Thermophysics, 24, 1155-1170'
  'B.-J. Lee, CALPHAD, 17 (1993) 251-268; revision of Fe-Cr and Fe -Ni liquid'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'B.-J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270
      (1986); CR-FE'
  'A. Dinsdale and T. Chart, MTDS NPL, Unpublished work (1986); CR -NI'
  'A. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); FE-NI'
 -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

 TCFE9   =  Steels/Fe-Alloys  v9.0
 TCFE10  =  Steels/Fe-Alloys  v10.0 SNAPSHOT
 TCFE8   =  Steels/Fe-Alloys  v8.1
 FROST1  =  FROST database v1.0
 TCFE7   =  Steels/Fe-Alloys  v7.0
 TCFE6   =  Steels/Fe-Alloys  v6.2
 TCFE5   =  Steels/Fe-Alloys  v5.0
 TCFE4   =  Steels/Fe-Alloys  v4.1
 TCFE3   =  Steels/Fe-Alloys  v3.1
 TCFE2   =  Steels/Fe-Alloys  v2.1
 TCFE1   =  Steels/Fe-Alloys  v1.0
 TCNI9   =  Ni-Alloys  v9.0 SNAPSHOT
 NI25    =  NI25 database
 TCNI8   =  Ni-Alloys  v8.1
 TCNI7   =  Ni-Alloys  v7.1
 TCNI6   =  Ni-Alloys  v6.0
 TCNI5   =  Ni-Alloys  v5.1
 TCNI4   =  Ni-Alloys  v4.0
 TCNI1   =  Ni-Alloys  v1.3
 TCAL5   =  Al-Alloys  v5.0
 TCAL4   =  Al-Alloys  v4.0
 TCAL3   =  Al-Alloys  v3.0
 TCAL2   =  Al-Alloys  v2.1
 TCAL1   =  Al-Alloys  v1.2
 TCMG4   =  Mg-Alloys  v4.0
 TCMG3   =  Mg-Alloys  v3.0
```

```
 TCMG2   =  Mg-Alloys  v2.0
 TCMG1   =  Mg-Alloys  v1.1
 TCTI1   =  Ti-Alloys  v1.0
 TCCU2   =  Cu-Alloys  v2.0
 TCCU1   =  Cu-Alloys  v1.0
 TCCC1   =  Cemented carbide  v1.0
 TCHEA2  =  High Entropy Alloy  v2.1
 TCHEA1  =  High Entropy Alloy  v1.0
 SSOL6   =  SGTE Alloy Solutions Database v6.0
 SSOL5   =  SGTE Alloy Solutions Database v5.0
 SSOL4   =  SGTE Alloy Solutions Database v4.9g
 SSOL2   =  SGTE Alloy Solutions Database v2.1
 SSUB6   =  SGTE Substances Database v6.0
 SSUB5   =  SGTE Substances Database v5.2
 SSUB4   =  SGTE Substances Database v4.1
 SSUB3   =  SGTE Substances Database v3.3
 SSUB2   =  SGTE Substances Database v2.2
 SNOB3   =  SGTE Noble Metal Alloys Database v3.1
 STBC2   =  SGTE Thermal Barrier Coating TDB v2.2
 STBC1   =  SGTE Thermal Barrier Coating TDB v1.1
 SALT1   =  SGTE Molten Salts Database v1.2
 SEMC2   =  TC Semi-Conductors  v2.1
 SLAG4   =  Fe-containing Slag  v4.1
 SLAG3   =  Fe-containing Slag  v3.2
 SLAG2   =  Fe-containing Slag  v2.2
 SLAG1   =  Fe-containing Slag  v1.2
 TCOX7   =  Metal Oxide Solutions  v7.0
 TCOX6   =  Metal Oxide Solutions  v6.0
 TCOX5   =  Metal Oxide Solutions  v5.1
 TCOX4   =  Metal Oxide Solutions  v4.1
 ION3    =  Ionic Solutions  v3.0
 ION2    =  Ionic Solutions  v2.6
 ION1    =  Ionic Solutions  v1.5
 NOX2    =  NPL Oxide Solutions Database v2.1
 TCNOBL1 =  Noble Metals Alloys v1.0
 TCSLD3  =  Solder Alloys  v3.2
 TCSLD2  =  Solder Alloys  v2.0
 TCSI1   =  Ultrapure Silicon  v1.2
 TCMP2   =  Materials Processing  v2.5
 TCES1   =  Combustion/Sintering  v1.1
 TCSC1   =  Super Conductor  v1.0
 TCFC1   =  SOFC Database v1.0
 NUMT2   =  Nuclear Materials  v2.1
 NUOX4   =  Nuclear Oxides  v4.2
 NUCL15  =  IRSN NUCLEA-15_4
 NUCL10  =  ThermoData NUCLEA Alloys-oxides TDB v10.2
 MEPH15  =  IRSN Mephista-15_1
 MEPH11  =  ThermoData MEPHISTA Nuclear Fuels TDB v11.2
 TCAQ3   =  Aqueous Solution  v3.0
 TCAQ2   =  Aqueous Solution  v2.6
 AQS2    =  TGG Aqueous Solution Database v2.6
 GCE2    =  TGG Geochemical/Environmental TDB v2.3
 FEDEMO  =  Iron Demo Database v2.0
 ALDEMO  =  Aluminum Demo Database v2.0
 NIDEMO  =  Nickel Demo Database v1.0
 CUDEMO  =  Copper Demo Database v1.0
 SLDEMO  =  Solder Demo Database v1.0
 OXDEMO  =  Oxide Demo Database v1.0
 SUBDEMO =  Substance Demo Database v1.0
 PTERN   =  Public Ternary Alloys TDB v1.3
 PAQ2    =  Public Aqueous Soln (SIT) TDB v2.4
 PG35    =  G35 Binary Semi-Conductors TDB v1.2
 PURE5   =  SGTE Unary (Pure Elements) TDB v5.1
 MOB2    =  Alloys Mobility  v2.7
 MOB1    =  Alloys Mobility  v1.3
 MOBFE1  =  Steels/Fe-Alloys Mobility  v1.0
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBNI4  =  Ni-Alloys Mobility  v4.0
 MOBNI3  =  Ni-Alloys Mobility  v3.1
 MOBNI2  =  Ni-Alloys Mobility  v2.4
 MOBNI1  =  Ni-Alloys Mobility  v1.0
 MOBAL3  =  Al-Alloys Mobility  v3.0
 MOBAL2  =  Al-Alloys Mobility  v2.0
 MOBAL1  =  Al-Alloys Mobility  v1.0
 MOBCU1  =  Cu-Alloys Mobility  v1.0
 MOBCU2  =  Cu-Alloys Mobility  v2.0
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBSLD1 =  Solder-Alloys Mobility  v1.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0 SNAPSHOT
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v1.0
 MFEDEMO =  Fe-Alloys Mobility demo database v2.0
 MNIDEMO =  Ni-Alloys Mobility demo database v1.0
 MCUDEMO =  Cu-Alloys Mobility demo database v1.0
 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
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 ....

 List of references for assessed data

  'This parameter has not been assessed'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Fe diffusion fcc Cr-Fe'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Ni diffusion fcc Cr-Ni'
  'B. Jonsson: Z. Metallkunde 86(1995)686-692; Cr, Fe and Ni diffusion fcc
```

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      Cr-Fe-Ni'
   'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
      -Ni'
   'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Ni self-diffusion'
   'B. Jonsson: ISIJ International, 35(1995)1415-1421; Cr, Fe and Ni
      diffusion bcc Cr-Fe-Ni'
   'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
      in bcc Fe'
 -OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP
APP: @@
APP: go d-m
 NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ LIST THE MOBILITIES IN THE LIQUID
DIC> @@
DIC> list-mobility-data
 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
 I AM SORRY BUT YOU MUST THEN REENTER ALL 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
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
 I AM SORRY BUT YOU MUST THEN REENTER ALL RANGES
 DQ(LIQUID&CR#1,FE;0) =
LOW TEMPERATURE LIMIT /298.15/: 298.15 +R*T*LN(1E-06); 6000 n
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
 I AM SORRY BUT YOU MUST THEN REENTER ALL RANGES
 DQ(LIQUID&CR#1,NI;0) =
LOW TEMPERATURE LIMIT /298.15/: 298.15 +R*T*LN(1E-06); 6000 n
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
 I AM SORRY BUT YOU MUST THEN REENTER ALL RANGES
 DQ(LIQUID&NI#1,CR;0) =
LOW TEMPERATURE LIMIT /298.15/: 298.15 +R*T*LN(1E-06); 6000 n
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
 I AM SORRY BUT YOU MUST THEN REENTER ALL RANGES
 DQ(LIQUID&NI#1,FE;0) =
LOW TEMPERATURE LIMIT /298.15/: 298.15 +R*T*LN(1E-06); 6000 n
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
 I AM SORRY BUT YOU MUST THEN REENTER ALL RANGES
 DQ(LIQUID&NI#1,NI;0) =
LOW TEMPERATURE LIMIT /298.15/: 298.15 +R*T*LN(1E-06); 6000 n
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
 I AM SORRY BUT YOU MUST THEN REENTER ALL RANGES
 DQ(LIQUID&FE#1,CR;0) =
LOW TEMPERATURE LIMIT /298.15/: 298.15 +R*T*LN(1E-06); 6000 n
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
 I AM SORRY BUT YOU MUST THEN REENTER ALL RANGES
 DQ(LIQUID&FE#1,FE;0) =
LOW TEMPERATURE LIMIT /298.15/: 298.15 +R*T*LN(1E-06); 6000 n
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
 I AM SORRY BUT YOU MUST THEN REENTER ALL RANGES
 DQ(LIQUID&FE#1,NI;0) =
LOW TEMPERATURE LIMIT /298.15/: 298.15 +R*T*LN(1E-06); 6000 n
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
 SETTING CHECK INTERFACE POSITION ON
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
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 /YES/: 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 (0 -> 0.5 -> 1): /.5/:
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /NO/:
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>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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
 single geometric dense at  0.10000E-03
 0.99375       62
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882254
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.10874528E-05 DT =  0.98745278E-06 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882254
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.30623583E-05 DT =  0.19749056E-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 =  0.70121695E-05 DT =  0.39498111E-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 =  0.14911792E-04 DT =  0.78996222E-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 =  0.30711036E-04 DT =  0.15799244E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882254
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.62309525E-04 DT =  0.31598489E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882254
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.12550650E-03 DT =  0.63196978E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882254
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.25190046E-03 DT =  0.12639396E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882254
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.50468837E-03 DT =  0.25278791E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                        NI = .0754116207882256
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.10102642E-02 DT =  0.50557582E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.20214158E-02 DT =  0.10111516E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                        NI = .0754116207882259
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.40437191E-02 DT =  0.20223033E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                        NI = .0754116207882259
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.80883257E-02 DT =  0.40446066E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992477  FE = .733068011219298
                        NI = .0754116207882252
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    1 seconds
 TIME =  0.16177539E-01 DT =  0.80892132E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992482  FE = .733068011219295
                        NI = .0754116207882228
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.32355965E-01 DT =  0.16178426E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992504  FE = .733068011219263
                        NI = .0754116207882329
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.64712818E-01 DT =  0.32356853E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992551  FE = .733068011219194
                        NI = .0754116207882548
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
```

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  CPU time used in timestep                    0 seconds
 TIME =  0.12942652     DT =  0.64713705E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .19152036799265  FE = .733068011219074
                        NI = .0754116207882761
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.25885393     DT =  0.12942741     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992726  FE = .733068011218895
                        NI = .0754116207883795
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.51770876     DT =  0.25885482     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992969  FE = .733068011218548
                        NI = .0754116207884827
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   1.0354184     DT =  0.51770964     SUM OF SQUARES =   0.0000000


output ignored...



... output resumed

 2.0863736475878 91E-015        4.787229045784939E-014        1.971385888754113E-
016       TIME =   199.16151     DT =   1.0000000     SUM OF SQUARES =  0.19713859E-15
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.10033934E-06 AND  -0.10033934E-06
 POSITION OF INTERFACE SMALTA / R_FCC_A1 IS   0.46441749E-06
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.11516775E-07 AND   0.11516775E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.10970287E-04
 U-FRACTION IN SYSTEM:  CR = .191211086169418  FE = .733433260812751
                        NI = .0753556530178301
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  32  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_FCC_A1

  CPU time used in timestep                    4 seconds
 3.780876991451475E-007        3.786514022577464E-007        3.780834027702343E-007        3.780917218658302E-007        3.779744598558534E-
007        2.326746685393648E-008        9.107557821247557E-010        7.162247005586656E-013        1.756975994127614E-
014        1.047100422739898E-015        5.726994848012839E-013        1.904683817878645E-
016       TIME =   200.00000     DT =  0.83849346     SUM OF SQUARES =  0.19046838E-15
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.85423816E-07 AND  -0.85423816E-07
 POSITION OF INTERFACE SMALTA / R_FCC_A1 IS   0.39279018E-06
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.13581454E-07 AND   0.13581454E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.10981675E-04
 U-FRACTION IN SYSTEM:  CR = .191211078394994  FE = .733433268342357
                        NI = .075355653262649
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 MUST SAVE WORKSPACE ON FILE
 WORKSPACE SAVED ON FILE
 RECLAIMING WORKSPACE
 DELETING TIME-RECORD FOR TIME    170.39980
 DELETING TIME-RECORD FOR TIME    170.48379
 DELETING TIME-RECORD FOR TIME    170.48379
 DELETING TIME-RECORD FOR TIME    170.48379
 DELETING TIME-RECORD FOR TIME    170.48379
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 DELETING TIME-RECORD FOR TIME    170.48381
 DELETING TIME-RECORD FOR TIME    170.48384
 DELETING TIME-RECORD FOR TIME    170.48389
 DELETING TIME-RECORD FOR TIME    170.48399
 DELETING TIME-RECORD FOR TIME    170.48419
 DELETING TIME-RECORD FOR TIME    170.48460
 DELETING TIME-RECORD FOR TIME    170.48542
 DELETING TIME-RECORD FOR TIME    170.48706
 DELETING TIME-RECORD FOR TIME    170.49034
 DELETING TIME-RECORD FOR TIME    170.49689
 DELETING TIME-RECORD FOR TIME    170.51000
 DELETING TIME-RECORD FOR TIME    170.53621
 DELETING TIME-RECORD FOR TIME    170.58864
 DELETING TIME-RECORD FOR TIME    170.69350
 DELETING TIME-RECORD FOR TIME    170.90322
 DELETING TIME-RECORD FOR TIME    171.32265
 DELETING TIME-RECORD FOR TIME    172.16151
 DELETING TIME-RECORD FOR TIME    173.16151
 DELETING TIME-RECORD FOR TIME    174.16151
 DELETING TIME-RECORD FOR TIME    175.16151
 DELETING TIME-RECORD FOR TIME    176.16151
 DELETING TIME-RECORD FOR TIME    177.16151
 DELETING TIME-RECORD FOR TIME    178.16151
 DELETING TIME-RECORD FOR TIME    179.16151
 DELETING TIME-RECORD FOR TIME    180.16151
 DELETING TIME-RECORD FOR TIME    181.16151
 DELETING TIME-RECORD FOR TIME    182.16151
 DELETING TIME-RECORD FOR TIME    183.16151
 DELETING TIME-RECORD FOR TIME    184.16151
 DELETING TIME-RECORD FOR TIME    185.16151
 DELETING TIME-RECORD FOR TIME    186.16151
 DELETING TIME-RECORD FOR TIME    187.16151
 DELETING TIME-RECORD FOR TIME    188.16151
 DELETING TIME-RECORD FOR TIME    189.16151
 DELETING TIME-RECORD FOR TIME    190.16151
 DELETING TIME-RECORD FOR TIME    191.16151
 DELETING TIME-RECORD FOR TIME    192.16151
 DELETING TIME-RECORD FOR TIME    193.16151
 DELETING TIME-RECORD FOR TIME    194.16151
 DELETING TIME-RECORD FOR TIME    195.16151
 DELETING TIME-RECORD FOR TIME    196.16151
 DELETING TIME-RECORD FOR TIME    197.16151
 DELETING TIME-RECORD FOR TIME    198.16151

 KEEPING TIME-RECORD FOR TIME    199.16151
 AND FOR TIME                    200.00000
 WORKSPACE RECLAIMED

 TIMESTEP AT     200.000000     SELECTED

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

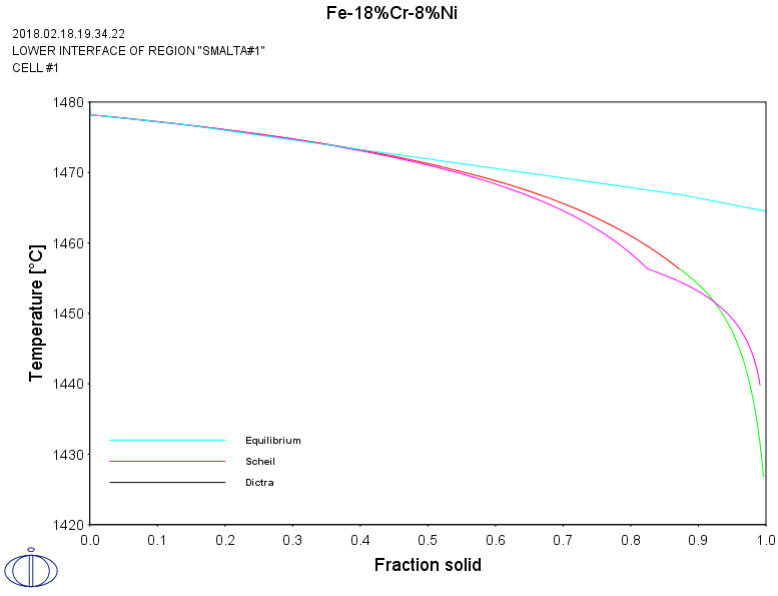
```
DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ THE SIMULATION IS FINISHED
DIC> @@
DIC>
DIC> set-inter
 --OK---
DIC>
```

exb4c-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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: plo
```

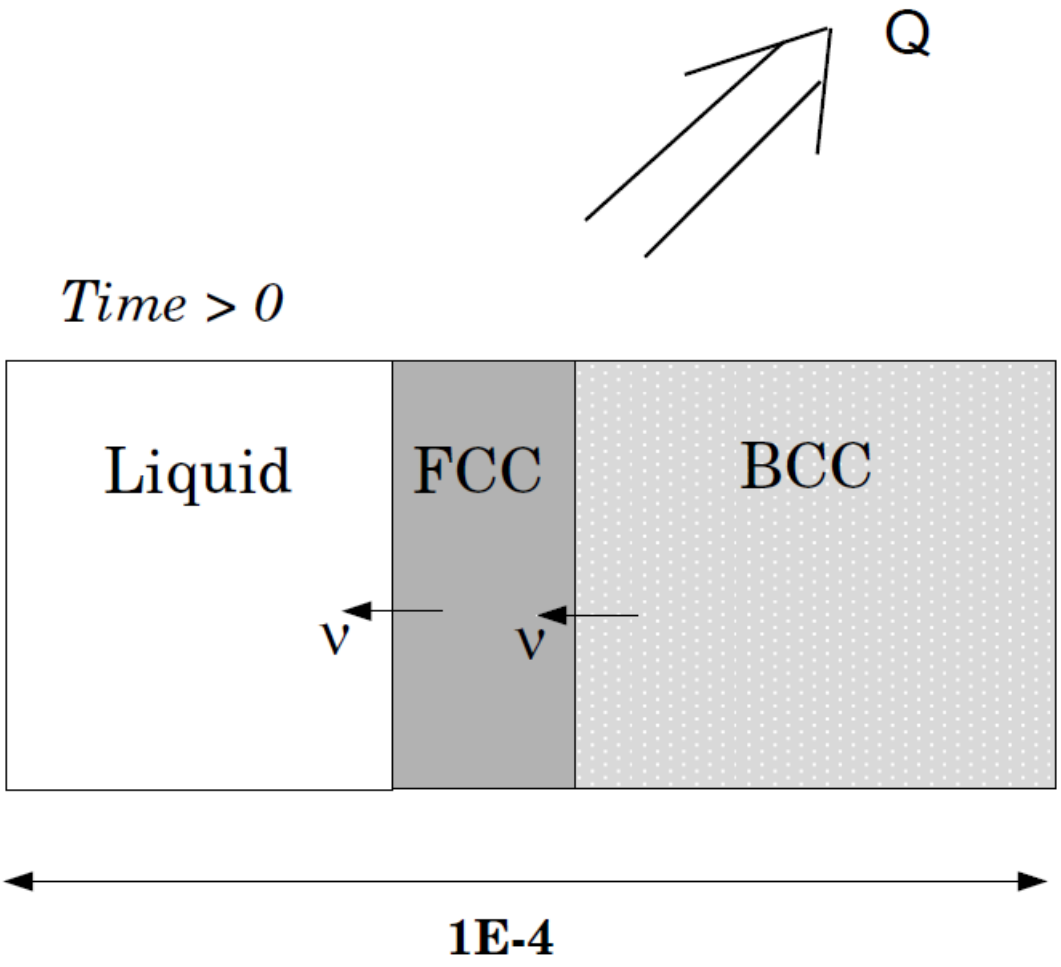



```
POST-1:
POST-1:
POST-1:
POST-1: set-inter
 --OK---
POST-1:
```

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

```
About Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri Feb 16 15:22:08 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

 VA                     /-  DEFINED
 L12_FCC                B2_BCC                 DICTRA_FCC_A1
   REJECTED
TDB_TCFE9:
TDB_TCFE9: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA
TDB_TCFE9: sw fedemo
 Current database: Iron Demo Database v2.0

 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
 LIQUID:L               BCC_A2                 CHI_A12
 FCC_A1                 HCP_A3                 LAVES_PHASE_C14
 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
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'X.-G. Lu, M. Selleby, B. Sundman, CALPHAD, 29 (2005) 49-55; Fe P-T diagram'
  'J. Brillo and I. Egry, Int. J. Thermophysics, 24, 1155-1170'
  'B.-J. Lee, CALPHAD, 17 (1993) 251-268; revision of Fe-Cr and Fe -Ni liquid'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'B.-J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270
      (1986); CR-FE'
  'A. Dinsdale and T. Chart, MTDS NPL, Unpublished work (1986); CR -NI'
  'A. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); FE-NI'
 -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

 TCFE9    =  Steels/Fe-Alloys  v9.0
 TCFE10   =  Steels/Fe-Alloys  v10.0 SNAPSHOT
 TCFE8    =  Steels/Fe-Alloys  v8.1
 FROST1   =  FROST database v1.0
 TCFE7    =  Steels/Fe-Alloys  v7.0
 TCFE6    =  Steels/Fe-Alloys  v6.2
 TCFE5    =  Steels/Fe-Alloys  v5.0
 TCFE4    =  Steels/Fe-Alloys  v4.1
 TCFE3    =  Steels/Fe-Alloys  v3.1
 TCFE2    =  Steels/Fe-Alloys  v2.1
 TCFE1    =  Steels/Fe-Alloys  v1.0
 TCNI9    =  Ni-Alloys  v9.0 SNAPSHOT
 NI25     =  NI25 database
 TCNI8    =  Ni-Alloys  v8.1
 TCNI7    =  Ni-Alloys  v7.1
 TCNI6    =  Ni-Alloys  v6.0
 TCNI5    =  Ni-Alloys  v5.1
 TCNI4    =  Ni-Alloys  v4.0
 TCNI1    =  Ni-Alloys  v1.3
 TCAL5    =  Al-Alloys  v5.0
 TCAL4    =  Al-Alloys  v4.0
 TCAL3    =  Al-Alloys  v3.0
 TCAL2    =  Al-Alloys  v2.1
 TCAL1    =  Al-Alloys  v1.2
 TCMG4    =  Mg-Alloys  v4.0
 TCMG3    =  Mg-Alloys  v3.0
 TCMG2    =  Mg-Alloys  v2.0
 TCMG1    =  Mg-Alloys  v1.1
 TCTI1    =  Ti-Alloys  v1.0
 TCCU2    =  Cu-Alloys  v2.0
```

```
 TCCU1   =  Cu-Alloys  v1.0
 TCCC1   =  Cemented carbide  v1.0
 TCHEA2  =  High Entropy Alloy  v2.1
 TCHEA1  =  High Entropy Alloy  v1.0
 SSOL6   =  SGTE Alloy Solutions Database v6.0
 SSOL5   =  SGTE Alloy Solutions Database v5.0
 SSOL4   =  SGTE Alloy Solutions Database v4.9g
 SSOL2   =  SGTE Alloy Solutions Database v2.1
 SSUB6   =  SGTE Substances Database v6.0
 SSUB5   =  SGTE Substances Database v5.2
 SSUB4   =  SGTE Substances Database v4.1
 SSUB3   =  SGTE Substances Database v3.3
 SSUB2   =  SGTE Substances Database v2.2
 SNOB3   =  SGTE Noble Metal Alloys Database v3.1
 STBC2   =  SGTE Thermal Barrier Coating TDB v2.2
 STBC1   =  SGTE Thermal Barrier Coating TDB v1.1
 SALT1   =  SGTE Molten Salts Database v1.2
 SEMC2   =  TC Semi-Conductors  v2.1
 SLAG4   =  Fe-containing Slag  v4.1
 SLAG3   =  Fe-containing Slag  v3.2
 SLAG2   =  Fe-containing Slag  v2.2
 SLAG1   =  Fe-containing Slag  v1.2
 TCOX7   =  Metal Oxide Solutions  v7.0
 TCOX6   =  Metal Oxide Solutions  v6.0
 TCOX5   =  Metal Oxide Solutions  v5.1
 TCOX4   =  Metal Oxide Solutions  v4.1
 ION3    =  Ionic Solutions  v3.0
 ION2    =  Ionic Solutions  v2.6
 ION1    =  Ionic Solutions  v1.5
 NOX2    =  NPL Oxide Solutions Database v2.1
 TCNOBL1 =  Noble Metals Alloys v1.0
 TCSLD3  =  Solder Alloys  v3.2
 TCSLD2  =  Solder Alloys  v2.0
 TCSI1   =  Ultrapure Silicon  v1.2
 TCMP2   =  Materials Processing  v2.5
 TCES1   =  Combustion/Sintering  v1.1
 TCSC1   =  Super Conductor  v1.0
 TCFC1   =  SOFC Database v1.0
 NUMT2   =  Nuclear Materials  v2.1
 NUOX4   =  Nuclear Oxides  v4.2
 NUCL15  =  IRSN NUCLEA-15_4
 NUCL10  =  ThermoData NUCLEA Alloys-oxides TDB v10.2
 MEPH15  =  IRSN Mephista-15_1
 MEPH11  =  ThermoData MEPHISTA Nuclear Fuels TDB v11.2
 TCAQ3   =  Aqueous Solution  v3.0
 TCAQ2   =  Aqueous Solution  v2.6
 AQS2    =  TGG Aqueous Solution Database v2.6
 GCE2    =  TGG Geochemical/Environmental TDB v2.3
 FEDEMO  =  Iron Demo Database v2.0
 ALDEMO  =  Aluminum Demo Database v2.0
 NIDEMO  =  Nickel Demo Database v1.0
 CUDEMO  =  Copper Demo Database v1.0
 SLDEMO  =  Solder Demo Database v1.0
 OXDEMO  =  Oxide Demo Database v1.0
 SUBDEMO =  Substance Demo Database v1.0
 PTERN   =  Public Ternary Alloys TDB v1.3
 PAQ2    =  Public Aqueous Soln (SIT) TDB v2.4
 PG35    =  G35 Binary Semi-Conductors TDB v1.2
 PURE5   =  SGTE Unary (Pure Elements) TDB v5.1
 MOB2    =  Alloys Mobility  v2.7
 MOB1    =  Alloys Mobility  v1.3
 MOBFE1  =  Steels/Fe-Alloys Mobility  v1.0
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBNI4  =  Ni-Alloys Mobility  v4.0
 MOBNI3  =  Ni-Alloys Mobility  v3.1
 MOBNI2  =  Ni-Alloys Mobility  v2.4
 MOBNI1  =  Ni-Alloys Mobility  v1.0
 MOBAL3  =  Al-Alloys Mobility  v3.0
 MOBAL2  =  Al-Alloys Mobility  v2.0
 MOBAL1  =  Al-Alloys Mobility  v1.0
 MOBCU1  =  Cu-Alloys Mobility  v1.0
 MOBCU2  =  Cu-Alloys Mobility  v2.0
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBSLD1 =  Solder-Alloys Mobility  v1.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0 SNAPSHOT
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v1.0
 MFEDEMO =  Fe-Alloys Mobility demo database v2.0
 MNIDEMO =  Ni-Alloys Mobility demo database v1.0
 MCUDEMO =  Cu-Alloys Mobility demo database v1.0
 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
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 ....

 List of references for assessed data

  'This parameter has not been assessed'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Fe diffusion fcc Cr-Fe'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Ni diffusion fcc Cr-Ni'
  'B. Jonsson: Z. Metallkunde 86(1995)686-692; Cr, Fe and Ni diffusion fcc
      Cr-Fe-Ni'
  'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
      -Ni'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Ni self-diffusion'
```

```
  'B. Jonsson: ISIJ International, 35(1995)1415-1421; Cr, Fe and Ni
      diffusion bcc Cr-Fe-Ni'
  'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
      in bcc Fe'
 -OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP
APP: @@
APP: go d-m
 NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ EXTRACT HEAT 91.19 J/mole/s
DIC> @@
DIC> set-cond glob Q 0 91.19; * N

DIC>
DIC> @@
DIC> @@ ENTER AN INITIAL TEMPERATURE
DIC> @@
DIC> set-initial-temp 1900
DIC>
DIC> @@
DIC> @@ ENTER A REGION CALLED smalta
DIC> @@
DIC> enter-region smalta
DIC>
DIC> @@
DIC> @@ ENTER A GEOMETRIC GRID INTO THE REGION
DIC> @@
DIC> enter-grid
REGION NAME : /SMALTA/: smalta
WIDTH OF REGION /1/: 1e-4
TYPE /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
 SETTING CHECK INTERFACE POSITION ON
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 /YES/: 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 (0 -> 0.5 -> 1): /.5/:
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /NO/:
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>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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
 single geometric dense at  0.10000E-03
 0.92197       87
 TEMPERATURE:   1900.     ENTHALPY:  0.7394E+05
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                        NI = .0754116207882254
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 TEMPERATURE:   1900.     ENTHALPY:  0.7394E+05
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                        NI = .0754116207882254
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 3.863918610053681E-007        3.864691456620901E-007        3.837979016399162E-016        3.830845290529296E-025       TIME =  0.10000000E-
06 DT =  0.10000000E-06 SUM OF SQUARES =  0.38308453E-24
 TEMPERATURE:   1900.     ENTHALPY:  0.7394E+05
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                        NI = .0754116207882254
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 9.508207427607264E-018       TIME =  0.26002472E-05 DT =  0.25002472E-05 SUM OF SQUARES =  0.95082074E-17
 TEMPERATURE:   1900.     ENTHALPY:  0.7394E+05
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                        NI = .0754116207882254
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 3.803282971042906E-017       TIME =  0.76007416E-05 DT =  0.50004944E-05 SUM OF SQUARES =  0.38032830E-16
 TEMPERATURE:   1900.     ENTHALPY:  0.7394E+05
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                        NI = .0754116207882254
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 1.521313188417162E-016        1.521313188417162E-016


     ERROR RETURN FROM NS01A BECAUSE A NEARBY STATIONARY POINT OF F(X) IS PREDICTED

 *** ERROR  1890 IN DCNS01
 *** ERROR RETURN FROM NS01A
 1.521313188417162E-016        1.521313188417162E-016        1.521313188417162E-016        9.303850408268813E-020        1.431856390077847E-
016        3.399472344393975E-017        3.399472344393975E-017        1.089191126797645E-019        1.089191126797645E-
019        1.089191126797645E-019        1.089191126797645E-019        2.673347549794903E-017        1.089185930657826E-
019        1.089185930657826E-019        1.089185930657826E-019        1.089185930657826E-019        1.092210507539688E-
018        1.089191126797645E-019       TIME =  0.17601730E-04 DT =  0.10000989E-04 SUM OF SQUARES =  0.10891911E-18
 TEMPERATURE:   1900.     ENTHALPY:  0.7394E+05
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                        NI = .0754116207882254
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 1.666578502523493E-016        1.666578502523493E-016


     ERROR RETURN FROM NS01A BECAUSE A NEARBY STATIONARY POINT OF F(X) IS PREDICTED

 *** ERROR  1890 IN DCNS01
 *** ERROR RETURN FROM NS01A
 1.666578502523493E-016        1.666578502523493E-016        1.666578502523493E-016        1.352477274150108E-012        1.666578502523493E-
016        1.038241667728256E-035        1.038241667728256E-035        1.038241667728256E-035        1.038241667728256E-
035        1.038241667728256E-035        1.038241667728256E-035        1.038241667728256E-035        1.038241667728256E-
035        1.038241667728256E-035        1.038241667728256E-035        1.038241667728256E-035       TIME =  0.37603708E-04 DT =  0.20001978E-
04 SUM OF SQUARES =  0.10382417E-34
 TEMPERATURE:   1900.     ENTHALPY:  0.7394E+05
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                        NI = .0754116207882254
 TOTAL SIZE OF SYSTEM:  1E-04 [m]


output ignored...



... output resumed

 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.55694300E-05
 TEMPERATURE:   1705.     ENTHALPY:  0.5598E+05
 U-FRACTION IN SYSTEM:  CR = .191419766484522  FE = .73319305074855
                        NI = .075387182766928
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  2  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_FCC_A1

  CPU time used in timestep                    1 seconds
 2.851700635661659E-007        2.851708831145793E-007        2.851624308208675E-007        2.851128595190466E-007        3.297264654510150E-
008        3.644973198683710E-013        1.151450973113358E-
017       TIME =   196.69085     DT =  0.66250000     SUM OF SQUARES =  0.11514510E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.77639011E-07 AND   0.77639011E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.56208658E-05
 TEMPERATURE:   1704.     ENTHALPY:  0.5592E+05
 U-FRACTION IN SYSTEM:  CR = .191419766484524  FE = .733193050748551
                        NI = .0753871827669249
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  3  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_FCC_A1

  CPU time used in timestep                    1 seconds
 1.454026536091647E-006        1.454359117619401E-006        1.454001659786809E-006        1.453664261497834E-006        8.606587472876681E-
007        4.249638417202260E-007        3.262596954381343E-008        1.388431396930162E-012        1.963259591187198E-
```

```
017       TIME =   198.01585     DT =   1.3250000     SUM OF SQUARES =  0.19632596E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.91803141E-07 AND   0.91803141E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.57425050E-05
 TEMPERATURE:   1701.      ENTHALPY:  0.5580E+05
 U-FRACTION IN SYSTEM:  CR = .191419766484521  FE = .733193050748554
                        NI = .0753871827669252
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  10  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_FCC_A1

  CPU time used in timestep                      2 seconds
 1.244319273883474E-006        1.244443998637513E-006        1.244744746398433E-006        1.243773368185792E-006        8.842480260593866E-
007        5.113987890663018E-007        1.095007729722212E-007        1.184043441071940E-011        4.534939770399833E-
016        7.718568589832551E-020       TIME =   200.00000     DT =   1.9841508     SUM OF SQUARES =  0.77185686E-19
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.10665583E-06 AND   0.10665583E-06
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.59541262E-05
 TEMPERATURE:   1696.      ENTHALPY:  0.5562E+05
 U-FRACTION IN SYSTEM:  CR = .191419766484487  FE = .733193050748579
                        NI = .0753871827669334
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 MUST SAVE WORKSPACE ON FILE
 WORKSPACE SAVED ON FILE
 RECLAIMING WORKSPACE
 DELETING TIME-RECORD FOR TIME    194.62054
 DELETING TIME-RECORD FOR TIME    195.44866
 DELETING TIME-RECORD FOR TIME    195.53147
 DELETING TIME-RECORD FOR TIME    195.69710
 DELETING TIME-RECORD FOR TIME    196.02835
 DELETING TIME-RECORD FOR TIME    196.69085

 KEEPING TIME-RECORD FOR TIME    198.01585
 AND FOR TIME                    200.00000
 WORKSPACE RECLAIMED

 TIMESTEP AT     200.000000     SELECTED

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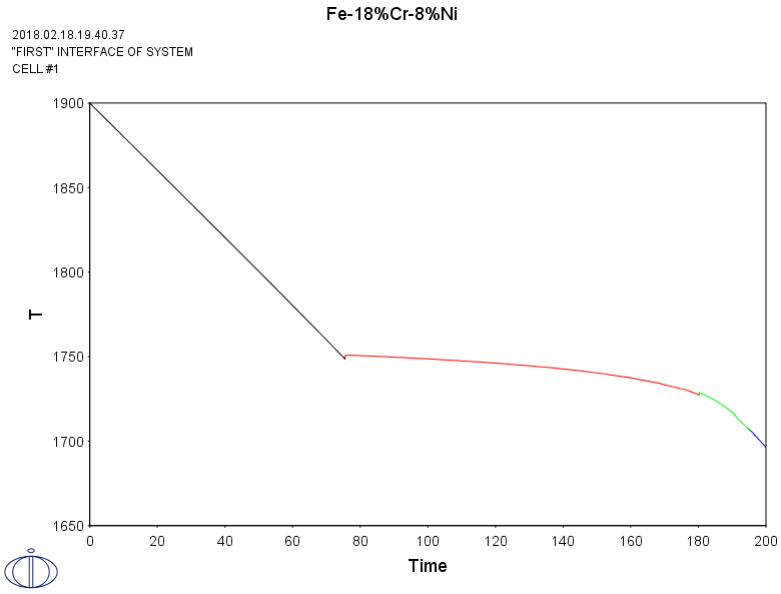
DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ THE SIMULATION IS FINISHED
DIC> @@
DIC>
DIC> set-inter
 --OK---
DIC>
```

exb4d-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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

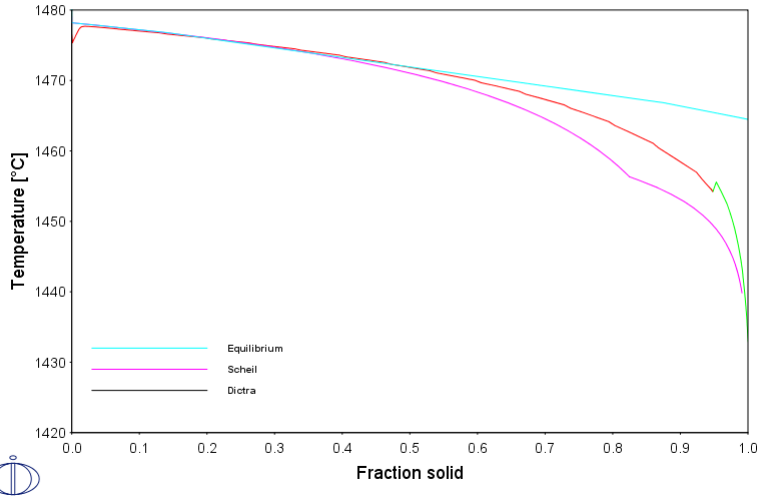
POST-1:
POST-1: set-title Fe-18%Cr-8%Ni
POST-1:
POST-1: @@
POST-1: @@ PLOT THE FRACTION OF SOLID AND COMPARE WITH SCHEIL-GULLIVER
POST-1: @@ SIMULATION AND EQUILIBRIUM SOLIDIFICATION (DATA ON FILE exb4.exp)
POST-1: @@
POST-1: s-d-a x time
  INFO: Time is set as independent variable
POST-1: s-d-a y T
POST-1: s-p-c inter first
POST-1: 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: plo
```

Fe-18%Cr-8%Ni

2018.02.18.19.40.38
LOWER INTERFACE OF REGION "SMALTA#1"
CELL #1

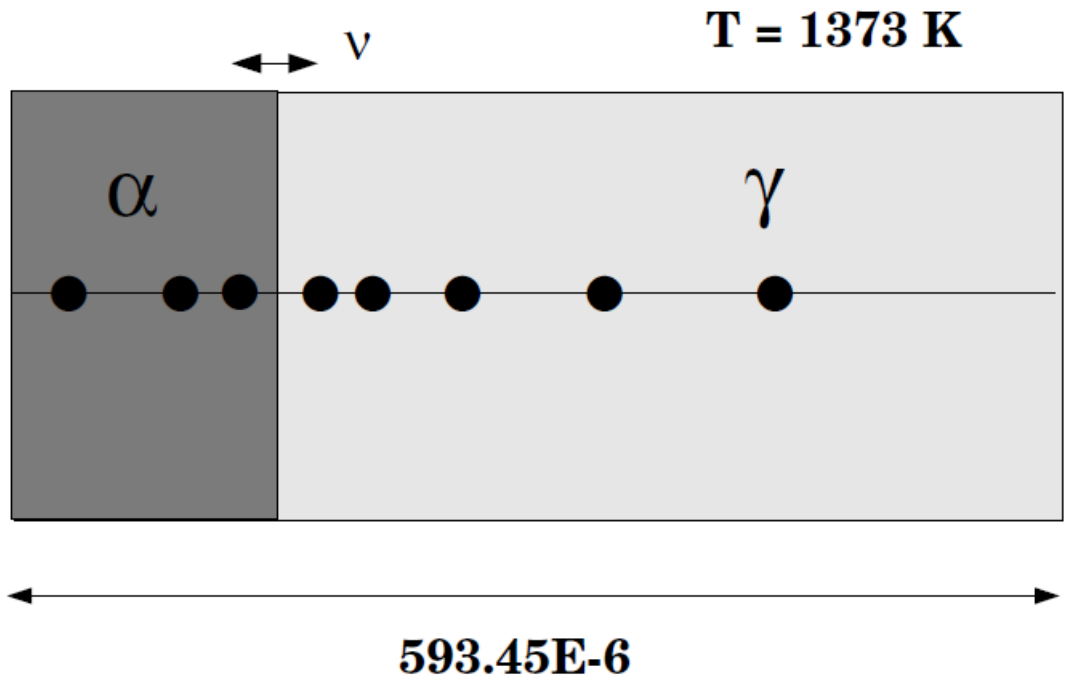



```
POST-1:
POST-1:
POST-1:
POST-1: set-inter
 --OK---
POST-1:
```

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

```
About License library version: 8.5.1.0017
 Linked: Fri Feb 16 15:22:08 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb5\setup.DCM" @@
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
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

 VA                        /-  DEFINED
 L12_FCC                   B2_BCC                    DICTRA_FCC_A1
   REJECTED
TDB_TCFE9: sw fedemo
 Current database: Iron Demo Database v2.0

 VA                        /-  DEFINED
TDB_FEDEMO: def-sys cr fe ni
 CR                        FE                        NI
   DEFINED
TDB_FEDEMO: rej-ph /all
 LIQUID:L                  BCC_A2                    CHI_A12
 FCC_A1                    HCP_A3                    LAVES_PHASE_C14
 SIGMA  REJECTED
TDB_FEDEMO: res-ph bcc,fcc
 BCC_A2                    FCC_A1  RESTORED
TDB_FEDEMO: get
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'X.-G. Lu, M. Selleby, B. Sundman, CALPHAD, 29 (2005) 49-55; Fe P-T diagram'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270
      (1986); CR-FE'
  'B.-J. Lee, CALPHAD, 17 (1993) 251-268; revision of Fe-Cr and Fe -Ni liquid'
  'B.-J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
  'A. Dinsdale and T. Chart, MTDS NPL, Unpublished work (1986); CR -NI'
  'A. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); FE-NI'
 -OK-
TDB_FEDEMO:
TDB_FEDEMO: app
 Use one of these databases

 TCFE9   =  Steels/Fe-Alloys  v9.0
 TCFE10  =  Steels/Fe-Alloys  v10.0 SNAPSHOT
 TCFE8   =  Steels/Fe-Alloys  v8.1
 FROST1  =  FROST database v1.0
 TCFE7   =  Steels/Fe-Alloys  v7.0
 TCFE6   =  Steels/Fe-Alloys  v6.2
 TCFE5   =  Steels/Fe-Alloys  v5.0
 TCFE4   =  Steels/Fe-Alloys  v4.1
 TCFE3   =  Steels/Fe-Alloys  v3.1
 TCFE2   =  Steels/Fe-Alloys  v2.1
 TCFE1   =  Steels/Fe-Alloys  v1.0
 TCNI9   =  Ni-Alloys  v9.0 SNAPSHOT
 NI25    =  NI25 database
 TCNI8   =  Ni-Alloys  v8.1
 TCNI7   =  Ni-Alloys  v7.1
 TCNI6   =  Ni-Alloys  v6.0
 TCNI5   =  Ni-Alloys  v5.1
 TCNI4   =  Ni-Alloys  v4.0
 TCNI1   =  Ni-Alloys  v1.3
 TCAL5   =  Al-Alloys  v5.0
 TCAL4   =  Al-Alloys  v4.0
 TCAL3   =  Al-Alloys  v3.0
 TCAL2   =  Al-Alloys  v2.1
 TCAL1   =  Al-Alloys  v1.2
 TCMG4   =  Mg-Alloys  v4.0
 TCMG3   =  Mg-Alloys  v3.0
 TCMG2   =  Mg-Alloys  v2.0
 TCMG1   =  Mg-Alloys  v1.1
 TCTI1   =  Ti-Alloys  v1.0
 TCCU2   =  Cu-Alloys  v2.0
 TCCU1   =  Cu-Alloys  v1.0
 TCCC1   =  Cemented carbide  v1.0
 TCHEA2  =  High Entropy Alloy  v2.1
 TCHEA1  =  High Entropy Alloy  v1.0
 SSOL6   =  SGTE Alloy Solutions Database v6.0
 SSOL5   =  SGTE Alloy Solutions Database v5.0
 SSOL4   =  SGTE Alloy Solutions Database v4.9g
 SSOL2   =  SGTE Alloy Solutions Database v2.1
 SSUB6   =  SGTE Substances Database v6.0
 SSUB5   =  SGTE Substances Database v5.2
 SSUB4   =  SGTE Substances Database v4.1
 SSUB3   =  SGTE Substances Database v3.3
 SSUB2   =  SGTE Substances Database v2.2
```

```
 SNOB3   =  SGTE Noble Metal Alloys Database v3.1
 STBC2   =  SGTE Thermal Barrier Coating TDB v2.2
 STBC1   =  SGTE Thermal Barrier Coating TDB v1.1
 SALT1   =  SGTE Molten Salts Database v1.2
 SEMC2   =  TC Semi-Conductors  v2.1
 SLAG4   =  Fe-containing Slag  v4.1
 SLAG3   =  Fe-containing Slag  v3.2
 SLAG2   =  Fe-containing Slag  v2.2
 SLAG1   =  Fe-containing Slag  v1.2
 TCOX7   =  Metal Oxide Solutions  v7.0
 TCOX6   =  Metal Oxide Solutions  v6.0
 TCOX5   =  Metal Oxide Solutions  v5.1
 TCOX4   =  Metal Oxide Solutions  v4.1
 ION3    =  Ionic Solutions  v3.0
 ION2    =  Ionic Solutions  v2.6
 ION1    =  Ionic Solutions  v1.5
 NOX2    =  NPL Oxide Solutions Database v2.1
 TCNOBL1 =  Noble Metals Alloys v1.0
 TCSLD3  =  Solder Alloys  v3.2
 TCSLD2  =  Solder Alloys  v2.0
 TCSI1   =  Ultrapure Silicon  v1.2
 TCMP2   =  Materials Processing  v2.5
 TCES1   =  Combustion/Sintering  v1.1
 TCSC1   =  Super Conductor  v1.0
 TCFC1   =  SOFC Database v1.0
 NUMT2   =  Nuclear Materials  v2.1
 NUOX4   =  Nuclear Oxides  v4.2
 NUCL15  =  IRSN NUCLEA-15_4
 NUCL10  =  ThermoData NUCLEA Alloys-oxides TDB v10.2
 MEPH15  =  IRSN Mephista-15_1
 MEPH11  =  ThermoData MEPHISTA Nuclear Fuels TDB v11.2
 TCAQ3   =  Aqueous Solution  v3.0
 TCAQ2   =  Aqueous Solution  v2.6
 AQS2    =  TGG Aqueous Solution Database v2.6
 GCE2    =  TGG Geochemical/Environmental TDB v2.3
 FEDEMO  =  Iron Demo Database v2.0
 ALDEMO  =  Aluminum Demo Database v2.0
 NIDEMO  =  Nickel Demo Database v1.0
 CUDEMO  =  Copper Demo Database v1.0
 SLDEMO  =  Solder Demo Database v1.0
 OXDEMO  =  Oxide Demo Database v1.0
 SUBDEMO =  Substance Demo Database v1.0
 PTERN   =  Public Ternary Alloys TDB v1.3
 PAQ2    =  Public Aqueous Soln (SIT) TDB v2.4
 PG35    =  G35 Binary Semi-Conductors TDB v1.2
 PURE5   =  SGTE Unary (Pure Elements) TDB v5.1
 MOB2    =  Alloys Mobility  v2.7
 MOB1    =  Alloys Mobility  v1.3
 MOBFE1  =  Steels/Fe-Alloys Mobility  v1.0
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBNI4  =  Ni-Alloys Mobility  v4.0
 MOBNI3  =  Ni-Alloys Mobility  v3.1
 MOBNI2  =  Ni-Alloys Mobility  v2.4
 MOBNI1  =  Ni-Alloys Mobility  v1.0
 MOBAL3  =  Al-Alloys Mobility  v3.0
 MOBAL2  =  Al-Alloys Mobility  v2.0
 MOBAL1  =  Al-Alloys Mobility  v1.0
 MOBCU1  =  Cu-Alloys Mobility  v1.0
 MOBCU2  =  Cu-Alloys Mobility  v2.0
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBSLD1 =  Solder-Alloys Mobility  v1.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0 SNAPSHOT
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v1.0
 MFEDEMO =  Fe-Alloys Mobility demo database v2.0
 MNIDEMO =  Ni-Alloys Mobility demo database v1.0
 MCUDEMO =  Cu-Alloys Mobility demo database v1.0
 USER    =  User defined Database

DATABASE NAME /FEDEMO/: mfedemo
 Current database: Fe-Alloys Mobility demo database v2.0

 VA  DEFINED
APP: def-sys cr fe ni
 CR                     FE                     NI
   DEFINED
APP: rej-ph /all
 BCC_A2                 FCC_A1  REJECTED
APP: res-ph bcc,fcc
 BCC_A2                 FCC_A1  RESTORED
APP: get
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'This parameter has not been assessed'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Fe diffusion fcc Cr-Fe'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Ni diffusion fcc Cr-Ni'
  'B. Jonsson: Z. Metallkunde 86(1995)686-692; Cr, Fe and Ni diffusion fcc
      Cr-Fe-Ni'
  'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
      -Ni'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Ni self-diffusion'
  'B. Jonsson: ISIJ International, 35(1995)1415-1421; Cr, Fe and Ni
      diffusion bcc Cr-Fe-Ni'
  'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
      in bcc Fe'
 -OK-
APP:
APP: @@
APP: @@ GO TO THE DICTRA MODULE TO SET UP THE SIMULATION
APP: @@
APP: go d-m
 NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ SET THE GLOBAL CONDITIONS
DIC> @@
```

```
DIC> set-cond glob T 0 1373; * N

DIC>
DIC> @@
DIC> @@ ENTER TWO REGIONS, ONE FOR EACH PHASE
DIC> @@
DIC> enter-region alpha
DIC> enter-region gamma
ATTACH TO REGION NAMED /ALPHA/:
ATTACHED TO THE RIGHT OF ALPHA /YES/:
DIC> @@
DIC> @@ ENTER THE GRID SIZE AND SPACINGS
DIC> @@
DIC> enter-grid alpha  93.45E-6 AUTO
DIC> enter-grid gamma 500.0E-6 AUTO
DIC>
DIC> @@
DIC> @@ SPECIFY WHICH PHASE GOES INTO WHICH REGION
DIC> @@
DIC> enter-phase act alpha  matrix bcc
DIC> enter-phase act gamma matrix fcc
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITIONS IN THE PHASES
DIC> @@ IT IS IMPORTANT NOT TO PUT 0%NI IN PHASE BCC,
DIC> @@ ENTER SOME SMALL VALUE INSTEAD
DIC> @@
DIC> enter-composition
REGION NAME : /ALPHA/: alpha
PHASE NAME: /BCC_A2/: bcc
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-f
PROFILE FOR /CR/: cr lin  .38 .38
PROFILE FOR /NI/: ni lin  1e-5 1e-5
DIC>
DIC> enter-composition
REGION NAME : /GAMMA/: gamma
PHASE NAME: /FCC_A1/: fcc
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-f
PROFILE FOR /CR/: cr lin .27 .27
PROFILE FOR /NI/: ni lin .28 .28
DIC>
DIC> @@
DIC> @@ SPECIFY THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 36E5
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /360000/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC> SAVE exb5 Y
DIC>
DIC> set-inter
 --OK---
DIC>
```

exb5-run

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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
 single geometric dense at  0.93450E-04
 0.80000       36
 Region: GAMMA
 single geometric dense at   0.0000
  1.2500      103
  Trying old scheme                      4
 GENERATING STARTING VALUES FOR CELL #  1 INTERFACE #  2
 DETERMINING INITIAL EQUILIBRIUM VALUES
CALCULATING STARTING VALUES:       9   EQUILIBRIUM CALCULATIONS
 *** ERROR  1611 IN QTHISS
 *** TOO MANY ITERATIONS
 Give the command INFO TROUBLE for help
 DONE     6 OUT OF     9
 *** ERROR  1611 IN QTHISS
 *** TOO MANY ITERATIONS
 Give the command INFO TROUBLE for help
 DONE     9 OUT OF     9                                                    try                      1  failed
  try                     2  failed
  try                     3  failed
 DETERMINED ACTIVITIES  ACR(NI) 2.00457405352E-04

  UNABLE TO OBTAIN GOOD STARTING VALUE USING THE OLD SCHEME
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 = .223047485172706
 TOTAL SIZE OF SYSTEM:  5.9345E-04 [m]
 U-FRACTION IN SYSTEM:  CR = .305280432605602  FE = .471672082221692
                        NI = .223047485172706
 TOTAL SIZE OF SYSTEM:  5.9345E-04 [m]
 3.503057562902913E-002        3.503838978364429E-002        3.503070722844563E-002        6.010860840116191E-004        4.996070361075793E-
004        3.843182361484345E-004        2.949921646937419E-004        2.951292562679729E-004        1.282229555240126E-
004        1.268212026678937E-007        1.765332679167226E-009        4.480619344654895E-011        2.125046441002659E-
015        7.823058275186145E-022       TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =  0.78230583E-21
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.16001447     AND   0.16001447
 POSITION OF INTERFACE ALPHA / GAMMA IS   0.93466001E-04
 U-FRACTION IN SYSTEM:  CR = .305280432536186  FE = .471672082122531
                        NI = .223047485341282
 TOTAL SIZE OF SYSTEM:  5.9345E-04 [m]
  26  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: GAMMA

  CPU time used in timestep                    1 seconds
 9.795982825774254E-004        9.797942119996134E-004        9.795987026447346E-004        1.691332024217569E-012        1.336248638663800E-
012        1.296755492972891E-012        1.534999402036739E-012        6.680078110408412E-012        1.211461393523816E-
012        1.208868024354182E-012        1.209218283081458E-012        6.030069487016950E-012        1.204231816459639E-
012        1.202965651061900E-012        1.202807755374170E-012        5.949304372240396E-012        1.202017591598718E-
012        1.201381990581038E-012        1.200629548694862E-012        5.941375509837813E-012        1.199444091669443E-
012        1.197808643807507E-012        1.194411667821751E-012        5.934987263075989E-012        1.188089742024129E-
012        1.175555822806514E-012        1.150437977125342E-012        5.896773996143438E-012

output ignored...



... output resumed

 2.975976620426760E-012        3.931638072329925E-019       TIME =   2202068.9     DT =   360000.00     SUM OF SQUARES =  0.39316381E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.76088558E-11 AND  -0.76088558E-11
 POSITION OF INTERFACE ALPHA / GAMMA IS   0.95399216E-04
 U-FRACTION IN SYSTEM:  CR = .30528044499911  FE = .471672025911522
                        NI = .223047529089368
 TOTAL SIZE OF SYSTEM:  5.9345E-04 [m]
  7  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: GAMMA

  CPU time used in timestep                    1 seconds
 1.859732029877999E-006        1.862546550414088E-006        1.855096410819417E-006        1.312282436255117E-008        2.801684163890738E-
009        2.762662017971759E-013        5.231291158935700E-
022       TIME =   2562068.9     DT =   360000.00     SUM OF SQUARES =  0.52312912E-21
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.64451770E-11 AND  -0.64451770E-11
 POSITION OF INTERFACE ALPHA / GAMMA IS   0.93078952E-04
 U-FRACTION IN SYSTEM:  CR = .305280445370872  FE = .471672025256904
                        NI = .223047529372225
 TOTAL SIZE OF SYSTEM:  5.9345E-04 [m]
  6  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: GAMMA

  CPU time used in timestep                    2 seconds
 6.449616370182997E-007        6.463791775320258E-007        6.422623646262826E-007        3.405505750689575E-009        6.550220994884708E-
010        9.333631752488630E-015        4.177582806767291E-
022       TIME =   2922068.9     DT =   360000.00     SUM OF SQUARES =  0.41775828E-21
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.58182489E-11 AND  -0.58182489E-11
 POSITION OF INTERFACE ALPHA / GAMMA IS   0.90984382E-04
 U-FRACTION IN SYSTEM:  CR = .305280445548385  FE = .471672025176166
                        NI = .223047529275448
 TOTAL SIZE OF SYSTEM:  5.9345E-04 [m]
  7  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: GAMMA
```

```
  CPU time used in timestep                    1 seconds
 3.680698764738160E-007        3.690426708596007E-007        3.660556407863467E-007        1.728115014843000E-009        3.136194763808131E-
010        1.475858477781552E-015        2.893927018201920E-
023       TIME =    3282068.9     DT =    360000.00     SUM OF SQUARES =  0.28939270E-22
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.53569641E-11 AND  -0.53569641E-11
 POSITION OF INTERFACE ALPHA / GAMMA IS   0.89055875E-04
 U-FRACTION IN SYSTEM:  CR = .305280446127722  FE = .47167202349365
                        NI = .223047530378628
 TOTAL SIZE OF SYSTEM:  5.9345E-04 [m]
  5  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: GAMMA

  CPU time used in timestep                    1 seconds
 4.278373565459864E-009        4.280902901842744E-009        4.297285706959512E-009        1.879840611235033E-009        8.591834998963679E-
010        4.289222548337157E-016        1.381416581816048E-
024       TIME =    3600000.0     DT =    317931.12     SUM OF SQUARES =  0.13814166E-23
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.49338740E-11 AND  -0.49338740E-11
 POSITION OF INTERFACE ALPHA / GAMMA IS   0.87487243E-04
 U-FRACTION IN SYSTEM:  CR = .30528044638003  FE = .471672022864279
                        NI = .223047530755692
 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    0.93355784E-05
 DELETING TIME-RECORD FOR TIME    0.27806735E-04
 DELETING TIME-RECORD FOR TIME    0.64749049E-04
 DELETING TIME-RECORD FOR TIME    0.13863368E-03
 DELETING TIME-RECORD FOR TIME    0.28640293E-03
 DELETING TIME-RECORD FOR TIME    0.58194144E-03
 DELETING TIME-RECORD FOR TIME    0.11730185E-02
 DELETING TIME-RECORD FOR TIME    0.23551725E-02
 DELETING TIME-RECORD FOR TIME    0.47194806E-02
 DELETING TIME-RECORD FOR TIME    0.94480967E-02
 DELETING TIME-RECORD FOR TIME    0.18905329E-01
 DELETING TIME-RECORD FOR TIME    0.37819794E-01
 DELETING TIME-RECORD FOR TIME    0.75648723E-01
 DELETING TIME-RECORD FOR TIME    0.15130658
 DELETING TIME-RECORD FOR TIME    0.19274610
 DELETING TIME-RECORD FOR TIME    0.21544345
 DELETING TIME-RECORD FOR TIME    0.26083817
 DELETING TIME-RECORD FOR TIME    0.35162760
 DELETING TIME-RECORD FOR TIME    0.40135502
 DELETING TIME-RECORD FOR TIME    0.50080986
 DELETING TIME-RECORD FOR TIME    0.69971953
 DELETING TIME-RECORD FOR TIME    0.91386552
 DELETING TIME-RECORD FOR TIME     1.3421575
 DELETING TIME-RECORD FOR TIME     2.0765292
 DELETING TIME-RECORD FOR TIME     3.2890531
 DELETING TIME-RECORD FOR TIME     5.5909634
 DELETING TIME-RECORD FOR TIME     10.194784
 DELETING TIME-RECORD FOR TIME     13.853759
 DELETING TIME-RECORD FOR TIME     21.171708
 DELETING TIME-RECORD FOR TIME     35.807606
 DELETING TIME-RECORD FOR TIME     65.079402
 DELETING TIME-RECORD FOR TIME     89.577448
 DELETING TIME-RECORD FOR TIME     138.57354
 DELETING TIME-RECORD FOR TIME     236.56573
 DELETING TIME-RECORD FOR TIME     319.77973
 DELETING TIME-RECORD FOR TIME     486.20775
 DELETING TIME-RECORD FOR TIME     761.28537
 DELETING TIME-RECORD FOR TIME     1232.2152
 DELETING TIME-RECORD FOR TIME     2093.9211
 DELETING TIME-RECORD FOR TIME     3662.4504
 DELETING TIME-RECORD FOR TIME     6799.5089
 DELETING TIME-RECORD FOR TIME     13073.626
 DELETING TIME-RECORD FOR TIME     25621.860
 DELETING TIME-RECORD FOR TIME     50718.328
 DELETING TIME-RECORD FOR TIME     100911.26
 DELETING TIME-RECORD FOR TIME     201297.14
 DELETING TIME-RECORD FOR TIME     402068.88
 DELETING TIME-RECORD FOR TIME     762068.88
 DELETING TIME-RECORD FOR TIME     1122068.9
 DELETING TIME-RECORD FOR TIME     1482068.9
 DELETING TIME-RECORD FOR TIME     1842068.9
 DELETING TIME-RECORD FOR TIME     2202068.9
 DELETING TIME-RECORD FOR TIME     2562068.9
 DELETING TIME-RECORD FOR TIME     2922068.9

 KEEPING TIME-RECORD FOR TIME     3282068.9
 AND FOR TIME                     3600000.0
 WORKSPACE RECLAIMED

 TIMESTEP AT     3600000.00     SELECTED

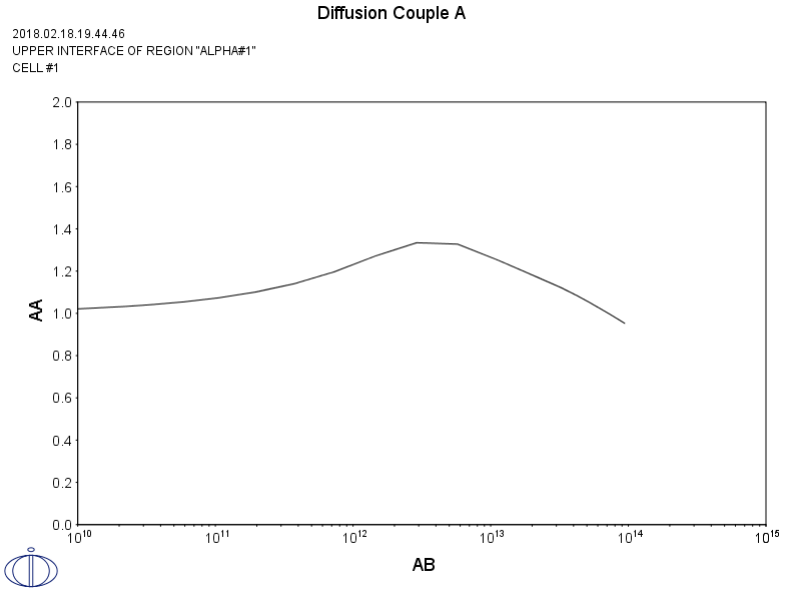
DIC> set-inter
 --OK---
DIC>
```

exb5-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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

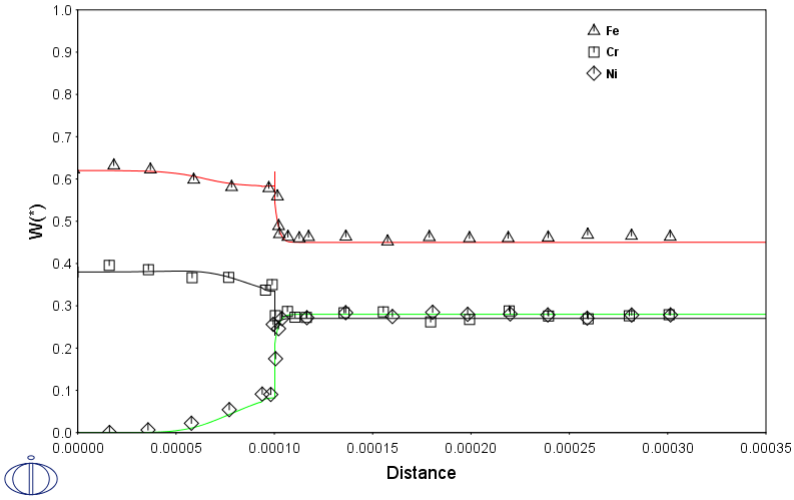
POST-1:
POST-1: set-title Diffusion Couple A
POST-1:
POST-1: @@
POST-1: @@ WE ARE INTERESTED IN THE POSITION OF THE UPPER INTERFACE OF REGION ALPHA
POST-1: @@
POST-1: s-p-c interf alpha upper
POST-1:
POST-1: @@
POST-1: @@ l0 IS THE INITIAL THICKNESS USED FOR NORMALIZATION
POST-1: @@
POST-1: enter func 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: plo
```




```
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: plo
```

Diffusion Couple A

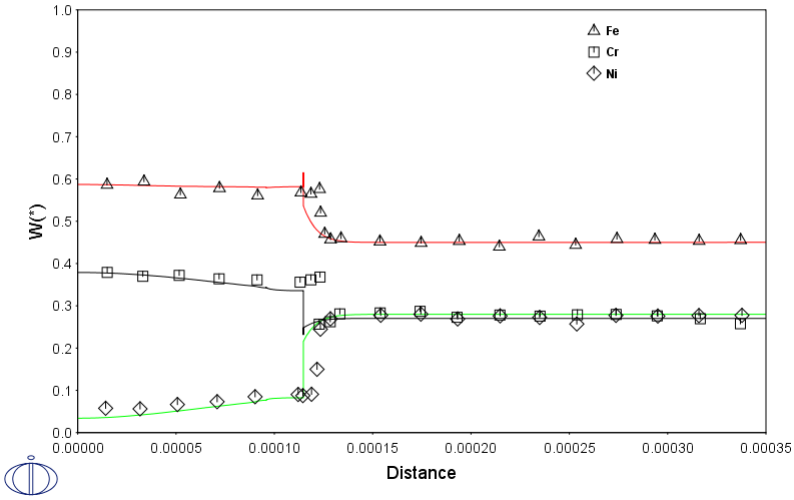
2018.02.18.19.44.46
Time = 3600
CELL #1



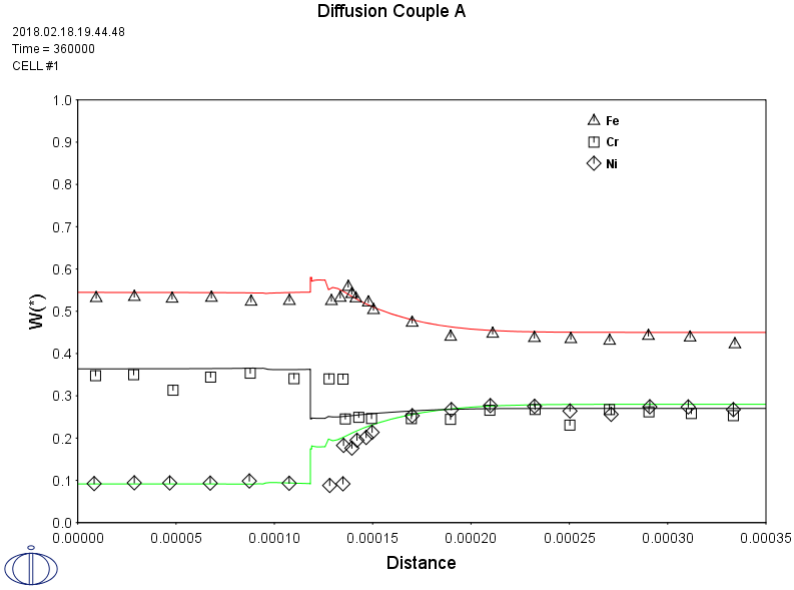
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: s-p-c time 36000
POST-1: app y exb5.exp 0; 2
POST-1: plo

Diffusion Couple A

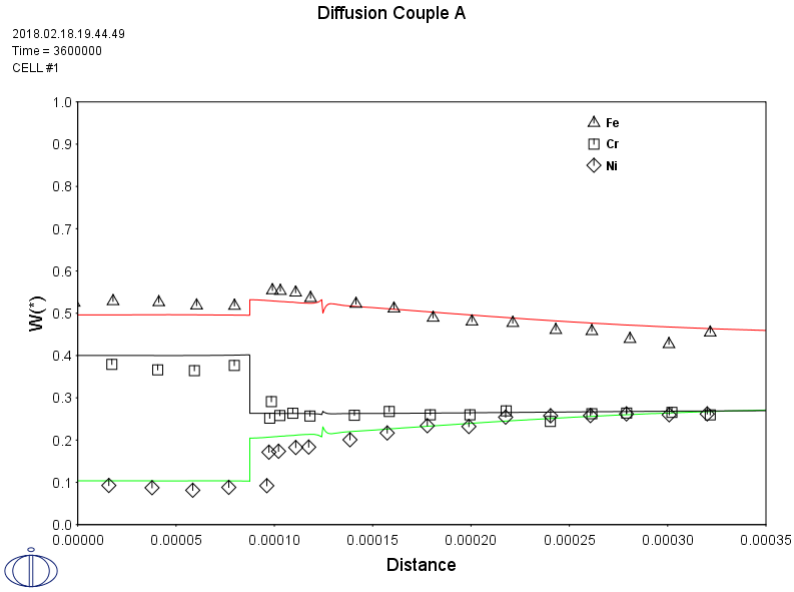
2018.02.18.19.44.47
Time = 36000
CELL #1



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: plo



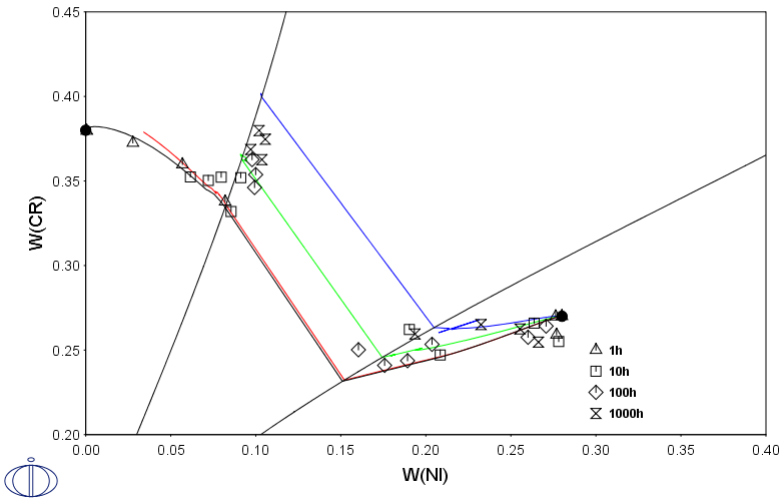

```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: s-p-c time 3600000
POST-1: app y exb5.exp 0; 4
POST-1: plo
```




```
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: plo
```

Diffusion Couple A

2018.02.18.19.44.49
Time = 3600,36000,360000,3600000
CELL #1

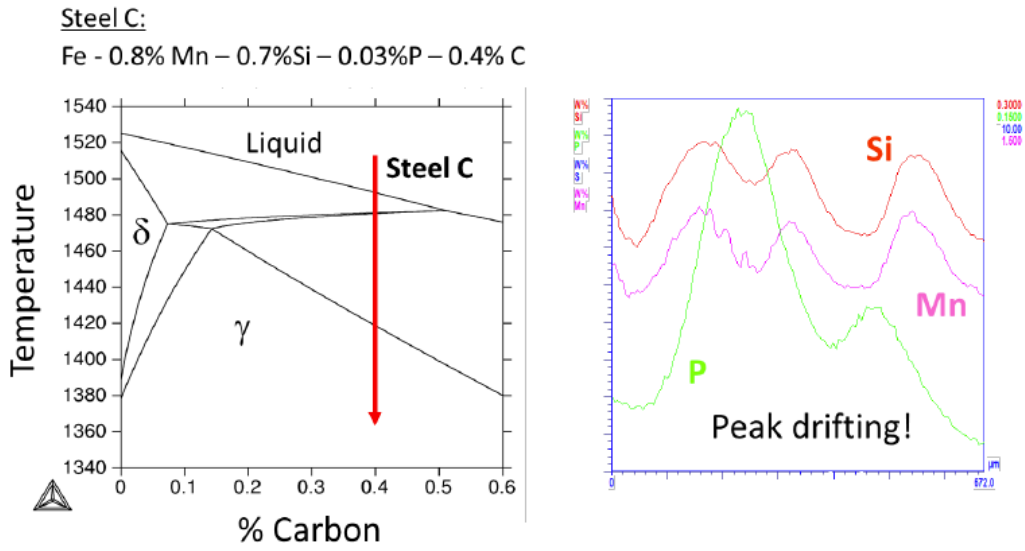


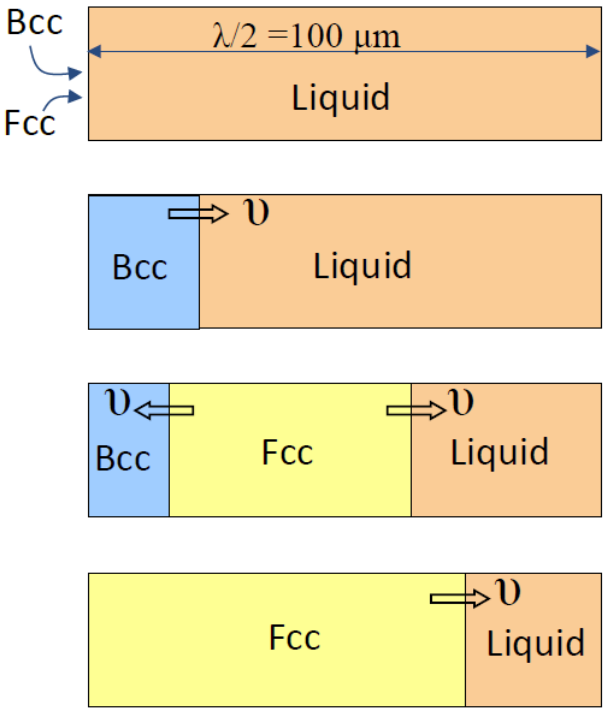
POST-1:
POST-1:
POST-1:
POST-1: set-inter
--OK---
POST-1:

Example exb6

Micro-segregation of phosphorus

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





exb6-setup

```
About Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri Feb 16 15:22:08 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb6\setup.DCM" @@
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
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

 VA                     /-  DEFINED
 L12_FCC                B2_BCC                  DICTRA_FCC_A1
   REJECTED
TDB_TCFE9:
TDB_TCFE9: @@ USE A TCFE DATABASE FOR THERMODYNAMIC DATA
TDB_TCFE9: sw tcfe7
 Current database: Steels/Fe-Alloys  v7.0

 VA  DEFINED
 L12_FCC                B2_BCC                  B2_VACANCY
 HIGH_SIGMA             DICTRA_FCC_A1  REJECTED
TDB_TCFE7:
TDB_TCFE7: @@ DEFINE THE SYSTEM TO WORK WITH
TDB_TCFE7: def-sys fe c si mn p
 FE                     C                       SI
 MN                     P  DEFINED
TDB_TCFE7:
TDB_TCFE7: @@ EXCLUDE THE THERMODYNAMIC DATA FOR THE PHASES THAT ARE NOT NEEDED
TDB_TCFE7: rej ph /all
 GAS:G                  LIQUID:L                BCC_A2
 FCC_A1                 HCP_A3                  DIAMOND_FCC_A4
 RED_P                  WHITE_P                 GRAPHITE
 CEMENTITE              M23C6                   M7C3
 M5C2                   KSI_CARBIDE             A1_KAPPA
 KAPPA                  FE4N_LP1                FECN_CHI
 LAVES_PHASE_C14        M3SI                    G_PHASE
 CR3SI                  FE2SI                   MSI
 M5SI3                  AL4C3                   FE8SI2C
 SIC                    FEP                     CU3P
 M2P                    M3P  REJECTED
TDB_TCFE7: res ph fcc liq bcc
 FCC_A1                 LIQUID:L                BCC_A2
   RESTORED
TDB_TCFE7:
TDB_TCFE7: @@ RETRIEVE DATA FROM THE DATABASE FILE
TDB_TCFE7: get
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'
  'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C
     -FE'
  'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
  'J. Grobner, H.L. Lukas and F. Aldinger, Calphad, 20 (1996), 247-254; Si-C
     and Al-Si-C'
  'W. Huang, Calphad, 13 (1989), 243-252; TRITA-MAC 388 (rev 1989); FE-MN'
  'J.-H. Shim, C.-S. Oh and D.N. Lee, J. Korean Inst. Met. Mater., 34 (1996),
      1385-1393; Fe-P'
  'J. Lacaze and B. Sundman, Metall. Mater. Trans. A, 22A (1991), 2211-2223;
     Fe-Si and Fe-Si-C'
  'J. Miettinen and B. Hallstedt, Calphad, 22 (1998), 231-256; Fe-Si and Fe
     -Si-C'
  'J.E. Tibballs, SI Norway (1991) Rep. 890221-5; Mn-Si'
  'P. Franke, estimated parameter within SGTE, 2008; Fe-Mn-C'
  'J.-H. Shim, H.-J. Chung and D.N. Lee, Z. fur Metallkde., (1999); Fe-C-P'
  'B. Sundman, 1999, revision of the liquid Fe-Si-C description'
  'NPL, unpublished work (1989); C-Mn-Si'
  'A. Forsberg and J. Agren, J. Phase Equil., 14 (1993), 354-363; Fe-Mn-Si'
  'B. Uhrenius (1993-1994), International journal of refractory metals and
     hard mater, Vol. 12, pp. 121-127; Molar volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
     Molar volumes'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
  'W. Huang, Metall. Trans. A, 21A (1990), 2115-2123; TRITA-MAC 411 (Rev
     1989); C-FE-MN'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
 -OK-
TDB_TCFE7:
TDB_TCFE7: @@
TDB_TCFE7: @@ MOBILITY/DIFFUSIVITY DATA ARE STORED IN A SEPARATE DATABASE FILE.
TDB_TCFE7: @@ SWITCH TO A MOBILITY DATABASE AND APPEND THE DATA.
TDB_TCFE7: @@
TDB_TCFE7: app
 Use one of these databases

 TCFE9   =  Steels/Fe-Alloys  v9.0
 TCFE10  =  Steels/Fe-Alloys  v10.0 SNAPSHOT
 TCFE8   =  Steels/Fe-Alloys  v8.1
 FROST1  =  FROST database v1.0
 TCFE7   =  Steels/Fe-Alloys  v7.0
 TCFE6   =  Steels/Fe-Alloys  v6.2
 TCFE5   =  Steels/Fe-Alloys  v5.0
 TCFE4   =  Steels/Fe-Alloys  v4.1
 TCFE3   =  Steels/Fe-Alloys  v3.1
 TCFE2   =  Steels/Fe-Alloys  v2.1
```

```
 TCFE1   =  Steels/Fe-Alloys  v1.0
 TCNI9   =  Ni-Alloys  v9.0 SNAPSHOT
 NI25    =  NI25 database
 TCNI8   =  Ni-Alloys  v8.1
 TCNI7   =  Ni-Alloys  v7.1
 TCNI6   =  Ni-Alloys  v6.0
 TCNI5   =  Ni-Alloys  v5.1
 TCNI4   =  Ni-Alloys  v4.0
 TCNI1   =  Ni-Alloys  v1.3
 TCAL5   =  Al-Alloys  v5.0
 TCAL4   =  Al-Alloys  v4.0
 TCAL3   =  Al-Alloys  v3.0
 TCAL2   =  Al-Alloys  v2.1
 TCAL1   =  Al-Alloys  v1.2
 TCMG4   =  Mg-Alloys  v4.0
 TCMG3   =  Mg-Alloys  v3.0
 TCMG2   =  Mg-Alloys  v2.0
 TCMG1   =  Mg-Alloys  v1.1
 TCTI1   =  Ti-Alloys  v1.0
 TCCU2   =  Cu-Alloys  v2.0
 TCCU1   =  Cu-Alloys  v1.0
 TCCC1   =  Cemented carbide  v1.0
 TCHEA2  =  High Entropy Alloy  v2.1
 TCHEA1  =  High Entropy Alloy  v1.0
 SSOL6   =  SGTE Alloy Solutions Database v6.0
 SSOL5   =  SGTE Alloy Solutions Database v5.0
 SSOL4   =  SGTE Alloy Solutions Database v4.9g
 SSOL2   =  SGTE Alloy Solutions Database v2.1
 SSUB6   =  SGTE Substances Database v6.0
 SSUB5   =  SGTE Substances Database v5.2
 SSUB4   =  SGTE Substances Database v4.1
 SSUB3   =  SGTE Substances Database v3.3
 SSUB2   =  SGTE Substances Database v2.2
 SNOB3   =  SGTE Noble Metal Alloys Database v3.1
 STBC2   =  SGTE Thermal Barrier Coating TDB v2.2
 STBC1   =  SGTE Thermal Barrier Coating TDB v1.1
 SALT1   =  SGTE Molten Salts Database v1.2
 SEMC2   =  TC Semi-Conductors  v2.1
 SLAG4   =  Fe-containing Slag  v4.1
 SLAG3   =  Fe-containing Slag  v3.2
 SLAG2   =  Fe-containing Slag  v2.2
 SLAG1   =  Fe-containing Slag  v1.2
 TCOX7   =  Metal Oxide Solutions  v7.0
 TCOX6   =  Metal Oxide Solutions  v6.0
 TCOX5   =  Metal Oxide Solutions  v5.1
 TCOX4   =  Metal Oxide Solutions  v4.1
 ION3    =  Ionic Solutions  v3.0
 ION2    =  Ionic Solutions  v2.6
 ION1    =  Ionic Solutions  v1.5
 NOX2    =  NPL Oxide Solutions Database v2.1
 TCNOBL1 =  Noble Metals Alloys v1.0
 TCSLD3  =  Solder Alloys  v3.2
 TCSLD2  =  Solder Alloys  v2.0
 TCSI1   =  Ultrapure Silicon  v1.2
 TCMP2   =  Materials Processing  v2.5
 TCES1   =  Combustion/Sintering  v1.1
 TCSC1   =  Super Conductor  v1.0
 TCFC1   =  SOFC Database v1.0
 NUMT2   =  Nuclear Materials  v2.1
 NUOX4   =  Nuclear Oxides  v4.2
 NUCL15  =  IRSN NUCLEA-15_4
 NUCL10  =  ThermoData NUCLEA Alloys-oxides TDB v10.2
 MEPH15  =  IRSN Mephista-15_1
 MEPH11  =  ThermoData MEPHISTA Nuclear Fuels TDB v11.2
 TCAQ3   =  Aqueous Solution  v3.0
 TCAQ2   =  Aqueous Solution  v2.6
 AQS2    =  TGG Aqueous Solution Database v2.6
 GCE2    =  TGG Geochemical/Environmental TDB v2.3
 FEDEMO  =  Iron Demo Database v2.0
 ALDEMO  =  Aluminum Demo Database v2.0
 NIDEMO  =  Nickel Demo Database v1.0
 CUDEMO  =  Copper Demo Database v1.0
 SLDEMO  =  Solder Demo Database v1.0
 OXDEMO  =  Oxide Demo Database v1.0
 SUBDEMO =  Substance Demo Database v1.0
 PTERN   =  Public Ternary Alloys TDB v1.3
 PAQ2    =  Public Aqueous Soln (SIT) TDB v2.4
 PG35    =  G35 Binary Semi-Conductors TDB v1.2
 PURE5   =  SGTE Unary (Pure Elements) TDB v5.1
 MOB2    =  Alloys Mobility  v2.7
 MOB1    =  Alloys Mobility  v1.3
 MOBFE1  =  Steels/Fe-Alloys Mobility  v1.0
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBNI4  =  Ni-Alloys Mobility  v4.0
 MOBNI3  =  Ni-Alloys Mobility  v3.1
 MOBNI2  =  Ni-Alloys Mobility  v2.4
 MOBNI1  =  Ni-Alloys Mobility  v1.0
 MOBAL3  =  Al-Alloys Mobility  v3.0
 MOBAL2  =  Al-Alloys Mobility  v2.0
 MOBAL1  =  Al-Alloys Mobility  v1.0
 MOBCU1  =  Cu-Alloys Mobility  v1.0
 MOBCU2  =  Cu-Alloys Mobility  v2.0
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBSLD1 =  Solder-Alloys Mobility  v1.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0 SNAPSHOT
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v1.0
 MFEDEMO =  Fe-Alloys Mobility demo database v2.0
 MNIDEMO =  Ni-Alloys Mobility demo database v1.0
 MCUDEMO =  Cu-Alloys Mobility demo database v1.0
 USER    =  User defined Database

DATABASE NAME /TCFE7/: mobfe2
 Current database: Steels/Fe-Alloys Mobility  v2.0
   TCS Steel Mobility Database Version 2.0 from 2011-12-09.

 VA  DEFINED
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 ....

 List of references for assessed data

  'This parameter has not been assessed'
  'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'
  'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
      -Ni'
  'Bae et al.: Z. Metallkunde 91(2000)672-674; fcc Fe-Mn
       Mn-Ni'
  'V. V. Mural and P. L. Gruzin, Phys. Met. Metallogr. (English Transl.) 17
      (5) (1964)154.; Impurity diff of P in fcc Fe.'
  'D. Bergner et al., Defect and Diffusion Forum 66-69(1989)409. Impurity
      diffusion of Si in fcc Fe.'
  'B. Jonsson: Z. Metallkunde 85(1994)498-501; C and N diffusion in bcc Cr
      -Fe-Ni'
  'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
      in bcc Fe'
  'B. Jonsson: Unpublished research bcc Fe-Si 1994'
  'Assessed from data presented in Landholt-Bornstein, Vol. 26, ed. H.
      Mehrer, springer (1990); Impurity diff of Mn in bcc Fe.'
  'Assessed from data presented in Landholt-Bornstein, Vol. 26, ed. H.
      Mehrer, springer (1990); Impurity diff of P in bcc Fe.'
 -OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP
APP: @@
APP: go d-m
 NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> @@ LOWER THE TEMPERATURE TO A RATE OF 0.2 K/s
DIC> @@
DIC> set-cond glob T 0 1780-0.2*TIME; * N

DIC>
DIC> @@
DIC> @@ ENTER A REGION CALLED smalta
DIC> @@
DIC> enter-region smalta
DIC>
DIC> @@
DIC> @@ ENTER A DOUBLE GEOMETRIC GRID INTO THE REGION
DIC> @@
DIC> enter-grid
REGION NAME : /SMALTA/: smalta
WIDTH OF REGION /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
 SETTING CHECK INTERFACE POSITION ON
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 /YES/: 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 (0 -> 0.5 -> 1): /.5/:
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /NO/:
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>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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
 single geometric dense at   0.0000
  1.0846       88
 U-FRACTION IN SYSTEM:  C = .0185375871047351  FE = .97748186120908
                        MN = .00810568126669965  P = 5.39133528237326E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 U-FRACTION IN SYSTEM:  C = .0185375871047351  FE = .97748186120908
                        MN = .00810568126669965  P = 5.39133528237326E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0185375871047351  FE = .977481861209079
                        MN = .00810568126669965  P = 5.39133528237326E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.26002472E-05 DT =  0.25002472E-05 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                    0 seconds
 TIME =  0.76007416E-05 DT =  0.50004944E-05 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0185375871047351  FE = .97748186120908
                        MN = .00810568126669965  P = 5.39133528237326E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.17601730E-04 DT =  0.10000989E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0185375871047351  FE = .97748186120908
                        MN = .00810568126669965  P = 5.39133528237326E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.37603708E-04 DT =  0.20001978E-04 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 =  0.77607664E-04 DT =  0.40003955E-04 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                    0 seconds
 TIME =  0.15761557E-03 DT =  0.80007911E-04 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                    0 seconds
 TIME =  0.31763140E-03 DT =  0.16001582E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0185375871047351  FE = .97748186120908
                        MN = .00810568126669965  P = 5.39133528237326E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.63766304E-03 DT =  0.32003164E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0185375871047351  FE = .97748186120908
                        MN = .00810568126669965  P = 5.39133528237326E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.12777263E-02 DT =  0.64006329E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0185375871047351  FE = .97748186120908
                        MN = .00810568126669965  P = 5.39133528237326E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.25578529E-02 DT =  0.12801266E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0185375871047351  FE = .97748186120908
                        MN = .00810568126669966  P = 5.39133528237326E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.51181060E-02 DT =  0.25602531E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0185375871047351  FE = .97748186120908
                        MN = .00810568126669966  P = 5.39133528237326E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    1 seconds
 TIME =  0.10238612E-01 DT =  0.51205063E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .018537587104735  FE = .97748186120908
                        MN = .00810568126669965  P = 5.39133528237326E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.20479625E-01 DT =  0.10241013E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .018537587104735  FE = .97748186120908
                        MN = .00810568126669965  P = 5.39133528237325E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.40961650E-01 DT =  0.20482025E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .018537587104735  FE = .97748186120908
                        MN = .00810568126669964  P = 5.39133528237325E-04
                        SI = .0138733239959838
```

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 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.81925700E-01 DT =  0.40964050E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0185375871047351  FE = .97748186120908
                        MN = .00810568126669966  P = 5.39133528237326E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.16385380     DT =  0.81928101E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0185375871047351  FE = .977481861209079
                        MN = .00810568126669971  P = 5.3913352823733E-04
                        SI = .0138733239959839
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.32771000     DT =  0.16385620     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0185375871047351  FE = .977481861209079
                        MN = .0081056812666997  P = 5.39133528237328E-04
                        SI = .013873323995984
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.65542241     DT =  0.32771240     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0185375871047355  FE = .977481861209078
                        MN = .00810568126669991  P = 5.39133528237341E-04


output ignored...


... output resumed

 DELETING TIME-RECORD FOR TIME    896.69665
 DELETING TIME-RECORD FOR TIME    911.69665
 DELETING TIME-RECORD FOR TIME    926.69665
 DELETING TIME-RECORD FOR TIME    941.69665
 DELETING TIME-RECORD FOR TIME    956.69665
 DELETING TIME-RECORD FOR TIME    971.69665
 DELETING TIME-RECORD FOR TIME    986.69665
 DELETING TIME-RECORD FOR TIME    1001.6966
 DELETING TIME-RECORD FOR TIME    1016.6966
 DELETING TIME-RECORD FOR TIME    1031.6966
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 DELETING TIME-RECORD FOR TIME    1331.6966
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 DELETING TIME-RECORD FOR TIME    1496.6966
 DELETING TIME-RECORD FOR TIME    1511.6966
 DELETING TIME-RECORD FOR TIME    1526.6966
 DELETING TIME-RECORD FOR TIME    1541.6966
 DELETING TIME-RECORD FOR TIME    1556.6966
 DELETING TIME-RECORD FOR TIME    1571.6966
 DELETING TIME-RECORD FOR TIME    1586.6966
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 DELETING TIME-RECORD FOR TIME    1646.6966
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 DELETING TIME-RECORD FOR TIME    1811.6966
 DELETING TIME-RECORD FOR TIME    1826.6966
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 DELETING TIME-RECORD FOR TIME    1976.6966
 DELETING TIME-RECORD FOR TIME    1991.6966
 DELETING TIME-RECORD FOR TIME    2006.6966
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 DELETING TIME-RECORD FOR TIME    2036.6966
 DELETING TIME-RECORD FOR TIME    2051.6966
 DELETING TIME-RECORD FOR TIME    2066.6966
 DELETING TIME-RECORD FOR TIME    2081.6966
 DELETING TIME-RECORD FOR TIME    2096.6966
 DELETING TIME-RECORD FOR TIME    2111.6966
 DELETING TIME-RECORD FOR TIME    2126.6966
 DELETING TIME-RECORD FOR TIME    2141.6966
 DELETING TIME-RECORD FOR TIME    2156.6966
```

```
 DELETING TIME-RECORD FOR TIME    2171.6966
 DELETING TIME-RECORD FOR TIME    2186.6966
 DELETING TIME-RECORD FOR TIME    2201.6966
 DELETING TIME-RECORD FOR TIME    2216.6966
 DELETING TIME-RECORD FOR TIME    2231.6966
 DELETING TIME-RECORD FOR TIME    2246.6966
 DELETING TIME-RECORD FOR TIME    2261.6966
 DELETING TIME-RECORD FOR TIME    2276.6966
 DELETING TIME-RECORD FOR TIME    2291.6966
 DELETING TIME-RECORD FOR TIME    2306.6966
 DELETING TIME-RECORD FOR TIME    2321.6966
 DELETING TIME-RECORD FOR TIME    2336.6966
 DELETING TIME-RECORD FOR TIME    2351.6966
 DELETING TIME-RECORD FOR TIME    2366.6966
 DELETING TIME-RECORD FOR TIME    2381.6966
 DELETING TIME-RECORD FOR TIME    2396.6966
 DELETING TIME-RECORD FOR TIME    2411.6966
 DELETING TIME-RECORD FOR TIME    2426.6966
 DELETING TIME-RECORD FOR TIME    2441.6966
 DELETING TIME-RECORD FOR TIME    2456.6966
 DELETING TIME-RECORD FOR TIME    2471.6966
 DELETING TIME-RECORD FOR TIME    2486.6966
 DELETING TIME-RECORD FOR TIME    2501.6966
 DELETING TIME-RECORD FOR TIME    2516.6966
 DELETING TIME-RECORD FOR TIME    2531.6966
 DELETING TIME-RECORD FOR TIME    2546.6966
 DELETING TIME-RECORD FOR TIME    2561.6966
 DELETING TIME-RECORD FOR TIME    2576.6966
 DELETING TIME-RECORD FOR TIME    2591.6966
 DELETING TIME-RECORD FOR TIME    2606.6966
 DELETING TIME-RECORD FOR TIME    2621.6966
 DELETING TIME-RECORD FOR TIME    2636.6966
 DELETING TIME-RECORD FOR TIME    2651.6966
 DELETING TIME-RECORD FOR TIME    2666.6966
 DELETING TIME-RECORD FOR TIME    2681.6966
 DELETING TIME-RECORD FOR TIME    2696.6966
 DELETING TIME-RECORD FOR TIME    2711.6966
 DELETING TIME-RECORD FOR TIME    2726.6966
 DELETING TIME-RECORD FOR TIME    2741.6966
 DELETING TIME-RECORD FOR TIME    2756.6966
 DELETING TIME-RECORD FOR TIME    2771.6966
 DELETING TIME-RECORD FOR TIME    2786.6966
 DELETING TIME-RECORD FOR TIME    2801.6966
 DELETING TIME-RECORD FOR TIME    2816.6966
 DELETING TIME-RECORD FOR TIME    2831.6966
 DELETING TIME-RECORD FOR TIME    2846.6966
 DELETING TIME-RECORD FOR TIME    2861.6966
 DELETING TIME-RECORD FOR TIME    2876.6966
 DELETING TIME-RECORD FOR TIME    2891.6966
 DELETING TIME-RECORD FOR TIME    2906.6966
 DELETING TIME-RECORD FOR TIME    2921.6966
 DELETING TIME-RECORD FOR TIME    2936.6966
 DELETING TIME-RECORD FOR TIME    2951.6966
 DELETING TIME-RECORD FOR TIME    2966.6966
 DELETING TIME-RECORD FOR TIME    2981.6966

 KEEPING TIME-RECORD FOR TIME    2996.6966
 AND FOR TIME                    3000.0000
 WORKSPACE RECLAIMED

 TIMESTEP AT     3000.00000     SELECTED

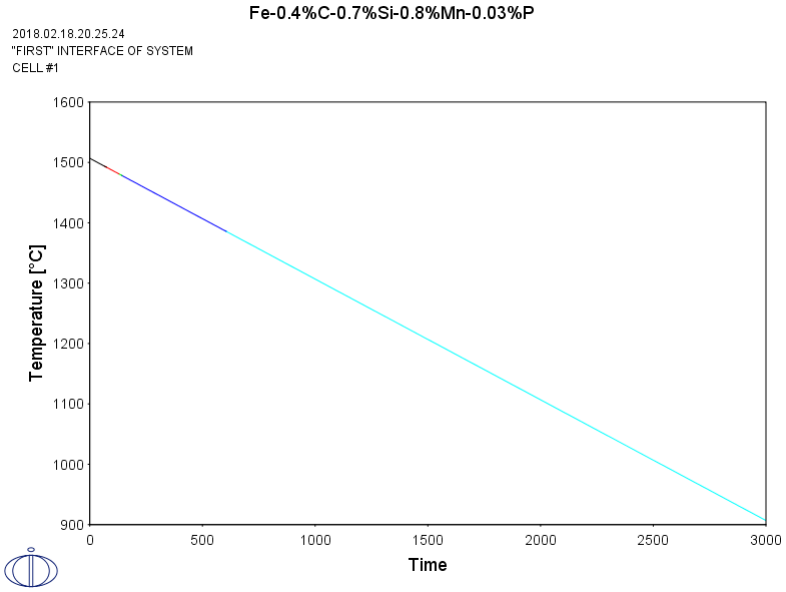
DIC> set-inter
 --OK---
DIC>
```

exb6-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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

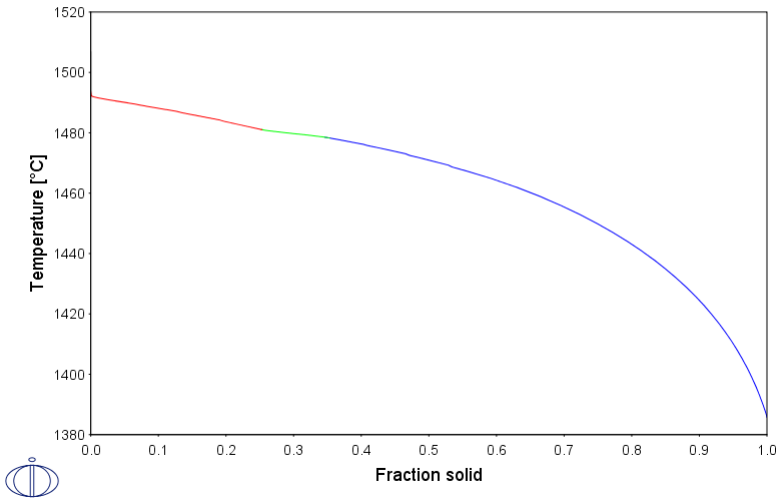
POST-1:
POST-1: set-title Fe-0.4%C-0.7%Si-0.8%Mn-0.03%P
POST-1:
POST-1: s-d-a y t-c
POST-1: s-d-a x time
  INFO: Time is set as independent variable
POST-1: s-p-c interf first
POST-1: plot
```




```
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: plot
```

Fe-0.4%C-0.7%Si-0.8%Mn-0.03%P

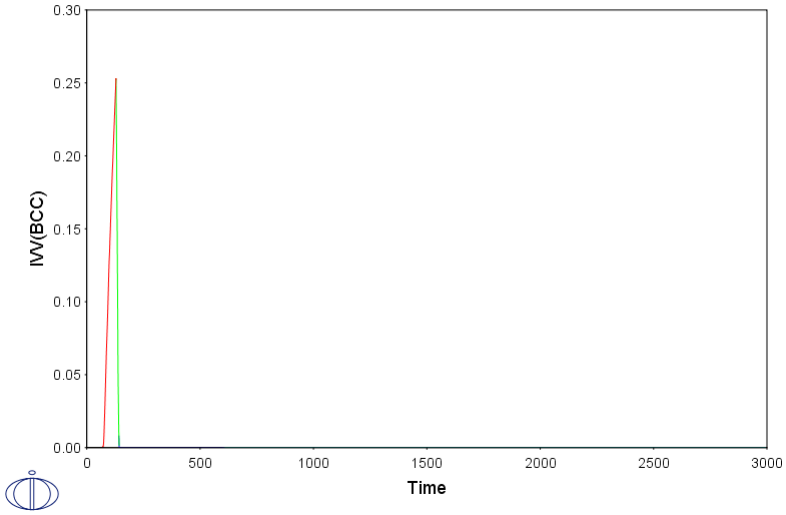
2018.02.18.20.25.27
LOWER INTERFACE OF REGION "SMALTA#1"
CELL #1



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: plot

Fe-0.4%C-0.7%Si-0.8%Mn-0.03%P

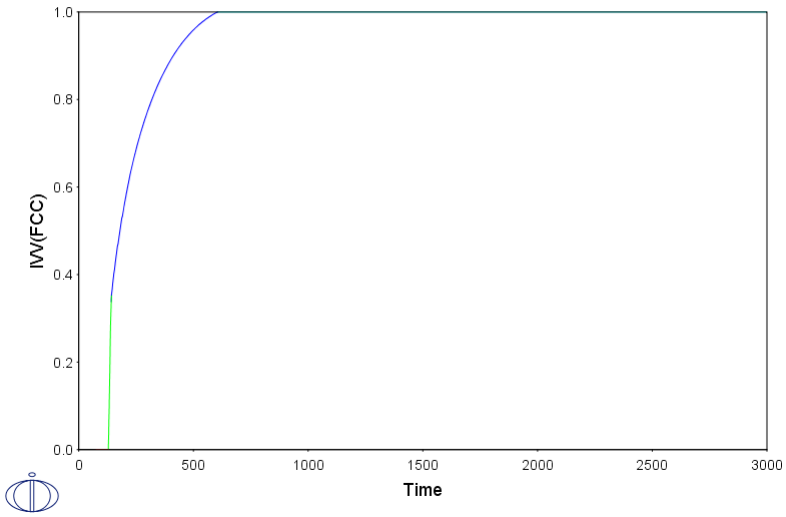
2018.02.18.20.25.30
CELL #1



POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: s-d-a y ivv(fcc)
POST-1: plot

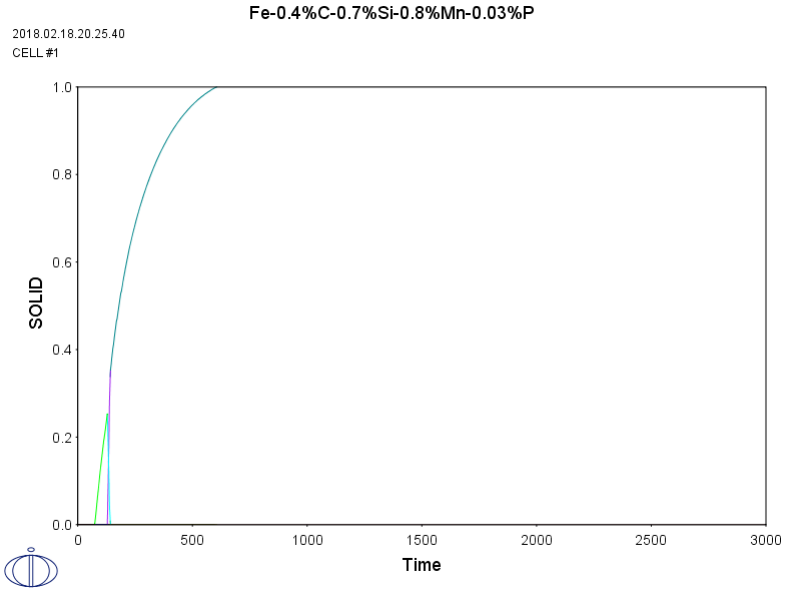
Fe-0.4%C-0.7%Si-0.8%Mn-0.03%P

2018.02.18.20.25.34
CELL #1

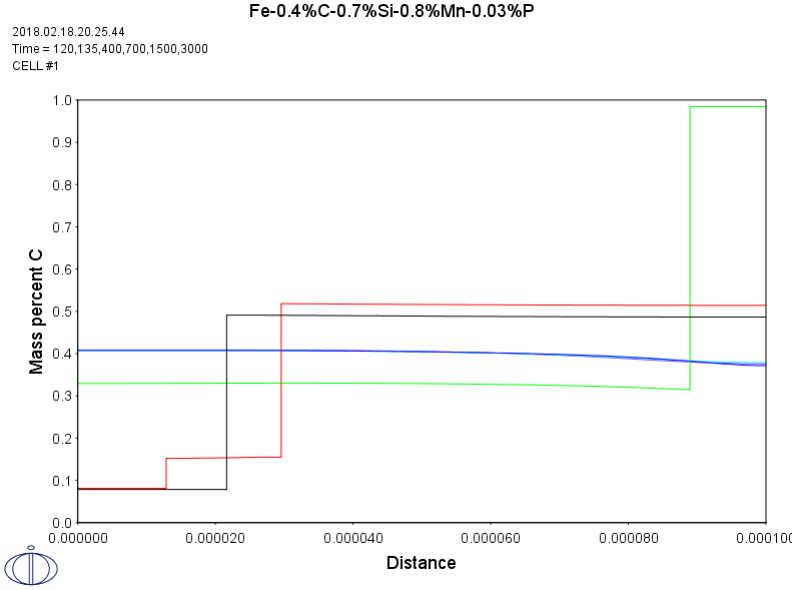


POST-1:
POST-1:Hit RETURN to continue
POST-1: ent table solid

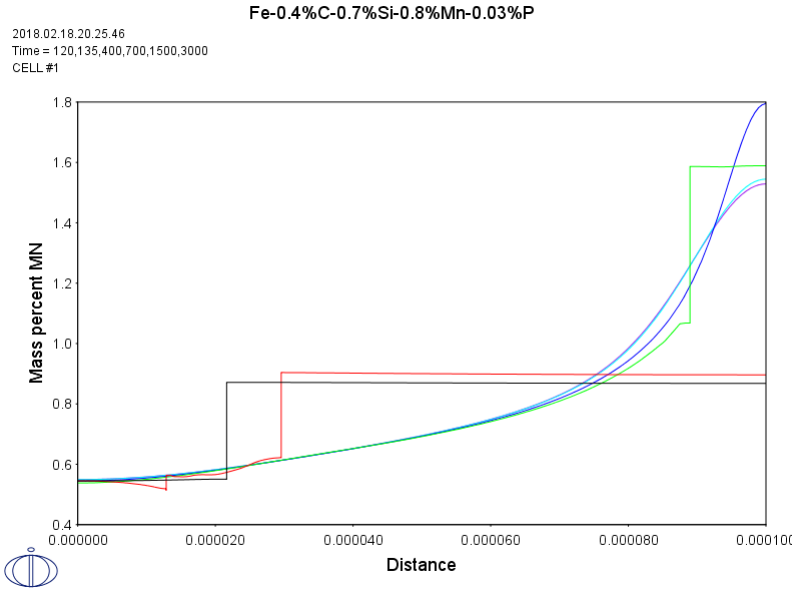
```
Variable(s) ivv(bcc) ivv(fcc)
POST-1:
POST-1: s-d-a y solid
COLUMN NUMBER /*/:
POST-1:
POST-1: plot
```



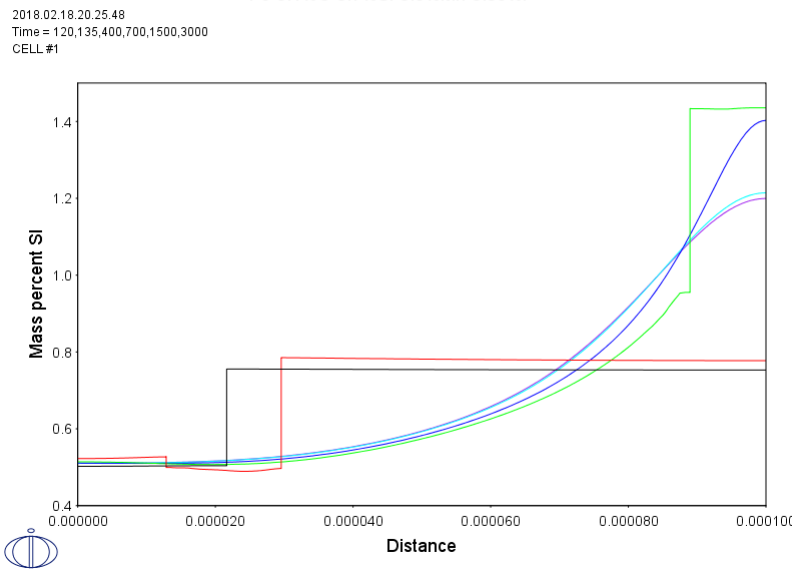

```
POST-1:
POST-1:Hit RETURN to continue
POST-1: s-d-a y w-p c
POST-1: s-d-a x dis gl
  INFO: Distance is set as independent variable
POST-1: s-p-c time 120,135,400,700,1500,3000
POST-1:
POST-1: plot
```



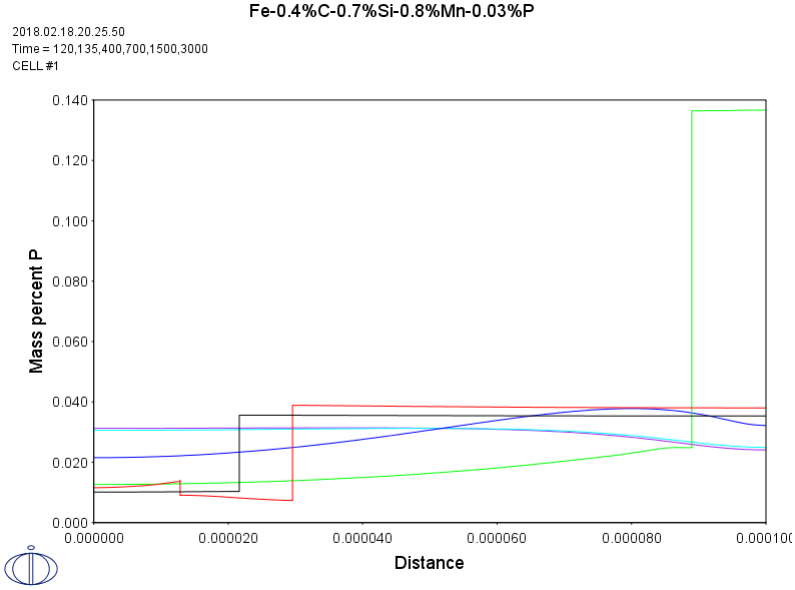

```
POST-1:
POST-1:Hit RETURN to continue
POST-1: s-d-a y w-p mn
POST-1: plot
```



POST-1:
POST-1:Hit RETURN to continue
POST-1: s-d-a y w-p si
POST-1: plot

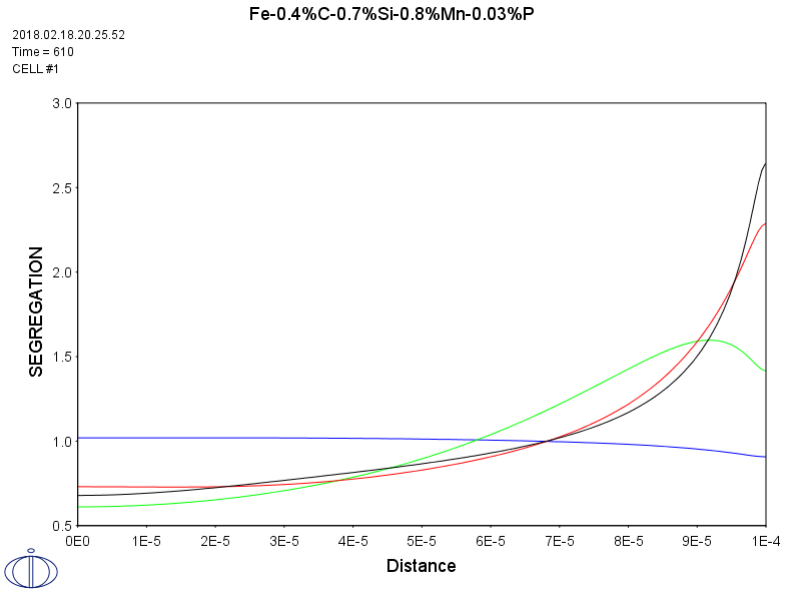


POST-1:
POST-1:Hit RETURN to continue
POST-1: s-d-a y w-p p
POST-1: plot

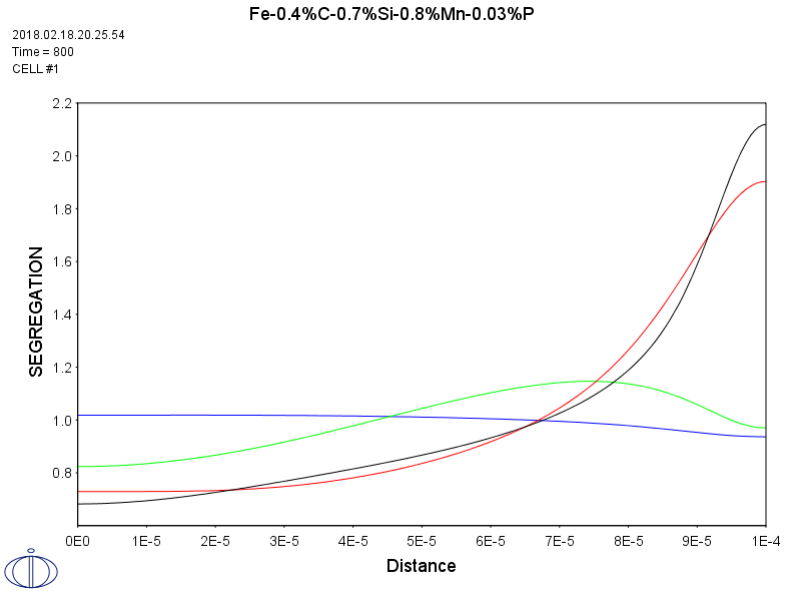


POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: ent function mnn
FUNCTION: w(mn)/0.008
&
POST-1: ent function sin

```
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: plot
```



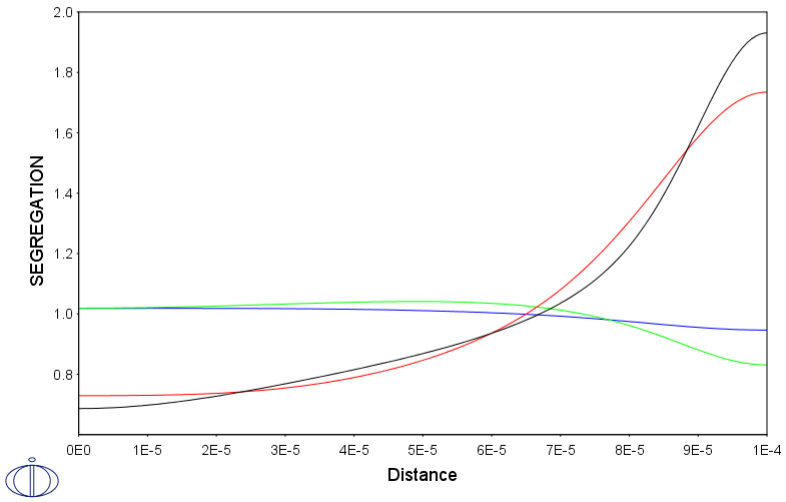

```
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: s-p-c time 800
POST-1: plot
```




```
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: s-p-c time 1500
POST-1: plot
```

Fe-0.4%C-0.7%Si-0.8%Mn-0.03%P

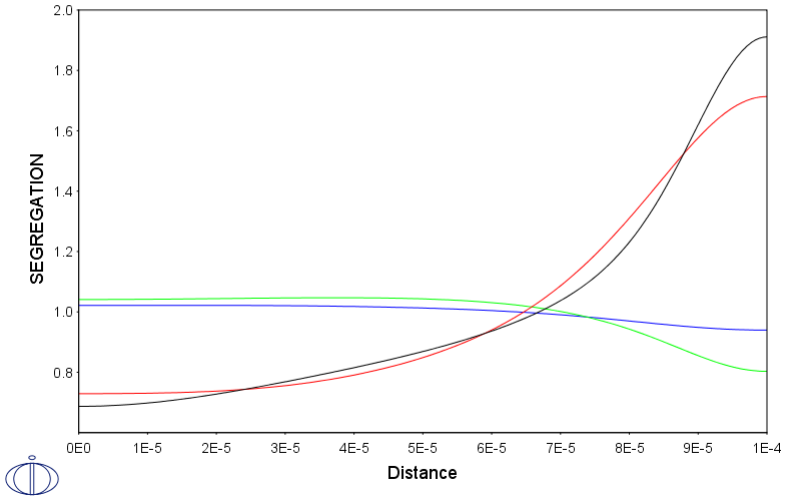
2018.02.18.20.25.55
Time = 1500
CELL #1



POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: s-p-c time 3000
POST-1: plot

Fe-0.4%C-0.7%Si-0.8%Mn-0.03%P

2018.02.18.20.25.57
Time = 3000
CELL #1

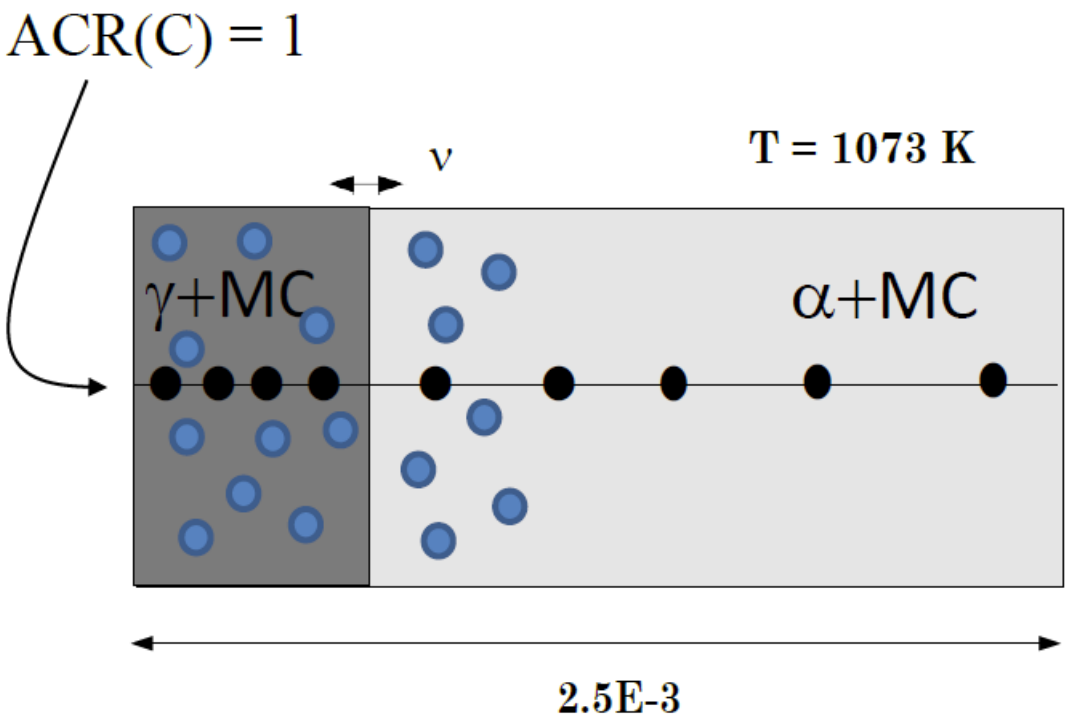


POST-1:
POST-1:Hit RETURN to continue
POST-1: set-inter
--OK---
POST-1:

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

```
About License library version: 8.5.1.0017
 Linked: Fri Feb 16 15:22:08 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb7\setup.DCM" @@
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
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

 VA                     /-  DEFINED
 L12_FCC                B2_BCC                  DICTRA_FCC_A1
   REJECTED
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ USE A TCFE DATABASE FOR THERMODYNAMIC DATA
TDB_TCFE9: @@
TDB_TCFE9: sw tcfe7
 Current database: Steels/Fe-Alloys  v7.0

 VA  DEFINED
 L12_FCC                B2_BCC                  B2_VACANCY
 HIGH_SIGMA             DICTRA_FCC_A1  REJECTED
TDB_TCFE7:
TDB_TCFE7: @@
TDB_TCFE7: @@ DEFINE THE SYSTEM TO WORK WITH
TDB_TCFE7: @@
TDB_TCFE7: def-species fe c nb
 FE                     C                       NB
   DEFINED
TDB_TCFE7:
TDB_TCFE7: @@
TDB_TCFE7: @@ EXCLUDE THE THERMODYNAMIC DATA FOR THE PHASES THAT ARE NOT NEEDED
TDB_TCFE7: @@
TDB_TCFE7: rej ph * all
 GAS:G                  LIQUID:L                BCC_A2
 FCC_A1                 HCP_A3                  DIAMOND_FCC_A4
 GRAPHITE               CEMENTITE               M23C6
 M7C3                   M6C                     M5C2
 KSI_CARBIDE            A1_KAPPA                KAPPA
 Z_PHASE                FE4N_LP1                FECN_CHI
 SIGMA                  MU_PHASE                LAVES_PHASE_C14
 G_PHASE                CR3SI                   NBNI3
   REJECTED
TDB_TCFE7: res ph fcc bcc grap
 FCC_A1                 BCC_A2                  GRAPHITE
   RESTORED
TDB_TCFE7:
TDB_TCFE7: @@
TDB_TCFE7: @@ RETRIEVE DATA FROM THE DATABASE FILE
TDB_TCFE7: @@
TDB_TCFE7: get
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'
  'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
  'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C
      -FE'
  'B.-J. Lee, estimated parameter 1999'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
      Molar volumes'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
  'S. Canderyd, Report IM-2005-109, Stockholm, Sweden; Fe-Nb-C'
  'W. Huang, Zeitschrift fur Metallkunde, Vol. 6 (1990), pp. 397-404; Fe-Nb-C'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'B. Uhrenius (1993-1994), International journal of refractory metals and
      hard mater, Vol. 12, pp. 121-127; Molar volumes'
  'B.-J. Lee, Metall. Mater. Trans. A, 32A, 2423-39(2001); Fe-Nb'
 -OK-
TDB_TCFE7:
TDB_TCFE7: @@
TDB_TCFE7: @@ NOW APPEND A SSUB DATABASE FROM WHICH WE READ THE THERMODYNAMIC
TDB_TCFE7: @@ DESCRIPTION OF NIOBIUM CARBIDE
TDB_TCFE7: @@
TDB_TCFE7:
TDB_TCFE7: app SSUB5
 Current database: SGTE Substances Database v5.2

 VA  DEFINED
APP: def-sys  fe c nb
 FE                     C                       NB
   DEFINED
APP: rej ph *
 GAS:G                  GRAPHITE                GRAPHITE_L
 DIAMOND                C0_749NB1_S             C0_877NB1_S
 C0_98NB1_S             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 ....

 List of references for assessed data

   C1NB1 I. BARIN 3rd. Edition
      C1NB1 NbC
      Data taken from BARIN 3rd. Ed. (1995)
 -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 mobfe2
 Current database: Steels/Fe-Alloys Mobility  v2.0
   TCS Steel Mobility Database Version 2.0 from 2011-12-09.

 VA  DEFINED
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 ....

 List of references for assessed data

  'This parameter has not been assessed'
  'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'
  'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
      -Ni'
  'J. Geise and Ch. Herzig, Z. Metallkd. 76(1985)622.; Impurity diffusion of
      Nb in fcc Fe.'
  'Assessed from data presented by B. B. Yu and R. F. Davis J. Phys. Chem.
      Solids 40(1979)997.; C Self-Diff in NbC.'
  'B. Jonsson: Z. Metallkunde 85(1994)498-501; C and N diffusion in bcc Cr
      -Fe-Ni'
  'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
      in bcc Fe'
  'R. F. Peart, Acta Metall. 10(1962)519.; Impurity diffusion of Fe in bcc
      Nb.'
  'Assessed from data presented in Landholt-Bornstein, Vol. 26, ed. H.
      Mehrer, springer (1990); Impurity diff of Nb in bcc Fe.'
  'R. E. Einziger et al., Phys. Rev. B 17(1978)440.; self-diffusion of Nb in
      bcc Nb.'
 -OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP
APP: @@
APP: go d-m
 NO TIME STEP DEFINED
 *** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
 *** ENTERING C1NB1_S AS A DIFFUSION NONE PHASE
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 1073.15; * N

DIC>
DIC> @@
DIC> @@ ENTER REGIONS ferr AND aus
DIC> @@
DIC> enter-region
REGION NAME : ferr
DIC>
DIC> ent-reg
REGION NAME : aus
ATTACH TO REGION NAMED /FERR/: ferr
ATTACHED TO THE RIGHT OF FERR /YES/: n
DIC>
DIC> @@
DIC> @@ ENTER GRIDS INTO REGIONS
DIC> @@
DIC> enter-grid
REGION NAME : /AUS/: ferr
WIDTH OF REGION /1/: 2.499999e-3
TYPE /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
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
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-07/: 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>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb7\run.DCM"DIC> @@
DIC> @@ READ THE SET UP FROM FILE AND START THE SIMULATION
DIC> @@
DIC>
DIC> go d-m
 TIME STEP AT TIME  0.00000E+00
 *** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
 *** ENTERING C1NB1_S AS A DIFFUSION NONE PHASE
DIC> read exb7
 OK
DIC> sim yes
 Region: AUS
 double geometric
 dense at outer boundaries, coarse at  0.50000E-09
lower part   1.0800       16
upper part  0.92593       16
 Region: FERR
 single geometric dense at   0.0000
  1.0800      114
 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)
 Saving results
 ----------------------------------
  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
 Stage 1
 Evaluating Jacobian
Iteration #   1 sum residual **2:   0.44222132E+15
Iteration #   2 sum residual **2:   0.43975158E+15
 Evaluating Jacobian
Iteration #   3 sum residual **2:   0.51145294E+15
 Reducing dt to   5.000000000000000E-009
 Stage 1
 Evaluating Jacobian
Iteration #   1 sum residual **2:   0.10858850E+15
Iteration #   2 sum residual **2:   0.10768159E+15
 Evaluating Jacobian
Iteration #   3 sum residual **2:   0.47896705E+14
 Error                    408
 Reducing dt to   2.500000000000000E-009
 Stage 1
 Evaluating Jacobian
Iteration #   1 sum residual **2:   0.26436925E+14
Iteration #   2 sum residual **2:   0.26156665E+14
Iteration #   3 sum residual **2:   0.19671471E+14
Iteration #   4 sum residual **2:   0.15909309E+14
Iteration #   5 sum residual **2:   0.13449818E+14
Iteration #   6 sum residual **2:   0.11738463E+14
Iteration #   7 sum residual **2:   0.10482765E+14
Iteration #   8 sum residual **2:   0.95259408E+13
Iteration #   9 sum residual **2:   0.87784754E+13
Iteration #  10 sum residual **2:   0.81854606E+13
Iteration #  11 sum residual **2:   0.77115365E+13
Iteration #  12 sum residual **2:   0.73332751E+13
Iteration #  13 sum residual **2:   0.70494151E+13
Iteration #  14 sum residual **2:   0.67771939E+13
Iteration #  15 sum residual **2:   0.66328406E+13
Iteration #  16 sum residual **2:   0.65465027E+13
 Error                    408
 Reducing dt to   1.250000000000000E-009
 Stage 1
 Evaluating Jacobian
Iteration #   1 sum residual **2:   0.63517503E+13
Iteration #   2 sum residual **2:   0.48482644E+13
Iteration #   3 sum residual **2:   0.37734642E+13
Iteration #   4 sum residual **2:   0.30347657E+13
Iteration #   5 sum residual **2:   0.25629830E+13
Iteration #   6 sum residual **2:   0.22401447E+13
Iteration #   7 sum residual **2:   0.20098774E+13
Iteration #   8 sum residual **2:   0.18423841E+13
Iteration #   9 sum residual **2:   0.17206673E+13
Iteration #  10 sum residual **2:   0.16346439E+13
Iteration #  11 sum residual **2:   0.15783334E+13
 Error                    408
 Reducing dt to   6.250000000000000E-010
 Stage 1
 Evaluating Jacobian
Iteration #   1 sum residual **2:   0.15173761E+13
Iteration #   2 sum residual **2:   0.92807494E+12
Iteration #   3 sum residual **2:   0.68227945E+12
Iteration #   4 sum residual **2:   0.55087278E+12
Iteration #   5 sum residual **2:   0.47067619E+12
Iteration #   6 sum residual **2:   0.41909384E+12
Iteration #   7 sum residual **2:   0.38590443E+12
Iteration #   8 sum residual **2:   0.36635838E+12
 Error                    408
 Reducing dt to   3.125000000000000E-010
 Stage 1
 Evaluating Jacobian
Iteration #   1 sum residual **2:   0.27840998E+12
Iteration #   2 sum residual **2:   0.17201055E+12
Iteration #   3 sum residual **2:   0.12687021E+12
Iteration #   4 sum residual **2:   0.10303215E+12
Iteration #   5 sum residual **2:   0.89261308E+11
 Error                    408
 Reducing dt to   1.562500000000000E-010
 Stage 1
 Evaluating Jacobian
Iteration #   1 sum residual **2:   0.50738890E+11
```

```
Iteration #   2 sum residual **2:   0.30812257E+11
Iteration #   3 sum residual **2:   0.22477716E+11
Iteration #   4 sum residual **2:   0.18061437E+11
 Error                    408
 Reducing dt to   7.812500000000000E-011
 Stage 1
 Evaluating Jacobian
Iteration #   1 sum residual **2:   0.84899306E+10
Iteration #   2 sum residual **2:   0.46952010E+10
Iteration #   3 sum residual **2:   0.31616839E+10
 Error                    408
 Reducing dt to   3.906250000000000E-011
 Stage 1
 Evaluating Jacobian
Iteration #   1 sum residual **2:   0.14543949E+10
Iteration #   2 sum residual **2:   0.60577985E+09
 Error                    408
 Reducing dt to   1.953125000000000E-011
 Stage 1
 Evaluating Jacobian
Iteration #   1 sum residual **2:   0.18465102E+09
Iteration #   2 sum residual **2:    44022478.
Iteration #   3 sum residual **2:    10202979.
Iteration #   4 sum residual **2:    2204131.6
 Error                    408
 Reducing dt to   9.765625000000000E-012
 Stage 1


output ignored...



... output resumed

 DELETING TIME-RECORD FOR TIME    27256.351
 DELETING TIME-RECORD FOR TIME    27291.247
 DELETING TIME-RECORD FOR TIME    27342.250
 DELETING TIME-RECORD FOR TIME    27406.675
 DELETING TIME-RECORD FOR TIME    27449.624
 DELETING TIME-RECORD FOR TIME    27492.574
 DELETING TIME-RECORD FOR TIME    27535.524
 DELETING TIME-RECORD FOR TIME    27578.473
 DELETING TIME-RECORD FOR TIME    27621.423
 DELETING TIME-RECORD FOR TIME    27664.373
 DELETING TIME-RECORD FOR TIME    27707.322
 DELETING TIME-RECORD FOR TIME    27750.272
 DELETING TIME-RECORD FOR TIME    27793.222
 DELETING TIME-RECORD FOR TIME    27846.909
 DELETING TIME-RECORD FOR TIME    27889.858
 DELETING TIME-RECORD FOR TIME    27975.758
 DELETING TIME-RECORD FOR TIME    28018.708
 DELETING TIME-RECORD FOR TIME    28061.657
 DELETING TIME-RECORD FOR TIME    28104.607
 DELETING TIME-RECORD FOR TIME    28147.557
 DELETING TIME-RECORD FOR TIME    28190.506
 DELETING TIME-RECORD FOR TIME    28233.456
 DELETING TIME-RECORD FOR TIME    28276.406
 DELETING TIME-RECORD FOR TIME    28319.355
 DELETING TIME-RECORD FOR TIME    28356.936
 DELETING TIME-RECORD FOR TIME    28394.517
 DELETING TIME-RECORD FOR TIME    28432.098
 DELETING TIME-RECORD FOR TIME    28469.679
 DELETING TIME-RECORD FOR TIME    28507.260
 DELETING TIME-RECORD FOR TIME    28544.841
 DELETING TIME-RECORD FOR TIME    28582.422
 DELETING TIME-RECORD FOR TIME    28620.003
 DELETING TIME-RECORD FOR TIME    28657.584
 DELETING TIME-RECORD FOR TIME    28695.165
 DELETING TIME-RECORD FOR TIME    28732.746
 DELETING TIME-RECORD FOR TIME    28770.327
 DELETING TIME-RECORD FOR TIME    28807.908
 DELETING TIME-RECORD FOR TIME    28845.489
 DELETING TIME-RECORD FOR TIME    28883.070
 DELETING TIME-RECORD FOR TIME    28920.651
 DELETING TIME-RECORD FOR TIME    28958.232
 DELETING TIME-RECORD FOR TIME    28995.813
 DELETING TIME-RECORD FOR TIME    29033.394
 DELETING TIME-RECORD FOR TIME    29070.975
 DELETING TIME-RECORD FOR TIME    29105.871
 DELETING TIME-RECORD FOR TIME    29140.768
 DELETING TIME-RECORD FOR TIME    29175.664
 DELETING TIME-RECORD FOR TIME    29210.561
 DELETING TIME-RECORD FOR TIME    29285.723
 DELETING TIME-RECORD FOR TIME    29328.673
 DELETING TIME-RECORD FOR TIME    29371.622
 DELETING TIME-RECORD FOR TIME    29414.572
 DELETING TIME-RECORD FOR TIME    29457.522
 DELETING TIME-RECORD FOR TIME    29500.471
 DELETING TIME-RECORD FOR TIME    29543.421
 DELETING TIME-RECORD FOR TIME    29586.371
 DELETING TIME-RECORD FOR TIME    29629.320
 DELETING TIME-RECORD FOR TIME    29672.270
 DELETING TIME-RECORD FOR TIME    29715.220
 DELETING TIME-RECORD FOR TIME    29758.169
 DELETING TIME-RECORD FOR TIME    29801.119
 DELETING TIME-RECORD FOR TIME    29838.700
 DELETING TIME-RECORD FOR TIME    29876.281
 DELETING TIME-RECORD FOR TIME    29913.862
 DELETING TIME-RECORD FOR TIME    29951.443
 DELETING TIME-RECORD FOR TIME    29989.024
 DELETING TIME-RECORD FOR TIME    30026.605
 DELETING TIME-RECORD FOR TIME    30064.186
 DELETING TIME-RECORD FOR TIME    30101.767
 DELETING TIME-RECORD FOR TIME    30139.348
 DELETING TIME-RECORD FOR TIME    30176.929
 DELETING TIME-RECORD FOR TIME    30214.510
 DELETING TIME-RECORD FOR TIME    30252.091
 DELETING TIME-RECORD FOR TIME    30289.671
 DELETING TIME-RECORD FOR TIME    30327.252
 DELETING TIME-RECORD FOR TIME    30364.833
 DELETING TIME-RECORD FOR TIME    30402.414
 DELETING TIME-RECORD FOR TIME    30439.995
 DELETING TIME-RECORD FOR TIME    30477.576
 DELETING TIME-RECORD FOR TIME    30515.157
 DELETING TIME-RECORD FOR TIME    30552.738
```

```
 DELETING TIME-RECORD FOR TIME    30590.319
 DELETING TIME-RECORD FOR TIME    30627.900
 DELETING TIME-RECORD FOR TIME    30665.481
 DELETING TIME-RECORD FOR TIME    30703.062
 DELETING TIME-RECORD FOR TIME    30740.643
 DELETING TIME-RECORD FOR TIME    30778.224
 DELETING TIME-RECORD FOR TIME    30815.805
 DELETING TIME-RECORD FOR TIME    30853.386
 DELETING TIME-RECORD FOR TIME    30890.967
 DELETING TIME-RECORD FOR TIME    30928.548
 DELETING TIME-RECORD FOR TIME    30966.129
 DELETING TIME-RECORD FOR TIME    31003.710
 DELETING TIME-RECORD FOR TIME    31041.291
 DELETING TIME-RECORD FOR TIME    31078.872
 DELETING TIME-RECORD FOR TIME    31116.453
 DELETING TIME-RECORD FOR TIME    31154.034
 DELETING TIME-RECORD FOR TIME    31191.615
 DELETING TIME-RECORD FOR TIME    31229.196
 DELETING TIME-RECORD FOR TIME    31266.777
 DELETING TIME-RECORD FOR TIME    31304.357
 DELETING TIME-RECORD FOR TIME    31341.938
 DELETING TIME-RECORD FOR TIME    31379.519
 DELETING TIME-RECORD FOR TIME    31417.100
 DELETING TIME-RECORD FOR TIME    31454.681
 DELETING TIME-RECORD FOR TIME    31492.262
 DELETING TIME-RECORD FOR TIME    31529.843
 DELETING TIME-RECORD FOR TIME    31567.424
 DELETING TIME-RECORD FOR TIME    31605.005
 DELETING TIME-RECORD FOR TIME    31642.586
 DELETING TIME-RECORD FOR TIME    31677.483
 DELETING TIME-RECORD FOR TIME    31712.379
 DELETING TIME-RECORD FOR TIME    31747.276
 DELETING TIME-RECORD FOR TIME    31795.594
 DELETING TIME-RECORD FOR TIME    31838.544
 DELETING TIME-RECORD FOR TIME    31881.494
 DELETING TIME-RECORD FOR TIME    31924.443
 DELETING TIME-RECORD FOR TIME    31967.393
 DELETING TIME-RECORD FOR TIME    32010.343
 DELETING TIME-RECORD FOR TIME    32053.292
 DELETING TIME-RECORD FOR TIME    32096.242
 DELETING TIME-RECORD FOR TIME    32139.192
 DELETING TIME-RECORD FOR TIME    32182.141
 DELETING TIME-RECORD FOR TIME    32225.091
 DELETING TIME-RECORD FOR TIME    32268.041
 DELETING TIME-RECORD FOR TIME    32310.990
 DELETING TIME-RECORD FOR TIME    32348.571

 KEEPING TIME-RECORD FOR TIME    32386.152
 AND FOR TIME                    32400.000
 WORKSPACE RECLAIMED
 -------------------------------------------------
 INTERPOLATION SCHEME USED THIS FRACTION OF
 THE ALLOCATED MEMORY:   0.979204858989315
 EFFICIENCY FACTOR:    31.4799576717506
 MEMORY FRACTION USAGE PER BRANCH:
   1.00000000000000
  0.906424464627948
   1.00000000000000
 -------------------------------------------------
 DEALLOCATING
 -------------------------------------------------

 TIMESTEP AT     32400.0000     SELECTED

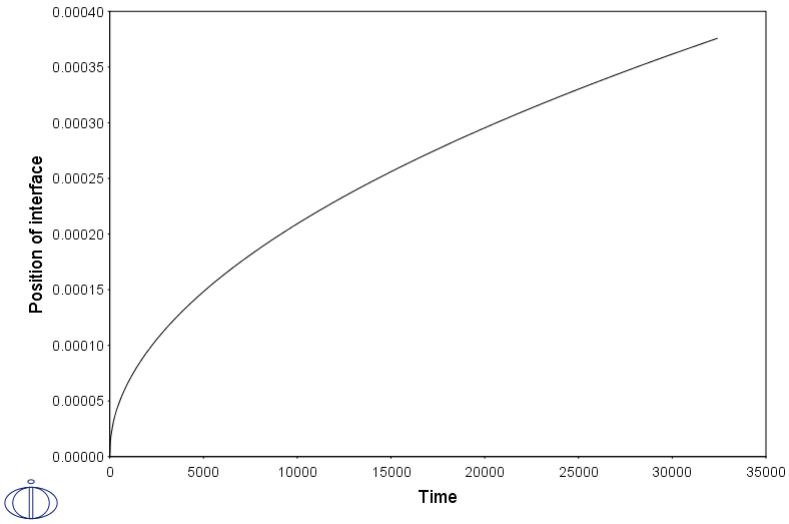
DIC>
DIC> set-inter
 --OK---
DIC>
```

exb7-plot

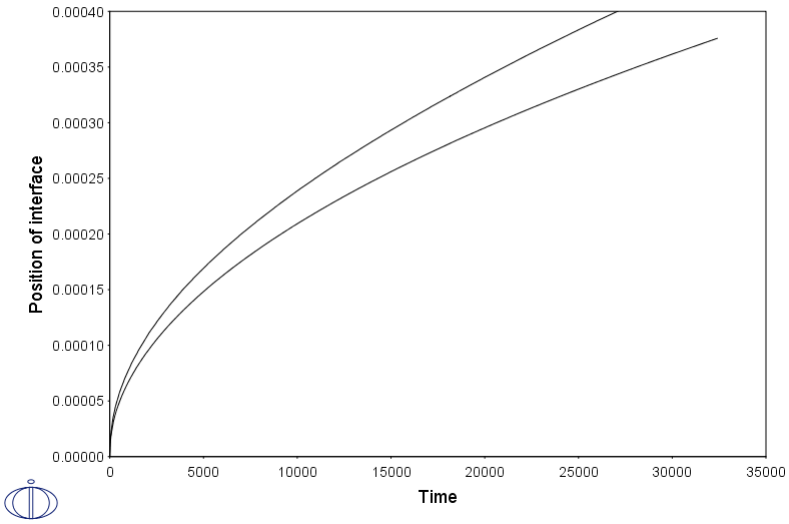
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb7\plot.DCM"DIC>
DIC>
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  3.24000E+04
 *** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
 *** ENTERING C1NB1_S 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
   2018.02.18.20.44.43
   UPPER INTERFACE OF REGION "AUS#1"
   CELL #1
```



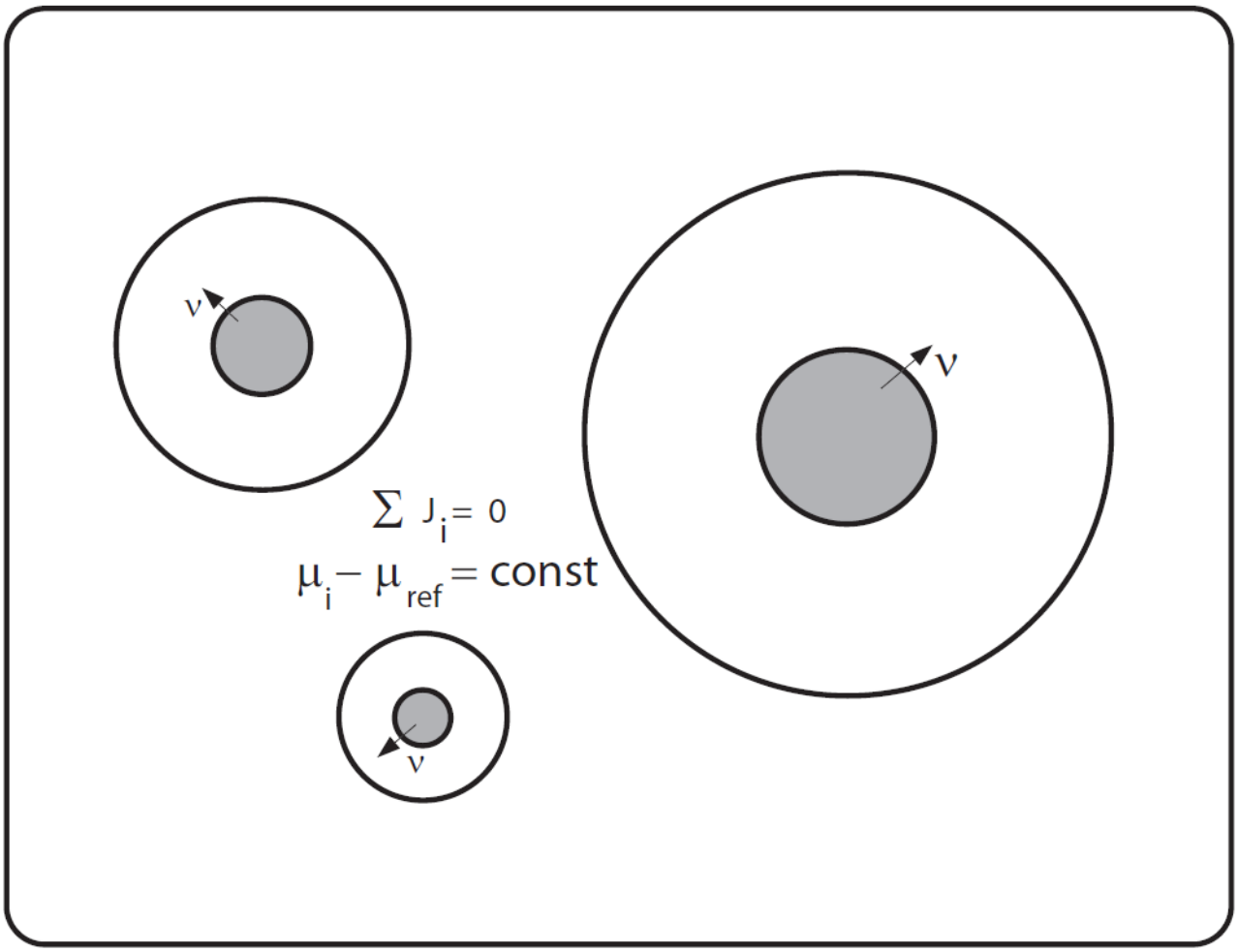

```
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ APPEND DATA FROM A CORRESPONDING SIMULATION
POST-1: @@ WITHOUT NIOBIUM
POST-1: @@
POST-1:
POST-1: app y fec.exp 0
DATASET NUMBER(s): /-1/: 1
POST-1:
POST-1: plot
   2018.02.18.20.44.49
   UPPER INTERFACE OF REGION "AUS#1"
   CELL #1
```




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

--OK---
POST-1:

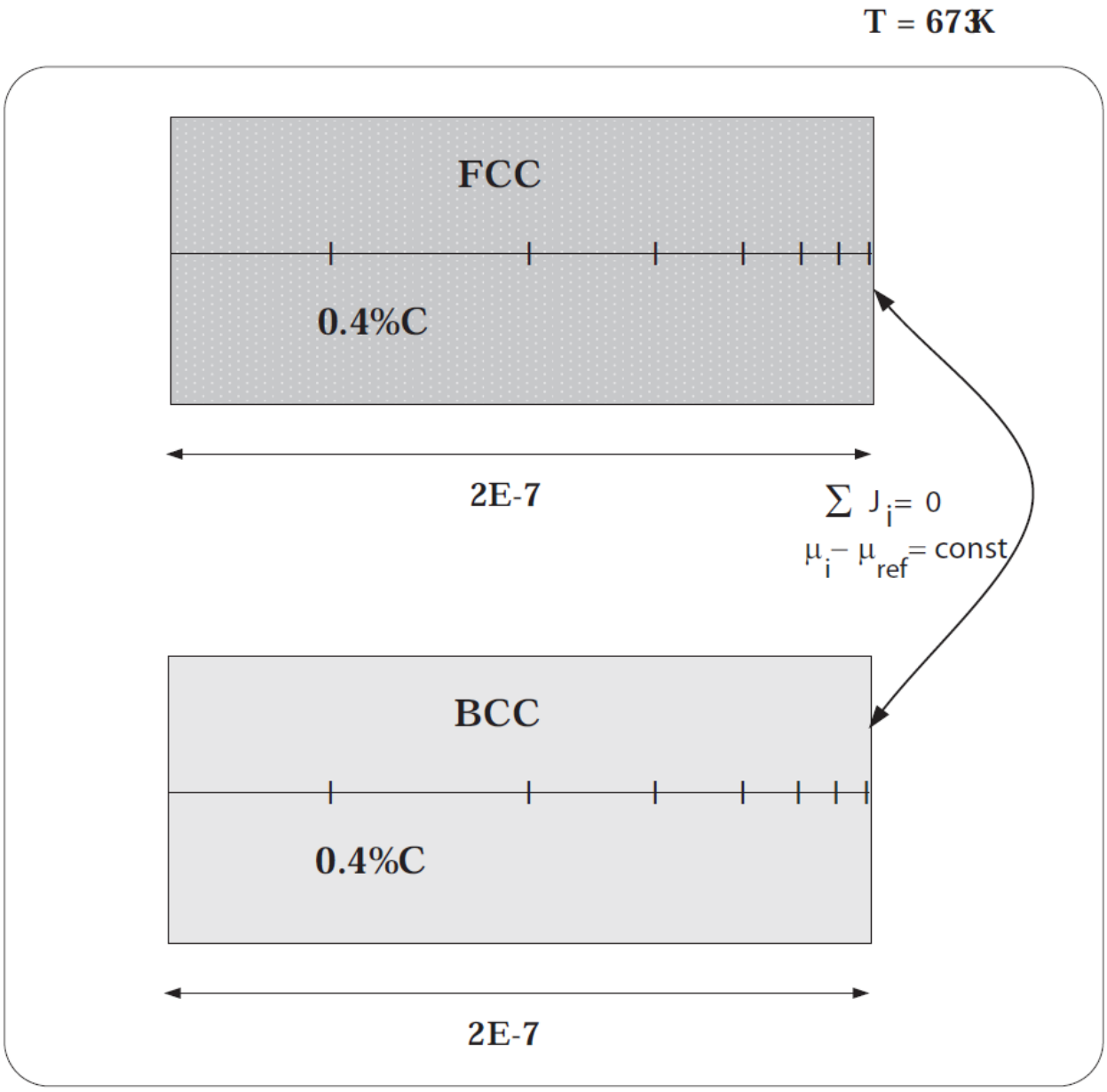
Cell Calculations



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

```
About Stockholm, Sweden

 Software  (build 12987) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri Feb 16 15:22:08 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exc1\setup.DCM" ?@@
 NO SUCH COMMAND, USE HELP
SYS: @@ Cell calculation.
SYS: @@ Carbon cannon in ferrite/austenite: Fe-C system, 2-cell calculation
SYS: @@ This example simulates what happens to a ferrite plate that has
SYS: @@ inherited the carbon content of its parent austenite. The ferrite
SYS: @@ plate formed is embedded in an austenite matrix. This setup
SYS: @@ corresponds to a proposed mechanism for formation of Widmannstätten
SYS: @@ ferrite or for the ferrite phase of the bainite structure. It is
SYS: @@ assumed that the phase boundary between ferrite and austenite is
SYS: @@ immobile, this is achieved in the simulation by putting the ferrite
SYS: @@ and the austenite in two different cells. See also M. Hillert,
SYS: @@ L. Höglund and J. Ågren: 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
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

 VA                     /-  DEFINED
 L12_FCC                B2_BCC                 DICTRA_FCC_A1
   REJECTED
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA
TDB_TCFE9: @@
TDB_TCFE9: sw fedemo
 Current database: Iron Demo Database v2.0

 VA                     /-  DEFINED
TDB_FEDEMO: def-sys fe c
 FE                     C  DEFINED
TDB_FEDEMO: rej ph * all
 GAS:G                  LIQUID:L               BCC_A2
 CEMENTITE              DIAMOND_FCC_A4         FCC_A1
 GRAPHITE               HCP_A3                 KSI_CARBIDE
 LAVES_PHASE_C14        M23C6                  M5C2
 M7C3   REJECTED
TDB_FEDEMO: res ph fcc,bcc
 FCC_A1                 BCC_A2  RESTORED
TDB_FEDEMO: get
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'P. Franke, Estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
  'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'X.-G. Lu, M. Selleby, B. Sundman, CALPHAD, 29 (2005) 49-55; Fe P-T diagram'
  'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
 -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 v2.0

 VA  DEFINED
APP: def-sys fe c
 FE                     C  DEFINED
APP: rej ph * all
 BCC_A2                 FCC_A1  REJECTED
APP: res ph fcc,bcc
 FCC_A1                 BCC_A2  RESTORED
APP: get
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'This parameter has not been assessed'
  'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'
  'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
      -Ni'
  'B. Jonsson: Z. Metallkunde 85(1994)498-501; C and N diffusion in bcc Cr
      -Fe-Ni'
  'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
      in bcc Fe'
 -OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR
APP: @@
APP: go d-m
```

```
 NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 673; * N

DIC>
DIC> @@
DIC> @@ IN THE FIRST CELL
DIC> @@
DIC> @@ ENTER REGION aus CONTAINING AUSTENITE
DIC> @@ ENTER A GEOMETRICAL GRID INTO THAT REGION
DIC> @@ ENTER THE INITIAL COMPOSITION INTO THE AUSTENITE
DIC> @@
DIC> enter-region aus
DIC> enter-grid aus  0.2e-6 AUTO
DIC> enter-phase act aus  matrix fcc_a1#1
DIC>
DIC> enter-composition
REGION NAME : /AUS/: aus
PHASE NAME: /FCC_A1/: fcc_a1#1
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: c
TYPE /LINEAR/: lin 0.4 0.4
DIC>
DIC> @@
DIC> @@ IN THE SECOND CELL
DIC> @@
DIC> create-new-cell
CELL DISTRIBUTION FACTOR /1/: 1
 CREATING NEW CELL, NUMBER:  2
 CELL   2 SELECTED
DIC-2>
DIC-2> @@
DIC-2> @@ ENTER REGION fer CONTAINING FERRITE
DIC-2> @@ ENTER A GEOMETRICAL GRID INTO THAT REGION
DIC-2> @@ ENTER THE INITIAL COMPOSITION INTO THE FERRITE
DIC-2> @@
DIC-2> enter-region fer
DIC-2>
DIC-2>
DIC-2>
DIC-2> enter-grid fer  0.2e-6 AUTO
DIC-2> enter-phase act fer  matrix bcc_a2#1
DIC-2>
DIC-2> enter-composition
REGION NAME : /FER/: fer
PHASE NAME: /BCC_A2/: bcc_a2#1
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: c
TYPE /LINEAR/: lin 0.4 0.4
DIC-2>
DIC-2> @@
DIC-2> @@ SET THE SIMULATION TIME AND OTHER SIMULATION PARAMETERS
DIC-2> @@
DIC-2> set-simulation-time
END TIME FOR INTEGRATION /.1/: 0.5
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /.05/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC-2>
DIC-2>
DIC-2>
DIC-2> @@
DIC-2> @@ USE IMPLICIT (1) TIME INTEGRATION
DIC-2> @@
DIC-2> set-simulation-cond
NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /NO/:
VARY POTENTIALS OR ACTIVITIES OR LNAC : /POTENTIAL/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (0 -> 0.5 -> 1): /.5/: 1.0
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /NO/:
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>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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
 single geometric dense at  0.20000E-06
 0.89105       93
 Region: FER
 single geometric dense at  0.20000E-06
 0.96940       72
 U-FRACTION IN SYSTEM:  C = .0186733111178274  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
 U-FRACTION IN SYSTEM:  C = .0186733111178274  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
 2.570491440876833E-002        2.570457646507204E-002        1.632468496708230E-002        1.481595250675601E-003        4.374341462051788E-
005        2.088305124067901E-007        2.465148837668976E-011        1.324756764297081E-017       TIME =  0.10000000E-06 DT =  0.10000000E-
06 SUM OF SQUARES =  0.13247568E-16
 U-FRACTION IN SYSTEM:  C = .0186733111178092  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    0 seconds
 1.721271285522132E-002        1.721309826251375E-002        1.320114685474547E-003        1.780264104372174E-004        4.883616119764177E-
006        2.701426733646338E-008        4.894446543282404E-012        5.060987976361818E-018       TIME =  0.30000000E-06 DT =  0.20000000E-
06 SUM OF SQUARES =  0.50609880E-17
 U-FRACTION IN SYSTEM:  C = .0186733111178317  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    1 seconds
 1.723030673037079E-002        1.722973038975870E-002        6.546665653188744E-004        1.540163381854436E-005        9.847914086370379E-
009        1.575452822349616E-013        1.593769930090315E-021       TIME =  0.70000000E-06 DT =  0.40000000E-
06 SUM OF SQUARES =  0.15937699E-20
 U-FRACTION IN SYSTEM:  C = .0186733111783162  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    0 seconds
 2.046536420972098E-003        2.046359859030639E-003        1.093843934644341E-005        4.894916965478312E-008        1.003356508283692E-
012        9.302414829459864E-020       TIME =  0.15000000E-05 DT =  0.80000000E-06 SUM OF SQUARES =  0.93024148E-19
 U-FRACTION IN SYSTEM:  C = .0186733111783284  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    1 seconds
 1.307886964750396E-003        1.307786277164665E-003        8.937183842406468E-006        4.994501913148052E-008        1.605937233342920E-
012        2.925328975717250E-019       TIME =  0.31000000E-05 DT =  0.16000000E-05 SUM OF SQUARES =  0.29253290E-18
 U-FRACTION IN SYSTEM:  C = .0186733111783716  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    0 seconds
 5.482172962189864E-004        5.481699846891220E-004        2.979475699821687E-006        1.354117993457866E-008        2.862902386732131E-
013        2.781528300460643E-020       TIME =  0.63000000E-05 DT =  0.32000000E-05 SUM OF SQUARES =  0.27815283E-19
 U-FRACTION IN SYSTEM:  C = .0186733111783983  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    1 seconds
 2.615717394236350E-002        2.615484476818204E-002        1.336512838121405E-004        5.745045707598120E-007        1.084421168367715E-
011        8.892868844306621E-019       TIME =  0.12700000E-04 DT =  0.64000000E-05 SUM OF SQUARES =  0.88928688E-18
 U-FRACTION IN SYSTEM:  C = .0186733111784285  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    0 seconds
 1.276911017788254E-002        1.276795521545566E-002        6.327039393406848E-005        2.645588403126521E-007        4.737846880516210E-
012        3.569977336034442E-019       TIME =  0.25500000E-04 DT =  0.12800000E-04 SUM OF SQUARES =  0.35699773E-18
 U-FRACTION IN SYSTEM:  C = .0186733111784667  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    1 seconds
 6.319101225966472E-003        6.318525707093593E-003        3.090594428117439E-005        1.275882533925475E-007        2.220821508127569E-
012        1.611800391932045E-019       TIME =  0.51100000E-04 DT =  0.25600000E-04 SUM OF SQUARES =  0.16118004E-18
 U-FRACTION IN SYSTEM:  C = .0186733111785181  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    0 seconds


output ignored...



... output resumed

  CPU time used in timestep                    1 seconds
 1.041680260932563E-005        1.044882763923012E-005        2.674505246573720E-011        6.870659146256508E-
017       TIME =  0.19801409     DT =  0.25429002E-01 SUM OF SQUARES =  0.68706591E-16
 U-FRACTION IN SYSTEM:  C = .0186734961934036  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    1 seconds
 2.750911886267648E-005        2.755302229687276E-005        1.960583380456374E-010        2.118675333162608E-015        3.859697201540206E-
026       TIME =  0.22607048     DT =  0.28056387E-01 SUM OF SQUARES =  0.38596972E-25
 U-FRACTION IN SYSTEM:  C = .0186734961934041  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    1 seconds
 5.476254514334582E-005        5.481399792191551E-005        9.961828823810722E-010        3.090901447690774E-014        1.568808231454754E-
023       TIME =  0.25814941     DT =  0.32078937E-01 SUM OF SQUARES =  0.15688082E-22
 U-FRACTION IN SYSTEM:  C = .01867349619341  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    0 seconds
 1.037340039671143E-004        1.037913251929635E-004        5.850917451587556E-009        4.334007629790979E-013        1.607062125161847E-
021       TIME =  0.29683922     DT =  0.38689804E-01 SUM OF SQUARES =  0.16070621E-20
 U-FRACTION IN SYSTEM:  C = .0186734961934866  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    1 seconds
 1.750218760511170E-004        1.750799684339703E-004        2.677121614192444E-008        4.755031610811476E-012        1.228186568924781E-
019       TIME =  0.34683922     DT =  0.50000000E-01 SUM OF SQUARES =  0.12281866E-18
 U-FRACTION IN SYSTEM:  C = .0186734961943616  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    1 seconds
 1.655026934031139E-005        1.656587674570809E-005        2.354174427019946E-010        5.748241630297222E-015        2.866681598955606E-
024       TIME =  0.39683922     DT =  0.50000000E-01 SUM OF SQUARES =  0.28666816E-23
 U-FRACTION IN SYSTEM:  C = .0186734961943642  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    1 seconds
 2.721459416064997E-006        2.715794026107815E-006        1.265798785600308E-011        3.005751528023248E-
017       TIME =  0.44683922     DT =  0.50000000E-01 SUM OF SQUARES =  0.30057515E-16
 U-FRACTION IN SYSTEM:  C = .0186734961806575  FE = 1
```

```
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    0 seconds
 2.924257073550977E-005        2.922561803227903E-005        1.420221635556956E-009        5.383694526367622E-014        1.053517999033209E-
022       TIME =  0.49683922     DT =  0.50000000E-01 SUM OF SQUARES =  0.10535180E-21
 U-FRACTION IN SYSTEM:  C = .0186734961806317  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    1 seconds
 1.311639930578495E-002        1.311509713869623E-002        1.933611102012263E-005        2.528801921586462E-008        6.842159294738176E-
014        9.431797172291871E-023       TIME =  0.50000000     DT =  0.31607821E-02 SUM OF SQUARES =  0.94317972E-22
 U-FRACTION IN SYSTEM:  C = .0186734961806332  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   0.45184716E-01
 DELETING TIME-RECORD FOR TIME   0.64717392E-01
 DELETING TIME-RECORD FOR TIME   0.84711978E-01
 DELETING TIME-RECORD FOR TIME   0.10530467
 DELETING TIME-RECORD FOR TIME   0.12664930
 DELETING TIME-RECORD FOR TIME   0.14896624
 DELETING TIME-RECORD FOR TIME   0.17258509
 DELETING TIME-RECORD FOR TIME   0.19801409
 DELETING TIME-RECORD FOR TIME   0.22607048
 DELETING TIME-RECORD FOR TIME   0.25814941
 DELETING TIME-RECORD FOR TIME   0.29683922
 DELETING TIME-RECORD FOR TIME   0.34683922
 DELETING TIME-RECORD FOR TIME   0.39683922
 DELETING TIME-RECORD FOR TIME   0.44683922

 KEEPING TIME-RECORD FOR TIME   0.49683922
 AND FOR TIME                   0.50000000
 WORKSPACE RECLAIMED

 TIMESTEP AT    0.500000000     SELECTED

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

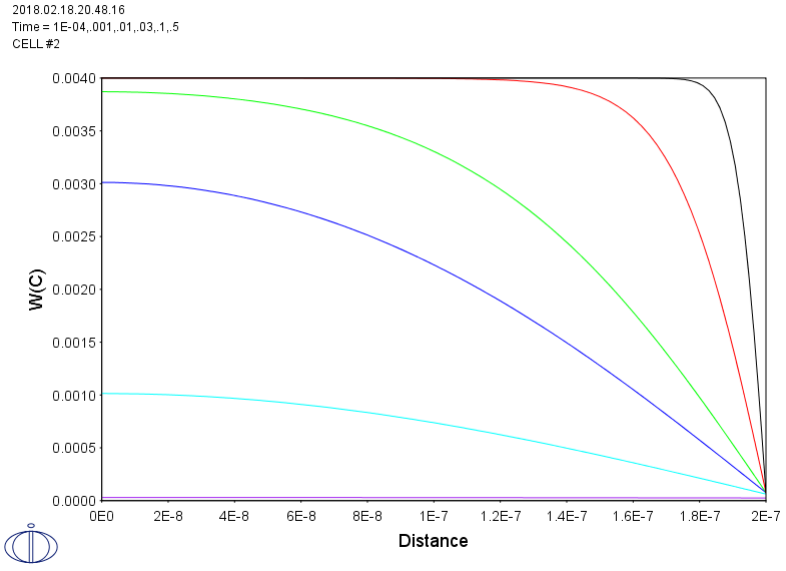
exc1-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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: plo
```

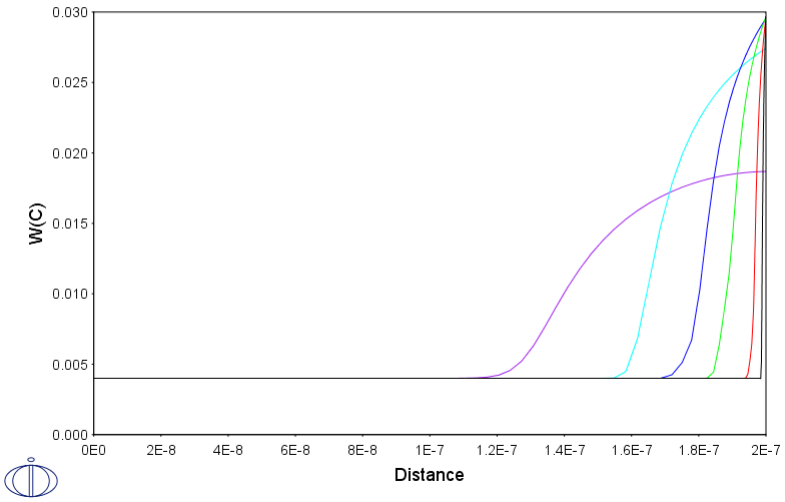
Figure c1.1




```
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: plo
```

Figure c1.2

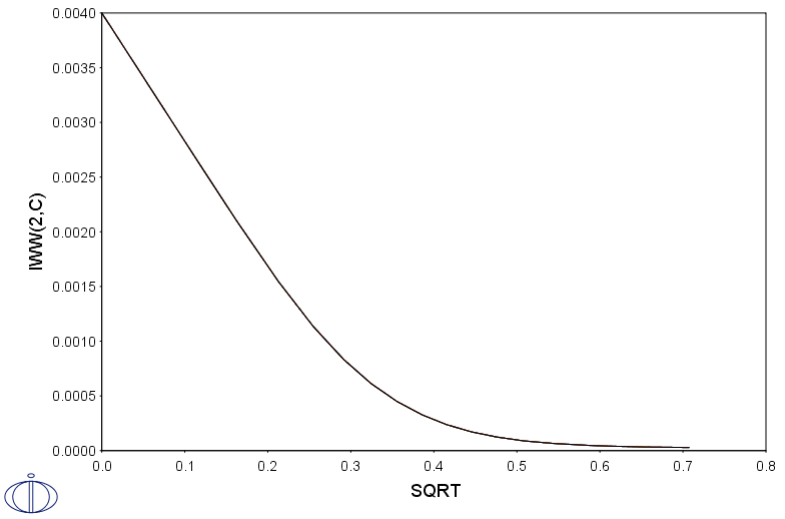
2018.02.18.20.48.16
Time = 1E-04,.001,.01,.03,.1,.5
CELL #1




```
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: plo
```

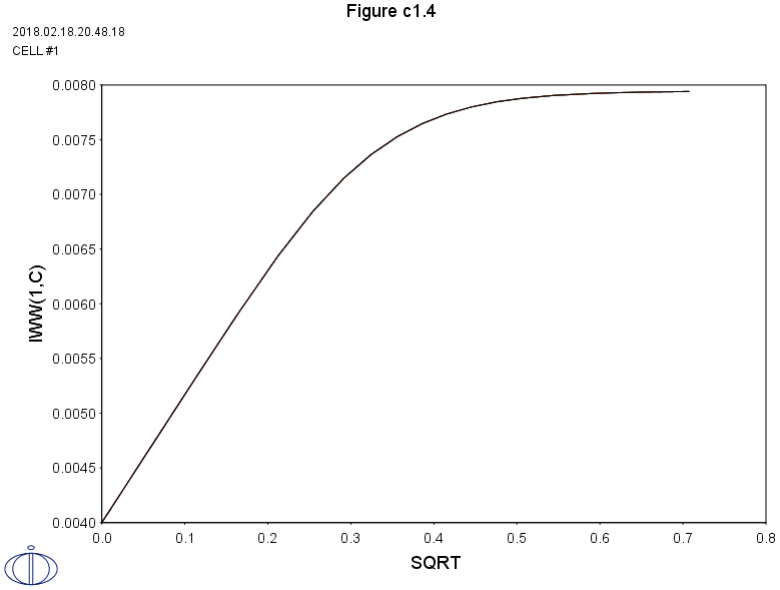
Figure c1.3

2018.02.18.20.48.17
CELL #2



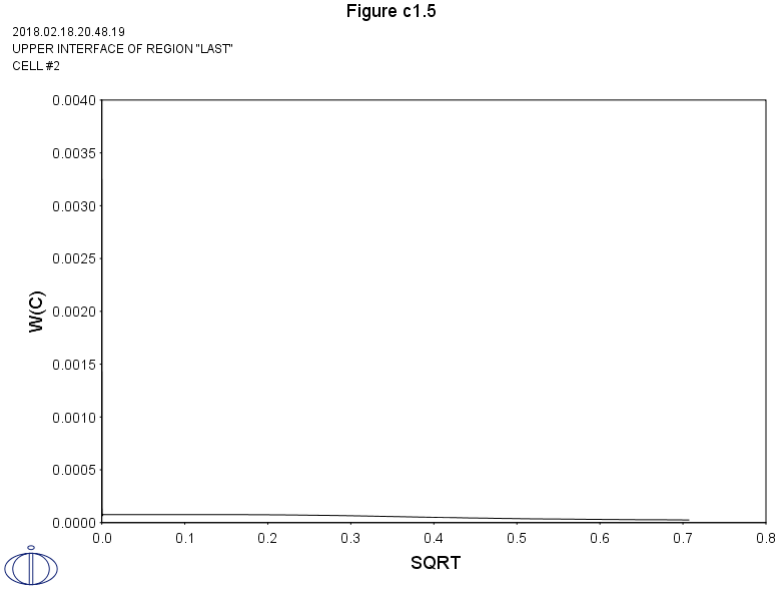

```
POST-2:
POST-2:
POST-2:
POST-2:@?<_hit_return_to_continue_>
POST-2:
POST-2: @@
POST-2: @@ DO THE SAME THING FOR THE AUSTENITE
POST-2: @@
POST-2: sel-cell 1
 CELL    1 SELECTED
POST-1: s-d-a y iww(1,c)
POST-1: set-title Figure c1.4
POST-1: plo
```

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: plo
```

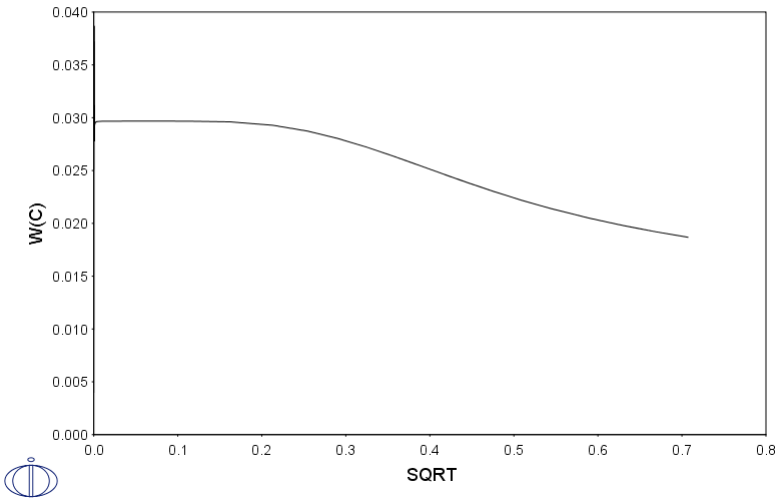
Figure c1.5




```
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: plo
```

Figure c1.6

2018.02.18.20.48.19
UPPER INTERFACE OF REGION "LAST"
CELL #1

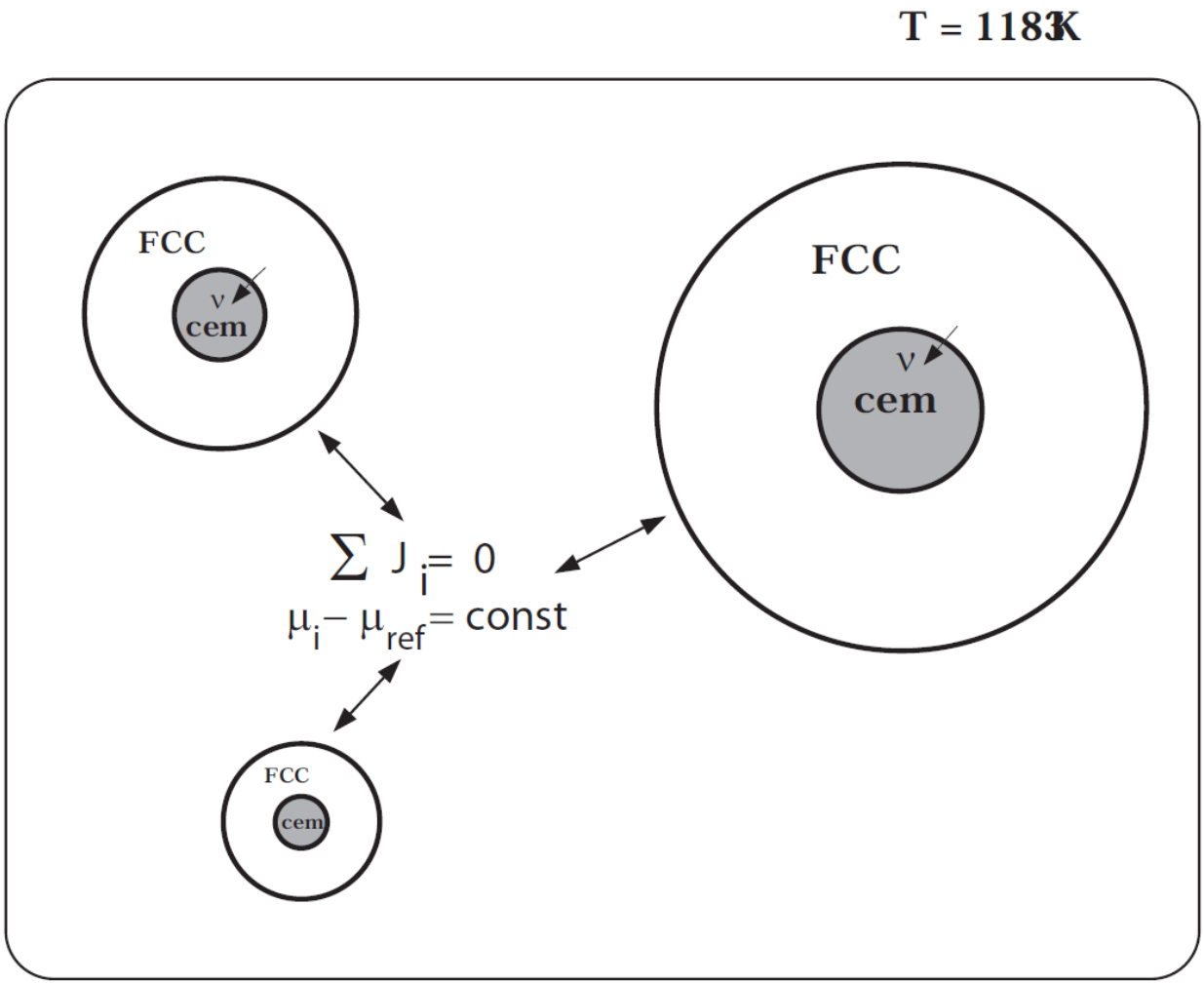



```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: set-inter
 --OK---
POST-1:
```

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

```
About Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri Feb 16 15:22:08 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exc2\setup.DCM" ?@@
 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. Höglund, B. Jönsson and J. Ågren:
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
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

 VA                     /-  DEFINED
 L12_FCC                B2_BCC                 DICTRA_FCC_A1
   REJECTED
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA
TDB_TCFE9: @@
TDB_TCFE9: switch fedemo
 Current database: Iron Demo Database v2.0

 VA                     /-  DEFINED
TDB_FEDEMO: def-sys fe cr c
 FE                     CR                     C
   DEFINED
TDB_FEDEMO: rej ph * all
 GAS:G                  LIQUID:L               BCC_A2
 CEMENTITE              CHI_A12                DIAMOND_FCC_A4
 FCC_A1                 GRAPHITE               HCP_A3
 KSI_CARBIDE            LAVES_PHASE_C14        M23C6
 M3C2                   M5C2                   M7C3
 SIGMA  REJECTED
TDB_FEDEMO: res ph fcc cementite
 FCC_A1                 CEMENTITE  RESTORED
TDB_FEDEMO: get
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'B.-J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
  'P. Villars and L.D. Calvert (1985). Pearson`s handbook of
      crystallographic data for intermetallic phases. Metals park, Ohio.
      American Society for Metals; Molar volumes'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'B. Hallstedt, D. Djurovic, J. von Appen, R. Dronskowski, A. Dick, F.
      Koermann, T. Hickel, J. Neugebauer, CALPHAD, 34, 129 -33(2010); Fe-C'
  'A.V. Khvan, B. Hallstedt, C. Broeckmann, CALPHAD, 46, 24 -33(2014); Cr-Fe
      -C'
  'J. Bratberg, Z. Metallkd., 96 (2005) 335-344; Fe-Cr-Mo-C'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'X.-G. Lu, M. Selleby, B. Sundman, CALPHAD, 29 (2005) 49-55; Fe P-T diagram'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, 2016; FCC Fe-Cr-C and C-Cr-Ni'
  'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
  'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270
      (1986); CR-FE'
 -OK-
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE MOBILITY DATA
TDB_FEDEMO: @@
TDB_FEDEMO: app mobfe2
 Current database: Steels/Fe-Alloys Mobility  v2.0
   TCS Steel Mobility Database Version 2.0 from 2011-12-09.

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

 List of references for assessed data

  'This parameter has not been assessed'
```

```
  'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'
  'B. Jonsson: Z. Metallkunde 85(1994)502-509; C diffusion in fcc Cr-Fe-Ni'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Fe diffusion fcc Cr-Fe'
  'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
      -Ni'
  'This parameter has been estimated'
 -OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR
APP: @@
APP: go d-m
 NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@  ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob t 0 1183; * n

DIC>
DIC> @@------------------------------------------------------------------------
DIC> @@ CELL NUMBER ONE
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/: AUTO
DIC>
DIC> @@
DIC> @@ THE SIZE OF THE FCC REGION CAN BE CALCULATED FROM A MASS BALANCE
DIC> @@ AFTER ESTIMATING THE INITIAL COMPOSITIONS IN THE TWO PHASES.
DIC> @@
DIC> enter-grid
REGION NAME : /AUS/: aus
WIDTH OF REGION /1/: 7.1832993E-7
TYPE /LINEAR/: AUTO
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 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
DIC> @@-----------------------------------------------------------------
DIC> create-new-cell
CELL DISTRIBUTION FACTOR /1/: 2
 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 AUTO
DIC-2> enter-grid aus  3.0785568E-7 AUTO
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 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
DIC-2> @@-----------------------------------------------------------------
DIC-2> create-new-cell
CELL DISTRIBUTION FACTOR /1/: 3
 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 AUTO
DIC-3> enter-grid aus   5.3926054E-7 AUTO
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 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
DIC-3> @@-----------------------------------------------------------------
DIC-3>
DIC-3> @@
DIC-3> @@ SET TO A SPHERICAL GEOMETRY
DIC-3> @@
DIC-3> enter-geo 2
DIC-3>
DIC-3> @s-n-l
's-n-l' is not recognized as an internal or external command,
operable program or batch file.
DIC-3> @
DIC-3> @
DIC-3> @
DIC-3> @
DIC-3> @
DIC-3> @
DIC-3> @
DIC-3> @1E-3
'1E-3' is not recognized as an internal or external command,
operable program or batch file.
DIC-3>
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>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exc2\run.DCM"DIC-3>
DIC-3>
DIC-3> @@ exc2_run.DCM
DIC-3>
DIC-3> @@
DIC-3> @@ READ THE SET UP FROM FILE AND START THE SIMULATION
DIC-3> @@
DIC-3>
DIC-3> go d-m
 TIME STEP AT TIME  0.00000E+00
DIC-3> read exc2
 OK
DIC> sim yes
 Region: CARB
 single geometric dense at  0.70000E-06
 0.84611       96
 Region: AUS
 double geometric
 dense at outer boundaries, coarse at  0.35916E-06
lower part   1.0486       22
upper part  0.95367       22
 Region: CARB
 single geometric dense at  0.30000E-06
 0.86023       95
 Region: AUS
 double geometric
 dense at outer boundaries, coarse at  0.15393E-06
lower part   1.0067       22
upper part  0.99334       22
 Region: CARB
 single geometric dense at  0.52550E-06
 0.85084       96
 Region: AUS
 double geometric
 dense at outer boundaries, coarse at  0.26963E-06
lower part   1.0222       22
upper part  0.97828       22
  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
89434.0516915

  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
89434.0516915

  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
89434.0516915

 U-FRACTION IN SYSTEM:  C = .0406910187346776  CR = .0214382352304608
                        FE = .978561764900046
 TOTAL SIZE OF SYSTEM:  2.90023192349E-17 [m^3]
 U-FRACTION IN SYSTEM:  C = .0406910187346776  CR = .0214382352304608
                        FE = .978561764900046
 TOTAL SIZE OF SYSTEM:  2.90023192349E-17 [m^3]
 0.549881621022645        0.549917064641365        0.549938978099241        0.549921828506971        0.549881463442405        0.549881396770026
002        3.584789099736 41E-004        4.707896215169447E-005        1.368538548719131E-006        9.616968067506565E-
006        1.052143984005091E-006        9.010518126001122E-007        8.267746915912355E-007        8.321573838165257E-
007        8.024773009998710E-007        8.036126148068533E-007        7.984608479813919E-007        8.050009081216152E-
007        8.000667876669771E-007        7.984620140526977E-007        7.984782243626459E-007        8.003049929700262E-
007        8.048504050500911E-007        8.013658009077427E-007        7.869048260291603E-007        7.845298608518584E-
007        7.828052493081366E-007        7.795100507715870E-007        7.765420050192562E-007        7.772966895125170E-
007        7.719168100439892E-007        7.729228850442111E-007        7.669031199779128E-007        7.600329286473438E-
007        7.604611933884462E-007        7.600341337121120E-007        7.600503467478045E-007        7.525562577038541E-
007        7.561970193980981E-007        7.540768031118053E-007        7.401555177117967E-007        7.236762721884894E-
007        7.065875831403977E-007        6.785553058049482E-007        6.488672003692035E-007        6.495030277159912E-
007        5.991860198842355E-007        6.000961686264694E-007        5.458302380562768E-007        4.547576422565395E-
007        4.549588595027279E-007        4.547588559509569E-007        4.547750687468223E-007        3.591727483757561E-
007        3.588608067310060E-007        3.590808326814583E-007        5.291229251797131E-007

output ignored...



... output resumed

  CPU time used in timestep                    7 seconds
 5.620581424891137E-003        5.620581564388538E-003        5.620581508537940E-003        5.620540923880623E-003        5.620520505914677E-
003        5.620326414263263E-003        5.619702649084130E-003        7.742050606249825E-005        1.323439267523031E-
007        5.817710003152266E-011        5.515829749944256E-015        2.174892940297279E-
018       TIME =    7809.6319     DT =    1000.0000     SUM OF SQUARES =  0.21748929E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.11246961E-10 AND  -0.11246961E-10
 POSITION OF INTERFACE CARB / AUS IS   0.41766602E-06
 CELL # 3 VELOCITY AT INTERFACE # 2 IS  -0.12055364E-10 AND  -0.12055364E-10
 POSITION OF INTERFACE CARB / AUS IS   0.24051287E-06
 U-FRACTION IN SYSTEM:  C = .0407685929205705  CR = .0215929494072436
                        FE = .978407050723264
 TOTAL SIZE OF SYSTEM:  2.90023192349E-17 [m^3]
  2  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUS

  CPU time used in timestep                    7 seconds
 7.934031240604640E-003        7.934031328174185E-003        7.934031262086262E-003        7.933988781095068E-003        7.933969458942978E-
003        7.933720822871469E-003        7.932958999150535E-003        1.064628757143287E-004        1.769185728713574E-
007        6.623928274324932E-011        8.284615497018037E-015        3.045150403943920E-
018       TIME =    8809.6319     DT =    1000.0000     SUM OF SQUARES =  0.30451504E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.10004228E-10 AND  -0.10004228E-10
 POSITION OF INTERFACE CARB / AUS IS   0.40766180E-06
 CELL # 3 VELOCITY AT INTERFACE # 2 IS  -0.11461628E-10 AND  -0.11461628E-10
 POSITION OF INTERFACE CARB / AUS IS   0.22905124E-06
 U-FRACTION IN SYSTEM:  C = .0407686429154155  CR = .0215927495127581
                        FE = .978407250617749
 TOTAL SIZE OF SYSTEM:  2.90023192349E-17 [m^3]
  CPU time used in timestep                    7 seconds
 1.006113374931269E-002        1.006113380991831E-002        1.006113374177700E-002        1.006109483355299E-002        1.006107935045509E-
002        1.006077875322448E-002        1.005989666807813E-002        1.098011320655540E-004        2.151159140861997E-
007        1.046557591121068E-010        1.820497473457117E-014        5.159997584024858E-
```

```
018       TIME =   9809.6319     DT =   1000.0000     SUM OF SQUARES =  0.51599976E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.90230963E-11 AND  -0.90230963E-11
 POSITION OF INTERFACE CARB / AUS IS   0.39863870E-06
 CELL # 3 VELOCITY AT INTERFACE # 2 IS  -0.11230209E-10 AND  -0.11230209E-10
 POSITION OF INTERFACE CARB / AUS IS   0.21782103E-06
 U-FRACTION IN SYSTEM:  C = .0407686754390633  CR = .021592605907101
                        FE = .978407394223406
 TOTAL SIZE OF SYSTEM:  2.90023192349E-17 [m^3]
  CPU time used in timestep                    6 seconds
 1.779068765597569E-003        1.779068879167698E-003        1.779068996862769E-003        1.779006723877378E-003        1.778982022365881E-
003        1.778992665887361E-003        1.778953539242408E-003        4.689999101035954E-004        1.299753080877434E-
005        1.326390437922909E-008        2.069343359129675E-012        1.247555139274113E-
016       TIME =   10000.000     DT =   190.36805     SUM OF SQUARES =  0.12475551E-15
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.74915641E-11 AND  -0.74915641E-11
 POSITION OF INTERFACE CARB / AUS IS   0.39721255E-06
 CELL # 3 VELOCITY AT INTERFACE # 2 IS  -0.86402264E-11 AND  -0.86402264E-11
 POSITION OF INTERFACE CARB / AUS IS   0.21617621E-06
 U-FRACTION IN SYSTEM:  C = .0407686958332996  CR = .021592572826188
                        FE = .978407427304319
 TOTAL SIZE OF SYSTEM:  2.90023192349E-17 [m^3]
 MUST SAVE WORKSPACE ON FILE
 WORKSPACE SAVED ON FILE
 RECLAIMING WORKSPACE
 DELETING TIME-RECORD FOR TIME    3160.9163
 DELETING TIME-RECORD FOR TIME    3467.4547
 DELETING TIME-RECORD FOR TIME    3467.4547
 DELETING TIME-RECORD FOR TIME    3467.4547
 DELETING TIME-RECORD FOR TIME    3467.4547
 DELETING TIME-RECORD FOR TIME    3467.4548
 DELETING TIME-RECORD FOR TIME    3467.4550
 DELETING TIME-RECORD FOR TIME    3467.4553
 DELETING TIME-RECORD FOR TIME    3467.4559
 DELETING TIME-RECORD FOR TIME    3467.4572
 DELETING TIME-RECORD FOR TIME    3467.4598
 DELETING TIME-RECORD FOR TIME    3467.4649
 DELETING TIME-RECORD FOR TIME    3467.4751
 DELETING TIME-RECORD FOR TIME    3467.4956
 DELETING TIME-RECORD FOR TIME    3467.5366
 DELETING TIME-RECORD FOR TIME    3467.6185
 DELETING TIME-RECORD FOR TIME    3467.7823
 DELETING TIME-RECORD FOR TIME    3468.1100
 DELETING TIME-RECORD FOR TIME    3468.7654
 DELETING TIME-RECORD FOR TIME    3470.0761
 DELETING TIME-RECORD FOR TIME    3472.6975
 DELETING TIME-RECORD FOR TIME    3477.9404
 DELETING TIME-RECORD FOR TIME    3488.4262
 DELETING TIME-RECORD FOR TIME    3509.3977
 DELETING TIME-RECORD FOR TIME    3551.3407
 DELETING TIME-RECORD FOR TIME    3635.2268
 DELETING TIME-RECORD FOR TIME    3802.9990
 DELETING TIME-RECORD FOR TIME    4138.5433
 DELETING TIME-RECORD FOR TIME    4809.6319
 DELETING TIME-RECORD FOR TIME    5809.6319
 DELETING TIME-RECORD FOR TIME    6809.6319
 DELETING TIME-RECORD FOR TIME    7809.6319
 DELETING TIME-RECORD FOR TIME    8809.6319

 KEEPING TIME-RECORD FOR TIME    9809.6319
 AND FOR TIME                    10000.000
 WORKSPACE RECLAIMED

 TIMESTEP AT     10000.0000     SELECTED

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

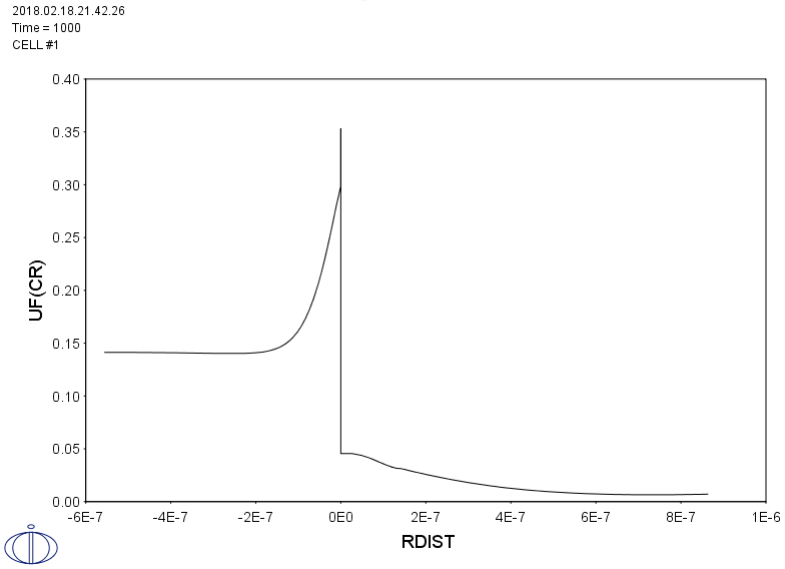
exc2-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exc2\plot.DCM"DIC>
DIC>
DIC> @@ exc2_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE c2
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  1.00000E+04
DIC> read exc2
 OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post

  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson

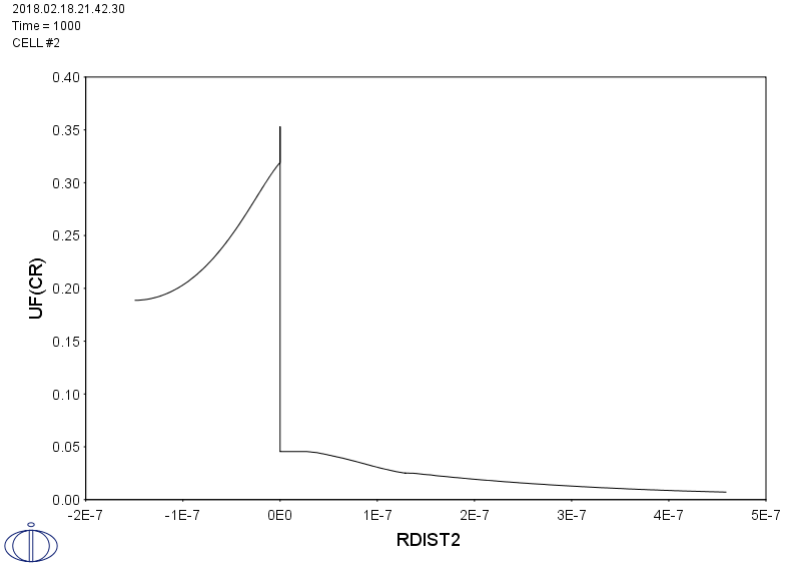
POST-1:
POST-1: @@
POST-1: @@ PLOT THE CHROMIUM CONCENTRATION PROFILES IN THE SAME WAY AS IN exb2
POST-1: @@ BUT NOW FOR EACH PARTICLE. LET US LOOK AT THE PROFILES AFTER 1000s.
POST-1: @@
POST-1:
POST-1: @@
POST-1: @@ FIRST CELL
POST-1: @@
POST-1: enter-symb
Function or table /FUNCTION/: func
NAME: rdist
FUNCTION: gd-poi(carb,u);
POST-1:
POST-1: s-d-a x rdist
POST-1:
POST-1: s-d-a y uf(cr)
POST-1:
POST-1: s-i-v
VARIABLE /TIME/: dist
DISTANCE : /GLOBAL/: glo
POST-1:
POST-1: s-p-c time 1000
POST-1:
POST-1: @@
POST-1: @@ SET THE TITLE ON THE PLOT
POST-1: @@
POST-1: set-title Figure C2.1
POST-1: plo
```

Figure C2.1



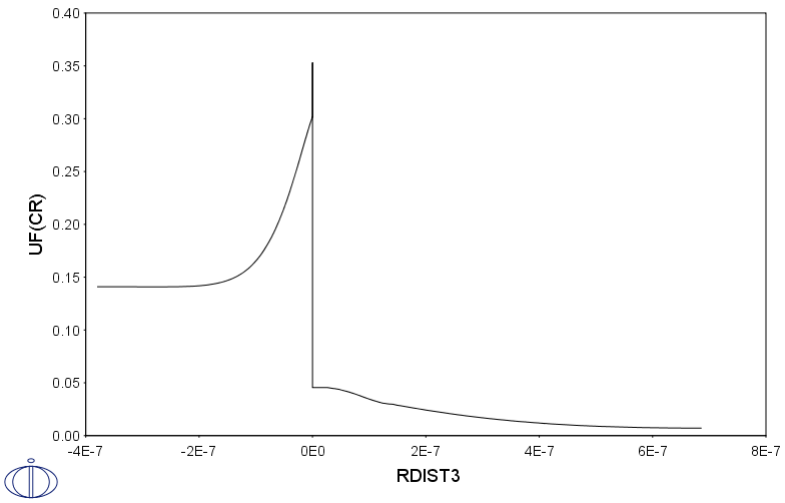

```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: @@
POST-1: @@ SELECT CELL 2
POST-1: @@
POST-1: select-cell
Number /NEXT/: 2
 CELL   2 SELECTED
POST-2:
POST-2: enter-symb
Function or table /FUNCTION/: func
NAME: rdist2
FUNCTION: gd-poi(carb,u);
POST-2:
POST-2: s-d-a x rdist2
POST-2:
POST-2: set-title Figure C2.2
POST-2: plo
```

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: plo
```

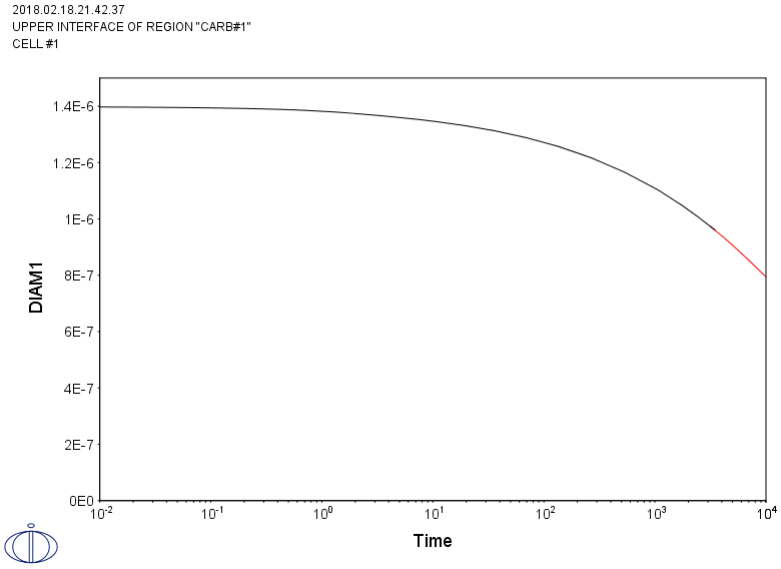
Figure C2.3




```
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:
```

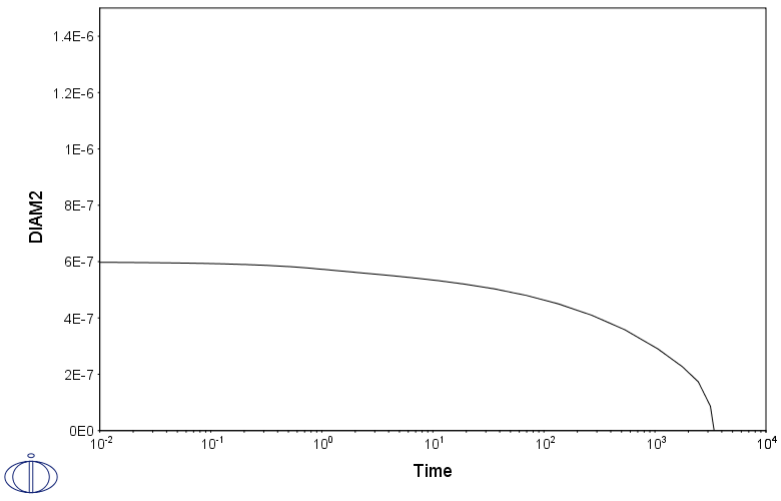
```
POST-1: s-p-c interf carb upp
POST-1:
POST-1: app n
POST-1: set-title Figure C2.4
POST-1: plo
```

Figure C2.4



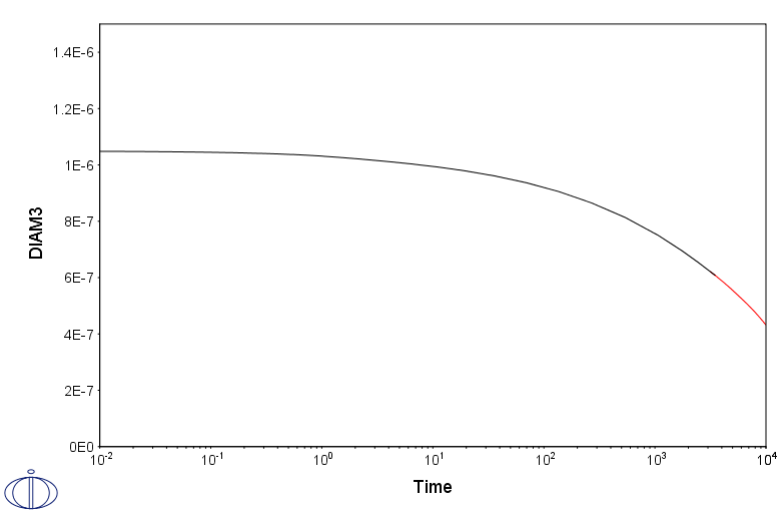

```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1:
POST-1: @@
POST-1: @@ SELECT CELL 2
POST-1: @@
POST-1: sel-cell 2
 CELL   2 SELECTED
POST-2:
POST-2: enter func diam2=2*poi(carb,u);
POST-2: s-d-a y diam2
POST-2: s-s-s y n 0 1.5e-6
POST-2:
POST-2: s-p-c interf carb upp
POST-2:
POST-2: set-title Figure C2.5
POST-2: plo
```

Figure C2.5



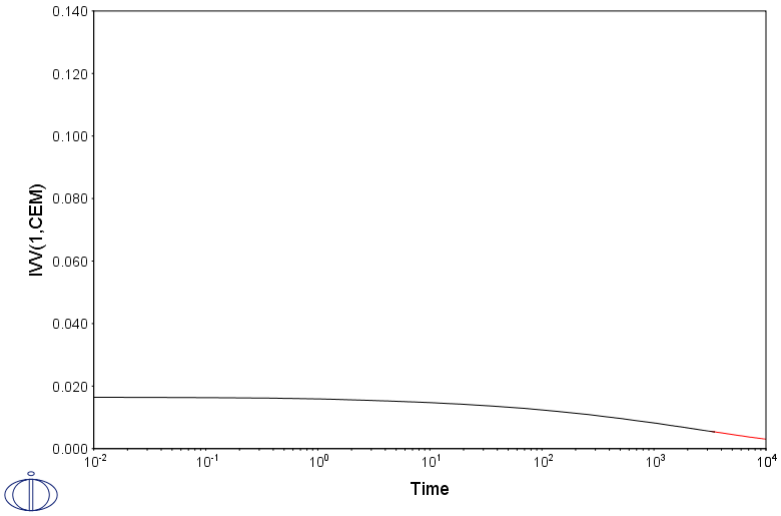

```
POST-2:
POST-2:
POST-2:
POST-2:
POST-2:@?<_hit_return_to_continue_>
POST-2:
POST-2: @@
POST-2: @@ SELECT CELL 3
POST-2: @@
POST-2: sel-cell 3
 CELL   3 SELECTED
POST-3:
POST-3: enter func diam3=2*poi(carb,u);
POST-3: s-d-a y diam3
POST-3: s-s-s y n 0 1.5e-6
POST-3:
POST-3: s-p-c interf carb upp
POST-3:
POST-3: set-title Figure C2.6
POST-3:
POST-3: plo
```

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: plo
```

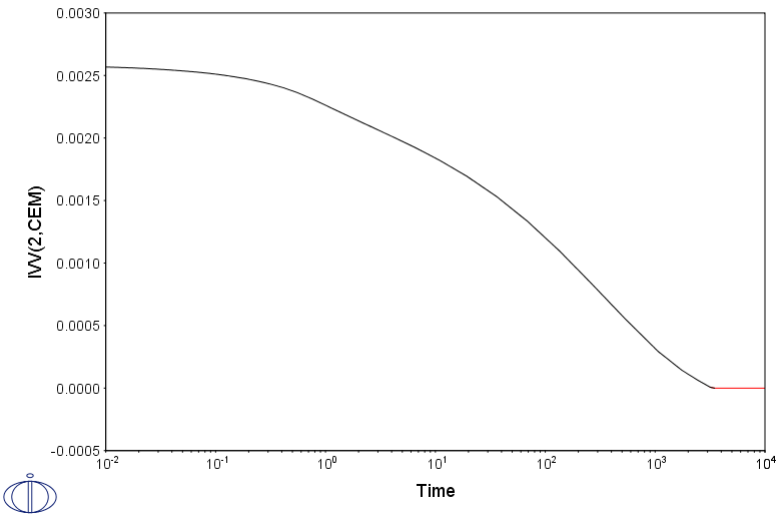
Figure C2.7




```
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: plo
```

Figure C2.8

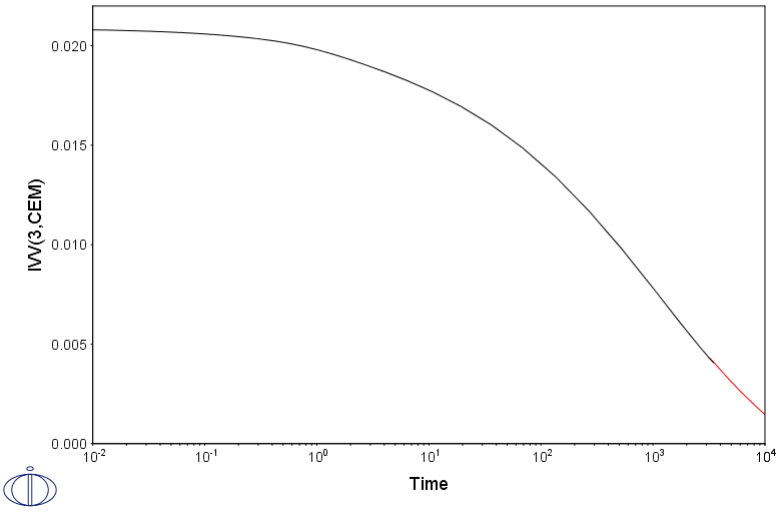
2018.02.18.21.43.00
CELL #3




```
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: plo
```

Figure C2.9

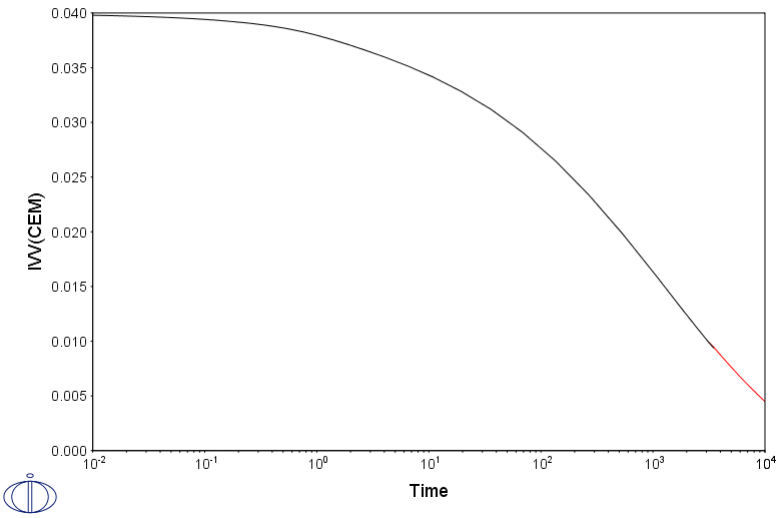
2018.02.18.21.43.10
CELL #3




```
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: plo
```

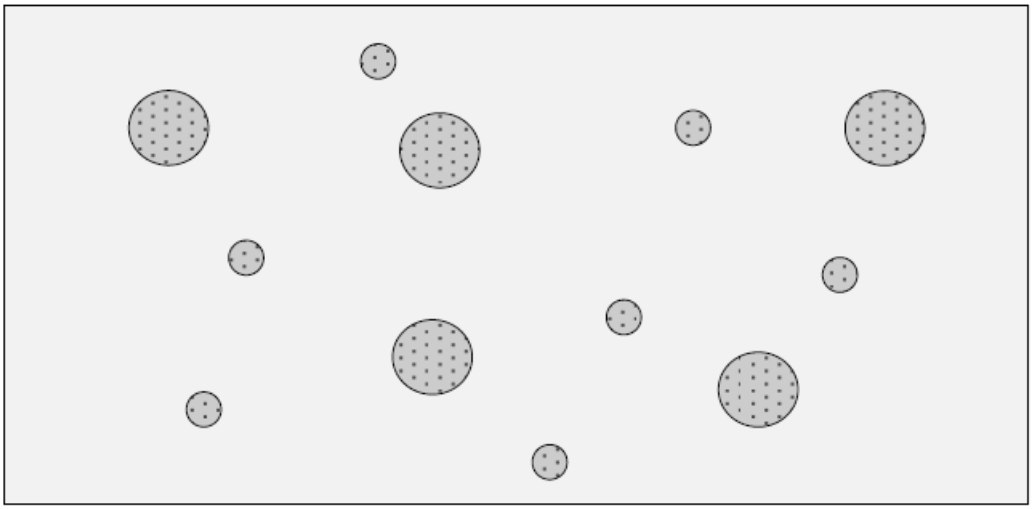
Figure C2.10

2018.02.18.21.43.19
CELL #3



POST-3:
POST-3:
POST-3:
POST-3:
POST-3:@?<_hit_return_to_continue_>
POST-3:
POST-3: set-inter
 --OK---
POST-3:

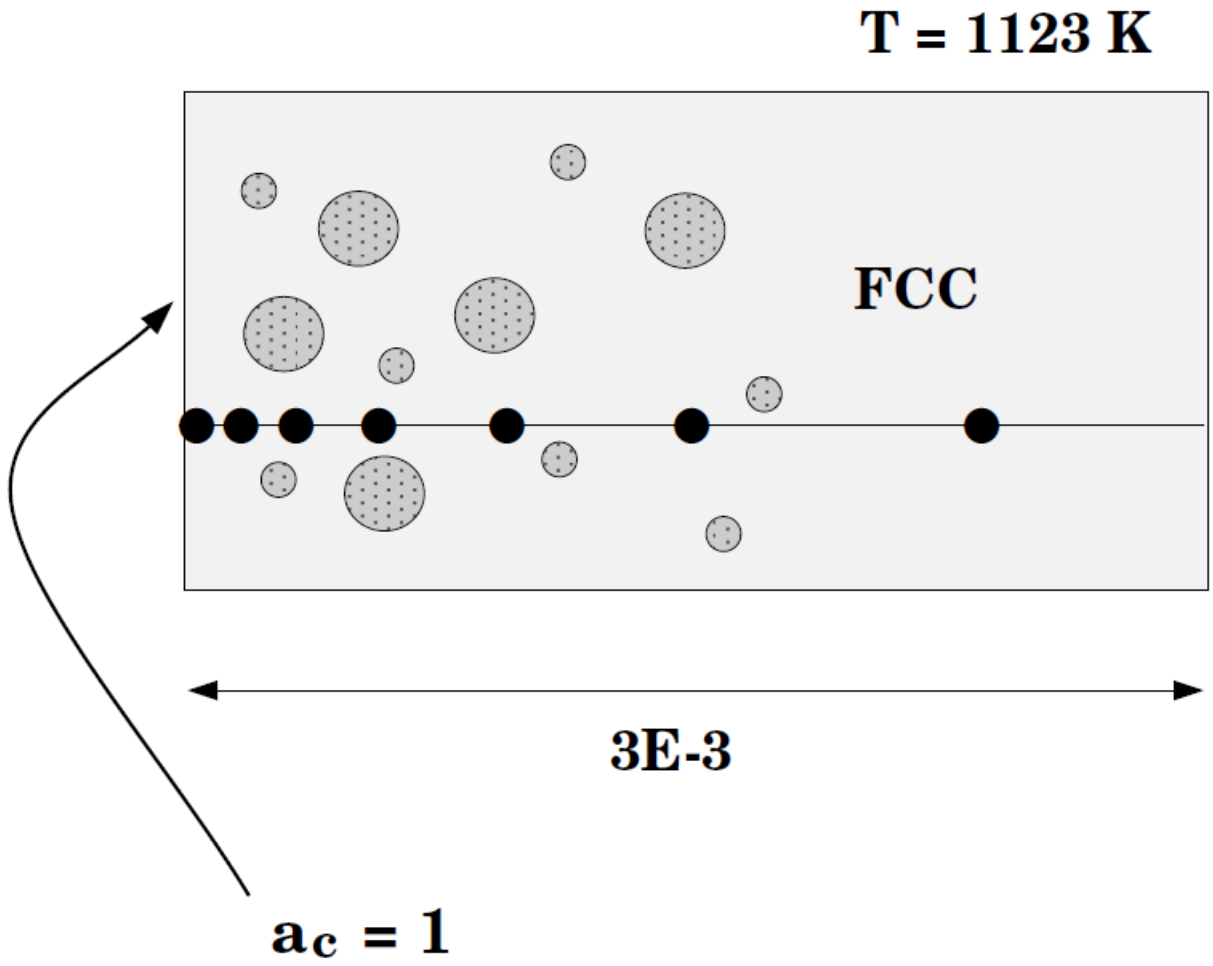
Diffusion in Dispersed Systems



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

```
About Linked: Fri Feb 16 15:22:08 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exd1a\setup.DCM" ?@@
 NO SUCH COMMAND, USE HELP
SYS: @@ Diffusion in dispersed systems.
SYS: @@ Carburization of Ni-25%Cr alloy: Dispersed system model
SYS: @@ This example is about carburization of a Ni-25Cr alloy.
SYS: @@ In this case the M3C2 and M7C3 carbides are entered as
SYS: @@ spheroid phases in a FCC matrix. This simulation can be run
SYS: @@ with either the DISPERSED SYSTEM MODEL or the HOMOGENIZATION MODEL.
SYS: @@ In this example the DISPERSED SYSTEM MODEL is used, which requires
SYS: @@ that the default HOMOGENIZATION MODEL is disabled.
SYS: @@ With the DISPERSED SYSTEM MODEL the command
SYS: @@ ENTER_LABYRINTH_FUNCTION is used to take into account the
SYS: @@ impeding effect of dispersed phases on long-range diffusion.
SYS: @@ For the HOMOGENIZATION MODEL the command
SYS: @@ ENTER_HOMOGENIZATION_FUNCTION should be used.
SYS: @@ This case is from A. Engström, L. Höglund and J. Ågren:
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
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

 VA                     /-  DEFINED
 L12_FCC                B2_BCC                 DICTRA_FCC_A1
   REJECTED
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ USE THE SSOL DATABASE FOR THERMODYNAMIC DATA
TDB_TCFE9: @@
TDB_TCFE9: sw ssol2
 Current database: SGTE Alloy Solutions Database v2.1

 VA  DEFINED
 B2_BCC                 L12_FCC                AL5FE4:
   REJECTED
 GAS:G                  AQUEOUS:A              WATER:A
   REJECTED
TDB_SSOL2: def-sys ni cr c
 NI                     CR                     C
   DEFINED
TDB_SSOL2: rej ph * all
 LIQUID:L               FCC_A1                 BCC_A2
 HCP_A3                 DIAMOND_A4             CHI_A12
 CBCC_A12               CUB_A13                SIGMA
 GRAPHITE               CEMENTITE              KSI_CARBIDE
 M23C6                  M7C3                   M3C2
 FE4N                   AL3NI2                 ALNI_B2
 CR3SI                  CRSI2  REJECTED
TDB_SSOL2: res ph fcc,m7c3,m3c2,grap
 FCC_A1                 M7C3                   M3C2
 GRAPHITE  RESTORED
TDB_SSOL2: get
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   'Byeong-Joo Lee, unpublished revision (1991); C-Cr-Fe-Ni'
   'Alan Dinsdale, SGTE Data for Pure Elements, NPL Report DMA(A)195
       September 1989'
   'Alan Dinsdale, SGTE Data for Pure Elements,
       Calphad Vol 15(1991) p 317-425,
       also in NPL Report DMA(A)195 Rev. August 1990'
   'A. Gabriel, C. Chatillon, I. Ansara, to be published in
       High Temp. Sci. (parameters listed in
       Calphad Vol 11 (1987) pp 203-218); C-NI'
   'A. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); CR-NI'
   'NPL, unpublished work (1989); C-Cr-Ni'
 -OK-
TDB_SSOL2:
TDB_SSOL2: @@
TDB_SSOL2: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE MOBILITY DATA
TDB_SSOL2: @@
TDB_SSOL2: app mob2
 Current database: Alloys Mobility  v2.7

 VA  DEFINED
 GAS:G  REJECTED
APP: def-sys ni c cr
 NI                     C                      CR
   DEFINED
APP: rej ph * all
 BCC_A2                 CEMENTITE              DIAMOND_A4
 FCC_A1                 M4N                    GRAPHITE
 HCP_A3                 KSI_CARBIDE            LIQUID:L
 M23C6                  M3C2                   M7C3
 SIGMA  REJECTED
APP: res ph fcc,m7c3,m3c2,grap
 FCC_A1                 M7C3                   M3C2
 GRAPHITE  RESTORED
APP: get
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....
```

```
 List of references for assessed data

   'This parameter has not been assessed'
   'B. Jonsson: Z. Metallkunde 85(1994)502-509;
      C diffusion in fcc Cr-Fe-Ni'
   'B. Jonsson: Scand. J. Metall. 24(1995)21-27;
      Cr and Fe diffusion fcc Cr-Fe'
   'B. Jonsson: Scand. J. Metall. 24(1995)21-27;
      Cr and Ni diffusion fcc Cr-Ni'
   'B. Jonsson: Scand. J. Metall. 24(1995)21-27;
      Ni self-diffusion'
 -OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR
APP: @@
APP: go d-m
 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
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
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 /NO/:
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 (0 -> 0.5 -> 1): /.5/:
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /NO/:
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>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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
 U-FRACTION IN SYSTEM:  C = 4.73399698964897E-06  CR = .273386070506604
                        NI = .726613929493396
 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 = 4.73399698964898E-06  CR = .273386070506604
                        NI = .726613929493396
 TOTAL SIZE OF SYSTEM:  .003 [m]
 TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = 7.37829265031503E-05  CR = .273386070506603
                        NI = .726613929493397
 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 = 1.07765273658403E-04  CR = .273386070506579
                        NI = .726613929493421
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.40010010     DT =  0.40000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = 1.29844980713891E-04  CR = .273386070500949
                        NI = .726613929499051
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   61.221707     DT =   60.821607     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = 1.67985911285438E-04  CR = .273386069358852
                        NI = .726613930641148
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   135.34814     DT =   74.126429     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = 2.08836403949596E-04  CR = .273386068335922
                        NI = .726613931664078
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   242.67634     DT =   107.32821     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = 2.57253556459827E-04  CR = .273386067317191
                        NI = .726613932682809
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1 seconds
 TIME =   408.61790     DT =   165.94156     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = 3.16829365327122E-04  CR = .273386066351575
                        NI = .726613933648425
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   677.99375     DT =   269.37585     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = 3.91398501422706E-04  CR = .273386065452222
                        NI = .726613934547778
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   1140.3108     DT =   462.31701     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = 4.86579533187512E-04  CR = .273386064383137
                        NI = .726613935616863
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   2003.0736     DT =   862.76284     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = 6.16999894543263E-04  CR = .273386063110096
                        NI = .726613936889904
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3701.3810     DT =   1698.3074     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = 8.03308317133761E-04  CR = .273386061634911
                        NI = .726613938365089
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   5501.3810     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = 9.81626963664688E-04  CR = .273386060762439
                        NI = .726613939237561
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   7301.3810     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0011473629203206  CR = .273386060181809
                        NI = .726613939818191
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1 seconds
 TIME =   9101.3810     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00130395620915009  CR = .273386059222275
                        NI = .726613940777725
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   10901.381     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00145171605713694  CR = .27338605759019
                        NI = .72661394240981
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   12701.381     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00159094848225919  CR = .273386055196014
```

```
                        NI = .726613944803986
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   14501.381     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00172523892272202  CR = .273386052870503
                        NI = .726613947129497
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   16281.441     DT =   1780.0601     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00185414605779616  CR = .273386050613403
                        NI = .726613949386597
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   17974.233     DT =   1692.7914     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00197453952520549  CR = .273386048403136
                        NI = .726613951596864
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1 seconds
 TIME =   19638.326     DT =   1664.0930     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00209171331269535  CR = .273386046243972
                        NI = .726613953756028
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   21359.693     DT =   1721.3670     SUM OF SQUARES =   0.0000000


output ignored...



... output resumed

  CPU time used in timestep                    0 seconds
 TIME =   3563759.7     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0315220916911913  CR = .273385942837795
                        NI = .726614057162205
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3565559.7     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0315300410032483  CR = .273385942809509
                        NI = .726614057190491
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1 seconds
 TIME =   3567359.7     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .031537988371072  CR = .273385942780993
                        NI = .726614057219007
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3569159.7     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0315459338120607  CR = .273385942752247
                        NI = .726614057247753
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3570959.7     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0315538773435958  CR = .273385942723271
                        NI = .726614057276729
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3572759.7     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0315618189830341  CR = .273385942694064
                        NI = .726614057305936
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3574559.7     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0315697587477025  CR = .273385942664627
                        NI = .726614057335374
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3576359.7     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0315776966548907  CR = .273385942634958
                        NI = .726614057365042
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1 seconds
 TIME =   3578159.7     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0315856327218464  CR = .273385942605058
                        NI = .726614057394942
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3579959.7     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0315935669657689  CR = .273385942574927
                        NI = .726614057425074
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3581759.7     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0316014994038048  CR = .273385942544563
                        NI = .726614057455437
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3583559.7     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0316094300530422  CR = .273385942513967
                        NI = .726614057486033
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3585359.7     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0316173589305068  CR = .273385942483139
                        NI = .726614057516861
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1 seconds
 TIME =   3587159.7     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0316252860531569  CR = .273385942452079
                        NI = .726614057547921
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3588959.7     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0316332114378796  CR = .273385942420785
                        NI = .726614057579215
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3590759.7     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0316411351014866  CR = .273385942389258
                        NI = .726614057610742
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3592559.7     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0316490570607107  CR = .273385942357497
                        NI = .726614057642503
```

```
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3594359.7     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0316569773322023  CR = .273385942325503
                        NI = .726614057674497
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1 seconds
 TIME =   3596159.7     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0316648959325256  CR = .273385942293274
                        NI = .726614057706726
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3597959.7     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0316728128781564  CR = .273385942260811
                        NI = .726614057739189
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3599759.7     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0316807281854782  CR = .273385942228113
                        NI = .726614057771886
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3600000.0     DT =   240.30748     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0316817891333221  CR = .273385942223672
                        NI = .726614057776328
 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    163559.69
 DELETING TIME-RECORD FOR TIME    341759.69
 DELETING TIME-RECORD FOR TIME    519959.69
 DELETING TIME-RECORD FOR TIME    698159.69
 DELETING TIME-RECORD FOR TIME    876359.69
 DELETING TIME-RECORD FOR TIME    1054559.7
 DELETING TIME-RECORD FOR TIME    1232759.7
 DELETING TIME-RECORD FOR TIME    1410959.7
 DELETING TIME-RECORD FOR TIME    1589159.7
 DELETING TIME-RECORD FOR TIME    1767359.7
 DELETING TIME-RECORD FOR TIME    1945559.7
 DELETING TIME-RECORD FOR TIME    2123759.7
 DELETING TIME-RECORD FOR TIME    2301959.7
 DELETING TIME-RECORD FOR TIME    2480159.7
 DELETING TIME-RECORD FOR TIME    2658359.7
 DELETING TIME-RECORD FOR TIME    2836559.7
 DELETING TIME-RECORD FOR TIME    3014759.7
 DELETING TIME-RECORD FOR TIME    3192959.7
 DELETING TIME-RECORD FOR TIME    3371159.7
 DELETING TIME-RECORD FOR TIME    3549359.7
 DELETING TIME-RECORD FOR TIME    3596159.7
 DELETING TIME-RECORD FOR TIME    3597959.7

 KEEPING TIME-RECORD FOR TIME    3599759.7
 AND FOR TIME                    3600000.0
 WORKSPACE RECLAIMED

 TIMESTEP AT     3600000.00     SELECTED

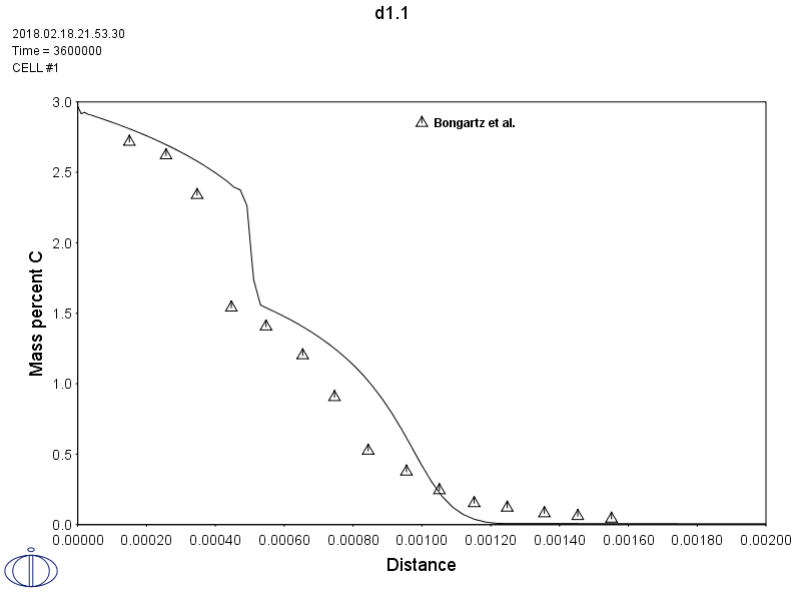
DIC>
DIC> set-inter
 --OK---
DIC>
```

exd1a-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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

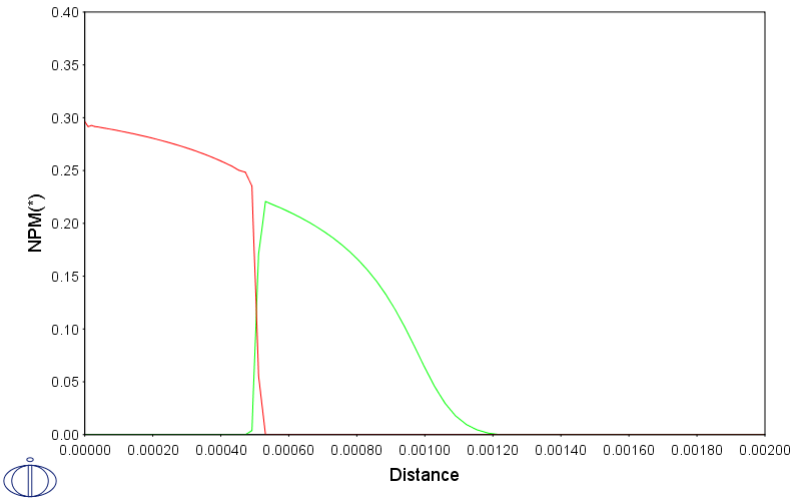
POST-1:
POST-1: @@
POST-1: @@ LOT THE TOTAL CARBON CONCENTRATION PROFILE
POST-1: @@
POST-1: s-d-a y w-p c
POST-1: s-d-a x distance global
  INFO: Distance is set as independent variable
POST-1: s-s-s x n 0 2e-3
POST-1: s-p-c time 3600000
POST-1:
POST-1: app y exd1.exp
PROLOGUE NUMBER: /0/: 1
DATASET 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
```

d1.2

2018.02.18.21.53.31
Time = 3600000
CELL #1

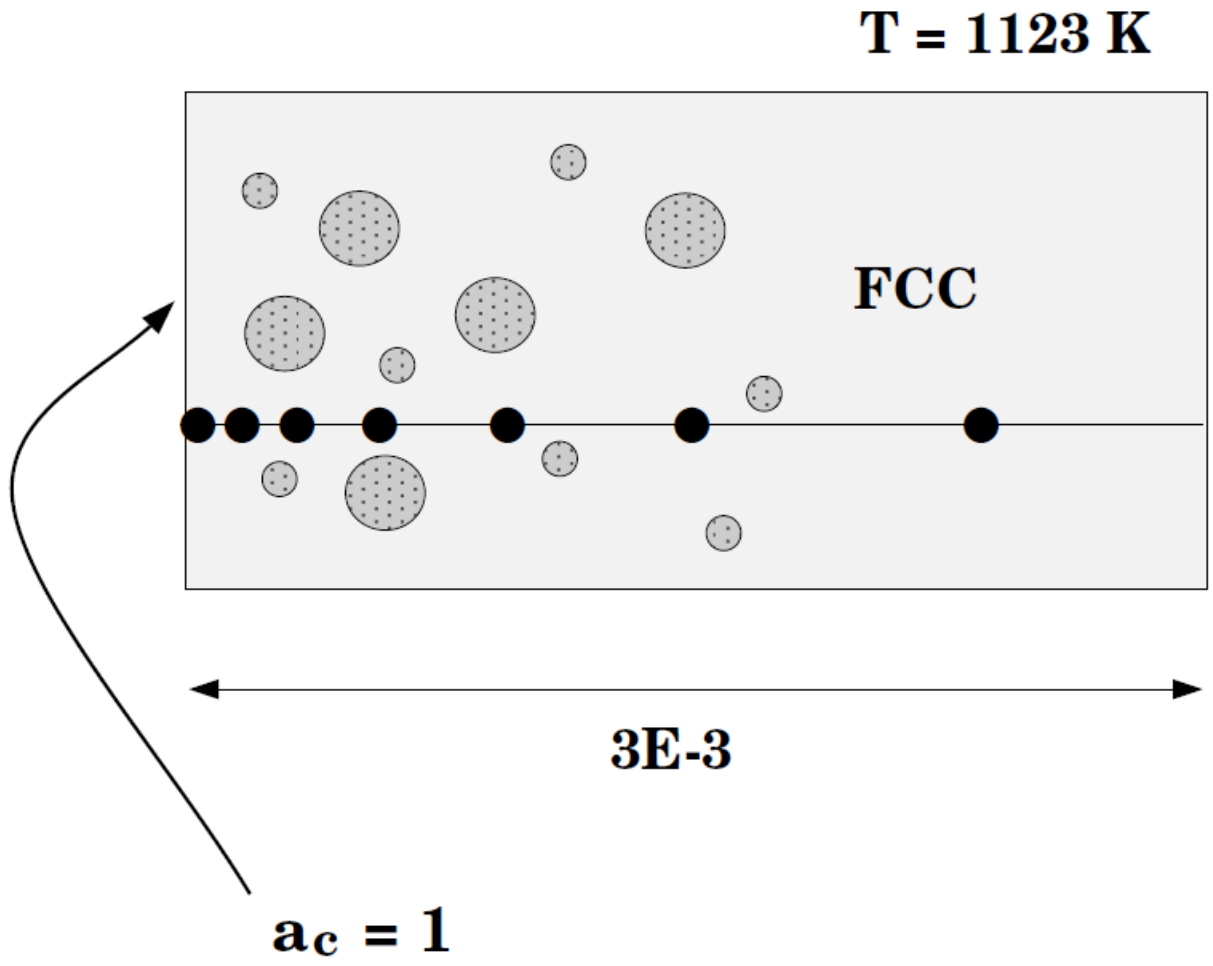



```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: set-inter
 --OK---
POST-1:
```

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

```
About Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 12987) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri Feb 16 15:22:08 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exd1b\setup.DCM"SYS: ?@@
 NO SUCH COMMAND, USE HELP
SYS: @@ Diffusion in dispersed systems.
SYS: @@ Carburization of Ni-25%Cr alloy: Homogenization model
SYS: @@ This example is about carburization of a Ni-25Cr alloy.
SYS: @@ In this case the M3C2 and M7C3 carbides are entered as
SYS: @@ spheroid phases in a FCC matrix. This case is from
SYS: @@ A. Engström, L. Höglund and J. Ågren: Metall.Trans. A,
SYS: @@ v.25A (1994), pp. 1127-1134.
SYS: @@ This simulation can be run with the DISPERSED SYSTEM MODEL or
SYS: @@ HOMOGENIZATION MODEL. The default HOMOGENIZATION MODEL is used
SYS: @@ and then ENTER_HOMOGENIZATION_FUNCTION should be used instead of
SYS: @@ ENTER_LABYRINTH_FUNCTION.
SYS: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exd1b_setup.DCM
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASE
SYS: @@
SYS: go da
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

 VA                       /-  DEFINED
 L12_FCC                  B2_BCC                   DICTRA_FCC_A1
   REJECTED
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ USE THE SSOL DATABASE FOR THERMODYNAMIC DATA
TDB_TCFE9: @@
TDB_TCFE9: sw ssol2
 Current database: SGTE Alloy Solutions Database v2.1

 VA  DEFINED
 B2_BCC                   L12_FCC                  AL5FE4:
   REJECTED
 GAS:G                    AQUEOUS:A                WATER:A
   REJECTED
TDB_SSOL2: def-sys ni cr c
 NI                       CR                       C
   DEFINED
TDB_SSOL2: rej ph * all
 LIQUID:L                 FCC_A1                   BCC_A2
 HCP_A3                   DIAMOND_A4               CHI_A12
 CBCC_A12                 CUB_A13                  SIGMA
 GRAPHITE                 CEMENTITE                KSI_CARBIDE
 M23C6                    M7C3                     M3C2
 FE4N                     AL3NI2                   ALNI_B2
 CR3SI                    CRSI2  REJECTED
TDB_SSOL2: res ph fcc,m7c3,m3c2,grap
 FCC_A1                   M7C3                     M3C2
 GRAPHITE  RESTORED
TDB_SSOL2: get
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   'Byeong-Joo Lee, unpublished revision (1991); C-Cr-Fe-Ni'
   'Alan Dinsdale, SGTE Data for Pure Elements, NPL Report DMA(A)195
       September 1989'
   'Alan Dinsdale, SGTE Data for Pure Elements,
       Calphad Vol 15(1991) p 317-425,
       also in NPL Report DMA(A)195 Rev. August 1990'
   'A. Gabriel, C. Chatillon, I. Ansara, to be published in
       High Temp. Sci. (parameters listed in
       Calphad Vol 11 (1987) pp 203-218); C-NI'
   'A. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); CR-NI'
   'NPL, unpublished work (1989); C-Cr-Ni'
 -OK-
TDB_SSOL2:
TDB_SSOL2: @@
TDB_SSOL2: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE MOBILITY DATA
TDB_SSOL2: @@
TDB_SSOL2: app mob2
 Current database: Alloys Mobility  v2.7

 VA  DEFINED
 GAS:G  REJECTED
APP: def-sys ni c cr
 NI                       C                        CR
   DEFINED
APP: rej ph * all
 BCC_A2                   CEMENTITE                DIAMOND_A4
 FCC_A1                   M4N                      GRAPHITE
 HCP_A3                   KSI_CARBIDE              LIQUID:L
 M23C6                    M3C2                     M7C3
 SIGMA  REJECTED
APP: res ph fcc,m7c3,m3c2,grap
 FCC_A1                   M7C3                     M3C2
 GRAPHITE  RESTORED
APP: get
 ELEMENTS .....
 SPECIES ......
 PHASES .......
```

```
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   'This parameter has not been assessed'
   'B. Jonsson: Z. Metallkunde 85(1994)502-509;
      C diffusion in fcc Cr-Fe-Ni'
   'B. Jonsson: Scand. J. Metall. 24(1995)21-27;
      Cr and Fe diffusion fcc Cr-Fe'
   'B. Jonsson: Scand. J. Metall. 24(1995)21-27;
      Cr and Ni diffusion fcc Cr-Ni'
   'B. Jonsson: Scand. J. Metall. 24(1995)21-27;
      Ni self-diffusion'
 -OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR
APP: @@
APP: go d-m
 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
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
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 /NO/:
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 (0 -> 0.5 -> 1): /.5/:
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /NO/:
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>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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
 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)
 Saving results
 ----------------------------------
  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
 Stage 1
 Stage 2
 Stage 3
 Moles of elements / mole fractions in system:
C    0.14201992E-07 /   0.47339748E-05
CR   0.82015821E-03 /   0.27338478
NI   0.21798418E-02 /   0.72661049

Time-step converged t0=   0.0000000     dt=  0.10000000E-06
 ----------------------------------
 Saving results
 ----------------------------------
Starting time-step t0=  0.10000000E-06 dt=  0.20000000E-06
 Stage 1
 Stage 2
 Stage 3
 Moles of elements / mole fractions in system:
C    0.14201993E-07 /   0.47339753E-05
CR   0.82015821E-03 /   0.27338478
NI   0.21798418E-02 /   0.72661049

Time-step converged t0=  0.10000000E-06 dt=  0.20000000E-06
 ----------------------------------
Starting time-step t0=  0.30000000E-06 dt=  0.40000000E-06
 Stage 1
 Evaluating Jacobian
Iteration #   1 sum residual **2:   0.85928988E-03
 Stage 2
 Stage 3
 Moles of elements / mole fractions in system:
C    0.14201996E-07 /   0.47339762E-05
CR   0.82015821E-03 /   0.27338478
NI   0.21798418E-02 /   0.72661049

Time-step converged t0=  0.30000000E-06 dt=  0.40000000E-06
 ----------------------------------
Starting time-step t0=  0.70000000E-06 dt=  0.80000000E-06
 Stage 1
Iteration #   1 sum residual **2:   0.14356446E-03
 Stage 2
 Stage 3
 Moles of elements / mole fractions in system:
C    0.14202001E-07 /   0.47339780E-05
CR   0.82015821E-03 /   0.27338478
NI   0.21798418E-02 /   0.72661049

Time-step converged t0=  0.70000000E-06 dt=  0.80000000E-06
 ----------------------------------
Starting time-step t0=  0.15000000E-05 dt=  0.16000000E-05
 Stage 1
Iteration #   1 sum residual **2:   0.61865070E-04
 Stage 2
 Stage 3
 Moles of elements / mole fractions in system:
C    0.14202012E-07 /   0.47339817E-05
CR   0.82015821E-03 /   0.27338478
NI   0.21798418E-02 /   0.72661049

Time-step converged t0=  0.15000000E-05 dt=  0.16000000E-05
 ----------------------------------
Starting time-step t0=  0.31000000E-05 dt=  0.32000000E-05
 Stage 1
Iteration #   1 sum residual **2:   0.42610973E-04
 Stage 2
 Stage 3
 Moles of elements / mole fractions in system:
C    0.14202034E-07 /   0.47339891E-05
CR   0.82015821E-03 /   0.27338478
NI   0.21798418E-02 /   0.72661049

Time-step converged t0=  0.31000000E-05 dt=  0.32000000E-05
 ----------------------------------
Starting time-step t0=  0.63000000E-05 dt=  0.64000000E-05
 Stage 1
Iteration #   1 sum residual **2:   0.35739934E-04
 Stage 2
 Stage 3
 Moles of elements / mole fractions in system:
C    0.14202079E-07 /   0.47340038E-05
CR   0.82015821E-03 /   0.27338478
NI   0.21798418E-02 /   0.72661049
```

```
Time-step converged t0=  0.63000000E-05 dt=  0.64000000E-05
 ----------------------------------
Starting time-step t0=  0.12700000E-04 dt=  0.12800000E-04
 Stage 1
Iteration #   1 sum residual **2:   0.32808897E-04
 Stage 2
 Stage 3
 Moles of elements / mole fractions in system:
C    0.14202167E-07 /   0.47340332E-05
CR   0.82015821E-03 /   0.27338478
NI   0.21798418E-02 /   0.72661049

Time-step converged t0=  0.12700000E-04 dt=  0.12800000E-04
 ----------------------------------
Starting time-step t0=  0.25500000E-04 dt=  0.25600000E-04
 Stage 1
Iteration #   1 sum residual **2:   0.31463321E-04
 Stage 2
 Stage 3
 Moles of elements / mole fractions in system:
C    0.14202343E-07 /   0.47340920E-05
CR   0.82015821E-03 /   0.27338478
NI   0.21798418E-02 /   0.72661049


output ignored...



... output resumed

 DELETING TIME-RECORD FOR TIME    3092410.2
 DELETING TIME-RECORD FOR TIME    3096275.7
 DELETING TIME-RECORD FOR TIME    3100141.2
 DELETING TIME-RECORD FOR TIME    3104006.6
 DELETING TIME-RECORD FOR TIME    3107872.1
 DELETING TIME-RECORD FOR TIME    3111737.6
 DELETING TIME-RECORD FOR TIME    3115603.0
 DELETING TIME-RECORD FOR TIME    3119468.5
 DELETING TIME-RECORD FOR TIME    3123334.0
 DELETING TIME-RECORD FOR TIME    3127199.5
 DELETING TIME-RECORD FOR TIME    3131064.9
 DELETING TIME-RECORD FOR TIME    3134930.4
 DELETING TIME-RECORD FOR TIME    3138795.9
 DELETING TIME-RECORD FOR TIME    3142661.3
 DELETING TIME-RECORD FOR TIME    3146526.8
 DELETING TIME-RECORD FOR TIME    3150392.3
 DELETING TIME-RECORD FOR TIME    3154257.7
 DELETING TIME-RECORD FOR TIME    3158123.2
 DELETING TIME-RECORD FOR TIME    3161988.7
 DELETING TIME-RECORD FOR TIME    3165854.2
 DELETING TIME-RECORD FOR TIME    3169719.6
 DELETING TIME-RECORD FOR TIME    3173585.1
 DELETING TIME-RECORD FOR TIME    3177450.6
 DELETING TIME-RECORD FOR TIME    3181316.0
 DELETING TIME-RECORD FOR TIME    3185181.5
 DELETING TIME-RECORD FOR TIME    3189047.0
 DELETING TIME-RECORD FOR TIME    3192912.5
 DELETING TIME-RECORD FOR TIME    3196777.9
 DELETING TIME-RECORD FOR TIME    3200643.4
 DELETING TIME-RECORD FOR TIME    3204508.9
 DELETING TIME-RECORD FOR TIME    3208374.3
 DELETING TIME-RECORD FOR TIME    3212239.8
 DELETING TIME-RECORD FOR TIME    3216105.3
 DELETING TIME-RECORD FOR TIME    3219970.7
 DELETING TIME-RECORD FOR TIME    3223836.2
 DELETING TIME-RECORD FOR TIME    3227701.7
 DELETING TIME-RECORD FOR TIME    3231567.2
 DELETING TIME-RECORD FOR TIME    3235432.6
 DELETING TIME-RECORD FOR TIME    3239298.1
 DELETING TIME-RECORD FOR TIME    3243163.6
 DELETING TIME-RECORD FOR TIME    3247029.0
 DELETING TIME-RECORD FOR TIME    3250894.5
 DELETING TIME-RECORD FOR TIME    3254760.0
 DELETING TIME-RECORD FOR TIME    3258625.5
 DELETING TIME-RECORD FOR TIME    3262490.9
 DELETING TIME-RECORD FOR TIME    3266356.4
 DELETING TIME-RECORD FOR TIME    3270221.9
 DELETING TIME-RECORD FOR TIME    3274087.3
 DELETING TIME-RECORD FOR TIME    3277952.8
 DELETING TIME-RECORD FOR TIME    3281818.3
 DELETING TIME-RECORD FOR TIME    3285683.7
 DELETING TIME-RECORD FOR TIME    3289549.2
 DELETING TIME-RECORD FOR TIME    3293414.7
 DELETING TIME-RECORD FOR TIME    3297280.2
 DELETING TIME-RECORD FOR TIME    3301145.6
 DELETING TIME-RECORD FOR TIME    3305011.1
 DELETING TIME-RECORD FOR TIME    3308876.6
 DELETING TIME-RECORD FOR TIME    3312742.0
 DELETING TIME-RECORD FOR TIME    3316607.5
 DELETING TIME-RECORD FOR TIME    3320473.0
 DELETING TIME-RECORD FOR TIME    3324338.5
 DELETING TIME-RECORD FOR TIME    3328203.9
 DELETING TIME-RECORD FOR TIME    3332069.4
 DELETING TIME-RECORD FOR TIME    3335934.9
 DELETING TIME-RECORD FOR TIME    3339800.3
 DELETING TIME-RECORD FOR TIME    3343665.8
 DELETING TIME-RECORD FOR TIME    3347531.3
 DELETING TIME-RECORD FOR TIME    3351396.7
 DELETING TIME-RECORD FOR TIME    3355262.2
 DELETING TIME-RECORD FOR TIME    3359127.7
 DELETING TIME-RECORD FOR TIME    3362993.2
 DELETING TIME-RECORD FOR TIME    3366858.6
 DELETING TIME-RECORD FOR TIME    3370724.1
 DELETING TIME-RECORD FOR TIME    3374589.6
 DELETING TIME-RECORD FOR TIME    3378455.0
 DELETING TIME-RECORD FOR TIME    3382320.5
 DELETING TIME-RECORD FOR TIME    3386186.0
 DELETING TIME-RECORD FOR TIME    3390051.5
 DELETING TIME-RECORD FOR TIME    3393916.9
 DELETING TIME-RECORD FOR TIME    3397782.4
 DELETING TIME-RECORD FOR TIME    3401647.9
 DELETING TIME-RECORD FOR TIME    3405513.3
 DELETING TIME-RECORD FOR TIME    3409378.8
 DELETING TIME-RECORD FOR TIME    3413244.3
```

```
 DELETING TIME-RECORD FOR TIME    3417109.7
 DELETING TIME-RECORD FOR TIME    3420975.2
 DELETING TIME-RECORD FOR TIME    3424840.7
 DELETING TIME-RECORD FOR TIME    3428706.2
 DELETING TIME-RECORD FOR TIME    3432571.6
 DELETING TIME-RECORD FOR TIME    3436437.1
 DELETING TIME-RECORD FOR TIME    3440302.6
 DELETING TIME-RECORD FOR TIME    3444168.0
 DELETING TIME-RECORD FOR TIME    3448033.5
 DELETING TIME-RECORD FOR TIME    3451899.0
 DELETING TIME-RECORD FOR TIME    3455764.5
 DELETING TIME-RECORD FOR TIME    3459629.9
 DELETING TIME-RECORD FOR TIME    3463495.4
 DELETING TIME-RECORD FOR TIME    3467360.9
 DELETING TIME-RECORD FOR TIME    3471226.3
 DELETING TIME-RECORD FOR TIME    3475091.8
 DELETING TIME-RECORD FOR TIME    3478957.3
 DELETING TIME-RECORD FOR TIME    3482822.7
 DELETING TIME-RECORD FOR TIME    3486688.2
 DELETING TIME-RECORD FOR TIME    3490553.7
 DELETING TIME-RECORD FOR TIME    3494419.2
 DELETING TIME-RECORD FOR TIME    3498284.6
 DELETING TIME-RECORD FOR TIME    3502150.1
 DELETING TIME-RECORD FOR TIME    3506015.6
 DELETING TIME-RECORD FOR TIME    3509881.0
 DELETING TIME-RECORD FOR TIME    3513746.5
 DELETING TIME-RECORD FOR TIME    3517612.0
 DELETING TIME-RECORD FOR TIME    3521477.5
 DELETING TIME-RECORD FOR TIME    3525342.9
 DELETING TIME-RECORD FOR TIME    3529208.4
 DELETING TIME-RECORD FOR TIME    3533073.9
 DELETING TIME-RECORD FOR TIME    3536939.3
 DELETING TIME-RECORD FOR TIME    3540804.8
 DELETING TIME-RECORD FOR TIME    3544670.3
 DELETING TIME-RECORD FOR TIME    3548535.7
 DELETING TIME-RECORD FOR TIME    3552401.2
 DELETING TIME-RECORD FOR TIME    3556266.7
 DELETING TIME-RECORD FOR TIME    3560132.2
 DELETING TIME-RECORD FOR TIME    3563997.6
 DELETING TIME-RECORD FOR TIME    3567863.1
 DELETING TIME-RECORD FOR TIME    3571728.6
 DELETING TIME-RECORD FOR TIME    3575594.0
 DELETING TIME-RECORD FOR TIME    3579459.5
 DELETING TIME-RECORD FOR TIME    3583325.0
 DELETING TIME-RECORD FOR TIME    3587190.4
 DELETING TIME-RECORD FOR TIME    3591055.9
 DELETING TIME-RECORD FOR TIME    3594921.4

 KEEPING TIME-RECORD FOR TIME    3598786.9
 AND FOR TIME                    3600000.0
 WORKSPACE RECLAIMED
 -------------------------------------------------
 INTERPOLATION SCHEME USED THIS FRACTION OF
 THE ALLOCATED MEMORY:   0.817338868519136
 EFFICIENCY FACTOR:    92.8870231802691
 -------------------------------------------------
 DEALLOCATING
 -------------------------------------------------

 TIMESTEP AT     3600000.00     SELECTED

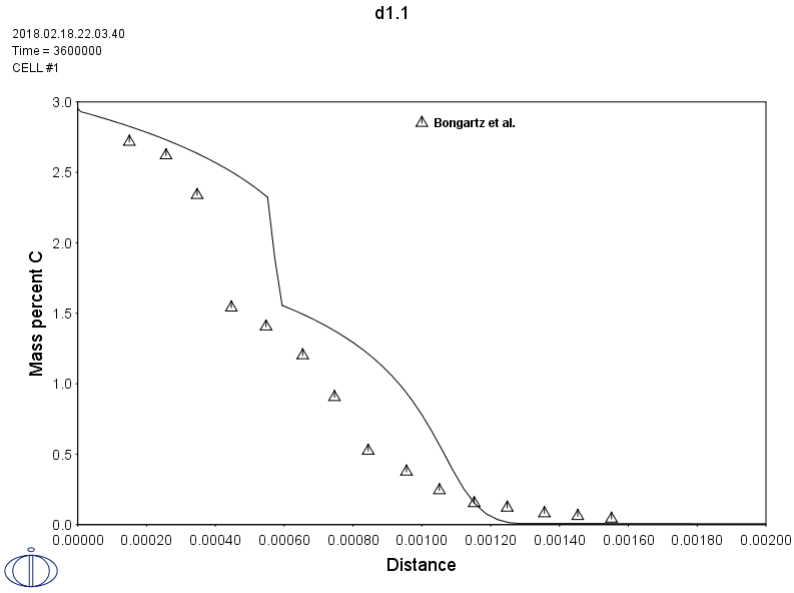
DIC>
DIC> set-inter
 --OK---
DIC>
```

exd1b-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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

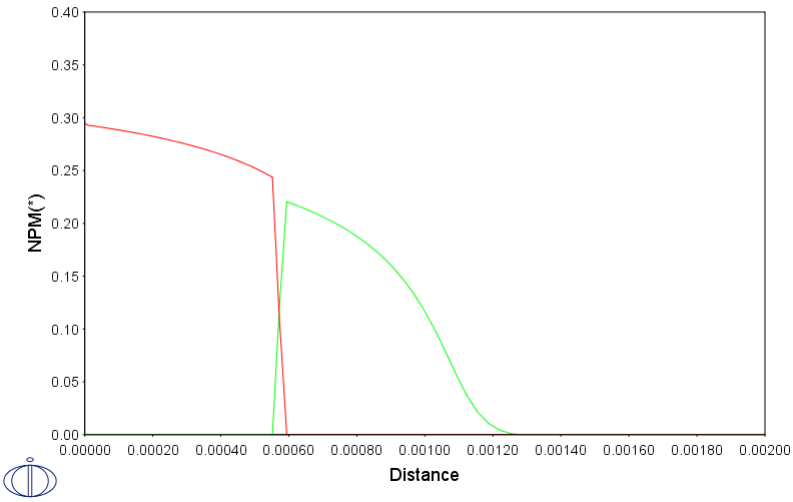
POST-1:
POST-1: @@
POST-1: @@ PLOT THE TOTAL CARBON CONCENTRATION PROFILE
POST-1: @@
POST-1: s-d-a y w-p c
POST-1: s-d-a x distance global
  INFO: Distance is set as independent variable
POST-1: s-s-s x n 0 2e-3
POST-1: s-p-c time 3600000
POST-1:
POST-1: app y exd1.exp
PROLOGUE NUMBER: /0/: 1
DATASET 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
```

d1.2

2018.02.18.22.03.46
Time = 3600000
CELL #1



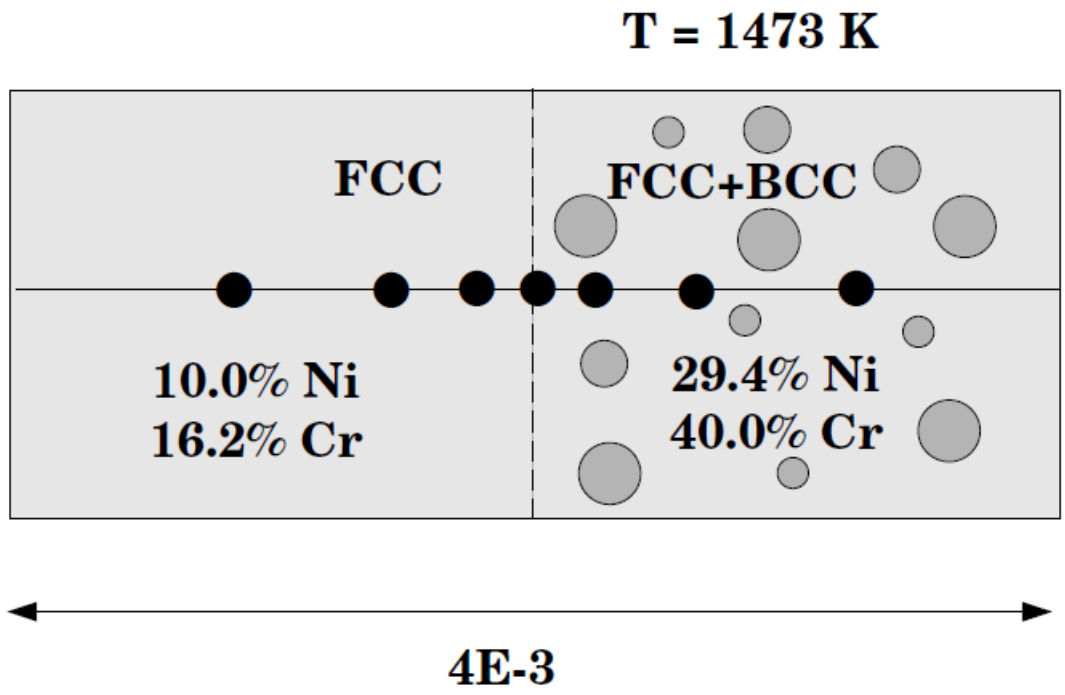

```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: set-inter
 --OK---
POST-1:
```

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

```
About License library version: 8.5.1.0017
 Linked: Fri Feb 16 15:22:08 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exd2a\setup.DCM"SYS: ?@@
 NO SUCH COMMAND, USE HELP
SYS: @@ Diffusion in dispersed systems.
SYS: @@ Diffusion couple of Fe-Cr-Ni alloys: Dispersed system model
SYS: @@ This example calculates the interdiffusion in a diffusion
SYS: @@ couple between a two-phase (FCC+BCC) and a single-phase (FCC)
SYS: @@ Fe-Ni-Cr alloy. This case is from A. Engström: Scand. J. Met., v. 24,
SYS: @@ 1995, pp.12-20. This simulation can be run with either the DISPERSED
SYS: @@ SYSTEM MODEL or the HOMOGENIZATION MODEL.
SYS: @@ In this example the DISPERSED SYSTEM MODEL is used, which requires
SYS: @@ that the default HOMOGENIZATION MODEL is disabled.
SYS: @@ With the DISPERSED SYSTEM MODEL the command
SYS: @@ ENTER_LABYRINTH_FUNCTION is used to take into account the
SYS: @@ impeding effect of dispersed phases on long-range diffusion.
SYS: @@ For the HOMOGENIZATION MODEL the command
SYS: @@ ENTER_HOMOGENIZATION_FUNCTION should be used.
SYS: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exd2_setup.DCM
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASE
SYS: @@
SYS: go da
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

 VA                     /-  DEFINED
 L12_FCC                B2_BCC                 DICTRA_FCC_A1
   REJECTED
TDB_TCFE9: sw fedemo
 Current database: Iron Demo Database v2.0

 VA                     /-  DEFINED
TDB_FEDEMO: def-sys fe ni cr
 FE                     NI                     CR
   DEFINED
TDB_FEDEMO: rej ph * all
 LIQUID:L               BCC_A2                 CHI_A12
 FCC_A1                 HCP_A3                 LAVES_PHASE_C14
 SIGMA  REJECTED
TDB_FEDEMO: res ph fcc,bcc
 FCC_A1                 BCC_A2  RESTORED
TDB_FEDEMO: get
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'X.-G. Lu, M. Selleby, B. Sundman, CALPHAD, 29 (2005) 49-55; Fe P-T diagram'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270
      (1986); CR-FE'
  'B.-J. Lee, CALPHAD, 17 (1993) 251-268; revision of Fe-Cr and Fe -Ni liquid'
  'B.-J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
  'A. Dinsdale and T. Chart, MTDS NPL, Unpublished work (1986); CR -NI'
  'A. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); FE-NI'
 -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 v2.0

 VA  DEFINED
APP: def-sys fe ni cr
 FE                     NI                     CR
   DEFINED
APP: rej ph * all
 BCC_A2                 FCC_A1  REJECTED
APP: res ph fcc,bcc
 FCC_A1                 BCC_A2  RESTORED
APP: get
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'This parameter has not been assessed'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Fe diffusion fcc Cr-Fe'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Ni diffusion fcc Cr-Ni'
  'B. Jonsson: Z. Metallkunde 86(1995)686-692; Cr, Fe and Ni diffusion fcc
      Cr-Fe-Ni'
  'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
      -Ni'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Ni self-diffusion'
  'B. Jonsson: ISIJ International, 35(1995)1415-1421; Cr, Fe and Ni
      diffusion bcc Cr-Fe-Ni'
  'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
      in bcc Fe'
 -OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR
```

```
APP: @@
APP: go d-m
 NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 1473; * N

DIC>
DIC> @@
DIC> @@ ENTER THE REGION fer
DIC> @@
DIC> enter-region fer
DIC>
DIC>
DIC> @@
DIC> @@ ENTER 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
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 /NO/:
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 (0 -> 0.5 -> 1): /.5/:
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /NO/:
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>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exd2a\run.DCM"DIC>
DIC>
DIC> @@ exd2_run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING THE SIMULATION OF EXAMPLE D2
DIC> @@
DIC>
DIC> @@
DIC> @@ READ THE SETUP FROM FILE AND START THE SIMULATION
DIC> @@
DIC>
DIC> go d-m
 TIME STEP AT TIME  0.00000E+00
DIC> read exd2
 OK
DIC> sim
 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 = .297842647356821  FE = .517227320600573
                        NI = .184930032042606
 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 = .297842648005432  FE = .517227319061159
                        NI = .18493003293341
 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 = .297842676377595  FE = .517227251840507
                        NI = .184930071781899
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0 seconds
 TIME =   281.72200     DT =   281.32190     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .29784776027007  FE = .517216317308823
                        NI = .184935922421107
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0 seconds
 TIME =   844.36579     DT =   562.64380     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297849615184738  FE = .517212946633455
                        NI = .184937438181807
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0 seconds
 TIME =   1969.6534     DT =   1125.2876     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297850550731969  FE = .517211426818701
                        NI = .18493802244933
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0 seconds
 TIME =   4220.2286     DT =   2250.5752     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297851119000635  FE = .517210569323814
                        NI = .18493831167555
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0 seconds
 TIME =   8721.3789     DT =   4501.1504     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297851494954329  FE = .517210020163945
                        NI = .184938484881725
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    1 seconds
 TIME =   13721.379     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297851732113685  FE = .517209740277055
                        NI = .184938527609259
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0 seconds
 TIME =   18721.379     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297851883453499  FE = .517209584045538
                        NI = .184938532500963
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0 seconds
 TIME =   23721.379     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297851977657541  FE = .517209483265981
                        NI = .184938539076478
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0 seconds
 TIME =   28721.379     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852029985815  FE = .517209412426198
                        NI = .184938557587987
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0 seconds
 TIME =   33721.379     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852049765999  FE = .517209361691084
                        NI = .184938588542917
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0 seconds
 TIME =   38721.379     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852045015463  FE = .517209326359902
                        NI = .184938628624635
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    1 seconds
 TIME =   43721.379     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .29785205230068  FE = .517209299378176
                        NI = .184938648321145
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0 seconds
 TIME =   48721.379     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852064900627  FE = .517209276184267
                        NI = .184938658915106
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0 seconds
 TIME =   53721.379     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852069935234  FE = .517209260646735
```

```
                        NI = .184938669418031
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0 seconds
 TIME =   58721.379     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852077632299  FE = .517209244116565
                        NI = .184938678251136
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0 seconds
 TIME =   63721.379     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852087307301  FE = .517209229697568
                        NI = .184938682995131
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0 seconds
 TIME =   68721.379     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852092166783  FE = .517209219703004
                        NI = .184938688130213
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    1 seconds
 TIME =   73721.379     DT =   5000.0000     SUM OF SQUARES =   0.0000000


output ignored...



... output resumed

 U-FRACTION IN SYSTEM:  CR = .297852035243513  FE = .517209097316324
                        NI = .184938867440163
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0 seconds
 TIME =   608721.38     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852040343797  FE = .517209095828386
                        NI = .184938863827817
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0 seconds
 TIME =   613721.38     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .29785204675644  FE = .517209094403579
                        NI = .184938858839982
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0 seconds
 TIME =   618721.38     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852053277425  FE = .51720909326324
                        NI = .184938853459336
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0 seconds
 TIME =   623721.38     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852059288634  FE = .517209092514252
                        NI = .184938848197115
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    1 seconds
 TIME =   628721.38     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852064436369  FE = .517209092217996
                        NI = .184938843345635
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0 seconds
 TIME =   633721.38     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852068500819  FE = .517209092415578
                        NI = .184938839083604
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0 seconds
 TIME =   638721.38     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852071392425  FE = .517209093083974
                        NI = .184938835523601
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0 seconds
 TIME =   643721.38     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852073681571  FE = .517209091807077
                        NI = .184938834511353
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0 seconds
 TIME =   648721.38     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852074518659  FE = .51720909119049
                        NI = .18493883429085
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    1 seconds
 TIME =   653721.38     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852073879942  FE = .517209091158213
                        NI = .184938834961845
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0 seconds
 TIME =   658721.38     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852071737167  FE = .517209091673281
                        NI = .184938836589552
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0 seconds
 TIME =   663721.38     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852068061577  FE = .517209092719113
                        NI = .18493883921931
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0 seconds
 TIME =   668721.38     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .29785206282492  FE = .517209094290084
                        NI = .184938842884996
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    1 seconds
 TIME =   673721.38     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852056000012  FE = .517209096387373
                        NI = .184938847612615
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0 seconds
 TIME =   678721.38     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852047560589  FE = .517209099016427
                        NI = .184938853422984
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0 seconds
 TIME =   683721.38     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852037481032  FE = .517209102185695
                        NI = .184938860333273
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0 seconds
 TIME =   688721.38     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852031720789  FE = .517209104528048
                        NI = .184938863751162
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0 seconds
```

```
 TIME =   693721.38     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852035106901  FE = .517209102778509
                        NI = .184938862114591
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    1 seconds
 TIME =   698721.38     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852041265549  FE = .517209100862487
                        NI = .184938857871964
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0 seconds
 TIME =   703721.38     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852048238891  FE = .517209099115038
                        NI = .184938852646072
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0 seconds
 TIME =   708721.38     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852055131586  FE = .517209097666857
                        NI = .184938847201557
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0 seconds
 TIME =   713721.38     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852061470614  FE = .517209096580512
                        NI = .184938841948874
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    1 seconds
 TIME =   718721.38     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852066979841  FE = .517209095891422
                        NI = .184938837128738
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0 seconds
 TIME =   720000.00     DT =   1278.6211     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .2978520717672  FE = .517209095429389
                        NI = .184938832803411
 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    468721.38
 DELETING TIME-RECORD FOR TIME    708721.38
 DELETING TIME-RECORD FOR TIME    713721.38

 KEEPING TIME-RECORD FOR TIME    718721.38
 AND FOR TIME                    720000.00
 WORKSPACE RECLAIMED

 TIMESTEP AT     720000.000     SELECTED

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

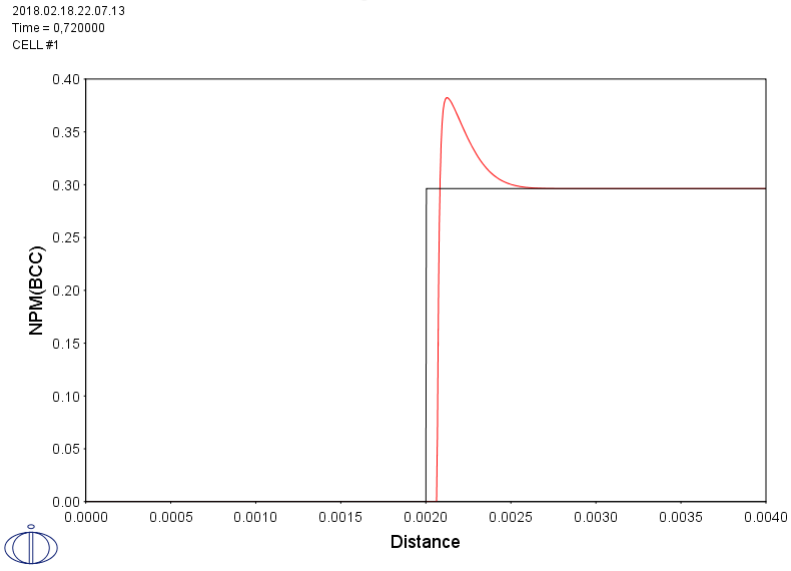
exd2a-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exd2a\plot.DCM"DIC>
DIC>
DIC> @@ exd2_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE D2
DIC> @@
DIC> @@ ENTER THE DICTRA MODULE AND SPECIFY THE STORE-RESULT FILE
DIC> @@
DIC>
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: pl
```

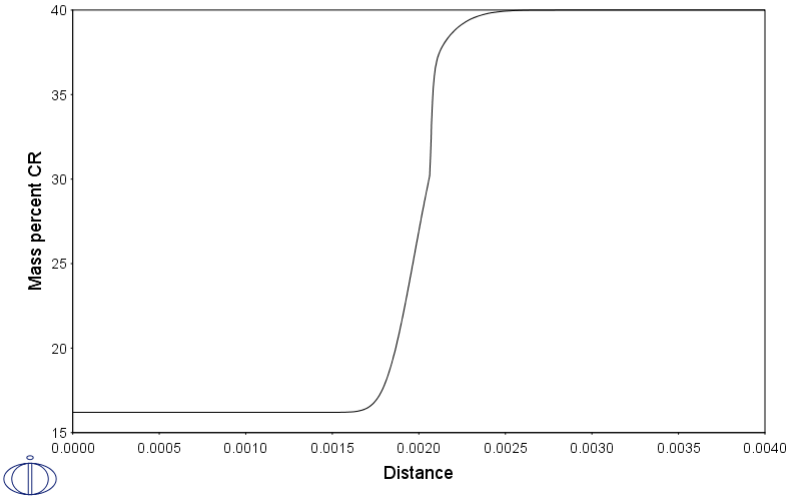
Figure D2.1




```
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: pl
```

Figure D2.2

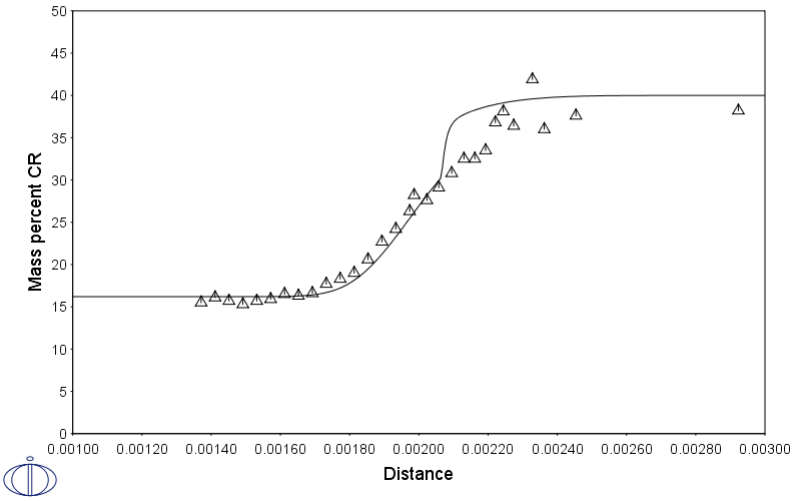
2018.02.18.22.07.14
Time = 720000
CELL #1




```
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: pl
```

Figure D2.3

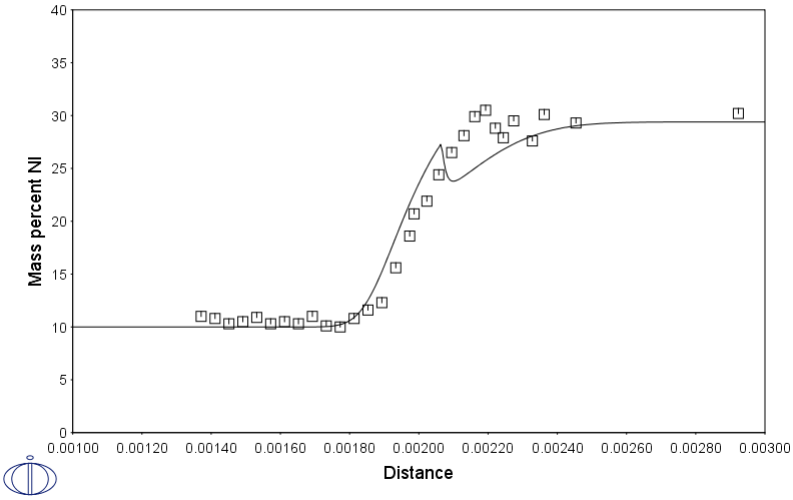
2018.02.18.22.07.14
Time = 720000
CELL #1




```
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: pl
```

Figure D2.4

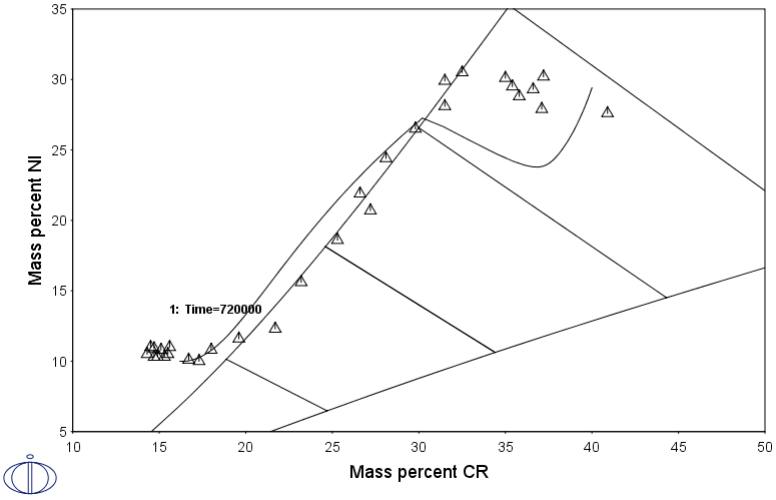
2018.02.18.22.07.15
Time = 720000
CELL #1




```
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: pl
```

Figure D2.5

2018.02.18.22.07.15
Time = 720000
CELL #1



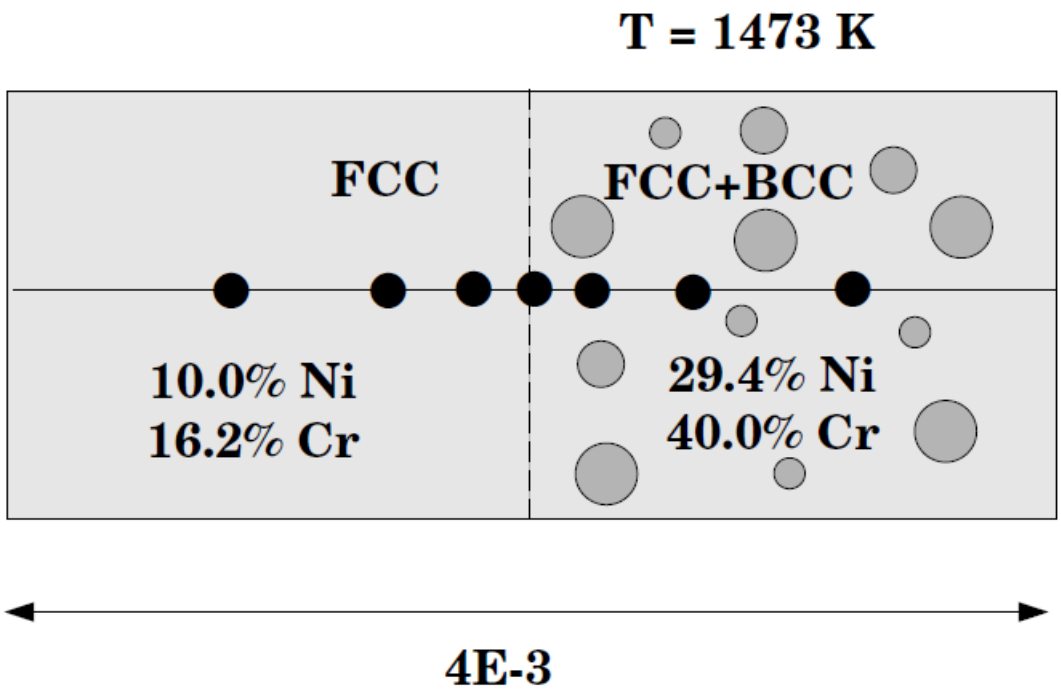

```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1: set-interactive
 --OK---
POST-1:
```

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

```
About Linked: Fri Feb 16 15:22:08 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exd2b\setup.DCM" ?@@
 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. Engström: 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
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

 VA                     /-  DEFINED
 L12_FCC                B2_BCC                 DICTRA_FCC_A1
   REJECTED
TDB_TCFE9: sw fedemo
 Current database: Iron Demo Database v2.0

 VA                     /-  DEFINED
TDB_FEDEMO: def-sys fe ni cr
 FE                     NI                     CR
   DEFINED
TDB_FEDEMO: rej ph * all
 LIQUID:L               BCC_A2                 CHI_A12
 FCC_A1                 HCP_A3                 LAVES_PHASE_C14
 SIGMA  REJECTED
TDB_FEDEMO: res ph fcc,bcc
 FCC_A1                 BCC_A2  RESTORED
TDB_FEDEMO: get
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'X.-G. Lu, M. Selleby, B. Sundman, CALPHAD, 29 (2005) 49-55; Fe P-T diagram'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270
      (1986); CR-FE'
  'B.-J. Lee, CALPHAD, 17 (1993) 251-268; revision of Fe-Cr and Fe -Ni liquid'
  'B.-J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
  'A. Dinsdale and T. Chart, MTDS NPL, Unpublished work (1986); CR -NI'
  'A. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); FE-NI'
 -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 v2.0

 VA  DEFINED
APP: def-sys fe ni cr
 FE                     NI                     CR
   DEFINED
APP: rej ph * all
 BCC_A2                 FCC_A1  REJECTED
APP: res ph fcc,bcc
 FCC_A1                 BCC_A2  RESTORED
APP: get
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'This parameter has not been assessed'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Fe diffusion fcc Cr-Fe'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Ni diffusion fcc Cr-Ni'
  'B. Jonsson: Z. Metallkunde 86(1995)686-692; Cr, Fe and Ni diffusion fcc
      Cr-Fe-Ni'
  'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
      -Ni'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Ni self-diffusion'
  'B. Jonsson: ISIJ International, 35(1995)1415-1421; Cr, Fe and Ni
      diffusion bcc Cr-Fe-Ni'
  'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
      in bcc Fe'
 -OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR
APP: @@
APP: go d-m
 NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
```

```
DIC> set-cond glob T 0 1473; * N

DIC>
DIC> @@
DIC> @@ ENTER THE REGION fer
DIC> @@
DIC> enter-region fer
DIC>
DIC>
DIC> @@
DIC> @@ ENTER 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
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 /NO/: 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 (0 -> 0.5 -> 1): /.5/: 1
MAX TIMESTEP CHANGE PER TIMESTEP : /2/: 2
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /NO/: 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>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exd2b\run.DCM"DIC>
DIC>
DIC> @@ exd2_run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING THE SIMULATION OF EXAMPLE D2
DIC> @@
DIC>
DIC> @@
DIC> @@ READ THE SETUP FROM FILE AND START THE SIMULATION
DIC> @@
DIC>
DIC> go d-m
 TIME STEP AT TIME  0.00000E+00
DIC> read exd2
 OK
DIC> sim
 STARTING SIMULATION USING HOMOGENIZATION MODEL
 ----------------------------------------------
 Saving results
 ----------------------------------
  WARNING:BCC_A2 HAS NO VOLUME FRACTION, CREATING ONE
Starting time-step t0=   0.0000000     dt=  0.10000000E-06
 Stage 1
 Stage 2
 Stage 3
 Moles of elements / mole fractions in system:
CR   0.11913706E-02 /   0.29784265
FE   0.20689093E-02 /   0.51722732
NI   0.73972013E-03 /   0.18493003

Time-step converged t0=   0.0000000     dt=  0.10000000E-06
 ----------------------------------
 Saving results
 ----------------------------------
Starting time-step t0=  0.10000000E-06 dt=  0.20000000E-06
 Stage 1
 Stage 2
 Stage 3
 Moles of elements / mole fractions in system:
CR   0.11913706E-02 /   0.29784265
FE   0.20689093E-02 /   0.51722732
NI   0.73972013E-03 /   0.18493003

Time-step converged t0=  0.10000000E-06 dt=  0.20000000E-06
 ----------------------------------
Starting time-step t0=  0.30000000E-06 dt=  0.40000000E-06
 Stage 1
 Stage 2
 Stage 3
 Moles of elements / mole fractions in system:
CR   0.11913706E-02 /   0.29784265
FE   0.20689093E-02 /   0.51722732
NI   0.73972013E-03 /   0.18493003

Time-step converged t0=  0.30000000E-06 dt=  0.40000000E-06
 ----------------------------------
Starting time-step t0=  0.70000000E-06 dt=  0.80000000E-06
 Stage 1
 Stage 2
 Stage 3
 Moles of elements / mole fractions in system:
CR   0.11913706E-02 /   0.29784265
FE   0.20689093E-02 /   0.51722732
NI   0.73972013E-03 /   0.18493003

Time-step converged t0=  0.70000000E-06 dt=  0.80000000E-06
 ----------------------------------
Starting time-step t0=  0.15000000E-05 dt=  0.16000000E-05
 Stage 1
 Stage 2
 Stage 3
 Moles of elements / mole fractions in system:
CR   0.11913706E-02 /   0.29784265
FE   0.20689093E-02 /   0.51722732
NI   0.73972013E-03 /   0.18493003

Time-step converged t0=  0.15000000E-05 dt=  0.16000000E-05
 ----------------------------------
Starting time-step t0=  0.31000000E-05 dt=  0.32000000E-05
 Stage 1
 Stage 2
 Stage 3
 Moles of elements / mole fractions in system:
CR   0.11913706E-02 /   0.29784265
FE   0.20689093E-02 /   0.51722732
NI   0.73972013E-03 /   0.18493003

Time-step converged t0=  0.31000000E-05 dt=  0.32000000E-05
 ----------------------------------
Starting time-step t0=  0.63000000E-05 dt=  0.64000000E-05
 Stage 1
 Stage 2
 Stage 3
 Moles of elements / mole fractions in system:
CR   0.11913706E-02 /   0.29784265
FE   0.20689093E-02 /   0.51722732
NI   0.73972013E-03 /   0.18493003

Time-step converged t0=  0.63000000E-05 dt=  0.64000000E-05
 ----------------------------------
Starting time-step t0=  0.12700000E-04 dt=  0.12800000E-04
 Stage 1
 Stage 2
 Stage 3
 Moles of elements / mole fractions in system:
CR   0.11913706E-02 /   0.29784265
FE   0.20689093E-02 /   0.51722732
NI   0.73972013E-03 /   0.18493003

Time-step converged t0=  0.12700000E-04 dt=  0.12800000E-04
 ----------------------------------
```

```
Starting time-step t0=  0.25500000E-04 dt=  0.25600000E-04
 Stage 1
 Stage 2
 Stage 3
 Moles of elements / mole fractions in system:
CR   0.11913706E-02 /   0.29784265
FE   0.20689093E-02 /   0.51722732
NI   0.73972013E-03 /   0.18493003

Time-step converged t0=  0.25500000E-04 dt=  0.25600000E-04
 ----------------------------------
Starting time-step t0=  0.51100000E-04 dt=  0.51200000E-04
 Stage 1
 Stage 2
 Stage 3
 Moles of elements / mole fractions in system:
CR   0.11913706E-02 /   0.29784265
FE   0.20689093E-02 /   0.51722732
NI   0.73972013E-03 /   0.18493003


output ignored...



... output resumed

 Stage 2
Iteration #   1 sum residual **2:    641.14263
Iteration #   2 sum residual **2:    27.481021
Iteration #   3 sum residual **2:   0.38755444E-01
 Stage 3
Iteration #   1 sum residual **2:    67.925276
Iteration #   2 sum residual **2:    2.2436106
Iteration #   3 sum residual **2:    1.2693144
 Moles of elements / mole fractions in system:
CR   0.11913706E-02 /   0.29784265
FE   0.20689093E-02 /   0.51722732
NI   0.73972013E-03 /   0.18493003

Time-step converged t0=   655895.19     dt=   27487.791
 ----------------------------------
 Saving results
 ----------------------------------
Starting time-step t0=   683382.98     dt=   36617.016
 Stage 1
Iteration #   1 sum residual **2:    1556545.3
Iteration #   2 sum residual **2:    1464876.5
Iteration #   3 sum residual **2:    1350823.3
Iteration #   4 sum residual **2:    632635.82
Iteration #   5 sum residual **2:    34965.417
Iteration #   6 sum residual **2:    7237.5103
Iteration #   7 sum residual **2:    6078.2733
Iteration #   8 sum residual **2:    140.00412
Iteration #   9 sum residual **2:    23.699209
Iteration #  10 sum residual **2:    4.9926134
Iteration #  11 sum residual **2:    3.9305885
Iteration #  12 sum residual **2:   0.96280135
 Stage 2
Iteration #   1 sum residual **2:    186.95702
Iteration #   2 sum residual **2:    48.200441
Iteration #   3 sum residual **2:    32.148971
Iteration #   4 sum residual **2:    1.3454838
 Stage 3
Iteration #   1 sum residual **2:    1100.7455
Iteration #   2 sum residual **2:    178.06850
Iteration #   3 sum residual **2:    23.045748
Iteration #   4 sum residual **2:   0.65872549
 Moles of elements / mole fractions in system:
CR   0.11913706E-02 /   0.29784265
FE   0.20689093E-02 /   0.51722732
NI   0.73972013E-03 /   0.18493003

Time-step converged t0=   683382.98     dt=   36617.016
 ----------------------------------
 Saving results
 ----------------------------------
 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    6496.1380
 DELETING TIME-RECORD FOR TIME    7355.1315
 DELETING TIME-RECORD FOR TIME    8214.1250
 DELETING TIME-RECORD FOR TIME    9073.1184
 DELETING TIME-RECORD FOR TIME    9932.1119
 DELETING TIME-RECORD FOR TIME    10791.105
 DELETING TIME-RECORD FOR TIME    11650.099
 DELETING TIME-RECORD FOR TIME    13368.086
 DELETING TIME-RECORD FOR TIME    15086.073
 DELETING TIME-RECORD FOR TIME    16804.060
 DELETING TIME-RECORD FOR TIME    18522.046
 DELETING TIME-RECORD FOR TIME    20240.033
 DELETING TIME-RECORD FOR TIME    21958.020
 DELETING TIME-RECORD FOR TIME    25393.994
 DELETING TIME-RECORD FOR TIME    28829.968
 DELETING TIME-RECORD FOR TIME    30547.955
 DELETING TIME-RECORD FOR TIME    33983.929
 DELETING TIME-RECORD FOR TIME    37419.903
 DELETING TIME-RECORD FOR TIME    40855.876
 DELETING TIME-RECORD FOR TIME    44291.850
 DELETING TIME-RECORD FOR TIME    51163.798
 DELETING TIME-RECORD FOR TIME    58035.746
 DELETING TIME-RECORD FOR TIME    64907.693
 DELETING TIME-RECORD FOR TIME    71779.641
 DELETING TIME-RECORD FOR TIME    78651.589
 DELETING TIME-RECORD FOR TIME    85523.536
 DELETING TIME-RECORD FOR TIME    88959.510
 DELETING TIME-RECORD FOR TIME    95831.458
```

```
 DELETING TIME-RECORD FOR TIME    109575.35
 DELETING TIME-RECORD FOR TIME    116447.30
 DELETING TIME-RECORD FOR TIME    130191.20
 DELETING TIME-RECORD FOR TIME    143935.09
 DELETING TIME-RECORD FOR TIME    147371.07
 DELETING TIME-RECORD FOR TIME    150807.04
 DELETING TIME-RECORD FOR TIME    154243.01
 DELETING TIME-RECORD FOR TIME    161114.96
 DELETING TIME-RECORD FOR TIME    174858.86
 DELETING TIME-RECORD FOR TIME    188602.75
 DELETING TIME-RECORD FOR TIME    216090.54
 DELETING TIME-RECORD FOR TIME    229834.44
 DELETING TIME-RECORD FOR TIME    243578.33
 DELETING TIME-RECORD FOR TIME    271066.12
 DELETING TIME-RECORD FOR TIME    277938.07
 DELETING TIME-RECORD FOR TIME    291681.97
 DELETING TIME-RECORD FOR TIME    319169.76
 DELETING TIME-RECORD FOR TIME    346657.55
 DELETING TIME-RECORD FOR TIME    374145.34
 DELETING TIME-RECORD FOR TIME    387889.23
 DELETING TIME-RECORD FOR TIME    394761.18
 DELETING TIME-RECORD FOR TIME    408505.08
 DELETING TIME-RECORD FOR TIME    422248.97
 DELETING TIME-RECORD FOR TIME    449736.76
 DELETING TIME-RECORD FOR TIME    463480.66
 DELETING TIME-RECORD FOR TIME    470352.61
 DELETING TIME-RECORD FOR TIME    477224.55
 DELETING TIME-RECORD FOR TIME    490968.45
 DELETING TIME-RECORD FOR TIME    518456.24
 DELETING TIME-RECORD FOR TIME    532200.14
 DELETING TIME-RECORD FOR TIME    545944.03
 DELETING TIME-RECORD FOR TIME    573431.82
 DELETING TIME-RECORD FOR TIME    600919.61
 DELETING TIME-RECORD FOR TIME    628407.40
 DELETING TIME-RECORD FOR TIME    642151.30
 DELETING TIME-RECORD FOR TIME    655895.19

 KEEPING TIME-RECORD FOR TIME    683382.98
 AND FOR TIME                    720000.00
 WORKSPACE RECLAIMED
 -------------------------------------------------
 INTERPOLATION SCHEME USED THIS FRACTION OF
 THE ALLOCATED MEMORY:   0.565747808406386
 EFFICIENCY FACTOR:    36.6497967359925
 -------------------------------------------------
 DEALLOCATING
 -------------------------------------------------

 TIMESTEP AT     720000.000     SELECTED

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

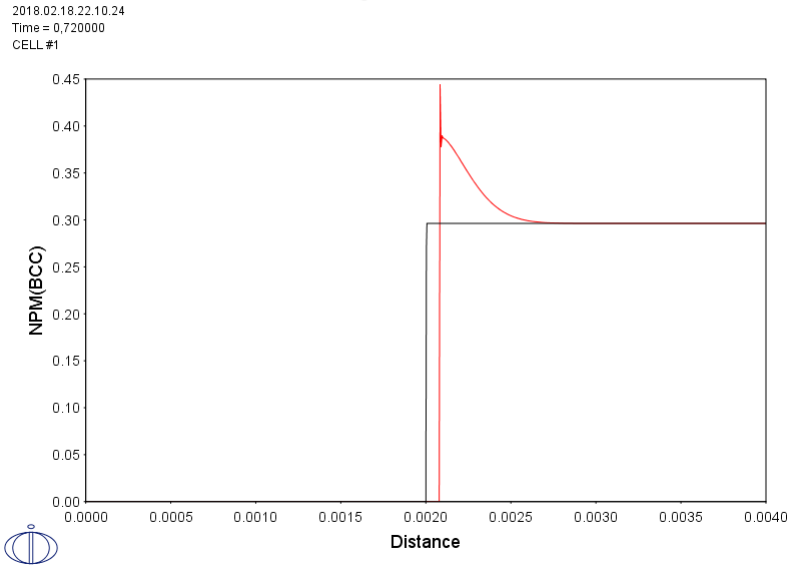
exd2b-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exd2b\plot.DCM"DIC>
DIC>
DIC> @@ exd2_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE D2
DIC> @@
DIC> @@ ENTER THE DICTRA MODULE AND SPECIFY THE STORE-RESULT FILE
DIC> @@
DIC>
DIC> go d-m
 TIME STEP AT TIME  7.20000E+05
DIC> read  exd2
 OK
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA POST PROCESSOR
DIC> @@
DIC> post

  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson

POST-1:
POST-1:
POST-1: @@
POST-1: @@ LET US FIRST SEE HOW THE FRACTION OF FERRITE  HAS CHANGED
POST-1: @@ AS A RESULT OF THE DIFFUSION
POST-1: @@
POST-1: s-d-a y npm(bcc)
POST-1: s-d-a x distance global
  INFO: Distance is set as independent variable
POST-1: s-p-c time 0 720000
POST-1: set-tit Figure D2.1
POST-1: pl
```

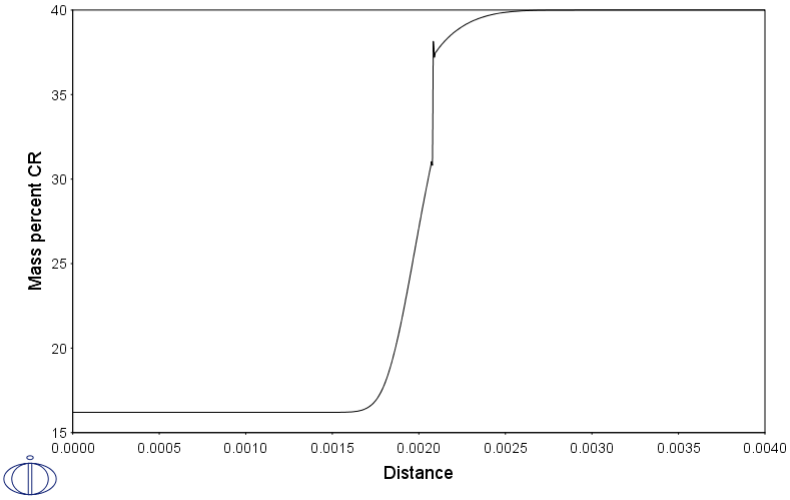
Figure D2.1




```
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: pl
```

Figure D2.2

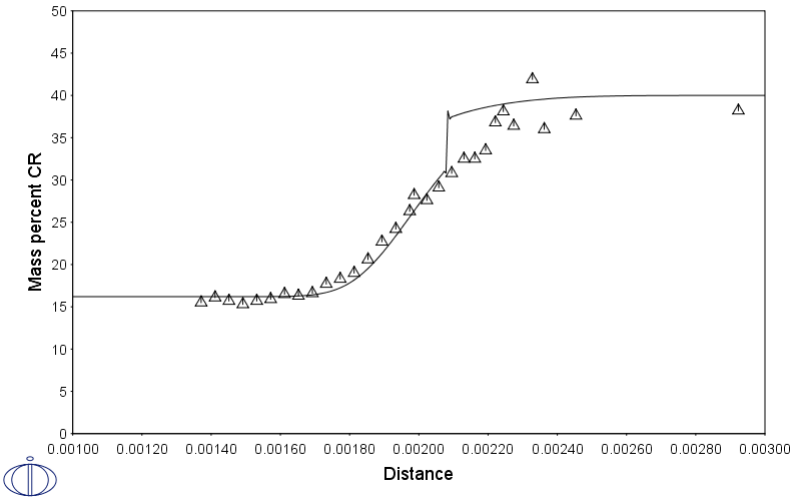
2018.02.18.22.10.26
Time = 720000
CELL #1




```
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: pl
```

Figure D2.3

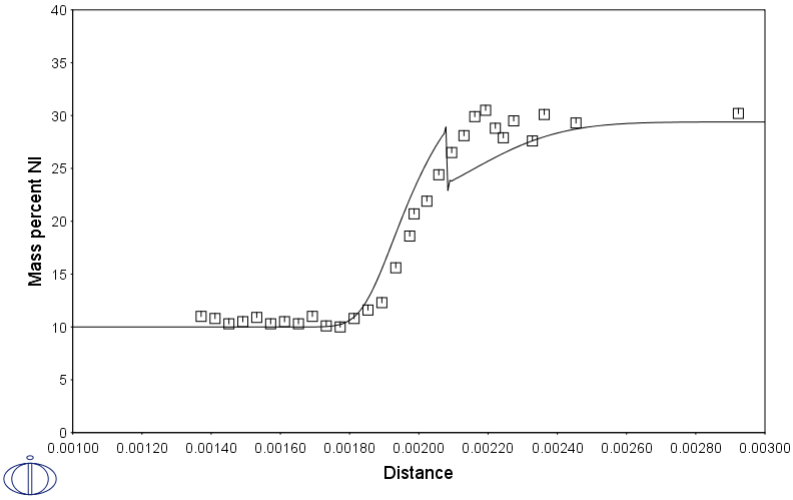
2018.02.18.22.10.27
Time = 720000
CELL #1




```
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: pl
```

Figure D2.4

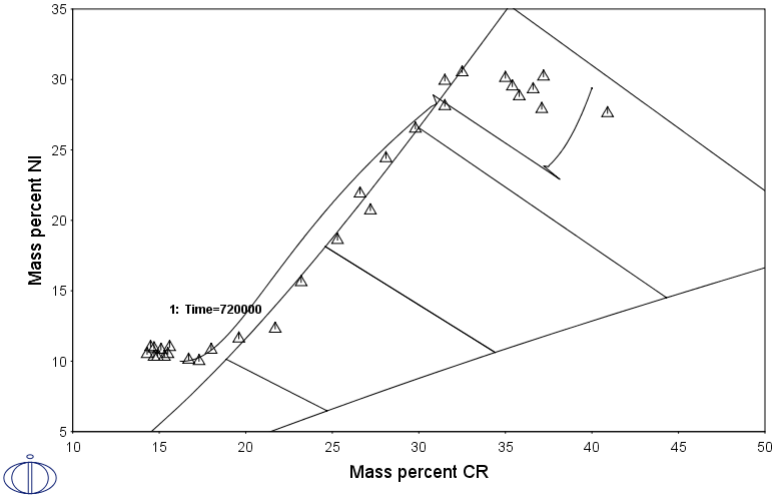
2018.02.18.22.10.29
Time = 720000
CELL #1




```
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: pl
```

Figure D2.5

2018.02.18.22.10.30
Time = 720000
CELL #1

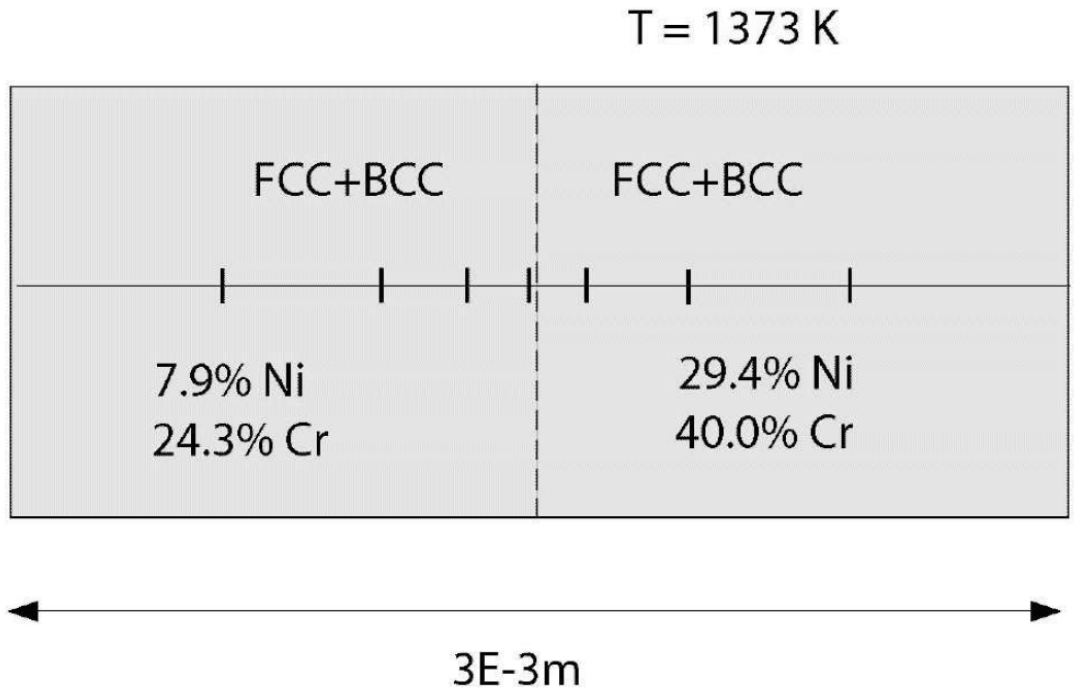



```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1: set-interactive
 --OK---
POST-1:
```

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

```
About License library version: 8.5.1.0017
 Linked: Fri Feb 16 15:22:08 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exd3\setup.DCM"SYS: ?@@
 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. Engström, Acta. Mater. v.54 (2006), pp. 2431-2439.
SYS: @@ Experimental data from A. Engström, 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
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

 VA                     /-  DEFINED
 L12_FCC                B2_BCC                 DICTRA_FCC_A1
   REJECTED
TDB_TCFE9: sw fedemo
 Current database: Iron Demo Database v2.0

 VA                     /-  DEFINED
TDB_FEDEMO: def-sys fe cr ni
 FE                     CR                     NI
   DEFINED
TDB_FEDEMO: rej-ph *
 LIQUID:L               BCC_A2                 CHI_A12
 FCC_A1                 HCP_A3                 LAVES_PHASE_C14
 SIGMA  REJECTED
TDB_FEDEMO: rest-ph bcc,fcc
 BCC_A2                 FCC_A1  RESTORED
TDB_FEDEMO: get
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'X.-G. Lu, M. Selleby, B. Sundman, CALPHAD, 29 (2005) 49-55; Fe P-T diagram'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270
      (1986); CR-FE'
  'B.-J. Lee, CALPHAD, 17 (1993) 251-268; revision of Fe-Cr and Fe -Ni liquid'
  'B.-J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
  'A. Dinsdale and T. Chart, MTDS NPL, Unpublished work (1986); CR -NI'
  'A. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); FE-NI'
 -OK-
TDB_FEDEMO:
TDB_FEDEMO: app mfedemo
 Current database: Fe-Alloys Mobility demo database v2.0

 VA  DEFINED
APP: def-sys fe cr ni
 FE                     CR                     NI
   DEFINED
APP: rej-ph *
 BCC_A2                 FCC_A1  REJECTED
APP: rest-ph bcc,fcc
 BCC_A2                 FCC_A1  RESTORED
APP: get
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'This parameter has not been assessed'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Fe diffusion fcc Cr-Fe'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Ni diffusion fcc Cr-Ni'
  'B. Jonsson: Z. Metallkunde 86(1995)686-692; Cr, Fe and Ni diffusion fcc
      Cr-Fe-Ni'
  'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
      -Ni'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Ni self-diffusion'
  'B. Jonsson: ISIJ International, 35(1995)1415-1421; Cr, Fe and Ni
      diffusion bcc Cr-Fe-Ni'
  'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
      in bcc Fe'
 -OK-
APP:
APP: go -m
 NO TIME STEP DEFINED
DIC>
DIC> set-cond glob T 0 1373.15; * N

DIC>
DIC> ent-geo 0
DIC>
```

```
DIC> ent-reg
REGION NAME : fecrni
DIC>
DIC> ent-grid
REGION NAME : /FECRNI/: fecrni
WIDTH OF REGION /1/: 3e-3
TYPE /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
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 /NO/: 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 (0 -> 0.5 -> 1): /.5/: .5
MAX TIMESTEP CHANGE PER TIMESTEP : /2/: 2
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /NO/: 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>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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
 STARTING SIMULATION USING HOMOGENIZATION MODEL
 ----------------------------------------------
 Saving results
 ----------------------------------
  WARNING:BCC_A2 HAS NO VOLUME FRACTION, CREATING ONE
Starting time-step t0=   0.0000000     dt=   1.0000000
 Stage 1
 Evaluating Jacobian
Iteration #   1 sum residual **2:   0.91200732E-03
 Stage 2
 Stage 3
 Moles of elements / mole fractions in system:
CR   0.10202298E-02 /   0.34007660
FE   0.14697902E-02 /   0.48993007
NI   0.50997997E-03 /   0.16999332

Time-step converged t0=   0.0000000     dt=   1.0000000
 ----------------------------------
 Saving results
 ----------------------------------
Starting time-step t0=   1.0000000     dt=   2.0000000
 Stage 1
Iteration #   1 sum residual **2:   0.49065622E-03
 Stage 2
 Stage 3
 Moles of elements / mole fractions in system:
CR   0.10202298E-02 /   0.34007660
FE   0.14697902E-02 /   0.48993007
NI   0.50997997E-03 /   0.16999332

Time-step converged t0=   1.0000000     dt=   2.0000000
 ----------------------------------
Starting time-step t0=   3.0000000     dt=   4.0000000
 Stage 1
Iteration #   1 sum residual **2:   0.35181588E-03
 Stage 2
 Stage 3
 Moles of elements / mole fractions in system:
CR   0.10202298E-02 /   0.34007660
FE   0.14697902E-02 /   0.48993007
NI   0.50997997E-03 /   0.16999332

Time-step converged t0=   3.0000000     dt=   4.0000000
 ----------------------------------
Starting time-step t0=   7.0000000     dt=   8.0000000
 Stage 1
Iteration #   1 sum residual **2:   0.32271218E-02
 Stage 2
 Stage 3
 Moles of elements / mole fractions in system:
CR   0.10202298E-02 /   0.34007660
FE   0.14697902E-02 /   0.48993007
NI   0.50997997E-03 /   0.16999332

Time-step converged t0=   7.0000000     dt=   8.0000000
 ----------------------------------
Starting time-step t0=   15.000000     dt=   16.000000
 Stage 1
Iteration #   1 sum residual **2:   0.82413380
 Stage 2
 Stage 3
 Moles of elements / mole fractions in system:
CR   0.10202298E-02 /   0.34007660
FE   0.14697902E-02 /   0.48993007
NI   0.50997997E-03 /   0.16999332

Time-step converged t0=   15.000000     dt=   16.000000
 ----------------------------------
Starting time-step t0=   31.000000     dt=   32.000000
 Stage 1
Iteration #   1 sum residual **2:    22.492550
Iteration #   2 sum residual **2:   0.41246053E-02
 Stage 2
Iteration #   1 sum residual **2:   0.24687442E-02
 Stage 3
 Moles of elements / mole fractions in system:
CR   0.10202298E-02 /   0.34007660
FE   0.14697902E-02 /   0.48993007
NI   0.50997997E-03 /   0.16999332

Time-step converged t0=   31.000000     dt=   32.000000
 ----------------------------------
Starting time-step t0=   63.000000     dt=   64.000000
 Stage 1
Iteration #   1 sum residual **2:    318.00997
Iteration #   2 sum residual **2:   0.11435874E-01
 Stage 2
Iteration #   1 sum residual **2:   0.11990052E-02
 Stage 3
 Moles of elements / mole fractions in system:
CR   0.10202298E-02 /   0.34007660
FE   0.14697902E-02 /   0.48993007
NI   0.50997997E-03 /   0.16999332

Time-step converged t0=   63.000000     dt=   64.000000
 ----------------------------------
Starting time-step t0=   127.00000     dt=   128.00000
 Stage 1
```

```
Iteration #   1 sum residual **2:    3329.2078
Iteration #   2 sum residual **2:    7.7906721
Iteration #   3 sum residual **2:   0.32771164E-02
 Stage 2
Iteration #   1 sum residual **2:   0.13169817
 Stage 3
Iteration #   1 sum residual **2:   0.20209404E-02
 Moles of elements / mole fractions in system:
CR   0.10202298E-02 /   0.34007660
FE   0.14697902E-02 /   0.48993007
NI   0.50997997E-03 /   0.16999332

Time-step converged t0=   127.00000     dt=   128.00000
 ----------------------------------
Starting time-step t0=   255.00000     dt=   256.00000
 Stage 1
Iteration #   1 sum residual **2:    24933.971
Iteration #   2 sum residual **2:    200.02314
Iteration #   3 sum residual **2:    2.7825925
Iteration #   4 sum residual **2:   0.14360047E-02
 Stage 2
Iteration #   1 sum residual **2:    6.6165731


output ignored...



... output resumed

Iteration #   1 sum residual **2:    5.0863916
Iteration #   2 sum residual **2:   0.71399236E-02
 Stage 2
Iteration #   1 sum residual **2:    5971.4116
Iteration #   2 sum residual **2:    1265.5268
Iteration #   3 sum residual **2:    266.01779
Iteration #   4 sum residual **2:    54.494203
Iteration #   5 sum residual **2:    10.332155
Iteration #   6 sum residual **2:    1.4118710
 Stage 3
Iteration #   1 sum residual **2:    18273.745
Iteration #   2 sum residual **2:    3873.9469
Iteration #   3 sum residual **2:    818.71032
Iteration #   4 sum residual **2:    171.24360
Iteration #   5 sum residual **2:    34.558136
Iteration #   6 sum residual **2:    6.2712291
Iteration #   7 sum residual **2:   0.63390019
 Moles of elements / mole fractions in system:
CR   0.10202298E-02 /   0.34007660
FE   0.14697902E-02 /   0.48993007
NI   0.50997997E-03 /   0.16999332

Time-step converged t0=   311295.00     dt=   16384.000
 ----------------------------------
 Saving results
 ----------------------------------
Starting time-step t0=   327679.00     dt=   16384.000
 Stage 1
Iteration #   1 sum residual **2:    172009.66
Iteration #   2 sum residual **2:    23342.198
Iteration #   3 sum residual **2:    6987.3141
Iteration #   4 sum residual **2:    541.32763
Iteration #   5 sum residual **2:    100.64340
Iteration #   6 sum residual **2:   0.32733569E-01
 Stage 2
Iteration #   1 sum residual **2:    10569.990
Iteration #   2 sum residual **2:    2929.6967
Iteration #   3 sum residual **2:    841.64359
Iteration #   4 sum residual **2:    232.15567
Iteration #   5 sum residual **2:    64.451542
Iteration #   6 sum residual **2:    16.244961
Iteration #   7 sum residual **2:    3.5432238
Iteration #   8 sum residual **2:   0.31909750
 Stage 3
Iteration #   1 sum residual **2:    21235.798
Iteration #   2 sum residual **2:    4571.0910
Iteration #   3 sum residual **2:    1020.7109
Iteration #   4 sum residual **2:    248.85990
Iteration #   5 sum residual **2:    69.980347
Iteration #   6 sum residual **2:    18.313420
Iteration #   7 sum residual **2:    4.1268621
Iteration #   8 sum residual **2:   0.40382679
 Moles of elements / mole fractions in system:
CR   0.10202298E-02 /   0.34007660
FE   0.14697902E-02 /   0.48993007
NI   0.50997997E-03 /   0.16999332

Time-step converged t0=   327679.00     dt=   16384.000
 ----------------------------------
 Saving results
 ----------------------------------
Starting time-step t0=   344063.00     dt=   15937.000
 Stage 1
Iteration #   1 sum residual **2:    10895.376
Iteration #   2 sum residual **2:    147.96473
Iteration #   3 sum residual **2:    1.3594067
Iteration #   4 sum residual **2:   0.92703049E-02
 Stage 2
Iteration #   1 sum residual **2:    7306.4604
Iteration #   2 sum residual **2:    1629.4028
Iteration #   3 sum residual **2:    366.42901
Iteration #   4 sum residual **2:    82.096557
Iteration #   5 sum residual **2:    18.503682
Iteration #   6 sum residual **2:    3.9577610
Iteration #   7 sum residual **2:   0.37067955
 Stage 3
Iteration #   1 sum residual **2:    22370.989
Iteration #   2 sum residual **2:    4974.7263
Iteration #   3 sum residual **2:    1104.1227
Iteration #   4 sum residual **2:    243.11191
Iteration #   5 sum residual **2:    52.266894
Iteration #   6 sum residual **2:    10.405947
Iteration #   7 sum residual **2:    1.5400717
 Moles of elements / mole fractions in system:
CR   0.10202298E-02 /   0.34007660
FE   0.14697902E-02 /   0.48993007
```

```
NI    0.50997997E-03 /   0.16999332

Time-step converged t0=   344063.00     dt=   15937.000
 -----------------------------------
 Saving results
 -----------------------------------
 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    10239.000
 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    65535.000
 DELETING TIME-RECORD FOR TIME    81919.000
 DELETING TIME-RECORD FOR TIME    98303.000
 DELETING TIME-RECORD FOR TIME    114687.00
 DELETING TIME-RECORD FOR TIME    131071.00
 DELETING TIME-RECORD FOR TIME    147455.00
 DELETING TIME-RECORD FOR TIME    163839.00
 DELETING TIME-RECORD FOR TIME    180223.00
 DELETING TIME-RECORD FOR TIME    196607.00
 DELETING TIME-RECORD FOR TIME    212991.00
 DELETING TIME-RECORD FOR TIME    229375.00
 DELETING TIME-RECORD FOR TIME    245759.00
 DELETING TIME-RECORD FOR TIME    262143.00
 DELETING TIME-RECORD FOR TIME    278527.00
 DELETING TIME-RECORD FOR TIME    294911.00
 DELETING TIME-RECORD FOR TIME    311295.00
 DELETING TIME-RECORD FOR TIME    327679.00

 KEEPING TIME-RECORD FOR TIME    344063.00
 AND FOR TIME                    360000.00
 WORKSPACE RECLAIMED
 ------------------------------------------------
 INTERPOLATION SCHEME USED THIS FRACTION OF
 THE ALLOCATED MEMORY:   0.381320622645912
 EFFICIENCY FACTOR:    7.09082167832168
 ------------------------------------------------
 DEALLOCATING
 ------------------------------------------------

 TIMESTEP AT     360000.000     SELECTED

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

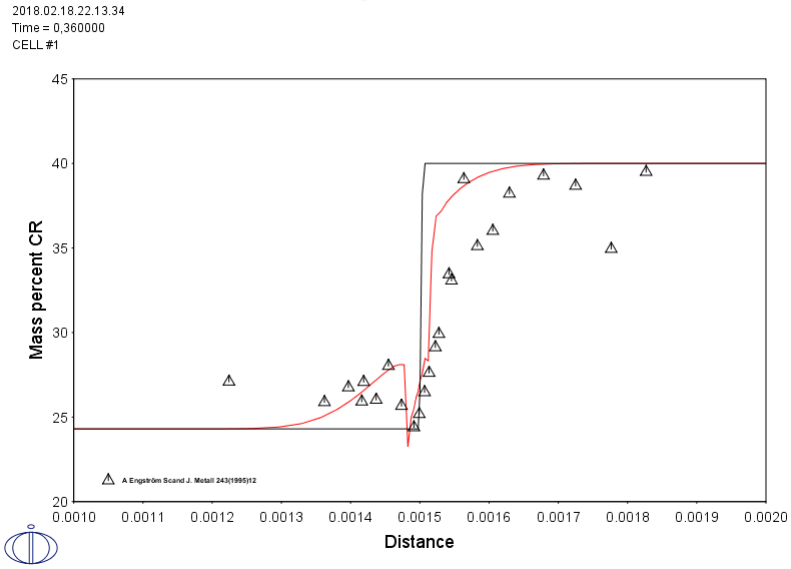
exd3-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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

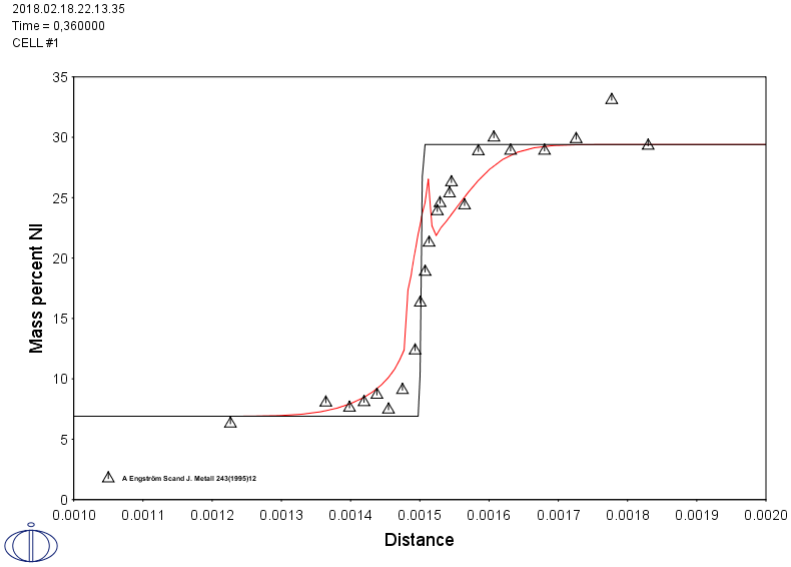
POST-1:
POST-1:
POST-1: @@
POST-1: @@ First study the composition profiles of Cr and Ni
POST-1: @@
POST-1: s-d-a x distance global
  INFO: Distance is set as independent variable
POST-1: s-d-a y w-p Cr
POST-1: s-p-c time 0 360000
POST-1: set-tit Figure D3.1
POST-1:
POST-1: app yes k5k7cr.exp 0; 1
POST-1:
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: plot
```

Figure D3.1



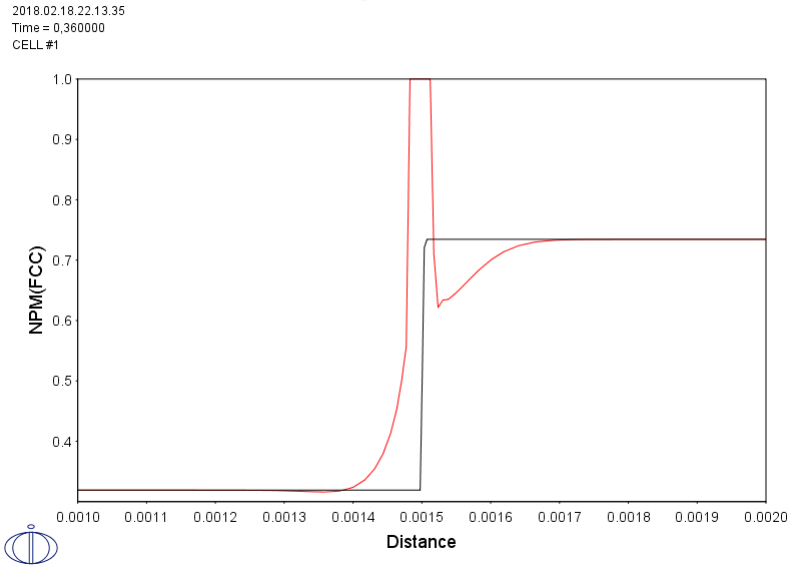

```
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1: s-d-a y w-p Ni
POST-1: set-tit Figure D3.2
POST-1:
POST-1: app yes k5k7ni.exp 0; 1
POST-1:
POST-1: s-s-s y n 0 35
POST-1:
POST-1: plot
```

Figure D3.2



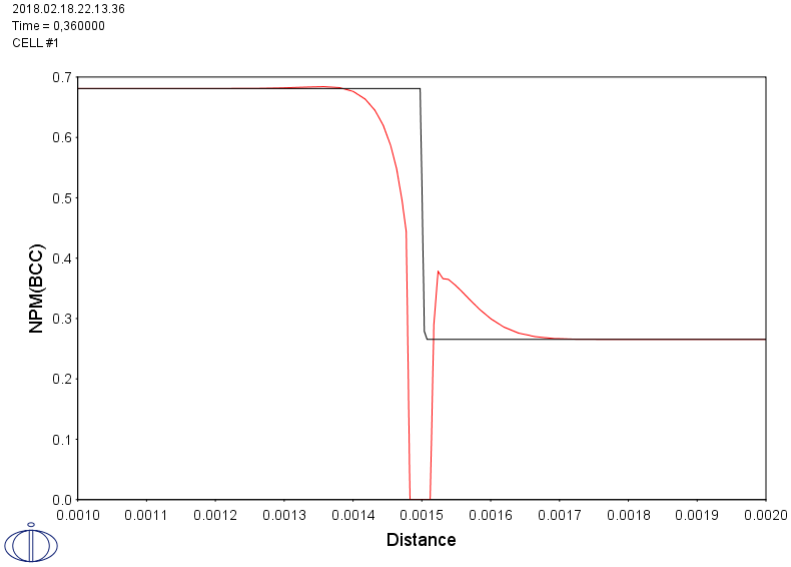

```
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1: @@
POST-1: @@ Then study the amount of FCC and BCC
POST-1: @@
POST-1: app no
POST-1: s-d-a y npm(fcc)
POST-1: set-tit Figure D3.3
POST-1: plot
```

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: plot
```

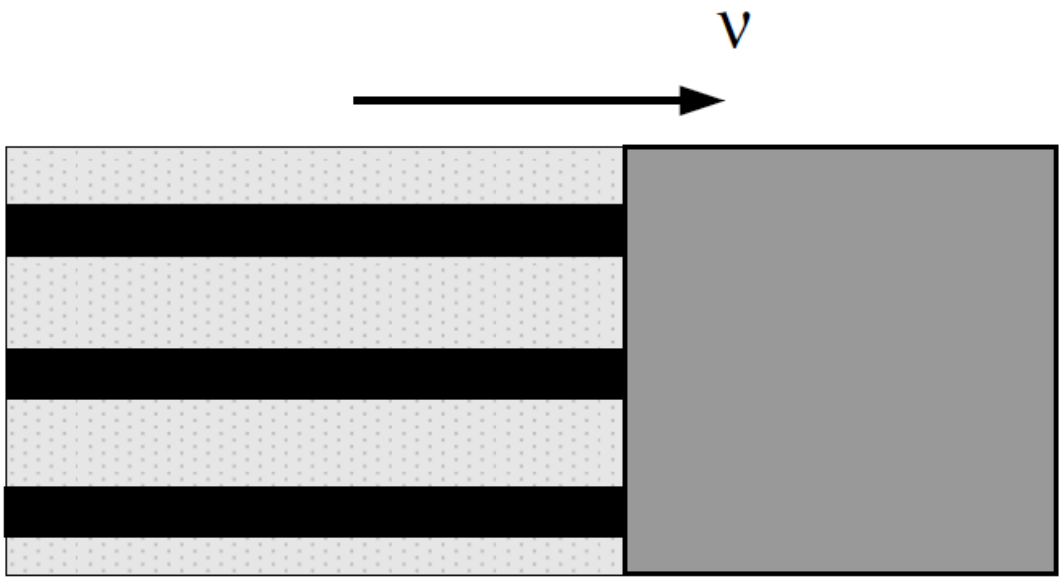
Figure D3.4




```
POST-1:
```

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

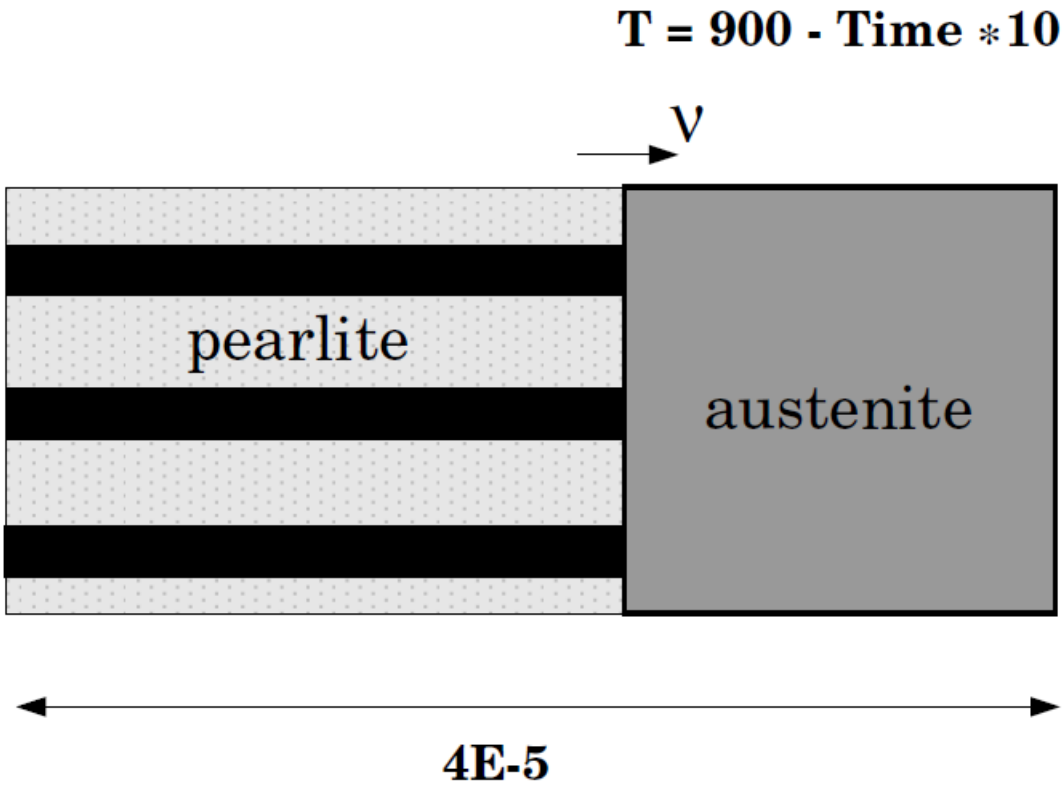
Cooperative Growth



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

```
About Linked: Fri Feb 16 15:22:08 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exe1\setup.DCM" ?@@
 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
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

 VA                     /-  DEFINED
 L12_FCC                B2_BCC                 DICTRA_FCC_A1
   REJECTED
TDB_TCFE9: sw tcfe7
 Current database: Steels/Fe-Alloys  v7.0

 VA  DEFINED
 L12_FCC                B2_BCC                 B2_VACANCY
 HIGH_SIGMA             DICTRA_FCC_A1  REJECTED
TDB_TCFE7:
TDB_TCFE7: @@
TDB_TCFE7: @@ DEFINE THE SYSTEM
TDB_TCFE7: @@
TDB_TCFE7: def-sys fe c mn
 FE                     C                      MN
   DEFINED
TDB_TCFE7:
TDB_TCFE7: @@
TDB_TCFE7: @@ KEEP ONLY THE AUSTENITE, FERRITE AND CEMENTITE PHASES
TDB_TCFE7: @@
TDB_TCFE7: rej-ph /all
 GAS:G                  LIQUID:L               BCC_A2
 FCC_A1                 HCP_A3                 DIAMOND_FCC_A4
 GRAPHITE               CEMENTITE              M23C6
 M7C3                   M5C2                   KSI_CARBIDE
 A1_KAPPA               KAPPA                  FE4N_LP1
 FECN_CHI               LAVES_PHASE_C14        G_PHASE
   REJECTED
TDB_TCFE7: rest-ph fcc,bcc,cem
 FCC_A1                 BCC_A2                 CEMENTITE
   RESTORED
TDB_TCFE7:
TDB_TCFE7: @@
TDB_TCFE7: @@ GET THE THERMODYNAMIC DATA
TDB_TCFE7: @@
TDB_TCFE7: get
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'
  'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
  'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C
      -FE'
  'W. Huang, Metall. Trans. A, 21A (1990), 2115-2123; TRITA-MAC 411 (Rev
      1989); C-FE-MN'
  'W. Huang, Calphad, 13 (1989), 243-252; TRITA-MAC 388 (rev 1989); FE-MN'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
      Molar volumes'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'P. Villars and L.D. Calvert (1985). Pearsons handbook of crystallographic
      data for intermetallic phases. Metals park, Ohio. American Society for
      Metals; Molar volumes'
 -OK-
TDB_TCFE7:
TDB_TCFE7: @@
TDB_TCFE7: @@ APPEND THE KINETIC DATA FROM THE MOBILITY DATABASE
TDB_TCFE7: @@
TDB_TCFE7: append mobfe2
 Current database: Steels/Fe-Alloys Mobility  v2.0
   TCS Steel Mobility Database Version 2.0 from 2011-12-09.

 VA  DEFINED
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 ....

 List of references for assessed data

  'This parameter has not been assessed'
```

```
  'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'
  'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
      -Ni'
  'Bae et al.: Z. Metallkunde 91(2000)672-674; fcc Fe-Mn
       Mn-Ni'
  'B. Jonsson: Z. Metallkunde 85(1994)498-501; C and N diffusion in bcc Cr
      -Fe-Ni'
  'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
      in bcc Fe'
  'Assessed from data presented in Landholt-Bornstein, Vol. 26, ed. H.
      Mehrer, springer (1990); Impurity diff of Mn in bcc Fe.'
 -OK-
APP:
APP: @@
APP: @@ ALL THE THERMODYNAMIC AND KINETIC DATA HAVE BEEN RETRIEVED.
APP: @@ GO TO THE DICTRA MONITOR TO SET UP YOUR PROBLEM.
APP: @@
APP: go d-m
 NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ SET THE CONDITION FOR TEMPERATURE
DIC> @@
DIC> set-cond glob t 0 900-time*10; * n

DIC>
DIC> @@
DIC> @@ ENTER A REGION
DIC> @@
DIC> enter-reg pearlite
DIC>
DIC> @@
DIC> @@ ENTER A SMALL INITIAL SIZE OF THE GRID IN THE 'PEARLITE' REGION
DIC> @@
DIC> enter-grid pearlite 5e-10 lin 5
DIC>
DIC> @@
DIC> @@ ENTER INTO THE 'PEARLITE' REGION THE PHASES 'BCC' AND 'CEM' AND SPECIFY
DIC> @@ THAT ARE PRESENT IN THE FORM OF A 'LAMELLAR AGGREGATE. SET THE STATUS
DIC> @@ TO 'ACTIVE'. SEVERAL PROMPTS FOLLOW ABOUT THE VALUES OF THE PARAMETERS
DIC> @@ IN THE PEARLITE GROWTH MODEL, FOR EXAMPLE AS SURFACE TENSION, OPTIMUM
DIC> @@ GROWTH RATE FACTOR, AND BOUNDARY DIFFUSION COEFFICIENTS.
DIC> @@
DIC> @@ CARBON(C) IS TREATED IN A SPECIAL WAY. IF 'AUTOMATIC' IS ENTERED
DIC> @@ THE DIFFUSION OF C IS CALCULATED ACCORDING TO AN EQUATION FOR
DIC> @@ MIXED BOUNDARY AND VOLUME DIFFUSION. YOU CAN CHOOSE BETWEEN
DIC> @@ MANUAL OR AUTOMATIC START VALUES FOR ALL VARIABLES EXCEPT THE GROWTH
DIC> @@ RATE. IN THIS EXAMPLE WE WILL TRY 1E-6
DIC> @@
DIC> @@ FOR MORE INFORMATION ABOUT THE PEARLITE GROWTH MODEL SEE
DIC> @@ B. JÖNSSON: 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>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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
  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   0.76465982E-05 AND   0.76465982E-05
 POSITION OF INTERFACE PEARLITE / AUSTENITE IS   0.50076466E-09
 U-FRACTION IN SYSTEM:  C = .0233843320030518  FE = .990707670399294
                        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                   0 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   0.76468335E-05 AND   0.76468335E-05
 POSITION OF INTERFACE PEARLITE / AUSTENITE IS   0.12654480E-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 =  0.13026424E-02 DT =  0.12025424E-02 SUM OF SQUARES =   0.0000000
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.76496630E-05 AND   0.76496630E-05
 POSITION OF INTERFACE PEARLITE / AUSTENITE IS   0.10464492E-07
 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
  2 GRIDPOINT(S) REMOVED FROM CELL#  1 REGION #  1
 TIME =  0.37077272E-02 DT =  0.24050848E-02 SUM OF SQUARES =   0.0000000
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.76553232E-05 AND   0.76553232E-05
 POSITION OF INTERFACE PEARLITE / AUSTENITE IS   0.28876193E-07
 U-FRACTION IN SYSTEM:  C = .0233843320030517  FE = .990707670399294
                        MN = .0092923297312127
 TOTAL SIZE OF SYSTEM:  2.68092626329E-13 [m^3]
  CPU time used in timestep                   0 seconds
  1 GRIDPOINT(S) REMOVED FROM CELL#  1 REGION #  1
 TIME =  0.85178967E-02 DT =  0.48101695E-02 SUM OF SQUARES =   0.0000000
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.76666480E-05 AND   0.76666480E-05
 POSITION OF INTERFACE PEARLITE / AUSTENITE IS   0.65754070E-07
 U-FRACTION IN SYSTEM:  C = .0233843320030517  FE = .990707670399295
                        MN = .0092923297312127
 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 =  0.18138236E-01 DT =  0.96203391E-02 SUM OF SQUARES =   0.0000000
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.76893156E-05 AND   0.76893156E-05
 POSITION OF INTERFACE PEARLITE / AUSTENITE IS   0.13972789E-06
 U-FRACTION IN SYSTEM:  C = .0233843320030517  FE = .990707670399294
                        MN = .00929232973121269
 TOTAL SIZE OF SYSTEM:  2.68092626329E-13 [m^3]
  CPU time used in timestep                   0 seconds
 TIME =  0.37378914E-01 DT =  0.19240678E-01 SUM OF SQUARES =   0.0000000
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.77347217E-05 AND   0.77347217E-05
 POSITION OF INTERFACE PEARLITE / AUSTENITE IS   0.28854918E-06
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399294
                        MN = .00929232973121269
 TOTAL SIZE OF SYSTEM:  2.68092626329E-13 [m^3]
  CPU time used in timestep                   0 seconds
 TIME =  0.75860270E-01 DT =  0.38481356E-01 SUM OF SQUARES =   0.0000000
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.78258159E-05 AND   0.78258159E-05
 POSITION OF INTERFACE PEARLITE / AUSTENITE IS   0.58969719E-06
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399294
                        MN = .00929232973121268
 TOTAL SIZE OF SYSTEM:  2.68092626329E-13 [m^3]
  CPU time used in timestep                   0 seconds
  1 GRIDPOINT(S) REMOVED FROM CELL#  1 REGION #  1
 TIME =  0.15282298     DT =  0.76962713E-01 SUM OF SQUARES =   0.0000000
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.80091146E-05 AND   0.80091146E-05
 POSITION OF INTERFACE PEARLITE / AUSTENITE IS   0.12061004E-05
 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
 TIME =  0.25282298     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.82494350E-05 AND   0.82494350E-05
 POSITION OF INTERFACE PEARLITE / AUSTENITE IS   0.20310439E-05
 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 =  0.35282298     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.84921077E-05 AND   0.84921077E-05
 POSITION OF INTERFACE PEARLITE / AUSTENITE IS   0.28802546E-05
 U-FRACTION IN SYSTEM:  C = .0233843320030515  FE = .990707670399295
                        MN = .00929232973121269
 TOTAL SIZE OF SYSTEM:  2.68092626329E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =  0.45282298     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.87370419E-05 AND   0.87370419E-05
 POSITION OF INTERFACE PEARLITE / AUSTENITE IS   0.37539588E-05
 U-FRACTION IN SYSTEM:  C = .0233843320030515  FE = .990707670399294
                        MN = .00929232973121275
 TOTAL SIZE OF SYSTEM:  2.68092626329E-13 [m^3]


output ignored...



... output resumed

 DELETING TIME-RECORD FOR TIME    2.9528230
 DELETING TIME-RECORD FOR TIME    3.0528230
 DELETING TIME-RECORD FOR TIME    3.1528230

 KEEPING TIME-RECORD FOR TIME    3.2528230
 AND FOR TIME                    3.3262605
 WORKSPACE RECLAIMED
  INFO: CELL   1 REGION AUSTENITE   DELETED
 U-FRACTION IN SYSTEM:  C = .0233843320030519  FE = .990707670399278
                        MN = .00929232973122969
 TOTAL SIZE OF SYSTEM:  2.67725268543E-13 [m^3]
 U-FRACTION IN SYSTEM:  C = .0233843320030519  FE = .990707670399278
                        MN = .00929232973122969
 TOTAL SIZE OF SYSTEM:  2.67725268543E-13 [m^3]
 TIME =   3.3262705     DT =  0.10000000E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030519  FE = .990707670399278
                        MN = .00929232973122969
 TOTAL SIZE OF SYSTEM:  2.67725268543E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   3.3362705     DT =  0.10000000E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030519  FE = .990707670399278
                        MN = .00929232973122969
 TOTAL SIZE OF SYSTEM:  2.67725268543E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   3.4362705     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030519  FE = .990707670399278
                        MN = .00929232973122969
 TOTAL SIZE OF SYSTEM:  2.67725268543E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   3.5362705     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030519  FE = .990707670399278
                        MN = .00929232973122969
 TOTAL SIZE OF SYSTEM:  2.67725268543E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   3.6362705     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030519  FE = .990707670399278
                        MN = .00929232973122969
 TOTAL SIZE OF SYSTEM:  2.67725268543E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   3.7362705     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030519  FE = .990707670399278
                        MN = .00929232973122969
 TOTAL SIZE OF SYSTEM:  2.67725268543E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   3.8362705     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030519  FE = .990707670399278
                        MN = .00929232973122969
 TOTAL SIZE OF SYSTEM:  2.67725268543E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   3.9362705     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030519  FE = .990707670399278
                        MN = .00929232973122969
 TOTAL SIZE OF SYSTEM:  2.67725268543E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   4.0362705     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030519  FE = .990707670399278
                        MN = .00929232973122969
 TOTAL SIZE OF SYSTEM:  2.67725268543E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   4.1362705     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030519  FE = .990707670399278
                        MN = .00929232973122969
 TOTAL SIZE OF SYSTEM:  2.67725268543E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   4.2362705     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030519  FE = .990707670399278
                        MN = .00929232973122969
 TOTAL SIZE OF SYSTEM:  2.67725268543E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   4.3362705     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030519  FE = .990707670399278
                        MN = .00929232973122969
 TOTAL SIZE OF SYSTEM:  2.67725268543E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   4.4362705     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030519  FE = .990707670399278
                        MN = .00929232973122969
 TOTAL SIZE OF SYSTEM:  2.67725268543E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   4.5362705     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030519  FE = .990707670399278
                        MN = .00929232973122969
 TOTAL SIZE OF SYSTEM:  2.67725268543E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   4.6362705     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030519  FE = .990707670399278
                        MN = .00929232973122969
 TOTAL SIZE OF SYSTEM:  2.67725268543E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   4.7362705     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030519  FE = .990707670399278
                        MN = .00929232973122969
 TOTAL SIZE OF SYSTEM:  2.67725268543E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   4.8362705     DT =  0.10000000     SUM OF SQUARES =   0.0000000
```

```
 U-FRACTION IN SYSTEM:  C = .0233843320030519  FE = .990707670399278
                        MN = .00929232973122969
 TOTAL SIZE OF SYSTEM:  2.67725268543E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   4.9362705     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030519  FE = .990707670399278
                        MN = .00929232973122969
 TOTAL SIZE OF SYSTEM:  2.67725268543E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   5.0000000     DT =  0.63729517E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030519  FE = .990707670399278
                        MN = .00929232973122969
 TOTAL SIZE OF SYSTEM:  2.67725268543E-13 [m^3]
 MUST SAVE WORKSPACE ON FILE
 WORKSPACE SAVED ON FILE
 RECLAIMING WORKSPACE
 DELETING TIME-RECORD FOR TIME    3.2528230
 DELETING TIME-RECORD FOR TIME    3.3262605
 DELETING TIME-RECORD FOR TIME    3.3262705
 DELETING TIME-RECORD FOR TIME    3.3362705
 DELETING TIME-RECORD FOR TIME    3.4362705
 DELETING TIME-RECORD FOR TIME    3.5362705
 DELETING TIME-RECORD FOR TIME    3.6362705
 DELETING TIME-RECORD FOR TIME    3.7362705
 DELETING TIME-RECORD FOR TIME    3.8362705
 DELETING TIME-RECORD FOR TIME    3.9362705
 DELETING TIME-RECORD FOR TIME    4.0362705
 DELETING TIME-RECORD FOR TIME    4.1362705
 DELETING TIME-RECORD FOR TIME    4.2362705
 DELETING TIME-RECORD FOR TIME    4.3362705
 DELETING TIME-RECORD FOR TIME    4.4362705
 DELETING TIME-RECORD FOR TIME    4.5362705
 DELETING TIME-RECORD FOR TIME    4.6362705
 DELETING TIME-RECORD FOR TIME    4.7362705
 DELETING TIME-RECORD FOR TIME    4.8362705

 KEEPING TIME-RECORD FOR TIME    4.9362705
 AND FOR TIME                    5.0000000
 WORKSPACE RECLAIMED

 TIMESTEP AT     5.00000000     SELECTED

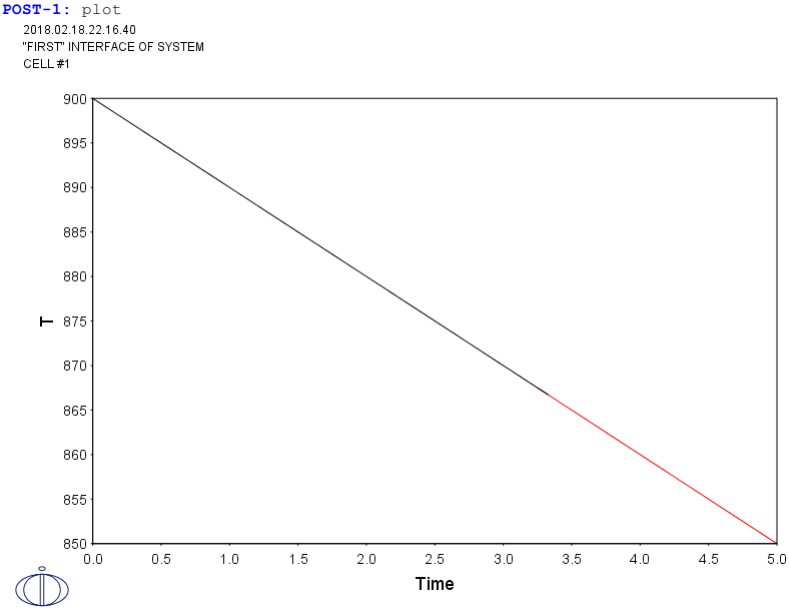
DIC>
DIC> @@
DIC> @@ THE SIMULATION IS FINISHED
DIC> @@
DIC>
DIC> set-inter
 --OK---
DIC>
```

exe1-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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

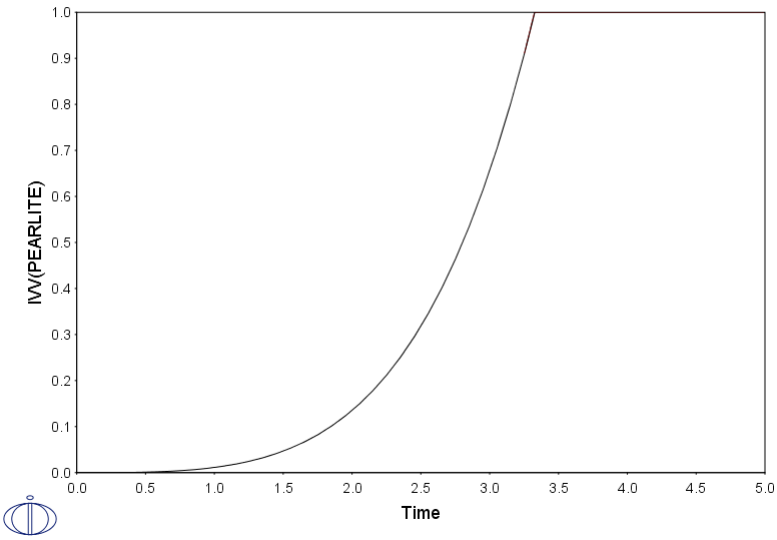
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson

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: plot
```



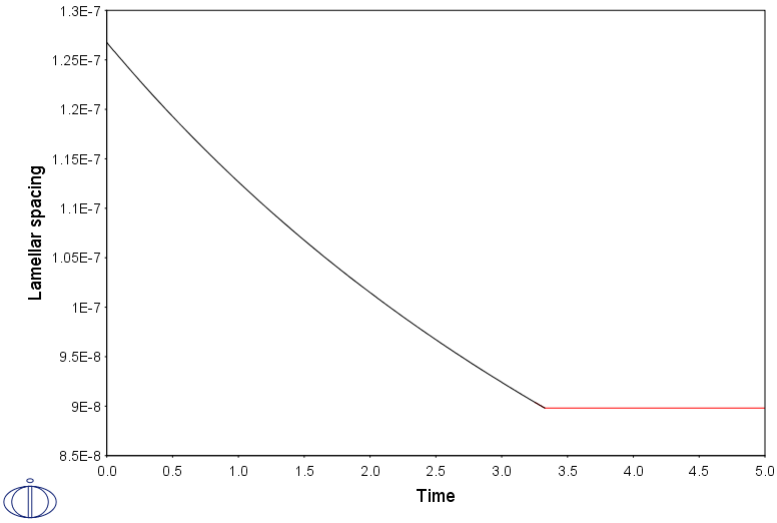

```
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ NOW PLOT THE FRACTION OF PEARLITE VS. TIME
POST-1: @@
POST-1: s-d-a y ivv(pearlite)
POST-1:
POST-1: plot
```

2018.02.18.22.16.41
CELL #1



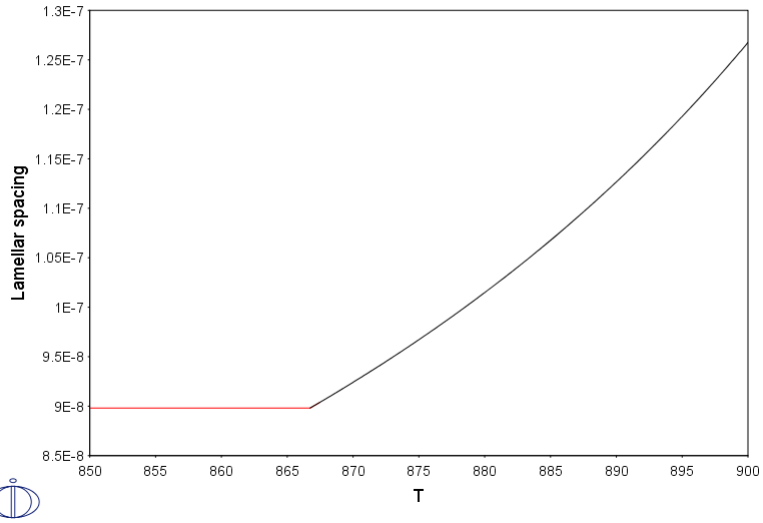
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ PLOT THE LAMELLAR SPACING AS A FUNCTION OF TIME
POST-1: @@
POST-1: s-d-a
AXIS (X, Y OR Z) : y
VARIABLE : lamellar-sp
IN REGION: /*/: pearlite
POST-1:
POST-1: s-p-c
CONDITION /INTEGRAL/: interface
INTERFACE : pearlite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

2018.02.18.22.16.41
UPPER INTERFACE OF REGION "PEARLITE#1"
CELL #1



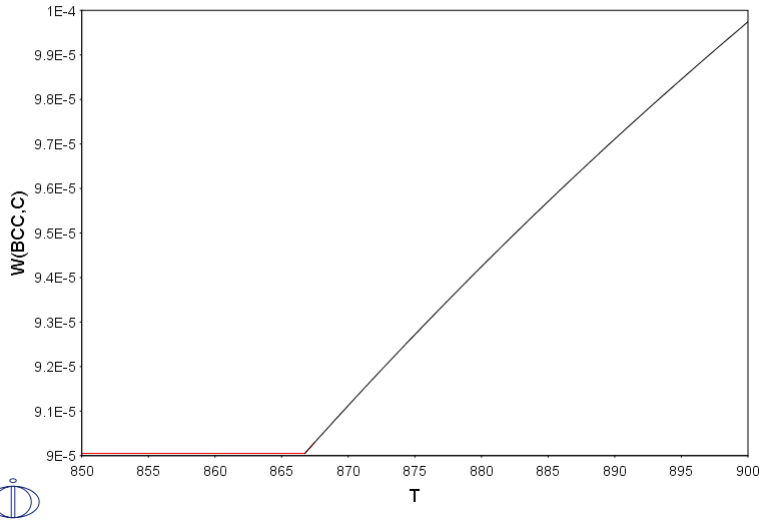
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ LET'S LOOK AT THE LAMELLAR SPACING VS. TEMPERATURE INSTEAD
POST-1: @@
POST-1: s-d-a x t
POST-1:
POST-1: s-p-c interface pearlite upper
POST-1:
POST-1: plot

2018.02.18.22.16.42
UPPER INTERFACE OF REGION "PEARLITE#1"
CELL #1



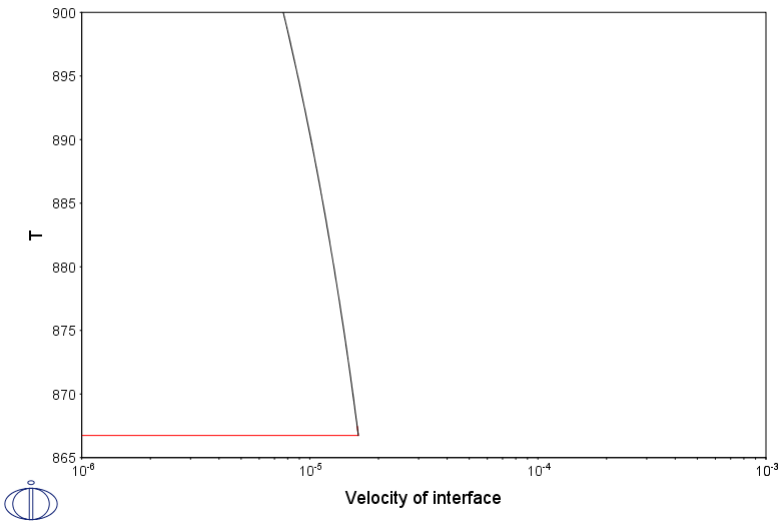
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ AND THE C COMPOSITION IN THE FERRITE VS. TEMP
POST-1: @@
POST-1: s-d-a y w(bcc,c)
POST-1:
POST-1:
POST-1: plot

2018.02.18.22.16.42
UPPER INTERFACE OF REGION "PEARLITE#1"
CELL #1



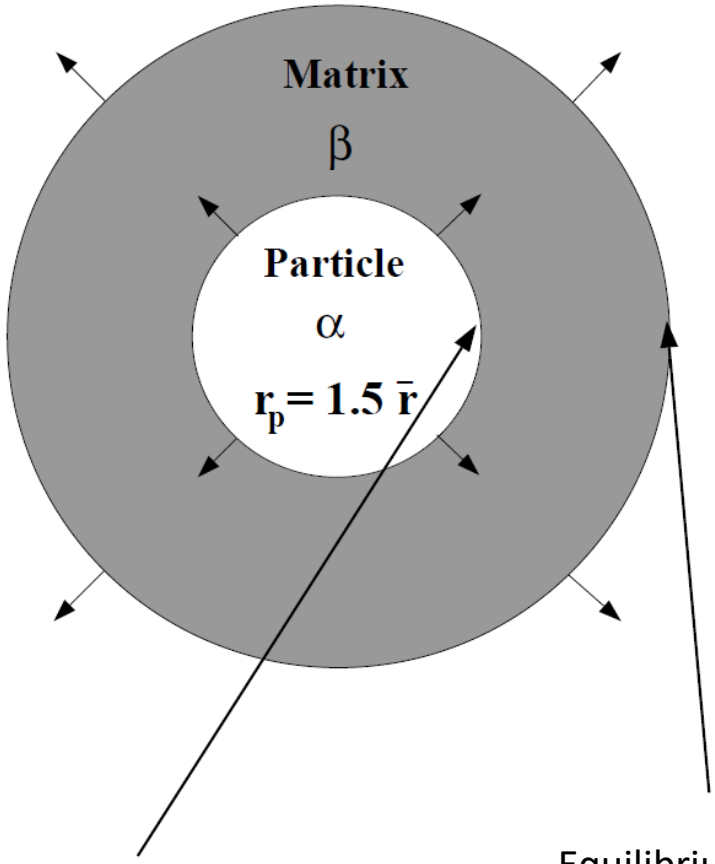
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ FINALLY, LET'S LOOK AT THE VELOCITY OF THE INTERFACE VS. TEMP
POST-1: @@
POST-1: s-d-a y t
POST-1: s-d-a x velocity
INTERFACE : pearlite
UPPER OR LOWER INTERFACE OF REGION PEARLITE#1 /LOWER/: upper
POST-1: set-ax-ty x log
POST-1: s-s-s x n 1e-6 1e-4
POST-1:
POST-1: plot

2018.02.18.22.16.43
UPPER INTERFACE OF REGION "PEARLITE#1"
CELL #1



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

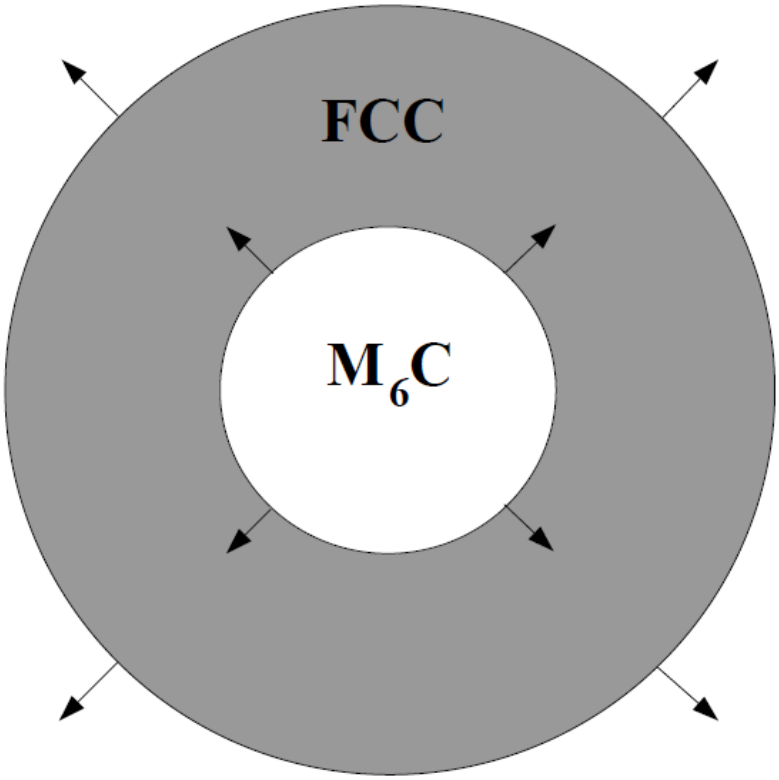
Equilibrium as defined by the average composition in the system.

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

```
About Stockholm, Sweden

 Software  (build 12987) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri Feb 16 15:22:08 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

 VA                     /-  DEFINED
 L12_FCC                B2_BCC                 DICTRA_FCC_A1
   REJECTED
TDB_TCFE9: switch tcfe7
 Current database: Steels/Fe-Alloys  v7.0

 VA  DEFINED
 L12_FCC                B2_BCC                 B2_VACANCY
 HIGH_SIGMA             DICTRA_FCC_A1  REJECTED
TDB_TCFE7: def-sys fe mo c
 FE                     MO                     C
   DEFINED
TDB_TCFE7: rej ph * all
 GAS:G                  LIQUID:L               BCC_A2
 FCC_A1                 HCP_A3                 DIAMOND_FCC_A4
 GRAPHITE               CEMENTITE              M23C6
 M7C3                   M6C                    M5C2
 M3C2                   MC_ETA                 MC_SHP
 KSI_CARBIDE            A1_KAPPA               KAPPA
 Z_PHASE                FE4N_LP1               FECN_CHI
 SIGMA                  MU_PHASE               P_PHASE
 R_PHASE                CHI_A12                LAVES_PHASE_C14
   REJECTED
TDB_TCFE7: res ph fcc m6c
 FCC_A1                 M6C  RESTORED
TDB_TCFE7: get
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'
  'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C
      -FE'
  'J-O. Andersson, Calphad, 12 (1988), 1-8; TRITA 0317 (1986); C-MO'
  'A. Fernandez Guillermet, Calphad, 6 (1982), 127-140; (sigma phase revised
      1986); TRITA-MAC 200 (1982); FE-MO'
  'J-O. Andersson, Calphad, 12 (1988), 9-23; TRITA 0321 (1986); C-FE-MO'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
      Molar volumes'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'S. Nagakura (1968), Transactions of the Iron and Steel Institute of Japan,
       Vol.8, pp. 265-294; Molar volumes'
  'Kupalova, IK and Pavlova, VI (988); High speed steels: Physical
      Properties, Prop. Data Update, 2, 67-78; Molar volumes'
 -OK-
TDB_TCFE7:
TDB_TCFE7: @@
TDB_TCFE7: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE MOBILITY DATA
TDB_TCFE7: @@
TDB_TCFE7: app
 Use one of these databases

 TCFE9   =  Steels/Fe-Alloys  v9.0
 TCFE10  =  Steels/Fe-Alloys  v10.0 SNAPSHOT
 TCFE8   =  Steels/Fe-Alloys  v8.1
 FROST1  =  FROST database v1.0
 TCFE7   =  Steels/Fe-Alloys  v7.0
 TCFE6   =  Steels/Fe-Alloys  v6.2
 TCFE5   =  Steels/Fe-Alloys  v5.0
 TCFE4   =  Steels/Fe-Alloys  v4.1
 TCFE3   =  Steels/Fe-Alloys  v3.1
 TCFE2   =  Steels/Fe-Alloys  v2.1
 TCFE1   =  Steels/Fe-Alloys  v1.0
 TCNI9   =  Ni-Alloys  v9.0 SNAPSHOT
 NI25    =  NI25 database
 TCNI8   =  Ni-Alloys  v8.1
 TCNI7   =  Ni-Alloys  v7.1
 TCNI6   =  Ni-Alloys  v6.0
 TCNI5   =  Ni-Alloys  v5.1
 TCNI4   =  Ni-Alloys  v4.0
 TCNI1   =  Ni-Alloys  v1.3
 TCAL5   =  Al-Alloys  v5.0
 TCAL4   =  Al-Alloys  v4.0
 TCAL3   =  Al-Alloys  v3.0
 TCAL2   =  Al-Alloys  v2.1
 TCAL1   =  Al-Alloys  v1.2
 TCMG4   =  Mg-Alloys  v4.0
 TCMG3   =  Mg-Alloys  v3.0
 TCMG2   =  Mg-Alloys  v2.0
 TCMG1   =  Mg-Alloys  v1.1
 TCTI1   =  Ti-Alloys  v1.0
 TCCU2   =  Cu-Alloys  v2.0
 TCCU1   =  Cu-Alloys  v1.0
```

```
 TCCC1   =  Cemented carbide  v1.0
 TCHEA2  =  High Entropy Alloy  v2.1
 TCHEA1  =  High Entropy Alloy  v1.0
 SSOL6   =  SGTE Alloy Solutions Database v6.0
 SSOL5   =  SGTE Alloy Solutions Database v5.0
 SSOL4   =  SGTE Alloy Solutions Database v4.9g
 SSOL2   =  SGTE Alloy Solutions Database v2.1
 SSUB6   =  SGTE Substances Database v6.0
 SSUB5   =  SGTE Substances Database v5.2
 SSUB4   =  SGTE Substances Database v4.1
 SSUB3   =  SGTE Substances Database v3.3
 SSUB2   =  SGTE Substances Database v2.2
 SNOB3   =  SGTE Noble Metal Alloys Database v3.1
 STBC2   =  SGTE Thermal Barrier Coating TDB v2.2
 STBC1   =  SGTE Thermal Barrier Coating TDB v1.1
 SALT1   =  SGTE Molten Salts Database v1.2
 SEMC2   =  TC Semi-Conductors  v2.1
 SLAG4   =  Fe-containing Slag  v4.1
 SLAG3   =  Fe-containing Slag  v3.2
 SLAG2   =  Fe-containing Slag  v2.2
 SLAG1   =  Fe-containing Slag  v1.2
 TCOX7   =  Metal Oxide Solutions  v7.0
 TCOX6   =  Metal Oxide Solutions  v6.0
 TCOX5   =  Metal Oxide Solutions  v5.1
 TCOX4   =  Metal Oxide Solutions  v4.1
 ION3    =  Ionic Solutions  v3.0
 ION2    =  Ionic Solutions  v2.6
 ION1    =  Ionic Solutions  v1.5
 NOX2    =  NPL Oxide Solutions Database v2.1
 TCNOBL1 =  Noble Metals Alloys v1.0
 TCSLD3  =  Solder Alloys  v3.2
 TCSLD2  =  Solder Alloys  v2.0
 TCSI1   =  Ultrapure Silicon  v1.2
 TCMP2   =  Materials Processing  v2.5
 TCES1   =  Combustion/Sintering  v1.1
 TCSC1   =  Super Conductor  v1.0
 TCFC1   =  SOFC Database v1.0
 NUMT2   =  Nuclear Materials  v2.1
 NUOX4   =  Nuclear Oxides  v4.2
 NUCL15  =  IRSN NUCLEA-15_4
 NUCL10  =  ThermoData NUCLEA Alloys-oxides TDB v10.2
 MEPH15  =  IRSN Mephista-15_1
 MEPH11  =  ThermoData MEPHISTA Nuclear Fuels TDB v11.2
 TCAQ3   =  Aqueous Solution  v3.0
 TCAQ2   =  Aqueous Solution  v2.6
 AQS2    =  TGG Aqueous Solution Database v2.6
 GCE2    =  TGG Geochemical/Environmental TDB v2.3
 FEDEMO  =  Iron Demo Database v2.0
 ALDEMO  =  Aluminum Demo Database v2.0
 NIDEMO  =  Nickel Demo Database v1.0
 CUDEMO  =  Copper Demo Database v1.0
 SLDEMO  =  Solder Demo Database v1.0
 OXDEMO  =  Oxide Demo Database v1.0
 SUBDEMO =  Substance Demo Database v1.0
 PTERN   =  Public Ternary Alloys TDB v1.3
 PAQ2    =  Public Aqueous Soln (SIT) TDB v2.4
 PG35    =  G35 Binary Semi-Conductors TDB v1.2
 PURE5   =  SGTE Unary (Pure Elements) TDB v5.1
 MOB2    =  Alloys Mobility  v2.7
 MOB1    =  Alloys Mobility  v1.3
 MOBFE1  =  Steels/Fe-Alloys Mobility  v1.0
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBNI4  =  Ni-Alloys Mobility  v4.0
 MOBNI3  =  Ni-Alloys Mobility  v3.1
 MOBNI2  =  Ni-Alloys Mobility  v2.4
 MOBNI1  =  Ni-Alloys Mobility  v1.0
 MOBAL3  =  Al-Alloys Mobility  v3.0
 MOBAL2  =  Al-Alloys Mobility  v2.0
 MOBAL1  =  Al-Alloys Mobility  v1.0
 MOBCU1  =  Cu-Alloys Mobility  v1.0
 MOBCU2  =  Cu-Alloys Mobility  v2.0
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBSLD1 =  Solder-Alloys Mobility  v1.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0 SNAPSHOT
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v1.0
 MFEDEMO =  Fe-Alloys Mobility demo database v2.0
 MNIDEMO =  Ni-Alloys Mobility demo database v1.0
 MCUDEMO =  Cu-Alloys Mobility demo database v1.0
 USER    =  User defined Database

DATABASE NAME /TCFE7/: mobfe2
 Current database: Steels/Fe-Alloys Mobility  v2.0
   TCS Steel Mobility Database Version 2.0 from 2011-12-09.

 VA  DEFINED
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
 *** M6C INPUT IGNORED
 FCC_A1  RESTORED
APP: get
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'This parameter has not been assessed'
  'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'
  'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
      -Ni'
  'H. Oikawa, Tech. Rept. Tohoku Univ., 48(1983)7.; Impurity diffusion of Mo
      in fcc Fe.'
 -OK-
APP:
```

```
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR
APP: @@
APP: go d-m
 NO TIME STEP DEFINED
 *** ENTERING M6C AS A DIFFUSION NONE PHASE
DIC>
DIC> @@
DIC> @@  ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> s-cond glob t 0 1173; * N

DIC>
DIC> @@
DIC> @@ ENTER REGIONS part AND aus
DIC> @@
DIC> enter-region
REGION NAME : part
DIC> enter-region aus
ATTACH TO REGION NAMED /PART/:
ATTACHED TO THE RIGHT OF PART /YES/:
DIC> @@
DIC> @@ ENTER 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>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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
 single geometric dense at  0.22800E-06
 0.80000       64
 Region: AUS
 single geometric dense at   0.0000
  1.0060       63
  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 = .0292387089677228
 TOTAL SIZE OF SYSTEM:  1.32376603026E-18 [m^3]
 U-FRACTION IN SYSTEM:  C = .0190652843033664  FE = .970761291162784
                        MO = .0292387089677228
 TOTAL SIZE OF SYSTEM:  1.32376603026E-18 [m^3]
 0.610222970497725        0.610391048253450        0.610222911134997        2.564830791787979E-002        2.191933775022290E-
003        1.266865136119346E-004        1.096501638371350E-003        1.278319034558927E-004        4.432656719961518E-
007        1.566395510936704E-009        1.947833880265816E-009        3.659995728395455E-009        1.418022229672293E-
009        1.309139620588423E-009        1.103985036086987E-009        3.800021162887927E-009        7.446660865207878E-
010        2.344009117646817E-010        1.080152646799767E-013        1.867047643211421E-018       TIME =  0.10000000E-06 DT =  0.10000000E-
06 SUM OF SQUARES =  0.18670476E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.50349420E-05 AND  -0.50349420E-05
 POSITION OF INTERFACE PART / AUS IS   0.22799950E-06
 U-FRACTION IN SYSTEM:  C = .0190659317665459  FE = .970759487634635
                        MO = .0292405124958722
 TOTAL SIZE OF SYSTEM:  1.32375726043E-18 [m^3]
  6  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: PART

  CPU time used in timestep                    1 seconds
 5.960105249474015E-005        5.961332411825232E-005        5.959460176685140E-005        3.934412729020296E-007        1.790897250277762E-
012        8.025303698046624E-020       SWITCHING ACTIVITIES FOR INTERFACE #2, CELL #1
 FROM: C  TO: MO

 TIME =  0.25446963E-05 DT =  0.24446963E-05 SUM OF SQUARES =  0.80253037E-19
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.39311816E-08 AND  -0.39311816E-08
 POSITION OF INTERFACE PART / AUS IS   0.22799949E-06
 U-FRACTION IN SYSTEM:  C = .0190664790765648  FE = .970759484142024
                        MO = .0292405159884825
 TOTAL SIZE OF SYSTEM:  1.32375709303E-18 [m^3]
  CPU time used in timestep                    0 seconds
 2.515003169879022E-008        2.515606839736259E-008        2.499418773175797E-008        2.005402508809647E-008        1.975188680744917E-
008        1.916893094188025E-008        1.798098166063758E-008        1.797987078560134E-008        1.576162116879742E-
008        1.172706230484645E-008        5.463976248626018E-009        5.470072379592426E-009        2.575739208186408E-
011        1.050353544654548E-019       TIME =  0.74340890E-05 DT =  0.48893927E-05 SUM OF SQUARES =  0.10503535E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.56316592E-09 AND  -0.56316592E-09
 POSITION OF INTERFACE PART / AUS IS   0.22799948E-06
 U-FRACTION IN SYSTEM:  C = .0190671017667952  FE = .970759483934874
                        MO = .0292405161956331
 TOTAL SIZE OF SYSTEM:  1.32375704507E-18 [m^3]
  CPU time used in timestep                    0 seconds
 4.332551967282598E-010        4.333461945146029E-010        4.418343369955179E-010        4.025620070840790E-010        4.017875831196053E-
010        4.002414387371992E-010        3.971401167325227E-010        3.975914295836094E-010        3.909910643665908E-
010        3.788198544736429E-010        3.550709191441153E-010        3.557264804400251E-010        3.098645677267985E-
010        2.286943575027542E-010        1.032590621477480E-010        1.037482117905484E-010        5.751503861739746E-
014        2.763822793450989E-024       TIME =  0.17212874E-04 DT =  0.97787853E-05 SUM OF SQUARES =  0.27638228E-23
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.11628456E-09 AND  -0.11628456E-09
 POSITION OF INTERFACE PART / AUS IS   0.22799948E-06
 U-FRACTION IN SYSTEM:  C = .0190679130625397  FE = .970759484400328
                        MO = .0292405157301795
 TOTAL SIZE OF SYSTEM:  1.32375702526E-18 [m^3]
  CPU time used in timestep                    1 seconds
 2.076847912747820E-011        2.077191339162079E-011        2.354369667011284E-011

output ignored...



... output resumed


  CPU time used in timestep                    1 seconds
 1.797896990453380E-009        1.817562512773176E-009        1.860191576603880E-009        1.285340664400574E-010        5.111582890912106E-
011        2.380129550930575E-017       TIME =   667998.25     DT =   100000.00     SUM OF SQUARES =  0.23801296E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.43742419E-13 AND   0.43742419E-13
 POSITION OF INTERFACE PART / AUS IS   0.26062097E-06
 U-FRACTION IN SYSTEM:  C = .0195372313730068  FE = .970698508146213
                        MO = .0293014919842948
 TOTAL SIZE OF SYSTEM:  1.97712789285E-18 [m^3]
  24  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: PART
  24  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUS

  CPU time used in timestep                    0 seconds
 1.233471697286479E-009        1.249173705752573E-009        1.284150172966186E-009        9.447077195244483E-011        3.990294095241907E-
011        1.009237030587298E-017       TIME =   767998.25     DT =   100000.00     SUM OF SQUARES =  0.10092370E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.42312933E-13 AND   0.42312933E-13
 POSITION OF INTERFACE PART / AUS IS   0.26485226E-06
 U-FRACTION IN SYSTEM:  C = .0195391105051876  FE = .970701112585041
                        MO = .0292988875454658
 TOTAL SIZE OF SYSTEM:  2.07499836302E-18 [m^3]
  23  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: PART
  22  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUS

  CPU time used in timestep                    0 seconds
 8.563550941427694E-010        8.689904479599197E-010        8.979024206738632E-010        6.898816135275240E-011        3.046766403834260E-
011        4.510099272753572E-018       TIME =   867998.25     DT =   100000.00     SUM OF SQUARES =  0.45100993E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.40994813E-13 AND   0.40994813E-13
 POSITION OF INTERFACE PART / AUS IS   0.26895174E-06
 U-FRACTION IN SYSTEM:  C = .0195409122716752  FE = .970703591885453
```

```
                       MO = .0292964082450549
 TOTAL SIZE OF SYSTEM:  2.17285021709E-18 [m^3]
  21  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: PART
  21  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUS

  CPU time used in timestep                    1 seconds
 5.974607342647882E-010        6.076711090577850E-010        6.316612824106478E-010        4.996744266686842E-011        2.282791334896858E-
011        1.268061141302764E-015        7.742683474201948E-
023       TIME =   967998.25     DT =   100000.00     SUM OF SQUARES =  0.77426835E-22
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.39774705E-13 AND   0.39774705E-13
 POSITION OF INTERFACE PART / AUS IS   0.27292922E-06
 U-FRACTION IN SYSTEM:  C = .0195426437607411  FE = .970705953695093
                       MO = .0292940464354147
 TOTAL SIZE OF SYSTEM:  2.27068437365E-18 [m^3]
  20  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: PART
  20  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUS

  CPU time used in timestep                    0 seconds
 7.325232698426969E-010        7.226212817693013E-010        6.940725678957351E-010        1.243095839897094E-013        8.495379236702611E-
021       TIME =   1000000.0     DT =   32001.747     SUM OF SQUARES =  0.84953792E-20
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.39032951E-13 AND   0.39032951E-13
 POSITION OF INTERFACE PART / AUS IS   0.27417834E-06
 U-FRACTION IN SYSTEM:  C = .0195446957121146  FE = .970707245727071
                       MO = .0292927544034362
 TOTAL SIZE OF SYSTEM:  2.30200418971E-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   0.25446963E-05
 DELETING TIME-RECORD FOR TIME   0.74340890E-05
 DELETING TIME-RECORD FOR TIME   0.17212874E-04
 DELETING TIME-RECORD FOR TIME   0.36770445E-04
 DELETING TIME-RECORD FOR TIME   0.75885586E-04
 DELETING TIME-RECORD FOR TIME   0.15411587E-03
 DELETING TIME-RECORD FOR TIME   0.31057643E-03
 DELETING TIME-RECORD FOR TIME   0.62349756E-03
 DELETING TIME-RECORD FOR TIME   0.12493398E-02
 DELETING TIME-RECORD FOR TIME   0.25010243E-02
 DELETING TIME-RECORD FOR TIME   0.50043934E-02
 DELETING TIME-RECORD FOR TIME   0.10011131E-01
 DELETING TIME-RECORD FOR TIME   0.20024608E-01
 DELETING TIME-RECORD FOR TIME   0.40051560E-01
 DELETING TIME-RECORD FOR TIME   0.80105465E-01
 DELETING TIME-RECORD FOR TIME   0.16021327
 DELETING TIME-RECORD FOR TIME   0.32042889
 DELETING TIME-RECORD FOR TIME   0.64086013
 DELETING TIME-RECORD FOR TIME    1.2817226
 DELETING TIME-RECORD FOR TIME    2.5634476
 DELETING TIME-RECORD FOR TIME    5.1268975
 DELETING TIME-RECORD FOR TIME    10.253797
 DELETING TIME-RECORD FOR TIME    20.507597
 DELETING TIME-RECORD FOR TIME    41.015196
 DELETING TIME-RECORD FOR TIME    82.030394
 DELETING TIME-RECORD FOR TIME    164.06079
 DELETING TIME-RECORD FOR TIME    328.12158
 DELETING TIME-RECORD FOR TIME    656.24317
 DELETING TIME-RECORD FOR TIME    1312.4863
 DELETING TIME-RECORD FOR TIME    2624.9727
 DELETING TIME-RECORD FOR TIME    5249.9454
 DELETING TIME-RECORD FOR TIME    10499.891
 DELETING TIME-RECORD FOR TIME    20999.782
 DELETING TIME-RECORD FOR TIME    41999.563
 DELETING TIME-RECORD FOR TIME    83999.126
 DELETING TIME-RECORD FOR TIME    167998.25
 DELETING TIME-RECORD FOR TIME    267998.25
 DELETING TIME-RECORD FOR TIME    367998.25
 DELETING TIME-RECORD FOR TIME    467998.25
 DELETING TIME-RECORD FOR TIME    567998.25
 DELETING TIME-RECORD FOR TIME    667998.25
 DELETING TIME-RECORD FOR TIME    767998.25
 DELETING TIME-RECORD FOR TIME    867998.25

 KEEPING TIME-RECORD FOR TIME    967998.25
 AND FOR TIME                    1000000.0
 WORKSPACE RECLAIMED

 TIMESTEP AT     1000000.00     SELECTED

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

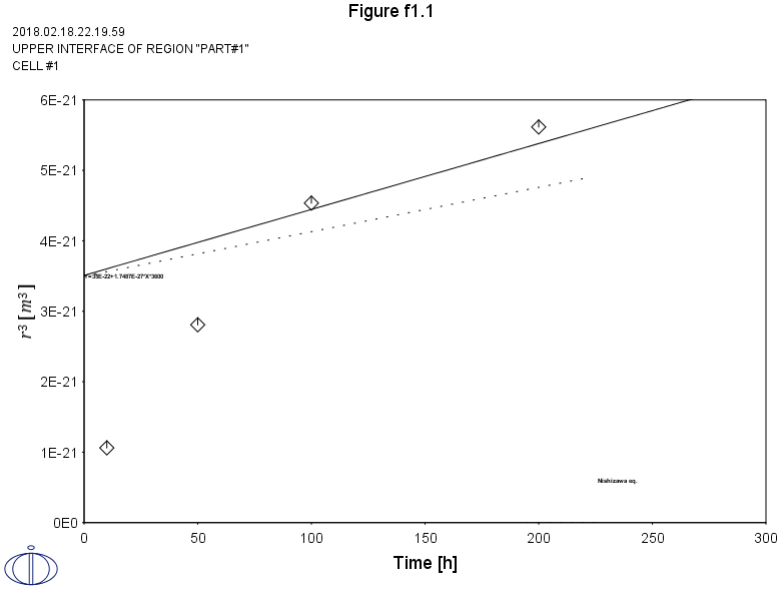
exf1-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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

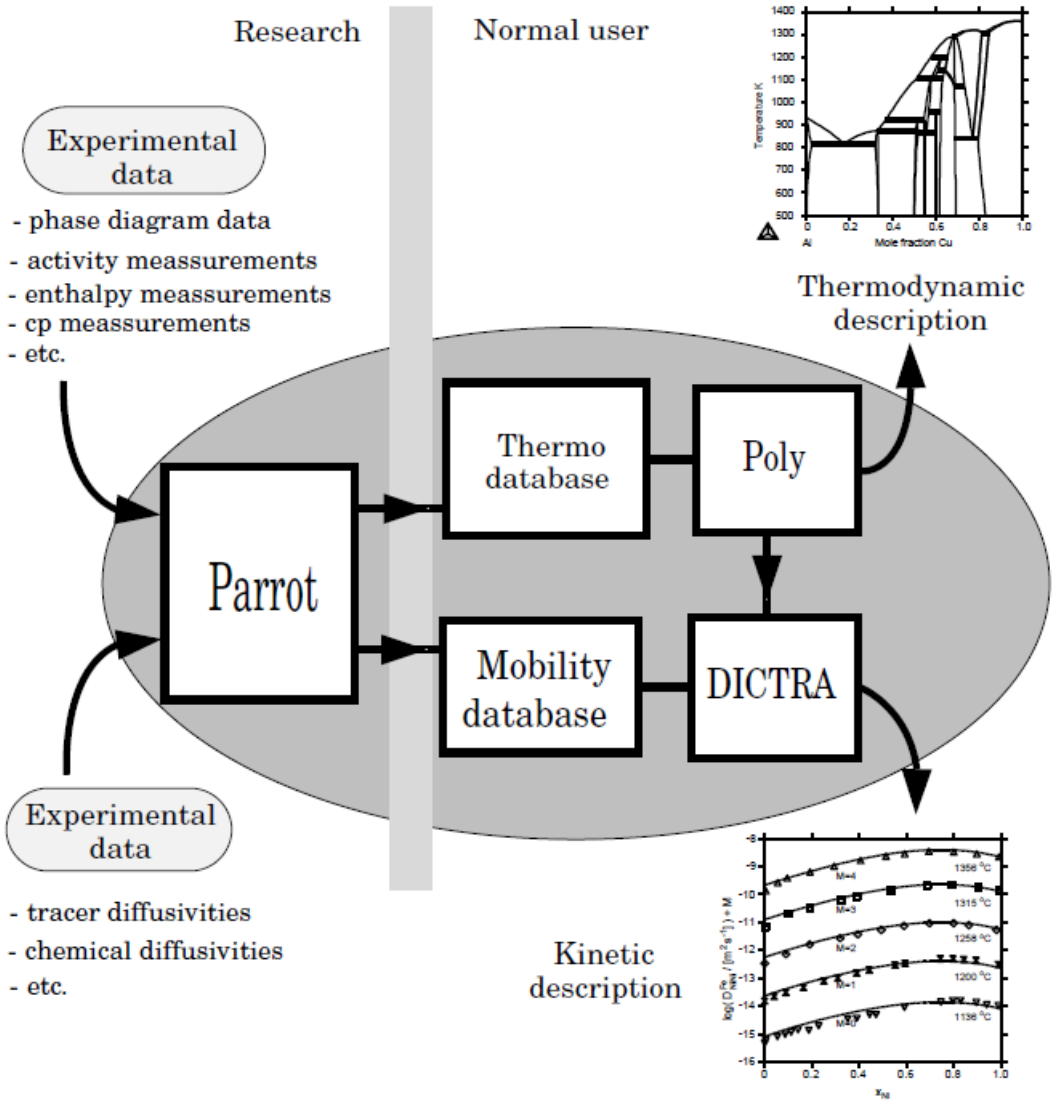
POST-1:
POST-1: @@
POST-1: @@ PLOT THE AVERAGE PARTICLE SIZE (CUBED) AS THIS ASSUMED TO
POST-1: @@ SCALE LINEARLY WITH TIME. THEN A FUNCTION IS ENTERED SO
POST-1: @@ THIS QUANTITY CAN BE ACCESSED. WE ALSO WANT TO PLOT THIS
POST-1: @@ QUANTITY VERSUS TIME (IN HOURS) SO A FUNCTION IS ENTERED.
POST-1: @@
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: 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:
```

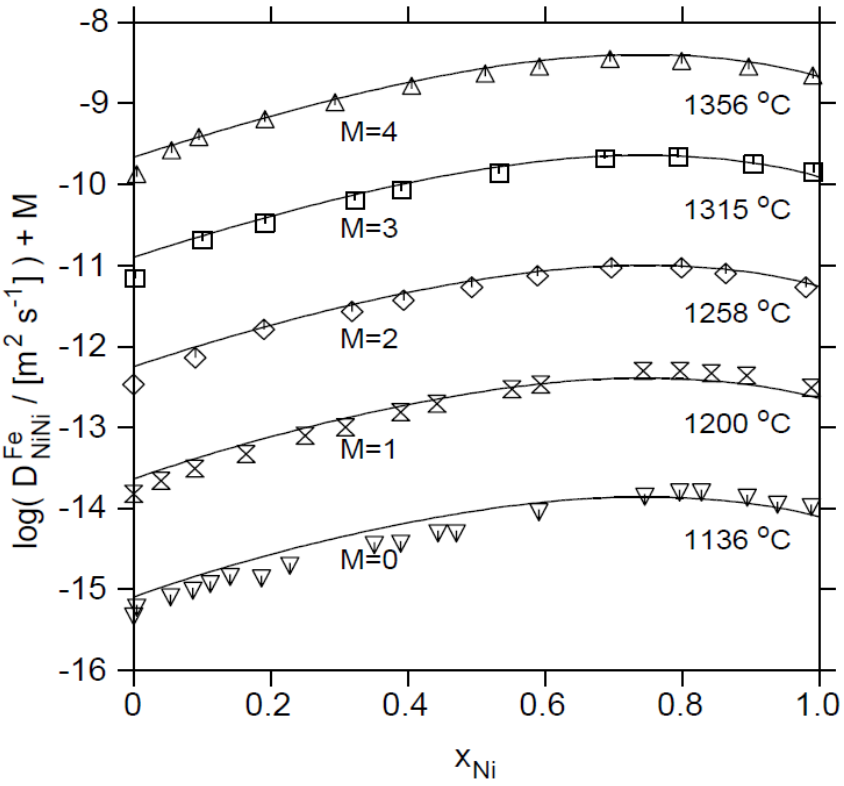
Kinetic Data



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

```
About Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 12987) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri Feb 16 15:22:08 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exg1\setup.DCM" @@
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
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

 VA                     /-  DEFINED
 L12_FCC                B2_BCC                 DICTRA_FCC_A1
   REJECTED
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ SELECT A DATABASE FOR THERMODYNAMIC DATA
TDB_TCFE9: @@
TDB_TCFE9: sw tcfe7
 Current database: Steels/Fe-Alloys  v7.0

 VA  DEFINED
 L12_FCC                B2_BCC                 B2_VACANCY
 HIGH_SIGMA             DICTRA_FCC_A1  REJECTED
TDB_TCFE7:
TDB_TCFE7: @@
TDB_TCFE7: @@ DEFINE THE SYSTEM TO WORK WITH
TDB_TCFE7: @@
TDB_TCFE7: def-sys fe ni
 FE                     NI  DEFINED
TDB_TCFE7:
TDB_TCFE7: @@
TDB_TCFE7: @@ EXCLUDE THE THERMODYNAMIC DATA FOR THE PHASES THAT ARE NOT NEEDED
TDB_TCFE7: @@
TDB_TCFE7: rej ph * all
 LIQUID:L               BCC_A2                 FCC_A1
 HCP_A3                 A1_KAPPA               KAPPA
 LAVES_PHASE_C14        NBNI3                  NI3TI
   REJECTED
TDB_TCFE7: res ph fcc
 FCC_A1  RESTORED
TDB_TCFE7:
TDB_TCFE7: @@
TDB_TCFE7: @@ RETRIEVE DATA FROM THE DATABASE FILE
TDB_TCFE7: @@
TDB_TCFE7: get
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'
  'A. Dinsdale, T. Chart, MTDS NPL, unpublished work (1986); FE-NI'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
      Molar volumes'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
 -OK-
TDB_TCFE7:
TDB_TCFE7: @@
TDB_TCFE7: @@ MOBILITY/DIFFUSIVITY DATA ARE STORED IN A SEPARATE DATABASE FILE.
TDB_TCFE7: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE DATA
TDB_TCFE7: @@
TDB_TCFE7: app
 Use one of these databases

 TCFE9   =  Steels/Fe-Alloys  v9.0
 TCFE10  =  Steels/Fe-Alloys  v10.0 SNAPSHOT
 TCFE8   =  Steels/Fe-Alloys  v8.1
 FROST1  =  FROST database v1.0
 TCFE7   =  Steels/Fe-Alloys  v7.0
 TCFE6   =  Steels/Fe-Alloys  v6.2
 TCFE5   =  Steels/Fe-Alloys  v5.0
 TCFE4   =  Steels/Fe-Alloys  v4.1
 TCFE3   =  Steels/Fe-Alloys  v3.1
 TCFE2   =  Steels/Fe-Alloys  v2.1
 TCFE1   =  Steels/Fe-Alloys  v1.0
 TCNI9   =  Ni-Alloys  v9.0 SNAPSHOT
 NI25    =  NI25 database
 TCNI8   =  Ni-Alloys  v8.1
 TCNI7   =  Ni-Alloys  v7.1
 TCNI6   =  Ni-Alloys  v6.0
 TCNI5   =  Ni-Alloys  v5.1
 TCNI4   =  Ni-Alloys  v4.0
 TCNI1   =  Ni-Alloys  v1.3
 TCAL5   =  Al-Alloys  v5.0
 TCAL4   =  Al-Alloys  v4.0
 TCAL3   =  Al-Alloys  v3.0
 TCAL2   =  Al-Alloys  v2.1
 TCAL1   =  Al-Alloys  v1.2
 TCMG4   =  Mg-Alloys  v4.0
 TCMG3   =  Mg-Alloys  v3.0
```

```
 TCMG2   =  Mg-Alloys  v2.0
 TCMG1   =  Mg-Alloys  v1.1
 TCTI1   =  Ti-Alloys  v1.0
 TCCU2   =  Cu-Alloys  v2.0
 TCCU1   =  Cu-Alloys  v1.0
 TCCC1   =  Cemented carbide  v1.0
 TCHEA2  =  High Entropy Alloy  v2.1
 TCHEA1  =  High Entropy Alloy  v1.0
 SSOL6   =  SGTE Alloy Solutions Database v6.0
 SSOL5   =  SGTE Alloy Solutions Database v5.0
 SSOL4   =  SGTE Alloy Solutions Database v4.9g
 SSOL2   =  SGTE Alloy Solutions Database v2.1
 SSUB6   =  SGTE Substances Database v6.0
 SSUB5   =  SGTE Substances Database v5.2
 SSUB4   =  SGTE Substances Database v4.1
 SSUB3   =  SGTE Substances Database v3.3
 SSUB2   =  SGTE Substances Database v2.2
 SNOB3   =  SGTE Noble Metal Alloys Database v3.1
 STBC2   =  SGTE Thermal Barrier Coating TDB v2.2
 STBC1   =  SGTE Thermal Barrier Coating TDB v1.1
 SALT1   =  SGTE Molten Salts Database v1.2
 SEMC2   =  TC Semi-Conductors  v2.1
 SLAG4   =  Fe-containing Slag  v4.1
 SLAG3   =  Fe-containing Slag  v3.2
 SLAG2   =  Fe-containing Slag  v2.2
 SLAG1   =  Fe-containing Slag  v1.2
 TCOX7   =  Metal Oxide Solutions  v7.0
 TCOX6   =  Metal Oxide Solutions  v6.0
 TCOX5   =  Metal Oxide Solutions  v5.1
 TCOX4   =  Metal Oxide Solutions  v4.1
 ION3    =  Ionic Solutions  v3.0
 ION2    =  Ionic Solutions  v2.6
 ION1    =  Ionic Solutions  v1.5
 NOX2    =  NPL Oxide Solutions Database v2.1
 TCNOBL1 =  Noble Metals Alloys v1.0
 TCSLD3  =  Solder Alloys  v3.2
 TCSLD2  =  Solder Alloys  v2.0
 TCSI1   =  Ultrapure Silicon  v1.2
 TCMP2   =  Materials Processing  v2.5
 TCES1   =  Combustion/Sintering  v1.1
 TCSC1   =  Super Conductor  v1.0
 TCFC1   =  SOFC Database v1.0
 NUMT2   =  Nuclear Materials  v2.1
 NUOX4   =  Nuclear Oxides  v4.2
 NUCL15  =  IRSN NUCLEA-15_4
 NUCL10  =  ThermoData NUCLEA Alloys-oxides TDB v10.2
 MEPH15  =  IRSN Mephista-15_1
 MEPH11  =  ThermoData MEPHISTA Nuclear Fuels TDB v11.2
 TCAQ3   =  Aqueous Solution  v3.0
 TCAQ2   =  Aqueous Solution  v2.6
 AQS2    =  TGG Aqueous Solution Database v2.6
 GCE2    =  TGG Geochemical/Environmental TDB v2.3
 FEDEMO  =  Iron Demo Database v2.0
 ALDEMO  =  Aluminum Demo Database v2.0
 NIDEMO  =  Nickel Demo Database v1.0
 CUDEMO  =  Copper Demo Database v1.0
 SLDEMO  =  Solder Demo Database v1.0
 OXDEMO  =  Oxide Demo Database v1.0
 SUBDEMO =  Substance Demo Database v1.0
 PTERN   =  Public Ternary Alloys TDB v1.3
 PAQ2    =  Public Aqueous Soln (SIT) TDB v2.4
 PG35    =  G35 Binary Semi-Conductors TDB v1.2
 PURE5   =  SGTE Unary (Pure Elements) TDB v5.1
 MOB2    =  Alloys Mobility  v2.7
 MOB1    =  Alloys Mobility  v1.3
 MOBFE1  =  Steels/Fe-Alloys Mobility  v1.0
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBNI4  =  Ni-Alloys Mobility  v4.0
 MOBNI3  =  Ni-Alloys Mobility  v3.1
 MOBNI2  =  Ni-Alloys Mobility  v2.4
 MOBNI1  =  Ni-Alloys Mobility  v1.0
 MOBAL3  =  Al-Alloys Mobility  v3.0
 MOBAL2  =  Al-Alloys Mobility  v2.0
 MOBAL1  =  Al-Alloys Mobility  v1.0
 MOBCU1  =  Cu-Alloys Mobility  v1.0
 MOBCU2  =  Cu-Alloys Mobility  v2.0
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBSLD1 =  Solder-Alloys Mobility  v1.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0 SNAPSHOT
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v1.0
 MFEDEMO =  Fe-Alloys Mobility demo database v2.0
 MNIDEMO =  Ni-Alloys Mobility demo database v1.0
 MCUDEMO =  Cu-Alloys Mobility demo database v1.0
 USER    =  User defined Database

DATABASE NAME /TCFE7/: mobfe2
 Current database: Steels/Fe-Alloys Mobility  v2.0
   TCS Steel Mobility Database Version 2.0 from 2011-12-09.

 VA  DEFINED
APP: def-sys fe ni
 FE                     NI  DEFINED
APP: rej ph * all
 BCC_A2                 FCC_A1                 HCP_A3
 LIQUID:L  REJECTED
APP: res ph fcc
 FCC_A1  RESTORED
APP: get
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'This parameter has not been assessed'
  'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
      -Ni'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Ni self-diffusion'
 -OK-
APP:
```

```
APP: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP
APP: @@
APP: go d-m
 NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ LIST MOBILITY DATA
DIC> @@
DIC> list-mob-data
 Sorry, LIST-DATA disabled for this database
DIC>
DIC>
DIC>
DIC>@?<Hit_return_to_continue>
DIC>
DIC> @@
DIC> @@ CHECK THE DIFFUSIVITES
DIC> @@
DIC> check
 AMBIGUOUS COMMAND, USE HELP
DIC>
DIC> fcc
 NO SUCH COMMAND, USE HELP
DIC> fe
 NO SUCH COMMAND, USE HELP
DIC> 0.3
 NO SUCH COMMAND, USE HELP
DIC> 101325
 NO SUCH COMMAND, USE HELP
DIC> 1409
 NO SUCH COMMAND, USE HELP
DIC> dl
 NO SUCH COMMAND, USE HELP
DIC>
DIC>
DIC>@?<Hit_return_to_continue>
DIC>
DIC> @@
DIC> @@ USE STEPPING IN POLY-3 TO CALCULATE THE DIFFUSIVITIES VS. COMPOSITION
DIC> @@
DIC> go p-3
POLY_3: s-c t=1409,p=101325,n=1,x(ni)=0.3
POLY_3: 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_3:
POLY_3: s-a-v
Axis number: /1/: 1
Condition /NONE/: x(ni)
Min value /0/: 0
Max value /1/: 1
Increment /.025/: 1e-3
POLY_3:
POLY_3: step
Option? /NORMAL/: normal
 No initial equilibrium, using default
 Step will start from axis value   0.300000
...OK

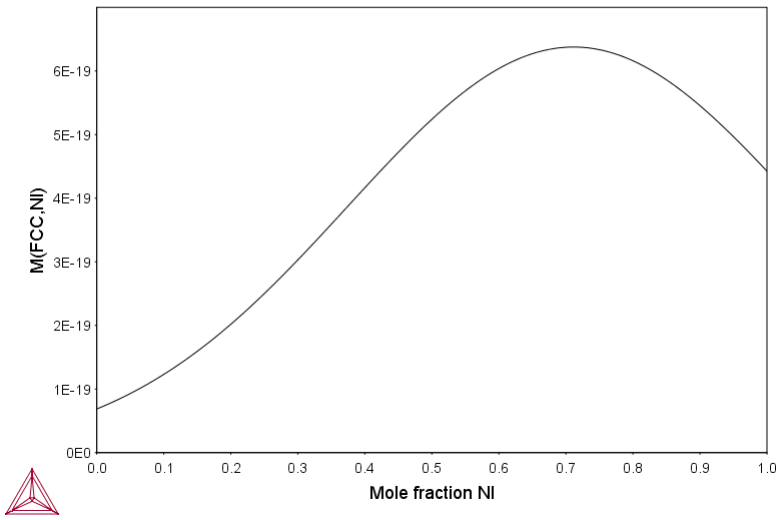
 Phase Region from   0.300000     for:
     FCC_A1
 Global test at  3.08000E-01 .... OK
 Global test at  3.18000E-01 .... OK
 Global test at  3.28000E-01 .... OK
 Global test at  3.38000E-01 .... OK
 Global test at  3.48000E-01 .... OK
 Global test at  3.58000E-01 .... OK
 Global test at  3.68000E-01 .... 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\developer\Documents\RESULT_002.POLY3
POLY_3:
POLY_3: @@
POLY_3: @@ ENTER THE POST PROCESSOR AND PLOT THE RESULT
POLY_3: @@
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2

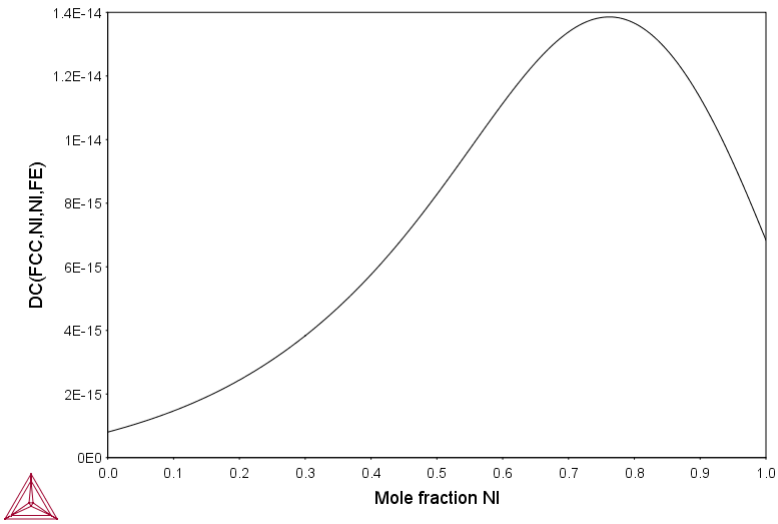
POST:
POST:
POST:
POST: @@
POST: @@ PLOT THE MOBILITY OF Ni VS. X(Ni)
POST: @@
POST: s-d-a y m(fcc,ni)
POST: s-d-a x m-f ni
POST:
POST: plot
   2018.02.18.22.21.23
   MOBFE2: FE, NI
   T=1409, P=1.01325E5, N=1
```




```
POST:
POST:
POST:
POST:@?<Hit_return_to_continue>
```

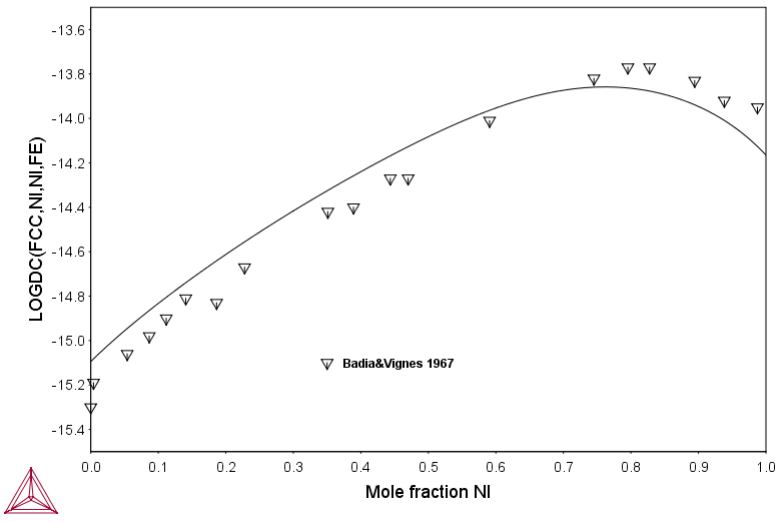
```
POST:
POST: @@
POST: @@ THEN PLOT THE DIFFUSIVITY OF Ni VS. X(Ni)
POST: @@
POST: s-d-a y dc(fcc,ni,ni,fe)
POST:
POST: plot
```

2018.02.18.22.21.23
MOBFE2: FE, NI
T=1409, P=1.01325E5, N=1




```
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: plot
```

2018.02.18.22.21.24
MOBFE2: FE, NI
T=1409, P=1.01325E5, N=1

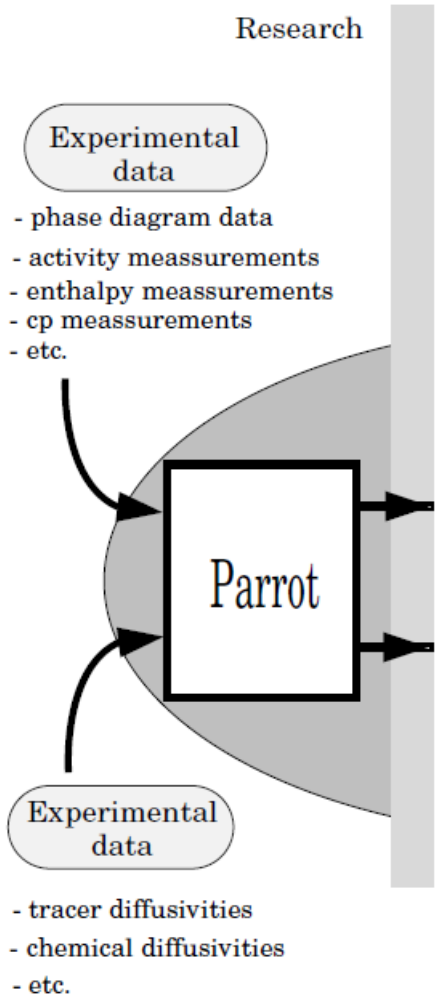



```
POST:
POST:
POST:@?<Hit_return_to_continue>
POST:
POST: set-inter
POST:
```

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

```
About License library version: 8.5.1.0017
 Linked: Fri Feb 16 15:22:08 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exg2\setup.DCM"SYS: ?@@
 NO SUCH COMMAND, USE HELP
SYS: @@ Kinetic data example.
SYS: @@ Optimization of mobilities in Ni-Al fcc alloys
SYS: @@ A file for reading thermodynamic data and setting up the kinetic
SYS: @@ parameters that are needed for an optimization of the FCC phase
SYS: @@ in the binary Ni-Al system.
SYS: @@ See also A. Engström and J. Ågren: ("Assessment of Diffusional
SYS: @@ Mobilities in Face-Centered Cubic Ni-Cr-Al Alloys" in
SYS: @@ Z. Metallkunde, Feb. 1996).
SYS: ------------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exg2_setup.DCM
SYS:
SYS: @@
SYS: @@ RETRIEVE THERMODYNAMIC DATA FROM A USER-DEFINED DATABASE
SYS: @@
SYS: go data
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

 VA                     /-  DEFINED
 L12_FCC                B2_BCC                 DICTRA_FCC_A1
   REJECTED
TDB_TCFE9: sw us tdata
 Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

 VA  DEFINED
TDB_USER: def-sys el
ELEMENTS: 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
ELEMENTS: 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 ....

 List of references for assessed data

   'This parameter has not been assessed'
   'A. Engstrom and J. Agren: Z. Metallkunde 87(1996)92-97;
      Al, Cr and Ni diffusion in fcc Al-Cr-Ni'
   'B. Jonsson: Scand. J. Metall. 24(1995)21-27;
      Ni self-diffusion'
 -OK-
APP:
APP: @@
APP: @@ GO TO THE DICTRA MODULE AND DEFINE THE KINETIC PARAMETERS. THE
APP: @@ VARIABLES V1,V2,V3 AND V4 ARE TO BE OPTIMIZED. NOTE THAT IF
APP: @@ YOU ARE OPTIMIZING PARAMETERS FOR A PHASE WITH MAGNETIC
APP: @@ CONTRIBUTION. I.E. USING BOTH MF- AND MQ-PARAMETERS, YOU
APP: @@ MIGHT HAVE TO ENTER THE PARROT MODULE AND GO BACK BEFORE
APP: @@ ENTERING PARAMETERS CONTAINING VARIABLES.
APP: @@
APP: go dic_par

 PARROT  VERSION 5.3d RUNNING ON PC/WINDOWS NT

 Developed at the Division of Physical Metallurgy
 Royal Institute of Technology Stockholm, Sweden

PARROT:
PARROT:
PARROT: go d-m
 NO TIME STEP DEFINED
DIC>
DIC> @@ MOBILITY OF Al IN Al
DIC> ENTER-MOB-DATA
PARAMETER: MQ(FCC_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:AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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
 S-C X(AL)=.1716
 EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.02:.1
 CREATE_NEW 0028,1


output ignored...



... output resumed

 V3     -1.32972463E+05   -1.32959167E+05   -1.32959167E+05    3.97449919E+00    3.97449919E+00
    3.97449919E+00    3.97449919E+00    3.97449919E+00    3.97449919E+00    3.97449919E+00
    3.97449919E+00    3.97449919E+00    3.97449919E+00    3.97449919E+00    3.97449919E+00
    3.97449919E+00    3.97449919E+00    3.97449919E+00    3.97449919E+00    3.97449919E+00
    3.97449919E+00    3.97449919E+00    3.97449919E+00
 V4      7.81857805E+01    7.81857805E+01    7.81857805E+01    4.46532140E+00    4.46532140E+00
    4.46532140E+00    4.46532140E+00    4.46532140E+00    4.46532140E+00    4.46532140E+00
    4.46532140E+00    4.46532140E+00    4.46532140E+00    4.46532140E+00    4.46532140E+00
    4.46532140E+00    4.46532140E+00    4.46532140E+00    4.46532140E+00    4.46532140E+00
    4.46532140E+00    4.46532140E+00    4.46532140E+00

 NUMBER OF OPTIMIZING VARIABLES :   4
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   2.02977003E+01 TO   2.02976923E+01
 DEGREES OF FREEDOM  113.  REDUCED SUM OF SQUARES   1.79625595E-01


 Sorry, LIST-DATA disabled for this database

 ======  BLOCK NUMBER  1

 DEFINED CONSTANTS
    P0=101325
10 LOGDC(F...,AL,NI)=-12.6       -12.56      0.10      4.3827E-02  0.4383
11 LOGDC(F...,AL,NI)=-12.56      -12.55      0.10      1.2341E-02  0.1234
12 LOGDC(F...,AL,NI)=-12.65      -12.53      0.10      0.1167       1.167
13 LOGDC(F...,AL,NI)=-12.52      -12.51      0.10      5.8843E-03  5.8843E-02
14 LOGDC(F...,AL,NI)=-12.52      -12.51      0.10      5.8843E-03  5.8843E-02
15 LOGDC(F...,AL,NI)=-12.48      -12.49      0.10     -8.4123E-03 -8.4123E-02
16 LOGDC(F...,AL,NI)=-12.43      -12.46      0.10     -2.6851E-02 -0.2685
17 LOGDC(F...,AL,NI)=-12.41      -12.43      0.10     -1.7821E-02 -0.1782
18 LOGDC(F...,AL,NI)=-12.37      -12.39      0.10     -2.3493E-02 -0.2349
19 LOGDC(F...,AL,NI)=-12.32      -12.36      0.10     -3.8626E-02 -0.3863
20 LOGDC(F...,AL,NI)=-12.28      -12.33      0.10     -5.1933E-02 -0.5193
21 LOGDC(F...,AL,NI)=-12.24      -12.29      0.10     -5.4919E-02 -0.5492
22 LOGDC(F...,AL,NI)=-12.2       -12.26      0.10     -5.5128E-02 -0.5513
23 LOGDC(F...,AL,NI)=-12.18      -12.22      0.10     -4.3400E-02 -0.4340
24 LOGDC(F...,AL,NI)=-12.16      -12.18      0.10     -2.2927E-02 -0.2293
25 LOGDC(F...,AL,NI)=-12.1       -12.14      0.10     -3.6888E-02 -0.3689
26 LOGDC(F...,AL,NI)=-12.08      -12.10      0.10     -1.9703E-02 -0.1970
27 LOGDC(F...,AL,NI)=-12.02      -12.04      0.10     -2.2272E-02 -0.2227
28 LOGDC(F...,AL,NI)=-11.98      -11.99      0.10     -9.0917E-03 -9.0917E-02
29 LOGDC(F...,AL,NI)=-11.94      -11.95      0.10     -9.1618E-03 -9.1618E-02
30 LOGDC(F...,AL,NI)=-13         -12.86      0.10      0.1360       1.360
31 LOGDC(F...,AL,NI)=-12.96      -12.85      0.10      0.1059       1.059
32 LOGDC(F...,AL,NI)=-12.92      -12.84      0.10      8.4799E-02  0.8480
33 LOGDC(F...,AL,NI)=-12.9       -12.82      0.10      8.2549E-02  0.8255
34 LOGDC(F...,AL,NI)=-12.77      -12.79      0.10     -1.5173E-02 -0.1517
35 LOGDC(F...,AL,NI)=-12.74      -12.75      0.10     -1.1192E-02 -0.1119
36 LOGDC(F...,AL,NI)=-12.82      -12.72      0.10      9.5223E-02  0.9522
37 LOGDC(F...,AL,NI)=-12.82      -12.72      0.10      9.5223E-02  0.9522
38 LOGDC(F...,AL,NI)=-12.69      -12.68      0.10      5.7856E-03  5.7856E-02
39 LOGDC(F...,AL,NI)=-12.65      -12.65      0.10      2.6229E-03  2.6229E-02
40 LOGDC(F...,AL,NI)=-12.64      -12.62      0.10      1.9222E-02  0.1922
41 LOGDC(F...,AL,NI)=-12.61      -12.58      0.10      2.8492E-02  0.2849
42 LOGDC(F...,AL,NI)=-12.55      -12.54      0.10      9.2091E-03  9.2091E-02
43 LOGDC(F...,AL,NI)=-12.53      -12.51      0.10      2.1034E-02  0.2103
44 LOGDC(F...,AL,NI)=-12.47      -12.47      0.10      2.0402E-03  2.0402E-02
45 LOGDC(F...,AL,NI)=-12.41      -12.42      0.10     -1.0621E-02 -0.1062
46 LOGDC(F...,AL,NI)=-12.38      -12.38      0.10     -1.6323E-04 -1.6323E-03
47 LOGDC(F...,AL,NI)=-12.36      -12.32      0.10      3.6256E-02  0.3626
48 LOGDC(F...,AL,NI)=-12.36      -12.32      0.10      3.6256E-02  0.3626
49 LOGDC(F...,AL,NI)=-12.3       -12.27      0.10      3.0494E-02  0.3049
50 LOGDC(F...,AL,NI)=-13.23      -13.19      0.10      3.8416E-02  0.3842
51 LOGDC(F...,AL,NI)=-13.23      -13.19      0.10      3.8416E-02  0.3842
52 LOGDC(F...,AL,NI)=-13.19      -13.18      0.10      1.3209E-02  0.1321
53 LOGDC(F...,AL,NI)=-13.15      -13.16      0.10     -5.5530E-03 -5.5530E-02
54 LOGDC(F...,AL,NI)=-13.12      -13.13      0.10     -1.4736E-02 -0.1474
55 LOGDC(F...,AL,NI)=-13.09      -13.10      0.10     -1.2913E-02 -0.1291
56 LOGDC(F...,AL,NI)=-13.06      -13.07      0.10     -6.9397E-03 -6.9397E-02
57 LOGDC(F...,AL,NI)=-13.02      -13.04      0.10     -1.5971E-02 -0.1597
58 LOGDC(F...,AL,NI)=-12.99      -13.00      0.10     -1.0672E-02 -0.1067
59 LOGDC(F...,AL,NI)=-12.96      -12.96      0.10      8.0069E-04  8.0069E-03
60 LOGDC(F...,AL,NI)=-12.91      -12.93      0.10     -2.0470E-02 -0.2047
61 LOGDC(F...,AL,NI)=-12.88      -12.89      0.10     -7.3947E-03 -7.3947E-02
62 LOGDC(F...,AL,NI)=-12.86      -12.85      0.10      1.4312E-02  0.1431
63 LOGDC(F...,AL,NI)=-12.86      -12.85      0.10      1.4312E-02  0.1431
64 LOGDC(F...,AL,NI)=-12.83      -12.81      0.10      1.7076E-02  0.1708
65 LOGDC(F...,AL,NI)=-12.8       -12.77      0.10      2.9558E-02  0.2956
66 LOGDC(F...,AL,NI)=-12.75      -12.72      0.10      2.5293E-02  0.2529
67 LOGDC(F...,AL,NI)=-12.71      -12.68      0.10      2.6861E-02  0.2686
68 LOGDC(F...,AL,NI)=-12.67      -12.63      0.10      4.4033E-02  0.4403
70 LOGDC(F...,AL,NI)=-13.5       -13.54      0.10     -4.2456E-02 -0.4246
71 LOGDC(F...,AL,NI)=-13.47      -13.53      0.10     -5.5160E-02 -0.5516
72 LOGDC(F...,AL,NI)=-13.45      -13.50      0.10     -5.0384E-02 -0.5038
73 LOGDC(F...,AL,NI)=-13.42      -13.48      0.10     -5.6139E-02 -0.5614
74 LOGDC(F...,AL,NI)=-13.39      -13.44      0.10     -5.3034E-02 -0.5303
75 LOGDC(F...,AL,NI)=-13.36      -13.40      0.10     -4.3865E-02 -0.4386
76 LOGDC(F...,AL,NI)=-13.34      -13.37      0.10     -3.0943E-02 -0.3094
77 LOGDC(F...,AL,NI)=-13.31      -13.33      0.10     -2.0539E-02 -0.2054
78 LOGDC(F...,AL,NI)=-13.24      -13.29      0.10     -5.0311E-02 -0.5031
79 LOGDC(F...,AL,NI)=-13.22      -13.26      0.10     -4.1318E-02 -0.4132
80 LOGDC(F...,AL,NI)=-13.19      -13.22      0.10     -2.6230E-02 -0.2623
```

81	LOGDC(F...,AL,NI)=-13.13	-13.17	0.10	-4.3098E-02	-0.4310
82	LOGDC(F...,AL,NI)=-13.12	-13.14	0.10	-1.9773E-02	-0.1977
83	LOGDC(F...,AL,NI)=-13.08	-13.09	0.10	-1.4457E-02	-0.1446
84	LOGDC(F...,AL,NI)=-13.04	-13.05	0.10	-9.4618E-03	-9.4618E-02
85	LOGDC(F...,AL,NI)=-13.03	-13.01	0.10	2.2404E-02	0.2240
90	LOGDC(F...,AL,NI)=-13.97	-13.92	0.10	5.1241E-02	0.5124
91	LOGDC(F...,AL,NI)=-13.92	-13.90	0.10	2.0497E-02	0.2050
92	LOGDC(F...,AL,NI)=-13.88	-13.87	0.10	9.3920E-03	9.3920E-02
93	LOGDC(F...,AL,NI)=-13.85	-13.84	0.10	5.2264E-03	5.2264E-02
94	LOGDC(F...,AL,NI)=-13.82	-13.81	0.10	1.1044E-02	0.1104
95	LOGDC(F...,AL,NI)=-13.78	-13.77	0.10	1.3352E-02	0.1335
96	LOGDC(F...,AL,NI)=-13.9	-13.74	0.10	0.1640	1.640
97	LOGDC(F...,AL,NI)=-13.85	-13.69	0.10	0.1576	1.576
98	LOGDC(F...,AL,NI)=-13.65	-13.65	0.10	1.5604E-03	1.5604E-02
99	LOGDC(F...,AL,NI)=-13.62	-13.62	0.10	4.9052E-03	4.9052E-02
100	LOGDC(F...,AL,NI)=-13.57	-13.57	0.10	-9.5589E-04	-9.5589E-03
101	LOGDC(F...,AL,NI)=-13.52	-13.53	0.10	-5.4819E-03	-5.4819E-02
102	LOGDC(F...,AL,NI)=-13.47	-13.49	0.10	-2.0262E-02	-0.2026
103	LOGDC(F...,AL,NI)=-13.45	-13.45	0.10	4.9628E-03	4.9628E-02
104	LOGDC(F...,AL,NI)=-13.4	-13.40	0.10	2.8073E-03	2.8073E-02
110	LOGDC(F...,AL,NI)=-14.32	-14.32	0.10	-3.9760E-03	-3.9760E-02
111	LOGDC(F...,AL,NI)=-14.32	-14.30	0.10	1.9307E-02	0.1931
112	LOGDC(F...,AL,NI)=-14.28	-14.27	0.10	1.0664E-02	0.1066
113	LOGDC(F...,AL,NI)=-14.25	-14.24	0.10	8.9412E-03	8.9412E-02
114	LOGDC(F...,AL,NI)=-14.22	-14.20	0.10	1.8329E-02	0.1833
115	LOGDC(F...,AL,NI)=-14.17	-14.16	0.10	1.2994E-02	0.1299
116	LOGDC(F...,AL,NI)=-14.15	-14.12	0.10	3.0489E-02	0.3049
117	LOGDC(F...,AL,NI)=-14.1	-14.07	0.10	2.5593E-02	0.2559
118	LOGDC(F...,AL,NI)=-14.03	-14.03	0.10	-1.4483E-03	-1.4483E-02
119	LOGDC(F...,AL,NI)=-14	-14.00	0.10	2.7074E-03	2.7074E-02
120	LOGDC(F...,AL,NI)=-13.95	-13.95	0.10	-1.9282E-03	-1.9282E-02
121	LOGDC(F...,AL,NI)=-13.9	-13.91	0.10	-5.2349E-03	-5.2349E-02
122	LOGDC(F...,AL,NI)=-13.85	-13.87	0.10	-1.6645E-02	-0.1665
130	LOGDC(F...,AL,NI)=-14.73	-14.76	0.10	-3.0493E-02	-0.3049
131	LOGDC(F...,AL,NI)=-14.71	-14.73	0.10	-2.3757E-02	-0.2376
132	LOGDC(F...,AL,NI)=-14.68	-14.70	0.10	-1.9446E-02	-0.1945
133	LOGDC(F...,AL,NI)=-14.66	-14.67	0.10	-8.5997E-03	-8.5997E-02
134	LOGDC(F...,AL,NI)=-14.61	-14.63	0.10	-1.5314E-02	-0.1531
135	LOGDC(F...,AL,NI)=-14.61	-14.63	0.10	-1.5314E-02	-0.1531
136	LOGDC(F...,AL,NI)=-14.58	-14.58	0.10	3.4408E-03	3.4408E-02
137	LOGDC(F...,AL,NI)=-14.54	-14.54	0.10	3.3897E-03	3.3897E-02
138	LOGDC(F...,AL,NI)=-14.5	-14.49	0.10	9.2113E-03	9.2113E-02
139	LOGDC(F...,AL,NI)=-14.46	-14.44	0.10	1.5390E-02	0.1539
140	LOGDC(F...,AL,NI)=-14.41	-14.41	0.10	1.6005E-03	1.6005E-02
141	LOGDC(F...,AL,NI)=-14.35	-14.36	0.10	-1.1351E-02	-0.1135
142	LOGDC(F...,AL,NI)=-14.27	-14.31	0.10	-4.1487E-02	-0.4149
143	LOGDC(F...,AL,NI)=-14.2	-14.27	0.10	-7.4774E-02	-0.7477

PARROT:
PARROT:
PARROT: set-inter
 --OK---
PARROT:

exg2-plot

```
PARROT:AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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
POLY_3: s-c n=1,p=101325,t=1573
POLY_3: s-c x(al)=.1
POLY_3: 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_3: add,,
POLY_3:
POLY_3: s-a-v 1 x(al) 0.0001 .20 0.001,,,,
POLY_3: 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\developer\Documents\RESULT_002.POLY3
POLY_3: @@
POLY_3: @@ REPEATE THE PROCEDURE FOR SOME OTHER TEMPERATURES
POLY_3: @@
POLY_3: s-c t=1523,x(al)=.1
POLY_3: 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_3: s-a-v 1 x(al) 0.0001 .20 0.001,,,,
POLY_3: 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\developer\Documents\RESULT_002.POLY3
POLY_3: s-c t=1473,x(al)=.1
POLY_3: 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_3: s-a-v 1 x(al) 0.0001 .20 0.001,,,,
POLY_3: 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\developer\Documents\RESULT_002.POLY3
POLY_3: s-c t=1423,x(al)=.1
POLY_3: 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_3: s-a-v 1 x(al) 0.0001 .20 0.001,,,,
POLY_3: 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\developer\Documents\RESULT_002.POLY3
POLY_3: s-c t=1373,x(al)=.1
POLY_3: 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_3: s-a-v 1 x(al) 0.0001 .20 0.001,,,,
POLY_3: 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\developer\Documents\RESULT_002.POLY3
POLY_3: s-c t=1323,x(al)=.1
POLY_3: 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_3: s-a-v 1 x(al) 0.0001 .20 0.001,,,,
POLY_3: 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\developer\Documents\RESULT_002.POLY3
POLY_3: s-c t=1273,x(al)=.1
POLY_3: 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_3: s-a-v 1 x(al) 0.0001 .20 0.001,,,,
POLY_3: 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

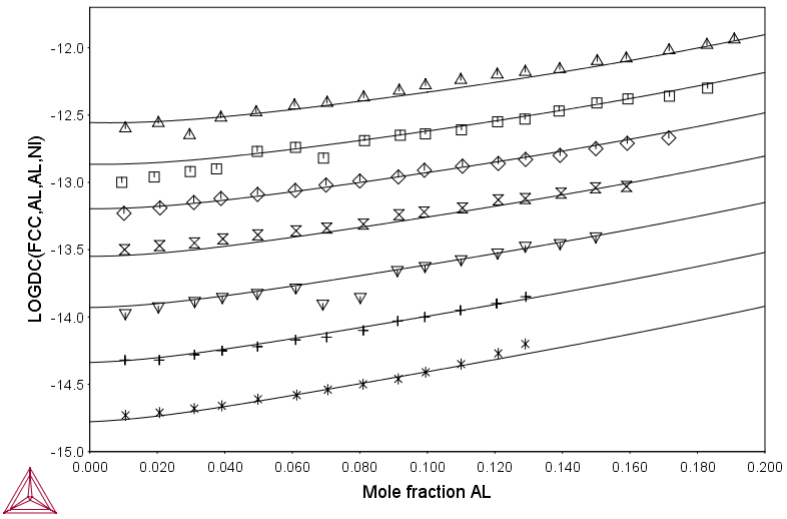
 Phase Region from   0.100000     for:
     FCC_A1
 Global test at  9.20000E-02 .... OK
 Global test at  8.20000E-02 .... OK
 Global test at  7.20000E-02 .... OK
 Global test at  6.20000E-02 .... OK
 Global test at  5.20000E-02 .... OK
 Global test at  4.20000E-02 .... OK
 Global test at  3.20000E-02 .... 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\developer\Documents\RESULT_002.POLY3
POLY_3: @@
POLY_3: @@ ENTER THE POST MODULE, PLOT THE DIFFUSIVITY ON THE Y-AXIS
POLY_3: @@ AND MOLE-FRACTION Al ON THE X-AXIS.
POLY_3: @@
POLY_3: 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
```

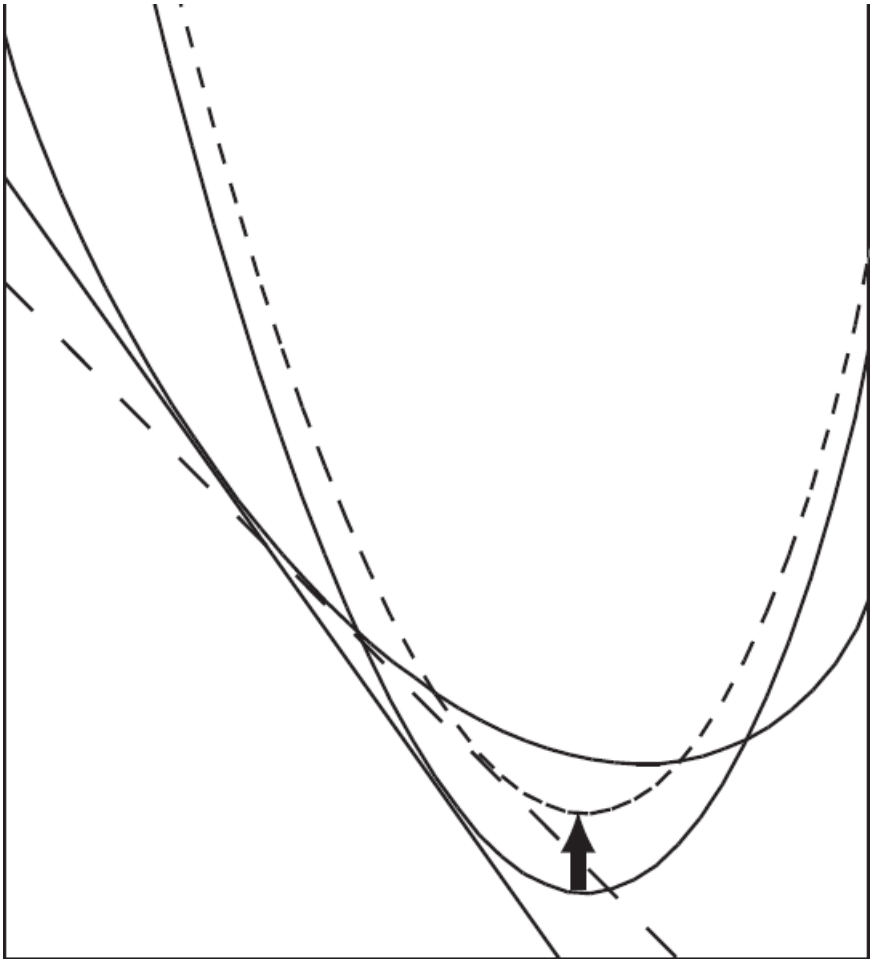
COMMAND NOT SUPPORTED IN THIS PLOT DRIVER
POST: s-s-s y n -15 -11.7
POST: s-t-m-s y
COMMAND NOT SUPPORTED IN THIS PLOT DRIVER
POST: plo

2018.02.18.22.24.24
MOB2: AL, NI
T=1273, N=1., P=1.01325E5



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

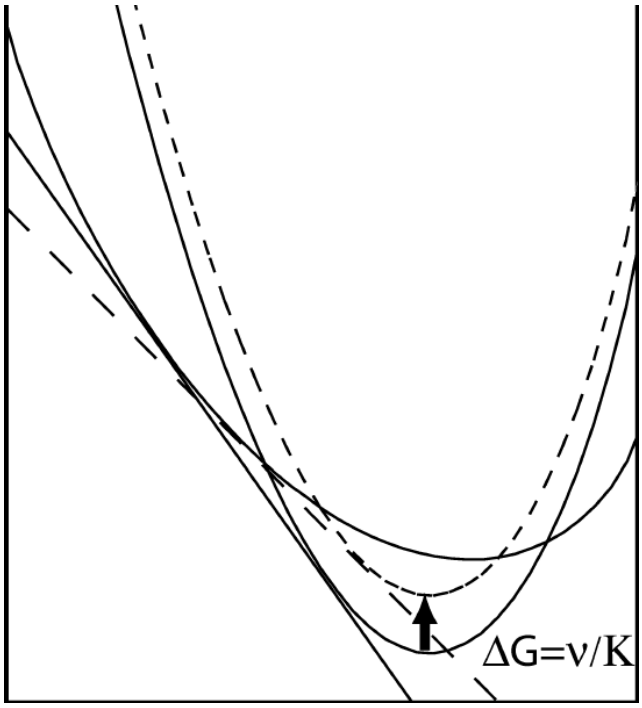
Deviation From Local Equilibrium



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

```
About
SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

 VA                     /-  DEFINED
 L12_FCC                B2_BCC                 DICTRA_FCC_A1
   REJECTED
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE THE DATA
TDB_TCFE9: @@
TDB_TCFE9: sw FEDEMO
 Current database: Iron Demo Database v2.0

 VA                     /-  DEFINED
TDB_FEDEMO: def-sys fe c
 FE                     C  DEFINED
TDB_FEDEMO: rej ph * all
 GAS:G                  LIQUID:L               BCC_A2
 CEMENTITE              DIAMOND_FCC_A4         FCC_A1
 GRAPHITE               HCP_A3                 KSI_CARBIDE
 LAVES_PHASE_C14        M23C6                  M5C2
 M7C3  REJECTED
TDB_FEDEMO: res ph bcc fcc
 BCC_A2                 FCC_A1  RESTORED
TDB_FEDEMO: get
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'P. Franke, Estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
  'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'X.-G. Lu, M. Selleby, B. Sundman, CALPHAD, 29 (2005) 49-55; Fe P-T diagram'
  'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
 -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 v2.0

 VA  DEFINED
APP: def-sys fe c
 FE                     C  DEFINED
APP: rej ph * all
 BCC_A2                 FCC_A1  REJECTED
APP: res ph bcc fcc
 BCC_A2                 FCC_A1  RESTORED
APP: get
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'This parameter has not been assessed'
  'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'
  'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
      -Ni'
  'B. Jonsson: Z. Metallkunde 85(1994)498-501; C and N diffusion in bcc Cr
      -Fe-Ni'
  'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
      in bcc Fe'
 -OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR
APP: @@
APP: go d-m
 NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 1000; * N

DIC>
DIC> @@
DIC> @@ START BY ENTERING THE REGIONS ferrite AND austenite WHERE
DIC> @@ THE BCC AND FCC PHASES ARE PUT, RESPECTIVELY. THE FERRITE REGION IS
DIC> @@ ASSUMED INITIALLY TO BE VERY THIN, 1E-9 METERS.
DIC> @@
DIC> enter-region
REGION NAME : ferrite
DIC>
```

```
DIC> enter-region
REGION NAME : austenite
ATTACH TO REGION NAMED /FERRITE/:
ATTACHED TO THE RIGHT OF FERRITE /YES/:
DIC>
DIC> @@
DIC> @@ ENTER GRIDS INTO THE REGIONS
DIC> @@
DIC> enter-grid
REGION NAME : /FERRITE/: ferrite
WIDTH OF REGION /1/: 1e-9
TYPE /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>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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
 single geometric dense at  0.10000E-08
 0.99998       24
 Region: AUSTENITE
 single geometric dense at   0.0000
  1.0666       84
  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]
 2.137709938668809E-004        2.137625593908550E-004         13.8289495127833        2.120998911211383E-004        2.112667987639259E-
004        2.108508673392353E-004        2.106430553153946E-004        2.104353457505012E-004        2.101948160083122E-
004        2.097141691516830E-004        2.087545259495225E-004        2.068418415894586E-004        2.030428810465509E-
004        1.955505926692782E-004        1.809885467492963E-004        1.535545782472665E-004        1.054471345952774E-
004        3.627422069935879E-005         13.8289494178875        3.615700697463181E-005        3.609847124386777E-
005        3.606922116142028E-005        3.605460056591150E-005        3.603998293423047E-005        3.602477904360235E-
005        3.599438088533936E-005        3.593362306058377E-005        3.581226137811151E-005        3.557015388125908E-
005        3.508840236026233E-005        3.413475320871956E-005        3.226687046760648E-005        2.868876723327018E-
005        2.216320975615694E-005        1.163469076818617E-005         7.48347199232498        1.161266684728771E-
005        1.160166271119065E-005        1.159616259921805E-005        1.159341303224015E-005        1.159066379128802E-
005        1.158790570211405E-005        1.158239050832246E-005        1.157136405908550E-005        1.154932691389981E-
005        1.150531563662104E-005        1.141754513473569E-005        1.124301234138844E-005        1.089797959650757E-
005        1.022404547389298E-005        1.490118083345267E-002        1.019021771314144E-005        1.017332485335765E-
005        1.016488367857833E-005        1.016066440497390E-005        1.015644600723762E-005        1.015204959594981E-
005        1.014325962855260E-005        1.012569111466427E-005        1.009059977048929E-005        1.002059981643303E-
005        9.881330845574529E-006        4.762707187234291E-006        4.438313610609329E-003        2.058831409609227E-
006        2.181365147016879E-007        6.215863080991705E-009        1.005966849204609E-011        2.807707691965722E-
008        1.740878263349759E-015        2.916483860250238E-008        3.123181243512367E-019       TIME =  0.10000000E-06 DT =  0.10000000E-
06 SUM OF SQUARES =  0.31231812E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS    4.9961063     AND    4.9961063
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.50061063E-06
 U-FRACTION IN SYSTEM:  C = 9.00101592838844E-04  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-06 [m]
  19  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: FERRITE
   3  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUSTENITE

  CPU time used in timestep                    0 seconds


output ignored...



... output resumed

TIME =  0.24974221E-02 DT =  0.18903334E-05 SUM OF SQUARES =  0.87185504E-22
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.83033491E-03 AND   0.83033491E-03
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.93676977E-06
 U-FRACTION IN SYSTEM:  C = 8.98900758877953E-04  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-06 [m]
  CPU time used in timestep                    1 seconds
 7.855361881346131E-008        7.845488659855833E-008        2.895741754987094E-010        1.377397370732311E-012        3.298868967596615E-
017       TIME =  0.24986191E-02 DT =  0.11969964E-05 SUM OF SQUARES =  0.32988690E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.95215869E-03 AND   0.95215869E-03
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.93790950E-06
 U-FRACTION IN SYSTEM:  C = 8.98953464809454E-04  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-06 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: FERRITE

  CPU time used in timestep                    0 seconds
 1.224778860998174E-007        1.223249305229064E-007        2.395848834555112E-010        6.518470747369290E-013        4.308904388595452E-
018       TIME =  0.24993550E-02 DT =  0.73586367E-06 SUM OF SQUARES =  0.43089044E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.10897992E-02 AND   0.10897992E-02
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.93871144E-06
 U-FRACTION IN SYSTEM:  C = 8.98994454594015E-04  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-06 [m]
  CPU time used in timestep                    0 seconds
 3.060424563913232E-007        3.057378465845341E-007        3.253009099214644E-010        5.404686073474901E-013        1.316128993548938E-
018       TIME =  0.24997404E-02 DT =  0.38538368E-06 SUM OF SQUARES =  0.13161290E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.12900930E-02 AND   0.12900930E-02
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.93920862E-06
 U-FRACTION IN SYSTEM:  C = 8.99052133144654E-04  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-06 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: FERRITE

  CPU time used in timestep                    1 seconds
 3.534167246769511E-007        3.530042245676402E-007        1.634702116437679E-010        8.223209437291750E-014        2.121677259154539E-
020       TIME =  0.24999375E-02 DT =  0.19709680E-06 SUM OF SQUARES =  0.21216773E-19
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.14857381E-02 AND   0.14857381E-02
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.93950146E-06
 U-FRACTION IN SYSTEM:  C = 8.99110496797815E-04  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-06 [m]
  CPU time used in timestep                    0 seconds
```

```
 1.382362431546073E-006        1.381359929145516E-006        1.794347463483156E-010        9.495490590523165E-015        3.811431082021190E-
022       TIME =  0.25000000E-02 DT =  0.62515089E-07 SUM OF SQUARES =  0.38114311E-21
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.18529405E-02 AND   0.18529405E-02
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.93961729E-06
 U-FRACTION IN SYSTEM:  C = 8.99171776165061E-04  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-06 [m]
 MUST SAVE WORKSPACE ON FILE
 WORKSPACE SAVED ON FILE
 RECLAIMING WORKSPACE
 DELETING TIME-RECORD FOR TIME    0.0000000
 DELETING TIME-RECORD FOR TIME   0.10000000E-06
 DELETING TIME-RECORD FOR TIME   0.30000000E-06
 DELETING TIME-RECORD FOR TIME   0.70000000E-06
 DELETING TIME-RECORD FOR TIME   0.15000000E-05
 DELETING TIME-RECORD FOR TIME   0.28565340E-05
 DELETING TIME-RECORD FOR TIME   0.52015355E-05
 DELETING TIME-RECORD FOR TIME   0.98915385E-05
 DELETING TIME-RECORD FOR TIME   0.19271544E-04
 DELETING TIME-RECORD FOR TIME   0.33687180E-04
 DELETING TIME-RECORD FOR TIME   0.53417475E-04
 DELETING TIME-RECORD FOR TIME   0.78654357E-04
 DELETING TIME-RECORD FOR TIME   0.10952898E-03
 DELETING TIME-RECORD FOR TIME   0.14613093E-03
 DELETING TIME-RECORD FOR TIME   0.18853080E-03
 DELETING TIME-RECORD FOR TIME   0.23679894E-03
 DELETING TIME-RECORD FOR TIME   0.29104868E-03
 DELETING TIME-RECORD FOR TIME   0.35145422E-03
 DELETING TIME-RECORD FOR TIME   0.41823577E-03
 DELETING TIME-RECORD FOR TIME   0.48723333E-03
 DELETING TIME-RECORD FOR TIME   0.55628734E-03
 DELETING TIME-RECORD FOR TIME   0.62546243E-03
 DELETING TIME-RECORD FOR TIME   0.69481214E-03
 DELETING TIME-RECORD FOR TIME   0.76438006E-03
 DELETING TIME-RECORD FOR TIME   0.83419596E-03
 DELETING TIME-RECORD FOR TIME   0.90425844E-03
 DELETING TIME-RECORD FOR TIME   0.97473720E-03
 DELETING TIME-RECORD FOR TIME   0.10456577E-02
 DELETING TIME-RECORD FOR TIME   0.11169996E-02
 DELETING TIME-RECORD FOR TIME   0.11887867E-02
 DELETING TIME-RECORD FOR TIME   0.12609691E-02
 DELETING TIME-RECORD FOR TIME   0.13331751E-02
 DELETING TIME-RECORD FOR TIME   0.14056136E-02
 DELETING TIME-RECORD FOR TIME   0.14782826E-02
 DELETING TIME-RECORD FOR TIME   0.15511175E-02
 DELETING TIME-RECORD FOR TIME   0.16239994E-02
 DELETING TIME-RECORD FOR TIME   0.16973709E-02
 DELETING TIME-RECORD FOR TIME   0.17714236E-02
 DELETING TIME-RECORD FOR TIME   0.18459453E-02
 DELETING TIME-RECORD FOR TIME   0.19208358E-02
 DELETING TIME-RECORD FOR TIME   0.19960898E-02
 DELETING TIME-RECORD FOR TIME   0.20715732E-02
 DELETING TIME-RECORD FOR TIME   0.21477958E-02
 DELETING TIME-RECORD FOR TIME   0.22245450E-02
 DELETING TIME-RECORD FOR TIME   0.23020845E-02
 DELETING TIME-RECORD FOR TIME   0.23637495E-02
 DELETING TIME-RECORD FOR TIME   0.24066138E-02
 DELETING TIME-RECORD FOR TIME   0.24364991E-02
 DELETING TIME-RECORD FOR TIME   0.24572377E-02
 DELETING TIME-RECORD FOR TIME   0.24715984E-02
 DELETING TIME-RECORD FOR TIME   0.24814555E-02
 DELETING TIME-RECORD FOR TIME   0.24881136E-02
 DELETING TIME-RECORD FOR TIME   0.24925865E-02
 DELETING TIME-RECORD FOR TIME   0.24955318E-02
 DELETING TIME-RECORD FOR TIME   0.24974221E-02
 DELETING TIME-RECORD FOR TIME   0.24986191E-02
 DELETING TIME-RECORD FOR TIME   0.24993550E-02
 DELETING TIME-RECORD FOR TIME   0.24997404E-02

 KEEPING TIME-RECORD FOR TIME   0.24999375E-02
 AND FOR TIME                   0.25000000E-02
 WORKSPACE RECLAIMED

 TIMESTEP AT    0.250000000E-02 SELECTED

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

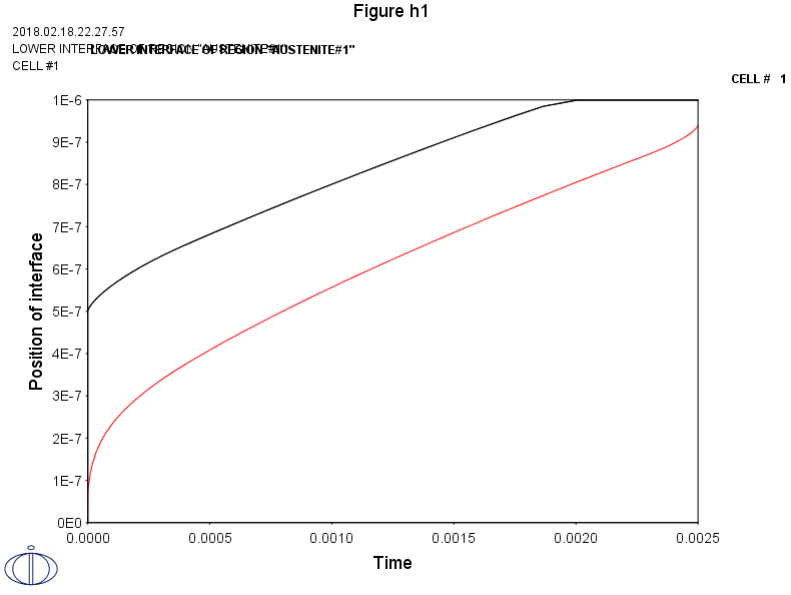
exh1-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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: plot
```

Figure h1

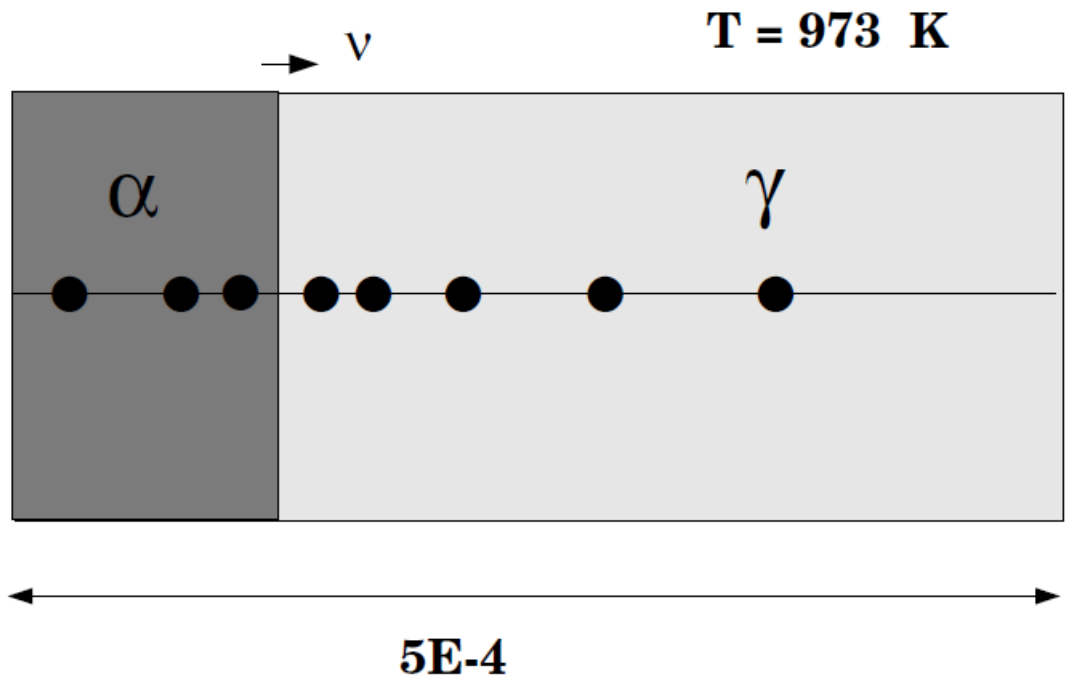



```
POST-1:
POST-1:
POST-1: set-inter
 --OK---
POST-1:
```

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

```
AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

 VA                     /-  DEFINED
 L12_FCC                B2_BCC                 DICTRA_FCC_A1
   REJECTED
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ SELECT A DATABASE FOR THERMODYNAMIC DATA
TDB_TCFE9: @@
TDB_TCFE9: sw fedemo
 Current database: Iron Demo Database v2.0

 VA                     /-  DEFINED
TDB_FEDEMO: def-sys fe ni c
 FE                     NI                     C
   DEFINED
TDB_FEDEMO: rej ph * all
 GAS:G                  LIQUID:L               BCC_A2
 CEMENTITE              DIAMOND_FCC_A4         FCC_A1
 GRAPHITE               HCP_A3                 KSI_CARBIDE
 LAVES_PHASE_C14        M23C6                  M5C2
 M7C3  REJECTED
TDB_FEDEMO: res ph bcc fcc
 BCC_A2                 FCC_A1  RESTORED
TDB_FEDEMO: get
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'P. Franke, Estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
  'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'A. Gabriel, C. Chatillon, and I. Ansara, published in High Temp. Sci.
      (Parameters listed in CALPHAD, 11 (1987) 203-218); C-NI'
  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'X.-G. Lu, M. Selleby, B. Sundman, CALPHAD, 29 (2005) 49-55; Fe P-T diagram'
  'A. Gabriel, P. Gustafson, and I. Ansara, CALPHAD, 11 (1987) 203 -218;
      TRITA-MAC 285 (1986); C-FE-NI'
  'A. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); FE-NI'
  'B.-J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
 -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 v2.0

 VA  DEFINED
APP: def-sys fe ni c
 FE                     NI                     C
   DEFINED
APP: rej ph * all
 BCC_A2                 FCC_A1  REJECTED
APP: res ph bcc fcc
 BCC_A2                 FCC_A1  RESTORED
APP: get
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'This parameter has not been assessed'
  'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'
  'B. Jonsson: Z. Metallkunde 85(1994)502-509; C diffusion in fcc Cr-Fe-Ni'
  'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
      -Ni'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Ni self-diffusion'
  'B. Jonsson: Z. Metallkunde 85(1994)498-501; C and N diffusion in bcc Cr
      -Fe-Ni'
  'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
      in bcc Fe'
  'B. Jonsson: ISIJ International, 35(1995)1415-1421; Cr, Fe and Ni
      diffusion bcc Cr-Fe-Ni'
 -OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR
APP: @@
APP: go d-m
 NO TIME STEP DEFINED
```

```
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 973; * N

DIC>
DIC> @@
DIC> @@ START BY ENTERING THE REGIONS ferrite AND austenite WHERE THE
DIC> @@ BCC AND FCC PHASES ARE PUT, RESPECTIVELY. THE FERRITE REGION IS
DIC> @@ ASSUMED INITIALLY TO BE VERY THIN, 1E-9 METERS.
DIC> @@
DIC> enter-region
REGION NAME : ferrite
DIC>
DIC> enter-region
REGION NAME : austenite
ATTACH TO REGION NAMED /FERRITE/:
ATTACHED TO THE RIGHT OF FERRITE /YES/:
DIC>
DIC> @@
DIC> @@ ENTER GRIDS INTO THE REGIONS
DIC> @@
DIC> enter-grid
REGION NAME : /FERRITE/: ferrite
WIDTH OF REGION /1/: 1e-9
TYPE /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>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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
 single geometric dense at  0.10000E-08
 0.99997       24
 Region: AUSTENITE
 single geometric dense at   0.0000
  1.1602       98
  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 = .00412262676333  FE = .980742621143594
                        NI = .0192573788564064
 TOTAL SIZE OF SYSTEM:  5.0001E-05 [m]
 U-FRACTION IN SYSTEM:  C = .00412262676333  FE = .980742621143594
                        NI = .0192573788564064
 TOTAL SIZE OF SYSTEM:  5.0001E-05 [m]
  13403.6958745548         13403.6958745560         13396.6824657623         181.652814770282         1.24966106488886         3.83383219646144
003        1.422760580718459E-005        4.522508972366437E-007        2.881050295641052E-014       TIME =  0.10000000E-06 DT =  0.10000000E-
06 SUM OF SQUARES =  0.28810503E-13
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.20145484E-01 AND   0.20145484E-01
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.30145484E-08
 U-FRACTION IN SYSTEM:  C = .00412273714809213  FE = .980742621143594
                        NI = .0192573788564064
 TOTAL SIZE OF SYSTEM:  5.0001E-05 [m]
  11  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUSTENITE

  CPU time used in timestep                    1 seconds
  13162.2365646424         13162.2365643854         13155.2460353378         172.785301156287         1.16153449406453         4.14451529695564
003        1.903400929927317E-003        2.796599852470772E-006        4.535465713686845E-007       1.548523392974097E-
009        7.179394106722943E-013       TIME =  0.20000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =  0.71793941E-12
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.28504281E-02 AND   0.28504281E-02
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.32995912E-08
 U-FRACTION IN SYSTEM:  C = .0041227339976926  FE = .980742621143594
                        NI = .0192573788564064
 TOTAL SIZE OF SYSTEM:  5.0001E-05 [m]
  CPU time used in timestep                    1 seconds
  12924.7969674917         12924.7969674983         12917.8299122818         164.371511428355         1.07976181183378         5.304376025252446
002        1.617763291090644E-004        1.560234792169188E-007        1.263010294691756E-003       6.312094358667842E-
016       TIME =  0.35656740E-06 DT =  0.15656740E-06 SUM OF SQUARES =  0.63120944E-15

output ignored...


... output resumed

 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.12884768E-04
 U-FRACTION IN SYSTEM:  C = .0041285513124062  FE = .980742621143594
                        NI = .0192573788564066
 TOTAL SIZE OF SYSTEM:  5.0001E-05 [m]
  12  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: FERRITE

  CPU time used in timestep                    1 seconds
  6134.60951334714         6134.60951334916         6128.88995331608         24.2689880423745         6.413322587234534E-
002        8.380054130777078E-004        3.990463092669323E-006        5.061492706429104E-011       1.608627863480817E-
003        4.006995280253253E-019       TIME =   41.718584     DT =   3.7168197     SUM OF SQUARES =  0.40069953E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.19118081E-06 AND   0.19118081E-06
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.13595352E-04
 U-FRACTION IN SYSTEM:  C = .00412892447597106  FE = .980742621143594
                        NI = .0192573788564067
 TOTAL SIZE OF SYSTEM:  5.0001E-05 [m]
  14  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: FERRITE

  CPU time used in timestep                    2 seconds
  6019.29790049546         6019.29790049063         6013.61359254264         23.1752709709811         5.988602697692924E-
002        6.191106944735658E-004        3.230252858632872E-006        5.179354754507486E-011       1.618147713604299E-
003        1.911118310035563E-020       TIME =   45.525738     DT =   3.8071537     SUM OF SQUARES =  0.19111183E-19
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.18327242E-06 AND   0.18327242E-06
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.14293099E-04
 U-FRACTION IN SYSTEM:  C = .0041292702380182  FE = .980742621143594
                        NI = .0192573788564067
 TOTAL SIZE OF SYSTEM:  5.0001E-05 [m]
  15  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: FERRITE
```

```
  CPU time used in timestep                    2 seconds
  5906.07319969691         5906.07319970334         5900.42420053078         22.1323492422866        5.592493008005637E-
002        1.888924989415762E-003        1.151756461771691E-006        1.342514614055690E-010        1.162544015976054E-
003        2.594038400966300E-019       TIME =   49.001916     DT =   3.4761784     SUM OF SQUARES =  0.25940384E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.18070690E-06 AND   0.18070690E-06
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.14921268E-04
 U-FRACTION IN SYSTEM:  C = .00412980312099469  FE = .980742621143594
                        NI = .0192573788564067
 TOTAL SIZE OF SYSTEM:  5.0001E-05 [m]
  12  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: FERRITE

  CPU time used in timestep                    2 seconds
  5794.90030702191         5794.90030702416         5789.28666554113         21.1377744513434        5.223026175570823E-
002        1.429845859724257E-002        3.466078132925075E-005        1.478441856462062E-007        1.640219090103663E-
003        7.286653961560384E-018       TIME =   50.000000     DT =  0.99808403     SUM OF SQUARES =  0.72866540E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.23051013E-06 AND   0.23051013E-06
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.15151336E-04
 U-FRACTION IN SYSTEM:  C = .0041309481336738  FE = .980742621143594
                        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   0.35656740E-06
 DELETING TIME-RECORD FOR TIME   0.63794974E-06
 DELETING TIME-RECORD FOR TIME   0.11506591E-05
 DELETING TIME-RECORD FOR TIME   0.21687314E-05
 DELETING TIME-RECORD FOR TIME   0.42048761E-05
 DELETING TIME-RECORD FOR TIME   0.82771656E-05
 DELETING TIME-RECORD FOR TIME   0.15887371E-04
 DELETING TIME-RECORD FOR TIME   0.25918565E-04
 DELETING TIME-RECORD FOR TIME   0.39472933E-04
 DELETING TIME-RECORD FOR TIME   0.59571679E-04
 DELETING TIME-RECORD FOR TIME   0.95661762E-04
 DELETING TIME-RECORD FOR TIME   0.16784193E-03
 DELETING TIME-RECORD FOR TIME   0.31220226E-03
 DELETING TIME-RECORD FOR TIME   0.60092292E-03
 DELETING TIME-RECORD FOR TIME   0.11783643E-02
 DELETING TIME-RECORD FOR TIME   0.20786157E-02
 DELETING TIME-RECORD FOR TIME   0.34937926E-02
 DELETING TIME-RECORD FOR TIME   0.60665663E-02
 DELETING TIME-RECORD FOR TIME   0.11212114E-01
 DELETING TIME-RECORD FOR TIME   0.21503208E-01
 DELETING TIME-RECORD FOR TIME   0.40842356E-01
 DELETING TIME-RECORD FOR TIME   0.75054322E-01
 DELETING TIME-RECORD FOR TIME   0.13545785
 DELETING TIME-RECORD FOR TIME   0.24516935
 DELETING TIME-RECORD FOR TIME   0.44180830
 DELETING TIME-RECORD FOR TIME   0.79606820
 DELETING TIME-RECORD FOR TIME    1.4337573
 DELETING TIME-RECORD FOR TIME    2.5843697
 DELETING TIME-RECORD FOR TIME    4.6661977
 DELETING TIME-RECORD FOR TIME    6.9580953
 DELETING TIME-RECORD FOR TIME    9.4344356
 DELETING TIME-RECORD FOR TIME    12.083242
 DELETING TIME-RECORD FOR TIME    14.887008
 DELETING TIME-RECORD FOR TIME    17.833560
 DELETING TIME-RECORD FOR TIME    20.908984
 DELETING TIME-RECORD FOR TIME    24.107288
 DELETING TIME-RECORD FOR TIME    27.422352
 DELETING TIME-RECORD FOR TIME    30.849994
 DELETING TIME-RECORD FOR TIME    34.377834
 DELETING TIME-RECORD FOR TIME    38.001764
 DELETING TIME-RECORD FOR TIME    41.718584
 DELETING TIME-RECORD FOR TIME    45.525738

 KEEPING TIME-RECORD FOR TIME    49.001916
 AND FOR TIME                    50.000000
 WORKSPACE RECLAIMED

 TIMESTEP AT     50.0000000     SELECTED

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

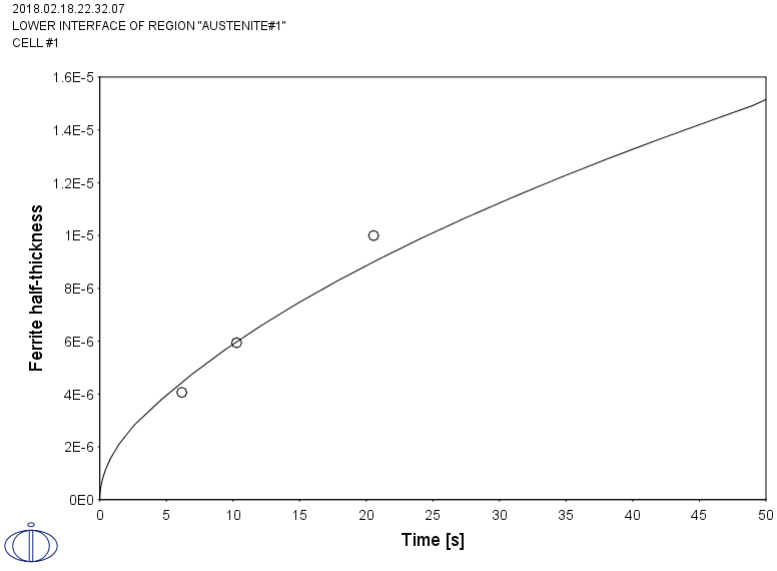
exh2-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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: plot
```

Figure h2



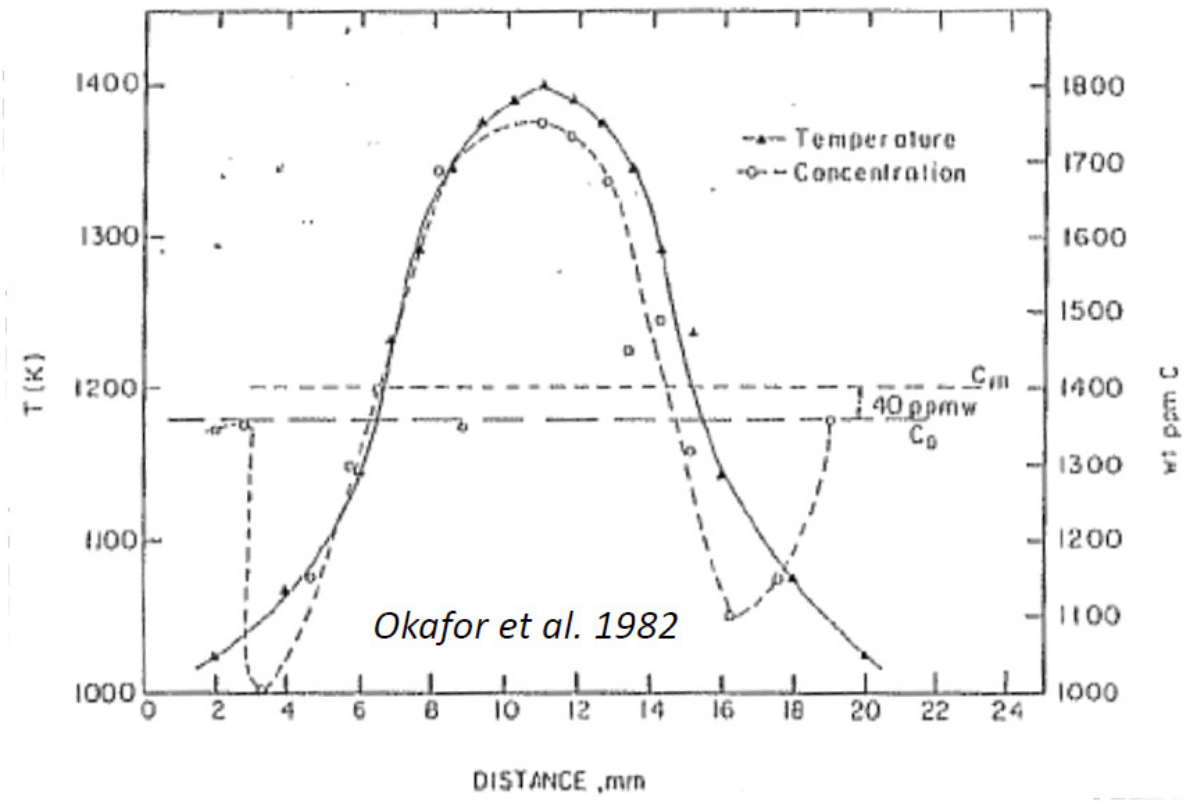

```
POST-1:
POST-1:
POST-1:
POST-1: set-inter
 --OK---
POST-1:
```

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

```
About Linked: Fri Feb 16 15:22:08 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

 VA                     /-  DEFINED
 L12_FCC                B2_BCC                 DICTRA_FCC_A1
   REJECTED
TDB_TCFE9: sw fedemo
 Current database: Iron Demo Database v2.0

 VA                     /-  DEFINED
TDB_FEDEMO: def-sys fe ni c
 FE                     NI                     C
   DEFINED
TDB_FEDEMO: rej ph * all
 GAS:G                  LIQUID:L               BCC_A2
 CEMENTITE              DIAMOND_FCC_A4         FCC_A1
 GRAPHITE               HCP_A3                 KSI_CARBIDE
 LAVES_PHASE_C14        M23C6                  M5C2
 M7C3   REJECTED
TDB_FEDEMO: res ph fcc graph
 FCC_A1                 GRAPHITE  RESTORED
TDB_FEDEMO: get
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'B.-J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
  'A. Gabriel, C. Chatillon, and I. Ansara, published in High Temp. Sci.
      (Parameters listed in CALPHAD, 11 (1987) 203-218); C-NI'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'X.-G. Lu, M. Selleby, B. Sundman, CALPHAD, 29 (2005) 49-55; Fe P-T diagram'
  'A. Gabriel, P. Gustafson, and I. Ansara, CALPHAD, 11 (1987) 203 -218;
      TRITA-MAC 285 (1986); C-FE-NI'
  'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
  'A. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); FE-NI'
  'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121 -127; Molar
      volumes'
 -OK-
TDB_FEDEMO: app mfedemo
 Current database: Fe-Alloys Mobility demo database v2.0

 VA  DEFINED
APP: def-sys fe ni c
 FE                     NI                     C
   DEFINED
APP: rej ph * all
 BCC_A2                 FCC_A1  REJECTED
APP: res ph fcc
 FCC_A1  RESTORED
APP: get
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'This parameter has not been assessed'
  'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'
  'B. Jonsson: Z. Metallkunde 85(1994)502-509; C diffusion in fcc Cr-Fe-Ni'
  'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
      -Ni'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Ni self-diffusion'
 -OK-
APP:
APP: go d-m
 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>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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 grid   75
 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 = .00662305741857947  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 = .00662305741857947  FE = .68534915460493
                        NI = .31465084539507
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    0 seconds
 TIME =   1600.4001     DT =   1600.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0066230574185794  FE = .68534915460493
                        NI = .31465084539507
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    0 seconds
 TIME =   75752.427     DT =   74152.027     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741850892  FE = .68534915460493
                        NI = .31465084539507
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    1 seconds
 TIME =   224056.48     DT =   148304.05     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741822253  FE = .68534915460493
                        NI = .31465084539507
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    0 seconds
 TIME =   520664.59     DT =   296608.11     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741822208  FE = .68534915460493
                        NI = .31465084539507
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    0 seconds
 TIME =   1113880.8     DT =   593216.22     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741822194  FE = .68534915460493
                        NI = .31465084539507
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    1 seconds
 TIME =   2300313.2     DT =   1186432.4     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741819878  FE = .68534915460493
                        NI = .31465084539507
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    0 seconds
 TIME =   4673178.1     DT =   2372864.9     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741817995  FE = .68534915460493
                        NI = .31465084539507
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    1 seconds
 TIME =   7599334.5     DT =   2926156.3     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741819184  FE = .68534915460493
                        NI = .31465084539507
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    0 seconds
 TIME =   10079984.     DT =   2480649.1     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741819794  FE = .68534915460493
                        NI = .31465084539507
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    0 seconds
 TIME =   12348045.     DT =   2268061.6     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741820075  FE = .68534915460493
                        NI = .31465084539507
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    1 seconds
 TIME =   14506749.     DT =   2158703.9     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741820244  FE = .68534915460493
                        NI = .31465084539507
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    0 seconds
 TIME =   16599481.     DT =   2092732.2     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741820524  FE = .68534915460493
                        NI = .31465084539507
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    1 seconds
 TIME =   18648923.     DT =   2049441.3     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741790953  FE = .685349154604931
                        NI = .31465084539507
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    0 seconds
 TIME =   20668354.     DT =   2019431.3     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741737831  FE = .685349154604931
                        NI = .31465084539507
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    0 seconds
 TIME =   22666114.     DT =   1997759.7     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741692653  FE = .68534915460493
                        NI = .31465084539507
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    1 seconds
 TIME =   24647703.     DT =   1981589.3     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741653748  FE = .68534915460493
                        NI = .31465084539507
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    0 seconds
```

```
TIME =   26616876.     DT =   1969173.4     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00662305741462012  FE = .685349154604931
                       NI = .31465084539507
TOTAL SIZE OF SYSTEM:  .025 [m]
 CPU time used in timestep                    0 seconds
TIME =   28576276.     DT =   1959399.6     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00662305741590643  FE = .68534915460493
                       NI = .31465084539507
TOTAL SIZE OF SYSTEM:  .025 [m]
 CPU time used in timestep                    1 seconds
TIME =   30527808.     DT =   1951532.4     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00662305741564765  FE = .68534915460493
                       NI = .31465084539507
TOTAL SIZE OF SYSTEM:  .025 [m]
 CPU time used in timestep                    0 seconds
TIME =   32472884.     DT =   1945075.6     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00662305741542058  FE = .68534915460493
                       NI = .31465084539507
TOTAL SIZE OF SYSTEM:  .025 [m]
 CPU time used in timestep                    0 seconds
TIME =   34412572.     DT =   1939688.3     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00662305741522016  FE = .68534915460493
                       NI = .31465084539507
TOTAL SIZE OF SYSTEM:  .025 [m]
 CPU time used in timestep                    1 seconds
TIME =   36347704.     DT =   1935131.5     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00662305741504403  FE = .68534915460493
                       NI = .31465084539507
TOTAL SIZE OF SYSTEM:  .025 [m]
 CPU time used in timestep                    0 seconds
TIME =   38278937.     DT =   1931233.7     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00662305741488843  FE = .68534915460493
                       NI = .31465084539507
TOTAL SIZE OF SYSTEM:  .025 [m]
 CPU time used in timestep                    0 seconds
TIME =   40206807.     DT =   1927869.8     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00662305741474968  FE = .68534915460493
                       NI = .31465084539507
TOTAL SIZE OF SYSTEM:  .025 [m]
 CPU time used in timestep                    1 seconds
TIME =   42131753.     DT =   1924946.2     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00662305741462626  FE = .68534915460493
                       NI = .31465084539507
TOTAL SIZE OF SYSTEM:  .025 [m]
 CPU time used in timestep                    0 seconds
TIME =   44054144.     DT =   1922391.1     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00662305741451708  FE = .68534915460493
                       NI = .31465084539507
TOTAL SIZE OF SYSTEM:  .025 [m]
 CPU time used in timestep                    0 seconds
TIME =   45974292.     DT =   1920148.0     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00662305741441852  FE = .68534915460493
                       NI = .31465084539507
TOTAL SIZE OF SYSTEM:  .025 [m]
 CPU time used in timestep                    1 seconds
TIME =   47614300.     DT =   1640007.6     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00662305741434809  FE = .685349154604931
                       NI = .31465084539507
TOTAL SIZE OF SYSTEM:  .025 [m]
 CPU time used in timestep                    0 seconds
TIME =   48910464.     DT =   1296163.5     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00662305741430267  FE = .68534915460493
                       NI = .31465084539507
TOTAL SIZE OF SYSTEM:  .025 [m]
 CPU time used in timestep                    0 seconds
TIME =   49749384.     DT =   838920.23     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00662305741428061  FE = .68534915460493
                       NI = .31465084539507
TOTAL SIZE OF SYSTEM:  .025 [m]
 CPU time used in timestep                    1 seconds
TIME =   50000000.     DT =   250616.21     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00662305741428022  FE = .68534915460493
                       NI = .31465084539507
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    1600.4001
DELETING TIME-RECORD FOR TIME    75752.427
DELETING TIME-RECORD FOR TIME    224056.48
DELETING TIME-RECORD FOR TIME    520664.59
DELETING TIME-RECORD FOR TIME    1113880.8
DELETING TIME-RECORD FOR TIME    2300313.2
DELETING TIME-RECORD FOR TIME    4673178.1
DELETING TIME-RECORD FOR TIME    7599334.5
DELETING TIME-RECORD FOR TIME    10079984.
DELETING TIME-RECORD FOR TIME    12348045.
DELETING TIME-RECORD FOR TIME    14506749.
DELETING TIME-RECORD FOR TIME    16599481.
DELETING TIME-RECORD FOR TIME    18648923.
DELETING TIME-RECORD FOR TIME    20668354.
DELETING TIME-RECORD FOR TIME    22666114.
DELETING TIME-RECORD FOR TIME    24647703.
DELETING TIME-RECORD FOR TIME    26616876.
DELETING TIME-RECORD FOR TIME    28576276.
DELETING TIME-RECORD FOR TIME    30527808.
DELETING TIME-RECORD FOR TIME    32472884.
DELETING TIME-RECORD FOR TIME    34412572.
DELETING TIME-RECORD FOR TIME    36347704.
DELETING TIME-RECORD FOR TIME    38278937.
DELETING TIME-RECORD FOR TIME    40206807.
DELETING TIME-RECORD FOR TIME    42131753.
DELETING TIME-RECORD FOR TIME    44054144.
DELETING TIME-RECORD FOR TIME    45974292.
DELETING TIME-RECORD FOR TIME    47614300.
DELETING TIME-RECORD FOR TIME    48910464.

KEEPING TIME-RECORD FOR TIME    49749384.
AND FOR TIME                    50000000.
WORKSPACE RECLAIMED

TIMESTEP AT     50000000.0     SELECTED
```

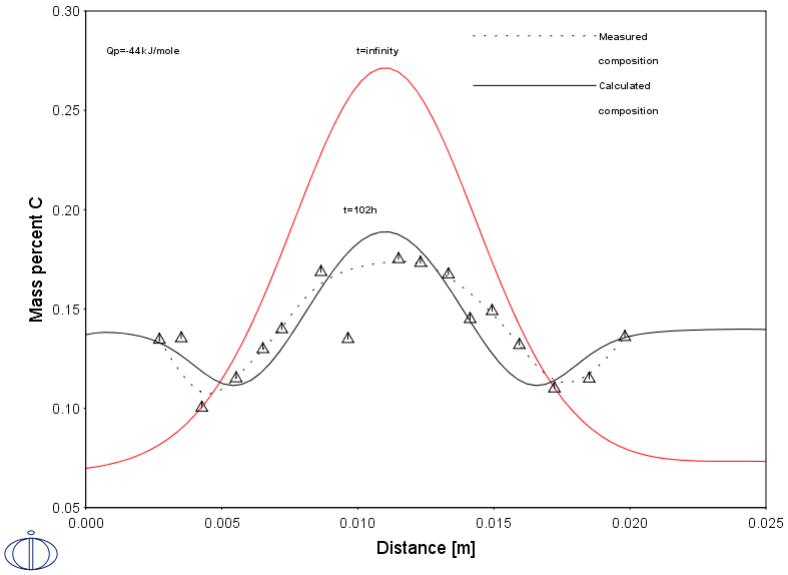
```
DIC>
DIC> set-inter
 --OK---
DIC>
```

exh3-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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

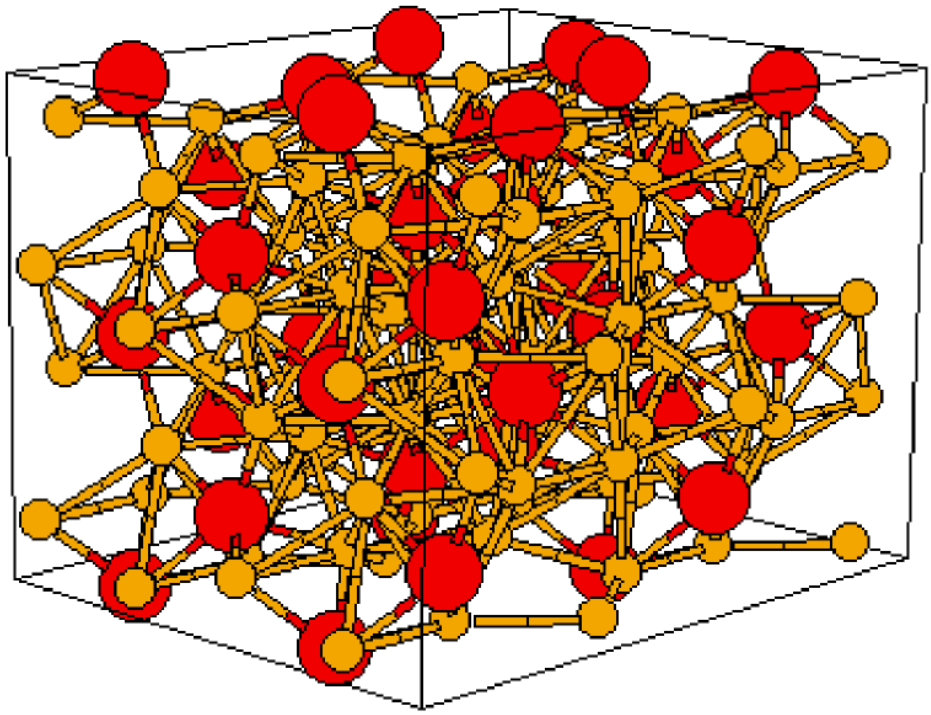
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson

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: plot
```




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

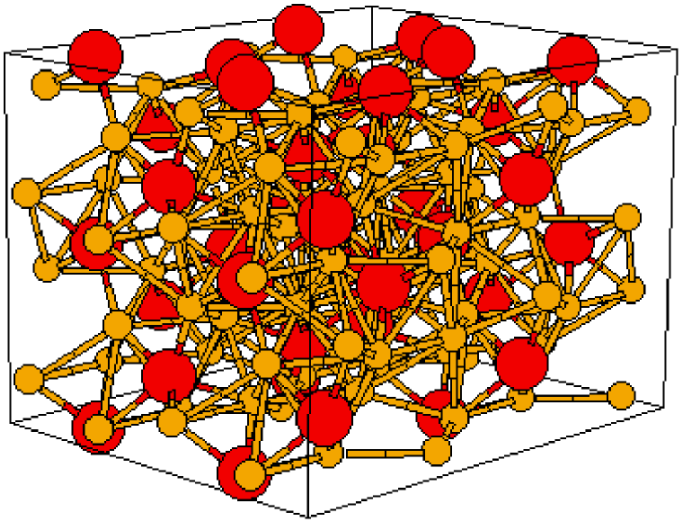
Diffusion in Complex Phases



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

```
About License library version: 8.5.1.0017
 Linked: Fri Feb 16 15:22:08 2018

SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exi1\setup.DCM" @@
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
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

 VA                       /-  DEFINED
 L12_FCC                  B2_BCC                   DICTRA_FCC_A1
   REJECTED
TDB_TCFE9: sw user AlFeNi-data.TDB
 Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

 VA  DEFINED
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
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....
 INFO: Forcing option USE_POLY3 for complex phase B2_ORD
 -OK-
TDB_USER: go -m
 NO TIME STEP DEFINED
DIC> set-cond glob T 0 1277; * N

DIC>
DIC> enter-region beta
DIC>
DIC> enter-grid beta
WIDTH OF REGION /1/: 2e-3
TYPE /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
 INFO: PHASE HAS DISORDERED CONTRIBUTION
 FORCED STARTING VALUES ARE ENABLED
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);
 Forcing automatic start values
 Automatic start values will be set
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 Forcing automatic start values
 Automatic start values will be set
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>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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
 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                   1 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                   0 seconds
 TIME =  0.40010010     DT =  0.40000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  AL = .429499345639258  FE = .290517917020317
                        NI = .279982737340426
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                   0 seconds
 TIME =   513.08856     DT =   512.68846     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  AL = .429499345639248  FE = .290517917020326
                        NI = .279982737340426
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                   1 seconds
 TIME =   1538.4655     DT =   1025.3769     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  AL = .429499345639233  FE = .290517917020342
                        NI = .279982737340425
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                   1 seconds
 TIME =   3589.2193     DT =   2050.7538     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  AL = .429499345639231  FE = .290517917020344
                        NI = .279982737340425
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                   1 seconds
 TIME =   7690.7270     DT =   4101.5077     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  AL = .429499345639227  FE = .290517917020345
                        NI = .279982737340428
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                   2 seconds
 TIME =   15893.742     DT =   8203.0154     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  AL = .429499345639233  FE = .290517917020341
                        NI = .279982737340426
 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 = .290517917020362
                        NI = .279982737340428
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                   2 seconds
 TIME =   65111.835     DT =   32812.062     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  AL = .429499345639174  FE = .290517917020382
                        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 = .290517917020496
                        NI = .279982737340415
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                   2 seconds
 TIME =   134231.83     DT =   34560.000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  AL = .429499345639132  FE = .290517917020483
                        NI = .279982737340386
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                   2 seconds
 TIME =   168791.83     DT =   34560.000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  AL = .429499345639167  FE = .290517917020446
                        NI = .279982737340387
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                   2 seconds
 TIME =   203351.83     DT =   34560.000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  AL = .429499345639157  FE = .290517917020456
                        NI = .279982737340388
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                   1 seconds
 TIME =   237911.83     DT =   34560.000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  AL = .429499345639151  FE = .290517917020441
                        NI = .279982737340408
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                   2 seconds
 TIME =   272471.83     DT =   34560.000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  AL = .429499345639151  FE = .290517917020425
                        NI = .279982737340423
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                   2 seconds
 TIME =   307031.83     DT =   34560.000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  AL = .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                    2 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

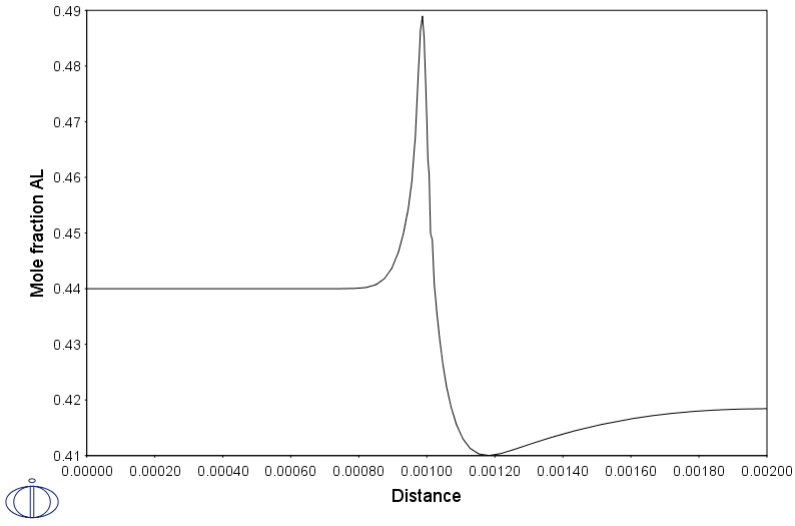
DIC>
DIC> set-inter
 --OK---
DIC>
```

exi1-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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

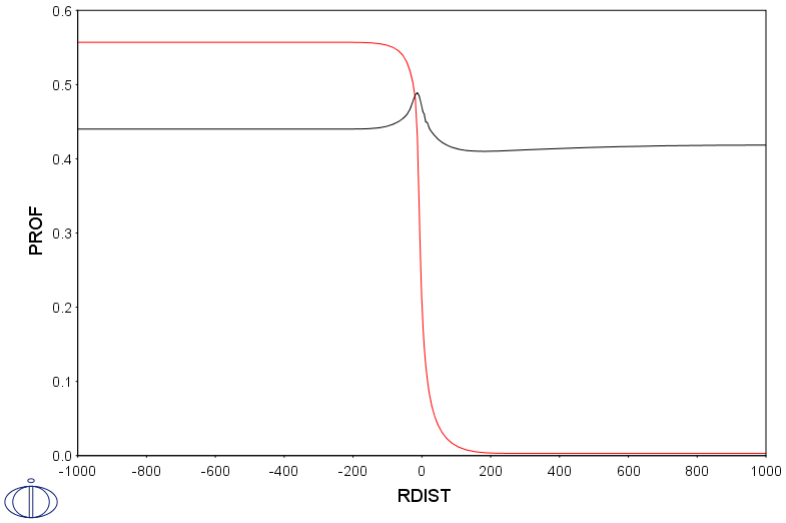
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson

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: plot
   2018.02.18.22.38.40
   Time = 345600
   CELL #1
```



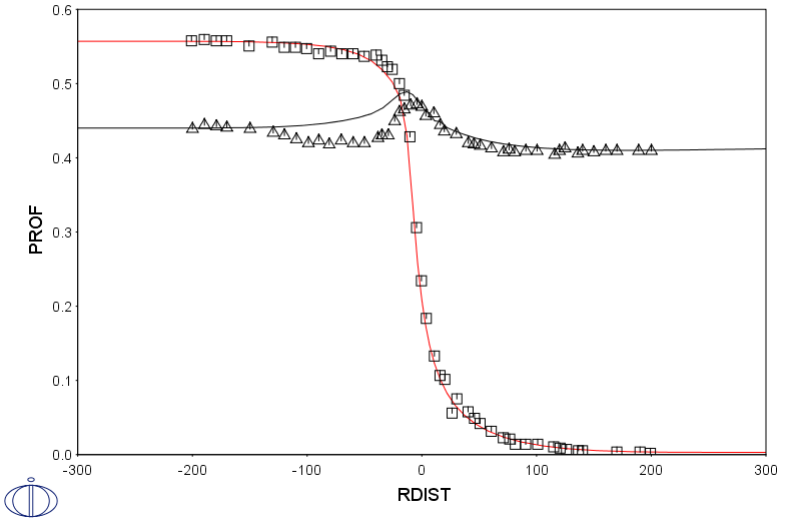

```
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: ent tab prof
Variable(s) x(al) x(ni)
POST-1:
POST-1: ent fun rdist
FUNCTION: 1e6*(gd-10e-4)
&
POST-1: s-d-a y prof
COLUMN NUMBER /*/: 1 2
POST-1:
POST-1: s-d-a x rdist
POST-1:
POST-1: plo
```

2018.02.18.22.38.40
Time = 345600
CELL #1



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: plot

2018.02.18.22.38.41
Time = 345600
CELL #1



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

About Linked: Fri Feb 16 15:22:08 2018

```
SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exi2\setup.DCM" @@
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
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

 VA                     /-  DEFINED
 L12_FCC                B2_BCC                 DICTRA_FCC_A1
   REJECTED
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA
TDB_TCFE9: @@
TDB_TCFE9: switch FEDEMO
 Current database: Iron Demo Database v2.0

 VA                     /-  DEFINED
TDB_FEDEMO: def-sys fe c
 FE                     C  DEFINED
TDB_FEDEMO: rej ph * all
 GAS:G                  LIQUID:L               BCC_A2
 CEMENTITE              DIAMOND_FCC_A4         FCC_A1
 GRAPHITE               HCP_A3                 KSI_CARBIDE
 LAVES_PHASE_C14        M23C6                  M5C2
 M7C3  REJECTED
TDB_FEDEMO: res ph bcc fcc cementite grap
 BCC_A2                 FCC_A1                 CEMENTITE
 GRAPHITE  RESTORED
TDB_FEDEMO: get
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES .....
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'P. Franke, Estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
  'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'X.-G. Lu, M. Selleby, B. Sundman, CALPHAD, 29 (2005) 49-55; Fe P-T diagram'
  'B. Hallstedt, D. Djurovic, J. von Appen, R. Dronskowski, A. Dick, F.
      Koermann, T. Hickel, J. Neugebauer, CALPHAD, 34, 129 -33(2010); Fe-C'
  'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
  'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121 -127; Molar
      volumes'
 -OK-
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE MOBILITY DATA
TDB_FEDEMO: @@
TDB_FEDEMO: app user cembccstoik.TDB
 Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

 VA  DEFINED
TDB_APP: def-sys fe c
 FE                     C  DEFINED
TDB_APP: rej ph * all
 BCC_A2                 CEMENTITE  REJECTED
TDB_APP: res ph fcc bcc cementite
 *** FCC INPUT IGNORED
 BCC_A2                 CEMENTITE  RESTORED
TDB_APP: get
 ELEMENTS .....
 SPECIES .....
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data


 *** ERROR  1000 IN TDBGRT
 *** NO REFERENCE FILE

 *** ERROR  1000 IN TDBGRT
 *** NO REFERENCE FILE
 -OK-
TDB_APP:
TDB_APP: @@
TDB_APP: @@ ENTER THE DICTRA MONITOR
TDB_APP: @@
```

```
TDB_APP: go d-m
 NO TIME STEP DEFINED
 *** ENTERING FCC_A1 AS A DIFFUSION NONE PHASE
 *** 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>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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 FCC_A1 AS A DIFFUSION NONE PHASE
 *** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
DIC> read exi2
 OK
DIC>
DIC> @@
DIC> @@ START THE SIMULATION
DIC> @@
DIC> sim
 Region: FER
 single geometric dense at  0.33000E-05
 0.91945       87
 Region: CARB
 double geometric
 dense at outer boundaries, coarse at  0.50000E-12
lower part   1.2500        9
upper part  0.80000        9
  Trying old scheme                    3
 U-FRACTION IN SYSTEM:  C = 4.6598005784384E-05  FE = 1
 TOTAL SIZE OF SYSTEM:  3.300001E-06 [m]
 U-FRACTION IN SYSTEM:  C = 4.6598005784384E-05  FE = 1
 TOTAL SIZE OF SYSTEM:  3.300001E-06 [m]
 0.111094107740055        0.111116327660160        1.168933545308438E-022       TIME =  0.10000000E-06 DT =  0.10000000E-
06 SUM OF SQUARES =  0.11689335E-21
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.55732855E-06 AND  -0.55732855E-06
 POSITION OF INTERFACE FER / CARB IS   0.32999999E-05
 U-FRACTION IN SYSTEM:  C = 4.65969237107415E-05  FE = 1
 TOTAL SIZE OF SYSTEM:  3.300001E-06 [m]
  2  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: FER

  CPU time used in timestep                    0 seconds
 1.985503622653894E-006        1.986016682715920E-006        8.569005889170424E-023       TIME =  0.25999666E-05 DT =  0.24999666E-
05 SUM OF SQUARES =  0.85690059E-22
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.12341808E-06 AND  -0.12341808E-06
 POSITION OF INTERFACE FER / CARB IS   0.32999996E-05
 U-FRACTION IN SYSTEM:  C = 4.66223850218017E-05  FE = 1
 TOTAL SIZE OF SYSTEM:  3.300001E-06 [m]
  CPU time used in timestep                    0 seconds
 9.632817666940026E-007        9.640732404382950E-007        1.188374989701993E-025       TIME =  0.75998999E-05 DT =  0.49999333E-
05 SUM OF SQUARES =  0.11883750E-24
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.91502734E-07 AND  -0.91502734E-07
 POSITION OF INTERFACE FER / CARB IS   0.32999992E-05
 U-FRACTION IN SYSTEM:  C = 4.66617913784151E-05  FE = 1
 TOTAL SIZE OF SYSTEM:  3.300001E-06 [m]
  CPU time used in timestep                    0 seconds
 5.520598281728834E-007        5.525040595679586E-007        1.288882881968142E-026       TIME =  0.17599767E-04 DT =  0.99998666E-
05 SUM OF SQUARES =  0.12888829E-25
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.67380405E-07 AND  -0.67380405E-07
 POSITION OF INTERFACE FER / CARB IS   0.32999985E-05
 U-FRACTION IN SYSTEM:  C = 4.67208116371187E-05  FE = 1
 TOTAL SIZE OF SYSTEM:  3.300001E-06 [m]
  CPU time used in timestep                    0 seconds
 3.294904029785897E-007        3.297431202262137E-007        1.269811257175113E-026       TIME =  0.37599500E-04 DT =  0.19999733E-
04 SUM OF SQUARES =  0.12698113E-25
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.48810906E-07 AND  -0.48810906E-07
 POSITION OF INTERFACE FER / CARB IS   0.32999975E-05
 U-FRACTION IN SYSTEM:  C = 4.68069809139129E-05  FE = 1
 TOTAL SIZE OF SYSTEM:  3.300001E-06 [m]
  CPU time used in timestep                    0 seconds
 1.842051604935253E-007        1.843420424813243E-007        3.758018249556124E-025       TIME =  0.77598966E-04 DT =  0.39999466E-
04 SUM OF SQUARES =  0.37580182E-24
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.34957854E-07 AND  -0.34957854E-07
 POSITION OF INTERFACE FER / CARB IS   0.32999961E-05
 U-FRACTION IN SYSTEM:  C = 4.69308608646658E-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
 9.778279830287753E-008        9.785422392329824E-008        1.355451665779685E-025       TIME =  0.15759790E-03 DT =  0.79998933E-
04 SUM OF SQUARES =  0.13554517E-24
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.24876846E-07 AND  -0.24876846E-07
 POSITION OF INTERFACE FER / CARB IS   0.32999941E-05
 U-FRACTION IN SYSTEM:  C = 4.71074840882462E-05  FE = 1
 TOTAL SIZE OF SYSTEM:  3.300001E-06 [m]
  49  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: CARB

  CPU time used in timestep                    0 seconds
 5.038045599773962E-006        5.041694015305950E-006        4.707624364821560E-025       TIME =  0.31759576E-03 DT =  0.15999787E-
03 SUM OF SQUARES =  0.47076244E-24
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.17645081E-07 AND  -0.17645081E-07
 POSITION OF INTERFACE FER / CARB IS   0.32999913E-05
 U-FRACTION IN SYSTEM:  C = 4.73582549999065E-05  FE = 1
 TOTAL SIZE OF SYSTEM:  3.300001E-06 [m]


output ignored...



... output resumed

TIME =   3142.1594     DT =   900.00000     SUM OF SQUARES =  0.30225501E-26
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.44854482E-11 AND  -0.44854482E-11
 POSITION OF INTERFACE FER / CARB IS   0.32722305E-05
 U-FRACTION IN SYSTEM:  C = .00283057618776405  FE = 1
 TOTAL SIZE OF SYSTEM:  3.300001E-06 [m]
  55  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: CARB

  CPU time used in timestep                    1 seconds
```

```
 3.512901236764630E-008        3.518395504960265E-008        9.614405727817597E-
029       TIME =   4042.1594     DT =   900.00000     SUM OF SQUARES =  0.96144057E-28
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.38334138E-11 AND  -0.38334138E-11
 POSITION OF INTERFACE FER / CARB IS   0.32687804E-05
 U-FRACTION IN SYSTEM:  C = .00317904137490816  FE = 1
 TOTAL SIZE OF SYSTEM:  3.300001E-06 [m]
  9  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: CARB

  CPU time used in timestep                    0 seconds
 1.337273690876802E-008        1.340171249585930E-008        1.438406288208647E-
026       TIME =   4942.1594     DT =   900.00000     SUM OF SQUARES =  0.14384063E-25
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.34097971E-11 AND  -0.34097971E-11
 POSITION OF INTERFACE FER / CARB IS   0.32657116E-05
 U-FRACTION IN SYSTEM:  C = .00348899893656266  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
 6.238597393059804E-009        6.256204153119521E-009        5.571054466188241E-
030       TIME =   5842.1594     DT =   900.00000     SUM OF SQUARES =  0.55710545E-29
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.31046285E-11 AND  -0.31046285E-11
 POSITION OF INTERFACE FER / CARB IS   0.32629174E-05
 U-FRACTION IN SYSTEM:  C = .00377121604704412  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
 3.280281446289517E-009        3.291907995765650E-009        1.610509839104679E-
030       TIME =   6742.1594     DT =   900.00000     SUM OF SQUARES =  0.16105098E-29
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.28707015E-11 AND  -0.28707015E-11
 POSITION OF INTERFACE FER / CARB IS   0.32603338E-05
 U-FRACTION IN SYSTEM:  C = .00403216870914912  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
 1.864873578096803E-007        1.872981047449765E-007        1.864276412969093E-
029       TIME =   7642.1594     DT =   900.00000     SUM OF SQUARES =  0.18642764E-28
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.26837249E-11 AND  -0.26837249E-11
 POSITION OF INTERFACE FER / CARB IS   0.32579185E-05
 U-FRACTION IN SYSTEM:  C = .00427612481768502  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
 1.118941665788623E-007        1.124814013240834E-007        7.257773708191617E-
030       TIME =   8542.1594     DT =   900.00000     SUM OF SQUARES =  0.72577737E-29
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.25296909E-11 AND  -0.25296909E-11
 POSITION OF INTERFACE FER / CARB IS   0.32556417E-05
 U-FRACTION IN SYSTEM:  C = .00450607892012097  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
 6.975845435923255E-008        7.019562001951880E-008        7.183192071095221E-
030       TIME =   9000.0000     DT =   457.84063     SUM OF SQUARES =  0.71831921E-29
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.23998555E-11 AND  -0.23998555E-11
 POSITION OF INTERFACE FER / CARB IS   0.32545430E-05
 U-FRACTION IN SYSTEM:  C = .00461705531635601  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   0.25999666E-05
 DELETING TIME-RECORD FOR TIME   0.75998999E-05
 DELETING TIME-RECORD FOR TIME   0.17599767E-04
 DELETING TIME-RECORD FOR TIME   0.37599500E-04
 DELETING TIME-RECORD FOR TIME   0.77598966E-04
 DELETING TIME-RECORD FOR TIME   0.15759790E-03
 DELETING TIME-RECORD FOR TIME   0.31759576E-03
 DELETING TIME-RECORD FOR TIME   0.63759149E-03
 DELETING TIME-RECORD FOR TIME   0.12775830E-02
 DELETING TIME-RECORD FOR TIME   0.25575659E-02
 DELETING TIME-RECORD FOR TIME   0.51175317E-02
 DELETING TIME-RECORD FOR TIME   0.10237463E-01
 DELETING TIME-RECORD FOR TIME   0.20477327E-01
 DELETING TIME-RECORD FOR TIME   0.40957054E-01
 DELETING TIME-RECORD FOR TIME   0.81916507E-01
 DELETING TIME-RECORD FOR TIME   0.16383541
 DELETING TIME-RECORD FOR TIME   0.32767323
 DELETING TIME-RECORD FOR TIME   0.65534886
 DELETING TIME-RECORD FOR TIME    1.3107001
 DELETING TIME-RECORD FOR TIME    2.6214026
 DELETING TIME-RECORD FOR TIME    5.2428076
 DELETING TIME-RECORD FOR TIME    10.485618
 DELETING TIME-RECORD FOR TIME    20.971238
 DELETING TIME-RECORD FOR TIME    41.942478
 DELETING TIME-RECORD FOR TIME    83.884958
 DELETING TIME-RECORD FOR TIME    167.76992
 DELETING TIME-RECORD FOR TIME    335.53984
 DELETING TIME-RECORD FOR TIME    671.07968
 DELETING TIME-RECORD FOR TIME    1342.1594
 DELETING TIME-RECORD FOR TIME    2242.1594
 DELETING TIME-RECORD FOR TIME    3142.1594
 DELETING TIME-RECORD FOR TIME    4042.1594
 DELETING TIME-RECORD FOR TIME    4942.1594
 DELETING TIME-RECORD FOR TIME    5842.1594
 DELETING TIME-RECORD FOR TIME    6742.1594
 DELETING TIME-RECORD FOR TIME    7642.1594

 KEEPING TIME-RECORD FOR TIME    8542.1594
 AND FOR TIME                    9000.0000
 WORKSPACE RECLAIMED

 TIMESTEP AT     9000.00000     SELECTED

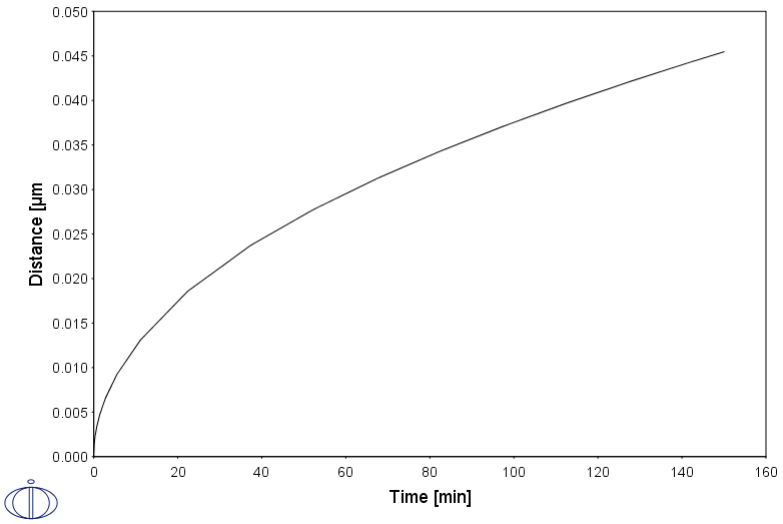
DIC>
DIC> set-inter
 --OK---
DIC>
```

exi2-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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 FCC_A1 AS A DIFFUSION NONE PHASE
 *** 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

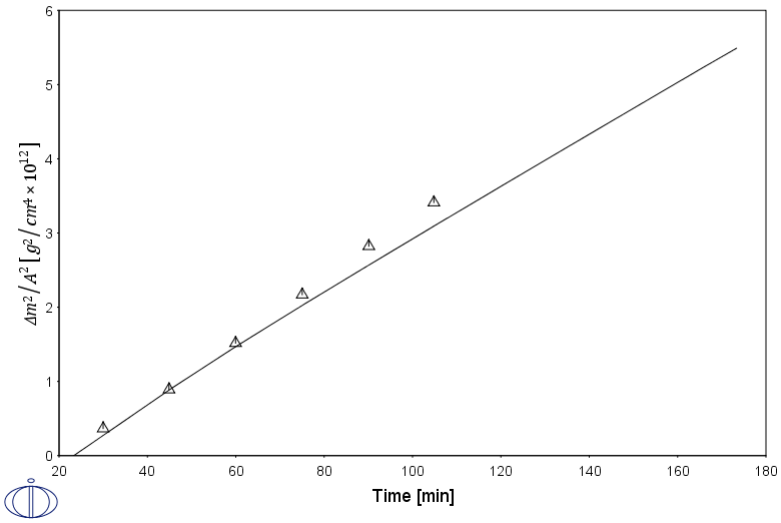
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson

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 [?m]
POST-1:
POST-1: plot
   2018.02.18.22.41.40
   "FIRST" INTERFACE OF SYSTEM
   CELL #1
```




```
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: plot
```

2018.02.18.22.41.41
"FIRST" INTERFACE OF SYSTEM
CELL #1

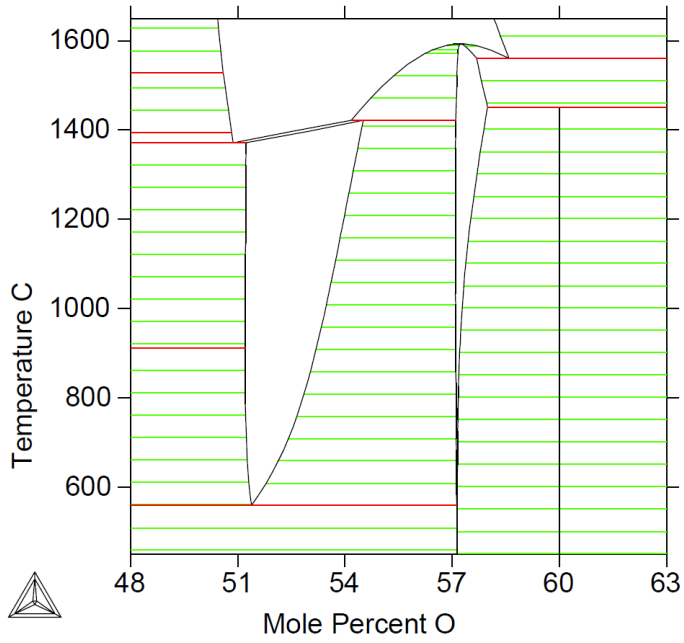


POST-1:
POST-1:
POST-1: set-inter
--OK---
POST-1:

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

```
About Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 12987) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri Feb 16 15:22:08 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

 VA                     /-  DEFINED
 L12_FCC                B2_BCC                 DICTRA_FCC_A1
   REJECTED
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ SELECT A USER DATABASE FOR READING THE THERMODYNAMIC DATA
TDB_TCFE9: @@
TDB_TCFE9: sw user FeO.TDB
 Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

 VA                     /-  DEFINED
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
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 Reference REF368     missing close to line                   55
 Reference REF304     missing close to line                   63
 Reference REF420     missing close to line                   65
 Reference REF420     missing close to line                   67
 Reference REF368     missing close to line                   69
 Reference REF368     missing close to line                   70
 Reference REF368     missing close to line                   72
 Reference REF418     missing close to line                   74
 Reference REF418     missing close to line                   76
 Reference REF304     missing close to line                   78
 Reference REF30      missing close to line                   86
 Reference REF30      missing close to line                   88
 Reference REF30      missing close to line                   90
 Reference REF420     missing close to line                   92
 Reference REF420     missing close to line                   94
 Reference REF30      missing close to line                   96
 Reference REF30      missing close to line                   98
 Reference REF30      missing close to line                  100
 Reference REF420     missing close to line                  102
 Reference REF420     missing close to line                  104
 Reference REF30      missing close to line                  106
 Reference REF30      missing close to line                  108
 Reference REF30      missing close to line                  110
 Reference REF420     missing close to line                  112
 Reference REF420     missing close to line                  114
 Reference REF30      missing close to line                  116
 Reference REF30      missing close to line                  118
 Reference REF30      missing close to line                  120
 Reference REF420     missing close to line                  122
 Reference REF420     missing close to line                  124
 Reference REF30      missing close to line                  126
 Reference REF30      missing close to line                  128
 Reference REF30      missing close to line                  130
 Reference REF420     missing close to line                  132
 Reference REF420     missing close to line                  134
 Reference REF30      missing close to line                  136
 Reference REF30      missing close to line                  138
 Reference REF30      missing close to line                  140
 Reference REF420     missing close to line                  142
 Reference REF420     missing close to line                  144
 Reference REF30      missing close to line                  146
 Reference REF30      missing close to line                  148
 Reference REF30      missing close to line                  150
 Reference REF420     missing close to line                  152
 Reference REF420     missing close to line                  154
 Reference REF30      missing close to line                  156
 Reference REF30      missing close to line                  158
 Reference REF30      missing close to line                  160
 Reference REF420     missing close to line                  162
```

```
 Reference REF420     missing close to line                    164
 Reference REF30      missing close to line                    166
 Reference REF30      missing close to line                    168
 Reference REF30      missing close to line                    170
 Reference REF420     missing close to line                    172
 Reference REF420     missing close to line                    174
 Reference REF30      missing close to line                    176
 Reference REF30      missing close to line                    178
 Reference REF30      missing close to line                    180
 Reference REF420     missing close to line                    182
 Reference REF420     missing close to line                    184
 Reference REF30      missing close to line                    186
 Reference REF30      missing close to line                    188
 Reference REF30      missing close to line                    190
 Reference REF420     missing close to line                    192
 Reference REF420     missing close to line                    194
 Reference REF30      missing close to line                    196
 Reference REF30      missing close to line                    198
 Reference REF30      missing close to line                    200
 Reference REF420     missing close to line                    202
 Reference REF420     missing close to line                    204
 FUNCTIONS ....
 -OK-
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
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 ...
 FUNCTIONS ....

 List of references for assessed data


 *** ERROR  1000 IN TDBGRT
 *** NO REFERENCE FILE

 *** ERROR  1000 IN TDBGRT
 *** NO REFERENCE FILE
 -OK-
TDB_APP:
TDB_APP:
TDB_APP: @@
TDB_APP: @@ ENTER THE DICTRA MONITOR
TDB_APP: @@
TDB_APP: go d-m
 NO TIME STEP DEFINED
DIC>
DIC>
DIC> @@
DIC> @@  ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 823; * N

DIC>
DIC>
DIC> @@
DIC> @@  SET THE REFERENCE STATE FOR O TO O2 (GAS)
DIC> @@
DIC> set-ref o gas,,,,,,,
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE REGIONS fer AND sp
DIC> @@
DIC> ent-reg fer
DIC> ent-reg sp,,,,,,,,
DIC>
DIC>
DIC> @@
DIC> @@ ENTER PHASES INTO THE REGIONS
DIC> @@
DIC> ent-phase act fer matrix bcc#1
DIC> ent-phase act sp matrix spinel
DIC>
DIC>
DIC> @@
DIC> @@ ENTER GRIDS INTO THE REGIONS
DIC> @@
DIC>
DIC> @@
DIC> @@ ENTER A SIZE FOR THE FERRITE
DIC> @@
DIC> @@
DIC> ent-grid fer 4.99999e-3 AUTO
DIC>
```

```
DIC> @@
DIC> @@ ENTER A THIN INITIAL SIZE FOR THE OXIDE
DIC> @@
DIC> @@
DIC> ent-grid sp  1.00e-10 AUTO
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITIONS IN BCC
DIC> @@
DIC> ent-comp fer bcc#1 m-f
PROFILE FOR /O/: o lin 1e-9 1e-9
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITIONS IN THE OXIDE
DIC> @@
DIC> ent-comp sp spinel m-f
  this is a phase with charged species
  with more than 2 sublattices
PROFILE FOR /FE/: FE lin 4.28771E-01 4.28549E-01
DIC>
DIC>
DIC> @@
DIC> @@ ENTER A BOUNDARY CONDITION "GAS" ON THE UPPER (RIGHT-MOST) INTERFACE
DIC> @@ OF THE OXIDE. THIS ALLOWS THE SYSTEM TO EXPAND AND THE OXIDE LAYER
DIC> @@ TO GROW 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>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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
 single geometric dense at  0.50000E-02
 0.87386       95
 Region: SP
 double geometric
 dense at outer boundaries, coarse at  0.50000E-10
lower part   1.2500        9
upper part  0.80000        9
  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]
 0.347387301619340        0.347386528699253        0.347386701354488        4.618089872755317E-002        1.115577003344626E-
022       TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =  0.11155770E-21
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.39646054E-03 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49999900E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.66982674E-03 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.49999901E-02
 U-FRACTION IN SYSTEM:  FE = 0.99999998954903  O = 3.44015229571833E-08
 TOTAL SIZE OF SYSTEM:  .00499999012734 [m]
  10  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: FER

  CPU time used in timestep                    0 seconds
 1.5075552605990936E-005        1.507739146467480E-005        1.507822847287634E-005        2.226308397782723E-007        2.476318028538286E-
031       TIME =  0.30000000E-06 DT =  0.20000000E-06 SUM OF SQUARES =  0.24763180E-30
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.14849229E-03 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49999899E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.20393047E-03 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.49999901E-02
 U-FRACTION IN SYSTEM:  FE = 0.99999998713864  O = 4.25584032292646E-08
 TOTAL SIZE OF SYSTEM:  .00499999013842 [m]
  CPU time used in timestep                    1 seconds
 1.398975101859364E-008        1.397926494961065E-008        1.395940586724563E-008        3.137487096517389E-011        7.276780229330289E-
034       TIME =  0.70000000E-06 DT =  0.40000000E-06 SUM OF SQUARES =  0.72767802E-33
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.14913262E-03 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49999899E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.21655229E-03 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.49999902E-02
 U-FRACTION IN SYSTEM:  FE = 0.99999998167656  O = 5.9883649440439E-08
 TOTAL SIZE OF SYSTEM:  .00499999016539 [m]
  CPU time used in timestep                    0 seconds
 5.609742547589773E-007        5.611284846250793E-007        5.611264634536804E-007        2.444637655298936E-010        1.128709675659560E-
034       TIME =  0.15000000E-05 DT =  0.80000000E-06 SUM OF SQUARES =  0.11287097E-33
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.93393028E-04 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49999898E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.13339356E-03 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.49999902E-02
 U-FRACTION IN SYSTEM:  FE = 0.99999997507588  O = 8.12291255492651E-08
 TOTAL SIZE OF SYSTEM:  .00499999019739 [m]
  23  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    0 seconds
 8.108701239277702E-006        8.112502967450534E-006        8.112138099848266E-006        1.121067578002317E-008        3.531749267158546E-
032       TIME =  0.31000000E-05 DT =  0.16000000E-05 SUM OF SQUARES =  0.35317493E-31
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.70760985E-04 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49999897E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.10183290E-03 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.49999902E-02
 U-FRACTION IN SYSTEM:  FE = 0.99999996490465  O = 1.13820151455531E-07
 TOTAL SIZE OF SYSTEM:  .00499999024711 [m]
  35  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    0 seconds
 8.100481734301132E-006        8.103302413441165E-006        8.103162850361541E-006        7.195354227408064E-009        8.335665540551005E-
033       TIME =  0.63000000E-05 DT =  0.32000000E-05 SUM OF SQUARES =  0.83356655E-32
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.49011444E-04 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49999895E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.70269554E-04 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.49999903E-02
 U-FRACTION IN SYSTEM:  FE = 0.99999995092491  O = 1.5879999799066E-07
 TOTAL SIZE OF SYSTEM:  .00499999031513 [m]


output ignored...



... output resumed

 POSITION OF INTERFACE FER / SP IS   0.49497263E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.85406534E-09 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.50216007E-02
 U-FRACTION IN SYSTEM:  FE = .995601423066401  O = .0143132204538531
 TOTAL SIZE OF SYSTEM:  .005021600735 [m]
  23  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    1 seconds
 2.789556769619959E-007        2.794057581865568E-007        2.793655764673843E-007        3.800585456559765E-010        3.352321809449032E-
033       TIME =   56943.895     DT =   8640.0000     SUM OF SQUARES =  0.33523218E-32
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.54743813E-09 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49449965E-02
```

```
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.78319309E-09 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.50236377E-02
 U-FRACTION IN SYSTEM:  FE = .995194725257651  O = .0156544064682328
 TOTAL SIZE OF SYSTEM:  .00502363765793 [m]
  8  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    0 seconds
 1.595105700887269E-007        1.598217866941193E-007        1.597953811857604E-007        2.020602968532874E-010        1.098381921408345E-
034       TIME =   65583.895     DT =   8640.0000     SUM OF SQUARES =  0.10983819E-33
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.50751127E-09 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49406116E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.72677808E-09 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.50255321E-02
 U-FRACTION IN SYSTEM:  FE = .994817249746003  O = .0168979971926314
 TOTAL SIZE OF SYSTEM:  .0050255321232 [m]
  7  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    0 seconds
 9.568367501087622E-008        9.590684465888028E-008        9.588874684630677E-008        1.147888046775199E-010        1.391785311373588E-
034       TIME =   74223.895     DT =   8640.0000     SUM OF SQUARES =  0.13917853E-33
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.47495053E-09 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49365080E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.68062878E-09 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.50273092E-02
 U-FRACTION IN SYSTEM:  FE = .994463754813117  O = .0180617615442609
 TOTAL SIZE OF SYSTEM:  .00502730918328 [m]
  10  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    0 seconds
 5.962030960084013E-008        5.978502100270548E-008        5.977212458826642E-008        6.869420014653385E-011        2.456312995478252E-
033       TIME =   82863.895     DT =   8640.0000     SUM OF SQUARES =  0.24563130E-32
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.44778107E-09 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49326392E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.64203085E-09 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.50289875E-02
 U-FRACTION IN SYSTEM:  FE = .994130359456937  O = .0191587681410625
 TOTAL SIZE OF SYSTEM:  .00502898750134 [m]
  8  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    0 seconds
 9.162180973319777E-009        9.108164931689858E-009        9.224421743565125E-009        1.011580316905061E-011        2.783570622747177E-
034       TIME =   86400.000     DT =   3536.1047     SUM OF SQUARES =  0.27835706E-33
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.44500201E-09 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49310656E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.61834793E-09 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.50296005E-02
 U-FRACTION IN SYSTEM:  FE = .994008758985575  O = .0195911680901775
 TOTAL SIZE OF SYSTEM:  .00502960047066 [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

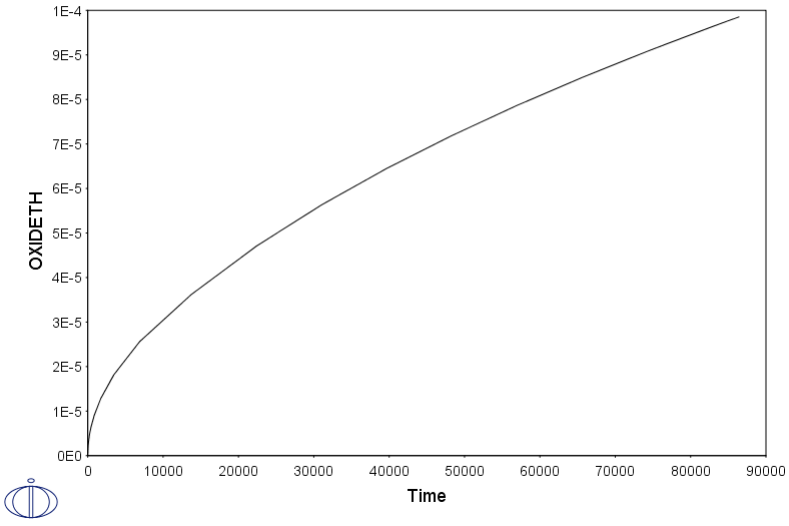
DIC>
DIC> set-inter
 --OK---
DIC>
```

exi3a-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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

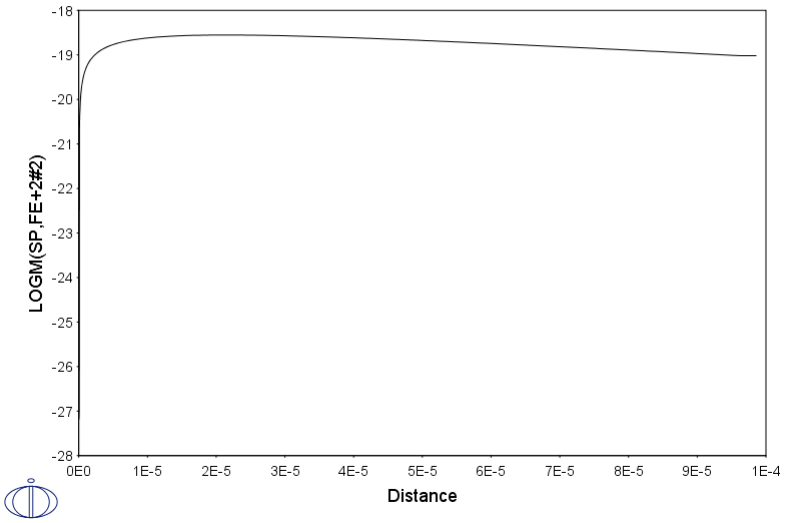
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson

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: plot
   2018.02.18.22.44.49
   UPPER INTERFACE OF REGION "SP#1"
   CELL #1
```



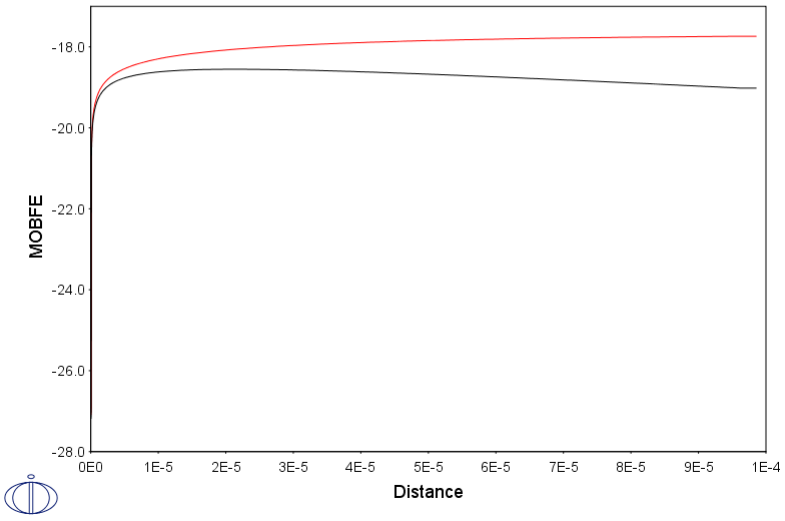

```
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: @@
POST-1: @@ NOW PLOT THE MOBILITY IN A SPINEL FOR Fe+2 ON THE SECOND SUBLATTICE
POST-1: @@
POST-1: s-d-a y logm(sp,fe+2#2)
POST-1:
POST-1: @@
POST-1: @@ LIMIT THE PLOT TO THE SPINEL PHASE
POST-1: @@
POST-1: s-d-a x dis local sp
  INFO: Distance is set as independent variable
POST-1:
POST-1: s-p-c time 86400
POST-1:
POST-1: plo
```

2018.02.18.22.44.50
Time = 86400
CELL #1



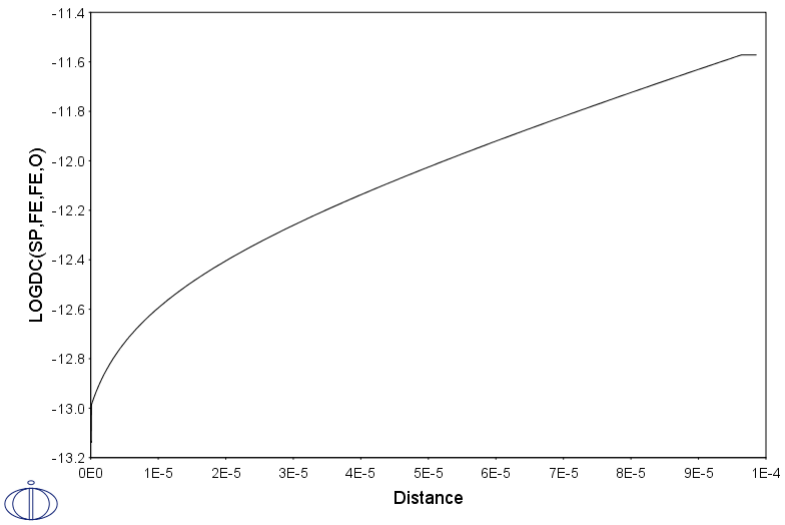
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: @@
POST-1: @@ COMPARE MOBILITIES IN A SPINEL FOR Fe+2 AND Fe+3 SPECIES PRESENT ON THE
POST-1: @@ SECOND SUBLATTICE. FOR THIS WE NEED TO ENTER A TABLE.
POST-1: @@
POST-1: ent table mobfe
Variable(s) logm(sp,fe+2#2) logm(sp,fe+3#2)
POST-1:
POST-1: s-d-a y mobfe
COLUMN NUMBER /*/:
POST-1:
POST-1: plot

2018.02.18.22.44.51
Time = 86400
CELL #1



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: plot

2018.02.18.22.44.52
Time = 86400
CELL #1

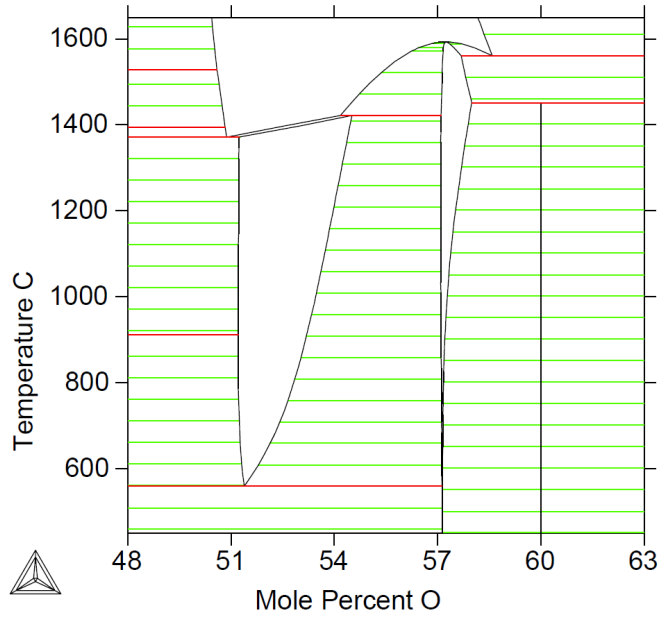


POST-1:
POST-1:
POST-1: set-inter
--OK---
POST-1:

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

```
About simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 12987) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri Feb 16 15:22:08 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exi3b\setup.DCM" @@
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
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

 VA                     /-  DEFINED
 L12_FCC                B2_BCC                 DICTRA_FCC_A1
   REJECTED
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ SELECT A USER DATABASE TO READ THE THERMODYNAMIC DATA
TDB_TCFE9: @@
TDB_TCFE9: sw user FeO.TDB
 Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

 VA                     /-  DEFINED
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
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 Reference REF368     missing close to line                    55
 Reference REF304     missing close to line                    63
 Reference REF420     missing close to line                    65
 Reference REF420     missing close to line                    67
 Reference REF368     missing close to line                    69
 Reference REF368     missing close to line                    70
 Reference REF368     missing close to line                    72
 Reference REF418     missing close to line                    74
 Reference REF418     missing close to line                    76
 Reference REF304     missing close to line                    78
 Reference REF30      missing close to line                    86
 Reference REF30      missing close to line                    88
 Reference REF30      missing close to line                    90
 Reference REF420     missing close to line                    92
 Reference REF420     missing close to line                    94
 Reference REF30      missing close to line                    96
 Reference REF30      missing close to line                    98
 Reference REF30      missing close to line                   100
 Reference REF420     missing close to line                   102
 Reference REF420     missing close to line                   104
 Reference REF30      missing close to line                   106
 Reference REF30      missing close to line                   108
 Reference REF30      missing close to line                   110
 Reference REF420     missing close to line                   112
 Reference REF420     missing close to line                   114
 Reference REF30      missing close to line                   116
 Reference REF30      missing close to line                   118
 Reference REF30      missing close to line                   120
 Reference REF420     missing close to line                   122
 Reference REF420     missing close to line                   124
 Reference REF30      missing close to line                   126
 Reference REF30      missing close to line                   128
 Reference REF30      missing close to line                   130
 Reference REF420     missing close to line                   132
 Reference REF420     missing close to line                   134
 Reference REF30      missing close to line                   136
 Reference REF30      missing close to line                   138
 Reference REF30      missing close to line                   140
 Reference REF420     missing close to line                   142
 Reference REF420     missing close to line                   144
 Reference REF30      missing close to line                   146
 Reference REF30      missing close to line                   148
 Reference REF30      missing close to line                   150
 Reference REF420     missing close to line                   152
 Reference REF420     missing close to line                   154
 Reference REF30      missing close to line                   156
```

```
 Reference REF30      missing close to line                   158
 Reference REF30      missing close to line                   160
 Reference REF420     missing close to line                   162
 Reference REF420     missing close to line                   164
 Reference REF30      missing close to line                   166
 Reference REF30      missing close to line                   168
 Reference REF30      missing close to line                   170
 Reference REF420     missing close to line                   172
 Reference REF420     missing close to line                   174
 Reference REF30      missing close to line                   176
 Reference REF30      missing close to line                   178
 Reference REF30      missing close to line                   180
 Reference REF420     missing close to line                   182
 Reference REF420     missing close to line                   184
 Reference REF30      missing close to line                   186
 Reference REF30      missing close to line                   188
 Reference REF30      missing close to line                   190
 Reference REF420     missing close to line                   192
 Reference REF420     missing close to line                   194
 Reference REF30      missing close to line                   196
 Reference REF30      missing close to line                   198
 Reference REF30      missing close to line                   200
 Reference REF420     missing close to line                   202
 Reference REF420     missing close to line                   204
 FUNCTIONS ....
 -OK-
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
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 ...
 FUNCTIONS ....

 List of references for assessed data


 *** ERROR  1000 IN TDBGRT
 *** NO REFERENCE FILE

 *** ERROR  1000 IN TDBGRT
 *** NO REFERENCE FILE
 -OK-
TDB_APP:
TDB_APP:
TDB_APP: @@
TDB_APP: @@ ENTER THE DICTRA MONITOR
TDB_APP: @@
TDB_APP: go d-m
 NO TIME STEP DEFINED
DIC>
DIC>
DIC> @@
DIC> @@  ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 823; * N

DIC>
DIC>
DIC> @@
DIC> @@  SET THE REFERENCE STATE FOR O TO O2 (GAS)
DIC> @@
DIC> set-ref o gas,,,,,,,
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE REGIONS fer AND sp
DIC> @@
DIC> ent-reg fer
DIC> ent-reg sp,,,,,,,,
DIC>
DIC>
DIC> @@
DIC> @@ ENTER PHASES INTO THE REGIONS
DIC> @@
DIC> ent-phase act fer matrix bcc#1
DIC> ent-phase act sp matrix spinel
DIC>
DIC>
DIC> @@
DIC> @@ ENTER GRIDS INTO THE REGIONS
DIC> @@
DIC>
DIC> @@
DIC> @@ ENTER A SIZE FOR THE FERRITE
DIC> @@
```

```
DIC> @@
DIC> ent-grid fer 4.99999e-3 AUTO
DIC>
DIC> @@
DIC> @@ ENTER A THIN INITIAL SIZE FOR THE OXIDE
DIC> @@
DIC> @@
DIC> ent-grid sp  1.00e-10 AUTO
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITIONS IN BCC
DIC> @@
DIC> ent-comp fer bcc#1 m-f
PROFILE FOR /O/: o lin 1e-9 1e-9
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITIONS IN THE OXIDE
DIC> @@
DIC> ent-comp sp spinel m-f
  this is a phase with charged species
  with more than 2 sublattices
PROFILE FOR /FE/: FE lin 4.28771E-01 4.28549E-01
DIC>
DIC>
DIC> @@
DIC> @@ ENTER A BOUNDARY CONDITION "GAS" ON THE UPPER (RIGHT-MOST) INTERFACE
DIC> @@ OF THE OXIDE. THIS ALLOWS THE SYSTEM TO EXPAND AND THE OXIDE LAYER
DIC> @@ TO GROW 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>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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
 single geometric dense at  0.50000E-02
 0.87386       95
 Region: SP
 double geometric
 dense at outer boundaries, coarse at  0.50000E-10
lower part   1.2500        9
upper part  0.80000        9
  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]
 6.141047161402763E-002        6.141016485504380E-002        6.141020906836839E-002        8.444643043596949E-003        1.457879775798498E-
024       TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =  0.14578798E-23
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.16337999E-03 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49999900E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.29859730E-03 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.49999901E-02
 U-FRACTION IN SYSTEM:  FE = 0.99999999230859  O = 2.69769194565743E-08
 TOTAL SIZE OF SYSTEM:  .00499999011352 [m]
  10  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: FER

  CPU time used in timestep                     0 seconds
 8.109452882793873E-006        8.108765481852460E-006        8.108714358263970E-006        3.429203689632118E-007        3.460921124583648E-
030       TIME =  0.30000000E-06 DT =  0.20000000E-06 SUM OF SQUARES =  0.34609211E-29
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.37478240E-03 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49999899E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.57006118E-03 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.49999902E-02
 U-FRACTION IN SYSTEM:  FE = 0.99999998461782  O = 4.97790566167421E-08
 TOTAL SIZE OF SYSTEM:  .00499999015258 [m]
  CPU time used in timestep                     0 seconds
 8.244220084356107E-006        8.245624820001861E-006        8.245834323740700E-006        5.265259157283041E-009        3.040545442780437E-
031       TIME =  0.70000000E-06 DT =  0.40000000E-06 SUM OF SQUARES =  0.30405454E-30
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.17607366E-03 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49999898E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.24106846E-03 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.49999902E-02
 U-FRACTION IN SYSTEM:  FE = 0.99999997890226  O = 6.90656000538019E-08
 TOTAL SIZE OF SYSTEM:  .00499999017858 [m]
  CPU time used in timestep                     0 seconds
 1.134920301888734E-007        1.135894804039261E-007        1.135506444176019E-007        5.608707817274067E-010        5.589428618385944E-
033       TIME =  0.15000000E-05 DT =  0.80000000E-06 SUM OF SQUARES =  0.55894286E-32
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.14432292E-03 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49999897E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.20898651E-03 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.49999902E-02
 U-FRACTION IN SYSTEM:  FE = 0.99999996836327  O = 1.02505972099334E-07
 TOTAL SIZE OF SYSTEM:  .00499999023031 [m]
  8  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                     1 seconds
 4.495117154993389E-007        4.496453319495406E-007        4.496431998391493E-007        2.514741666006164E-010        2.513206922058051E-
034       TIME =  0.31000000E-05 DT =  0.16000000E-05 SUM OF SQUARES =  0.25132069E-33
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.94208025E-04 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49999896E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.13424763E-03 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.49999903E-02
 U-FRACTION IN SYSTEM:  FE = 0.99999995509026  O = 1.45469731183719E-07
 TOTAL SIZE OF SYSTEM:  .00499999029437 [m]
  32  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                     0 seconds
 1.153179467205265E-005        1.153635784462131E-005        1.153592952376297E-005        1.797713989031012E-008        1.284911245787787E-
030       TIME =  0.63000000E-05 DT =  0.32000000E-05 SUM OF SQUARES =  0.12849112E-29
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.67615626E-04 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49999894E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.97021972E-04 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.49999904E-02
 U-FRACTION IN SYSTEM:  FE = 0.99999993575642  O = 2.07571156029763E-07
 TOTAL SIZE OF SYSTEM:  .00499999038847 [m]


output ignored...



... output resumed

 POSITION OF INTERFACE FER / SP IS   0.49333469E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.11009831E-08 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.50286092E-02
 U-FRACTION IN SYSTEM:  FE = .99418084422836  O = .0189442387183436
 TOTAL SIZE OF SYSTEM:  .00502860924784 [m]
  21  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                     1 seconds
 5.273117098378293E-007        5.281046129101103E-007        5.280427494561641E-007        7.076339562288592E-010        1.841670509320294E-
032       TIME =   56943.895      DT =   8640.0000      SUM OF SQUARES =  0.18416705E-31
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.70247282E-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 = .99366131709631  O = .020659486569886
 TOTAL SIZE OF SYSTEM:  .00503121911345 [m]
  9  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    0 seconds
 2.946689604425387E-007        2.952129684690918E-007        2.951641712357007E-007        3.823709736797433E-010        1.813082486708296E-
034       TIME =   65583.895     DT =   8640.0000     SUM OF SQUARES =  0.18130825E-33
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.64894663E-09 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49216707E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.92920435E-09 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.50336405E-02
 U-FRACTION IN SYSTEM:  FE = .993180429172029  O = .0222444823740345
 TOTAL SIZE OF SYSTEM:  .00503364054012 [m]
  8  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    1 seconds
 1.646046081816719E-007        1.649792107009017E-007        1.649481519432754E-007        1.988144432406818E-010        1.123208362097712E-
033       TIME =   74223.895     DT =   8640.0000     SUM OF SQUARES =  0.11232084E-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   0.86919604E-09 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.50359098E-02
 U-FRACTION IN SYSTEM:  FE = .992730593159095  O = .0237257189757379
 TOTAL SIZE OF SYSTEM:  .00503590981819 [m]
 11  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    1 seconds
 1.056445882444572E-007        1.059232720122668E-007        1.059039690796196E-007        1.220606026900290E-010        5.059327685939125E-
033       TIME =   82863.895     DT =   8640.0000     SUM OF SQUARES =  0.50593277E-32
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.57100511E-09 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49114966E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.81838278E-09 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.50380472E-02
 U-FRACTION IN SYSTEM:  FE = .992307543343385  O = .0251191391110857
 TOTAL SIZE OF SYSTEM:  .00503804716129 [m]
  7  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    0 seconds
 1.518627609602451E-008        1.512781289831391E-008        1.530717153876908E-008        1.085155039390110E-011        1.301507345230437E-
034       TIME =   86400.000     DT =   3536.1047     SUM OF SQUARES =  0.13015073E-33
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.56483678E-09 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49094993E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.78548555E-09 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.50388274E-02
 U-FRACTION IN SYSTEM:  FE = .992153350362077  O = .0256664807148033
 TOTAL SIZE OF SYSTEM:  .00503882739841 [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

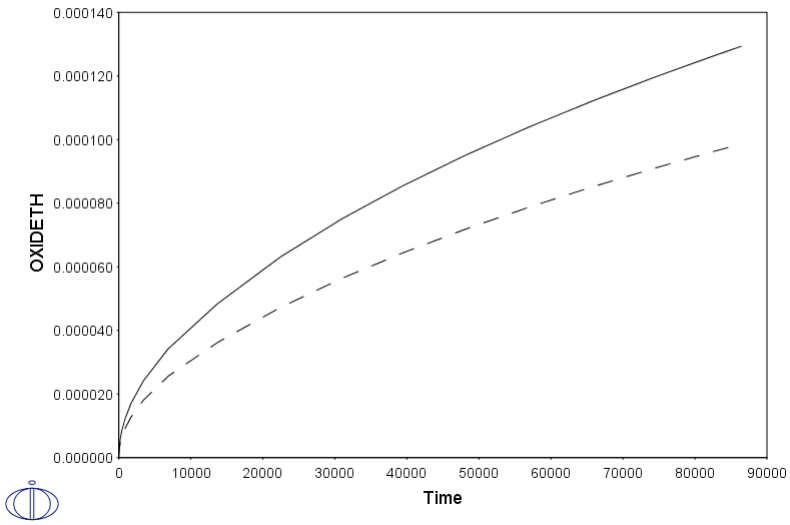
DIC>
DIC> set-inter
 --OK---
DIC>
```

exi3b-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\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: plot
  2018.02.18.22.48.16
  UPPER INTERFACE OF REGION "SP#1"
  CELL #1
```




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