Diffusion Module (DICTRA) Example Macros

Thermo-Calc Version 2019a

Thermo-Calc Software

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exa1

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

exa2a

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

exa2b

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

exa3

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

exa4

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

exa5

One-phase problem. Carburization of a binary Fe-0.15 wt% C alloy. A mixture of 40% N2 and 60% cracked methanol is used as carrier gas. The carburizing "carbon potential" in the gas is 0.85 wt%. A surface reaction controls the flux of C at the surface.

exa6

One-phase problem. Diffusion through a tube wall. A simple example about diffusion through a tube wall. The tube material is an Fe-0.6%Mn-0.7%Si-0.05%C alloy. On the inside wall a carbon activity of 0.9 is maintained whereas on the outside the C-activity is very low. This example demonstrates the use of the command SET-FIRST-INTERFACE as well as the MIXED boundary conditions.

exa7

One phase example. Homogenization heat treatment The initial segregation profile is created from a Scheil calculation (see macro create_initial_profile.TCM). The command INPUT_SCHEIL_PROFILE in the DICTRA MONITOR performs most of the set up. Only time and temperature must be entered after the INPUT_SCHEIL_PROFILE command is executed.

exb1a

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

exb1b

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

exb1c

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

exb2

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

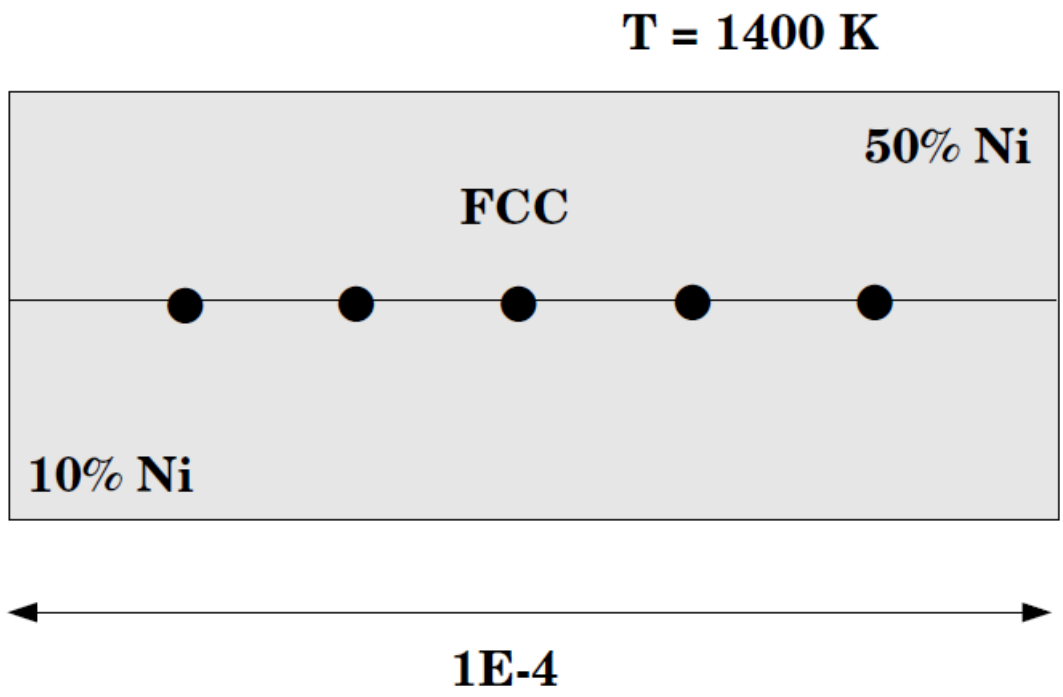
Diffusion in complex phases. Diffusion in iron oxide (FeO) This example shows the oxidation of an iron sample and the consequent growth of an oxide layer.

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

```
About License library version: 8.5.1.0017
 Linked: Wed Oct 31 13:18:51 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-
Examples\examples\exa1\setup.DCM.test"SYS:SYS:SYS:SYS:SYS:SYS: NO SUCH COMMAND, USE HELP
SYS:
SYS:SYS:SYS:SYS:MODULE NAME: 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:TDB_TCFE9:TDB_TCFE9: Use one of these databases

 TCFE9   =  Steels/Fe-Alloys  v9.0
 TCFE8   =  Steels/Fe-Alloys  v8.1
 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
 FEDAT   =  TCS/TT Steels Database v1.0
 TCNI9   =  Ni-Alloys  v9.0
 NI25    =  NI25 Database
 TCNI8   =  Ni-Alloys  v8.2
 TCNI7   =  Ni-Alloys  v7.2
 TCNI6   =  Ni-Alloys  v6.1
 TCNI5   =  Ni-Alloys  v5.1
 TCNI4   =  Ni-Alloys  v4.0
 TCNI1   =  Ni-Alloys  v1.3
 TCAL6   =  Al-Alloys  v6.0
 TCAL5   =  Al-Alloys  v5.1
 TCAL4   =  Al-Alloys  v4.0
 TCAL3   =  Al-Alloys  v3.0
 TCAL2   =  Al-Alloys  v2.1
 TCAL1   =  Al-Alloys  v1.2
 TCMG5   =  Mg-Alloys  v5.1
 TCMG4   =  Mg-Alloys  v4.0
 TCMG3   =  Mg-Alloys  v3.0
 TCMG2   =  Mg-Alloys  v2.0
 TCMG1   =  Mg-Alloys  v1.1
 TCTI2   =  Ti-Alloys  v2.0
 TCTI1   =  Ti-Alloys  v1.0
 TCCU2   =  Cu-Alloys  v2.0
 TCCU1   =  Cu-Alloys  v1.0
 TCCC1   =  Cemented carbide  v1.0
 TCHEA3  =  High Entropy Alloy  v3.1
 TCHEA2  =  High Entropy Alloy  v2.1.1
 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
 TCOX9   =  Metal Oxide Solutions  v9.0 SNAPSHOT
 TCOX8   =  Metal Oxide Solutions  v8.0
 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  v2.7
 AQS2    =  TGG Aqueous Solution Database v2.6
 GCE2    =  TGG Geochemical/Environmental TDB v2.3
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 ALDEMO  =  Aluminum Demo Database v3.0
 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  v1.1
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 MOBHEA1 =  High Entropy Alloys Mobility  v1.0
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
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 MOBTI2  =  Ti-Alloys Mobility  v2.0
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v2.0
 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/: Current database: Iron Demo Database v2.0

 VA                      /-  DEFINED
TDB_FEDEMO:
TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO:ELEMENTS: FE                      NI  DEFINED
TDB_FEDEMO:
TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO:ELEMENTS, SPECIES, PHASES, CONSTITUENT OR SYSTEM: /PHASES/:PHASES: LIQUID:L                BCC_A2
 HCP_A3                  LAVES_PHASE_C14  REJECTED
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 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'
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TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO: Use one of these databases

 TCFE9   =  Steels/Fe-Alloys  v9.0
 TCFE8   =  Steels/Fe-Alloys  v8.1
 TCFE7   =  Steels/Fe-Alloys  v7.0
 TCFE6   =  Steels/Fe-Alloys  v6.2
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 TCHEA3  =  High Entropy Alloy  v3.1
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 TCHEA1  =  High Entropy Alloy  v1.0
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 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
 TCOX9   =  Metal Oxide Solutions  v9.0 SNAPSHOT
 TCOX8   =  Metal Oxide Solutions  v8.0
 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  v2.7
 AQS2    =  TGG Aqueous Solution Database v2.6
 GCE2    =  TGG Geochemical/Environmental TDB v2.3
 FEDEMO  =  Iron Demo Database v2.0
 ALDEMO  =  Aluminum Demo Database v3.0
 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  v1.1
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBNI5  =  Ni-Alloys Mobility  v5.0
 MOBNI4  =  Ni-Alloys Mobility  v4.1
 MOBNI3  =  Ni-Alloys Mobility  v3.2
 MOBNI2  =  Ni-Alloys Mobility  v2.4
 MOBNI1  =  Ni-Alloys Mobility  v1.9
 MOBAL5  =  Al-Alloys Mobility  v5.0
 MOBAL4  =  Al-Alloys Mobility  v4.0
 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
 MOBHEA1 =  High Entropy Alloys Mobility  v1.0
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBSLD1 =  Solder-Alloys Mobility  v1.1
 MOBTI3  =  Ti-Alloys Mobility  v3.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v2.0
 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/: Current database: Fe-Alloys Mobility demo database v2.0

 VA  DEFINED
APP:ELEMENTS: FE                      NI  DEFINED
APP:ELEMENTS, SPECIES, PHASES, CONSTITUENT OR SYSTEM: /PHASES/:PHASES: BCC_A2                  FCC_A1  REJECTED
APP:
APP:ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /ELEMENTS/:PHASES: FCC_A1  RESTORED
APP:
APP: 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:APP:APP:MODULE NAME: NO TIME STEP DEFINED
DIC>
DIC>DIC>DIC>DIC>GLOBAL OR BOUNDARY CONDITION /GLOBAL/:VARIABLE :LOW TIME LIMIT /0/:T(TIME,X)=HIGH TIME LIMIT /*/:ANY MORE RANGES /N/:DIC>
DIC>DIC>DIC>DIC>REGION NAME :DIC>
DIC>DIC>DIC>DIC>DIC>DIC>REGION NAME : /AUSTENITE/:WIDTH OF REGION /1/:TYPE /LINEAR/:DIC>
DIC>
DIC>DIC>DIC>DIC>ACTIVE OR INACTIVE PHASE /ACTIVE/:REGION NAME : /AUSTENITE/:PHASE TYPE /MATRIX/:PHASE NAME: /NONE/:DIC>
DIC>DIC>DIC>DIC>DIC>REGION NAME : /AUSTENITE/:PHASE NAME: /FCC_A1/:DEPENDENT COMPONENT ? /NI/:COMPOSITION TYPE /MOLE_FRACTION/:PROFILE FOR /NI/
DIC>DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>END TIME FOR INTEGRATION /.1/:AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /100000/:
```

```
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC>DIC>DIC>DIC>DIC>
DIC> --OK---
DIC>
```

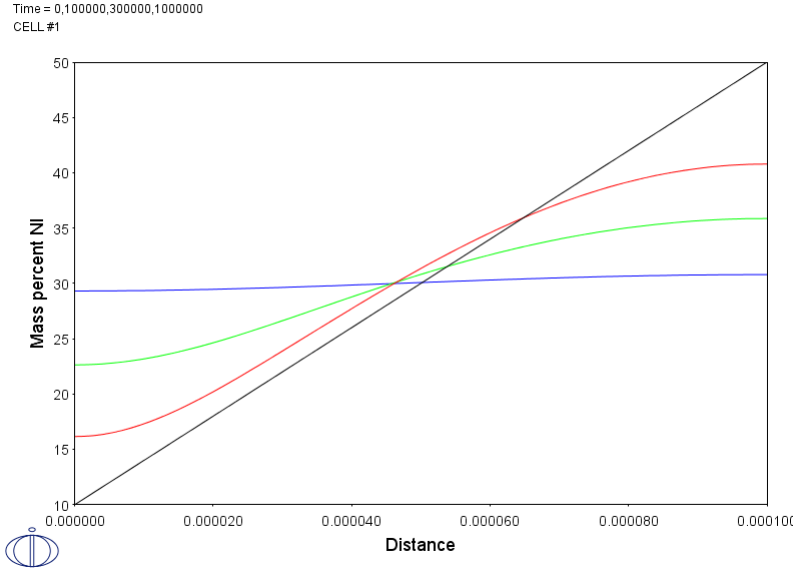
exa1-run

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa1\run.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>MODULE NAME: TIME STEP AT TIME  0.00000E+00
DIC>
DIC> OK
DIC>
DIC>DIC>DIC>DIC> 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                    0 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>DIC>DIC>
DIC> --OK---
DIC>
```

exa1-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa1\plot.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>MODULE NAME: TIME STEP AT TIME  1.00000E+06
DIC> OK
DIC>
DIC>DIC>DIC>DIC>  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:
POST-1:POST-1:POST-1:POST-1:AXIS (X, Y OR Z) :VARIABLE :  INFO: Distance is set as independent variable
DISTANCE : /GLOBAL/:POST-1:
POST-1:AXIS (X, Y OR Z) :VARIABLE :FOR COMPONENT :POST-1:
POST-1:CONDITION /TIME/:VALUE(S) /LAST/:POST-1:
POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```

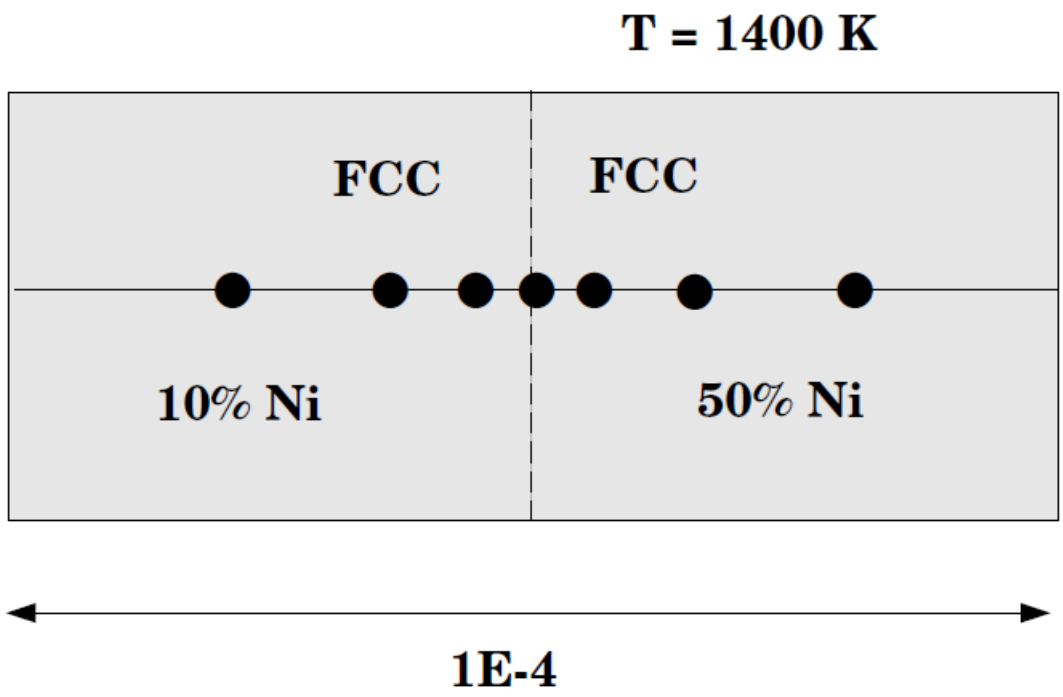



```
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: --OK---
POST-1:
```

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 License library version: 8.5.1.0017
 Linked: Wed Oct 31 13:18:51 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-
Examples\examples\exa2a\setup.DCM.test"SYS:SYS:SYS:SYS:SYS:SYS: NO SUCH COMMAND, USE HELP
SYS:
SYS:SYS:
SYS:SYS:SYS:SYS:SYS:
SYS:SYS:SYS:SYS:Heading:
SYS:SYS:SYS:SYS:   ... 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:TDB_TCFE9:TDB_TCFE9:   ... the command in full is SWITCH_DATABASE
 Current database: Iron Demo Database v2.0

 VA                       /-  DEFINED
TDB_FEDEMO:
TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO:   ... the command in full is DEFINE_SYSTEM
 FE                       NI  DEFINED
TDB_FEDEMO:
TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO:   ... the command in full is REJECT
 LIQUID:L                 BCC_A2                  FCC_A1
 HCP_A3                   LAVES_PHASE_C14  REJECTED
TDB_FEDEMO:   ... the command in full is RESTORE
 FCC_A1  RESTORED
TDB_FEDEMO:
TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO:   ... 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:TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO:   ... the command in full is APPEND_DATABASE
 Use one of these databases

 TCFE9   =  Steels/Fe-Alloys  v9.0
 TCFE8   =  Steels/Fe-Alloys  v8.1
 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
 FEDAT   =  TCS/TT Steels Database v1.0
 TCNI9   =  Ni-Alloys  v9.0
 NI25    =  NI25 Database
 TCNI8   =  Ni-Alloys  v8.2
 TCNI7   =  Ni-Alloys  v7.2
 TCNI6   =  Ni-Alloys  v6.1
 TCNI5   =  Ni-Alloys  v5.1
 TCNI4   =  Ni-Alloys  v4.0
 TCNI1   =  Ni-Alloys  v1.3
 TCAL6   =  Al-Alloys  v6.0
 TCAL5   =  Al-Alloys  v5.1
 TCAL4   =  Al-Alloys  v4.0
 TCAL3   =  Al-Alloys  v3.0
 TCAL2   =  Al-Alloys  v2.1
 TCAL1   =  Al-Alloys  v1.2
 TCMG5   =  Mg-Alloys  v5.1
 TCMG4   =  Mg-Alloys  v4.0
 TCMG3   =  Mg-Alloys  v3.0
 TCMG2   =  Mg-Alloys  v2.0
 TCMG1   =  Mg-Alloys  v1.1
 TCTI2   =  Ti-Alloys  v2.0
 TCTI1   =  Ti-Alloys  v1.0
 TCCU2   =  Cu-Alloys  v2.0
 TCCU1   =  Cu-Alloys  v1.0
 TCCC1   =  Cemented carbide  v1.0
 TCHEA3  =  High Entropy Alloy  v3.1
 TCHEA2  =  High Entropy Alloy  v2.1.1
 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
 TCOX9   =  Metal Oxide Solutions  v9.0 SNAPSHOT
 TCOX8   =  Metal Oxide Solutions  v8.0
 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  v2.7
 AQS2    =  TGG Aqueous Solution Database v2.6
 GCE2    =  TGG Geochemical/Environmental TDB v2.3
 FEDEMO  =  Iron Demo Database v2.0
 ALDEMO  =  Aluminum Demo Database v3.0
 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  v1.1
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBNI5  =  Ni-Alloys Mobility  v5.0
 MOBNI4  =  Ni-Alloys Mobility  v4.1
 MOBNI3  =  Ni-Alloys Mobility  v3.2
 MOBNI2  =  Ni-Alloys Mobility  v2.4
 MOBNI1  =  Ni-Alloys Mobility  v1.9
 MOBAL5  =  Al-Alloys Mobility  v5.0
 MOBAL4  =  Al-Alloys Mobility  v4.0
 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
 MOBHEA1 =  High Entropy Alloys Mobility  v1.0
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBSLD1 =  Solder-Alloys Mobility  v1.1
 MOBTI3  =  Ti-Alloys Mobility  v3.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v2.0
 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/: Current database: Fe-Alloys Mobility demo database v2.0

 VA  DEFINED
APP:   ... the command in full is DEFINE_SYSTEM
 FE                      NI  DEFINED
APP:   ... the command in full is REJECT
 BCC_A2                  FCC_A1  REJECTED
APP:   ... the command in full is RESTORE
 FCC_A1  RESTORED
APP:   ... 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:APP:APP:   ... the command in full is GOTO_MODULE
 NO TIME STEP DEFINED
DIC>
DIC>DIC>DIC>DIC>   ... the command in full is SET_CONDITION
GLOBAL OR BOUNDARY CONDITION /GLOBAL/:VARIABLE :LOW TIME LIMIT /0/:T(TIME,X)=HIGH TIME LIMIT /*/:ANY MORE RANGES /N/:DIC>
DIC>DIC>DIC>DIC>REGION NAME :DIC>
DIC>DIC>DIC>DIC>DIC>DIC>   ... the command in full is ENTER_GRID_COORDINATES
REGION NAME : /AUSTENITE/:WIDTH OF REGION /1/:TYPE /LINEAR/:NUMBER OF POINTS /50/:VALUE OF R IN THE GEOMETRICAL SERIE FOR LOWER PART OF REGION:
DIC>DIC>DIC>DIC>   ... the command in full is ENTER_PHASE_IN_REGION
ACTIVE OR INACTIVE PHASE /ACTIVE/:REGION NAME : /AUSTENITE/:PHASE TYPE /MATRIX/:PHASE NAME: /NONE/:DIC>
DIC>DIC>DIC>DIC>DIC>   ... the command in full is ENTER_COMPOSITIONS
REGION NAME : /AUSTENITE/:PHASE NAME: /FCC_A1/:DEPENDENT COMPONENT ? /NI/:COMPOSITION TYPE /MOLE_FRACTION/:PROFILE FOR /NI/:TYPE /LINEAR/:   ..
   ... 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
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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
```

```
   ... the command in full is COMPUTE_EQUILIBRIUM
   ... the command in full is COMPUTE_EQUILIBRIUM
   ... the command in full is COMPUTE_EQUILIBRIUM
```

```
DIC>
DIC>DIC>DIC>DIC>   ... the command in full is SAVE_WORKSPACES
DIC>
DIC>   ... the command in full is SET_INTERACTIVE
 --OK---
DIC>
```

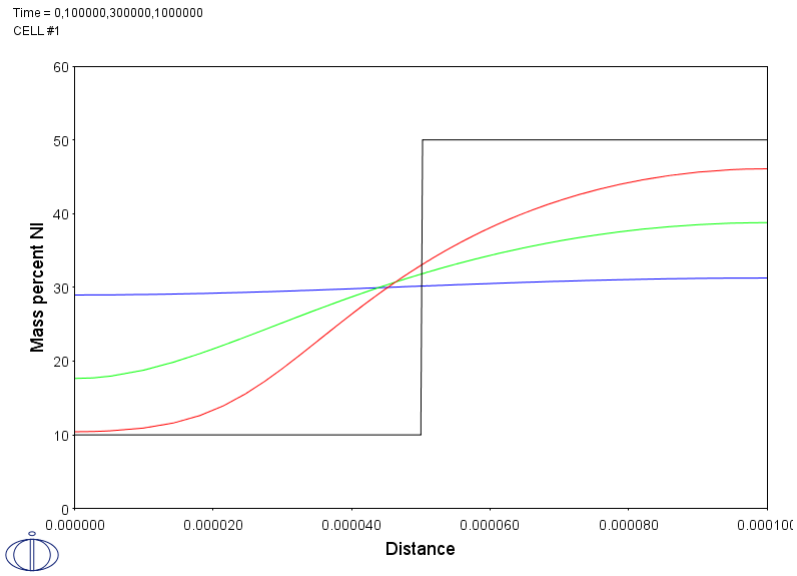
exa2a-run

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa2a\run.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>   ... the command in full is GOTO_MODULE
 TIME STEP AT TIME  0.00000E+00
DIC>
DIC>   ... 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>DIC>DIC>   ... 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
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    1 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                    0 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>DIC>DIC>
DIC>   ... the command in full is SET_INTERACTIVE
 --OK---
DIC>
```

exa2a-plot

```
DIC>AboutDIC>DIC>MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa2a\plot.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> AMBIGUOUS COMMAND, USE HELP
DIC>
DIC>DIC>DIC>DIC>   ... the command in full is GOTO_MODULE
 TIME STEP AT TIME  1.00000E+06
DIC>
DIC>   ... 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>DIC>DIC>   ... the command in full is POST_PROCESSOR
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:
POST-1:POST-1:POST-1:POST-1:   ... the command in full is SET_DIAGRAM_AXIS
AXIS (X, Y OR Z) :VARIABLE :  INFO: Distance is set as independent variable
   ... the command in full is SET_INDEPENDENT_VARIABLE
DISTANCE : /GLOBAL/:POST-1:
POST-1:   ... the command in full is SET_DIAGRAM_AXIS
AXIS (X, Y OR Z) :VARIABLE :FOR COMPONENT :POST-1:
POST-1:   ... the command in full is SET_PLOT_CONDITION
CONDITION /TIME/:VALUE(S) /LAST/:POST-1:
POST-1:POST-1:POST-1:POST-1:   ... the command in full is SET_SCALING_STATUS
AXIS (X, Y OR Z) :AUTOMATIC SCALING  (Y OR N) /N/:MIN VALUE :MAX VALUE :POST-1:
POST-1:
POST-1:POST-1:   ... the command in full is MAKE_EXPERIMENTAL_DATAFILE
POST-1:POST-1:
POST-1:   ... the command in full is PLOT_DIAGRAM
```

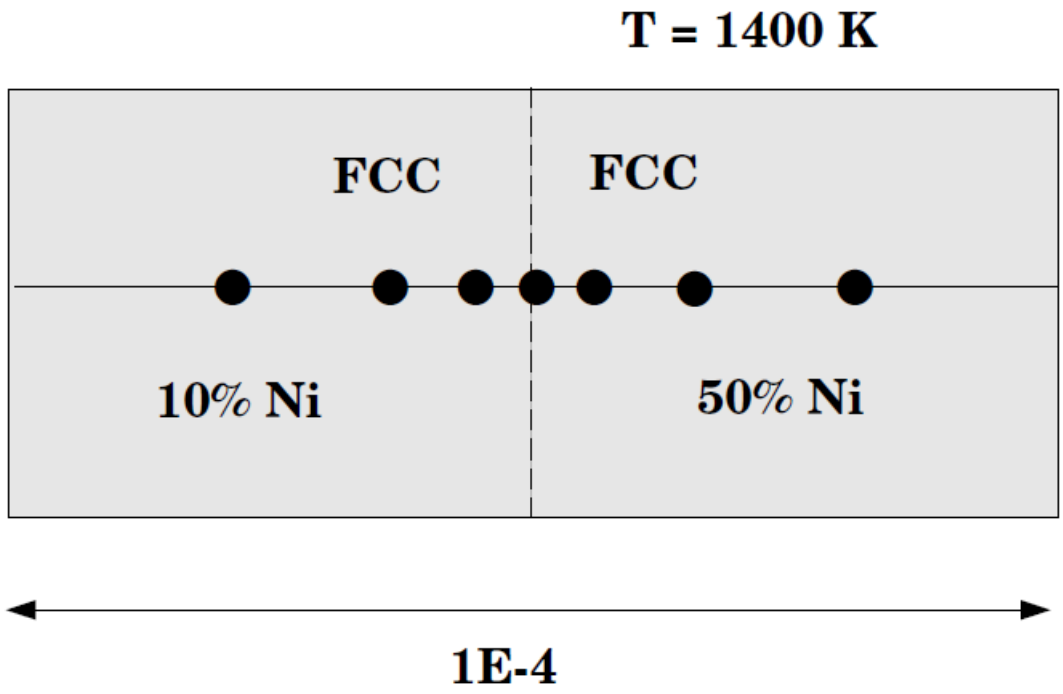



```
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1:   ... the command in full is SET_INTERACTIVE_MODE
 --OK---
POST-1:
```

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
 Software  (build 17825) 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: Wed Oct 31 13:18:51 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-
Examples\examples\exa2b\setup.DCM.test"SYS:SYS:SYS:SYS:SYS:SYS: NO SUCH COMMAND, USE HELP
SYS:
SYS:SYS:
SYS:SYS:SYS:SYS:Heading:
SYS:SYS:SYS:SYS:   ... 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:TDB_TCFE9:TDB_TCFE9:   ... 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:TDB_TCFE7:TDB_TCFE7:   ... the command in full is DEFINE_SYSTEM
 FE                      NI  DEFINED
TDB_TCFE7:
TDB_TCFE7:TDB_TCFE7:TDB_TCFE7:TDB_TCFE7:   ... 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:   ... the command in full is RESTORE
 FCC_A1  RESTORED
TDB_TCFE7:
TDB_TCFE7:TDB_TCFE7:TDB_TCFE7:TDB_TCFE7:   ... 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:TDB_TCFE7:TDB_TCFE7:TDB_TCFE7:   ... the command in full is APPEND_DATABASE
 Use one of these databases

 TCFE9   =  Steels/Fe-Alloys  v9.0
 TCFE8   =  Steels/Fe-Alloys  v8.1
 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
 FEDAT   =  TCS/TT Steels Database v1.0
 TCNI9   =  Ni-Alloys  v9.0
 NI25    =  NI25 Database
 TCNI8   =  Ni-Alloys  v8.2
 TCNI7   =  Ni-Alloys  v7.2
 TCNI6   =  Ni-Alloys  v6.1
 TCNI5   =  Ni-Alloys  v5.1
 TCNI4   =  Ni-Alloys  v4.0
 TCNI1   =  Ni-Alloys  v1.3
 TCAL6   =  Al-Alloys  v6.0
 TCAL5   =  Al-Alloys  v5.1
 TCAL4   =  Al-Alloys  v4.0
 TCAL3   =  Al-Alloys  v3.0
 TCAL2   =  Al-Alloys  v2.1
 TCAL1   =  Al-Alloys  v1.2
 TCMG5   =  Mg-Alloys  v5.1
 TCMG4   =  Mg-Alloys  v4.0
 TCMG3   =  Mg-Alloys  v3.0
 TCMG2   =  Mg-Alloys  v2.0
 TCMG1   =  Mg-Alloys  v1.1
 TCTI2   =  Ti-Alloys  v2.0
 TCTI1   =  Ti-Alloys  v1.0
 TCCU2   =  Cu-Alloys  v2.0
 TCCU1   =  Cu-Alloys  v1.0
 TCCC1   =  Cemented carbide  v1.0
 TCHEA3  =  High Entropy Alloy  v3.1
 TCHEA2  =  High Entropy Alloy  v2.1.1
 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
 TCOX9   =  Metal Oxide Solutions  v9.0 SNAPSHOT
 TCOX8   =  Metal Oxide Solutions  v8.0
 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  v2.7
 AQS2    =  TGG Aqueous Solution Database v2.6
 GCE2    =  TGG Geochemical/Environmental TDB v2.3
 FEDEMO  =  Iron Demo Database v2.0
 ALDEMO  =  Aluminum Demo Database v3.0
 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  v1.1
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBNI5  =  Ni-Alloys Mobility  v5.0
 MOBNI4  =  Ni-Alloys Mobility  v4.1
 MOBNI3  =  Ni-Alloys Mobility  v3.2
 MOBNI2  =  Ni-Alloys Mobility  v2.4
 MOBNI1  =  Ni-Alloys Mobility  v1.9
 MOBAL5  =  Al-Alloys Mobility  v5.0
 MOBAL4  =  Al-Alloys Mobility  v4.0
 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
 MOBHEA1 =  High Entropy Alloys Mobility  v1.0
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBSLD1 =  Solder-Alloys Mobility  v1.1
 MOBTI3  =  Ti-Alloys Mobility  v3.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v2.0
 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/: Current database: Steels/Fe-Alloys Mobility  v2.0
   TCS Steel Mobility Database Version 2.0 from 2011-12-09.

 VA  DEFINED
APP:   ... the command in full is DEFINE_SYSTEM
 FE                      NI  DEFINED
APP:   ... the command in full is REJECT
 BCC_A2                  FCC_A1                  HCP_A3
 LIQUID:L  REJECTED
APP:   ... the command in full is RESTORE
 FCC_A1  RESTORED
APP:   ... 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:APP:APP:   ... the command in full is GOTO_MODULE
 NO TIME STEP DEFINED
DIC>
DIC>DIC>DIC>DIC>   ... the command in full is SET_CONDITION
GLOBAL OR BOUNDARY CONDITION /GLOBAL/:VARIABLE :LOW TIME LIMIT /0/:T(TIME,X)=HIGH TIME LIMIT /*/:ANY MORE RANGES /N/:DIC>
DIC>DIC>DIC>DIC>REGION NAME :DIC>
DIC>DIC>DIC>DIC>DIC>DIC>   ... the command in full is ENTER_GRID_COORDINATES
REGION NAME : /AUSTENITE/:WIDTH OF REGION /1/:TYPE /LINEAR/:NUMBER OF POINTS /50/:VALUE OF R IN THE GEOMETRICAL SERIE FOR LOWER PART OF REGION:
DIC>DIC>DIC>DIC>   ... the command in full is ENTER_PHASE_IN_REGION
ACTIVE OR INACTIVE PHASE /ACTIVE/:REGION NAME : /AUSTENITE/:PHASE TYPE /MATRIX/:PHASE NAME: /NONE/:DIC>
DIC>DIC>DIC>DIC>DIC>   ... the command in full is ENTER_COMPOSITIONS
REGION NAME : /AUSTENITE/:PHASE NAME: /FCC_A1/:DEPENDENT COMPONENT ? /NI/:COMPOSITION TYPE /MOLE_FRACTION/:PROFILE FOR /NI/:TYPE /LINEAR/:   ..
   ... 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
   ... 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>DIC>DIC>
DIC>DIC>DIC>DIC>DIC>DIC>DIC>   ... 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/:MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /NO/:ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:DIC>DIC>END TIME FOR INTEGRATION /.
MAX TIMESTEP DURING INTEGRATION /100000/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC>DIC>DIC>   ... the command in full is SAVE_WORKSPACES
DIC>
DIC>   ... the command in full is SET_INTERACTIVE
 --OK---
DIC>
```

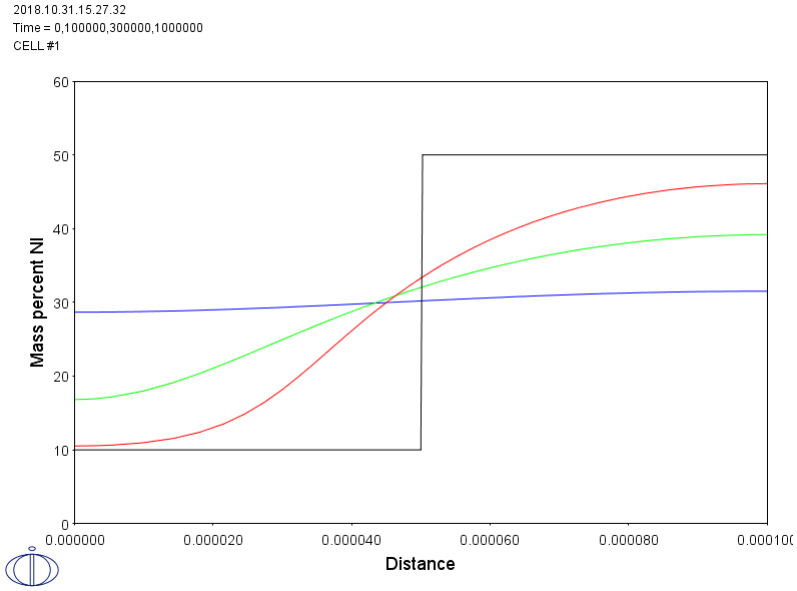
exa2b-run

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa2b\run.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> AMBIGUOUS COMMAND, USE HELP
DIC>
DIC>DIC>DIC>DIC>   ... the command in full is GOTO_MODULE
 TIME STEP AT TIME  0.00000E+00
DIC>   ... 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>DIC>DIC>   ... 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>DIC>DIC>
DIC>   ... the command in full is SET_INTERACTIVE
 --OK---
DIC>
```

exa2b-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa2b\plot.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> AMBIGUOUS COMMAND, USE HELP
DIC>
DIC>DIC>DIC>DIC>   ... the command in full is GOTO_MODULE
 TIME STEP AT TIME  1.00000E+06
DIC>   ... 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>DIC>DIC>   ... the command in full is POST_PROCESSOR
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:
POST-1:POST-1:POST-1:POST-1:   ... the command in full is SET_DIAGRAM_AXIS
AXIS (X, Y OR Z) :VARIABLE :  INFO: Distance is set as independent variable
   ... the command in full is SET_INDEPENDENT_VARIABLE
DISTANCE : /GLOBAL/:POST-1:
POST-1:   ... the command in full is SET_DIAGRAM_AXIS
AXIS (X, Y OR Z) :VARIABLE :FOR COMPONENT :POST-1:
POST-1:   ... the command in full is SET_PLOT_CONDITION
CONDITION /TIME/:VALUE(S) /LAST/:POST-1:
POST-1:POST-1:POST-1:POST-1:   ... the command in full is SET_SCALING_STATUS
AXIS (X, Y OR Z) :AUTOMATIC SCALING  (Y OR N) /N/:MIN VALUE :MAX VALUE :POST-1:
POST-1:
POST-1:POST-1:   ... the command in full is MAKE_EXPERIMENTAL_DATAFILE
POST-1:POST-1:
POST-1:   ... the command in full is PLOT_DIAGRAM
```



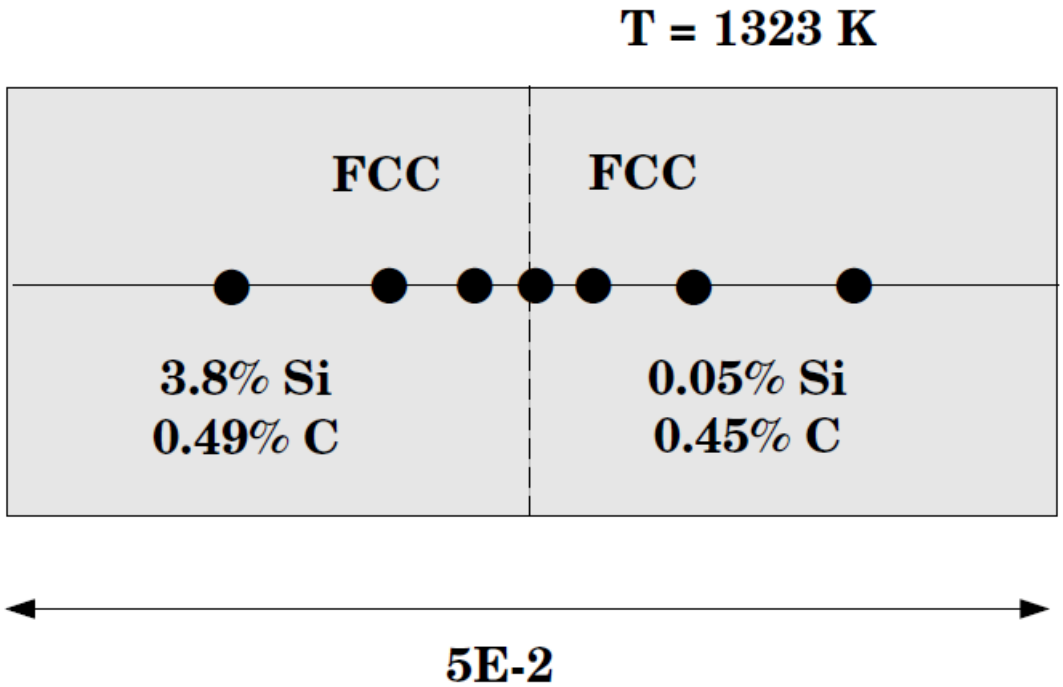

```
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1:   ... the command in full is SET_INTERACTIVE_MODE
 --OK---
POST-1:
```

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.test"SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: NO SUCH COMMAND, USE HELP
SYS:
SYS:SYS:
SYS:SYS:SYS:SYS:SYS:
SYS:SYS:SYS:SYS: 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:TDB_TCFE9:TDB_TCFE9: Current database: Steels/Fe-Alloys  v7.0

 VA  DEFINED
 L12_FCC                  B2_BCC                  B2_VACANCY
 HIGH_SIGMA               DICTRA_FCC_A1  REJECTED
TDB_TCFE7: FE                       SI                      C
   DEFINED
TDB_TCFE7: 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: FCC_A1  RESTORED
TDB_TCFE7: 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:TDB_TCFE7:TDB_TCFE7: Current database: Steels/Fe-Alloys Mobility  v2.0
   TCS Steel Mobility Database Version 2.0 from 2011-12-09.

 VA  DEFINED
APP: FE                     SI                      C
   DEFINED
APP: BCC_A2                 CEMENTITE               FCC_A1
 FE4N_LP1                 HCP_A3                  LIQUID:L
   REJECTED
APP: FCC_A1  RESTORED
APP: 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:APP:APP: NO TIME STEP DEFINED
DIC>
DIC>DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>REGION NAME :DIC>
DIC>DIC>DIC>DIC>DIC>REGION NAME : /AUSTENITE/:WIDTH OF REGION /1/:TYPE /LINEAR/:DIC>
DIC>DIC>DIC>DIC>ACTIVE OR INACTIVE PHASE /ACTIVE/:REGION NAME : /AUSTENITE/:PHASE TYPE /MATRIX/:PHASE NAME: /NONE/:DIC>
DIC>DIC>DIC>DIC>REGION NAME : /AUSTENITE/:PHASE NAME: /FCC_A1/:DEPENDENT COMPONENT ? /SI/:COMPOSITION TYPE /MOLE_FRACTION/:PROFILE FOR /C/:PROF
DIC>DIC>DIC>DIC>END TIME FOR INTEGRATION /.1/:AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /1E+09/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>DIC>
DIC> --OK---
DIC>
```

exa3-run

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa3\run.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  0.00000E+00
DIC>
DIC>DIC>DIC>DIC> OK
DIC>
DIC> 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 = .02153511228082  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 = .02153511228095  FE = .96291921367461
                        SI = .03708078632539
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                     1 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]
```

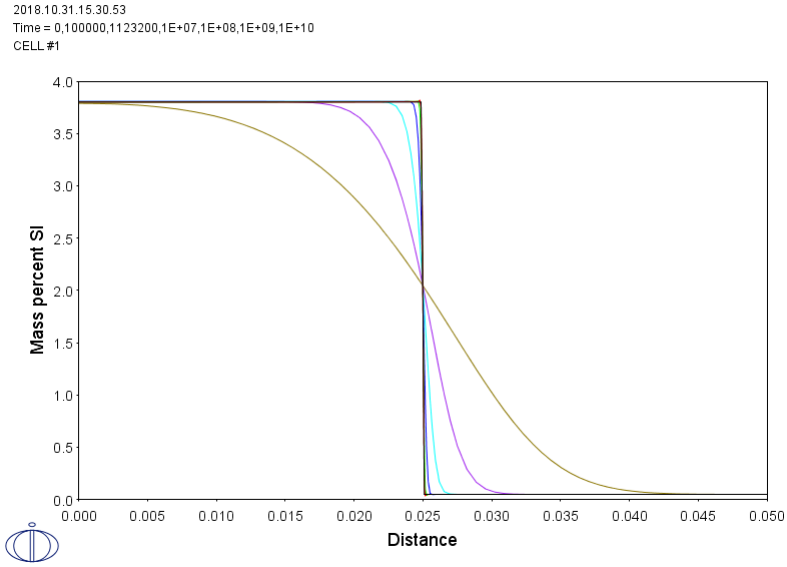
```
 CPU time used in timestep                    0 seconds
TIME =   2721755.3     DT =   1360887.8     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0215351122812751  FE = .96291921367461
                       SI = .03708078632539
TOTAL SIZE OF SYSTEM:  .05 [m]
 CPU time used in timestep                    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                    1 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                    0 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                    1 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                    0 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> --OK---
DIC>
```

exa3-plot

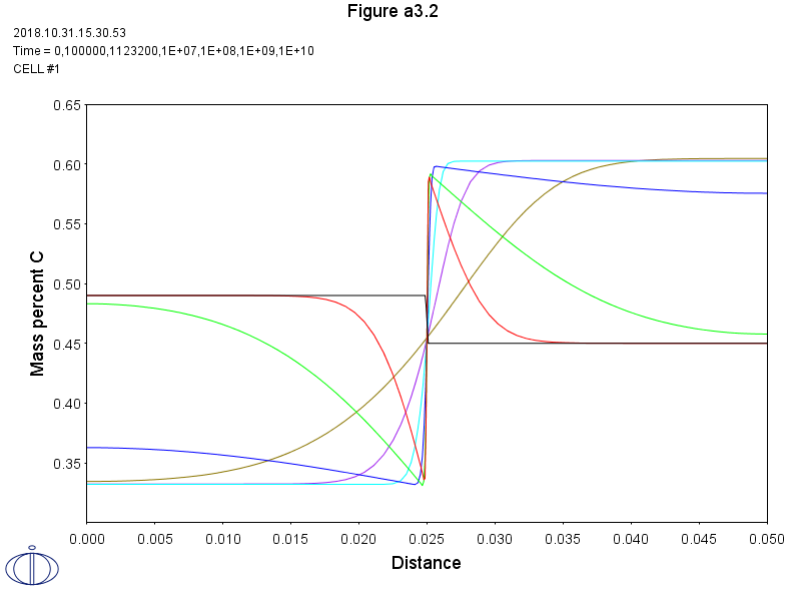
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa3\plot.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  1.00000E+10
DIC> OK
DIC>
DIC>DIC>DIC>DIC>  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:  INFO: Distance is set as independent variable
POST-1:POST-1:POST-1:
POST-1:POST-1:POST-1:POST-1:TITLE :POST-1:
POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```

Figure a3.1




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

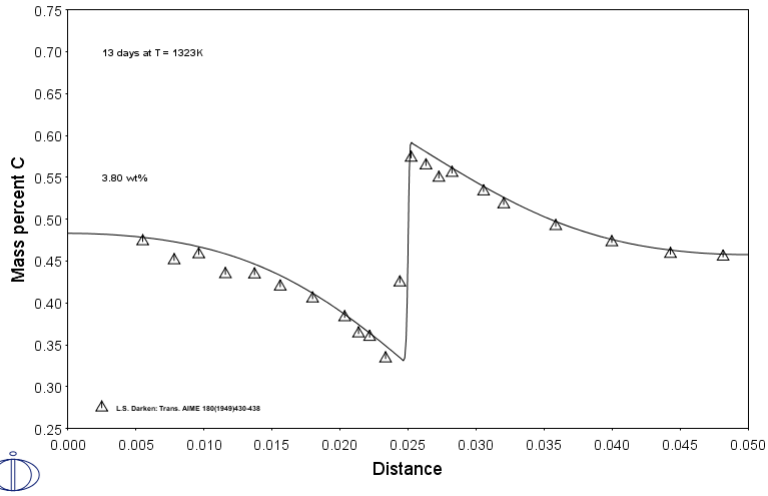
Figure a3.2




```
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:POST-1:POST-1:POST-1:POST-1:
POST-1:POST-1:
POST-1:AXIS (X, Y OR Z) :AUTOMATIC SCALING  (Y OR N) /N/:MIN VALUE :MAX VALUE :POST-1:
POST-1:POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```

Figure a3.3

2018.10.31.15.30.54
Time = 1123200
CELL #1

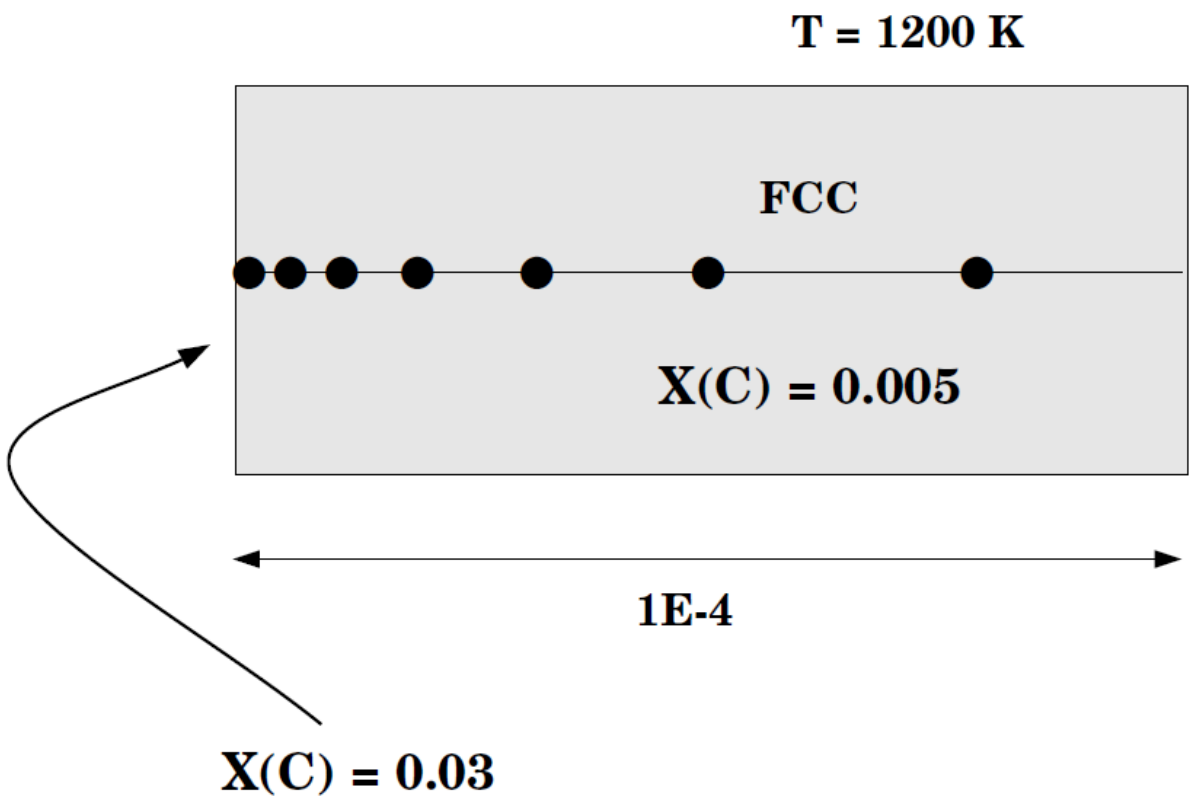



```
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1: --OK---
POST-1:
```

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 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Wed Oct 31 13:18:51 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-
Examples\examples\exa4\setup.DCM.test"SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: NO SUCH COMMAND, USE HELP
SYS:
SYS:SYS:
SYS:
SYS:SYS:SYS:SYS: THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

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

 VA                       /-  DEFINED
TDB_FEDEMO: FE                       C  DEFINED
TDB_FEDEMO: 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: FCC_A1  RESTORED
TDB_FEDEMO: 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: Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

 VA  DEFINED
TDB_APP: FE                       C  DEFINED
TDB_APP: FCC_A1  REJECTED
TDB_APP: FCC_A1  RESTORED
TDB_APP: ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....
 -OK-
TDB_APP:
TDB_APP:TDB_APP:TDB_APP:TDB_APP: NO TIME STEP DEFINED
DIC>
DIC>DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>REGION NAME :DIC>
DIC>DIC>DIC>DIC>DIC>DIC>DIC>REGION NAME : /STEEL/:WIDTH OF REGION /1/:TYPE /LINEAR/:DIC>
DIC>DIC>DIC>DIC>ACTIVE OR INACTIVE PHASE /ACTIVE/:REGION NAME : /STEEL/:PHASE TYPE /MATRIX/:PHASE NAME: /NONE/:DIC>
DIC>
DIC>DIC>DIC>DIC>REGION NAME : /STEEL/:PHASE NAME: /FCC_A1/:COMPOSITION TYPE /MOLE_FRACTION/:PROFILE FOR /C/:TYPE /LINEAR/:VALUE OF FIRST POINT
3/:DIC>
DIC>
DIC>DIC>DIC>DIC>GLOBAL OR BOUNDARY CONDITION /GLOBAL/:BOUNDARY /LOWER/:CONDITION TYPE /CLOSED_SYSTEM/:State variable expression #1 : /N=1/:Stat
DIC>
DIC>DIC>DIC>DIC>END TIME FOR INTEGRATION /.1/:AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /10/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC>
DIC>DIC>
DIC> --OK---
DIC>
```

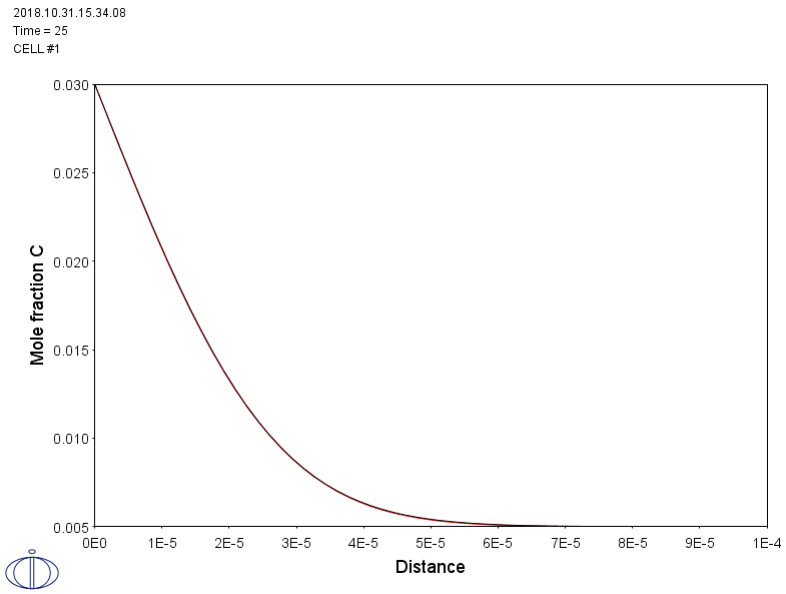
exa4-run

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa4\run.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  0.00000E+00
DIC> OK
DIC>
DIC>DIC>DIC>DIC> 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
```

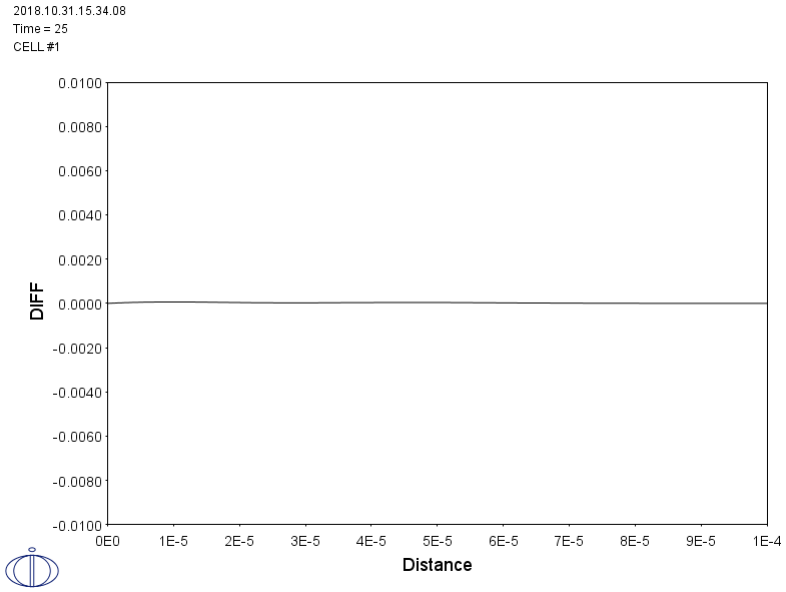
```
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    1 seconds
 TIME =   40.486185     DT =   10.000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0104363519865359  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    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>DIC>DIC>
DIC> --OK---
DIC>
```

exa4-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa4\plot.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  1.00000E+02
DIC> OK
DIC>
DIC>DIC>DIC>DIC>  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:POST-1:POST-1:POST-1:  INFO: Distance is set as independent variable
POST-1:POST-1:POST-1:
POST-1:POST-1:POST-1:POST-1:Function or table /FUNCTION/:NAME:FUNCTION:POST-1:
POST-1:POST-1:POST-1:POST-1:Function or table /FUNCTION/:NAME:Variable(s)POST-1:
POST-1:COLUMN NUMBER /*/:POST-1:
POST-1:AXIS (X, Y OR Z) :AUTOMATIC AXIS TEXT  (Y OR N) /N/:AXIS TEXT :POST-1:
POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```




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

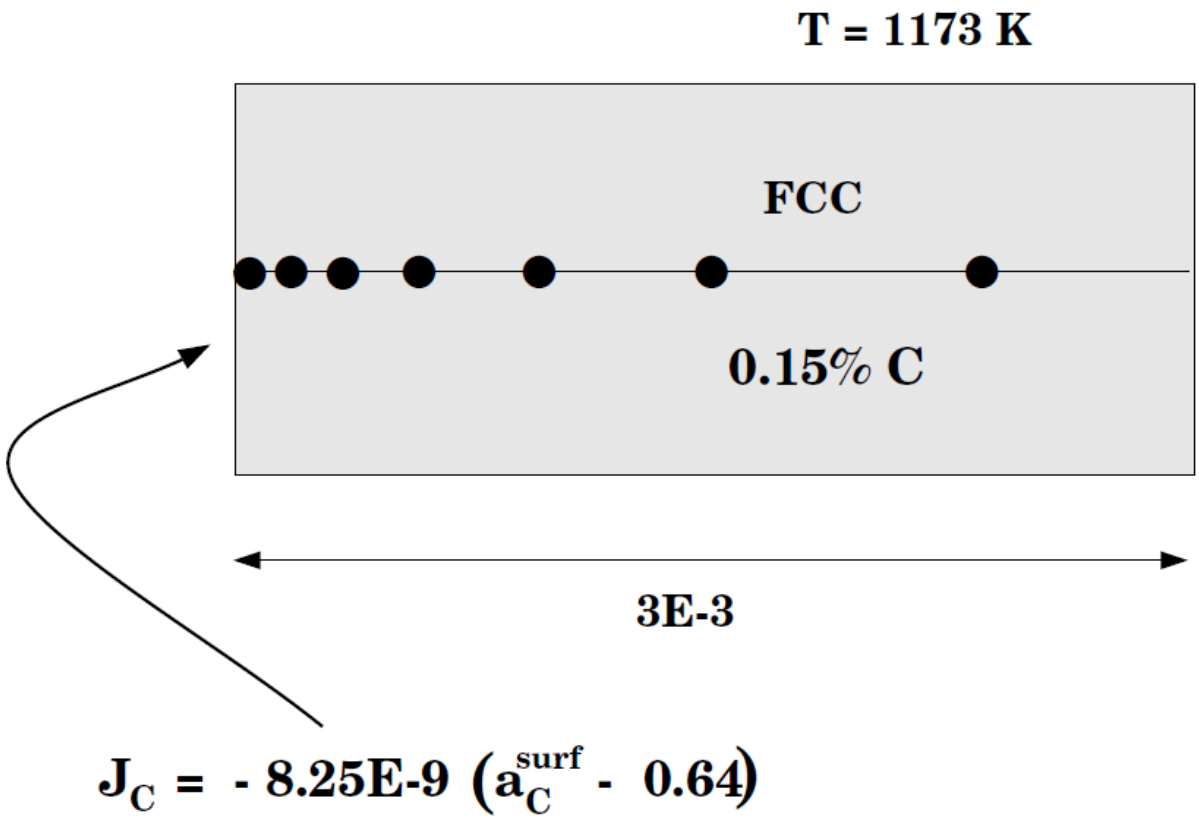



```
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: --OK---
POST-1:
```

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
SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa5\setup.DCM.test"SYS: NO SUCH COMMAND, USE HELP
SYS:SYS:SYS:SYS:SYS:SYS: NO SUCH COMMAND, USE HELP
SYS:
SYS:SYS:
SYS:SYS:SYS:SYS: THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

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

 VA                      /-  DEFINED
TDB_FEDEMO: FE                      C  DEFINED
TDB_FEDEMO: 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: FCC_A1                  GRAPHITE  RESTORED
TDB_FEDEMO: 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: Use one of these databases

 TCFE9   =  Steels/Fe-Alloys  v9.0
 TCFE8   =  Steels/Fe-Alloys  v8.1
 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
 FEDAT   =  TCS/TT Steels Database v1.0
 TCNI9   =  Ni-Alloys  v9.0
 NI25    =  NI25 Database
 TCNI8   =  Ni-Alloys  v8.2
 TCNI7   =  Ni-Alloys  v7.2
 TCNI6   =  Ni-Alloys  v6.1
 TCNI5   =  Ni-Alloys  v5.1
 TCNI4   =  Ni-Alloys  v4.0
 TCNI1   =  Ni-Alloys  v1.3
 TCAL6   =  Al-Alloys  v6.0
 TCAL5   =  Al-Alloys  v5.1
 TCAL4   =  Al-Alloys  v4.0
 TCAL3   =  Al-Alloys  v3.0
 TCAL2   =  Al-Alloys  v2.1
 TCAL1   =  Al-Alloys  v1.2
 TCMG5   =  Mg-Alloys  v5.1
 TCMG4   =  Mg-Alloys  v4.0
 TCMG3   =  Mg-Alloys  v3.0
 TCMG2   =  Mg-Alloys  v2.0
 TCMG1   =  Mg-Alloys  v1.1
 TCTI2   =  Ti-Alloys  v2.0
 TCTI1   =  Ti-Alloys  v1.0
 TCCU2   =  Cu-Alloys  v2.0
 TCCU1   =  Cu-Alloys  v1.0
 TCCC1   =  Cemented carbide  v1.0
 TCHEA3  =  High Entropy Alloy  v3.1
 TCHEA2  =  High Entropy Alloy  v2.1.1
 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
 TCOX9   =  Metal Oxide Solutions  v9.0 SNAPSHOT
 TCOX8   =  Metal Oxide Solutions  v8.0
 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  v2.7
 AQS2    =  TGG Aqueous Solution Database v2.6
 GCE2    =  TGG Geochemical/Environmental TDB v2.3
 FEDEMO  =  Iron Demo Database v2.0
 ALDEMO  =  Aluminum Demo Database v3.0
 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  v1.1
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBNI5  =  Ni-Alloys Mobility  v5.0
 MOBNI4  =  Ni-Alloys Mobility  v4.1
 MOBNI3  =  Ni-Alloys Mobility  v3.2
 MOBNI2  =  Ni-Alloys Mobility  v2.4
 MOBNI1  =  Ni-Alloys Mobility  v1.9
 MOBAL5  =  Al-Alloys Mobility  v5.0
 MOBAL4  =  Al-Alloys Mobility  v4.0
 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
 MOBHEA1 =  High Entropy Alloys Mobility  v1.0
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBSLD1 =  Solder-Alloys Mobility  v1.1
 MOBTI3  =  Ti-Alloys Mobility  v3.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v2.0
 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/: Current database: Fe-Alloys Mobility demo database v2.0

 VA  DEFINED
APP: FE                      C  DEFINED
APP: BCC_A2                  FCC_A1  REJECTED
APP: FCC_A1  RESTORED
APP: 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:APP:APP: NO TIME STEP DEFINED
 *** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>Component:Reference state:Temperature /*/:Pressure /100000/:DIC>
DIC>DIC>DIC>DIC>REGION NAME :DIC>
DIC>REGION NAME : /STEEL/:WIDTH OF REGION /1/:TYPE /LINEAR/:DIC>
DIC>ACTIVE OR INACTIVE PHASE /ACTIVE/:REGION NAME : /STEEL/:PHASE TYPE /MATRIX/:PHASE NAME: /NONE/:DIC>
DIC>REGION NAME : /STEEL/:PHASE NAME: /FCC_A1/:COMPOSITION TYPE /MOLE_FRACTION/:PROFILE FOR /C/:TYPE /LINEAR/:VALUE OF FIRST POINT :VALUE OF LA
DIC>DIC>DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>
```

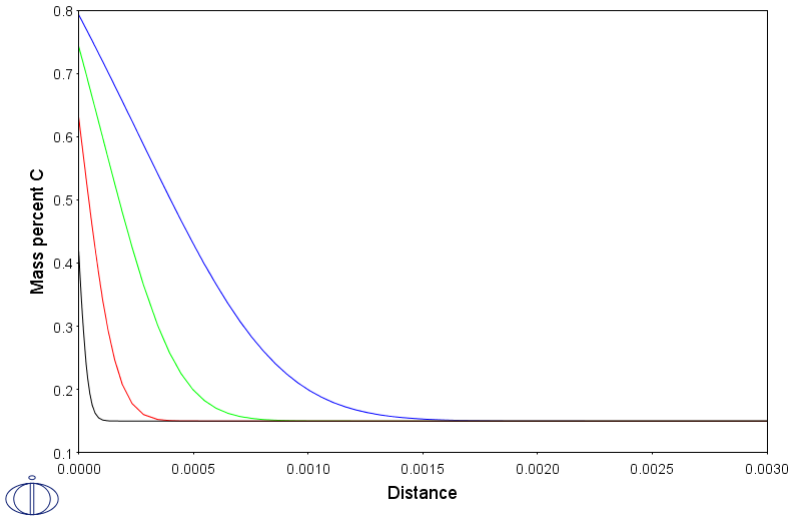
exa5-run

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa5\run.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  0.00000E+00
 *** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
DIC> OK
DIC>
DIC>DIC>DIC>DIC> 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 = .0069849596216772  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                    1 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                    0 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
```

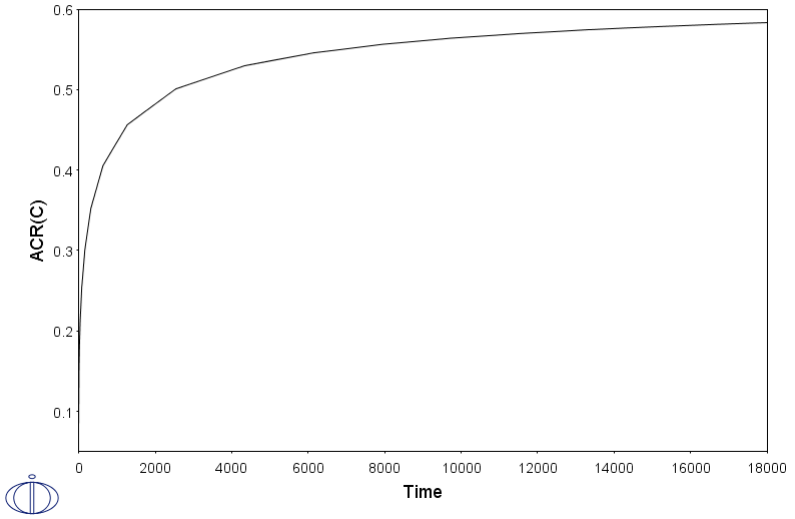
```
U-FRACTION IN SYSTEM:  C = .00703569376361486  FE = 1
TOTAL SIZE OF SYSTEM:  .003 [m]
 CPU time used in timestep                    0 seconds
TIME =   79.388998     DT =   39.694500     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00707989462116314  FE = 1
TOTAL SIZE OF SYSTEM:  .003 [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                    1 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                    0 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                    1 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> --OK---
DIC>
```

exa5-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa5\plot.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  1.80000E+04
 *** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
DIC> OK
DIC>
DIC>DIC>DIC>DIC>  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:POST-1:POST-1:POST-1:  INFO: Distance is set as independent variable
POST-1:POST-1:POST-1:
POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```

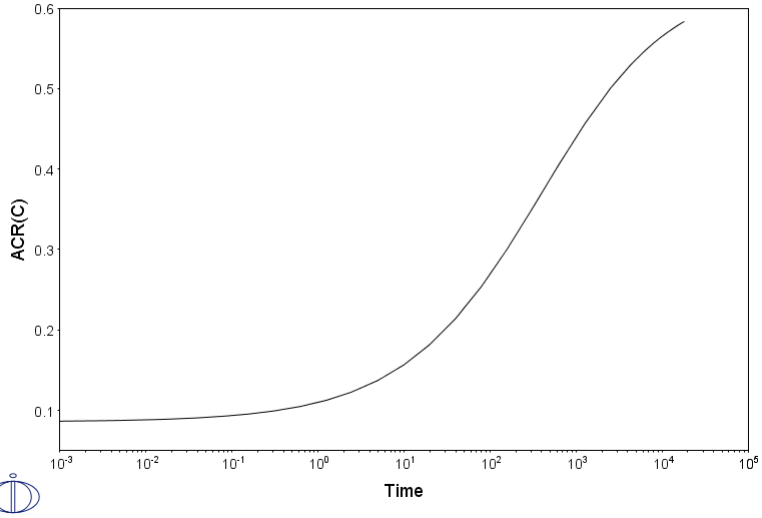



```
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:
POST-1:  INFO: Time is set as independent variable
POST-1:
POST-1:CONDITION /TIME/:INTERFACE :POST-1:
POST-1:
POST-1:POST-1:            OST-1:POST-1:
POST-1:
```



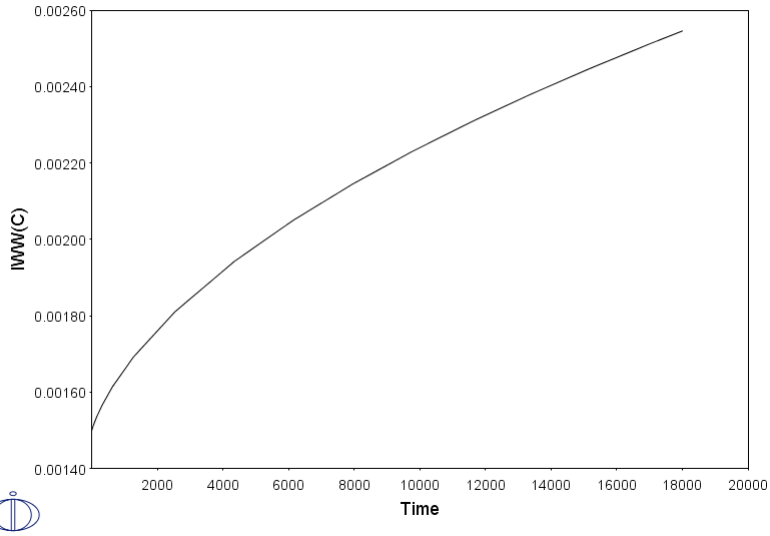

```
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1:POST-1:POST-1:POST-1:AXIS (X, Y OR Z) :AXIS TYPE /LINEAR/:POST-1:
POST-1:POST-1:
POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```

2018.10.31.15.37.26
"FIRST" INTERFACE OF SYSTEM
CELL #1




```
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:
POST-1:AXIS (X, Y OR Z) :AXIS TYPE /LINEAR/:POST-1:
POST-1:
POST-1:POST-1:            OST-1:POST-1:
POST-1:
```

2018.10.31.15.37.26
CELL #1

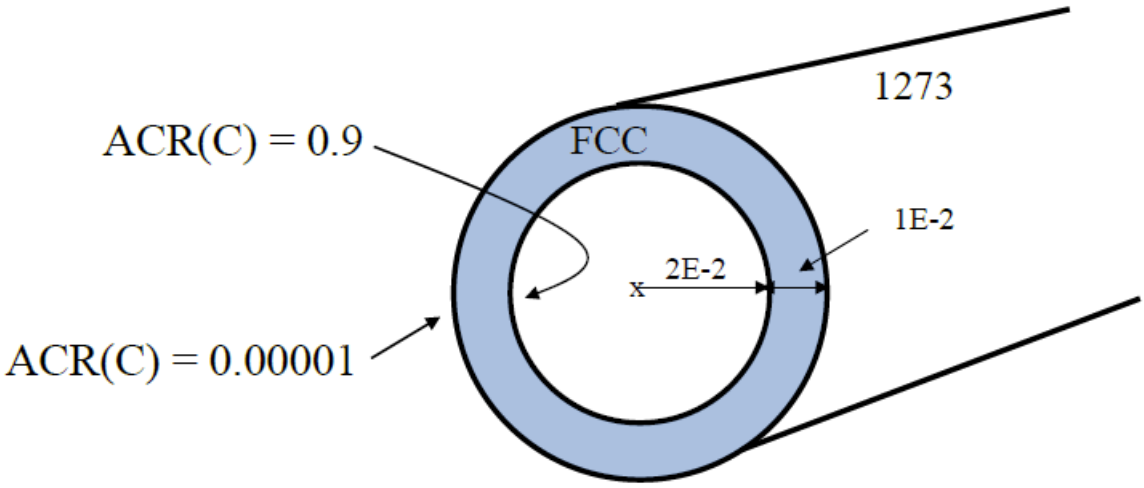



```
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1:
POST-1: --OK---
POST-1:
```

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 17825) 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: Wed Oct 31 13:18:51 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-
Examples\examples\exa6\setup.DCM.test"SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: NO SUCH COMMAND, USE HELP
SYS:
SYS:SYS:
SYS:
SYS:SYS:SYS:SYS: 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:TDB_TCFE9:TDB_TCFE9: Current database: Steels/Fe-Alloys  v7.0

 VA  DEFINED
 L12_FCC                  B2_BCC                  B2_VACANCY
 HIGH_SIGMA               DICTRA_FCC_A1  REJECTED
TDB_TCFE7: FE                       SI                      MN
 C  DEFINED
TDB_TCFE7: 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: FCC_A1                   GRAPHITE  RESTORED
TDB_TCFE7: 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:TDB_TCFE7:TDB_TCFE7: Use one of these databases

 TCFE9   =  Steels/Fe-Alloys  v9.0
 TCFE8   =  Steels/Fe-Alloys  v8.1
 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
 FEDAT   =  TCS/TT Steels Database v1.0
 TCNI9   =  Ni-Alloys  v9.0
 NI25    =  NI25 Database
 TCNI8   =  Ni-Alloys  v8.2
 TCNI7   =  Ni-Alloys  v7.2
 TCNI6   =  Ni-Alloys  v6.1
 TCNI5   =  Ni-Alloys  v5.1
 TCNI4   =  Ni-Alloys  v4.0
 TCNI1   =  Ni-Alloys  v1.3
 TCAL6   =  Al-Alloys  v6.0
 TCAL5   =  Al-Alloys  v5.1
 TCAL4   =  Al-Alloys  v4.0
 TCAL3   =  Al-Alloys  v3.0
 TCAL2   =  Al-Alloys  v2.1
 TCAL1   =  Al-Alloys  v1.2
 TCMG5   =  Mg-Alloys  v5.1
 TCMG4   =  Mg-Alloys  v4.0
 TCMG3   =  Mg-Alloys  v3.0
 TCMG2   =  Mg-Alloys  v2.0
 TCMG1   =  Mg-Alloys  v1.1
 TCTI2   =  Ti-Alloys  v2.0
 TCTI1   =  Ti-Alloys  v1.0
 TCCU2   =  Cu-Alloys  v2.0
 TCCU1   =  Cu-Alloys  v1.0
 TCCC1   =  Cemented carbide  v1.0
 TCHEA3  =  High Entropy Alloy  v3.1
 TCHEA2  =  High Entropy Alloy  v2.1.1
 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
 TCOX9   =  Metal Oxide Solutions  v9.0 SNAPSHOT
 TCOX8   =  Metal Oxide Solutions  v8.0
 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  v2.7
 AQS2    =  TGG Aqueous Solution Database v2.6
 GCE2    =  TGG Geochemical/Environmental TDB v2.3
 FEDEMO  =  Iron Demo Database v2.0
 ALDEMO  =  Aluminum Demo Database v3.0
 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  v1.1
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBNI5  =  Ni-Alloys Mobility  v5.0
 MOBNI4  =  Ni-Alloys Mobility  v4.1
 MOBNI3  =  Ni-Alloys Mobility  v3.2
 MOBNI2  =  Ni-Alloys Mobility  v2.4
 MOBNI1  =  Ni-Alloys Mobility  v1.9
 MOBAL5  =  Al-Alloys Mobility  v5.0
 MOBAL4  =  Al-Alloys Mobility  v4.0
 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
 MOBHEA1 =  High Entropy Alloys Mobility  v1.0
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBSLD1 =  Solder-Alloys Mobility  v1.1
 MOBTI3  =  Ti-Alloys Mobility  v3.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v2.0
 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/: Current database: Steels/Fe-Alloys Mobility  v2.0
   TCS Steel Mobility Database Version 2.0 from 2011-12-09.

 VA  DEFINED
APP: FE                      SI                      MN
 C  DEFINED
APP: BCC_A2                  CEMENTITE               FCC_A1
 FE4N_LP1                HCP_A3                  LIQUID:L
   REJECTED
APP: FCC_A1  RESTORED
APP: 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:APP:APP: NO TIME STEP DEFINED
 *** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
DIC>
DIC>DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>DIC>
```

```
DIC>DIC>DIC>DIC>REGION NAME : /AUS/:WIDTH OF REGION /1/:TYPE /LINEAR/:DIC>
DIC>DIC>DIC>DIC>GEOMETRICAL EXPONENT /0/:DIC>
DIC>DIC>DIC>DIC>COORDINATE FOR FIRST INTERFACE /0/:DIC>
DIC>DIC>DIC>DIC>ACTIVE OR INACTIVE PHASE /ACTIVE/:REGION NAME : /AUS/:PHASE TYPE /MATRIX/:PHASE NAME: /NONE/:DIC>
DIC>DIC>DIC>DIC>REGION NAME : /AUS/:PHASE NAME: /FCC_A1/:DEPENDENT COMPONENT ? /SI/:COMPOSITION TYPE /MOLE_FRACTION/:PROFILE FOR /C/:PROFILE FC
DIC>DIC>DIC>DIC>DIC>DIC>DIC>GLOBAL OR BOUNDARY CONDITION /GLOBAL/:BOUNDARY /LOWER/:CONDITION TYPE /CLOSED_SYSTEM/:Dependent substitutional elem
Dependent interstitial element:VA
TYPE OF CONDITION FOR COMPONENT C /ZERO_FLUX/:LOW TIME LIMIT /0/:ACR(C)
(TIME)=HIGH TIME LIMIT /*/:ANY MORE RANGES /N/:TYPE OF CONDITION FOR COMPONENT MN /ZERO_FLUX/:TYPE OF CONDITION FOR COMPONENT SI /ZERO_FLUX/:DI
DIC>GLOBAL OR BOUNDARY CONDITION /GLOBAL/:BOUNDARY /UPPER/:CONDITION TYPE /CLOSED_SYSTEM/:Dependent substitutional element:FE
Dependent interstitial element:VA
TYPE OF CONDITION FOR COMPONENT C /ZERO_FLUX/:LOW TIME LIMIT /0/:ACR(C)
(TIME)=HIGH TIME LIMIT /*/:ANY MORE RANGES /N/:TYPE OF CONDITION FOR COMPONENT MN /ZERO_FLUX/:TYPE OF CONDITION FOR COMPONENT SI /ZERO_FLUX/:DI
DIC>DIC>DIC>DIC>END TIME FOR INTEGRATION /.1/:AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /100000000/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC>DIC>DIC>DIC>DIC>
DIC> --OK---
DIC>
```

exa6-run

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa6\run.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  0.00000E+00
 *** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
DIC> OK
DIC>
DIC>DIC>DIC>DIC> 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                    1 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                    0 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                    1 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                    0 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                    1 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                    0 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                    1 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                    0 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                    1 seconds
 TIME =   400507.16     DT =   200255.11     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0130439049348442  FE = .490055682685357
                        MN = .00302988813193134  SI = .00691442924796516
```

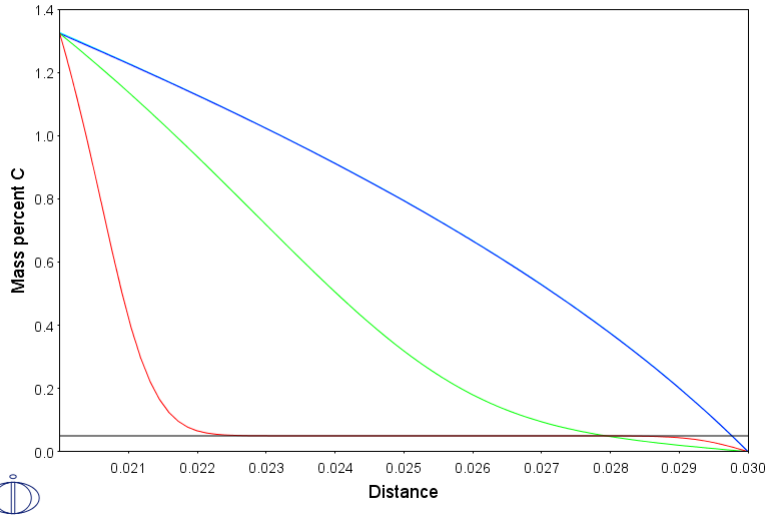
```
TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
 CPU time used in timestep                    0 seconds
TIME =   801017.38     DT =   400510.22     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0158210291341027  FE = .490055682685964
                       MN = .00302988813199274  SI = .00691442924729716
TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
 CPU time used in timestep                    0 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                    1 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 = .49005568269412
                       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 = .49005568270373
                       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                    0 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                    1 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 = .0030298882136918  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 = .49005568389079
                       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                    1 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                    0 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>DIC>DIC>
DIC> --OK---
DIC>
```

exa6-plot

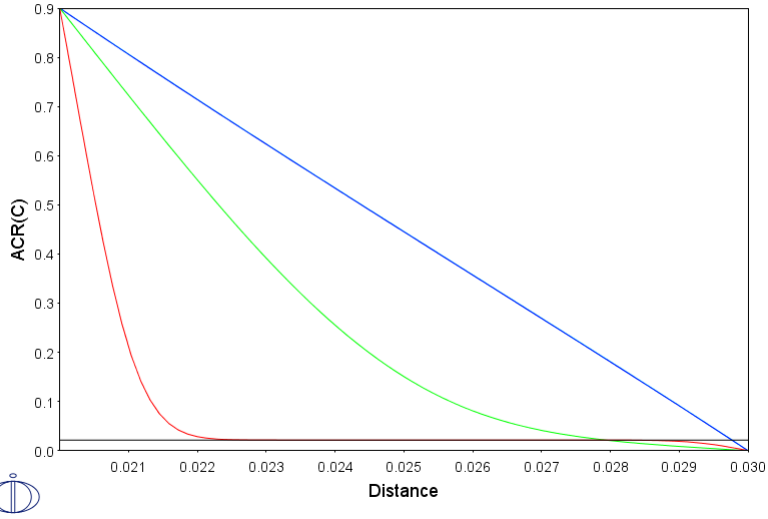
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa6\plot.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  1.00000E+09
 *** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
DIC> OK
DIC>
DIC>DIC>DIC>DIC>  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:
POST-1:POST-1:POST-1:POST-1:  INFO: Distance is set as independent variable
POST-1:POST-1:POST-1:
POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```

2018.10.31.15.40.57
Time = 0,10000,200000,1E+07,1E+09
CELL #1



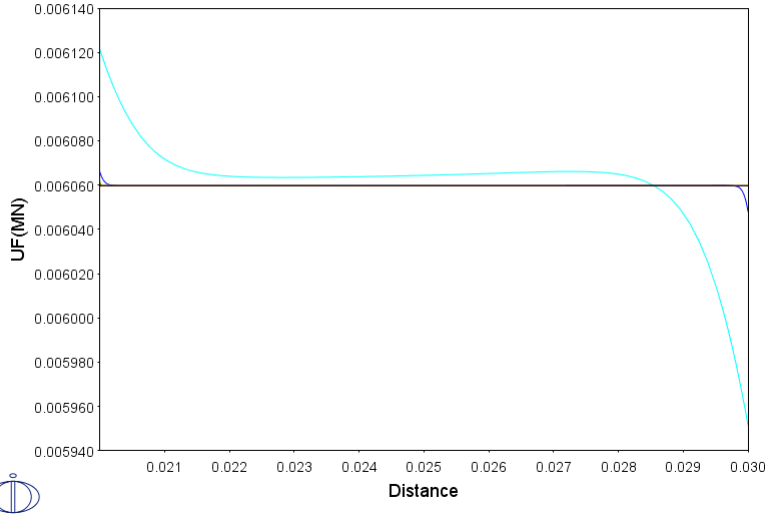

```
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:POST-1:
POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```

2018.10.31.15.40.59
Time = 0,10000,200000,1E+07,1E+09
CELL #1



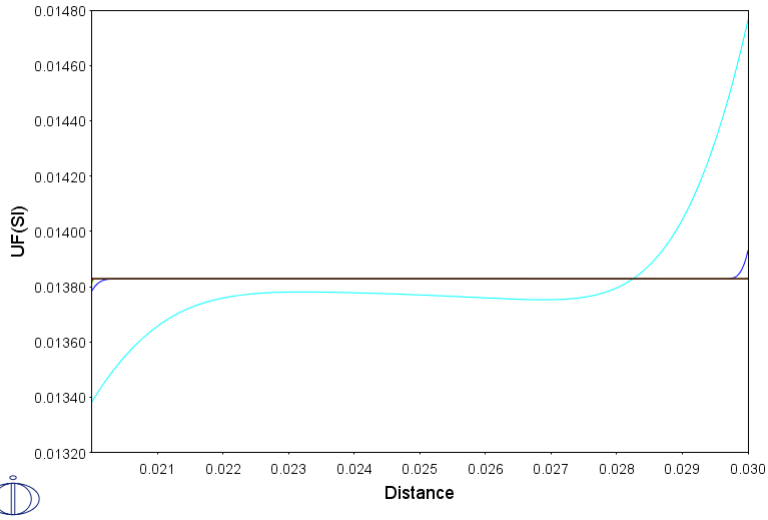

```
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:
POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```

2018.10.31.15.40.59
Time = 0,10000,200000,1E+07,1E+09
CELL #1



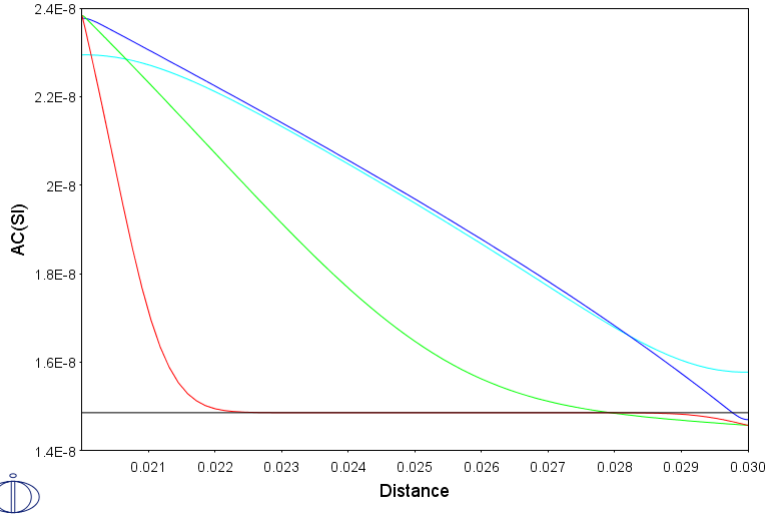

```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1:POST-1:
POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```

2018.10.31.15.41.00
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:POST-1:POST-1:POST-1:
POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```

2018.10.31.15.41.02
Time = 0,10000,200000,1E+07,1E+09
CELL #1



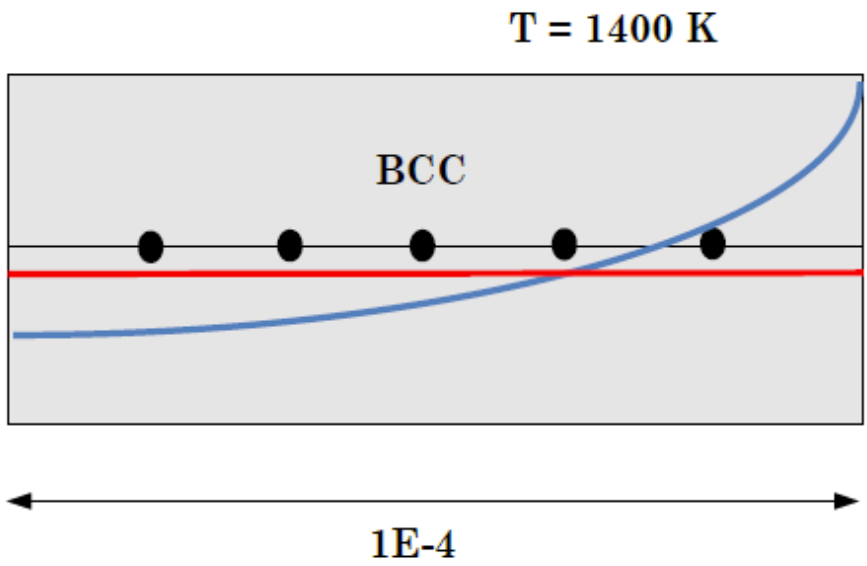

```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: --OK---
POST-1:
```

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 17825) 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: Wed Oct 31 13:18:51 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-
Examples\examples\exa7\setup.DCM.test"SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: NO SUCH COMMAND, USE HELP
SYS:
SYS:SYS: THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

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

 VA                      /-  DEFINED
TDB_FEDEMO: FE                      CR                      NI
 MN  DEFINED
TDB_FEDEMO: LIQUID:L                BCC_A2                  CHI_A12
 DIAMOND_FCC_A4          FCC_A1                  HCP_A3
 LAVES_PHASE_C14         SIGMA  REJECTED
TDB_FEDEMO: BCC_A2  RESTORED
TDB_FEDEMO: 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: Current database: Fe-Alloys Mobility demo database v2.0

 VA  DEFINED
APP: FE                     CR                      NI
 MN  DEFINED
APP: BCC_A2                 FCC_A1  REJECTED
APP: BCC_A2  RESTORED
APP: 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: NO TIME STEP DEFINED
DIC>
DIC>
DIC>DIC> INFO: SCHEIL_REGION CREATED
FILE NAME /XF.TXT/:ENTER WIDTH OF REGION /1/: INFO: LINEAR GRID IN SCHEIL_REGION ENTERED WITH 100 GRID POINTS
 ENTER MAIN SOLID SOLUTION PHASE
PHASE NAME: INFO: COMPOSITION PROFILE ENTERED IN REGION
SHOULD MORE PHASES BE ENTERED IN THE REGION /NO/: INFO: TO COMPLETE SETUP, ENTER TEMPERATURE AND
 SIMULATION TIME
DIC>
DIC>
DIC>DIC>GLOBAL OR BOUNDARY CONDITION /GLOBAL/:VARIABLE :LOW TIME LIMIT /0/:DIC>
DIC>
DIC>DIC>END TIME FOR INTEGRATION /.1/:AUTOMATIC TIMESTEP CONTROL /YES/:MAX TIMESTEP DURING INTEGRATION /360/:INITIAL TIMESTEP : /1E-
07/:SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:DIC>
DIC>
DIC>DIC>
DIC> --OK---
DIC>
```

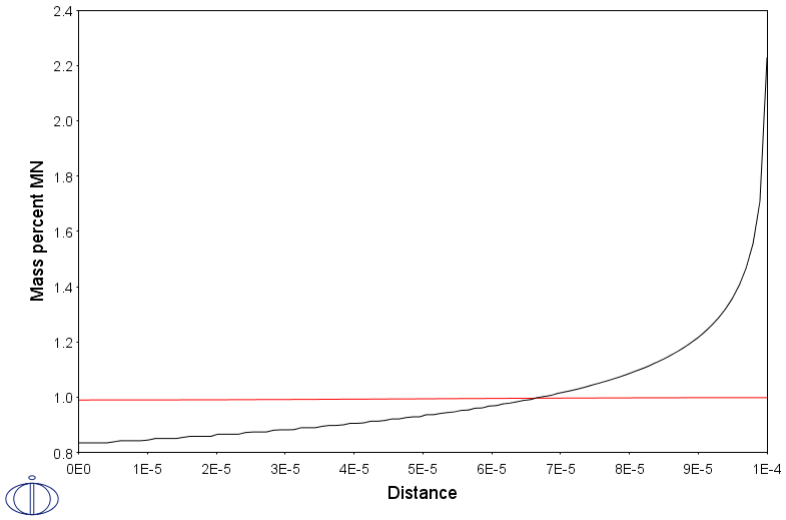
exa7-run

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa7\run.DCM.test"DIC> TIME STEP AT TIME  0.00000E+00
DIC>
DIC> OK
DIC>
DIC> 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                     1 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                     0 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                     1 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                     0 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                     1 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                     0 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                     1 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                     0 seconds
 TIME =   3600.0000     DT =   291.37940     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .180420497422138  FE = .796498787868426
```

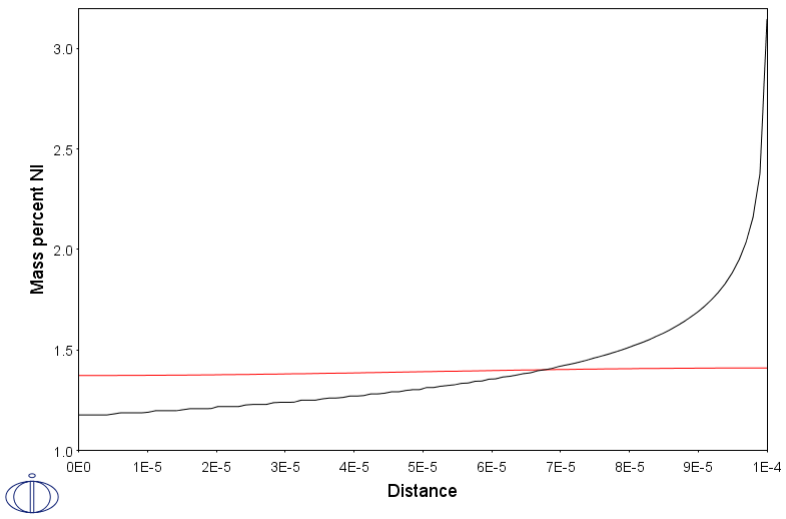
```
                        MN = .00999016878491876  NI = .0130905459245169
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 MUST SAVE WORKSPACE ON FILE
 WORKSPACE SAVED ON FILE
 RECLAIMING WORKSPACE
 DELETING TIME-RECORD FOR TIME    0.0000000
 DELETING TIME-RECORD FOR TIME   0.10000000E-06
 DELETING TIME-RECORD FOR 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> --OK---
DIC>
```

exa7-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa7\plot.DCM.test"DIC> TIME STEP AT TIME  3.60000E+03
DIC>
DIC> OK
DIC>
DIC>  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:POST-1:  INFO: Distance is set as independent variable
POST-1:POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```

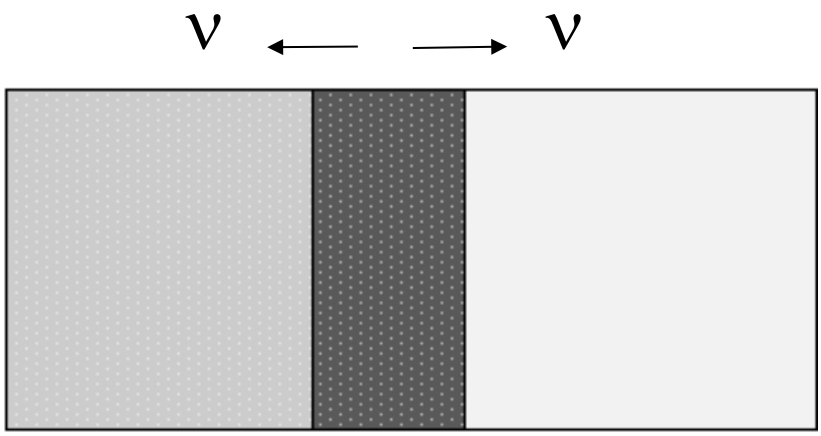



```
POST-1:
POST-1:POST-1:@?
POST-1:
POST-1:POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```




```
POST-1:
POST-1: --OK---
POST-1:
```

Moving Boundary Problems

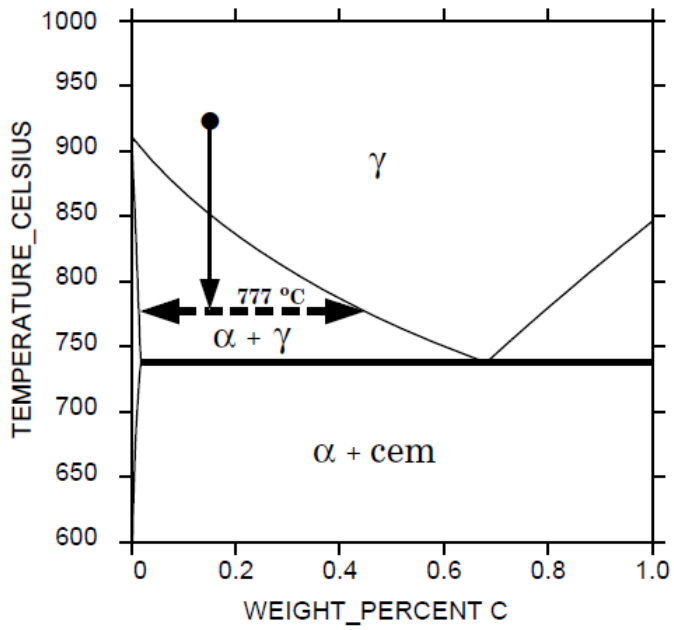


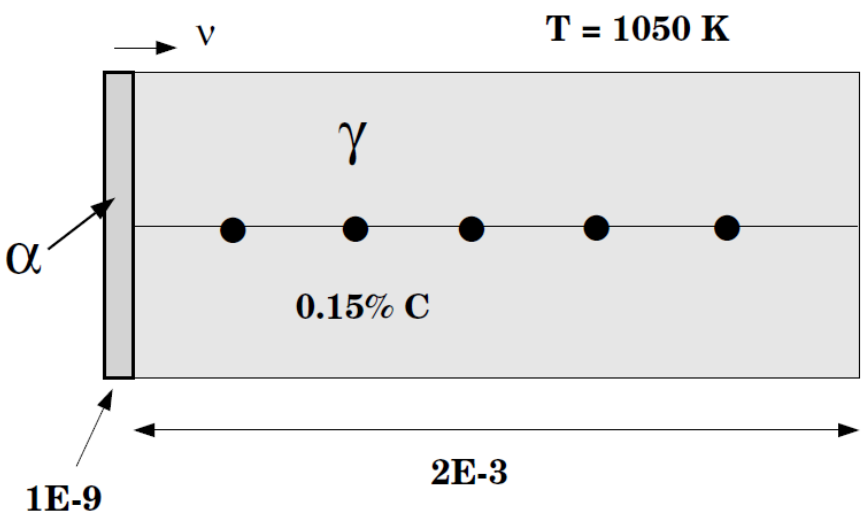
Example exb1a

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
SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-
Examples\examples\exb1a\setup.DCM.test"SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: NO SUCH COMMAND, USE HELP
SYS:
SYS:SYS:
SYS:
SYS:SYS:SYS:SYS: 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:TDB_TCFE9:TDB_TCFE9: Current database: Iron Demo Database v2.0

 VA                      /-  DEFINED
TDB_FEDEMO:
TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO: FE                      C  DEFINED
TDB_FEDEMO:
TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO: 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: FCC_A1                  BCC_A2  RESTORED
TDB_FEDEMO:
TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO: 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:TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO: Use one of these databases

 TCFE9   =  Steels/Fe-Alloys  v9.0
 TCFE8   =  Steels/Fe-Alloys  v8.1
 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
 FEDAT   =  TCS/TT Steels Database v1.0
 TCNI9   =  Ni-Alloys  v9.0
 NI25    =  NI25 Database
 TCNI8   =  Ni-Alloys  v8.2
 TCNI7   =  Ni-Alloys  v7.2
 TCNI6   =  Ni-Alloys  v6.1
 TCNI5   =  Ni-Alloys  v5.1
 TCNI4   =  Ni-Alloys  v4.0
 TCNI1   =  Ni-Alloys  v1.3
 TCAL6   =  Al-Alloys  v6.0
 TCAL5   =  Al-Alloys  v5.1
 TCAL4   =  Al-Alloys  v4.0
 TCAL3   =  Al-Alloys  v3.0
 TCAL2   =  Al-Alloys  v2.1
 TCAL1   =  Al-Alloys  v1.2
 TCMG5   =  Mg-Alloys  v5.1
 TCMG4   =  Mg-Alloys  v4.0
 TCMG3   =  Mg-Alloys  v3.0
 TCMG2   =  Mg-Alloys  v2.0
 TCMG1   =  Mg-Alloys  v1.1
 TCTI2   =  Ti-Alloys  v2.0
 TCTI1   =  Ti-Alloys  v1.0
 TCCU2   =  Cu-Alloys  v2.0
 TCCU1   =  Cu-Alloys  v1.0
 TCCC1   =  Cemented carbide  v1.0
 TCHEA3  =  High Entropy Alloy  v3.1
 TCHEA2  =  High Entropy Alloy  v2.1.1
 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
 TCOX9   =  Metal Oxide Solutions  v9.0 SNAPSHOT
 TCOX8   =  Metal Oxide Solutions  v8.0
 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  v2.7
 AQS2    =  TGG Aqueous Solution Database v2.6
 GCE2    =  TGG Geochemical/Environmental TDB v2.3
 FEDEMO  =  Iron Demo Database v2.0
 ALDEMO  =  Aluminum Demo Database v3.0
 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  v1.1
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBNI5  =  Ni-Alloys Mobility  v5.0
 MOBNI4  =  Ni-Alloys Mobility  v4.1
 MOBNI3  =  Ni-Alloys Mobility  v3.2
 MOBNI2  =  Ni-Alloys Mobility  v2.4
 MOBNI1  =  Ni-Alloys Mobility  v1.9
 MOBAL5  =  Al-Alloys Mobility  v5.0
 MOBAL4  =  Al-Alloys Mobility  v4.0
 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
 MOBHEA1 =  High Entropy Alloys Mobility  v1.0
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBSLD1 =  Solder-Alloys Mobility  v1.1
 MOBTI3  =  Ti-Alloys Mobility  v3.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v2.0
 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/: Current database: Fe-Alloys Mobility demo database v2.0

 VA  DEFINED
APP: FE                      C  DEFINED
APP: BCC_A2                  FCC_A1  REJECTED
APP: FCC_A1                  BCC_A2  RESTORED
APP: 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:APP:APP: NO TIME STEP DEFINED
DIC>
DIC>DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>DIC>DIC>REGION NAME :DIC>
DIC>REGION NAME :ATTACH TO REGION NAMED /FERRITE/:
ATTACHED TO THE RIGHT OF FERRITE /YES/:
DIC>
DIC>DIC>DIC>DIC>REGION NAME : /FERRITE/:WIDTH OF REGION /1/:TYPE /LINEAR/:DIC>
DIC>WIDTH OF REGION /1/:TYPE /LINEAR/:DIC>
DIC>DIC>DIC>DIC>ACTIVE OR INACTIVE PHASE /ACTIVE/:REGION NAME : /FERRITE/:PHASE TYPE /MATRIX/:PHASE NAME: /NONE/:DIC>
DIC>ACTIVE OR INACTIVE PHASE /ACTIVE/:REGION NAME : /AUSTENITE/:PHASE TYPE /MATRIX/:PHASE NAME: /NONE/:DIC>
DIC>
DIC>
DIC>DIC>DIC>DIC>REGION NAME : /FERRITE/:PHASE NAME: /BCC_A2/:COMPOSITION TYPE /MOLE_FRACTION/:PROFILE FOR /C/:TYPE /LINEAR/:VALUE OF FIRST POIN
2/:DIC>
DIC>DIC>DIC>DIC>REGION NAME : /AUSTENITE/:PHASE NAME: /FCC_A1/:COMPOSITION TYPE /MOLE_FRACTION/:PROFILE FOR /C/:TYPE /LINEAR/:VALUE OF FIRST PO
DIC>DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>END TIME FOR INTEGRATION /.1/:AUTOMATIC TIMESTEP CONTROL /YES/:MAX TIMESTEP DURING INTEGRATION /100000000/:INITIAL TIMESTEP : /
07/:SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:DIC>
DIC>
DIC>DIC>DIC>DIC>DIC>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/: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>DIC>DIC>
DIC> --OK---
DIC>
```

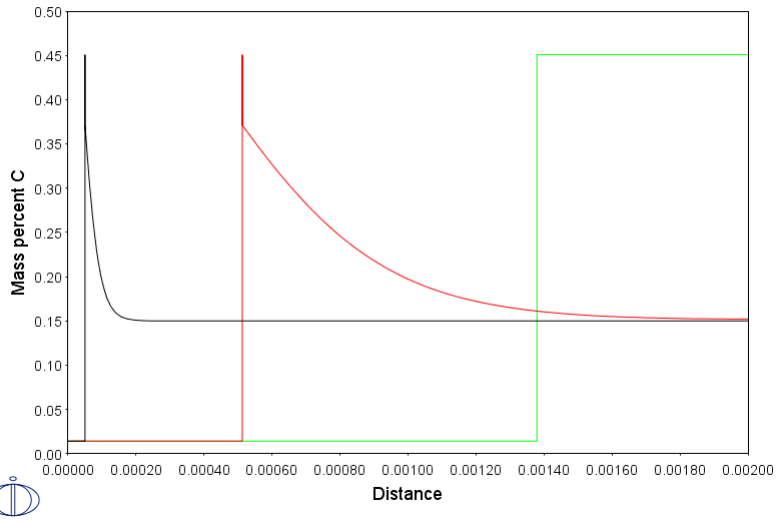
exb1a-run

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb1a\run.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  0.00000E+00
DIC> OK
DIC>
DIC>DIC>DIC>DIC> 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]
  CPU time used in timestep                     0 seconds
 9.829104754110936E-007        9.836537893098349E-007        1.102429090552512E-010        4.078551911522211E-014        1.058272452621317E-
021       TIME =  0.25500000E-02 DT =  0.12800000E-02 SUM OF SQUARES =  0.10582725E-20
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.18170713E-04 AND   0.18170713E-04
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.99390660E-07
 U-FRACTION IN SYSTEM:  C = .00698493641830885  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]


output ignored...



... output resumed

 2.107536493133355E-005        2.107957887942567E-005        1.857259034723269E-
023       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                     0 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
 1.197224211328478E-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
```

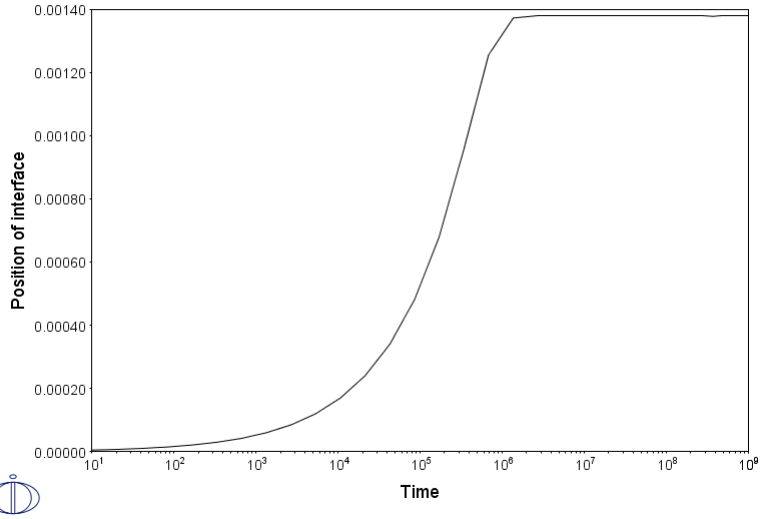
```
  CPU time used in timestep                    0 seconds
 2.955421017074509E-002        2.955388709148415E-002        2.998282669477928E-
017       TIME =  0.87592186E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.29982827E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.88900282E-15 AND  -0.88900282E-15
 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>DIC>DIC>
DIC> --OK---
DIC>
```

exb1a-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb1a\plot.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  1.00000E+09
DIC> OK
DIC>
DIC>DIC>DIC>DIC>  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:
POST-1:POST-1:POST-1:POST-1:  INFO: Distance is set as independent variable
POST-1:POST-1:POST-1:
POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```

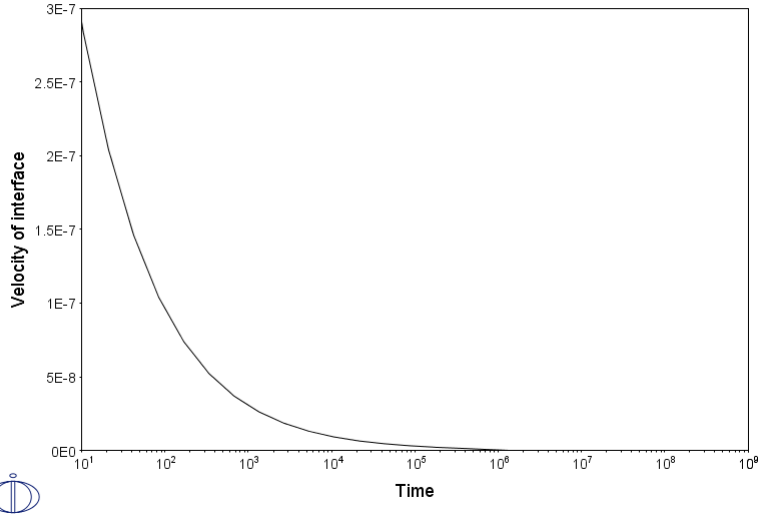



```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1:POST-1:POST-1:POST-1:  INFO: Time is set as independent variable
POST-1:VARIABLE :INTERFACE :UPPER OR LOWER INTERFACE OF REGION AUSTENITE#1 /LOWER/:POST-1:
POST-1:AXIS (X, Y OR Z) :AXIS TYPE /LINEAR/:POST-1:
POST-1:AXIS (X, Y OR Z) :AUTOMATIC SCALING  (Y OR N) /N/:MIN VALUE :MAX VALUE :POST-1:
POST-1:
POST-1:POST-1:            OST-1:POST-1:
POST-1:
```




```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1:POST-1:POST-1:POST-1:AXIS (X, Y OR Z) :VARIABLE :INTERFACE :UPPER OR LOWER INTERFACE OF REGION AUSTENITE#1 /LOWER/:POST-1:
POST-1:
POST-1:POST-1:            OST-1:POST-1:
POST-1:
```

2018.10.31.15.47.38
LOWER INTERFACE OF REGION "AUSTENITE#1"
CELL #1

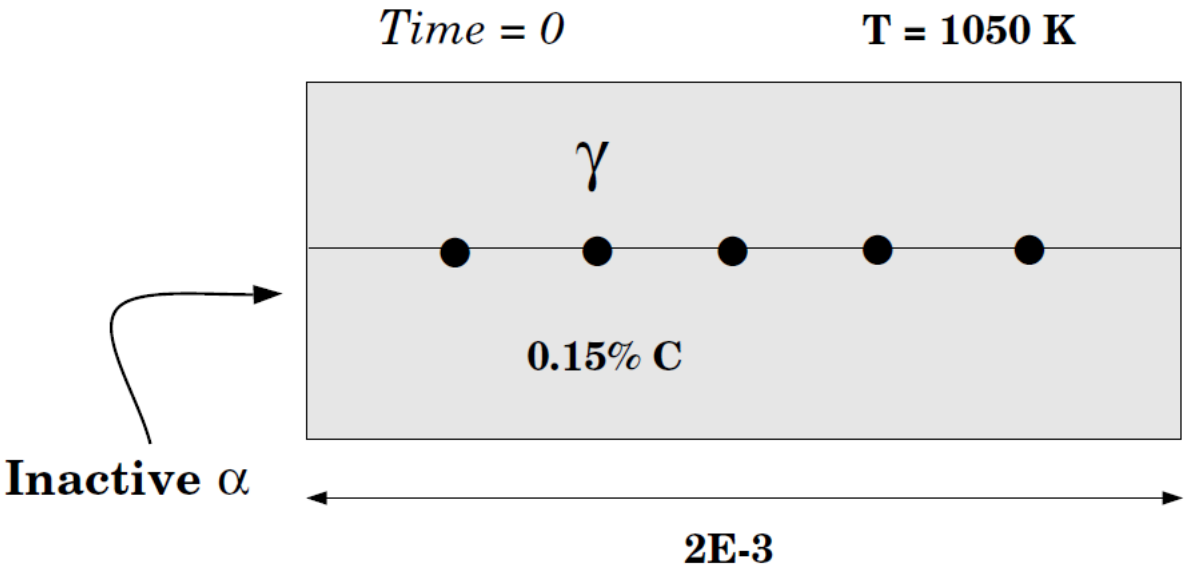


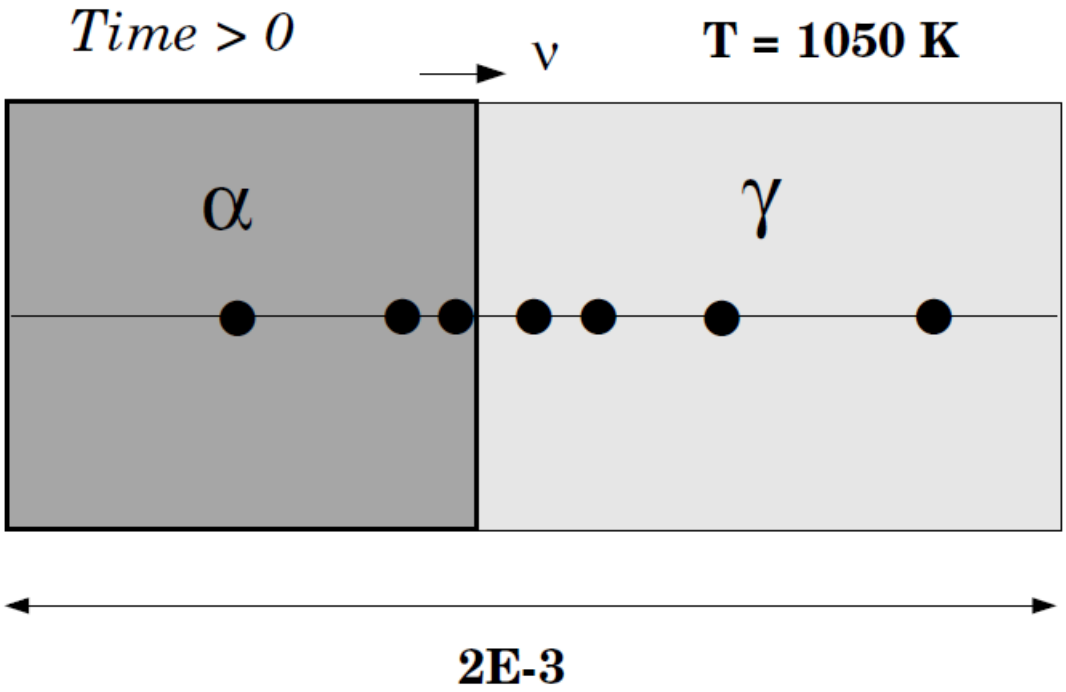

```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: --OK---
POST-1:
```

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
 Software  (build 17825) 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: Wed Oct 31 13:18:51 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-
Examples\examples\exb1b\setup.DCM.test"SYS:SYS:SYS:SYS:SYS:SYS: NO SUCH COMMAND, USE HELP
SYS:
SYS:SYS:
SYS:SYS:SYS:SYS: 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:TDB_TCFE9:TDB_TCFE9: Current database: Iron Demo Database v2.0

 VA                       /-  DEFINED
TDB_FEDEMO:
TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO: FE                       C  DEFINED
TDB_FEDEMO:
TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO: 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: FCC_A1                   BCC_A2  RESTORED
TDB_FEDEMO:
TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO: 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:TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO: Use one of these databases

 TCFE9   =  Steels/Fe-Alloys  v9.0
 TCFE8   =  Steels/Fe-Alloys  v8.1
 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
 FEDAT   =  TCS/TT Steels Database v1.0
 TCNI9   =  Ni-Alloys  v9.0
 NI25    =  NI25 Database
 TCNI8   =  Ni-Alloys  v8.2
 TCNI7   =  Ni-Alloys  v7.2
 TCNI6   =  Ni-Alloys  v6.1
 TCNI5   =  Ni-Alloys  v5.1
 TCNI4   =  Ni-Alloys  v4.0
 TCNI1   =  Ni-Alloys  v1.3
 TCAL6   =  Al-Alloys  v6.0
 TCAL5   =  Al-Alloys  v5.1
 TCAL4   =  Al-Alloys  v4.0
 TCAL3   =  Al-Alloys  v3.0
 TCAL2   =  Al-Alloys  v2.1
 TCAL1   =  Al-Alloys  v1.2
 TCMG5   =  Mg-Alloys  v5.1
 TCMG4   =  Mg-Alloys  v4.0
 TCMG3   =  Mg-Alloys  v3.0
 TCMG2   =  Mg-Alloys  v2.0
 TCMG1   =  Mg-Alloys  v1.1
 TCTI2   =  Ti-Alloys  v2.0
 TCTI1   =  Ti-Alloys  v1.0
 TCCU2   =  Cu-Alloys  v2.0
 TCCU1   =  Cu-Alloys  v1.0
 TCCC1   =  Cemented carbide  v1.0
 TCHEA3  =  High Entropy Alloy  v3.1
 TCHEA2  =  High Entropy Alloy  v2.1.1
 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
 TCOX9   =  Metal Oxide Solutions  v9.0 SNAPSHOT
 TCOX8   =  Metal Oxide Solutions  v8.0
 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  v2.7
 AQS2    =  TGG Aqueous Solution Database v2.6
 GCE2    =  TGG Geochemical/Environmental TDB v2.3
 FEDEMO  =  Iron Demo Database v2.0
 ALDEMO  =  Aluminum Demo Database v3.0
 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  v1.1
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBNI5  =  Ni-Alloys Mobility  v5.0
 MOBNI4  =  Ni-Alloys Mobility  v4.1
 MOBNI3  =  Ni-Alloys Mobility  v3.2
 MOBNI2  =  Ni-Alloys Mobility  v2.4
 MOBNI1  =  Ni-Alloys Mobility  v1.9
 MOBAL5  =  Al-Alloys Mobility  v5.0
 MOBAL4  =  Al-Alloys Mobility  v4.0
 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
 MOBHEA1 =  High Entropy Alloys Mobility  v1.0
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBSLD1 =  Solder-Alloys Mobility  v1.1
 MOBTI3  =  Ti-Alloys Mobility  v3.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v2.0
 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/: Current database: Fe-Alloys Mobility demo database v2.0

 VA  DEFINED
APP: FE                      C  DEFINED
APP: BCC_A2                  FCC_A1  REJECTED
APP: FCC_A1                  BCC_A2  RESTORED
APP: 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:APP:APP: NO TIME STEP DEFINED
DIC>
DIC>DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>REGION NAME :DIC>
DIC>DIC>DIC>DIC>REGION NAME : /AUSTENITE/:WIDTH OF REGION /1/:TYPE /LINEAR/:DIC>
DIC>DIC>DIC>DIC>ACTIVE OR INACTIVE PHASE /ACTIVE/:REGION NAME : /AUSTENITE/:PHASE TYPE /MATRIX/:PHASE NAME: /NONE/:DIC>
DIC>DIC>DIC>DIC>ACTIVE OR INACTIVE PHASE /ACTIVE/:ATTACH TO REGION NAMED /AUSTENITE/:ATTACHED TO THE RIGHT OF AUSTENITE /YES/:PHASE NAME: /NONE
05/:CONDITION TYPE /CLOSED_SYSTEM/:DIC>
DIC>DIC>DIC>DIC>REGION NAME : /AUSTENITE/:PHASE NAME: /FCC_A1/:COMPOSITION TYPE /MOLE_FRACTION/:PROFILE FOR /C/:TYPE /LINEAR/:VALUE OF FIRST PO
DIC>DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>END TIME FOR INTEGRATION /.1/:AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /100000000/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC>
DIC>DIC>DIC>DIC>DIC>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/: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>DIC>
 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> --OK---
DIC>
```

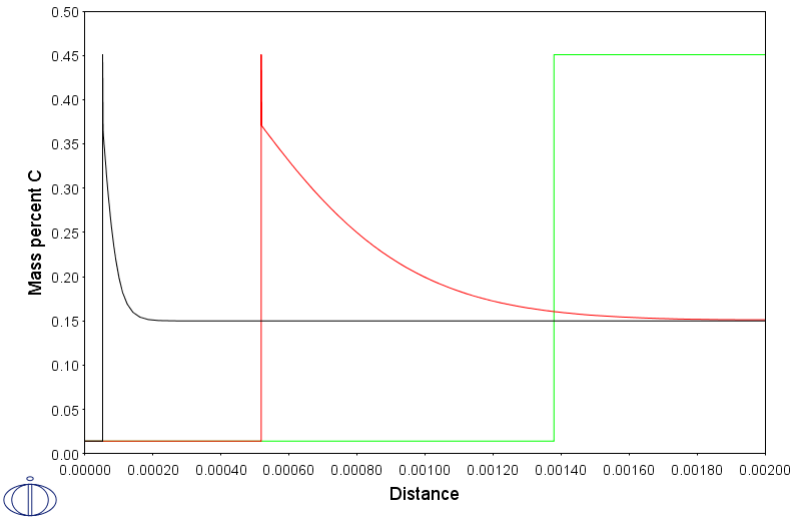
exb1b-run

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb1b\run.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  0.00000E+00
DIC> OK
DIC>
DIC>DIC>DIC>DIC> 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        2.363552975725973E-003        2.496385532063016E-003        2.363552975725973E-003        2.376826820350898E-
003        2.363552975725973E-003        2.369210192893830E-003        2.363552975725973E-003        2.366884139762012E-
003        2.363552975725973E-003        2.361884230806084E-003        2.361884230806084E-003        2.358736813613249E-
003        2.358736813613249E-003        2.400729508481361E-003        2.358736813613249E-003

output ignored...



... output resumed

 5.023044628187047E-005        1.556538506983708E-028       TIME =  0.50502330E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.15565385E-27
 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]
```

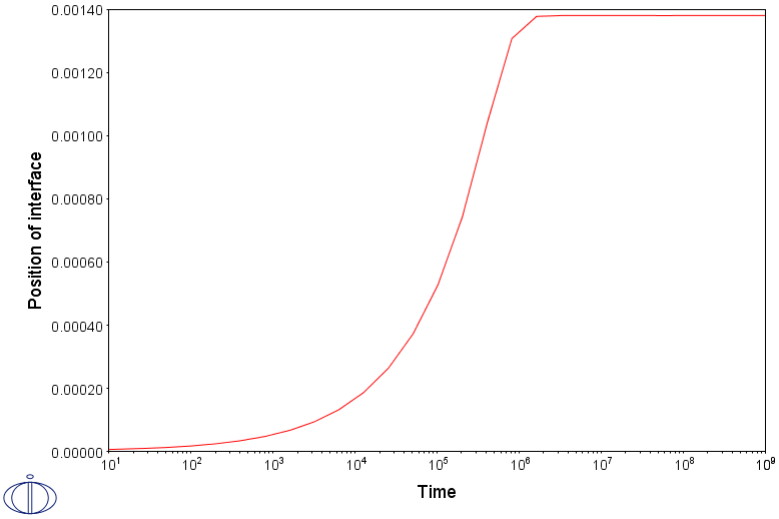
```
  2  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_BCC_A2

  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>DIC>DIC>
DIC> --OK---
DIC>
```

exb1b-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb1b\plot.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  1.00000E+09
DIC> OK
DIC>
DIC>DIC>DIC>DIC>  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:  INFO: Distance is set as independent variable
POST-1:POST-1:
POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```

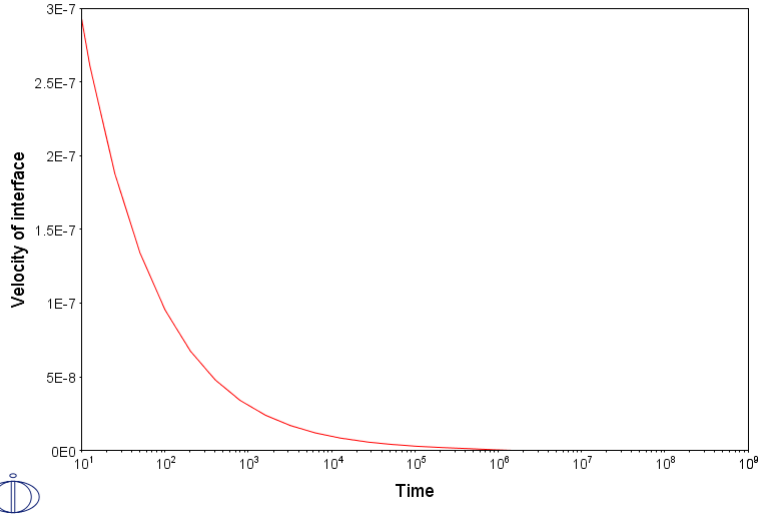



```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1:POST-1:POST-1:POST-1:  INFO: Time is set as independent variable
POST-1:VARIABLE :INTERFACE :UPPER OR LOWER INTERFACE OF REGION AUSTENITE#1 /LOWER/:POST-1:
POST-1:AXIS (X, Y OR Z) :AXIS TYPE /LINEAR/:POST-1:
POST-1:AXIS (X, Y OR Z) :AUTOMATIC SCALING  (Y OR N) /N/:MIN VALUE :MAX VALUE :POST-1:
POST-1:
POST-1:POST-1: ORKING ...          OST-1:POST-1:
POST-1:
```




```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1:POST-1:POST-1:POST-1:AXIS (X, Y OR Z) :VARIABLE :INTERFACE :UPPER OR LOWER INTERFACE OF REGION AUSTENITE#1 /LOWER/:POST-1:
POST-1:
POST-1:POST-1: ORKING ...          OST-1:POST-1:
POST-1:
```

2018.10.31.15.50.56
LOWER INTERFACE OF REGION "AUSTENITE#1"
CELL #1

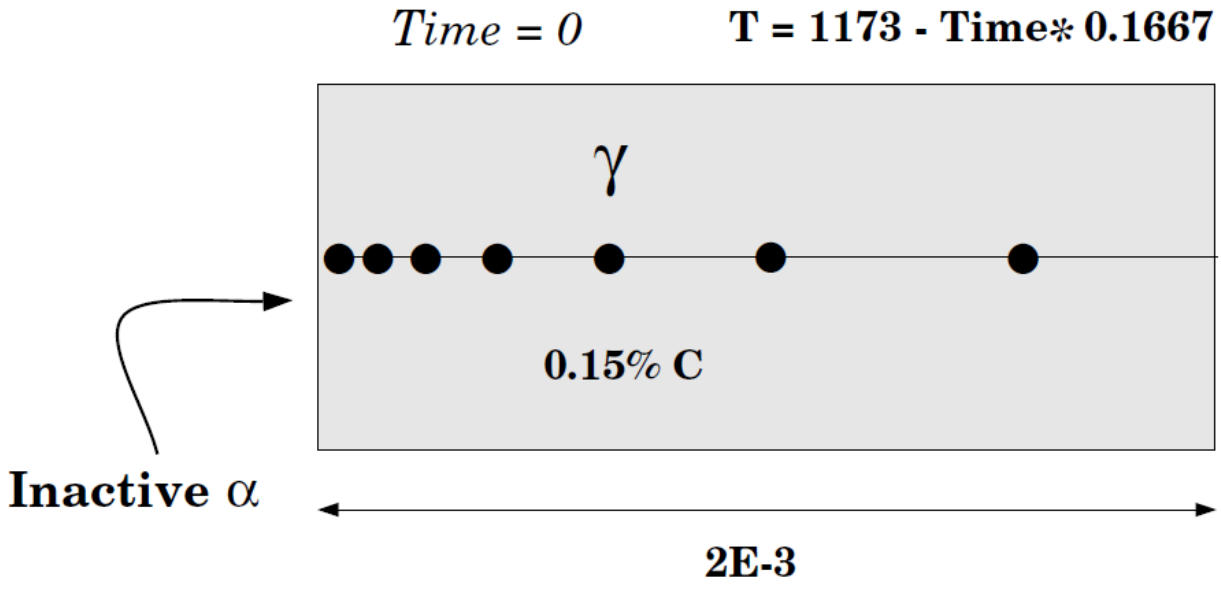


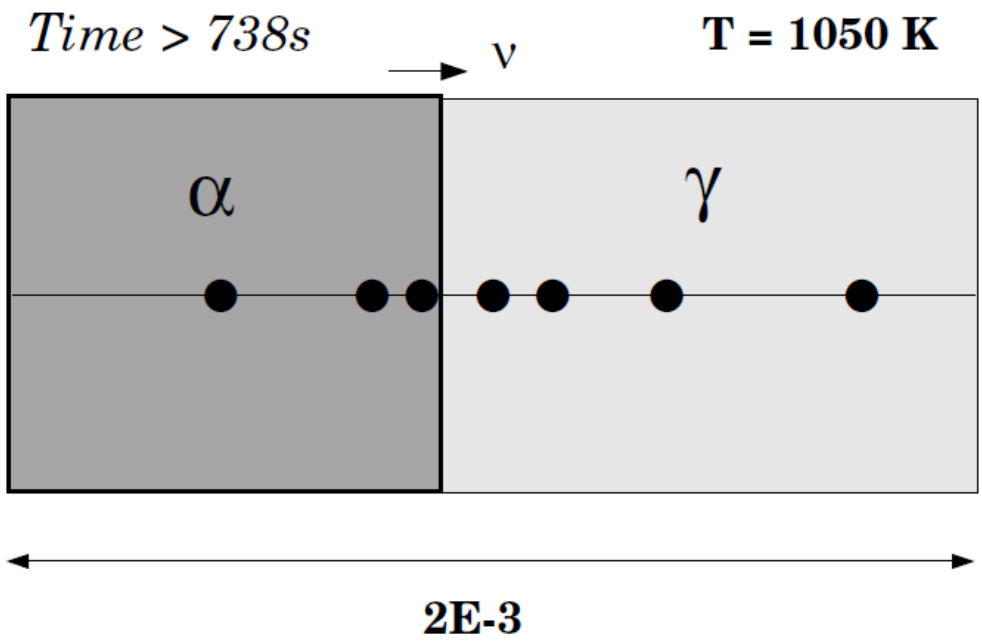

```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: --OK---
POST-1:
```

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

```
About Stockholm, Sweden

 Software  (build 17825) 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: Wed Oct 31 13:18:51 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-
Examples\examples\exb1c\setup.DCM.test"SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: NO SUCH COMMAND, USE HELP
SYS:
SYS:SYS:
SYS:SYS:SYS:SYS: 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:TDB_TCFE9:TDB_TCFE9: Current database: Iron Demo Database v2.0

 VA                       /-  DEFINED
TDB_FEDEMO:
TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO: FE                       C  DEFINED
TDB_FEDEMO:
TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO: 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: FCC_A1                   BCC_A2  RESTORED
TDB_FEDEMO:
TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO: 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:TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO: Use one of these databases

 TCFE9   =  Steels/Fe-Alloys  v9.0
 TCFE8   =  Steels/Fe-Alloys  v8.1
 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
 FEDAT   =  TCS/TT Steels Database v1.0
 TCNI9   =  Ni-Alloys  v9.0
 NI25    =  NI25 Database
 TCNI8   =  Ni-Alloys  v8.2
 TCNI7   =  Ni-Alloys  v7.2
 TCNI6   =  Ni-Alloys  v6.1
 TCNI5   =  Ni-Alloys  v5.1
 TCNI4   =  Ni-Alloys  v4.0
 TCNI1   =  Ni-Alloys  v1.3
 TCAL6   =  Al-Alloys  v6.0
 TCAL5   =  Al-Alloys  v5.1
 TCAL4   =  Al-Alloys  v4.0
 TCAL3   =  Al-Alloys  v3.0
 TCAL2   =  Al-Alloys  v2.1
 TCAL1   =  Al-Alloys  v1.2
 TCMG5   =  Mg-Alloys  v5.1
 TCMG4   =  Mg-Alloys  v4.0
 TCMG3   =  Mg-Alloys  v3.0
 TCMG2   =  Mg-Alloys  v2.0
 TCMG1   =  Mg-Alloys  v1.1
 TCTI2   =  Ti-Alloys  v2.0
 TCTI1   =  Ti-Alloys  v1.0
 TCCU2   =  Cu-Alloys  v2.0
 TCCU1   =  Cu-Alloys  v1.0
 TCCC1   =  Cemented carbide  v1.0
 TCHEA3  =  High Entropy Alloy  v3.1
 TCHEA2  =  High Entropy Alloy  v2.1.1
 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
 TCOX9   =  Metal Oxide Solutions  v9.0 SNAPSHOT
 TCOX8   =  Metal Oxide Solutions  v8.0
 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  v2.7
 AQS2    =  TGG Aqueous Solution Database v2.6
 GCE2    =  TGG Geochemical/Environmental TDB v2.3
 FEDEMO  =  Iron Demo Database v2.0
 ALDEMO  =  Aluminum Demo Database v3.0
 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  v1.1
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBNI5  =  Ni-Alloys Mobility  v5.0
 MOBNI4  =  Ni-Alloys Mobility  v4.1
 MOBNI3  =  Ni-Alloys Mobility  v3.2
 MOBNI2  =  Ni-Alloys Mobility  v2.4
 MOBNI1  =  Ni-Alloys Mobility  v1.9
 MOBAL5  =  Al-Alloys Mobility  v5.0
 MOBAL4  =  Al-Alloys Mobility  v4.0
 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
 MOBHEA1 =  High Entropy Alloys Mobility  v1.0
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBSLD1 =  Solder-Alloys Mobility  v1.1
 MOBTI3  =  Ti-Alloys Mobility  v3.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v2.0
 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/: Current database: Fe-Alloys Mobility demo database v2.0

 VA  DEFINED
APP: FE                      C  DEFINED
APP: BCC_A2                  FCC_A1  REJECTED
APP: FCC_A1                  BCC_A2  RESTORED
APP: 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:APP:APP: NO TIME STEP DEFINED
DIC>
DIC>DIC>DIC>DIC>DIC>DIC>GLOBAL OR BOUNDARY CONDITION /GLOBAL/:VARIABLE :LOW TIME LIMIT /0/:T(TIME,X)=HIGH TIME LIMIT /*/:ANY MORE RANGES /N/:T(
DIC>DIC>DIC>DIC>REGION NAME :DIC>
DIC>DIC>DIC>DIC>REGION NAME : /AUSTENITE/:WIDTH OF REGION /1/:TYPE /LINEAR/:DIC>
DIC>DIC>DIC>DIC>ACTIVE OR INACTIVE PHASE /ACTIVE/:REGION NAME : /AUSTENITE/:PHASE TYPE /MATRIX/:PHASE NAME: /NONE/:DIC>
DIC>DIC>DIC>DIC>ACTIVE OR INACTIVE PHASE /ACTIVE/:ATTACH TO REGION NAMED /AUSTENITE/:ATTACHED TO THE RIGHT OF AUSTENITE /YES/:PHASE NAME: /NONE
05/:CONDITION TYPE /CLOSED_SYSTEM/:DIC>
DIC>DIC>DIC>DIC>REGION NAME : /AUSTENITE/:PHASE NAME: /FCC_A1/:COMPOSITION TYPE /MOLE_FRACTION/:PROFILE FOR /C/:TYPE /LINEAR/:VALUE OF FIRST PO
DIC>DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>END TIME FOR INTEGRATION /.1/:AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /73.8/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC>DIC>DIC>DIC>DIC>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/: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>DIC>DIC>
DIC> --OK---
DIC>
```

exb1c-run

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb1c\run.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  0.00000E+00
DIC> OK
DIC>
DIC>DIC>DIC>DIC> 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]
```

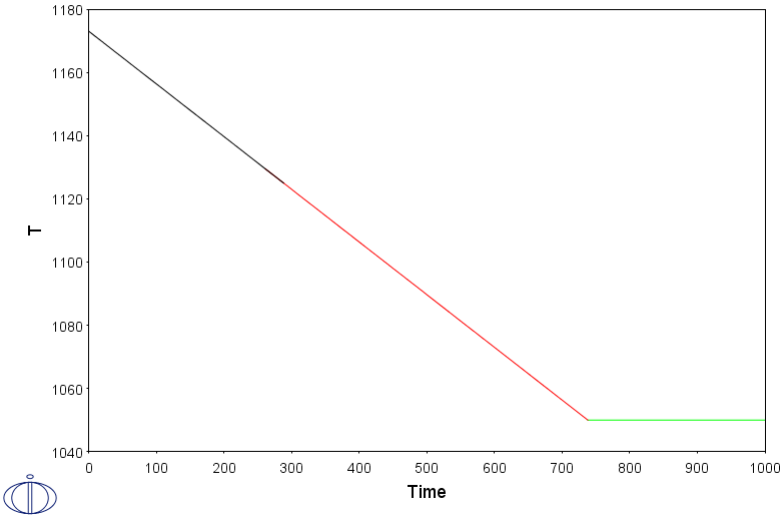
```
  CPU time used in timestep                    0 seconds
 TIME =   76.594946     DT =   36.900000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698495916383102  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    0 seconds
 TIME =   113.49495     DT =   36.900000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698495916383101  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    1 seconds
 TIME =   150.39495     DT =   36.900000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698495916383103  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    0 seconds
 TIME =   187.29495     DT =   36.900000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698495916383105  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    0 seconds
 TIME =   224.19495     DT =   36.900000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698495916383106  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]


output ignored...



... output resumed

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

  CPU time used in timestep                    0 seconds
 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                    1 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>DIC>DIC>
DIC> --OK---
DIC>
```

exb1c-plot

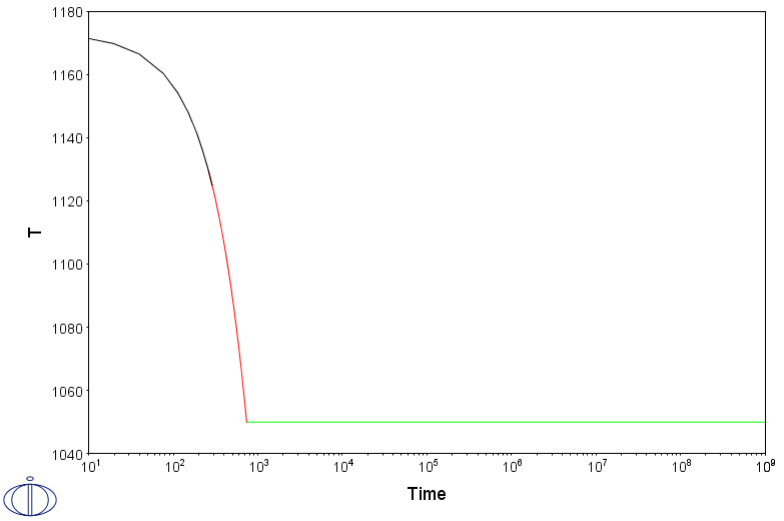
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb1c\plot.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  1.00000E+09
DIC> OK
DIC>
DIC>DIC>DIC>DIC>  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:  INFO: Time is set as independent variable
POST-1:CONDITION /TIME/:INTERFACE :UPPER OR LOWER INTERFACE OF REGION AUSTENITE#1 /LOWER/:POST-1:POST-1:
POST-1:
POST-1:POST-1: ORKING ...          OST-1:POST-1:
POST-1:
```

2018.10.31.15.54.15
LOWER INTERFACE OF REGION "AUSTENITE#1"
CELL #1



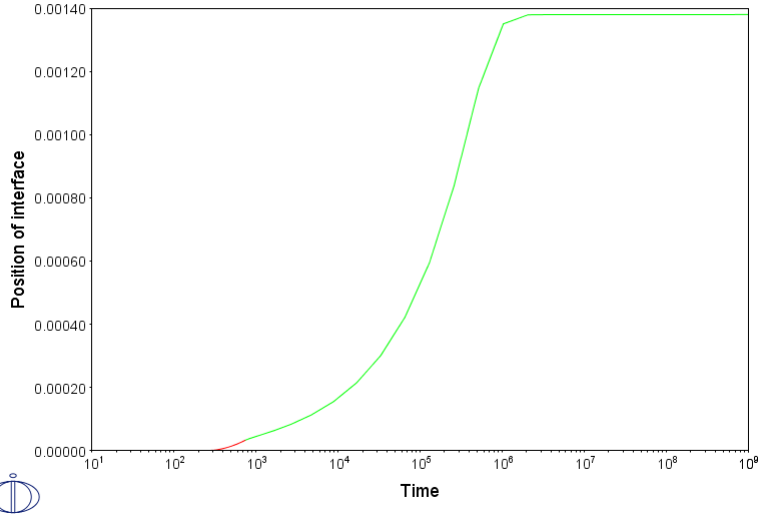

```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:
POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```

2018.10.31.15.54.15
LOWER INTERFACE OF REGION "AUSTENITE#1"
CELL #1



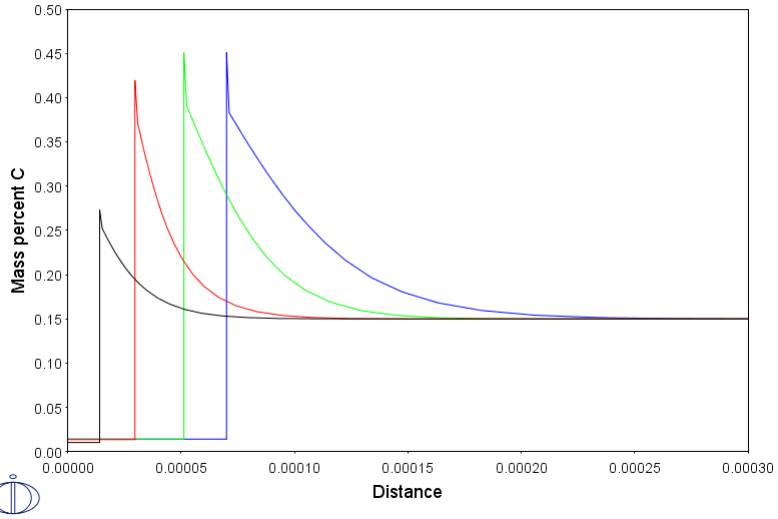

```
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1:POST-1:POST-1:POST-1:AXIS (X, Y OR Z) :VARIABLE :INTERFACE :UPPER OR LOWER INTERFACE OF REGION AUSTENITE#1 /LOWER/:POST-1:
POST-1:
POST-1:POST-1: ORKING ...          OST-1:POST-1:
POST-1:
```

2018.10.31.15.54.16
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:POST-1:POST-1:POST-1:  INFO: Distance is set as independent variable
POST-1:POST-1:POST-1:POST-1:
POST-1:
POST-1:POST-1: ORKING ...OST-1:POST-1:
POST-1:
```

2018.10.31.15.54.16
Time = 500,700,1200,2000
CELL #1

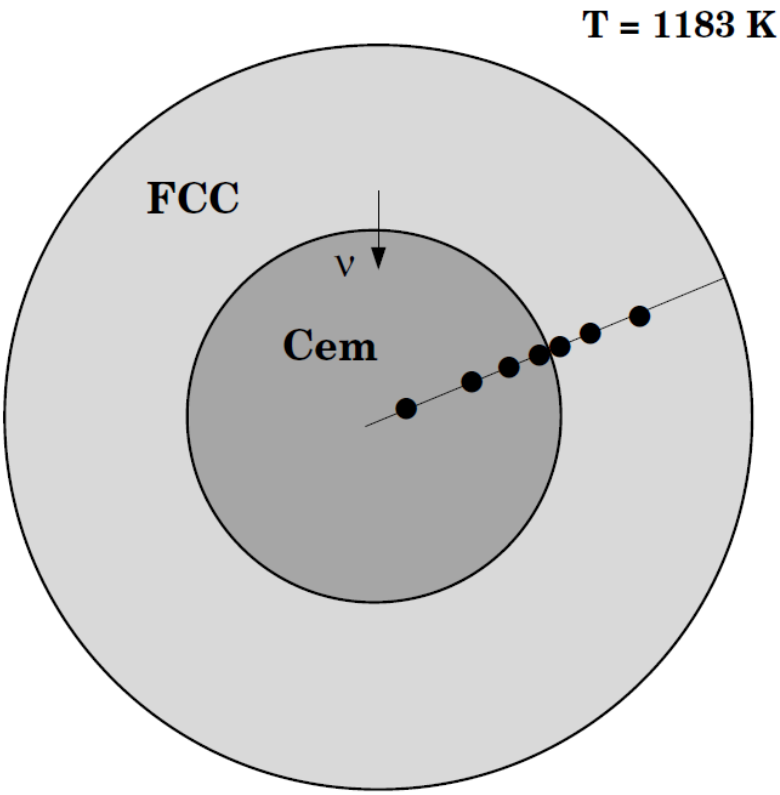



```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1: --OK---
POST-1:
```

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

```
AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb2\setup.DCM.test"SYS: NO SUCH COMMAND, USE HELP
SYS:SYS:SYS:SYS:SYS:SYS:SYS: NO SUCH COMMAND, USE HELP
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: 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:TDB_TCFE9:TDB_TCFE9: Current database: Iron Demo Database v2.0

 VA                       /-  DEFINED
TDB_FEDEMO: FE                       CR                      C
   DEFINED
TDB_FEDEMO: 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: FCC_A1                   BCC_A2                  CEMENTITE
   RESTORED
TDB_FEDEMO: 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:TDB_FEDEMO:TDB_FEDEMO: Current database: Steels/Fe-Alloys Mobility  v2.0
   TCS Steel Mobility Database Version 2.0 from 2011-12-09.

 VA  DEFINED
APP: FE                       CR                      C
   DEFINED
APP: BCC_A2                   CEMENTITE               FCC_A1
 FE4N_LP1                 HCP_A3                  LIQUID:L
   REJECTED
APP: FCC_A1                   CEMENTITE  RESTORED
APP: 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:APP:APP:
 POLY version  3.32
POLY_3:

POLY_3:POLY_3:POLY_3:POLY_3:POLY_3:POLY_3:
POLY_3:
POLY_3:POLY_3:POLY_3:POLY_3:
POLY_3:POLY_3:POLY_3:
POLY_3:POLY_3:POLY_3:
POLY_3:POLY_3:POLY_3:
POLY_3:POLY_3:POLY_3:
POLY_3:POLY_3:POLY_3:
POLY_3:
POLY_3:POLY_3:POLY_3:POLY_3: 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:POLY_3:POLY_3: RMAT=5.392487E-7
POLY_3: W(CEMENTITE,CR)=0.12581627
 W(BCC_A2,CR)=4.433258E-3
 W(BCC_A2,C)=1.510234E-4
POLY_3:
POLY_3:POLY_3:POLY_3:POLY_3:
POLY_3:
```

```
POLY_3:POLY_3:POLY_3:POLY_3: NO TIME STEP DEFINED
 *** ENTERING BCC_A2 AS A DIFFUSION NONE PHASE
DIC>
DIC>DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>REGION NAME :DIC>
DIC>REGION NAME :ATTACH TO REGION NAMED /CARB/:
ATTACHED TO THE RIGHT OF CARB /YES/:
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>DIC>DIC>REGION NAME : /CARB/:WIDTH OF REGION /1/:TYPE /LINEAR/:DIC>
DIC>DIC>DIC>DIC>DIC>REGION NAME : /AUS/:WIDTH OF REGION /1/:TYPE /LINEAR/:DIC>
DIC>DIC>DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>REGION NAME : /CARB/:PHASE NAME: /CEMENTITE/:COMPOSITION TYPE /MOLE_FRACTION/:PROFILE FOR /CR/:DIC>
DIC>REGION NAME : /AUS/:PHASE NAME: /FCC_A1#1/:DEPENDENT COMPONENT ? /FE/:COMPOSITION TYPE /MOLE_FRACTION/:PROFILE FOR /C/:PROFILE FOR /CR/:DIC
DIC>DIC>DIC>DIC>GEOMETRICAL EXPONENT /0/:DIC>
DIC>DIC>DIC>DIC>END TIME FOR INTEGRATION /.1/:AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /1000/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC>DIC>DIC>DIC>DIC>
DIC> --OK---
DIC>
```

exb2-run

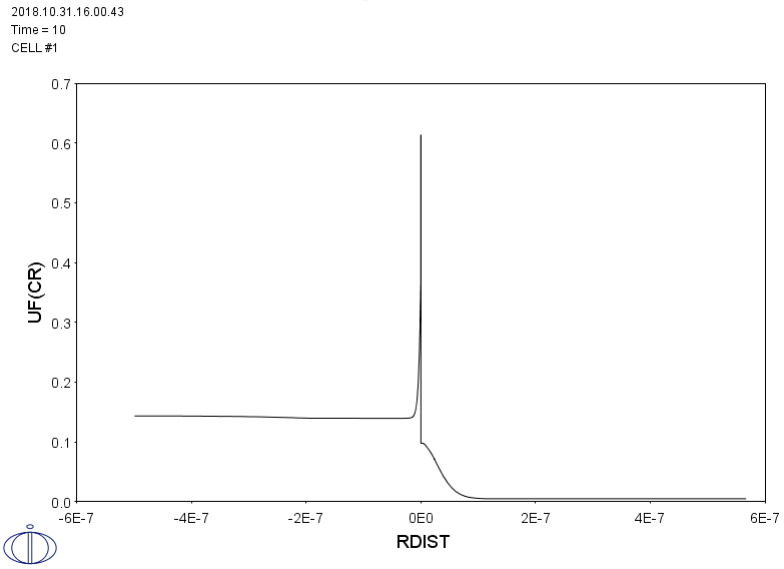
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb2\run.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC> TIME STEP AT TIME  0.00000E+00
 *** ENTERING BCC_A2 AS A DIFFUSION NONE PHASE
DIC> OK
DIC> Region: CARB
 single geometric dense at  0.52550E-06
 0.85084       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 = .0406910188418179  CR = .0214382349908299
                        FE = .978561765139677
 TOTAL SIZE OF SYSTEM:  5.0562665819E-18 [m^3]
 U-FRACTION IN SYSTEM:  C = .0406910188418179  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                     1 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                     0 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                     1 seconds
 3.788612455941237E-005        3.788586871828255E-005        3.788453387382108E-005        1.049991000427905E-005        1.697466271255278E-
008        3.616799432571808E-012        3.087812359916612E-015        2.462552467205662E-018       TIME =  0.31000000E-05 DT =  0.16000000E-
05 SUM OF SQUARES =  0.24625525E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.33005552E-05 AND  -0.33005552E-05


output ignored...



... output resumed

 9.369248327802317E-009        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                     2 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> --OK---
DIC>
```

exb2-plot

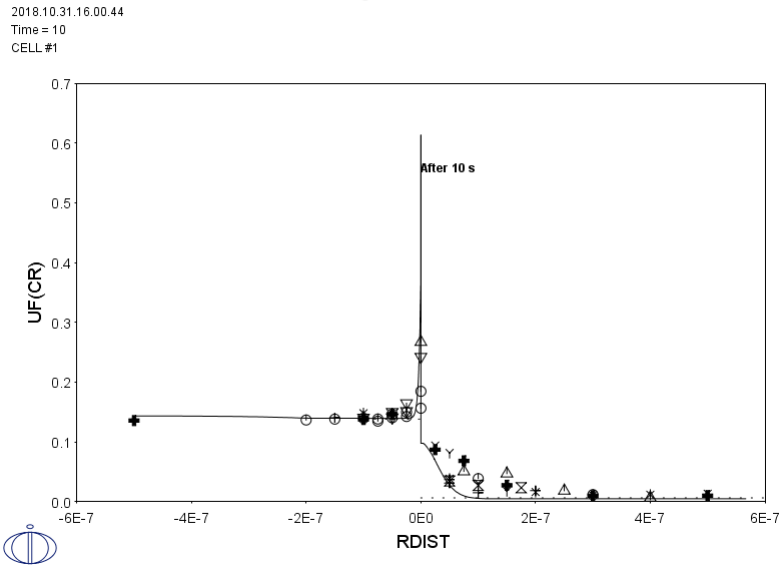
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb2\plot.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  1.00000E+04
 *** ENTERING BCC_A2 AS A DIFFUSION NONE PHASE
DIC> OK
DIC>
DIC>DIC>DIC>DIC>  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:Function or table /FUNCTION/:NAME:FUNCTION:POST-1:
POST-1:POST-1:
POST-1:VARIABLE /TIME/:DISTANCE : /GLOBAL/:POST-1:
POST-1:POST-1:
POST-1:POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:
POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```

Figure b2.1




```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:PROLOGUE NUMBER: /0/:DATASET NUMBER(s): /-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:POST-1:POST-1:PROLOGUE NUMBER: /0/:DATASET NUMBER(s): /-1/:POST-1:
POST-1:POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```

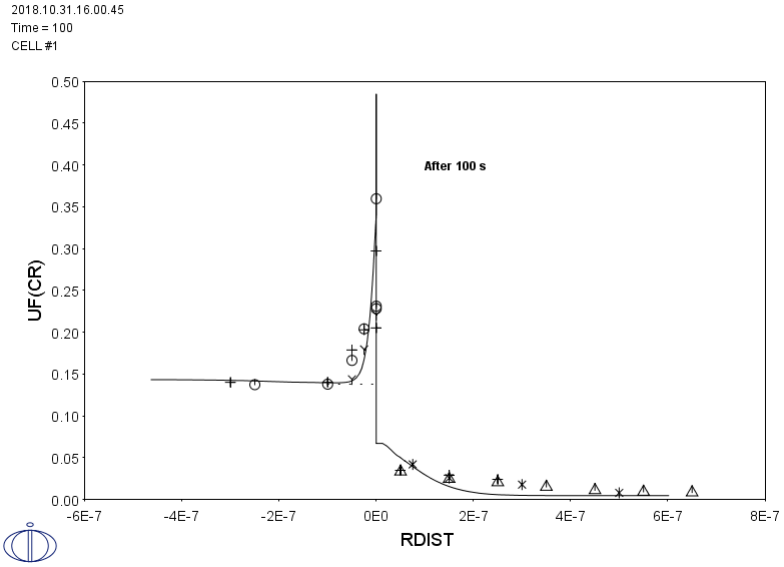
Figure b2.2




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

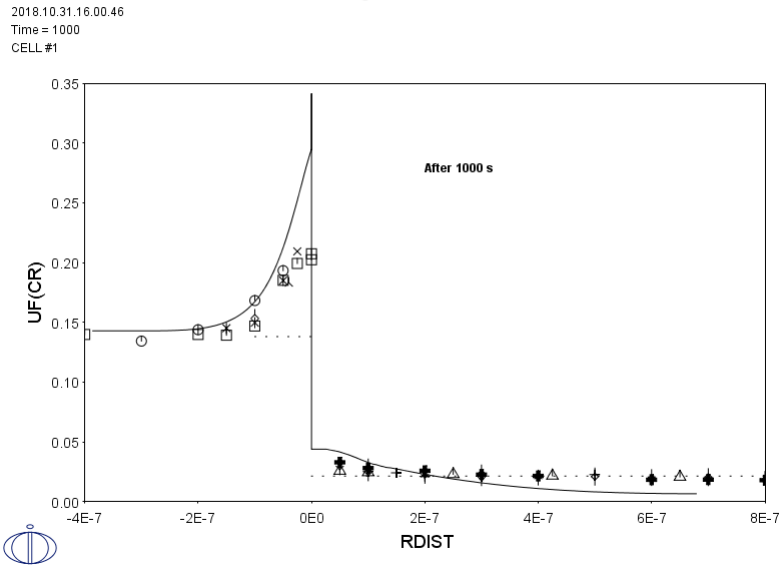
```
POST-1:POST-1:
POST-1:PROLOGUE NUMBER: /0/:DATASET NUMBER(s): /-1/:POST-1:
POST-1:POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```

Figure b2.3



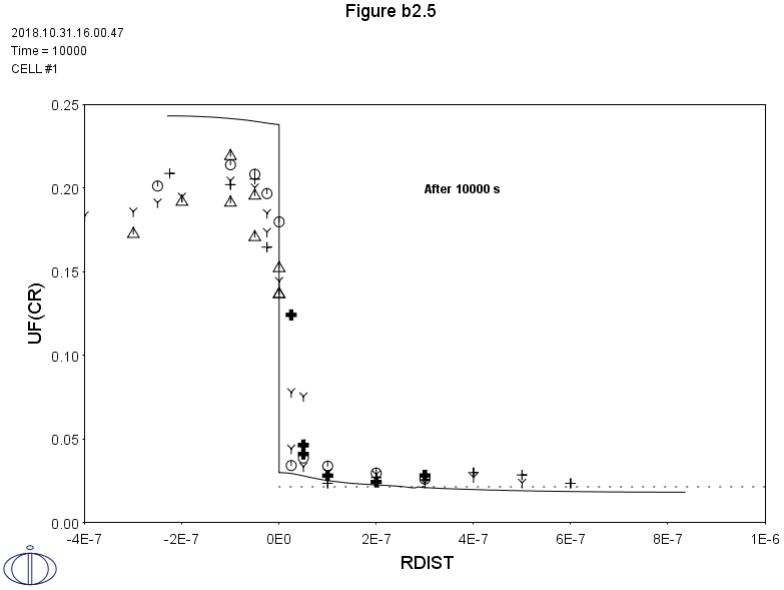

```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1:
POST-1:POST-1:
POST-1:PROLOGUE NUMBER: /0/:DATASET NUMBER(s): /-1/:POST-1:
POST-1:POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```

Figure b2.4



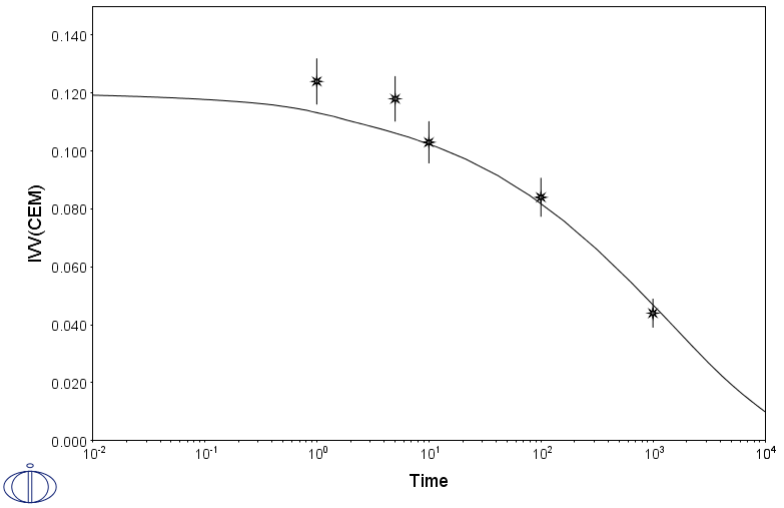

```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1:POST-1:
POST-1:PROLOGUE NUMBER: /0/:DATASET NUMBER(s): /-1/:POST-1:
POST-1:POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```

Figure b2.5




```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:
POST-1:  INFO: Time is set as independent variable
POST-1:POST-1:POST-1:
POST-1:POST-1:
POST-1:PROLOGUE NUMBER: /0/:DATASET NUMBER(s): /-1/:POST-1:
POST-1:POST-1:
POST-1:POST-1:            OST-1:POST-1:
POST-1:
```

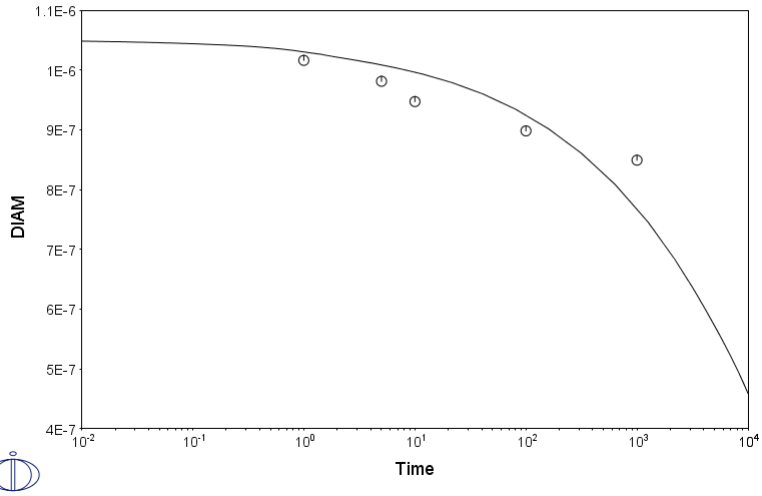
Figure b2.6




```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:
POST-1:POST-1:
POST-1:PROLOGUE NUMBER: /0/:DATASET NUMBER(s): /-1/:POST-1:
POST-1:POST-1:
POST-1:POST-1:            OST-1:POST-1:
POST-1:
```

Figure b2.7

2018.10.31.16.00.49
UPPER INTERFACE OF REGION "CARB#1"
CELL #1

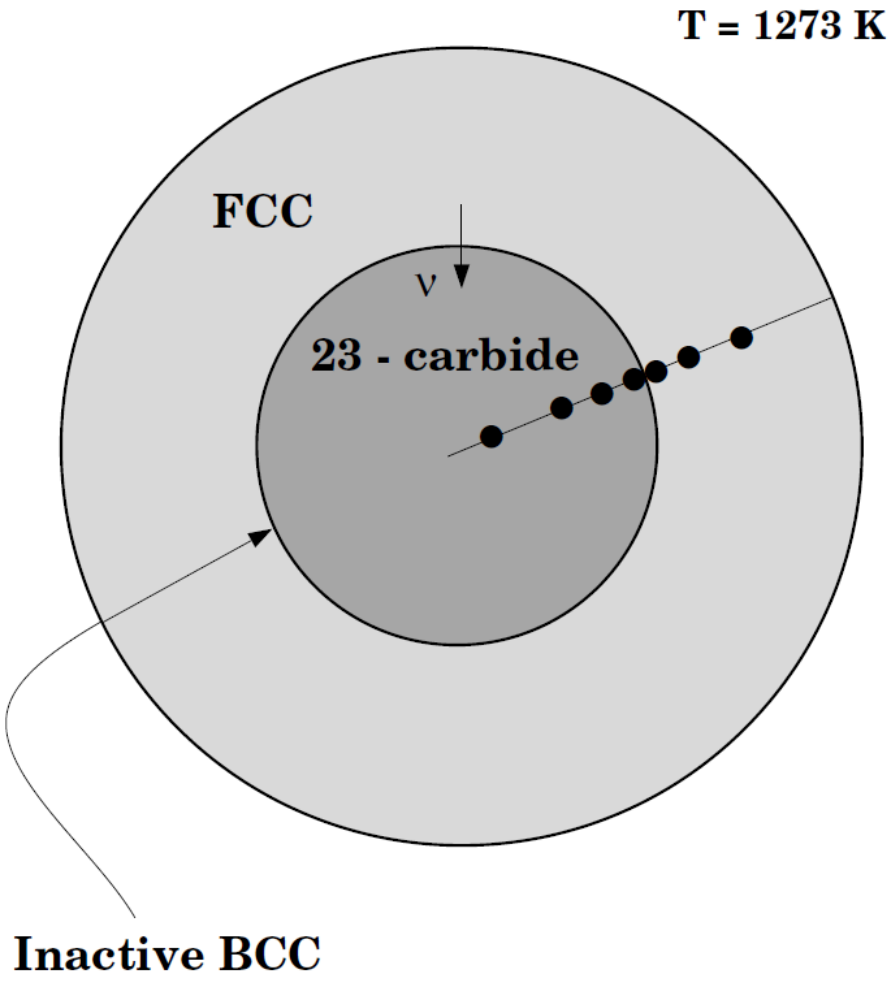



```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: --OK---
POST-1:
```

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

```
About Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Wed Oct 31 13:18:51 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb3\setup.DCM.test"SYS:
SYS:SYS:SYS:SYS:SYS:SYS: NO SUCH COMMAND, USE HELP
SYS:
SYS:SYS:SYS:SYS: 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:TDB_TCFE9:TDB_TCFE9: Current database: Iron Demo Database v2.0

 VA                       /-  DEFINED
TDB_FEDEMO: FE                       C                       CR
   DEFINED
TDB_FEDEMO: 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: FCC_A1                   BCC_A2                  M23C6
   RESTORED
TDB_FEDEMO: 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:TDB_FEDEMO:TDB_FEDEMO: Current database: Fe-Alloys Mobility demo database v2.0

 VA  DEFINED
APP: C                       CR                      FE
   DEFINED
APP: BCC_A2                  FCC_A1  REJECTED
APP: FCC_A1                  BCC_A2  RESTORED
APP: 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:APP:APP: NO TIME STEP DEFINED
 *** ENTERING M23C6 AS A DIFFUSION NONE PHASE
DIC>
DIC>
DIC>DIC>DIC>M[M23,C](T)=DIC>
DIC>M[M23,CR](T)=DIC>
DIC>M[M23,FE](T)=DIC>
DIC>DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>DIC>ATTACH TO REGION NAMED /CARBIDE/:
ATTACHED TO THE RIGHT OF CARBIDE /YES/:
DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>ACTIVE OR INACTIVE PHASE /ACTIVE/:REGION NAME : /CARBIDE/:PHASE TYPE /MATRIX/:PHASE NAM
DIC>ACTIVE OR INACTIVE PHASE /ACTIVE/:ATTACH TO REGION NAMED /MATRIX/:ATTACHED TO THE RIGHT OF MATRIX /YES/:PHASE NAME: /NONE/:DEPENDENT COMPON
05/:
CONDITION TYPE /CLOSED_SYSTEM/:DIC>
DIC>DIC>DIC>DIC>ACTIVE OR INACTIVE PHASE /ACTIVE/:REGION NAME : /CARBIDE/:PHASE TYPE /MATRIX/:PHASE NAME: /NONE/:DIC>
DIC>DIC>DIC>DIC>REGION NAME : /CARBIDE/:PHASE NAME: /M23C6/:DEPENDENT COMPONENT ? /FE/:COMPOSITION TYPE /MOLE_FRACTION/:PROFILE FOR /CR/:DIC>
DIC>
DIC>REGION NAME : /MATRIX/:PHASE NAME: /FCC_A1#1/:DEPENDENT COMPONENT ? /FE/:COMPOSITION TYPE /MOLE_FRACTION/:PROFILE FOR /C/:PROFILE FOR /CR/:
DIC>DIC>DIC>DIC>GEOMETRICAL EXPONENT /0/:DIC>
DIC>DIC>DIC>DIC>END TIME FOR INTEGRATION /.1/:AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /800/:
INITIAL TIMESTEP : /1E-07/:
```

```
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>DIC>DIC>DIC>DIC>
DIC>
DIC>
DIC> --OK---
DIC>
```

exb3-run

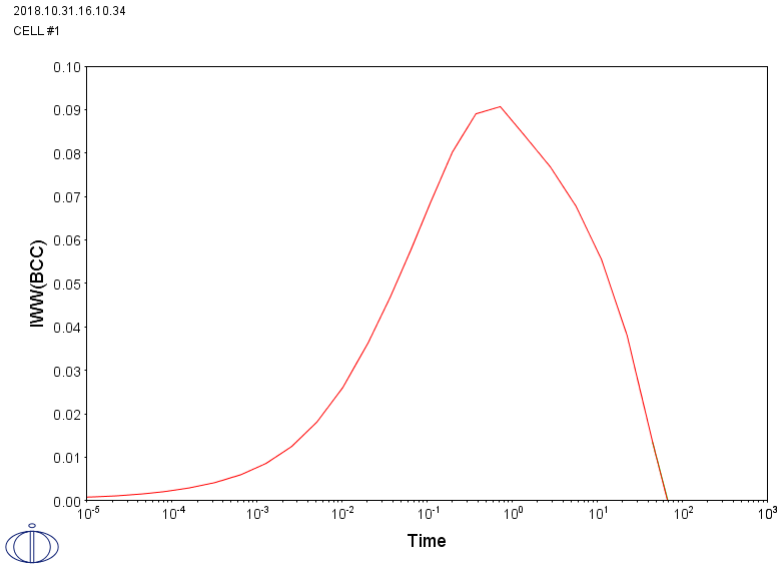
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb3\run.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  0.00000E+00
DIC> OK
DIC>
DIC>DIC>DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> Region: CARBIDE
 single geometric dense at  0.50000E-06
 0.83296       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        6.583132808814412E-007        2.505132181087267E-
010        2.332170771863875E-013        9.583970530938648E-018       TIME =  0.15000000E-05 DT =  0.80000000E-
06 SUM OF SQUARES =  0.95839705E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.15584668E-05 AND  -0.15584668E-05
 POSITION OF INTERFACE CARBIDE / MATRIX IS   0.49982392E-06
 U-FRACTION IN SYSTEM:  C = .0278774083426316  CR = .149918501535994
                        FE = .850081498594513
 TOTAL SIZE OF SYSTEM:  4.93068569406E-18 [m^3]
  CPU time used in timestep                     1 seconds
 6.464716141227625E-006        6.468802061244634E-006        6.464210848329603E-006        5.860745058484127E-008        8.514280777143424E-
012        1.149178417004620E-016

output ignored...



... output resumed

 1.864138773802530E-007        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                     2 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> --OK---
DIC>
```

exb3-plot

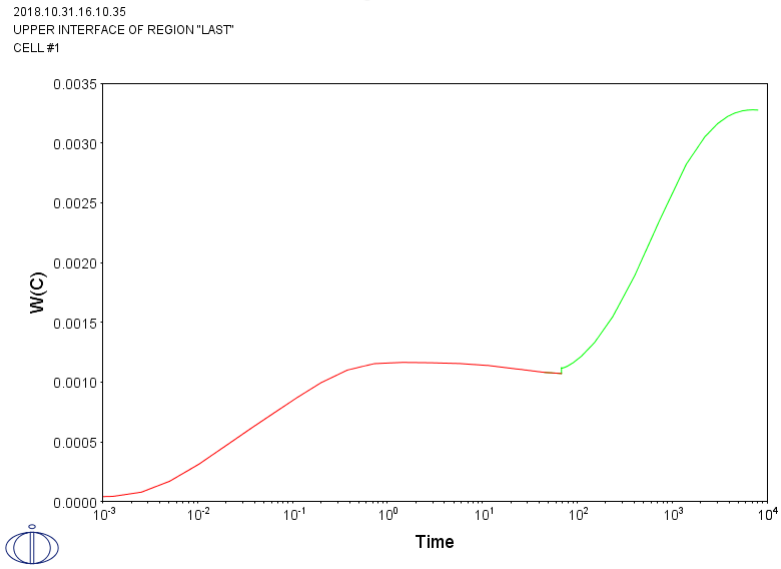
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb3\plot.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  8.00000E+03
DIC> OK
DIC>
DIC>DIC>DIC>DIC>  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:  INFO: Time is set as independent variable
POST-1:POST-1:POST-1:POST-1:
POST-1:POST-1:
POST-1:
POST-1:POST-1: ORKING ...          OST-1:POST-1:
POST-1:
```

Figure b3.1




```
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:
POST-1:POST-1:
POST-1:
POST-1:POST-1: ORKING ...          OST-1:POST-1:
POST-1:
```

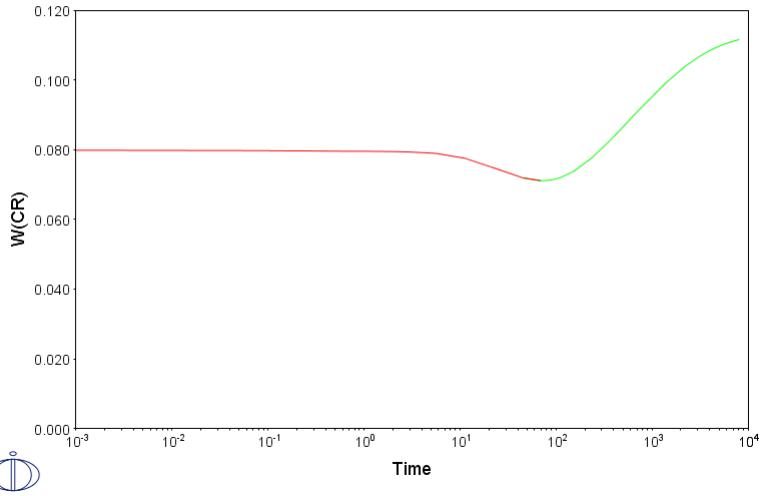
Figure b3.2




```
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1:POST-1:POST-1:
POST-1:POST-1:
POST-1:
POST-1:POST-1: ORKING ...          OST-1:POST-1:
POST-1:
```

Figure b3.3

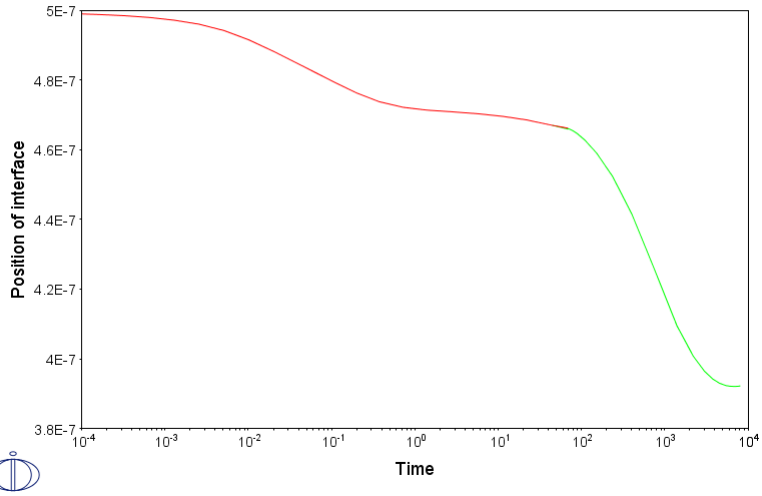
2018.10.31.16.10.36
UPPER INTERFACE OF REGION "LAST"
CELL #1




```
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:
POST-1:POST-1:
POST-1:
POST-1:POST-1: ORKING ...          OST-1:POST-1:
POST-1:
```

Figure b3.4

2018.10.31.16.10.37
UPPER INTERFACE OF REGION "CARBIDE#1"
CELL #1

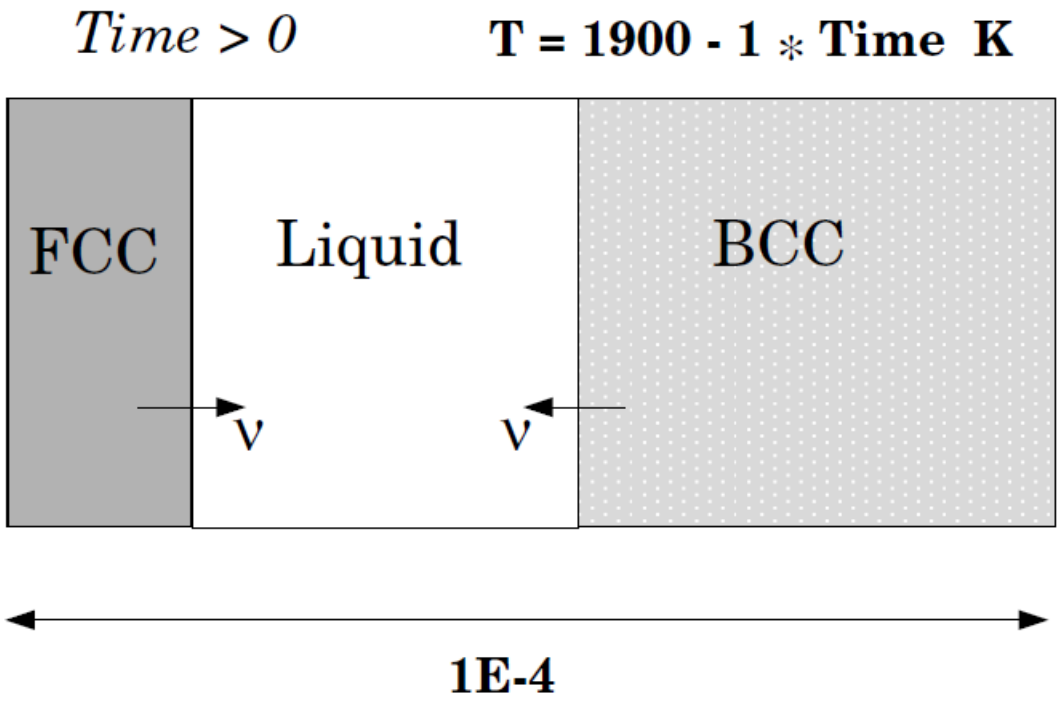



```
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1:
POST-1: --OK---
POST-1:
```

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
SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-
Examples\examples\exb4a\setup.DCM.test"SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: NO SUCH COMMAND, USE HELP
SYS:
SYS:SYS:
SYS:
SYS:SYS:SYS:SYS: 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: Current database: Iron Demo Database v2.0

 VA                      /-  DEFINED
TDB_FEDEMO:
TDB_FEDEMO:TDB_FEDEMO: FE                      NI                      CR
   DEFINED
TDB_FEDEMO:
TDB_FEDEMO:TDB_FEDEMO: LIQUID:L                BCC_A2                  CHI_A12
 FCC_A1                  HCP_A3                  LAVES_PHASE_C14
 SIGMA  REJECTED
TDB_FEDEMO: FCC_A1                  LIQUID:L                BCC_A2
   RESTORED
TDB_FEDEMO:
TDB_FEDEMO:TDB_FEDEMO: 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:TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO: Use one of these databases

 TCFE9   =  Steels/Fe-Alloys  v9.0
 TCFE8   =  Steels/Fe-Alloys  v8.1
 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
 FEDAT   =  TCS/TT Steels Database v1.0
 TCNI9   =  Ni-Alloys  v9.0
 NI25    =  NI25 Database
 TCNI8   =  Ni-Alloys  v8.2
 TCNI7   =  Ni-Alloys  v7.2
 TCNI6   =  Ni-Alloys  v6.1
 TCNI5   =  Ni-Alloys  v5.1
 TCNI4   =  Ni-Alloys  v4.0
 TCNI1   =  Ni-Alloys  v1.3
 TCAL6   =  Al-Alloys  v6.0
 TCAL5   =  Al-Alloys  v5.1
 TCAL4   =  Al-Alloys  v4.0
 TCAL3   =  Al-Alloys  v3.0
 TCAL2   =  Al-Alloys  v2.1
 TCAL1   =  Al-Alloys  v1.2
 TCMG5   =  Mg-Alloys  v5.1
 TCMG4   =  Mg-Alloys  v4.0
 TCMG3   =  Mg-Alloys  v3.0
 TCMG2   =  Mg-Alloys  v2.0
 TCMG1   =  Mg-Alloys  v1.1
 TCTI2   =  Ti-Alloys  v2.0
 TCTI1   =  Ti-Alloys  v1.0
 TCCU2   =  Cu-Alloys  v2.0
 TCCU1   =  Cu-Alloys  v1.0
 TCCC1   =  Cemented carbide  v1.0
 TCHEA3  =  High Entropy Alloy  v3.1
 TCHEA2  =  High Entropy Alloy  v2.1.1
 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
 TCOX9   =  Metal Oxide Solutions  v9.0 SNAPSHOT
 TCOX8   =  Metal Oxide Solutions  v8.0
 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  v2.7
 AQS2    =  TGG Aqueous Solution Database v2.6
 GCE2    =  TGG Geochemical/Environmental TDB v2.3
 FEDEMO  =  Iron Demo Database v2.0
 ALDEMO  =  Aluminum Demo Database v3.0
 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  v1.1
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBNI5  =  Ni-Alloys Mobility  v5.0
 MOBNI4  =  Ni-Alloys Mobility  v4.1
 MOBNI3  =  Ni-Alloys Mobility  v3.2
 MOBNI2  =  Ni-Alloys Mobility  v2.4
 MOBNI1  =  Ni-Alloys Mobility  v1.9
 MOBAL5  =  Al-Alloys Mobility  v5.0
 MOBAL4  =  Al-Alloys Mobility  v4.0
 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
 MOBHEA1 =  High Entropy Alloys Mobility  v1.0
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBSLD1 =  Solder-Alloys Mobility  v1.1
 MOBTI3  =  Ti-Alloys Mobility  v3.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v2.0
 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/: Current database: Steels/Fe-Alloys Mobility  v2.0
   TCS Steel Mobility Database Version 2.0 from 2011-12-09.

 VA  DEFINED
APP: FE                      NI                      CR
   DEFINED
APP: BCC_A2                  FCC_A1                  HCP_A3
 LIQUID:L  REJECTED
APP: FCC_A1                  LIQUID:L                BCC_A2
   RESTORED
APP: 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:APP:APP: NO TIME STEP DEFINED
DIC>
DIC>DIC>DIC>DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>REGION NAME : /SMALTA/:WIDTH OF REGION /1/:TYPE /LINEAR/:DIC>
DIC>
DIC>DIC>DIC>DIC>ACTIVE OR INACTIVE PHASE /ACTIVE/:REGION NAME : /SMALTA/:PHASE TYPE /MATRIX/:PHASE NAME: /NONE/: SETTING CHECK INTERFACE POSITI
DIC>
DIC>DIC>DIC>DIC>ACTIVE OR INACTIVE PHASE /ACTIVE/:ATTACH TO REGION NAMED /SMALTA/:ATTACHED TO THE RIGHT OF SMALTA /YES/:PHASE NAME: /NONE/:DEPE
05/:CONDITION TYPE /CLOSED_SYSTEM/:DIC>
DIC>ACTIVE OR INACTIVE PHASE /ACTIVE/:ATTACH TO REGION NAMED /SMALTA/:ATTACHED TO THE RIGHT OF SMALTA /YES/:PHASE NAME: /NONE/:DEPENDENT COMPON
05/:CONDITION TYPE /CLOSED_SYSTEM/:DIC>
DIC>DIC>DIC>DIC>REGION NAME : /SMALTA/:PHASE NAME: /LIQUID/:DEPENDENT COMPONENT ? /NI/:COMPOSITION TYPE /MOLE_FRACTION/:PROFILE FOR /CR/:PROFII
DIC>DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>END TIME FOR INTEGRATION /.1/:AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /20/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
```

```
DIC>
DIC>
DIC>DIC>DIC>DIC>DIC>DIC>NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /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>DIC>
DIC> --OK---
DIC>
```

exb4a-run

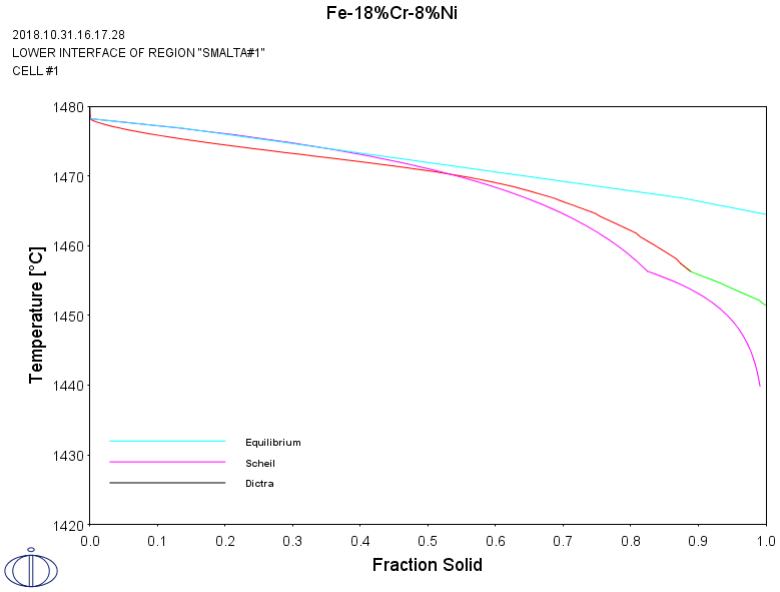
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb4a\run.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  0.00000E+00
DIC> OK
DIC>
DIC>DIC>DIC>DIC> Region: SMALTA
 double geometric
 dense at outer boundaries, coarse at  0.50000E-04
lower 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                     0 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                     1 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
                        NI = .0754116207882223
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   6.7168950     DT =   3.3584507     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .1915203679925  FE = .73306801121928
                        NI = .0754116207882197
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   13.433796     DT =   6.7169013     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992531  FE = .733068011219249
                        NI = .0754116207882203
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds


output ignored...



... output resumed


  CPU time used in timestep                    2 seconds
 5.468115123587098E-006        5.469005501550269E-006        5.464418165980488E-006        1.118094655563800E-009        3.575355512859289E-
013        3.426215582761858E-018       TIME =   178.06458     DT =   1.3107200     SUM OF SQUARES =  0.34262156E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.60685261E-07 AND  -0.60685261E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.64278280E-05
 U-FRACTION IN SYSTEM:  CR = .191499889761281  FE = .733100951194714
                        NI = .0753991590440045
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  2  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_BCC_A2

  CPU time used in timestep                    3 seconds
 1.043465747281716E-005        1.043461274515358E-005        1.042867238912182E-005        4.048704028578276E-007        3.645997347243329E-
011        3.665326621487055E-016        5.983933881146879E-
021       TIME =   180.68602     DT =   2.6214400     SUM OF SQUARES =  0.59839339E-20
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.43975057E-07 AND  -0.43975057E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.63125500E-05
 U-FRACTION IN SYSTEM:  CR = .191499889780548  FE = .733100951157363
                        NI = .0753991590620891
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  4  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_BCC_A2

  CPU time used in timestep                    2 seconds
 7.626170711708917E-006        7.626328577907376E-006        7.622924624592317E-006        1.047164370693728E-006        2.126150541302789E-
007        1.949493136601697E-012        5.084857751782888E-
017       TIME =   185.92890     DT =   5.2428800     SUM OF SQUARES =  0.50848578E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.16890984E-07 AND  -0.16890984E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.62239926E-05
 U-FRACTION IN SYSTEM:  CR = .191499889800969  FE = .733100951098935
                        NI = .0753991591000957
 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
 5.635431637144857E-006        5.635581541707952E-006        5.633975635379762E-006        2.455142061592187E-006        1.706419205906262E-
006        5.146048542485205E-007        4.638558717474289E-011        5.432539087909428E-015        2.050111139807171E-
018       TIME =   196.41466     DT =   10.485760     SUM OF SQUARES =  0.20501111E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.23379229E-07 AND   0.23379229E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.64691416E-05
 U-FRACTION IN SYSTEM:  CR = .191499889799974  FE = .733100951080359
                        NI = .0753991591196668
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  5  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_FCC_A1

  CPU time used in timestep                    3 seconds
 1.293394833256784E-005        1.293415435719968E-005        1.292908871017636E-005        2.670704853657980E-008        6.556916475792094E-
012        3.460497030648602E-018       TIME =   200.00000     DT =   3.5853393     SUM OF SQUARES =  0.34604970E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.18300843E-07 AND   0.18300843E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.65347563E-05
 U-FRACTION IN SYSTEM:  CR = .191499889800809  FE = .733100951073707
                        NI = .0753991591254837
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 MUST SAVE WORKSPACE ON FILE
 WORKSPACE SAVED ON FILE
 RECLAIMING WORKSPACE
 DELETING TIME-RECORD FOR TIME    175.05575
 DELETING TIME-RECORD FOR TIME    175.44315
 DELETING TIME-RECORD FOR TIME    175.44316
 DELETING TIME-RECORD FOR TIME    175.44318
 DELETING TIME-RECORD FOR TIME    175.44322
 DELETING TIME-RECORD FOR TIME    175.44330
 DELETING TIME-RECORD FOR TIME    175.44346
 DELETING TIME-RECORD FOR TIME    175.44378
 DELETING TIME-RECORD FOR TIME    175.44442
 DELETING TIME-RECORD FOR TIME    175.44570
 DELETING TIME-RECORD FOR TIME    175.44826
 DELETING TIME-RECORD FOR TIME    175.45338
 DELETING TIME-RECORD FOR TIME    175.46362
 DELETING TIME-RECORD FOR TIME    175.48410
 DELETING TIME-RECORD FOR TIME    175.52506
 DELETING TIME-RECORD FOR TIME    175.60698
 DELETING TIME-RECORD FOR TIME    175.77082
 DELETING TIME-RECORD FOR TIME    176.09850
 DELETING TIME-RECORD FOR TIME    176.75386
 DELETING TIME-RECORD FOR TIME    178.06458
 DELETING TIME-RECORD FOR TIME    180.68602
 DELETING TIME-RECORD FOR TIME    185.92890

 KEEPING TIME-RECORD FOR TIME    196.41466
 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> --OK---
DIC>
```

exb4a-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb4a\plot.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  2.00000E+02
DIC> OK
DIC>
DIC>DIC>DIC>DIC>  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:AXIS (X, Y OR Z) :AUTOMATIC AXIS TEXT  (Y OR N) /N/:AXIS TEXT :POST-1:
POST-1:POST-1:POST-1:
POST-1:POST-1:
POST-1:POST-1:
POST-1:POST-1: ORKING ...orking ...          OST-1:POST-1:
POST-1:
```

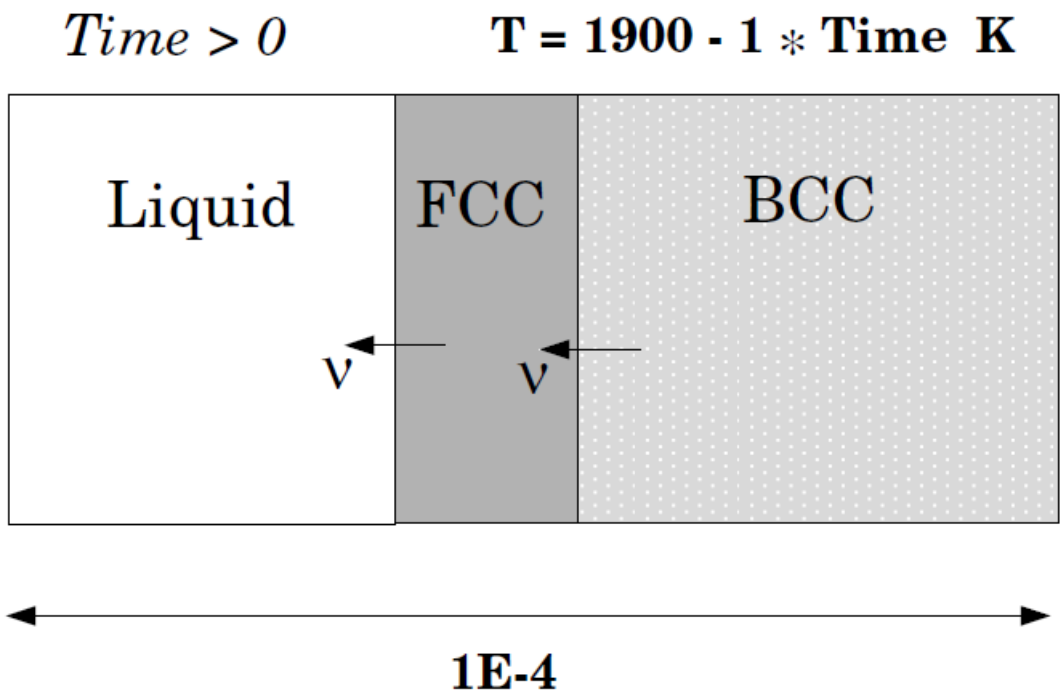



```
POST-1:
POST-1:
POST-1: --OK---
POST-1:
```

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 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Wed Oct 31 13:18:51 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-
Examples\examples\exb4b\setup.DCM.test"SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: NO SUCH COMMAND, USE HELP
SYS:
SYS:SYS:
SYS:
SYS:SYS:SYS:SYS: 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: Current database: Iron Demo Database v2.0

 VA                       /-  DEFINED
TDB_FEDEMO:
TDB_FEDEMO:TDB_FEDEMO: FE                      NI                      CR
   DEFINED
TDB_FEDEMO:
TDB_FEDEMO:TDB_FEDEMO: LIQUID:L                BCC_A2                  CHI_A12
 FCC_A1                   HCP_A3                  LAVES_PHASE_C14
 SIGMA  REJECTED
TDB_FEDEMO: FCC_A1                   LIQUID:L                BCC_A2
   RESTORED
TDB_FEDEMO:
TDB_FEDEMO:TDB_FEDEMO: 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:TDB_FEDEMO:TDB_FEDEMO: Use one of these databases

 TCFE9   =  Steels/Fe-Alloys  v9.0
 TCFE8   =  Steels/Fe-Alloys  v8.1
 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
 FEDAT   =  TCS/TT Steels Database v1.0
 TCNI9   =  Ni-Alloys  v9.0
 NI25    =  NI25 Database
 TCNI8   =  Ni-Alloys  v8.2
 TCNI7   =  Ni-Alloys  v7.2
 TCNI6   =  Ni-Alloys  v6.1
 TCNI5   =  Ni-Alloys  v5.1
 TCNI4   =  Ni-Alloys  v4.0
 TCNI1   =  Ni-Alloys  v1.3
 TCAL6   =  Al-Alloys  v6.0
 TCAL5   =  Al-Alloys  v5.1
 TCAL4   =  Al-Alloys  v4.0
 TCAL3   =  Al-Alloys  v3.0
 TCAL2   =  Al-Alloys  v2.1
 TCAL1   =  Al-Alloys  v1.2
 TCMG5   =  Mg-Alloys  v5.1
 TCMG4   =  Mg-Alloys  v4.0
 TCMG3   =  Mg-Alloys  v3.0
 TCMG2   =  Mg-Alloys  v2.0
 TCMG1   =  Mg-Alloys  v1.1
 TCTI2   =  Ti-Alloys  v2.0
 TCTI1   =  Ti-Alloys  v1.0
 TCCU2   =  Cu-Alloys  v2.0
 TCCU1   =  Cu-Alloys  v1.0
 TCCC1   =  Cemented carbide  v1.0
 TCHEA3  =  High Entropy Alloy  v3.1
 TCHEA2  =  High Entropy Alloy  v2.1.1
 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
 TCOX9   =  Metal Oxide Solutions  v9.0 SNAPSHOT
```

```
 TCOX8   =  Metal Oxide Solutions  v8.0
 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  v2.7
 AQS2    =  TGG Aqueous Solution Database v2.6
 GCE2    =  TGG Geochemical/Environmental TDB v2.3
 FEDEMO  =  Iron Demo Database v2.0
 ALDEMO  =  Aluminum Demo Database v3.0
 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  v1.1
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBNI5  =  Ni-Alloys Mobility  v5.0
 MOBNI4  =  Ni-Alloys Mobility  v4.1
 MOBNI3  =  Ni-Alloys Mobility  v3.2
 MOBNI2  =  Ni-Alloys Mobility  v2.4
 MOBNI1  =  Ni-Alloys Mobility  v1.9
 MOBAL5  =  Al-Alloys Mobility  v5.0
 MOBAL4  =  Al-Alloys Mobility  v4.0
 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
 MOBHEA1 =  High Entropy Alloys Mobility  v1.0
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBSLD1 =  Solder-Alloys Mobility  v1.1
 MOBTI3  =  Ti-Alloys Mobility  v3.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v2.0
 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/: Current database: Steels/Fe-Alloys Mobility  v2.0
   TCS Steel Mobility Database Version 2.0 from 2011-12-09.

 VA  DEFINED
APP: FE                      NI                      CR
   DEFINED
APP: BCC_A2                  FCC_A1                  HCP_A3
 LIQUID:L  REJECTED
APP: FCC_A1                  LIQUID:L                BCC_A2
   RESTORED
APP: 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:APP:APP: NO TIME STEP DEFINED
DIC>
DIC>DIC>DIC>DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>REGION NAME : /SMALTA/:WIDTH OF REGION /1/:TYPE /LINEAR/:DIC>
DIC>DIC>DIC>DIC>ACTIVE OR INACTIVE PHASE /ACTIVE/:REGION NAME : /SMALTA/:PHASE TYPE /MATRIX/:PHASE NAME: /NONE/: SETTING CHECK INTERFACE POSITI
DIC>
DIC>DIC>DIC>DIC>DIC>ACTIVE OR INACTIVE PHASE /ACTIVE/:ATTACH TO REGION NAMED /SMALTA/:ATTACHED TO THE RIGHT OF SMALTA /YES/:PHASE NAME: /NONE/:
05/:CONDITION TYPE /CLOSED_SYSTEM/:DIC>
DIC>ACTIVE OR INACTIVE PHASE /ACTIVE/:ATTACH TO REGION NAMED /SMALTA/:ATTACHED TO THE RIGHT OF SMALTA /YES/:PHASE NAME: /NONE/:DEPENDENT COMPON
05/:CONDITION TYPE /CLOSED_SYSTEM/:DIC>
DIC>DIC>DIC>DIC>REGION NAME : /SMALTA/:PHASE NAME: /LIQUID/:DEPENDENT COMPONENT ? /NI/:COMPOSITION TYPE /MOLE_FRACTION/:PROFILE FOR /CR/:PROFII
DIC>DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>END TIME FOR INTEGRATION /.1/:AUTOMATIC TIMESTEP CONTROL /YES/:
```

```
MAX TIMESTEP DURING INTEGRATION /20/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC>
DIC>DIC>DIC>DIC>DIC>DIC>NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /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>DIC>
DIC> --OK---
DIC>
```

exb4b-run

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb4b\run.DCM.test"DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  0.00000E+00
DIC> OK
DIC>
DIC>DIC>DIC>DIC> 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                    1 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                    0 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
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                        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
 U-FRACTION IN SYSTEM:  CR = .191520367992457  FE = .733068011219 33
                        NI = .075411620788214
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   5.2433960     DT =   2.6216992     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992452  FE = .733068011219344
                        NI = .0754116207882042
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   10.486794     DT =   5.2433984     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992378  FE = .733068011219438
                        NI = .0754116207881837
 TOTAL SIZE OF SYSTEM:  1E-04 [m]


output ignored...



... output resumed

TIME =   195.18556     DT =  0.65536000     SUM OF SQUARES =  0.27364281E-22
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.18539689E-07 AND  -0.18539689E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.94822735E-05
 U-FRACTION IN SYSTEM:  CR = .191136322949957  FE = .733496609558704
                        NI = .07536706749134
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_BCC_A2

  CPU time used in timestep                    3 seconds
 2.214709804724191E-007        2.215385460775575E-007        2.216770446930484E-007        2.115098746301935E-007        2.063345751411102E-
007        1.959186419863887E-007        1.733831856098066E-007        1.337618587931345E-007        1.336968776307525E-
007        6.882066398977718E-008        3.227571389056269E-009        1.153309295754278E-015        5.533414830454556E-
022       TIME =   196.49628     DT =   1.3107200     SUM OF SQUARES =  0.5533414 8E-21
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.60932674E-08 AND  -0.60932674E-08
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.94742869E-05
 U-FRACTION IN SYSTEM:  CR = .19113632294974  FE = .733496609558759
                        NI = .075367067491502
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_BCC_A2

  CPU time used in timestep                    3 seconds
 3.346201637143785E-007        3.346476224503627E-007        3.348322391428186E-007        3.159349557726709E-007        3.116732141995567E-
007        3.029833868982535E-007        2.854702000391888E-007        2.854481549448866E-007        2.523428583148455E-
007        1.918629925908208E-007        9.592570722039587E-008        9.594337528249705E-008        2.820922916010233E-
009        3.642727059548257E-016        9.495938467828619E-
025       TIME =   199.11772     DT =   2.6214400     SUM OF SQUARES =  0.94959385E-24
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.87055626E-08 AND   0.87055626E-08
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.94971080E-05
 U-FRACTION IN SYSTEM:  CR = .191136322957218  FE = .733496609557616
                        NI = .0753670674851663
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  27  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_FCC_A1

  CPU time used in timestep                    4 seconds
 9.465534019464837E-008        9.466872627447208E-008        9.512372799572881E-008        1.092918050164280E-009        9.467381643386949E-
010        6.854481393231618E-010        2.893324127957521E-010        1.625513485421880E-015        6.629915534430253E-
022       TIME =   200.00000     DT =  0.88228302     SUM OF SQUARES =  0.66299155E-21
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.36067991E-08 AND   0.36067991E-08
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.95002902E-05
 U-FRACTION IN SYSTEM:  CR = .191136322959274  FE = .733496609558258
                        NI = .075367067482468
 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>
```
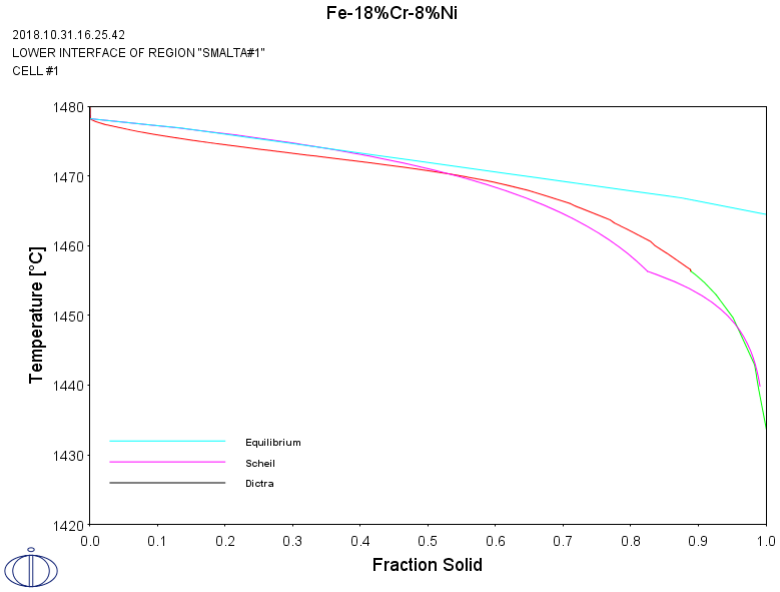

```
DIC>DIC>DIC>DIC>
DIC> --OK---
DIC>
```

exb4b-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb4b\plot.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  2.00000E+02
DIC> OK
DIC>
DIC>DIC>DIC>DIC>  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:
POST-1:POST-1:POST-1:
POST-1:POST-1:
POST-1:POST-1:
POST-1:POST-1: ORKING ...orking ...          OST-1:POST-1:
POST-1:
```

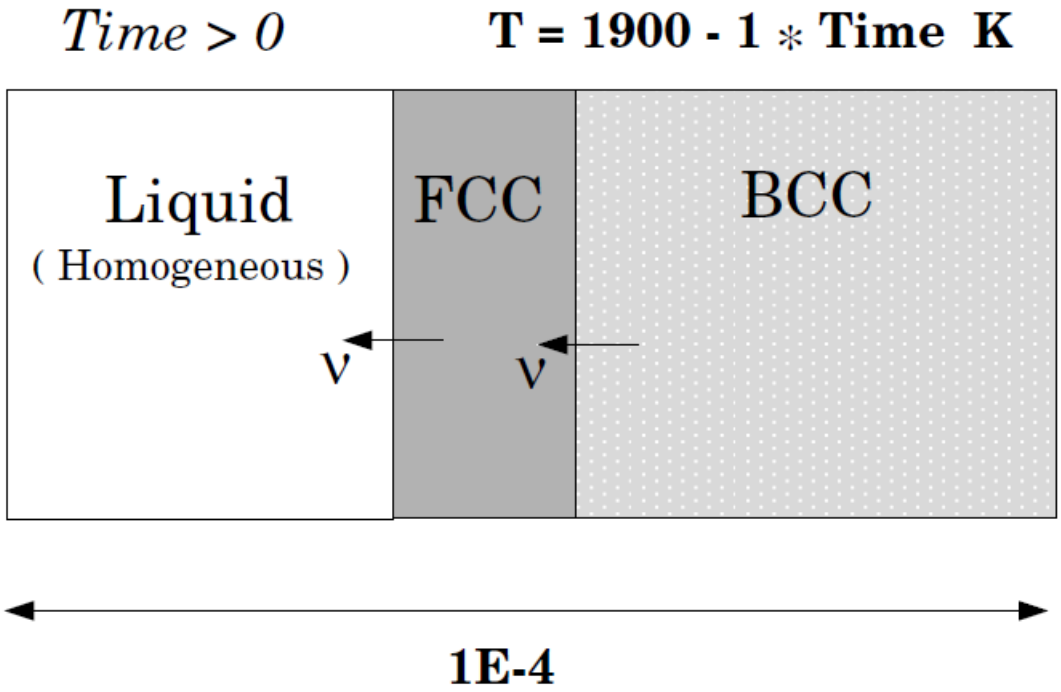



```
POST-1:
POST-1:
POST-1:
POST-1: --OK---
POST-1:
```

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 Linked: Wed Oct 31 13:18:51 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-
Examples\examples\exb4c\setup.DCM.test"SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: NO SUCH COMMAND, USE HELP
SYS:
SYS:SYS:
SYS:SYS:SYS:SYS: 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: Current database: Iron Demo Database v2.0

 VA                       /-  DEFINED
TDB_FEDEMO:
TDB_FEDEMO:TDB_FEDEMO: FE                       NI                      CR
   DEFINED
TDB_FEDEMO:
TDB_FEDEMO:TDB_FEDEMO: LIQUID:L                 BCC_A2                  CHI_A12
 FCC_A1                   HCP_A3                  LAVES_PHASE_C14
 SIGMA  REJECTED
TDB_FEDEMO: FCC_A1                   LIQUID:L                BCC_A2
   RESTORED
TDB_FEDEMO:
TDB_FEDEMO:TDB_FEDEMO: 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:TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO: Use one of these databases

 TCFE9   =  Steels/Fe-Alloys  v9.0
 TCFE8   =  Steels/Fe-Alloys  v8.1
 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
 FEDAT   =  TCS/TT Steels Database v1.0
 TCNI9   =  Ni-Alloys  v9.0
 NI25    =  NI25 Database
 TCNI8   =  Ni-Alloys  v8.2
 TCNI7   =  Ni-Alloys  v7.2
 TCNI6   =  Ni-Alloys  v6.1
 TCNI5   =  Ni-Alloys  v5.1
 TCNI4   =  Ni-Alloys  v4.0
 TCNI1   =  Ni-Alloys  v1.3
 TCAL6   =  Al-Alloys  v6.0
 TCAL5   =  Al-Alloys  v5.1
 TCAL4   =  Al-Alloys  v4.0
 TCAL3   =  Al-Alloys  v3.0
 TCAL2   =  Al-Alloys  v2.1
 TCAL1   =  Al-Alloys  v1.2
 TCMG5   =  Mg-Alloys  v5.1
 TCMG4   =  Mg-Alloys  v4.0
 TCMG3   =  Mg-Alloys  v3.0
 TCMG2   =  Mg-Alloys  v2.0
 TCMG1   =  Mg-Alloys  v1.1
 TCTI2   =  Ti-Alloys  v2.0
 TCTI1   =  Ti-Alloys  v1.0
 TCCU2   =  Cu-Alloys  v2.0
 TCCU1   =  Cu-Alloys  v1.0
 TCCC1   =  Cemented carbide  v1.0
 TCHEA3  =  High Entropy Alloy  v3.1
 TCHEA2  =  High Entropy Alloy  v2.1.1
 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
 TCOX9   =  Metal Oxide Solutions  v9.0 SNAPSHOT
 TCOX8   =  Metal Oxide Solutions  v8.0
 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  v2.7
 AQS2    =  TGG Aqueous Solution Database v2.6
 GCE2    =  TGG Geochemical/Environmental TDB v2.3
 FEDEMO  =  Iron Demo Database v2.0
 ALDEMO  =  Aluminum Demo Database v3.0
 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  v1.1
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBNI5  =  Ni-Alloys Mobility  v5.0
 MOBNI4  =  Ni-Alloys Mobility  v4.1
 MOBNI3  =  Ni-Alloys Mobility  v3.2
 MOBNI2  =  Ni-Alloys Mobility  v2.4
 MOBNI1  =  Ni-Alloys Mobility  v1.9
 MOBAL5  =  Al-Alloys Mobility  v5.0
 MOBAL4  =  Al-Alloys Mobility  v4.0
 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
 MOBHEA1 =  High Entropy Alloys Mobility  v1.0
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBSLD1 =  Solder-Alloys Mobility  v1.1
 MOBTI3  =  Ti-Alloys Mobility  v3.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v2.0
 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/: Current database: Steels/Fe-Alloys Mobility  v2.0
   TCS Steel Mobility Database Version 2.0 from 2011-12-09.

 VA  DEFINED
APP: FE                      NI                      CR
   DEFINED
APP: BCC_A2                  FCC_A1                  HCP_A3
 LIQUID:L  REJECTED
APP: FCC_A1                  LIQUID:L                BCC_A2
   RESTORED
APP: 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:APP:APP: NO TIME STEP DEFINED
DIC>
DIC>DIC>DIC>DIC> Sorry, LIST-DATA disabled for this database
DIC>
DIC>
DIC> NO SUCH COMMAND, USE HELP
DIC>
DIC>
DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>PARAMETER:
 *** ERROR, PLEASE RE-ENTER EACH PART SEPARATELY
IDENTIFIER:PHASE NAME:CONSTITUENT:INTERACTING CONSTITUENT:
  DQ(LIQUID&CR#1,CR;0) =  Sorry, database encrypted
DO YOU WANT TO CHANGE THE NUMBER OF RANGES /NO/: I AM SORRY BUT YOU MUST THEN REENTER ALL RANGES
 DQ(LIQUID&CR#1,CR;0) =
LOW TEMPERATURE LIMIT /298.15/:FUNCTION:HIGH TEMPERATURE LIMIT /6000/:ANY MORE RANGES /N/:DIC>
DIC>PARAMETER:  DQ(LIQUID&CR#1,FE;0) =  Sorry, database encrypted
DO YOU WANT TO CHANGE THE NUMBER OF RANGES /NO/: I AM SORRY BUT YOU MUST THEN REENTER ALL RANGES
```

```
 DQ(LIQUID&CR#1,FE;0) =
LOW TEMPERATURE LIMIT /298.15/:DIC>
DIC>  DQ(LIQUID&CR#1,NI;0) =  Sorry, database encrypted
DO YOU WANT TO CHANGE THE NUMBER OF RANGES /NO/: I AM SORRY BUT YOU MUST THEN REENTER ALL RANGES
 DQ(LIQUID&CR#1,NI;0) =
LOW TEMPERATURE LIMIT /298.15/:DIC>
DIC>  DQ(LIQUID&NI#1,CR;0) =  Sorry, database encrypted
DO YOU WANT TO CHANGE THE NUMBER OF RANGES /NO/: I AM SORRY BUT YOU MUST THEN REENTER ALL RANGES
 DQ(LIQUID&NI#1,CR;0) =
LOW TEMPERATURE LIMIT /298.15/:DIC>
DIC>  DQ(LIQUID&NI#1,FE;0) =  Sorry, database encrypted
DO YOU WANT TO CHANGE THE NUMBER OF RANGES /NO/: I AM SORRY BUT YOU MUST THEN REENTER ALL RANGES
 DQ(LIQUID&NI#1,FE;0) =
LOW TEMPERATURE LIMIT /298.15/:DIC>
DIC>  DQ(LIQUID&NI#1,NI;0) =  Sorry, database encrypted
DO YOU WANT TO CHANGE THE NUMBER OF RANGES /NO/: I AM SORRY BUT YOU MUST THEN REENTER ALL RANGES
 DQ(LIQUID&NI#1,NI;0) =
LOW TEMPERATURE LIMIT /298.15/:DIC>
DIC>  DQ(LIQUID&FE#1,CR;0) =  Sorry, database encrypted
DO YOU WANT TO CHANGE THE NUMBER OF RANGES /NO/: I AM SORRY BUT YOU MUST THEN REENTER ALL RANGES
 DQ(LIQUID&FE#1,CR;0) =
LOW TEMPERATURE LIMIT /298.15/:DIC>
DIC>  DQ(LIQUID&FE#1,FE;0) =  Sorry, database encrypted
DO YOU WANT TO CHANGE THE NUMBER OF RANGES /NO/: I AM SORRY BUT YOU MUST THEN REENTER ALL RANGES
 DQ(LIQUID&FE#1,FE;0) =
LOW TEMPERATURE LIMIT /298.15/:DIC>
DIC>  DQ(LIQUID&FE#1,NI;0) =  Sorry, database encrypted
DO YOU WANT TO CHANGE THE NUMBER OF RANGES /NO/: I AM SORRY BUT YOU MUST THEN REENTER ALL RANGES
 DQ(LIQUID&FE#1,NI;0) =
LOW TEMPERATURE LIMIT /298.15/:DIC>
DIC> AMBIGUOUS COMMAND, USE HELP
DIC>
DIC>
DIC> NO SUCH COMMAND, USE HELP
DIC>
DIC>
DIC>DIC>DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>REGION NAME : /SMALTA/:WIDTH OF REGION /1/:TYPE /LINEAR/:DIC>
DIC>DIC>DIC>DIC>ACTIVE OR INACTIVE PHASE /ACTIVE/:REGION NAME : /SMALTA/:PHASE TYPE /MATRIX/:PHASE NAME: /NONE/: SETTING CHECK INTERFACE POSITI
DIC>
DIC>DIC>DIC>DIC>DIC>ACTIVE OR INACTIVE PHASE /ACTIVE/:ATTACH TO REGION NAMED /SMALTA/:ATTACHED TO THE RIGHT OF SMALTA /YES/:PHASE NAME: /NONE/:
05/:CONDITION TYPE /CLOSED_SYSTEM/:DIC>
DIC>ACTIVE OR INACTIVE PHASE /ACTIVE/:ATTACH TO REGION NAMED /SMALTA/:ATTACHED TO THE RIGHT OF SMALTA /YES/:PHASE NAME: /NONE/:DEPENDENT COMPON
05/:CONDITION TYPE /CLOSED_SYSTEM/:DIC>
DIC>DIC>DIC>DIC>REGION NAME : /SMALTA/:PHASE NAME: /LIQUID/:DEPENDENT COMPONENT ? /NI/:COMPOSITION TYPE /MOLE_FRACTION/:PROFILE FOR /CR/:PROFII
DIC>DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>END TIME FOR INTEGRATION /.1/:AUTOMATIC TIMESTEP CONTROL /YES/:MAX TIMESTEP DURING INTEGRATION /20/:INITIAL TIMESTEP : /1E-
07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC>
DIC>
DIC>DIC>DIC>DIC>DIC>DIC>NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /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>DIC>
DIC> --OK---
DIC>
```

exb4c-run

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb4c\run.DCM.test"DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  0.00000E+00
DIC> OK
DIC>
DIC>DIC>DIC>DIC> 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                    1 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                    0 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]
  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
 U-FRACTION IN SYSTEM:  CR = .191520367993669  FE = .73306801121774
                        NI = .0754116207885905
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   2.0354184     DT =   1.0000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367995404  FE = .733068011215607
                        NI = .0754116207889895
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3.0354184     DT =   1.0000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367995681  FE = .733068011215
                        NI = .0754116207893191
 TOTAL SIZE OF SYSTEM:  1E-04 [m]


output ignored...



... output resumed

 1.720447645279585E-008        3.281288691361440E-009        6.971204257909571E-010        9.073690669303089E-011        7.873013728938335E-
016        1.985062366049126E-015        5.100018024183625E-014        1.255144131234050E-015        3.961787178348030E-
013        3.006043188658671E-016       TIME =   199.16151     DT =   1.0000000     SUM OF SQUARES =  0.30060432E-15
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.10033714E-06 AND  -0.10033714E-06
 POSITION OF INTERFACE SMALTA / R_FCC_A1 IS   0.46443259E-06
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.11516764E-07 AND   0.11516764E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.10970287E-04
 U-FRACTION IN SYSTEM:  CR = .191211085409268  FE = .733433262435344
                        NI = .0753556521553883
 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
 3.778400875658234E-007        3.784034986282486E-007        3.778357911569217E-007        3.777675929933972E-007        3.777268472362450E-
007        1.901293166793868E-008        6.349571562977370E-010        5.177766307993643E-013        3.465722682361440E-
016       TIME =   200.00000     DT =  0.83849346     SUM OF SQUARES =  0.34657227E-15
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.85428166E-07 AND  -0.85428166E-07
 POSITION OF INTERFACE SMALTA / R_FCC_A1 IS   0.39280163E-06
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.13581453E-07 AND   0.13581453E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.10981675E-04
 U-FRACTION IN SYSTEM:  CR = .191211077634819  FE = .733433269964699
                        NI = .0753556524004815
 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
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 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
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 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
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 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>
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DIC>
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DIC>
DIC>
DIC>DIC>DIC>DIC>
DIC> --OK---
DIC>
```
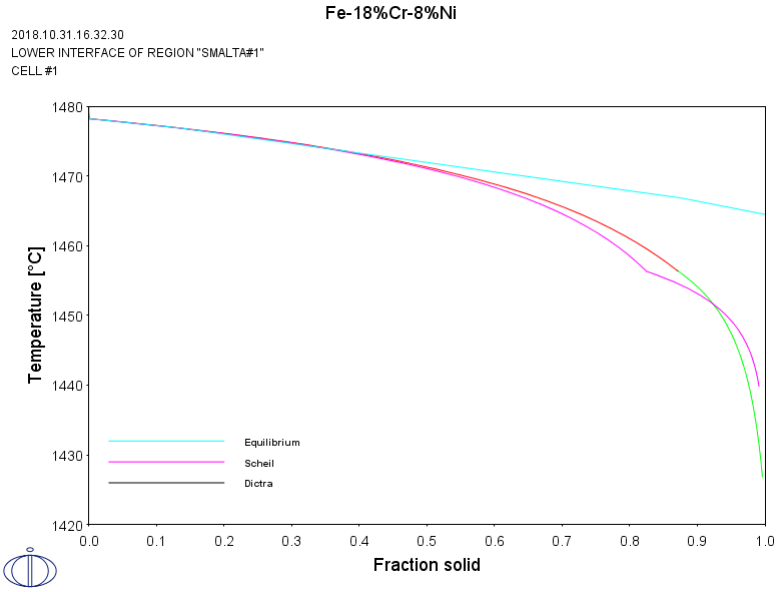

exb4c-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb4c\plot.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  2.00000E+02
DIC> OK
DIC>
DIC>DIC>DIC>DIC>  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:
POST-1:POST-1:POST-1:
POST-1:POST-1:
POST-1:POST-1:
POST-1:POST-1: ORKING ...          OST-1:POST-1:
POST-1:
```

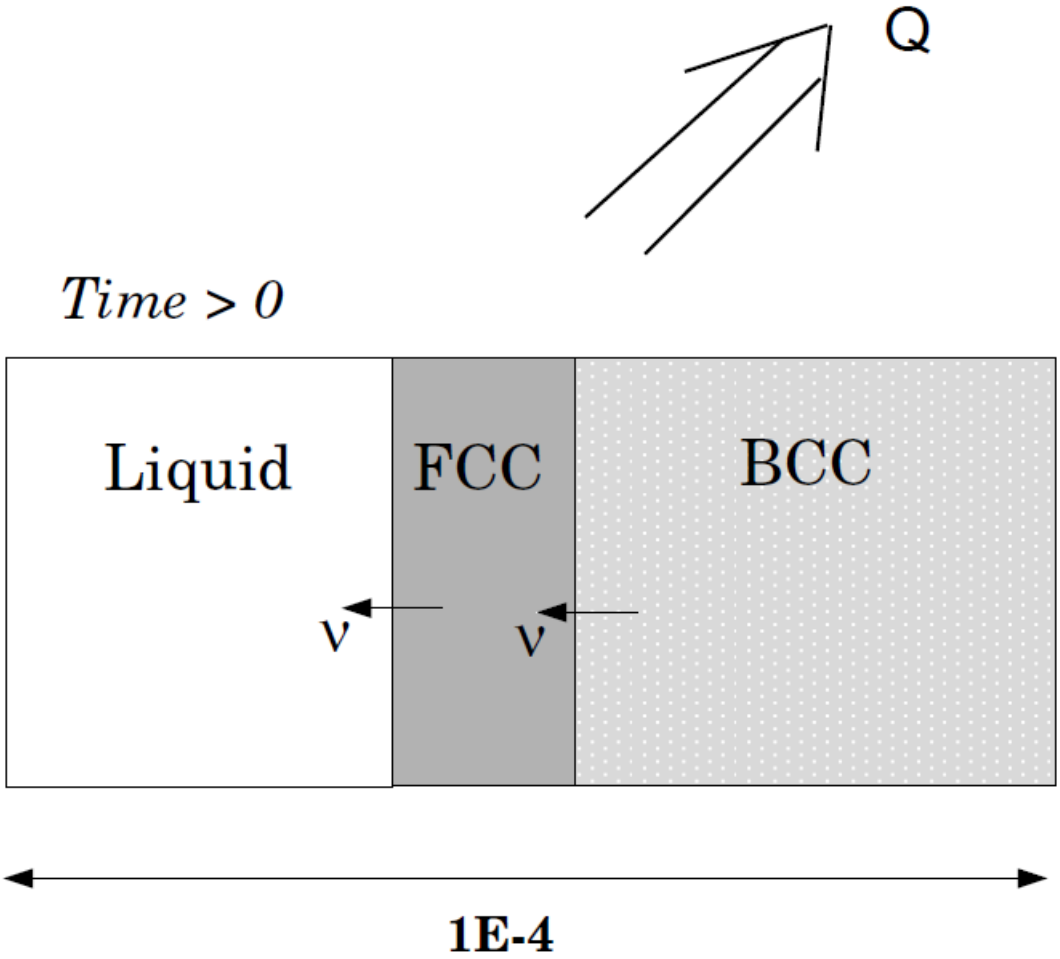



```
POST-1:
POST-1:
POST-1:
POST-1: --OK---
POST-1:
```

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 Linked: Wed Oct 31 13:18:51 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-
Examples\examples\exb4d\setup.DCM.test"SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: NO SUCH COMMAND, USE HELP
SYS:
SYS:SYS:
SYS:SYS:SYS:SYS: 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: Current database: Iron Demo Database v2.0

 VA                       /-  DEFINED
TDB_FEDEMO:
TDB_FEDEMO:TDB_FEDEMO: FE                       NI                       CR
   DEFINED
TDB_FEDEMO:
TDB_FEDEMO:TDB_FEDEMO: LIQUID:L                 BCC_A2                   CHI_A12
 FCC_A1                   HCP_A3                  LAVES_PHASE_C14
 SIGMA  REJECTED
TDB_FEDEMO: FCC_A1                   LIQUID:L                 BCC_A2
   RESTORED
TDB_FEDEMO:
TDB_FEDEMO:TDB_FEDEMO: 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:TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO: Use one of these databases

 TCFE9   =  Steels/Fe-Alloys  v9.0
 TCFE8   =  Steels/Fe-Alloys  v8.1
 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
 FEDAT   =  TCS/TT Steels Database v1.0
 TCNI9   =  Ni-Alloys  v9.0
 NI25    =  NI25 Database
 TCNI8   =  Ni-Alloys  v8.2
 TCNI7   =  Ni-Alloys  v7.2
 TCNI6   =  Ni-Alloys  v6.1
 TCNI5   =  Ni-Alloys  v5.1
 TCNI4   =  Ni-Alloys  v4.0
 TCNI1   =  Ni-Alloys  v1.3
 TCAL6   =  Al-Alloys  v6.0
 TCAL5   =  Al-Alloys  v5.1
 TCAL4   =  Al-Alloys  v4.0
 TCAL3   =  Al-Alloys  v3.0
 TCAL2   =  Al-Alloys  v2.1
 TCAL1   =  Al-Alloys  v1.2
 TCMG5   =  Mg-Alloys  v5.1
 TCMG4   =  Mg-Alloys  v4.0
 TCMG3   =  Mg-Alloys  v3.0
 TCMG2   =  Mg-Alloys  v2.0
 TCMG1   =  Mg-Alloys  v1.1
 TCTI2   =  Ti-Alloys  v2.0
 TCTI1   =  Ti-Alloys  v1.0
 TCCU2   =  Cu-Alloys  v2.0
 TCCU1   =  Cu-Alloys  v1.0
 TCCC1   =  Cemented carbide  v1.0
 TCHEA3  =  High Entropy Alloy  v3.1
 TCHEA2  =  High Entropy Alloy  v2.1.1
 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
 TCOX9   =  Metal Oxide Solutions  v9.0 SNAPSHOT
 TCOX8   =  Metal Oxide Solutions  v8.0
 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  v2.7
 AQS2    =  TGG Aqueous Solution Database v2.6
 GCE2    =  TGG Geochemical/Environmental TDB v2.3
 FEDEMO  =  Iron Demo Database v2.0
 ALDEMO  =  Aluminum Demo Database v3.0
 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  v1.1
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBNI5  =  Ni-Alloys Mobility  v5.0
 MOBNI4  =  Ni-Alloys Mobility  v4.1
 MOBNI3  =  Ni-Alloys Mobility  v3.2
 MOBNI2  =  Ni-Alloys Mobility  v2.4
 MOBNI1  =  Ni-Alloys Mobility  v1.9
 MOBAL5  =  Al-Alloys Mobility  v5.0
 MOBAL4  =  Al-Alloys Mobility  v4.0
 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
 MOBHEA1 =  High Entropy Alloys Mobility  v1.0
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBSLD1 =  Solder-Alloys Mobility  v1.1
 MOBTI3  =  Ti-Alloys Mobility  v3.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v2.0
 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/: Current database: Steels/Fe-Alloys Mobility  v2.0
   TCS Steel Mobility Database Version 2.0 from 2011-12-09.

 VA  DEFINED
APP: FE                      NI                      CR
   DEFINED
APP: BCC_A2                  FCC_A1                  HCP_A3
 LIQUID:L  REJECTED
APP: FCC_A1                  LIQUID:L                BCC_A2
   RESTORED
APP: 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:APP:APP: NO TIME STEP DEFINED
DIC>
DIC>DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>REGION NAME : /SMALTA/:WIDTH OF REGION /1/:TYPE /LINEAR/:DIC>
DIC>
DIC>DIC>DIC>DIC>ACTIVE OR INACTIVE PHASE /ACTIVE/:REGION NAME : /SMALTA/:PHASE TYPE /MATRIX/:PHASE NAME: /NONE/: SETTING CHECK INTERFACE POSITI
DIC>
DIC>DIC>DIC>DIC>DIC>ACTIVE OR INACTIVE PHASE /ACTIVE/:ATTACH TO REGION NAMED /SMALTA/:ATTACHED TO THE RIGHT OF SMALTA /YES/:PHASE NAME: /NONE/:
05/:CONDITION TYPE /CLOSED_SYSTEM/:DIC>
DIC>ACTIVE OR INACTIVE PHASE /ACTIVE/:ATTACH TO REGION NAMED /SMALTA/:ATTACHED TO THE RIGHT OF SMALTA /YES/:PHASE NAME: /NONE/:DEPENDENT COMPON
05/:CONDITION TYPE /CLOSED_SYSTEM/:DIC>
DIC>DIC>DIC>DIC>REGION NAME : /SMALTA/:PHASE NAME: /LIQUID/:DEPENDENT COMPONENT ? /NI/:COMPOSITION TYPE /MOLE_FRACTION/:PROFILE FOR /CR/:PROFII
DIC>DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>END TIME FOR INTEGRATION /.1/:AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /20/:
```

```
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC>
DIC>DIC>DIC>DIC>DIC>DIC>NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /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>DIC>
DIC> --OK---
DIC>
```

exb4d-run

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb4d\run.DCM.test"DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  0.00000E+00
DIC> OK
DIC>
DIC>DIC>DIC>DIC> 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                     1 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]
  CPU time used in timestep                     0 seconds
 6.085252910287480E-016        6.085252910287480E-016


     ERROR RETURN FROM NS01A BECAUSE A NEARBY STATIONARY POINT OF F(X) IS PREDICTED
 *** ERROR  1890 IN DCNS01: ERROR RETURN FROM NS01A
 6.085252910287480E-016        6.085252910287480E-016        6.085252910287480E-016        5.964155496588791E-012        6.085252910287480E-
016        7.556154069705013E-030        7.556154069705013E-030

output ignored...



... output resumed

 9.569144227234911E-017       TIME =   196.14562     DT =  0.33125000     SUM OF SQUARES =  0.95691442E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.67814979E-07 AND   0.67814979E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.53249251E-05
 TEMPERATURE:   1705.     ENTHALPY:  0.5597E+05
 U-FRACTION IN SYSTEM:  CR = .191421755402109  FE = .733187230135573
                        NI = .0753910144623178
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  8  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_FCC_A1

  CPU time used in timestep                     2 seconds
 2.844297053429026E-007        2.844299007588514E-007        2.844314872340127E-007        2.843725427290093E-007        4.091194466572615E-
009        1.266727083939472E-013        3.667458590054622E-
018       TIME =   196.80812     DT =  0.66250000     SUM OF SQUARES =  0.36674586E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.78154707E-07 AND   0.78154707E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.53767026E-05
 TEMPERATURE:   1703.     ENTHALPY:  0.5591E+05
 U-FRACTION IN SYSTEM:  CR = .191421755402118  FE = .733187230135566
                        NI = .0753910144623167
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  14  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_FCC_A1

  CPU time used in timestep                     1 seconds
 1.453047349768847E-006        1.453355027951001E-006        1.453304649612434E-006        1.452688436066125E-006        1.218715538639341E-
006        9.186360159089239E-007        5.848438219163468E-007        1.479303557692824E-007        8.990075078644068E-
012        2.448019339017669E-017       TIME =   198.13312     DT =   1.3250000     SUM OF SQUARES =  0.24480193E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.92557781E-07 AND   0.92557781E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.54993417E-05
 TEMPERATURE:   1700.     ENTHALPY:  0.5579E+05
 U-FRACTION IN SYSTEM:  CR = .191421755402141  FE = .733187230135558
                        NI = .0753910144623005
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  31  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_FCC_A1
```

```
  CPU time used in timestep                    2 seconds
 8.999406293435221E-007        8.999814837215278E-007        9.005659120744874E-007        8.995081212266609E-007        6.560707228970533E-
007        5.077534819765668E-007        2.056079421345099E-007        1.655906050325116E-011        2.930307509340963E-
016       TIME =   200.00000     DT =   1.8668831     SUM OF SQUARES =  0.29303075E-15
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.10625825E-06 AND   0.10625825E-06
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.56977134E-05
 TEMPERATURE:   1696.     ENTHALPY:  0.5562E+05
 U-FRACTION IN SYSTEM:  CR = .191421755402219  FE = .733187230135511
                        NI = .0753910144622697
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 MUST SAVE WORKSPACE ON FILE
 WORKSPACE SAVED ON FILE
 RECLAIMING WORKSPACE
 DELETING TIME-RECORD FOR TIME    194.73780
 DELETING TIME-RECORD FOR TIME    195.56593
 DELETING TIME-RECORD FOR TIME    195.64874
 DELETING TIME-RECORD FOR TIME    195.81437
 DELETING TIME-RECORD FOR TIME    196.14562
 DELETING TIME-RECORD FOR TIME    196.80812

 KEEPING TIME-RECORD FOR TIME    198.13312
 AND FOR TIME                    200.00000
 WORKSPACE RECLAIMED

 TIMESTEP AT     200.000000     SELECTED

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DIC>DIC>DIC>DIC>
DIC> --OK---
DIC>
```
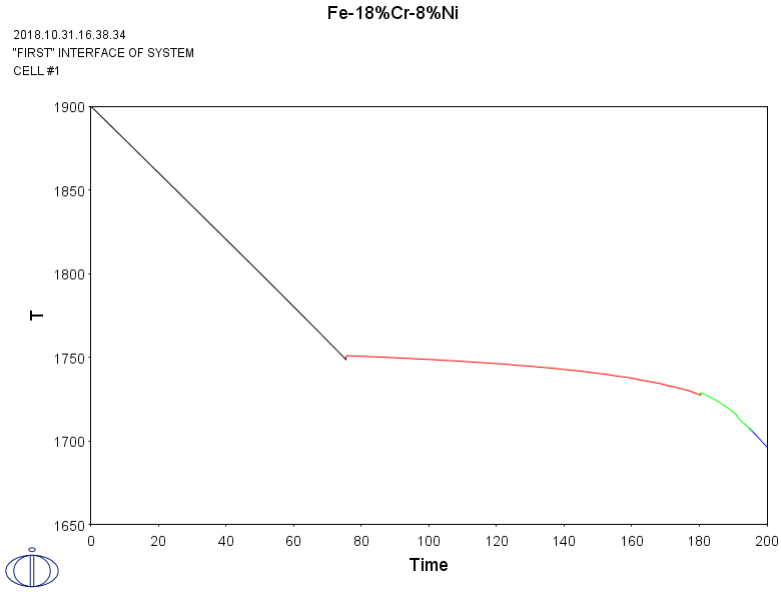
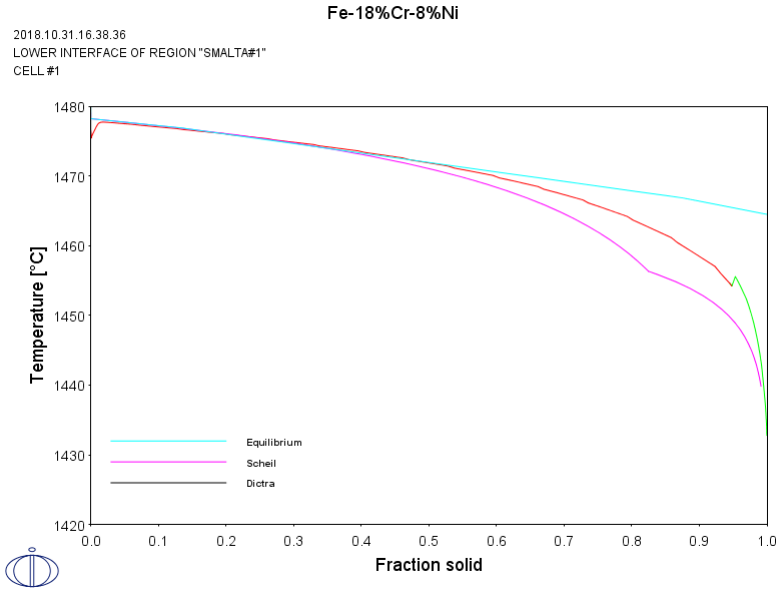

exb4d-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb4d\plot.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  2.00000E+02
DIC> OK
DIC>
DIC>DIC>DIC>DIC>  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:  INFO: Time is set as independent variable
POST-1:POST-1:POST-1:
POST-1:POST-1: ORKING ...orking ...          OST-1:POST-1:
POST-1:
```




```
POST-1:
POST-1:Hit RETURN to continue
POST-1:POST-1:POST-1:POST-1:POST-1:
POST-1:POST-1:POST-1:
POST-1:POST-1:
POST-1:POST-1:
POST-1:POST-1: ORKING ...orking ...          OST-1:POST-1:
POST-1:
```

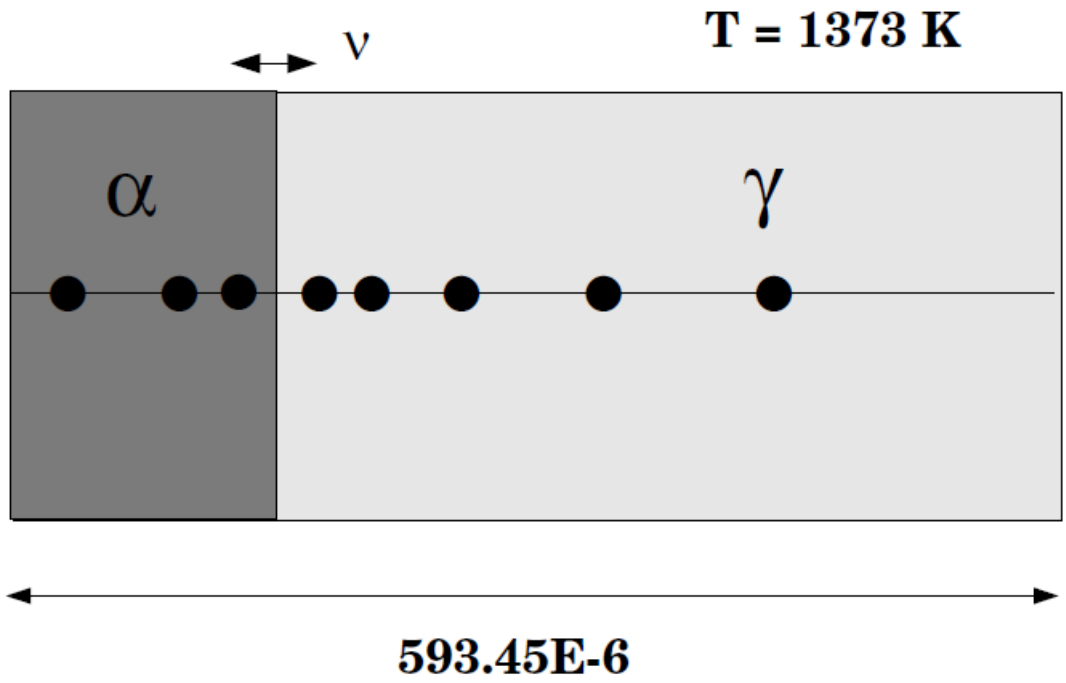



```
POST-1:
POST-1:
POST-1:
POST-1: --OK---
POST-1:
```

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
SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-
Examples\examples\exb5\setup.DCM.test"SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: NO SUCH COMMAND, USE HELP
SYS:
SYS:SYS:
SYS:SYS:SYS:SYS: THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

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

 VA                       /-  DEFINED
TDB_FEDEMO: CR                       FE                      NI
   DEFINED
TDB_FEDEMO: LIQUID:L                 BCC_A2                  CHI_A12
 FCC_A1                   HCP_A3                  LAVES_PHASE_C14
 SIGMA  REJECTED
TDB_FEDEMO: BCC_A2                   FCC_A1  RESTORED
TDB_FEDEMO: 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: Use one of these databases

 TCFE9   =  Steels/Fe-Alloys  v9.0
 TCFE8   =  Steels/Fe-Alloys  v8.1
 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
 FEDAT   =  TCS/TT Steels Database v1.0
 TCNI9   =  Ni-Alloys  v9.0
 NI25    =  NI25 Database
 TCNI8   =  Ni-Alloys  v8.2
 TCNI7   =  Ni-Alloys  v7.2
 TCNI6   =  Ni-Alloys  v6.1
 TCNI5   =  Ni-Alloys  v5.1
 TCNI4   =  Ni-Alloys  v4.0
 TCNI1   =  Ni-Alloys  v1.3
 TCAL6   =  Al-Alloys  v6.0
 TCAL5   =  Al-Alloys  v5.1
 TCAL4   =  Al-Alloys  v4.0
 TCAL3   =  Al-Alloys  v3.0
 TCAL2   =  Al-Alloys  v2.1
 TCAL1   =  Al-Alloys  v1.2
 TCMG5   =  Mg-Alloys  v5.1
 TCMG4   =  Mg-Alloys  v4.0
 TCMG3   =  Mg-Alloys  v3.0
 TCMG2   =  Mg-Alloys  v2.0
 TCMG1   =  Mg-Alloys  v1.1
 TCTI2   =  Ti-Alloys  v2.0
 TCTI1   =  Ti-Alloys  v1.0
 TCCU2   =  Cu-Alloys  v2.0
 TCCU1   =  Cu-Alloys  v1.0
 TCCC1   =  Cemented carbide  v1.0
 TCHEA3  =  High Entropy Alloy  v3.1
 TCHEA2  =  High Entropy Alloy  v2.1.1
 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
 TCOX9   =  Metal Oxide Solutions  v9.0 SNAPSHOT
 TCOX8   =  Metal Oxide Solutions  v8.0
 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  v2.7
 AQS2    =  TGG Aqueous Solution Database v2.6
 GCE2    =  TGG Geochemical/Environmental TDB v2.3
 FEDEMO  =  Iron Demo Database v2.0
 ALDEMO  =  Aluminum Demo Database v3.0
 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  v1.1
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBNI5  =  Ni-Alloys Mobility  v5.0
 MOBNI4  =  Ni-Alloys Mobility  v4.1
 MOBNI3  =  Ni-Alloys Mobility  v3.2
 MOBNI2  =  Ni-Alloys Mobility  v2.4
 MOBNI1  =  Ni-Alloys Mobility  v1.9
 MOBAL5  =  Al-Alloys Mobility  v5.0
 MOBAL4  =  Al-Alloys Mobility  v4.0
 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
 MOBHEA1 =  High Entropy Alloys Mobility  v1.0
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBSLD1 =  Solder-Alloys Mobility  v1.1
 MOBTI3  =  Ti-Alloys Mobility  v3.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v2.0
 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/: Current database: Fe-Alloys Mobility demo database v2.0

 VA  DEFINED
APP: CR                      FE                      NI
   DEFINED
APP: BCC_A2                  FCC_A1  REJECTED
APP: BCC_A2                  FCC_A1  RESTORED
APP: 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:APP:APP: NO TIME STEP DEFINED
DIC>
DIC>DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>DIC>ATTACH TO REGION NAMED /ALPHA/:
ATTACHED TO THE RIGHT OF ALPHA /YES/:
DIC>DIC>DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>DIC>DIC>REGION NAME : /ALPHA/:PHASE NAME: /BCC_A2/:DEPENDENT COMPONENT ? /NI/:COMPOSITION TYPE /MOLE_FRACTION/:PROFILE FOR /CR/
DIC>REGION NAME : /GAMMA/:PHASE NAME: /FCC_A1/:DEPENDENT COMPONENT ? /NI/:COMPOSITION TYPE /MOLE_FRACTION/:PROFILE FOR /CR/:PROFILE FOR /NI/:DI
DIC>DIC>DIC>DIC>END TIME FOR INTEGRATION /.1/:AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /360000/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC>DIC>
DIC> --OK---
DIC>
```

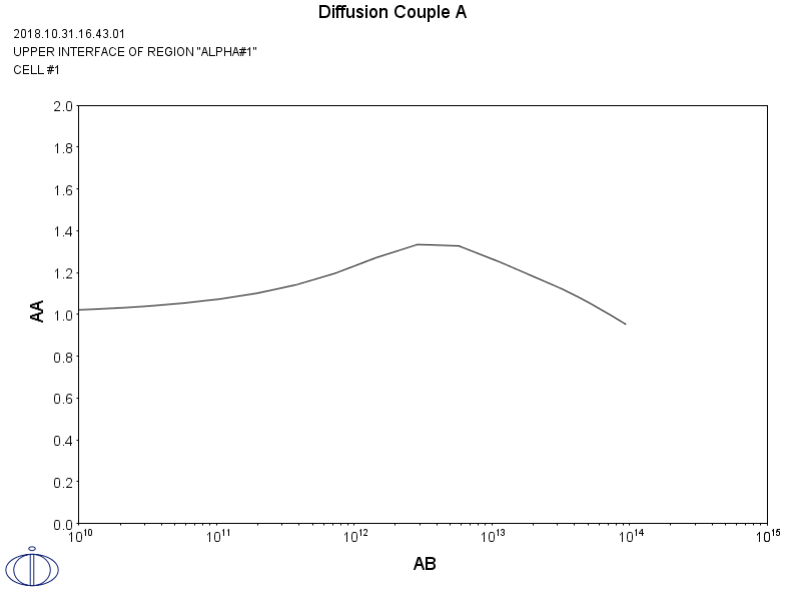
exb5-run

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb5\run.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  0.00000E+00
DIC> OK
DIC>
DIC>DIC>DIC>DIC> 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                     0 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        1.102521724323450E-
012        1.012598575344503E-012        8.579142826622250E-013        5.661502651298271E-012        6.016860883404360E-
013        2.433151163664946E-013        1.958409077926281E-014        1.188111053355531E-016       TIME =  0.93355784E-05 DT =  0.92355784E-
05 SUM OF SQUARES =  0.11881111E-15
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.96601163E-05 AND  -0.96601163E-05
 POSITION OF INTERFACE ALPHA / GAMMA IS   0.93465912E-04
 U-FRACTION IN SYSTEM:  CR = .305280432538621  FE = .471672082119085
                        NI = .223047485342294
 TOTAL SIZE OF SYSTEM:  5.9345E-04 [m]
  CPU time used in timestep                     1 seconds
 9.521906323698533E-005

output ignored...



... output resumed

 5.060724207762906E-009        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
```

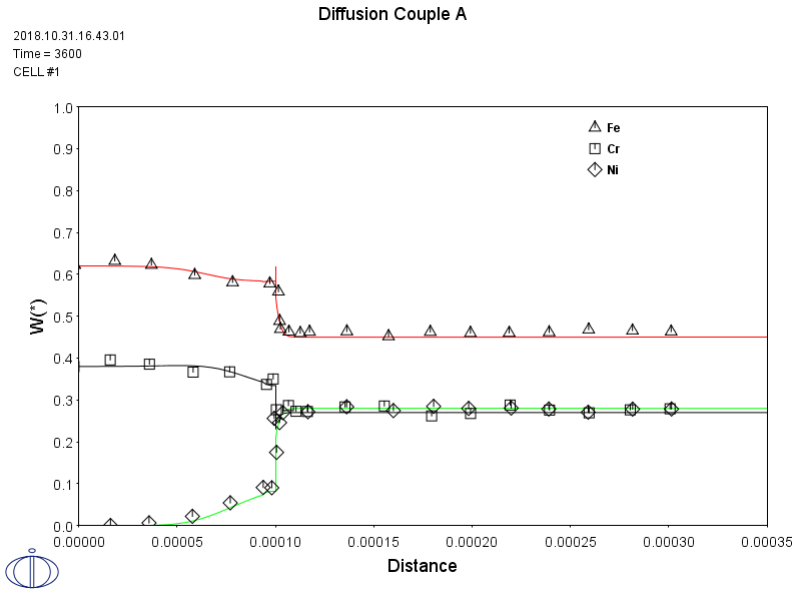
```
 TOTAL SIZE OF SYSTEM:  5.9345E-04 [m]
  5  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: GAMMA

  CPU time used in timestep                    2 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> --OK---
DIC>
```

exb5-plot

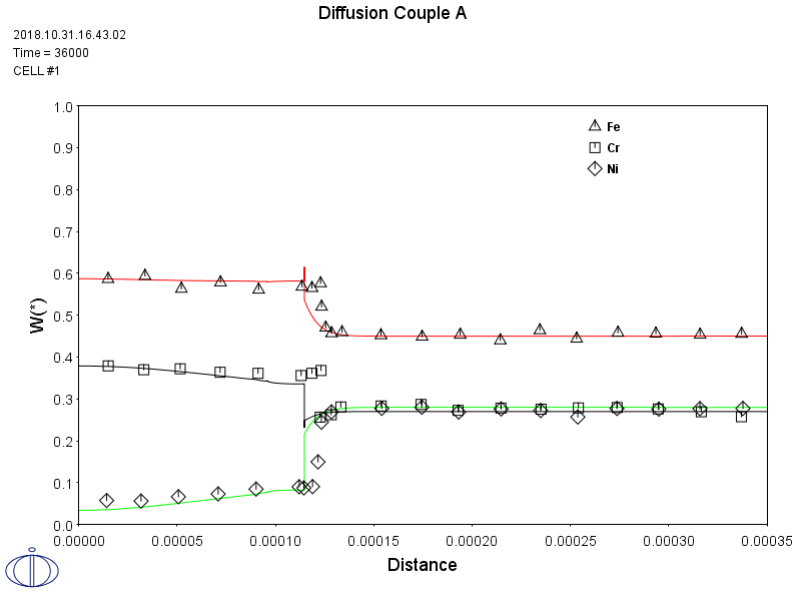
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb5\plot.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  3.60000E+06
DIC> OK
DIC>
DIC>DIC>DIC>DIC>  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:POST-1:POST-1:
POST-1:PROLOGUE NUMBER: /0/:DATASET NUMBER(s): /-1/:POST-1:
POST-1:
POST-1:POST-1:            OST-1:POST-1:
POST-1:
```



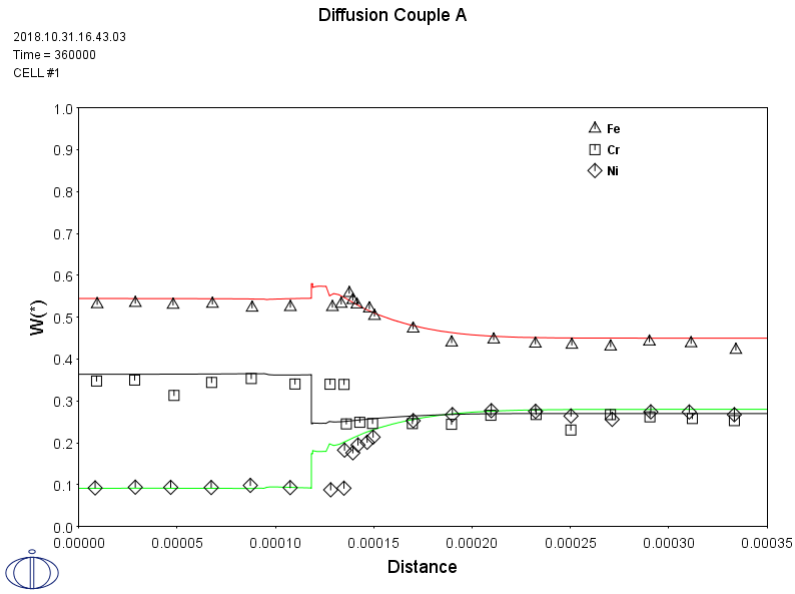

```
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1:POST-1:POST-1:POST-1:  INFO: Distance is set as independent variable
POST-1:POST-1:POST-1:
POST-1:POST-1:POST-1:
POST-1:POST-1:
POST-1:POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```



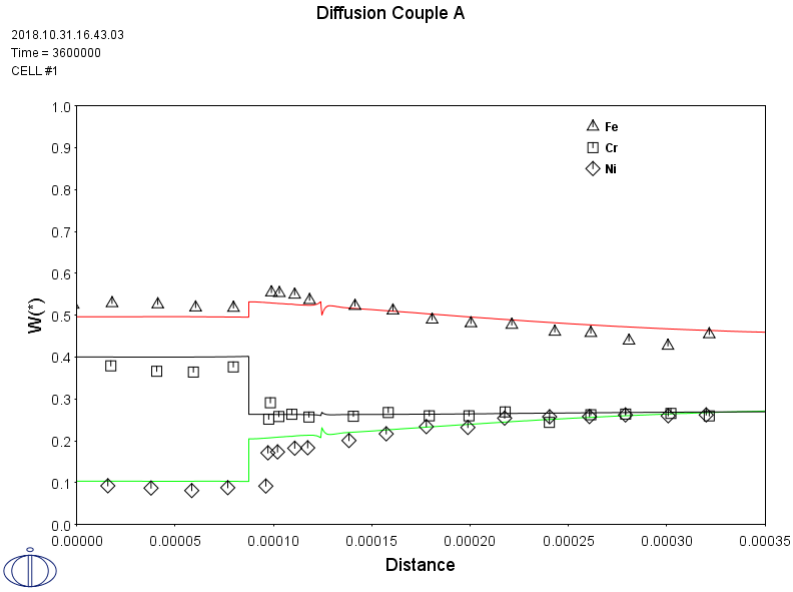

```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1:POST-1:POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```



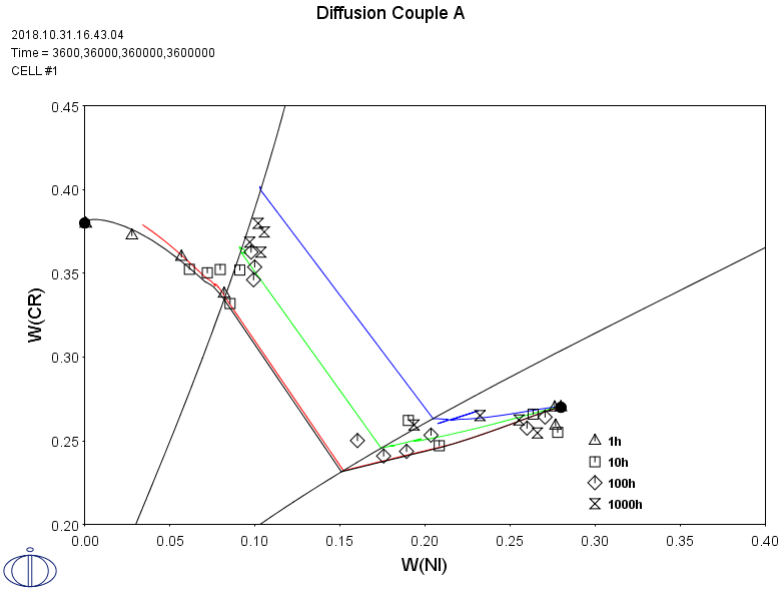

```
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1:POST-1:POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```




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




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

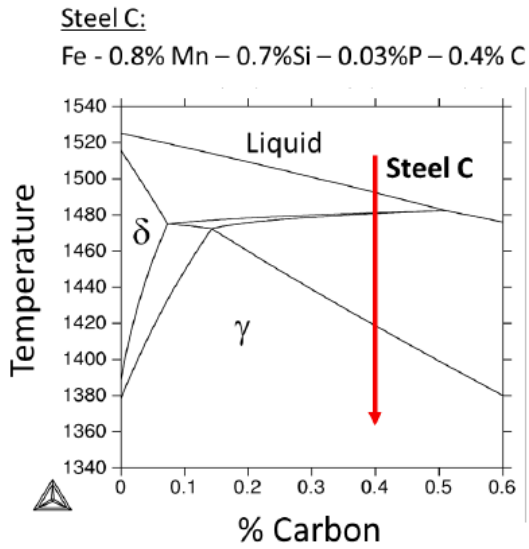


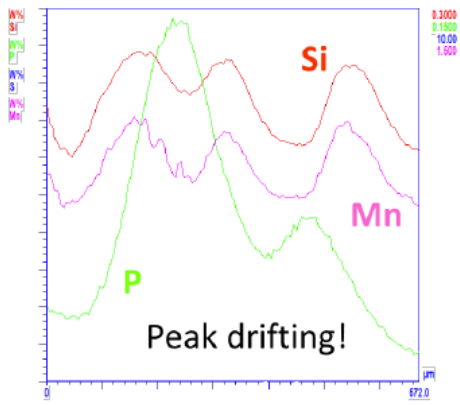

```
POST-1:
POST-1:
POST-1:
POST-1: --OK---
POST-1:
```

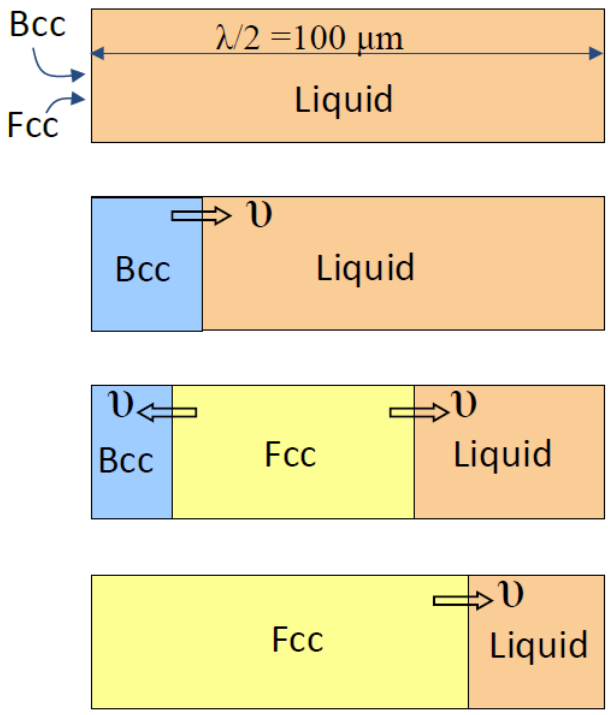
Example exb6

Micro-segregation of phosphorus

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







exb6-setup

```
About License library version: 8.5.1.0017
 Linked: Wed Oct 31 13:18:51 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-
Examples\examples\exb6\setup.DCM.test"SYS:SYS:SYS:SYS:SYS:SYS: NO SUCH COMMAND, USE HELP
SYS:
SYS:SYS:SYS:SYS: 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: 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: FE                     C                       SI
 MN                      P  DEFINED
TDB_TCFE7:
TDB_TCFE7:TDB_TCFE7: 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: FCC_A1                   LIQUID:L                BCC_A2
   RESTORED
TDB_TCFE7:
TDB_TCFE7:TDB_TCFE7: 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'
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      1989); C-FE-MN'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
 -OK-
TDB_TCFE7:
TDB_TCFE7:TDB_TCFE7:TDB_TCFE7:TDB_TCFE7:TDB_TCFE7: Use one of these databases

 TCFE9   =  Steels/Fe-Alloys  v9.0
 TCFE8   =  Steels/Fe-Alloys  v8.1
 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
 FEDAT   =  TCS/TT Steels Database v1.0
 TCNI9   =  Ni-Alloys  v9.0
 NI25    =  NI25 Database
 TCNI8   =  Ni-Alloys  v8.2
 TCNI7   =  Ni-Alloys  v7.2
 TCNI6   =  Ni-Alloys  v6.1
 TCNI5   =  Ni-Alloys  v5.1
 TCNI4   =  Ni-Alloys  v4.0
 TCNI1   =  Ni-Alloys  v1.3
 TCAL6   =  Al-Alloys  v6.0
 TCAL5   =  Al-Alloys  v5.1
 TCAL4   =  Al-Alloys  v4.0
 TCAL3   =  Al-Alloys  v3.0
 TCAL2   =  Al-Alloys  v2.1
 TCAL1   =  Al-Alloys  v1.2
 TCMG5   =  Mg-Alloys  v5.1
 TCMG4   =  Mg-Alloys  v4.0
 TCMG3   =  Mg-Alloys  v3.0
 TCMG2   =  Mg-Alloys  v2.0
 TCMG1   =  Mg-Alloys  v1.1
 TCTI2   =  Ti-Alloys  v2.0
 TCTI1   =  Ti-Alloys  v1.0
 TCCU2   =  Cu-Alloys  v2.0
 TCCU1   =  Cu-Alloys  v1.0
 TCCC1   =  Cemented carbide  v1.0
 TCHEA3  =  High Entropy Alloy  v3.1
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 TCHEA2  =  High Entropy Alloy  v2.1.1
 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
 TCOX9   =  Metal Oxide Solutions  v9.0 SNAPSHOT
 TCOX8   =  Metal Oxide Solutions  v8.0
 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  v2.7
 AQS2    =  TGG Aqueous Solution Database v2.6
 GCE2    =  TGG Geochemical/Environmental TDB v2.3
 FEDEMO  =  Iron Demo Database v2.0
 ALDEMO  =  Aluminum Demo Database v3.0
 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
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 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
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 MOBAL1  =  Al-Alloys Mobility  v1.0
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 MOBCU2  =  Cu-Alloys Mobility  v2.0
 MOBHEA1 =  High Entropy Alloys Mobility  v1.0
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBSLD1 =  Solder-Alloys Mobility  v1.1
 MOBTI3  =  Ti-Alloys Mobility  v3.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v2.0
 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/: Current database: Steels/Fe-Alloys Mobility  v2.0
   TCS Steel Mobility Database Version 2.0 from 2011-12-09.

 VA  DEFINED
APP: FE                     C                       SI
 MN                      P  DEFINED
APP: BCC_A2                 CEMENTITE               FCC_A1
 FE4N_LP1                HCP_A3                  LIQUID:L
   REJECTED
APP: FCC_A1                 LIQUID:L                BCC_A2
   RESTORED
APP: 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
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       Mn-Ni'
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      (5) (1964)154.; Impurity diff of P in fcc Fe.'
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      diffusion of Si in fcc Fe.'
  'B. Jonsson: Z. Metallkunde 85(1994)498-501; C and N diffusion in bcc Cr
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  'B. Jonsson: Unpublished research bcc Fe-Si 1994'
  'Assessed from data presented in Landholt-Bornstein, Vol. 26, ed. H.
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  'Assessed from data presented in Landholt-Bornstein, Vol. 26, ed. H.
      Mehrer, springer (1990); Impurity diff of P in bcc Fe.'
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DIC>
DIC>DIC>DIC>DIC>DIC>ACTIVE OR INACTIVE PHASE /ACTIVE/:ATTACH TO REGION NAMED /SMALTA/:ATTACHED TO THE RIGHT OF SMALTA /YES/:PHASE NAME: /NONE/:
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DIC>ACTIVE OR INACTIVE PHASE /ACTIVE/:ATTACH TO REGION NAMED /SMALTA/:ATTACHED TO THE RIGHT OF SMALTA /YES/:PHASE NAME: /NONE/:DEPENDENT COMPON
05/:CONDITION TYPE /CLOSED_SYSTEM/:DIC>
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DIC>DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>END TIME FOR INTEGRATION /.1/:AUTOMATIC TIMESTEP CONTROL /YES/:MAX TIMESTEP DURING INTEGRATION /300/:INITIAL TIMESTEP : /1E-
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SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
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FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /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>DIC>DIC>DIC>
DIC> --OK---
DIC>
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exb6-run

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DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb6\run.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC> TIME STEP AT TIME  0.00000E+00
DIC> OK
DIC> Region: SMALTA
 single geometric dense at   0.0000
  1.0846       88
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                        MN = .00810568126669965  P = 5.39133528237326E-04
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                        SI = .0138733239959838
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output ignored...


... output resumed

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 DELETING TIME-RECORD FOR TIME    1676.7174
 DELETING TIME-RECORD FOR TIME    1691.7174
 DELETING TIME-RECORD FOR TIME    1706.7174
 DELETING TIME-RECORD FOR TIME    1721.7174
 DELETING TIME-RECORD FOR TIME    1736.7174
 DELETING TIME-RECORD FOR TIME    1751.7174
 DELETING TIME-RECORD FOR TIME    1766.7174
 DELETING TIME-RECORD FOR TIME    1781.7174
 DELETING TIME-RECORD FOR TIME    1796.7174
 DELETING TIME-RECORD FOR TIME    1811.7174
 DELETING TIME-RECORD FOR TIME    1826.7174
 DELETING TIME-RECORD FOR TIME    1841.7174
 DELETING TIME-RECORD FOR TIME    1856.7174
 DELETING TIME-RECORD FOR TIME    1871.7174
 DELETING TIME-RECORD FOR TIME    1886.7174
 DELETING TIME-RECORD FOR TIME    1901.7174
 DELETING TIME-RECORD FOR TIME    1916.7174
 DELETING TIME-RECORD FOR TIME    1931.7174
 DELETING TIME-RECORD FOR TIME    1946.7174
 DELETING TIME-RECORD FOR TIME    1961.7174
 DELETING TIME-RECORD FOR TIME    1976.7174
 DELETING TIME-RECORD FOR TIME    1991.7174
 DELETING TIME-RECORD FOR TIME    2006.7174
 DELETING TIME-RECORD FOR TIME    2021.7174
 DELETING TIME-RECORD FOR TIME    2036.7174
 DELETING TIME-RECORD FOR TIME    2051.7174
 DELETING TIME-RECORD FOR TIME    2066.7174
 DELETING TIME-RECORD FOR TIME    2081.7174
 DELETING TIME-RECORD FOR TIME    2096.7174
 DELETING TIME-RECORD FOR TIME    2111.7174
 DELETING TIME-RECORD FOR TIME    2126.7174
 DELETING TIME-RECORD FOR TIME    2141.7174
```
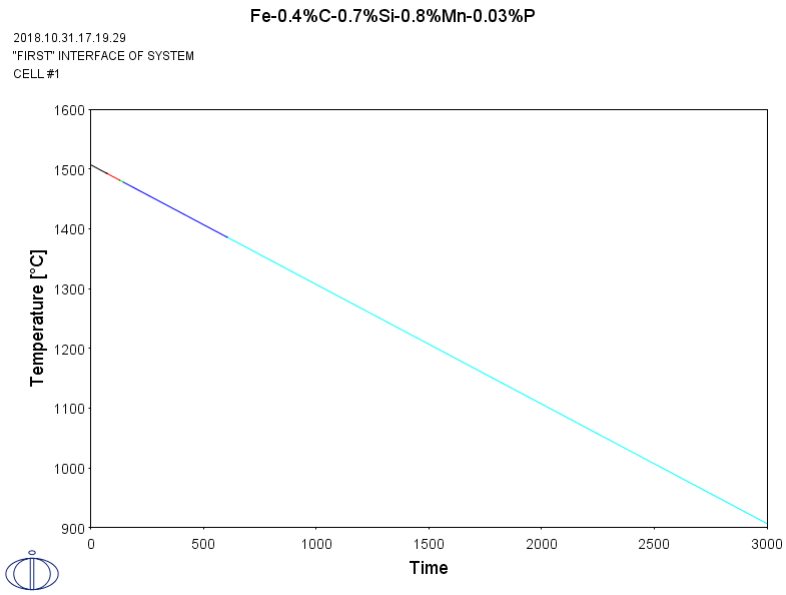
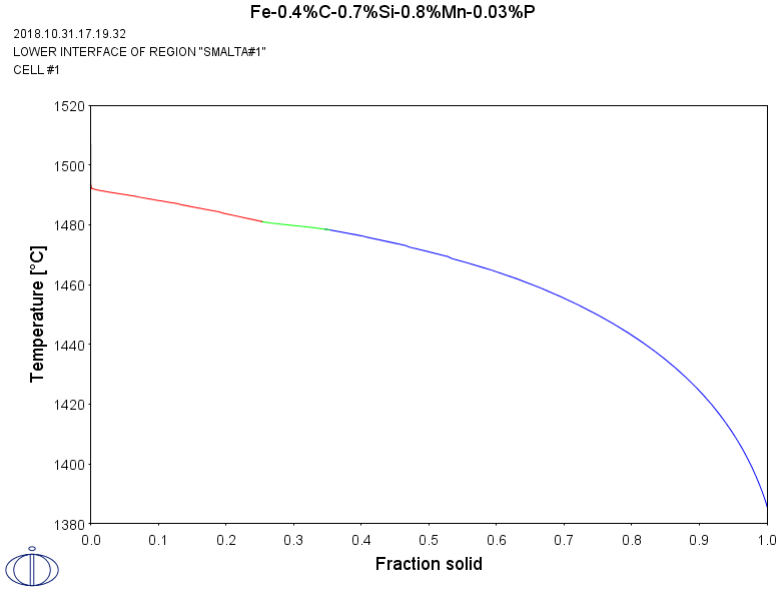

```
 DELETING TIME-RECORD FOR TIME    2156.7174
 DELETING TIME-RECORD FOR TIME    2171.7174
 DELETING TIME-RECORD FOR TIME    2186.7174
 DELETING TIME-RECORD FOR TIME    2201.7174
 DELETING TIME-RECORD FOR TIME    2216.7174
 DELETING TIME-RECORD FOR TIME    2231.7174
 DELETING TIME-RECORD FOR TIME    2246.7174
 DELETING TIME-RECORD FOR TIME    2261.7174
 DELETING TIME-RECORD FOR TIME    2276.7174
 DELETING TIME-RECORD FOR TIME    2291.7174
 DELETING TIME-RECORD FOR TIME    2306.7174
 DELETING TIME-RECORD FOR TIME    2321.7174
 DELETING TIME-RECORD FOR TIME    2336.7174
 DELETING TIME-RECORD FOR TIME    2351.7174
 DELETING TIME-RECORD FOR TIME    2366.7174
 DELETING TIME-RECORD FOR TIME    2381.7174
 DELETING TIME-RECORD FOR TIME    2396.7174
 DELETING TIME-RECORD FOR TIME    2411.7174
 DELETING TIME-RECORD FOR TIME    2426.7174
 DELETING TIME-RECORD FOR TIME    2441.7174
 DELETING TIME-RECORD FOR TIME    2456.7174
 DELETING TIME-RECORD FOR TIME    2471.7174
 DELETING TIME-RECORD FOR TIME    2486.7174
 DELETING TIME-RECORD FOR TIME    2501.7174
 DELETING TIME-RECORD FOR TIME    2516.7174
 DELETING TIME-RECORD FOR TIME    2531.7174
 DELETING TIME-RECORD FOR TIME    2546.7174
 DELETING TIME-RECORD FOR TIME    2561.7174
 DELETING TIME-RECORD FOR TIME    2576.7174
 DELETING TIME-RECORD FOR TIME    2591.7174
 DELETING TIME-RECORD FOR TIME    2606.7174
 DELETING TIME-RECORD FOR TIME    2621.7174
 DELETING TIME-RECORD FOR TIME    2636.7174
 DELETING TIME-RECORD FOR TIME    2651.7174
 DELETING TIME-RECORD FOR TIME    2666.7174
 DELETING TIME-RECORD FOR TIME    2681.7174
 DELETING TIME-RECORD FOR TIME    2696.7174
 DELETING TIME-RECORD FOR TIME    2711.7174
 DELETING TIME-RECORD FOR TIME    2726.7174
 DELETING TIME-RECORD FOR TIME    2741.7174
 DELETING TIME-RECORD FOR TIME    2756.7174
 DELETING TIME-RECORD FOR TIME    2771.7174
 DELETING TIME-RECORD FOR TIME    2786.7174
 DELETING TIME-RECORD FOR TIME    2801.7174
 DELETING TIME-RECORD FOR TIME    2816.7174
 DELETING TIME-RECORD FOR TIME    2831.7174
 DELETING TIME-RECORD FOR TIME    2846.7174
 DELETING TIME-RECORD FOR TIME    2861.7174
 DELETING TIME-RECORD FOR TIME    2876.7174
 DELETING TIME-RECORD FOR TIME    2891.7174
 DELETING TIME-RECORD FOR TIME    2906.7174
 DELETING TIME-RECORD FOR TIME    2921.7174
 DELETING TIME-RECORD FOR TIME    2936.7174
 DELETING TIME-RECORD FOR TIME    2951.7174
 DELETING TIME-RECORD FOR TIME    2966.7174
 DELETING TIME-RECORD FOR TIME    2981.7174

 KEEPING TIME-RECORD FOR TIME    2996.7174
 AND FOR TIME                    3000.0000
 WORKSPACE RECLAIMED

 TIMESTEP AT     3000.00000     SELECTED

DIC> --OK---
DIC>
```

exb6-plot

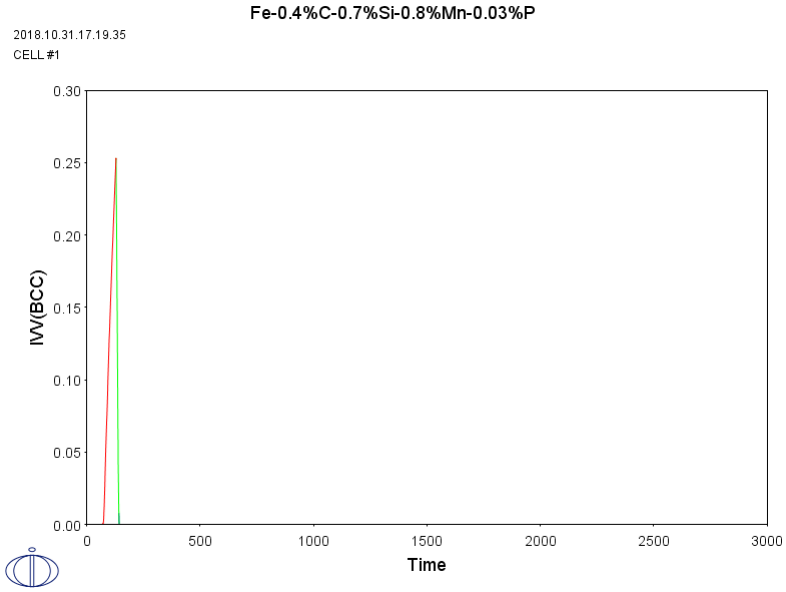
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb6\plot.DCM.test"DIC>
DIC>
DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  3.00000E+03
DIC> OK
DIC>
DIC>DIC>DIC>DIC>  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:POST-1:
POST-1:POST-1:  INFO: Time is set as independent variable
POST-1:POST-1:
POST-1:POST-1: ORKING ...orking ...          OST-1:POST-1:
POST-1:
```



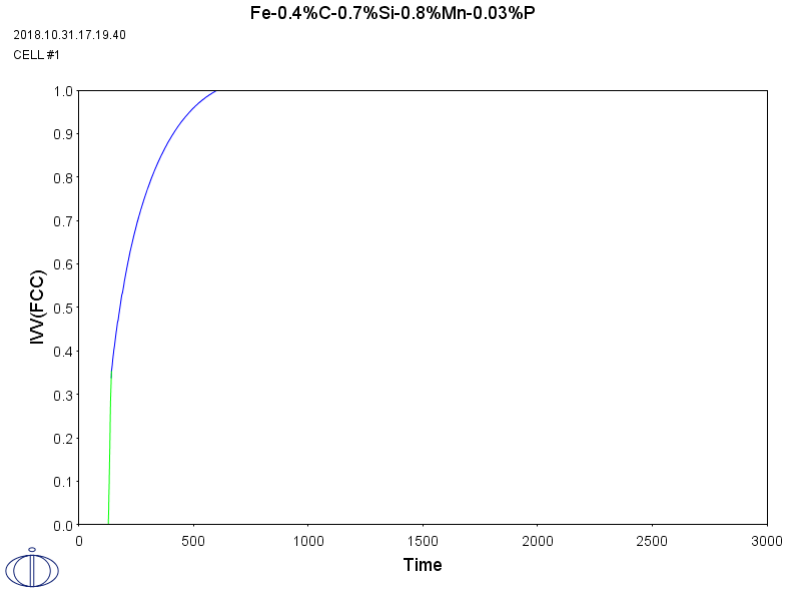

```
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:
POST-1:POST-1:
POST-1:
POST-1:POST-1:
POST-1:
POST-1:
POST-1:POST-1: ORKING ...orking ...          OST-1:POST-1:
POST-1:
```



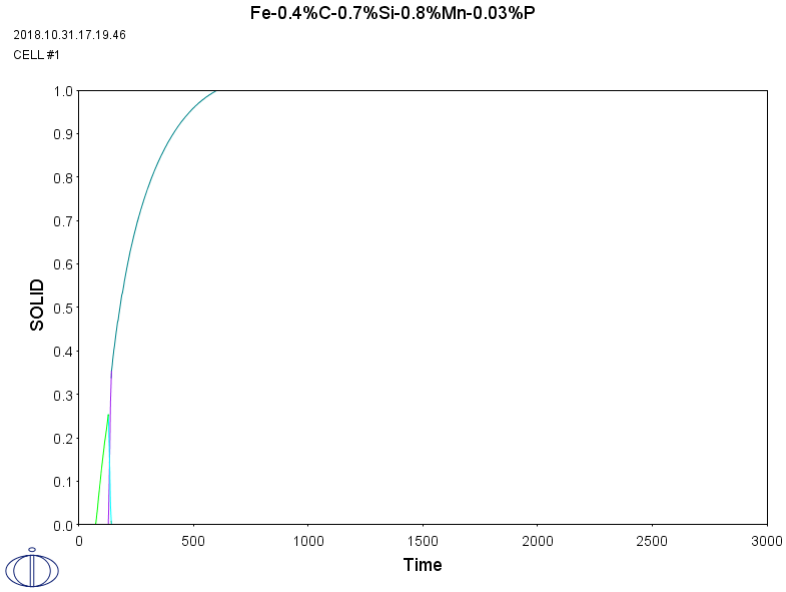

```
POST-1:
POST-1:Hit RETURN to continue
POST-1:POST-1:  INFO: Time is set as independent variable
POST-1:
POST-1:
POST-1:POST-1: ORKING ...orking ...          OST-1:POST-1:
POST-1:
```




```
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1:POST-1:
POST-1:POST-1: ORKING ...orking ...          OST-1:POST-1:
POST-1:
```

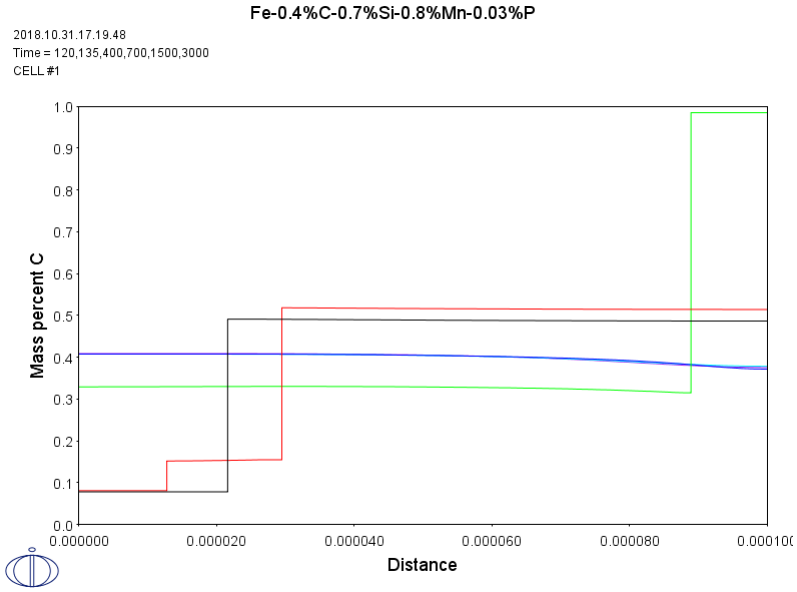



```
POST-1:
POST-1:Hit RETURN to continue
POST-1:Variable(s)POST-1:
POST-1:COLUMN NUMBER /*/:
POST-1:
POST-1:
POST-1:POST-1: ORKING ...orking ...          OST-1:POST-1:
POST-1:
```

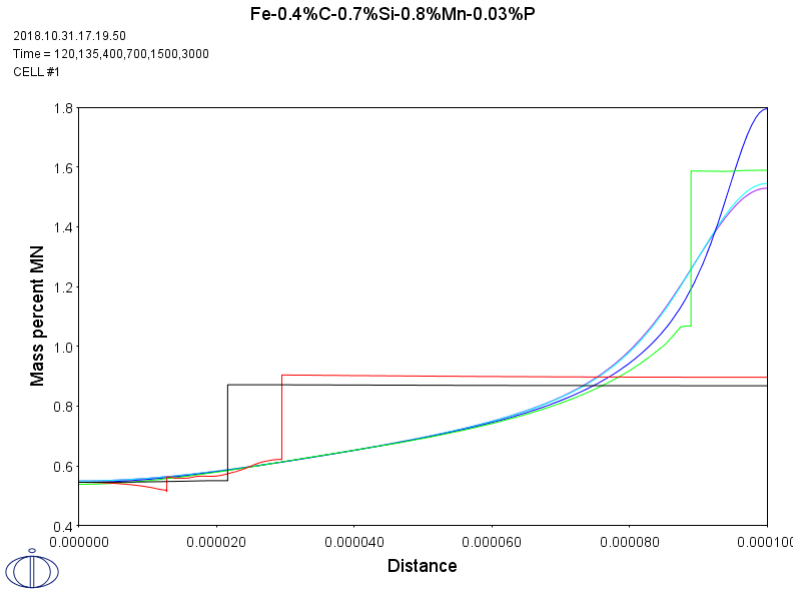



```
POST-1:
```

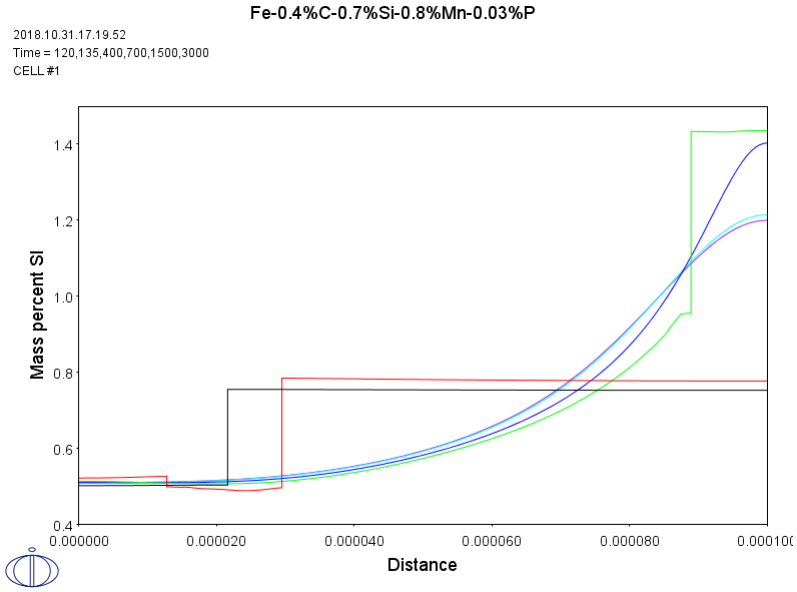
```
POST-1:Hit RETURN to continue
POST-1:POST-1:  INFO: Distance is set as independent variable
POST-1:POST-1:
POST-1:
POST-1:POST-1: ORKING ...orking ...OST-1:POST-1:
POST-1:
```



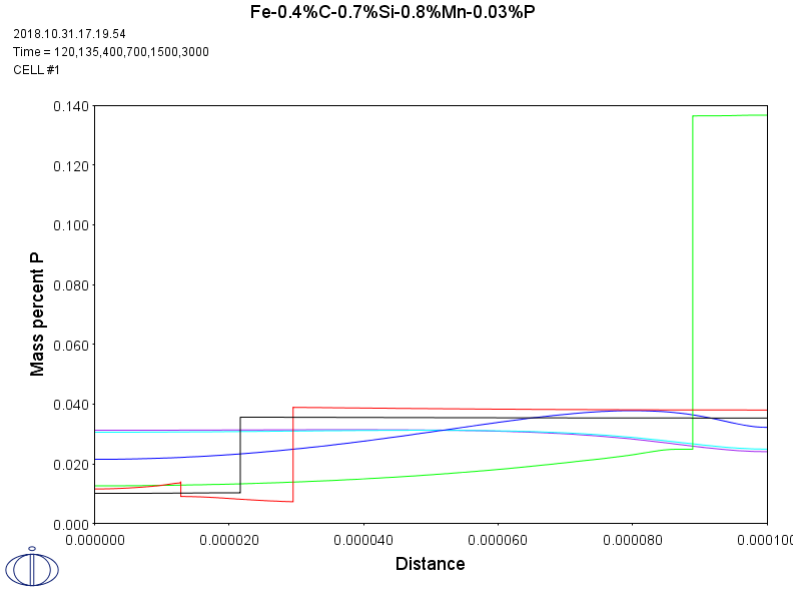

```
POST-1:
POST-1:Hit RETURN to continue
POST-1:POST-1:
POST-1:POST-1: ORKING ...orking ...OST-1:POST-1:
POST-1:
```



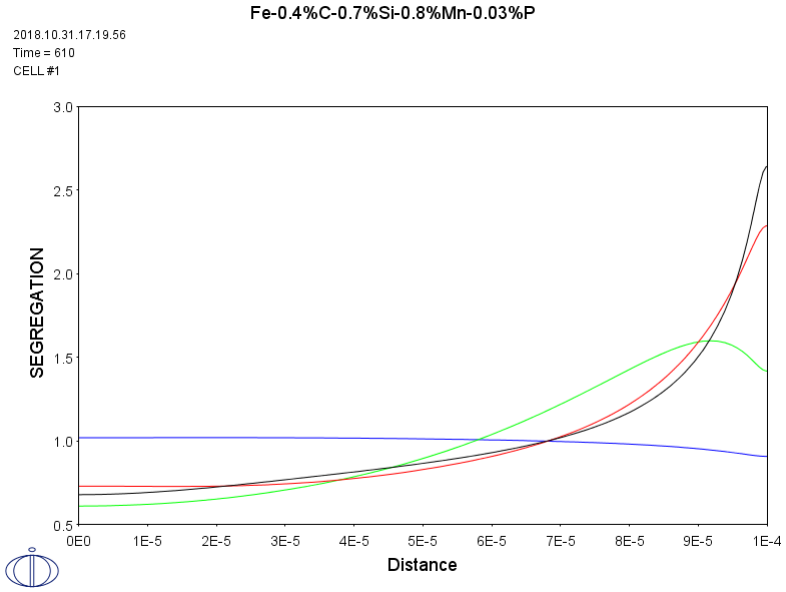

```
POST-1:
POST-1:Hit RETURN to continue
POST-1:POST-1:
POST-1:POST-1: ORKING ...orking ...OST-1:POST-1:
POST-1:
```



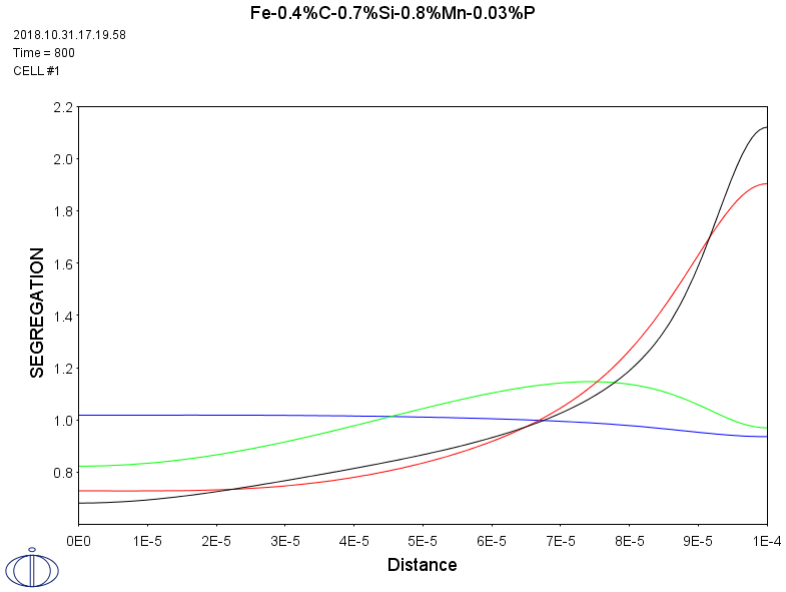

```
POST-1:
POST-1:Hit RETURN to continue
POST-1:POST-1:
POST-1:POST-1: ORKING ...orking ...OST-1:POST-1:
POST-1:
```



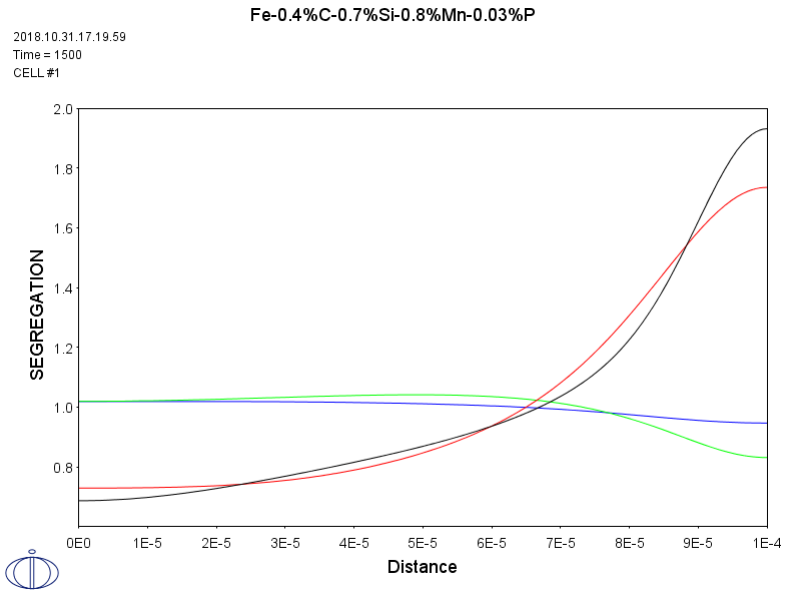

```
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1:FUNCTION:&
POST-1:FUNCTION:&
POST-1:FUNCTION:&
POST-1:FUNCTION:&
POST-1:Variable(s)POST-1:
POST-1:
POST-1:COLUMN NUMBER /*/:
POST-1:
POST-1:
POST-1:POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```




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

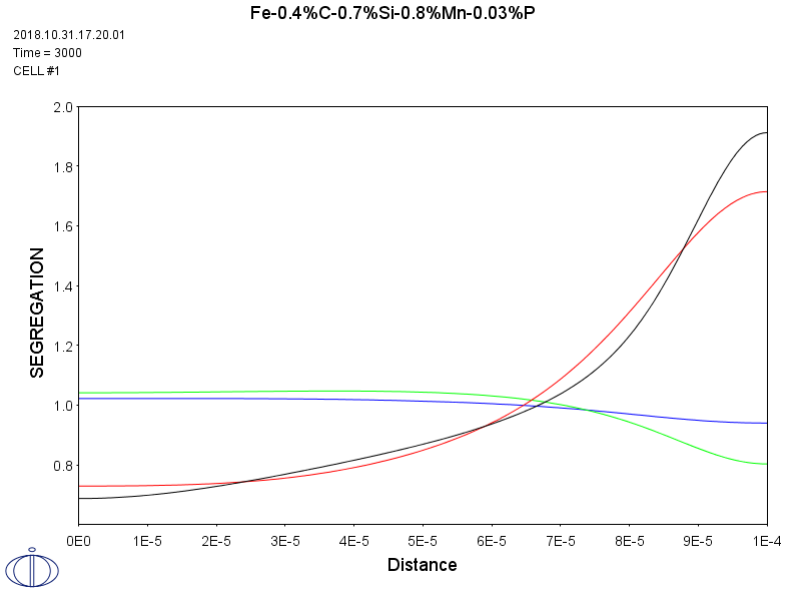



```
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1:POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```




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

```
POST-1:POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```

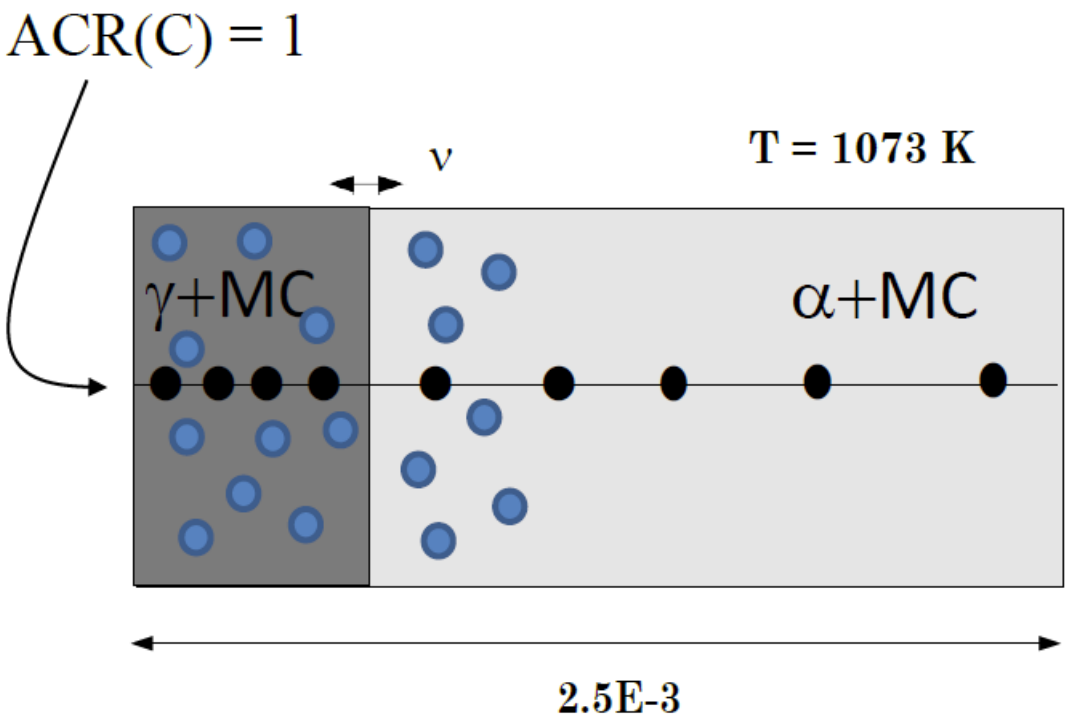



```
POST-1:
POST-1:Hit RETURN to continue
POST-1: --OK---
POST-1:
```

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
 Software  (build 17825) 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: Wed Oct 31 13:18:51 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb7\setup.DCM"SYS: @@
SYS: @@ Moving boundary problem.
SYS: @@ Moving boundary problem with multiple phases on each side
SYS: @@ This example shows how to enter dispersed phases on either side
SYS: @@ of a phase interface. The particular case shows how
SYS: @@ the kinetics of a ferrite to austenite transformation is
SYS: @@ affected by simultaneous precipitation of niobium carbide.
SYS: @@ The transformation is caused by carburization.
SYS: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASE
SYS: @@
SYS: go da
 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
```

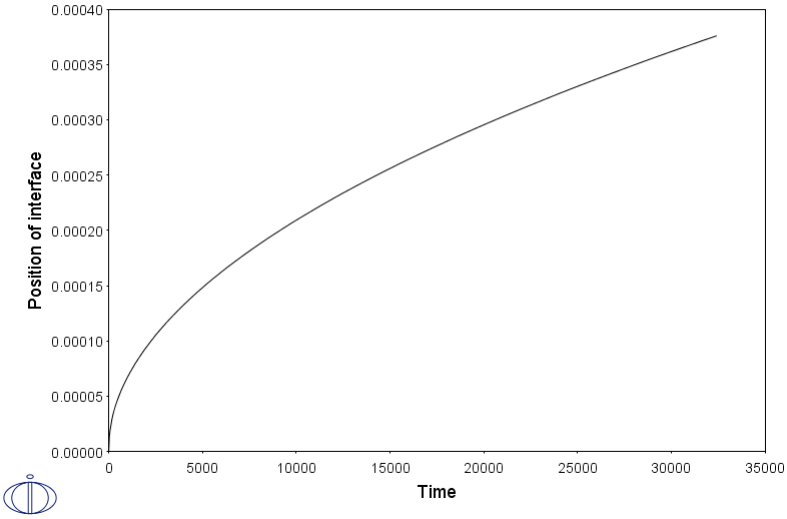
```
Iteration #   2 sum residual **2:   0.30812257E+11
Iteration #   3 sum residual **2:   0.22477716E+11
Iteration #   4 sum residual **2:   0.18061437E+11
 Error                     408
 Reducing dt to   7.812500000000000E-011
 Stage 1
 Evaluating Jacobian
Iteration #   1 sum residual **2:   0.84899306E+10
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    26503.389
 DELETING TIME-RECORD FOR TIME    26540.970
 DELETING TIME-RECORD FOR TIME    26578.551
 DELETING TIME-RECORD FOR TIME    26616.132
 DELETING TIME-RECORD FOR TIME    26653.713
 DELETING TIME-RECORD FOR TIME    26691.294
 DELETING TIME-RECORD FOR TIME    26728.875
 DELETING TIME-RECORD FOR TIME    26766.456
 DELETING TIME-RECORD FOR TIME    26801.353
 DELETING TIME-RECORD FOR TIME    26836.249
 DELETING TIME-RECORD FOR TIME    26871.146
 DELETING TIME-RECORD FOR TIME    26906.043
 DELETING TIME-RECORD FOR TIME    26943.624
 DELETING TIME-RECORD FOR TIME    27018.785
 DELETING TIME-RECORD FOR TIME    27104.685
 DELETING TIME-RECORD FOR TIME    27190.584
 DELETING TIME-RECORD FOR TIME    27276.483
 DELETING TIME-RECORD FOR TIME    27362.383
 DELETING TIME-RECORD FOR TIME    27448.282
 DELETING TIME-RECORD FOR TIME    27534.182
 DELETING TIME-RECORD FOR TIME    27620.081
 DELETING TIME-RECORD FOR TIME    27705.980
 DELETING TIME-RECORD FOR TIME    27791.880
 DELETING TIME-RECORD FOR TIME    27877.779
 DELETING TIME-RECORD FOR TIME    27931.466
 DELETING TIME-RECORD FOR TIME    27974.416
 DELETING TIME-RECORD FOR TIME    28017.365
 DELETING TIME-RECORD FOR TIME    28060.315
 DELETING TIME-RECORD FOR TIME    28103.265
 DELETING TIME-RECORD FOR TIME    28146.214
 DELETING TIME-RECORD FOR TIME    28189.164
 DELETING TIME-RECORD FOR TIME    28232.114
 DELETING TIME-RECORD FOR TIME    28275.063
 DELETING TIME-RECORD FOR TIME    28318.013
 DELETING TIME-RECORD FOR TIME    28360.963
 DELETING TIME-RECORD FOR TIME    28403.912
 DELETING TIME-RECORD FOR TIME    28438.809
 DELETING TIME-RECORD FOR TIME    28484.443
 DELETING TIME-RECORD FOR TIME    28527.393
 DELETING TIME-RECORD FOR TIME    28570.342
 DELETING TIME-RECORD FOR TIME    28613.292
 DELETING TIME-RECORD FOR TIME    28656.242
 DELETING TIME-RECORD FOR TIME    28699.191
 DELETING TIME-RECORD FOR TIME    28742.141
 DELETING TIME-RECORD FOR TIME    28785.091
 DELETING TIME-RECORD FOR TIME    28828.040
 DELETING TIME-RECORD FOR TIME    28870.990
 DELETING TIME-RECORD FOR TIME    28913.940
 DELETING TIME-RECORD FOR TIME    28948.836
 DELETING TIME-RECORD FOR TIME    28983.733
 DELETING TIME-RECORD FOR TIME    29021.314
 DELETING TIME-RECORD FOR TIME    29058.895
 DELETING TIME-RECORD FOR TIME    29096.476
 DELETING TIME-RECORD FOR TIME    29134.057
 DELETING TIME-RECORD FOR TIME    29171.638
 DELETING TIME-RECORD FOR TIME    29214.587
 DELETING TIME-RECORD FOR TIME    29279.012
 DELETING TIME-RECORD FOR TIME    29321.962
 DELETING TIME-RECORD FOR TIME    29364.911
 DELETING TIME-RECORD FOR TIME    29407.861
 DELETING TIME-RECORD FOR TIME    29450.811
 DELETING TIME-RECORD FOR TIME    29493.760
 DELETING TIME-RECORD FOR TIME    29536.710
 DELETING TIME-RECORD FOR TIME    29579.660
 DELETING TIME-RECORD FOR TIME    29622.609
 DELETING TIME-RECORD FOR TIME    29662.875
 DELETING TIME-RECORD FOR TIME    29727.299
 DELETING TIME-RECORD FOR TIME    29770.249
 DELETING TIME-RECORD FOR TIME    29813.199
 DELETING TIME-RECORD FOR TIME    29856.148
 DELETING TIME-RECORD FOR TIME    29899.098
 DELETING TIME-RECORD FOR TIME    29942.048
 DELETING TIME-RECORD FOR TIME    29984.997
 DELETING TIME-RECORD FOR TIME    30027.947
 DELETING TIME-RECORD FOR TIME    30070.897
 DELETING TIME-RECORD FOR TIME    30113.846
 DELETING TIME-RECORD FOR TIME    30156.796
 DELETING TIME-RECORD FOR TIME    30194.377
 DELETING TIME-RECORD FOR TIME    30231.958
 DELETING TIME-RECORD FOR TIME    30269.539
 DELETING TIME-RECORD FOR TIME    30307.120
```

```
 DELETING TIME-RECORD FOR TIME    30344.701
 DELETING TIME-RECORD FOR TIME    30382.282
 DELETING TIME-RECORD FOR TIME    30419.863
 DELETING TIME-RECORD FOR TIME    30457.444
 DELETING TIME-RECORD FOR TIME    30495.025
 DELETING TIME-RECORD FOR TIME    30532.606
 DELETING TIME-RECORD FOR TIME    30570.187
 DELETING TIME-RECORD FOR TIME    30607.767
 DELETING TIME-RECORD FOR TIME    30645.348
 DELETING TIME-RECORD FOR TIME    30682.929
 DELETING TIME-RECORD FOR TIME    30720.510
 DELETING TIME-RECORD FOR TIME    30758.091
 DELETING TIME-RECORD FOR TIME    30795.672
 DELETING TIME-RECORD FOR TIME    30833.253
 DELETING TIME-RECORD FOR TIME    30870.834
 DELETING TIME-RECORD FOR TIME    30908.415
 DELETING TIME-RECORD FOR TIME    30945.996
 DELETING TIME-RECORD FOR TIME    30983.577
 DELETING TIME-RECORD FOR TIME    31021.158
 DELETING TIME-RECORD FOR TIME    31058.739
 DELETING TIME-RECORD FOR TIME    31096.320
 DELETING TIME-RECORD FOR TIME    31133.901
 DELETING TIME-RECORD FOR TIME    31171.482
 DELETING TIME-RECORD FOR TIME    31209.063
 DELETING TIME-RECORD FOR TIME    31246.644
 DELETING TIME-RECORD FOR TIME    31284.225
 DELETING TIME-RECORD FOR TIME    31321.806
 DELETING TIME-RECORD FOR TIME    31359.387
 DELETING TIME-RECORD FOR TIME    31396.968
 DELETING TIME-RECORD FOR TIME    31434.549
 DELETING TIME-RECORD FOR TIME    31472.130
 DELETING TIME-RECORD FOR TIME    31509.711
 DELETING TIME-RECORD FOR TIME    31547.292
 DELETING TIME-RECORD FOR TIME    31584.873
 DELETING TIME-RECORD FOR TIME    31622.454
 DELETING TIME-RECORD FOR TIME    31660.034
 DELETING TIME-RECORD FOR TIME    31694.931
 DELETING TIME-RECORD FOR TIME    31729.828
 DELETING TIME-RECORD FOR TIME    31772.777
 DELETING TIME-RECORD FOR TIME    31837.202
 DELETING TIME-RECORD FOR TIME    31880.152
 DELETING TIME-RECORD FOR TIME    31966.051
 DELETING TIME-RECORD FOR TIME    32051.950
 DELETING TIME-RECORD FOR TIME    32137.850
 DELETING TIME-RECORD FOR TIME    32223.749
 DELETING TIME-RECORD FOR TIME    32309.648

 KEEPING TIME-RECORD FOR TIME    32395.548
 AND FOR TIME                    32400.000
 WORKSPACE RECLAIMED
 ------------------------------------------------
 INTERPOLATION SCHEME USED THIS FRACTION OF
 THE ALLOCATED MEMORY:    1.00000000000000
 EFFICIENCY FACTOR:    30.2326681183046
 MEMORY FRACTION USAGE PER BRANCH:
   1.00000000000000
   1.00000000000000
   1.00000000000000
 ------------------------------------------------
 DEALLOCATING
 ------------------------------------------------

 TIMESTEP AT     32400.0000     SELECTED

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

exb7-plot

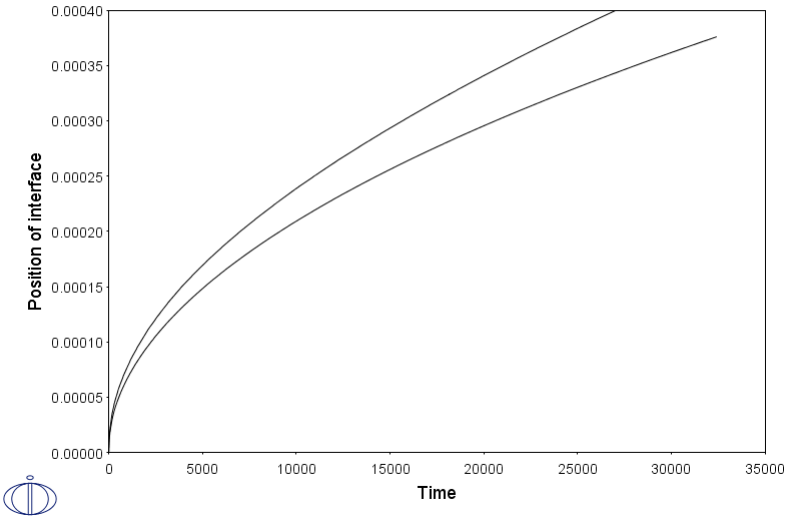
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb7\plot.DCM"DIC>
DIC>
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  3.24000E+04
 *** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
 *** ENTERING C1NB1_S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

2018.10.31.17.39.14
UPPER INTERFACE OF REGION "AUS#1"
CELL #1



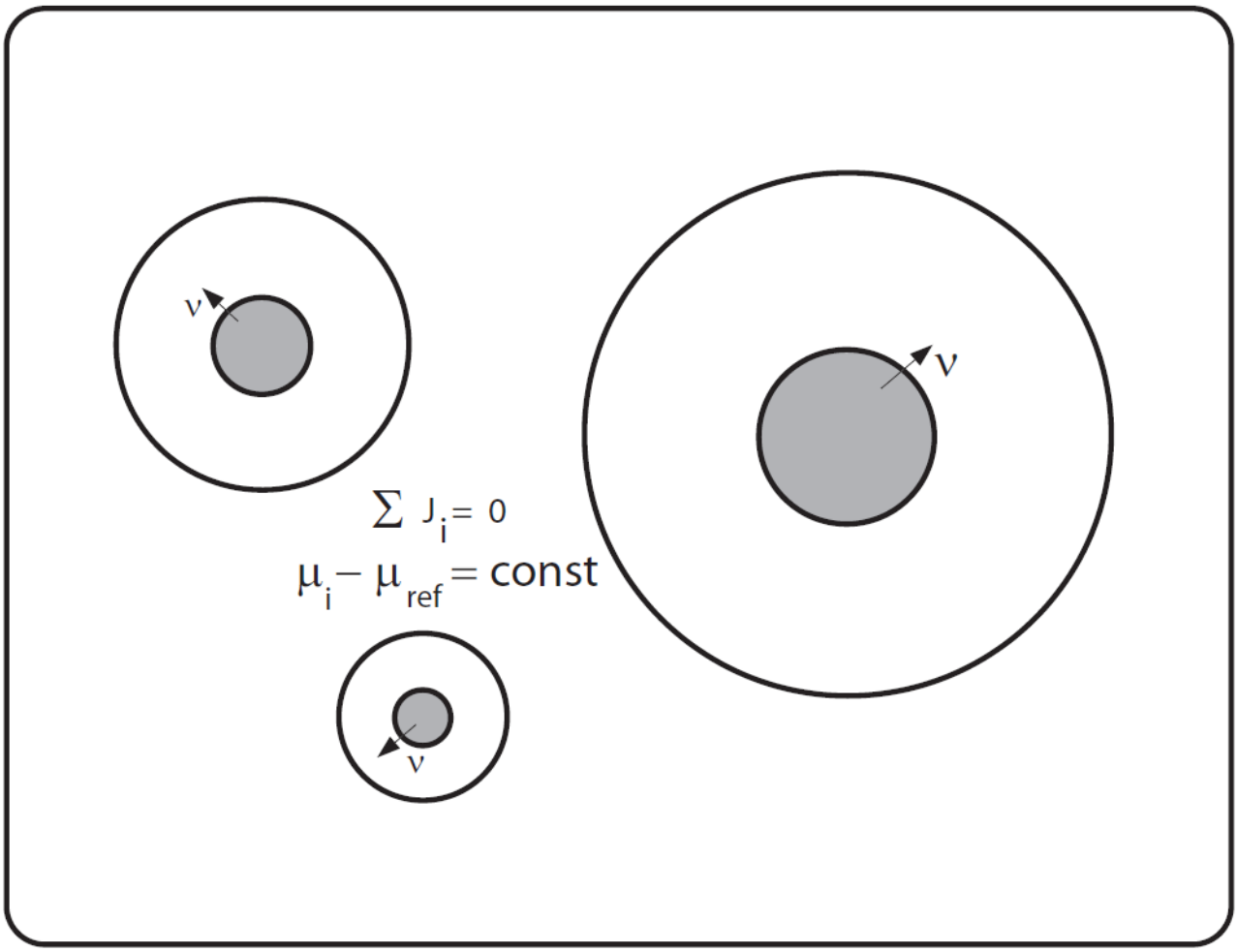

```
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ APPEND DATA FROM A CORRESPONDING SIMULATION
POST-1: @@ WITHOUT NIOBIUM
POST-1: @@
POST-1:
POST-1: app y fec.exp 0
DATASET NUMBER(s): /-1/: 1
POST-1:
POST-1: plot
```

2018.10.31.17.39.22
UPPER INTERFACE OF REGION "AUS#1"
CELL #1




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

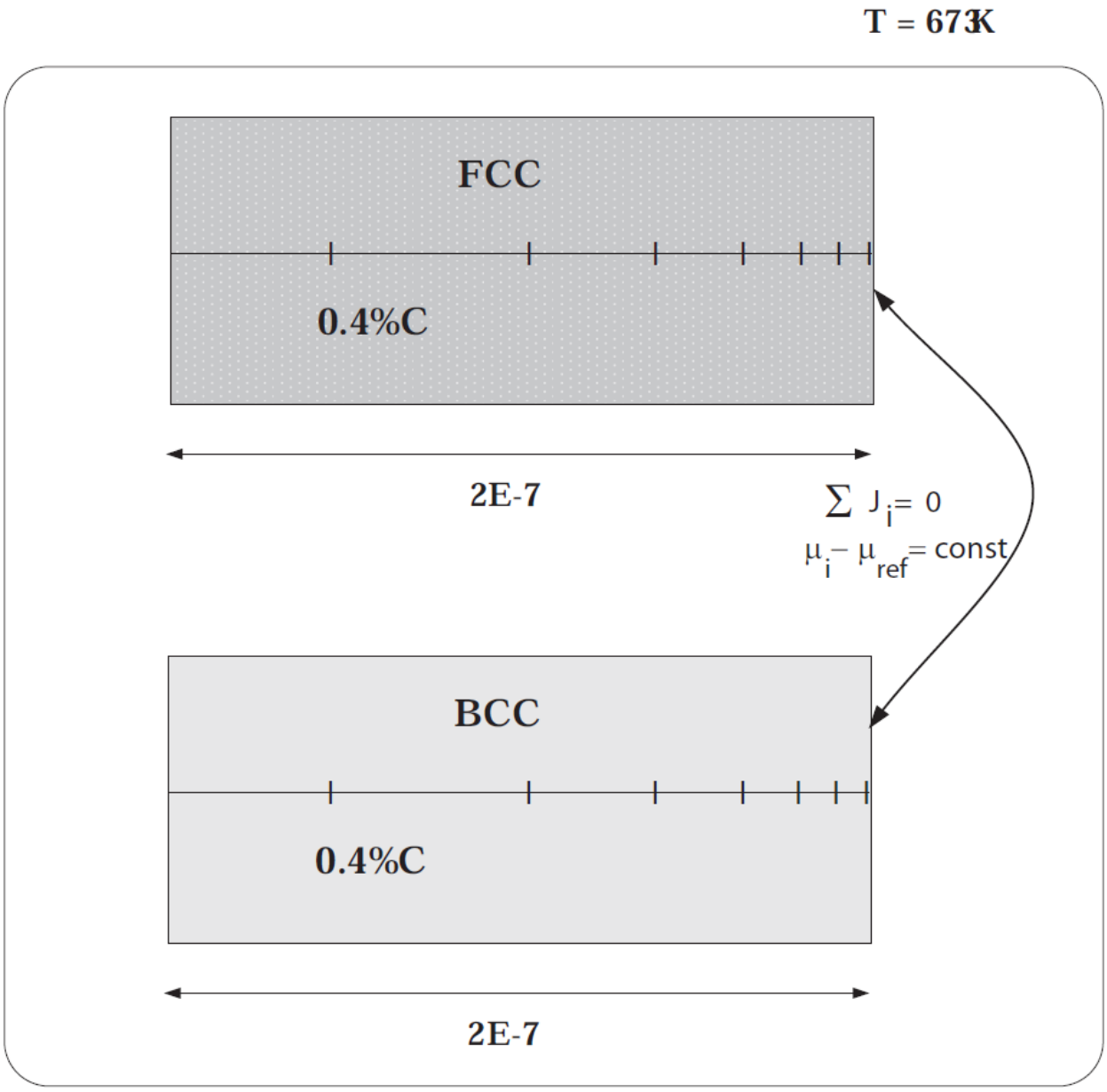
Cell Calculations



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 17825) 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: Wed Oct 31 13:18:51 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exc1\setup.DCM"SYS: ?@@
 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

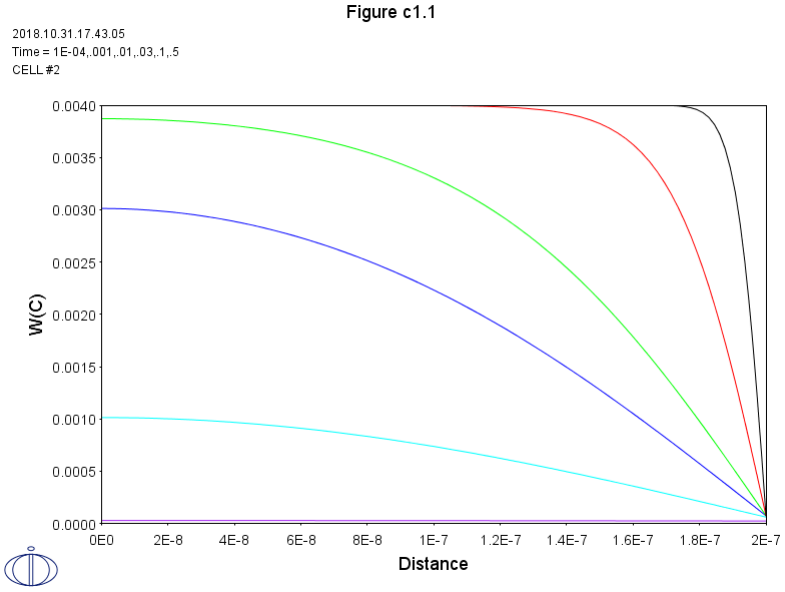
```
DIC-2>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exc1\run.DCM"DIC-2>
DIC-2>
DIC-2> @@ exc1_run.DCM
DIC-2>
DIC-2> @@
DIC-2> @@ READ THE WORKSPACE AND START THE SIMULATION
DIC-2> @@
DIC-2> go d-m
 TIME STEP AT TIME  0.00000E+00
DIC-2> read exc1
 OK
DIC> sim
 Region: 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 = .018673311178274  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
 U-FRACTION IN SYSTEM:  C = .018673311178274  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
 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 = .018673311178092  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 = .018673311178317  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                    1 seconds


output ignored...



... output resumed

  CPU time used in timestep                    0 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                    1 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                    0 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                    1 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                    0 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

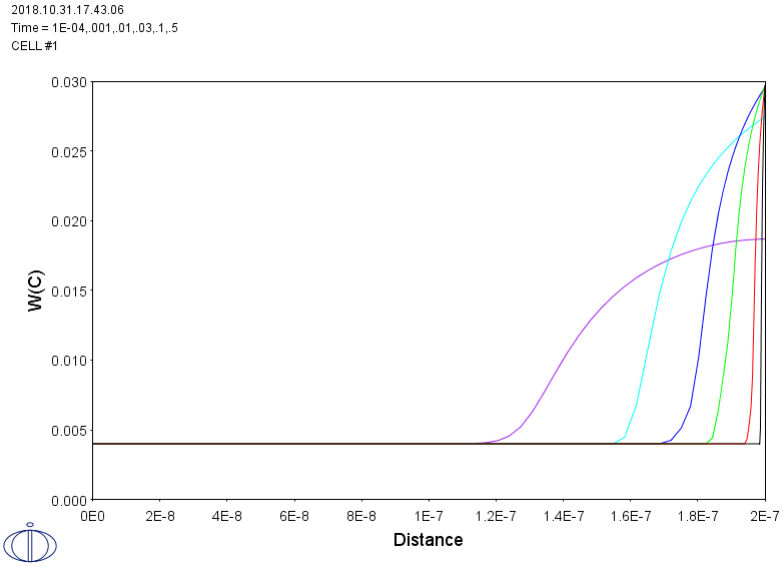
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exc1\plot.DCM"DIC>
DIC>
DIC> @@ exc1_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE c1
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go 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: plot
```

Figure c1.1



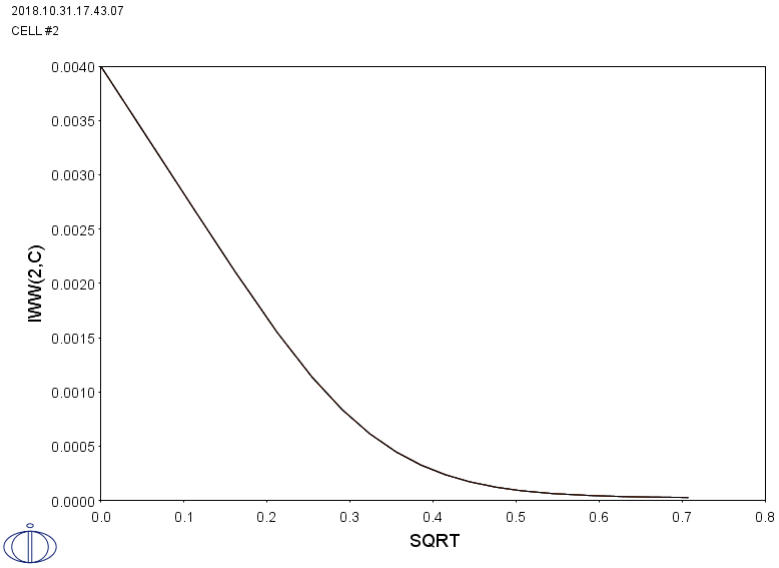

```
POST-2:
POST-2:
POST-2:
POST-2:@?<_hit_return_to_continue_>
POST-2:
POST-2: @@
POST-2: @@ DO THE SAME THING FOR THE AUSTENITE (CELL-1)
POST-2: @@
POST-2: select-cell
Number /NEXT/: 1
 CELL   1 SELECTED
POST-1: set-title Figure c1.2
POST-1: plot
```

Figure c1.2



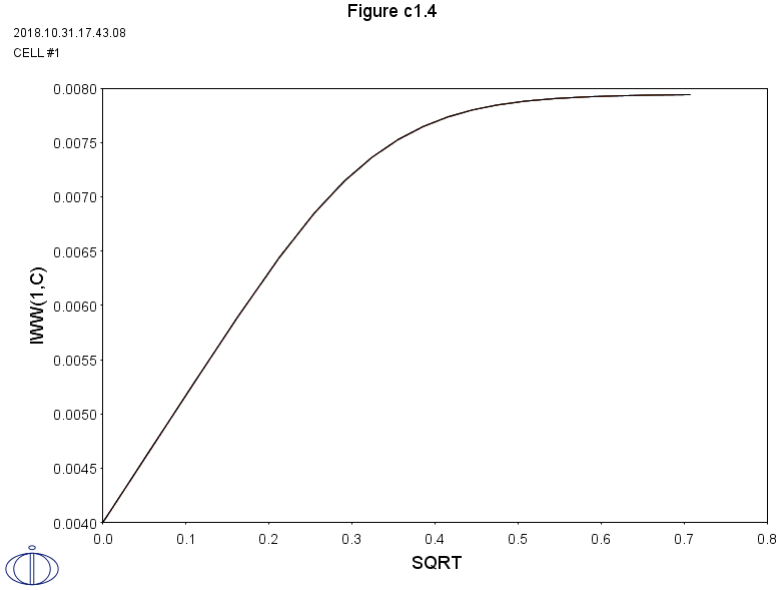

```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: @@
POST-1: @@ PLOT THE AVARAGE WEIGHT FRACTION OF CARBON IN FERRITE VS. SQUARE ROOT
POST-1: @@ OF TIME. START BY DEFINING A "SQUARE-ROOT-OF-TIME" FUNCTION.
POST-1: @@
POST-1: sel-cell 2
 CELL    2 SELECTED
POST-2: enter func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

Figure c1.3



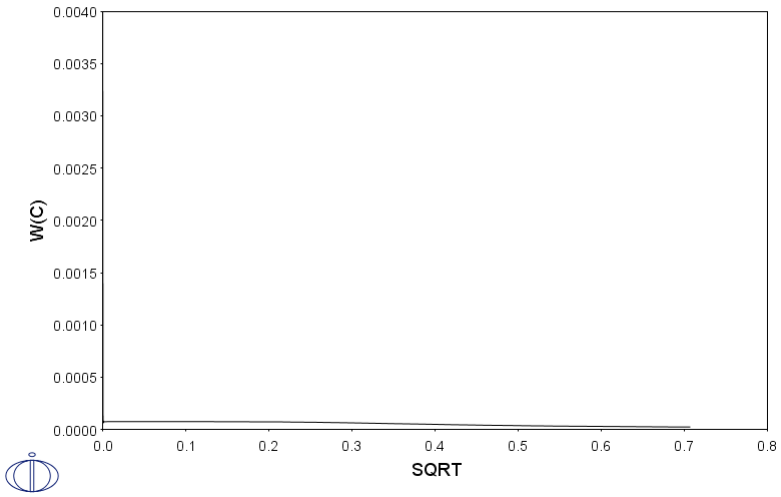

```
POST-2:
POST-2:
POST-2:
POST-2:@?<_hit_return_to_continue_>
POST-2:
POST-2: @@
POST-2: @@ DO THE SAME THING FOR THE AUSTENITE
POST-2: @@
POST-2: sel-cell 1
 CELL    1 SELECTED
POST-1: s-d-a y iww(1,c)
POST-1: set-title Figure c1.4
POST-1: plot
```

Figure c1.4




```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: @@
POST-1: @@ PLOT HOW THE CONCENTRATION IN FERRITE AT THE FERRITE/AUSTENITE BOUNDARY
POST-1: @@ V.S SQUARE ROOT OF TIME. THE  FERRITE/AUSTENITE BOUNDARY IS REPRESENTED
POST-1: @@ BY THE CELL BOUNDARY I.E. THE "LAST" INTERFACE.
POST-1: @@
POST-1: sel-cell 2
 CELL   2 SELECTED
POST-2: s-d-a y w(c)
POST-2: s-p-c interface last
POST-2: set-title Figure c1.5
POST-2: plot
```

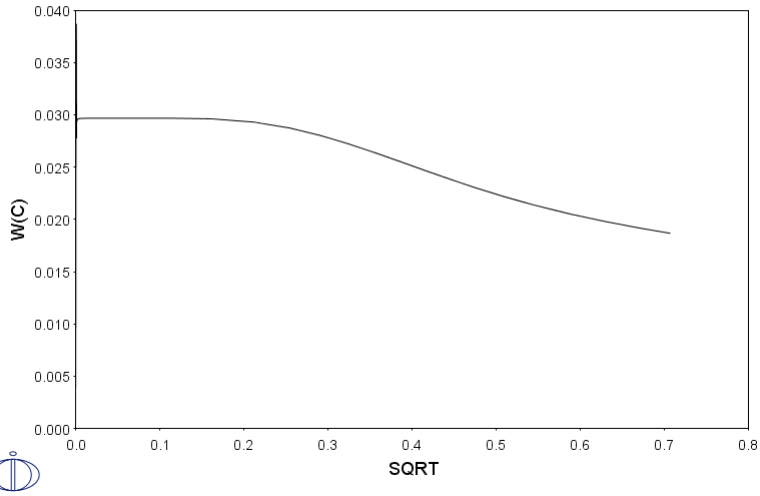
Figure c1.5




```
POST-2:
POST-2:
POST-2:
POST-2:@?<_hit_return_to_continue_>
POST-2:
POST-2: @@
POST-2: @@ DO THE SAME THING FOR THE AUSTENITE
POST-2: @@
POST-2: sel-cell 1
 CELL   1 SELECTED
POST-1: set-title Figure c1.6
POST-1: plot
```

Figure c1.6

2018.10.31.17.43.09
UPPER INTERFACE OF REGION "LAST"
CELL #1

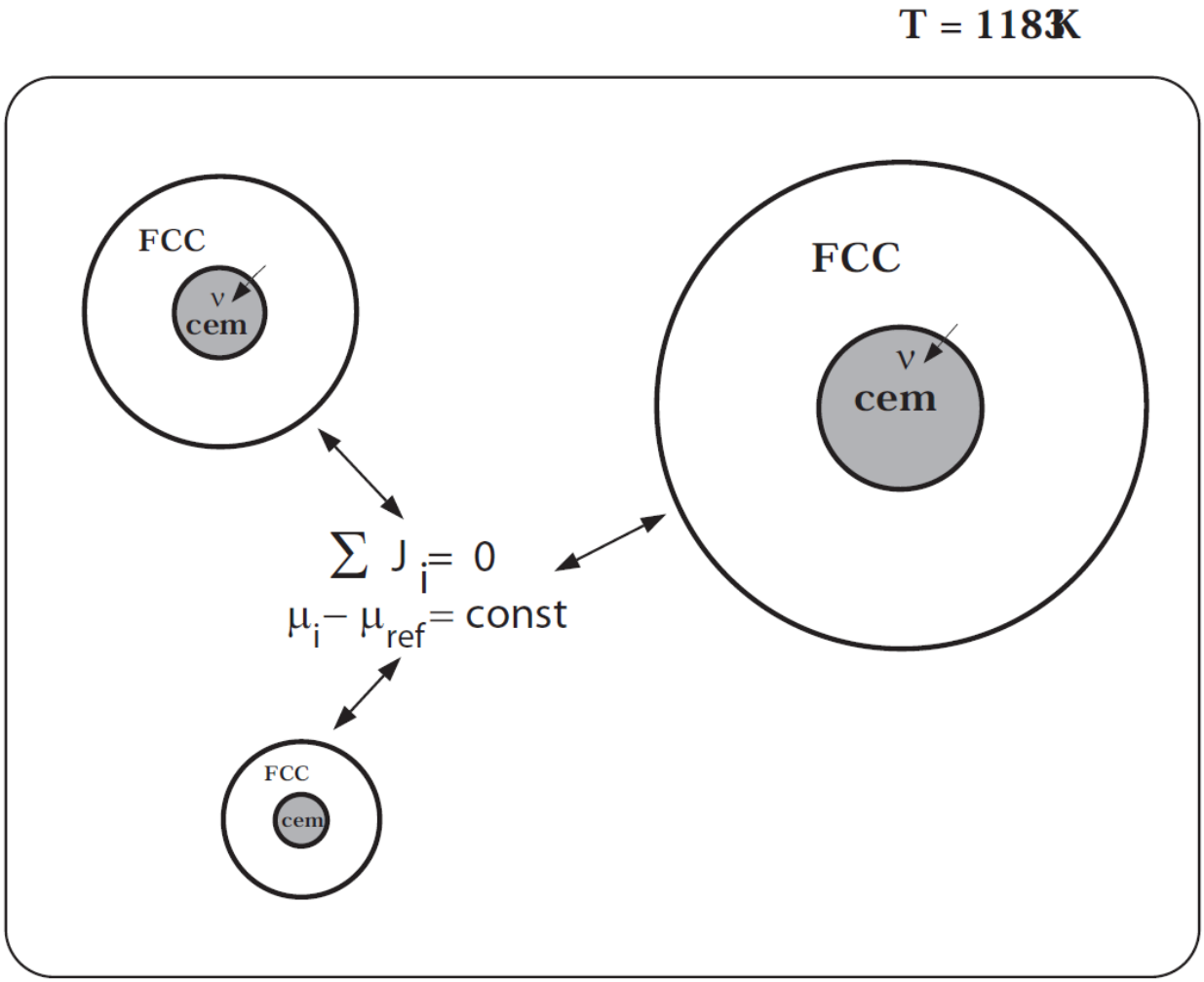



```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: set-inter
 --OK---
POST-1:
```

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
 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 17825) 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: Wed Oct 31 13:18:51 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exc2\setup.DCM"SYS: ?@@
 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

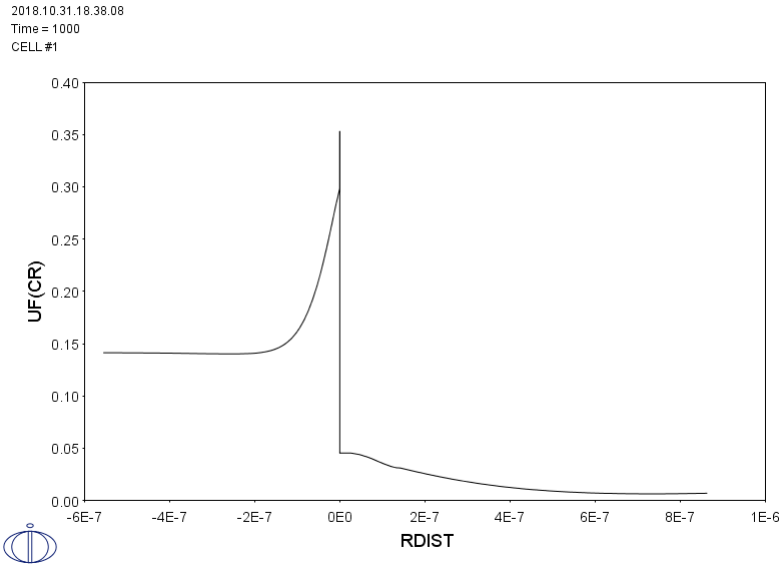
```
DIC-3>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exc2\run.DCM"DIC-3>
DIC-3>
DIC-3> @@ exc2_run.DCM
DIC-3>
DIC-3> @@
DIC-3> @@ READ THE SET UP FROM FILE AND START THE SIMULATION
DIC-3> @@
DIC-3>
DIC-3> go d-m
 TIME STEP AT TIME  0.00000E+00
DIC-3> read exc2
 OK
DIC> 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        3.584789099973641E-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        4.381093717681973E-
007        3.219088027645265E-007        2.868078269757498E-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

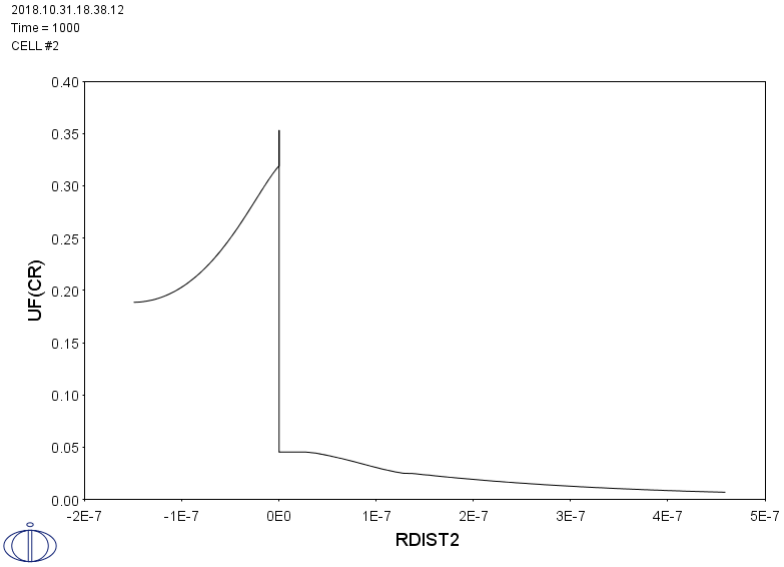
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exc2\plot.DCM"DIC>
DIC>
DIC> @@ exc2_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE c2
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go 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: plot
```

Figure C2.1



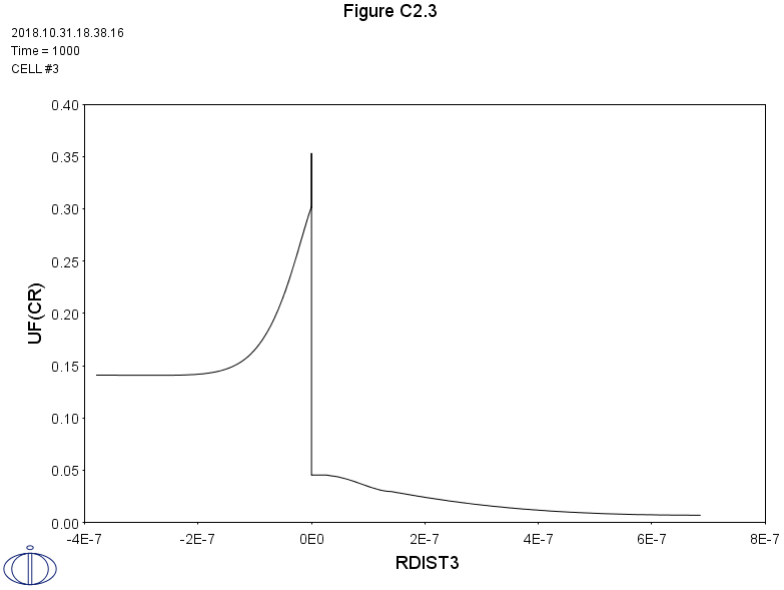

```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: @@
POST-1: @@ SELECT CELL 2
POST-1: @@
POST-1: select-cell
Number /NEXT/: 2
 CELL   2 SELECTED
POST-2:
POST-2: enter-symb
Function or table /FUNCTION/: func
NAME: rdist2
FUNCTION: gd-poi(carb,u);
POST-2:
POST-2: s-d-a x rdist2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

Figure C2.2




```
POST-2:
POST-2:
POST-2:
POST-2:@?<_hit_return_to_continue_>
POST-2:
POST-2: @@
POST-2: @@ SELECT CELL 3
POST-2: @@
POST-2: select-cell 3
 CELL   3 SELECTED
POST-3:
POST-3: enter-symb
Function or table /FUNCTION/: func
NAME: rdist3
FUNCTION: gd-poi(carb,u);
POST-3:
POST-3: s-d-a x rdist3
POST-3:
POST-3: set-title Figure C2.3
POST-3: plot
```

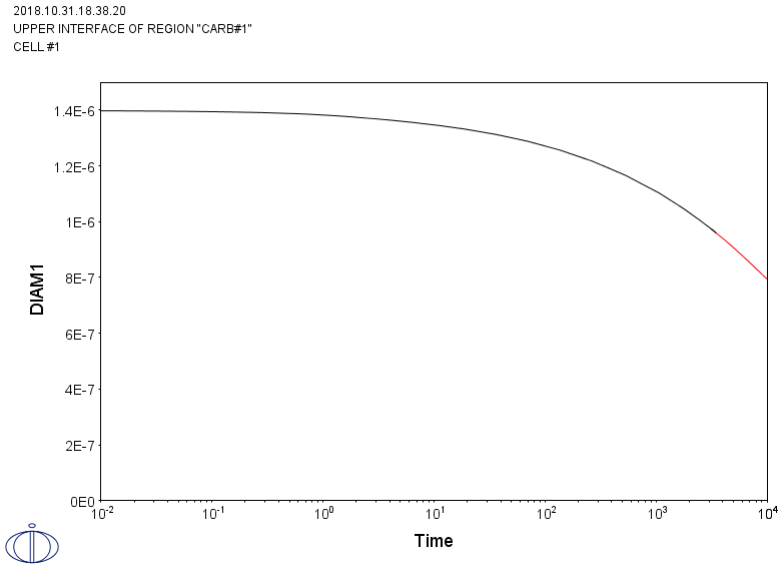
Figure C2.3




```
POST-3:
POST-3:
POST-3:
POST-3:
POST-3:@?<_hit_return_to_continue_>
POST-3:
POST-3:
POST-3: @@
POST-3: @@ ALSO PLOT HOW THE DIAMETER OF THE CEMENTITE PARTICLE VARIES
POST-3: @@ WITH TIME IN THE THREE CELLS
POST-3: @@
POST-3:
POST-3: @@
POST-3: @@ SELECT THE FIRST CELL
POST-3: @@
POST-3: sel-cell 1
 CELL   1 SELECTED
POST-1:
POST-1: s-d-a x time
  INFO: Time is set as independent variable
POST-1: s-s-s x n .01 10000
POST-1: set-axis-type x log
POST-1:
POST-1: enter func diam1=2*poi(carb,u);
POST-1: s-d-a y diam1
POST-1: s-s-s y n 0 1.5e-6
POST-1:
```

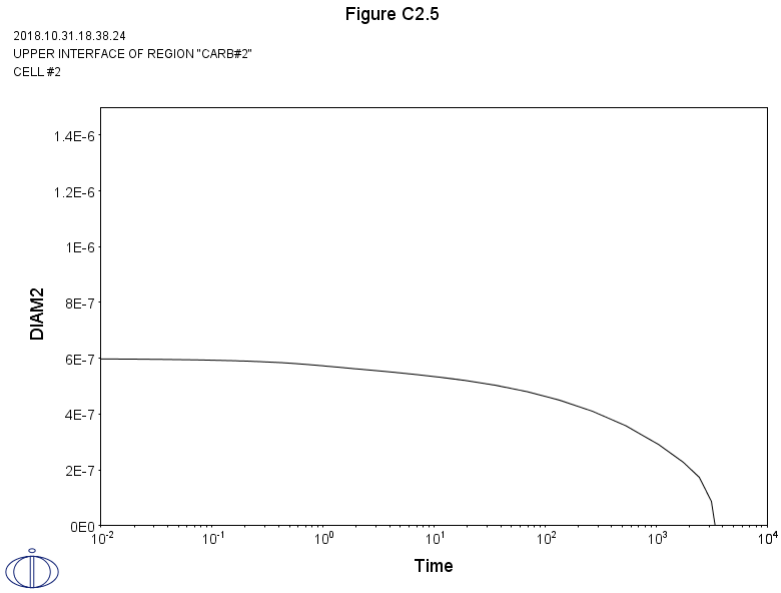
```
POST-1: s-p-c interf carb upp
POST-1:
POST-1: app n
POST-1: set-title Figure C2.4
POST-1: plot
```

Figure C2.4




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

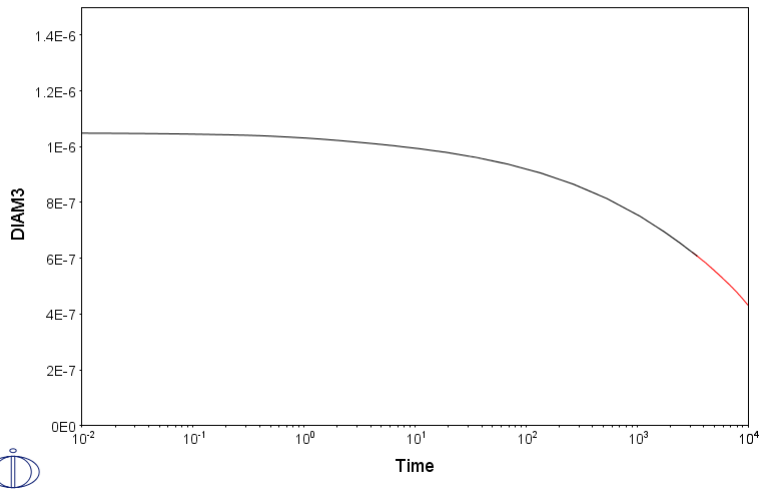
Figure C2.5




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

Figure C2.6

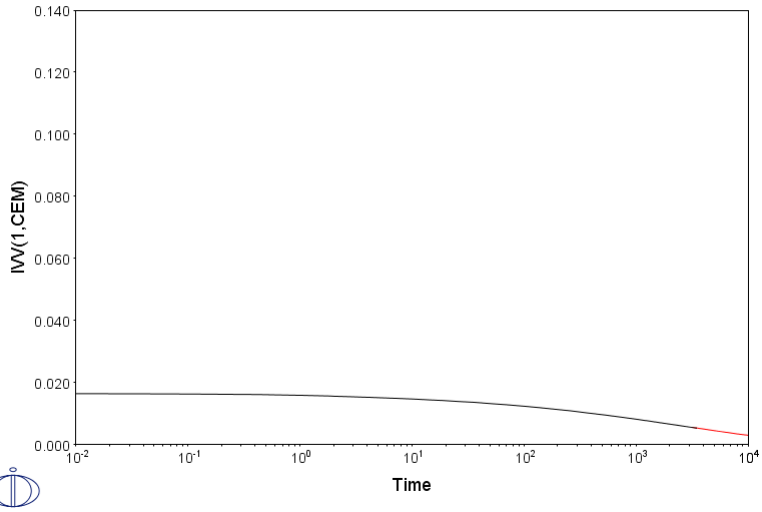
2018.10.31.18.38.28
UPPER INTERFACE OF REGION "CARB#3"
CELL #3




```
POST-3:
POST-3:
POST-3:
POST-3:
POST-3:@?<_hit_return_to_continue_>
POST-3:
POST-3: @@
POST-3: @@ NOW PLOT THE VOLUME FRACTION OF CEMENTITE IN THE THREE CELLS
POST-3: @@
POST-3: s-d-a x time
  INFO: Time is set as independent variable
POST-3: s-s-s x n .01 10000
POST-3: set-axis-type x log
POST-3:
POST-3: @@
POST-3: @@ CELL 1
POST-3: @@
POST-3: s-d-a y ivv(1,cem)
POST-3: s-s-s y n 0 0.14
POST-3:
POST-3: s-p-c integral
POST-3:
POST-3: set-title Figure C2.7
POST-3: plot
```

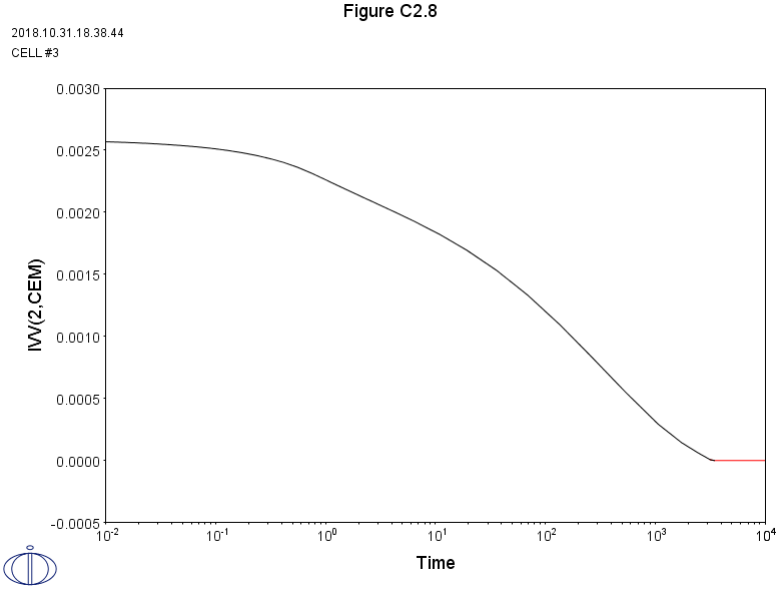
Figure C2.7

2018.10.31.18.38.35
CELL #3



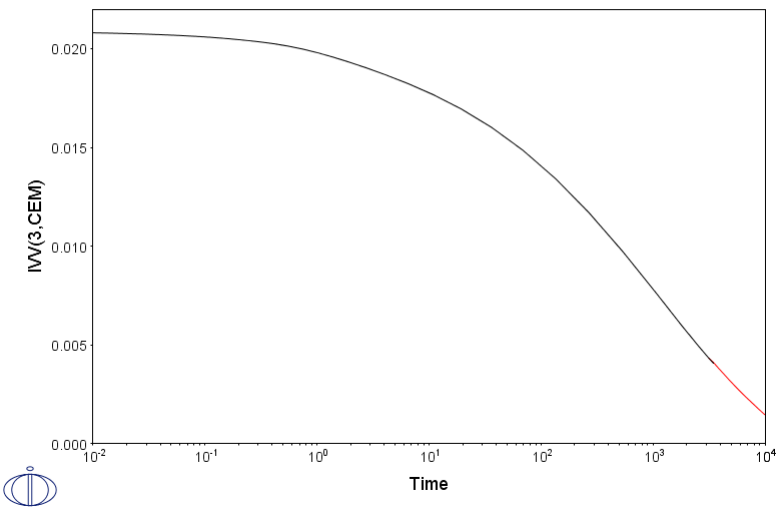

```
POST-3:
POST-3:
POST-3:
POST-3:
POST-3:@?<_hit_return_to_continue_>
POST-3:
POST-3: @@
POST-3: @@ CELL 2
POST-3: @@
POST-3: s-d-a y ivv(2,cem)
POST-3:
POST-3: set-title Figure C2.8
POST-3: plot
```

Figure C2.8




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

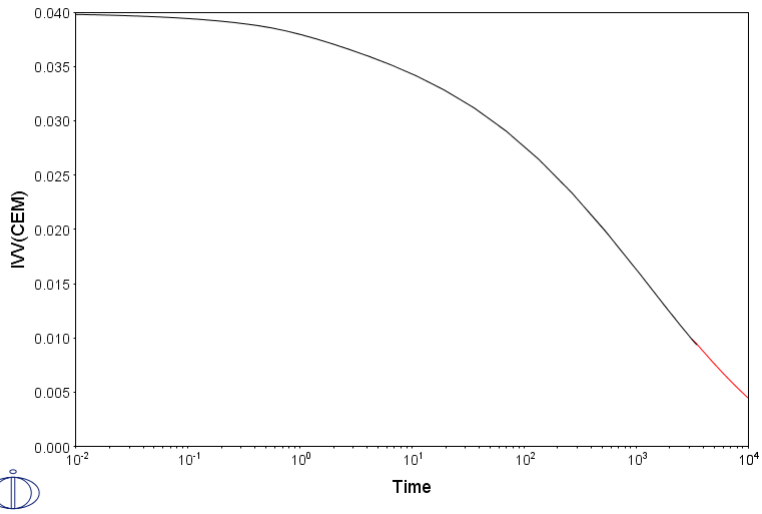
Figure C2.9




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

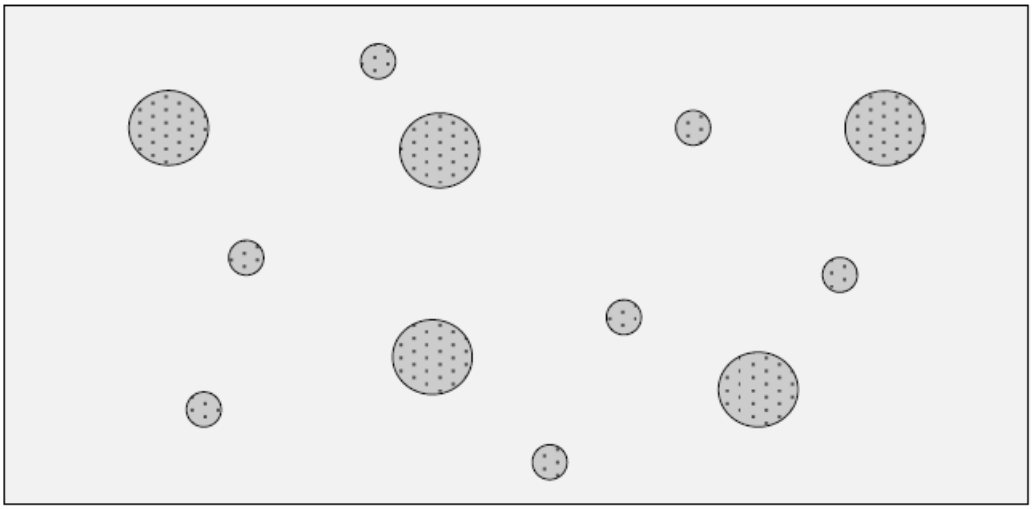
Figure C2.10

2018.10.31.18.39.05
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:
```

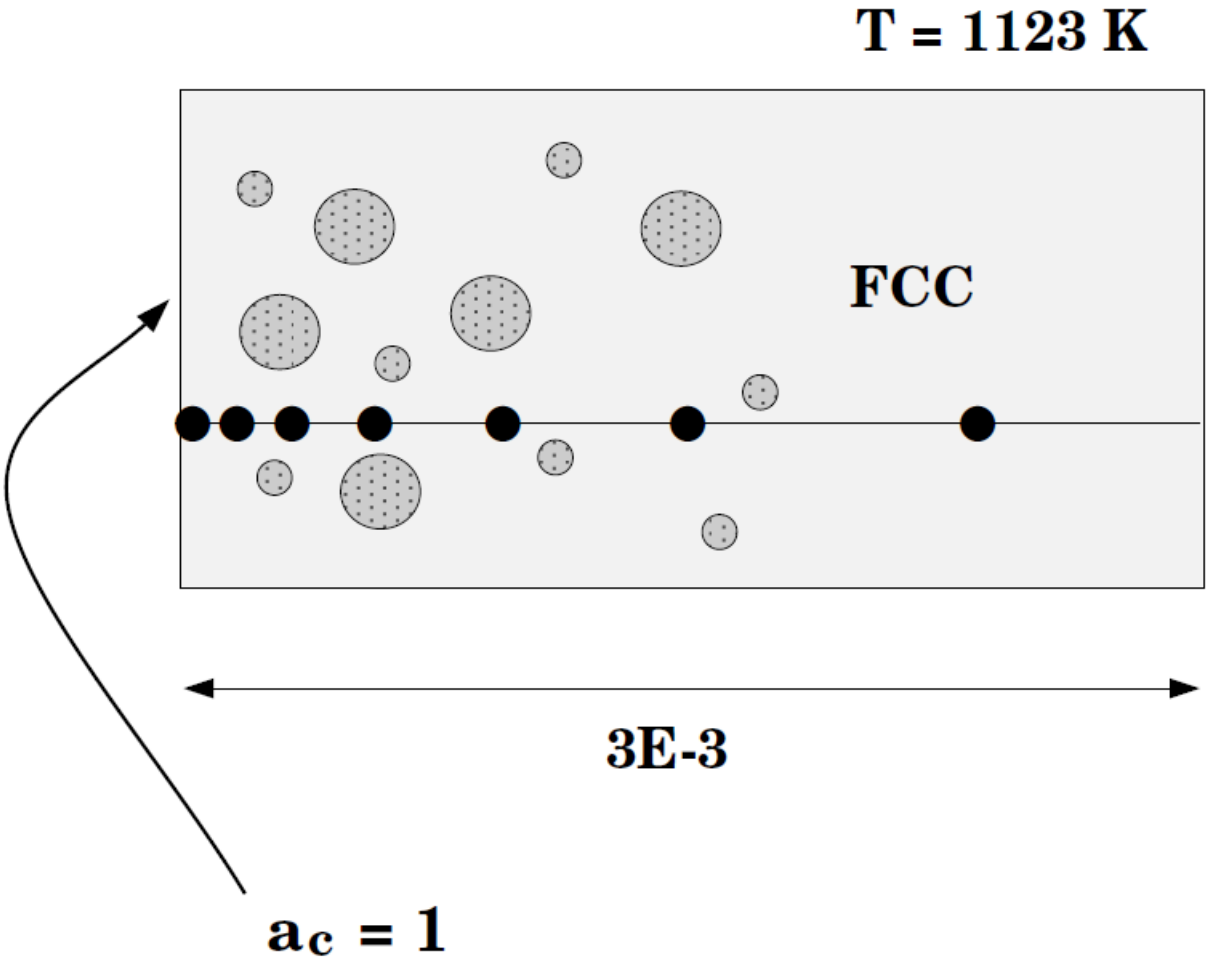
Diffusion in Dispersed Systems



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 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Wed Oct 31 13:18:51 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exd1a\setup.DCM"SYS: @@
SYS: @@ Diffusion in dispersed systems.
SYS: @@ Carburization of Ni-25%Cr alloy: Dispersed system model
SYS: @@ This example is about carburization of a Ni-25Cr alloy.
SYS: @@ In this case the M3C2 and M7C3 carbides are entered as
SYS: @@ spheroid phases in a FCC matrix. This simulation can be run
SYS: @@ with either the DISPERSED SYSTEM MODEL or the HOMOGENIZATION MODEL.
SYS: @@ In this example the DISPERSED SYSTEM MODEL is used, which requires
SYS: @@ that the default HOMOGENIZATION MODEL is disabled.
SYS: @@ With the DISPERSED SYSTEM MODEL the command
SYS: @@ ENTER_LABYRINTH_FUNCTION is used to take into account the
SYS: @@ impeding effect of dispersed phases on long-range diffusion.
SYS: @@ For the HOMOGENIZATION MODEL the command
SYS: @@ ENTER_HOMOGENIZATION_FUNCTION should be used.
SYS: @@ This case is from A. 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

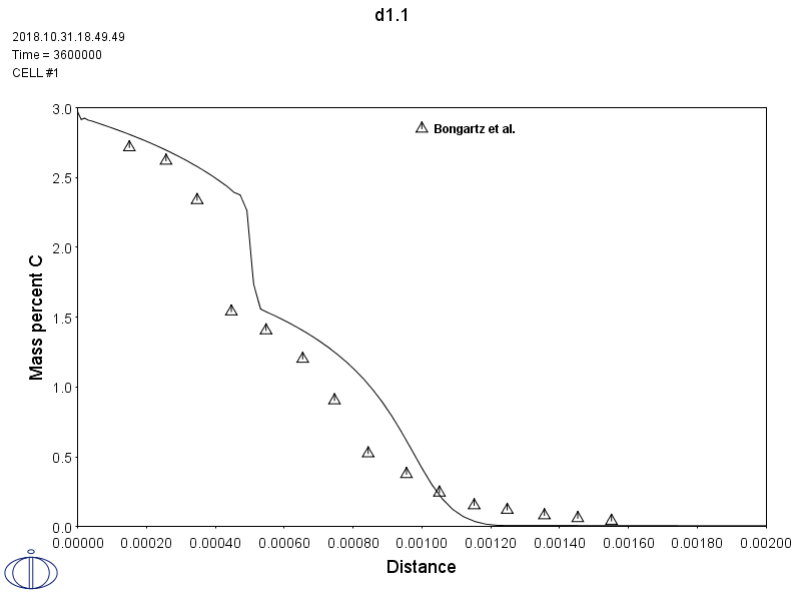
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exd1a\run.DCM"DIC>
DIC>
DIC> @@ exd1_run.DCM
DIC>
DIC> @@
DIC> @@ READ THE SETUP FILE AND START THE SIMULATION
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  0.00000E+00
 *** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
 *** ENTERING 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                    0 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                    1 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                    0 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                    1 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                    0 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                    1 seconds
TIME =   21359.693     DT =   1721.3670     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00220875177686407  CR = .273386044543294
                       NI = .726613955456706
TOTAL SIZE OF SYSTEM:  .003 [m]
 CPU time used in timestep                    0 seconds
TIME =   23159.693     DT =   1800.0000     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00232593131642948  CR = .273386043337658
                       NI = .726613956662342
TOTAL SIZE OF SYSTEM:  .003 [m]
 CPU time used in timestep                    0 seconds
TIME =   24959.693     DT =   1800.0000     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00243964458512875  CR = .273386042448499
                       NI = .726613957551501


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                    0 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                    1 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                    0 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                    1 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                    0 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                    1 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
```

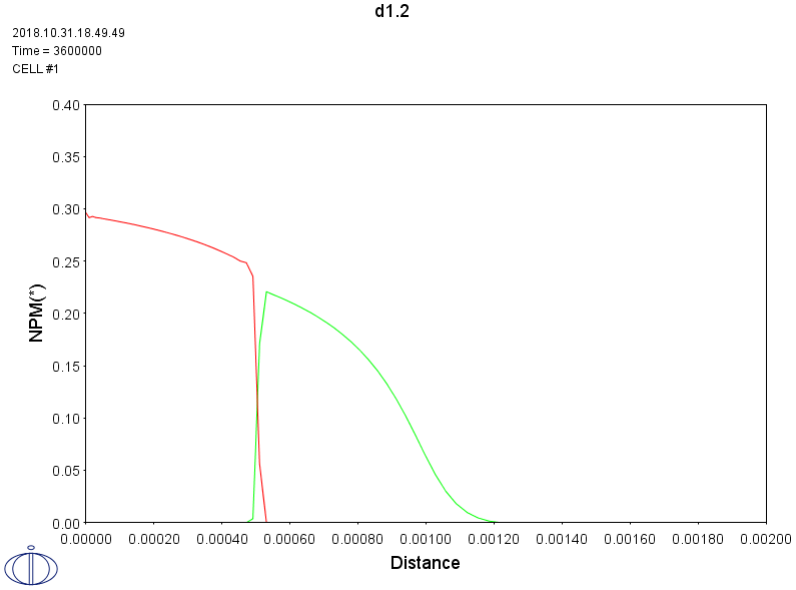
```
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3594359.7     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0316569773322023  CR = .273385942325503
                        NI = .726614057674497
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 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                    1 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
```

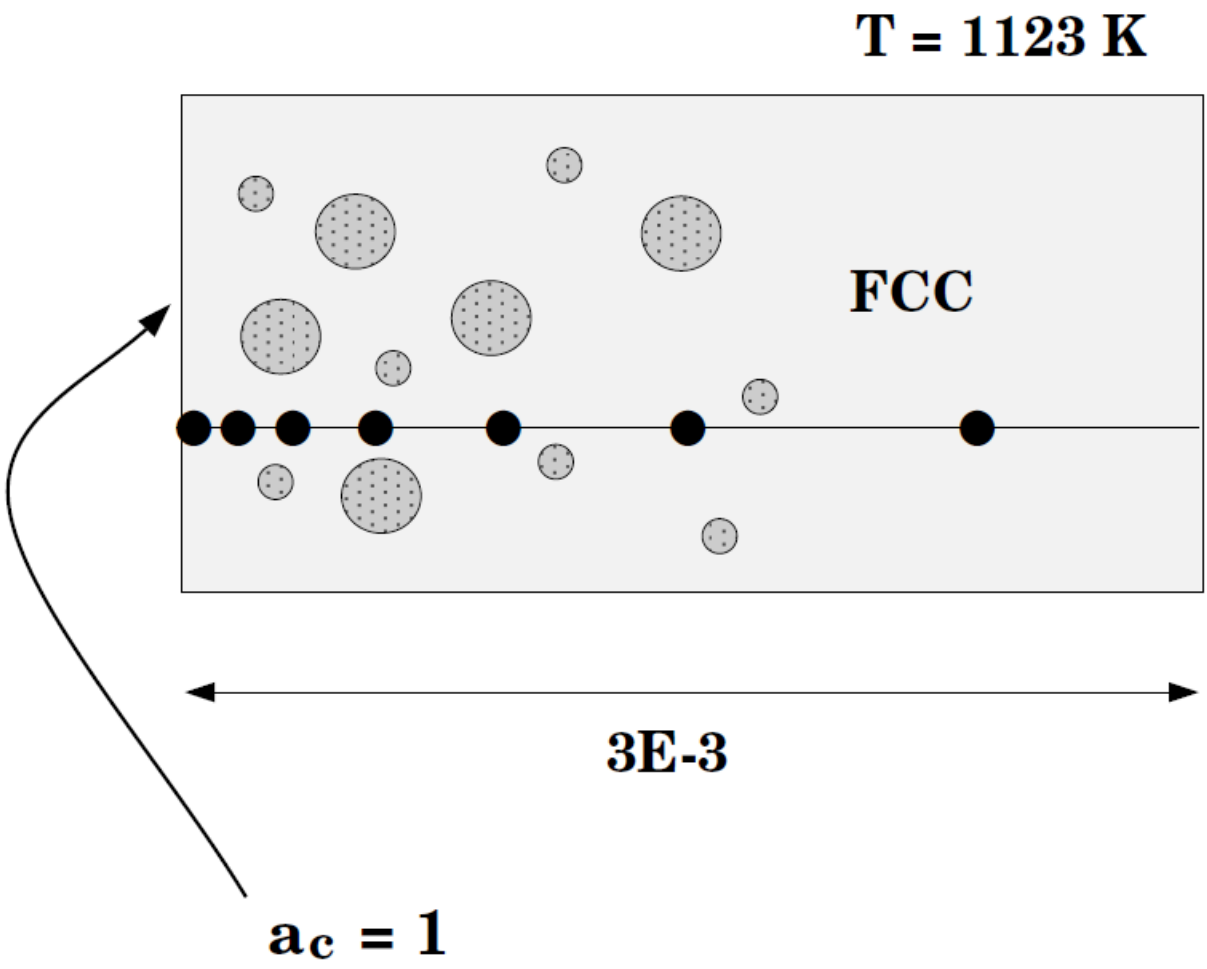



```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: set-inter
 --OK---
POST-1:
```

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 Linked: Wed Oct 31 13:18:51 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

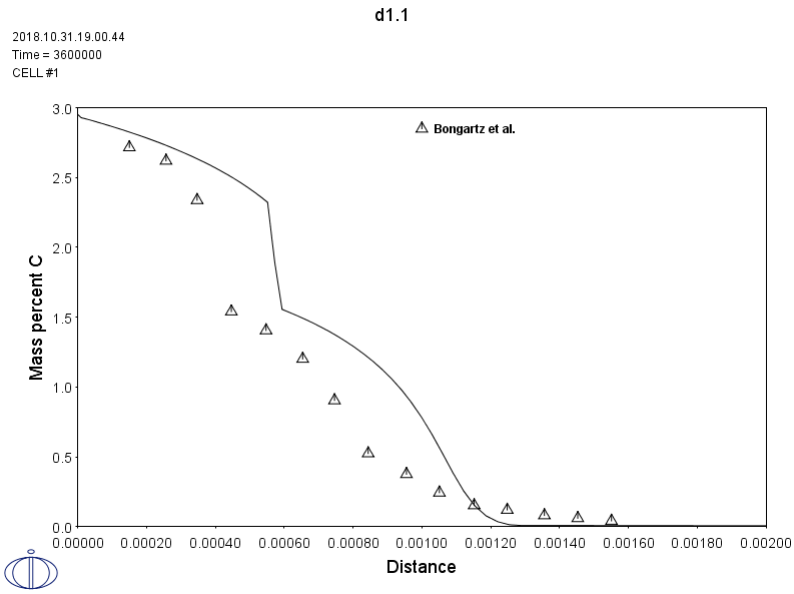
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exd1b\run.DCM"DIC>
DIC>
DIC> @@ exd1_run.DCM
DIC>
DIC> @@
DIC> @@ READ THE SETUP FILE AND START THE SIMULATION
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  0.00000E+00
 *** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
 *** ENTERING 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
Time-step converged t0=  0.25500000E-04 dt=  0.25600000E-04
 ----------------------------------
Starting time-step t0=  0.51100000E-04 dt=  0.51200000E-04
 Stage 1
Iteration #   1 sum residual **2:   0.30904909E-04
 Stage 2
 Stage 3
 Moles of elements / mole fractions in system:


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
```

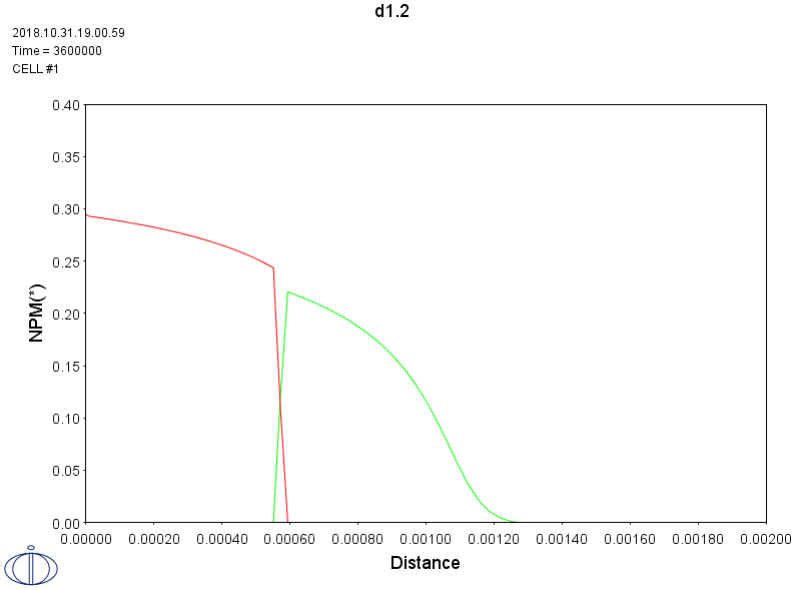
```
 DELETING TIME-RECORD FOR TIME    3417109.7
 DELETING TIME-RECORD FOR TIME    3420975.2
 DELETING TIME-RECORD FOR TIME    3424840.7
 DELETING TIME-RECORD FOR TIME    3428706.2
 DELETING TIME-RECORD FOR TIME    3432571.6
 DELETING TIME-RECORD FOR TIME    3436437.1
 DELETING TIME-RECORD FOR TIME    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:    1.00000000000000
 EFFICIENCY FACTOR:    91.5004394526733
 ------------------------------------------------
 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
```



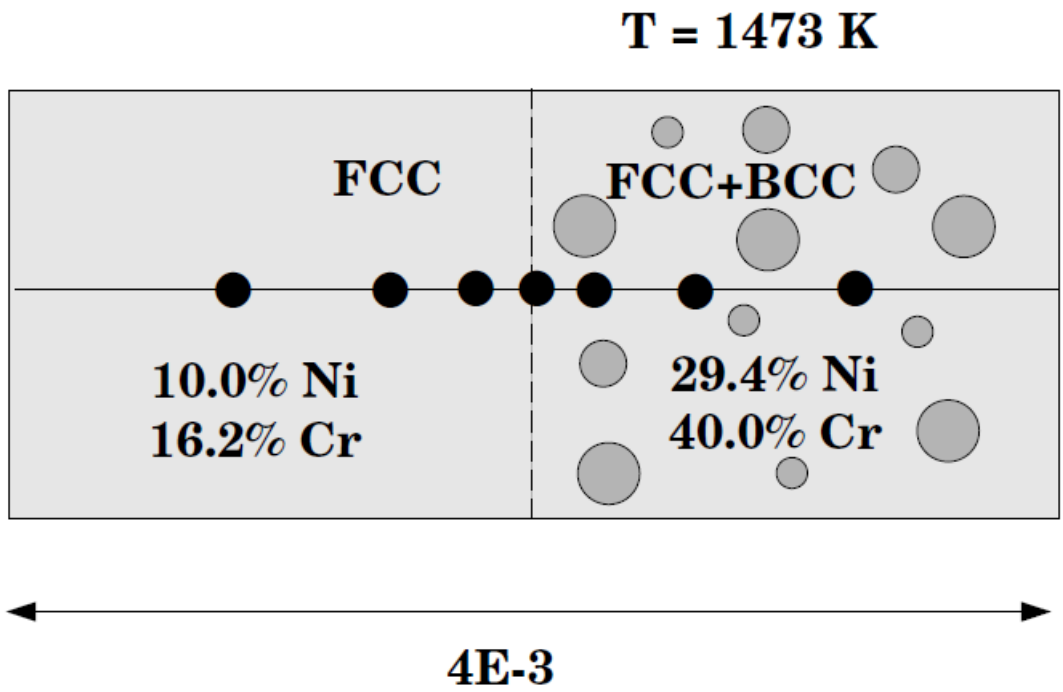

```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: set-inter
 --OK---
POST-1:
```

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 Software  (build 17825) 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: Wed Oct 31 13:18:51 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exd2a\setup.DCM"SYS: @@
SYS: @@ Diffusion in dispersed systems.
SYS: @@ Diffusion couple of Fe-Cr-Ni alloys: Dispersed system model
SYS: @@ This example calculates the interdiffusion in a diffusion
SYS: @@ couple between a two-phase (FCC+BCC) and a single-phase (FCC)
SYS: @@ Fe-Ni-Cr alloy. This case is from A. Engström: Scand. J. Met., v. 24,
SYS: @@ 1995, pp.12-20. This simulation can be run with either the DISPERSED
SYS: @@ SYSTEM MODEL or the HOMOGENIZATION MODEL.
SYS: @@ In this example the DISPERSED SYSTEM MODEL is used, which requires
SYS: @@ that the default HOMOGENIZATION MODEL is disabled.
SYS: @@ With the DISPERSED SYSTEM MODEL the command
SYS: @@ ENTER_LABYRINTH_FUNCTION is used to take into account the
SYS: @@ impeding effect of dispersed phases on long-range diffusion.
SYS: @@ For the HOMOGENIZATION MODEL the command
SYS: @@ ENTER_HOMOGENIZATION_FUNCTION should be used.
SYS: ------------------------------------------------------------------
 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                    1 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                    0 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                    1 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                    0 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                    1 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
```

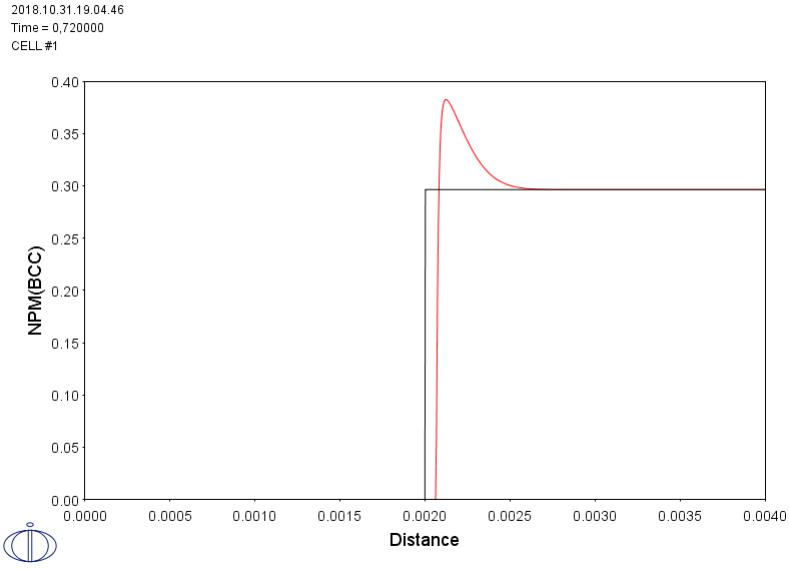
```
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0 seconds
 TIME =   63721.379     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852087307301  FE = .517209229697568
                        NI = .184938682995131
 TOTAL SIZE OF SYSTEM:  .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                    0 seconds
 TIME =   73721.379     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .29785209023541  FE = .517209210713481
                        NI = .184938699051109
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    1 seconds
 TIME =   78721.379     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852088278857  FE = .517209201664933


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                    0 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                    1 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

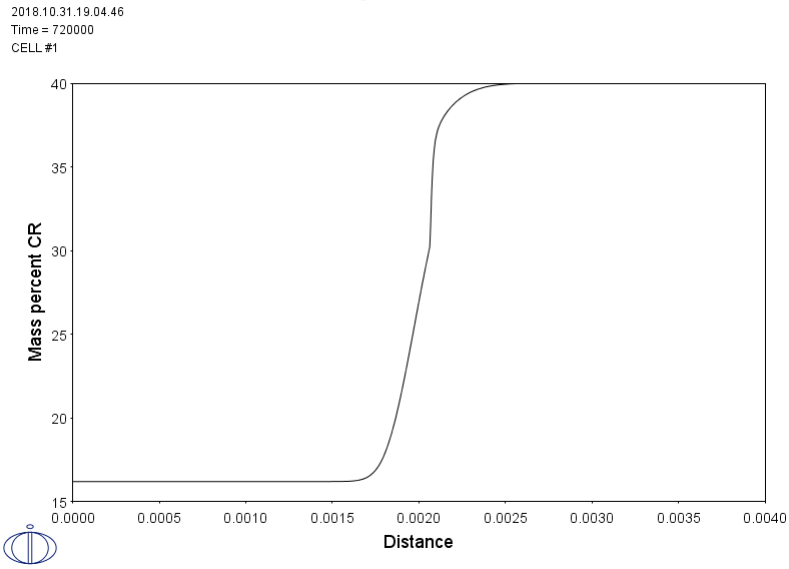
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exd2a\plot.DCM"DIC>
DIC>
DIC> @@ exd2_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE D2
DIC> @@
DIC> @@ ENTER THE DICTRA MODULE AND SPECIFY THE STORE-RESULT FILE
DIC> @@
DIC>
DIC> go d-m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

Figure D2.1



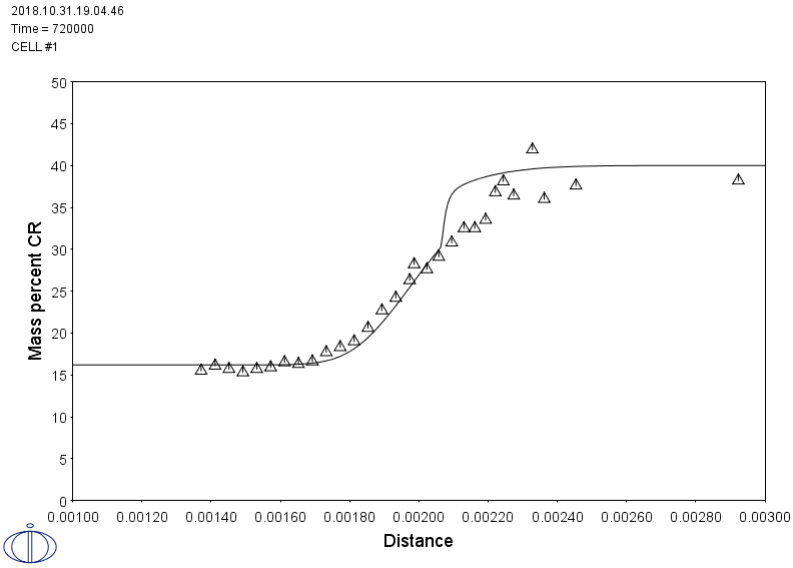

```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1: @@
POST-1: @@ NOW PLOT HOW THE AVERAGE Cr-CONCENTRATION VARIES WITH DISTANCE
POST-1: @@
POST-1: s-d-a y w-p cr
POST-1: s-p-c time last
POST-1: set-tit Figure D2.2
POST-1: plot
```

Figure D2.2



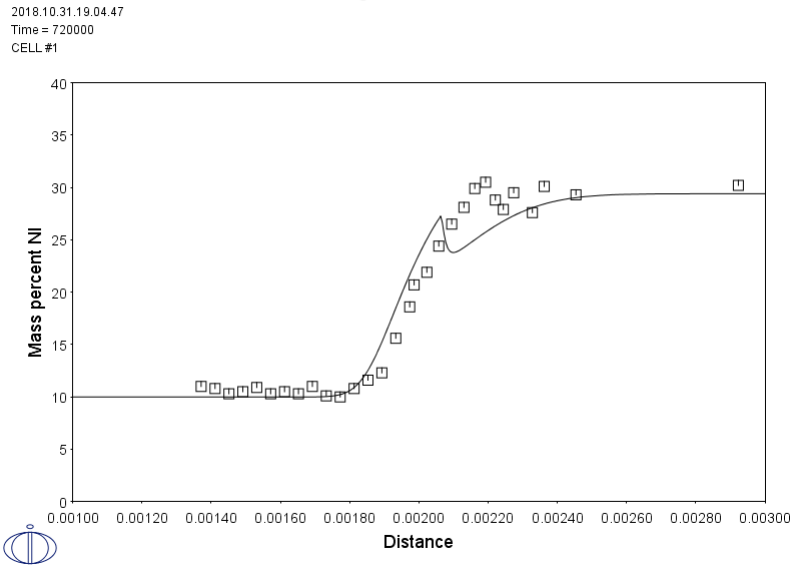
```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1: @@
POST-1: @@ NOW SELECT A BETTER SCALING AND APPEND THE EXPERIMENTAL DATA
POST-1: @@
POST-1:
POST-1: app y exd2.exp
PROLOGUE NUMBER: /0/: 1
DATASET NUMBER(s): /-1/: 4
POST-1:
POST-1: s-s-s y n 0 50
POST-1: s-s-s x n 10e-4 30e-4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

Figure D2.3




```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1: @@
POST-1: @@ NOW WE DO THE SAME FOR NICKEL
POST-1: @@
POST-1:
POST-1: s-d-a y w-p ni
POST-1:
POST-1: app y exd2.exp
PROLOGUE NUMBER: /1/: 1
DATASET NUMBER(s): /-1/: 5
POST-1:
POST-1: s-s-s x n 10e-4 30e-4
POST-1: s-s-s y n 0 40
POST-1:
POST-1: set-tit Figure D2.4
POST-1: plot
```

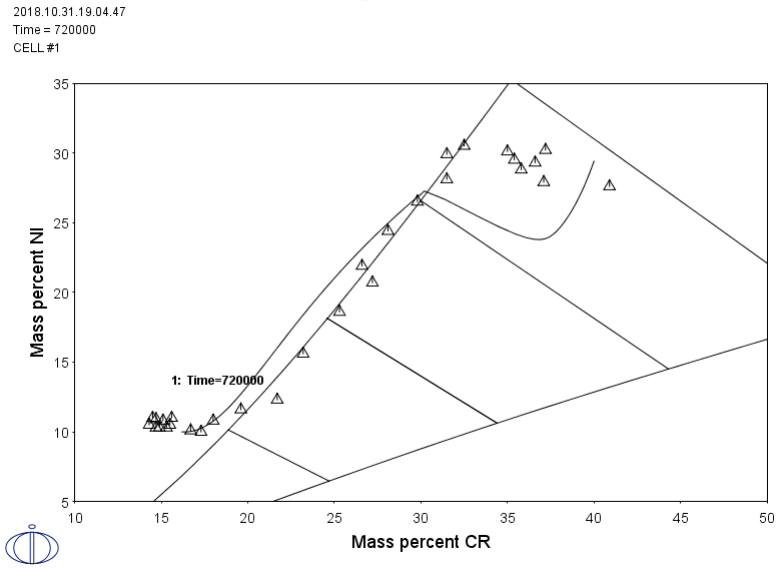
Figure D2.4




```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1: @@
POST-1: @@ LET US PLOT THE DIFFUSION PATH FOR THE COUPLE.
POST-1: @@ WE APPEND THE TERNARY PHASE-DIAGRAM CALCULATED IN THERMO-CALC
POST-1: @@ AND THE EXPERIMENTAL DATA
POST-1: @@
POST-1: s-d-a x w-p cr
POST-1: s-d-a y w-p ni
```

```
POST-1: s-i-v dis gl
POST-1: s-p-c time last
POST-1:
POST-1: app y exd2.exp
PROLOGUE NUMBER: /1/: 1
DATASET NUMBER(s): /-1/: 6 7 8
POST-1:
POST-1: s-s-s x n 10 50
POST-1: s-s-s y n 5 35
POST-1:
POST-1: set-tit Figure D2.5
POST-1: plot
```

Figure D2.5



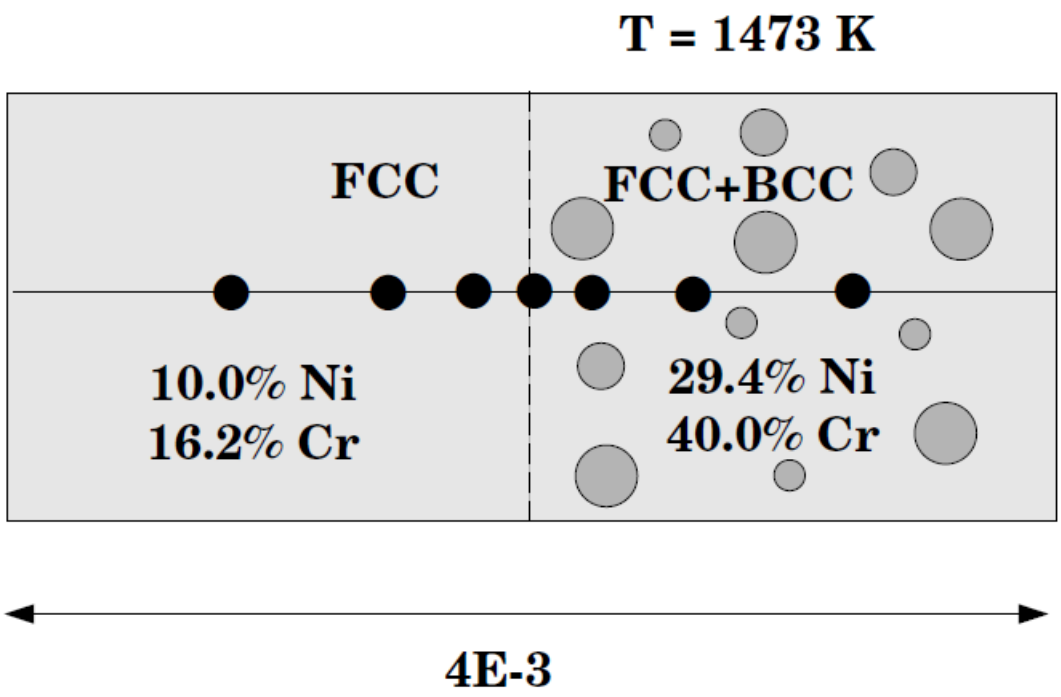

```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1: set-interactive
 --OK---
POST-1:
```

Example exd2b

Diffusion couple of Fe-Ni-Cr alloys: Homogenization model

This example calculates the interdiffusion in a diffusion couple between a two-phase (FCC+BCC) and a single-phase (FCC) Fe-Ni-Cr alloy. Initially it has a step profile. It is similar to exd2a except the default HOMOGENIZATION MODEL is used and then ENTER_HOMOGENIZATION_FUNCTION is used instead of ENTER_LABYRINTH_FUNCTION.

This case is from A. Engström: Scand. J. Met., vol. 24, 1995, pp.12-20.



exd2b-setup

```
About Linked: Wed Oct 31 13:18:51 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exd2b\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 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
```

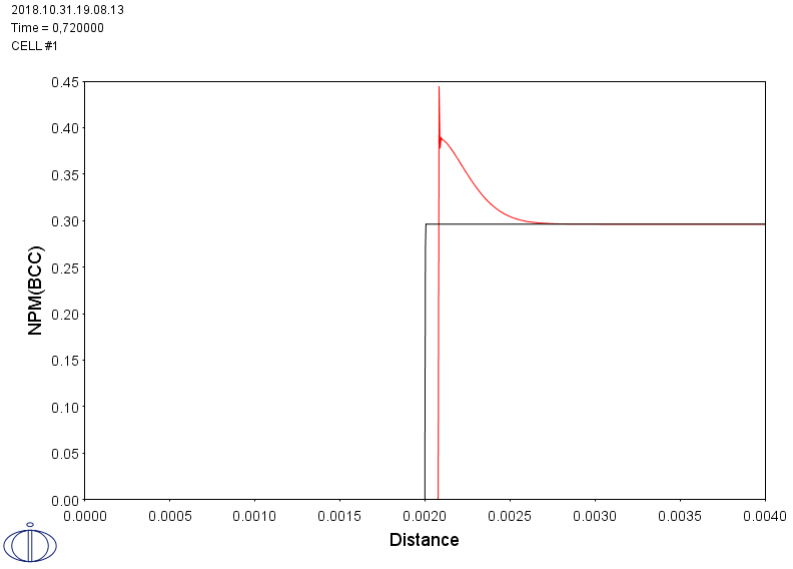
```
Time-step converged t0=  0.25500000E-04 dt=  0.25600000E-04
 ----------------------------------
Starting time-step t0=  0.51100000E-04 dt=  0.51200000E-04
 Stage 1
 Stage 2
 Stage 3
 Moles of elements / mole fractions in system:
CR   0.11913706E-02 /   0.29784265
FE   0.20689093E-02 /   0.51722732
NI   0.73972013E-03 /   0.18493003
Time-step converged t0=  0.51100000E-04 dt=  0.51200000E-04
 ----------------------------------
Starting time-step t0=  0.10230000E-03 dt=  0.10240000E-03
 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


output ignored...



... output resumed

Iteration #  14 sum residual **2:   0.61349107E-01
 Stage 2
Iteration #   1 sum residual **2:    83.644681
Iteration #   2 sum residual **2:    13.751199
Iteration #   3 sum residual **2:   0.16951888
 Stage 3
Iteration #   1 sum residual **2:    9.8444236
Iteration #   2 sum residual **2:    3.1206706
Iteration #   3 sum residual **2:   0.25006121
 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:    1585900.5
Iteration #   2 sum residual **2:    1496341.9
Iteration #   3 sum residual **2:    1360203.1
Iteration #   4 sum residual **2:    351907.37
Iteration #   5 sum residual **2:    19634.313
Iteration #   6 sum residual **2:    903.73486
Iteration #   7 sum residual **2:    680.84539
Iteration #   8 sum residual **2:    658.95302
Iteration #   9 sum residual **2:    644.28389
Iteration #  10 sum residual **2:    529.79761
Iteration #  11 sum residual **2:    17.588966
Iteration #  12 sum residual **2:    1.9463055
 Stage 2
Iteration #   1 sum residual **2:    141.26788
Iteration #   2 sum residual **2:    71.353255
Iteration #   3 sum residual **2:    12.036341
Iteration #   4 sum residual **2:    2.0004532
Iteration #   5 sum residual **2:   0.75629179E-02
 Stage 3
Iteration #   1 sum residual **2:    827.85449
Iteration #   2 sum residual **2:    121.13686
Iteration #   3 sum residual **2:    4.5534326
Iteration #   4 sum residual **2:   0.19172749
 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:    1.00000000000000
 EFFICIENCY FACTOR:    36.1555928865203
 ------------------------------------------------
 DEALLOCATING
 ------------------------------------------------

 TIMESTEP AT     720000.000     SELECTED

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

exd2b-plot

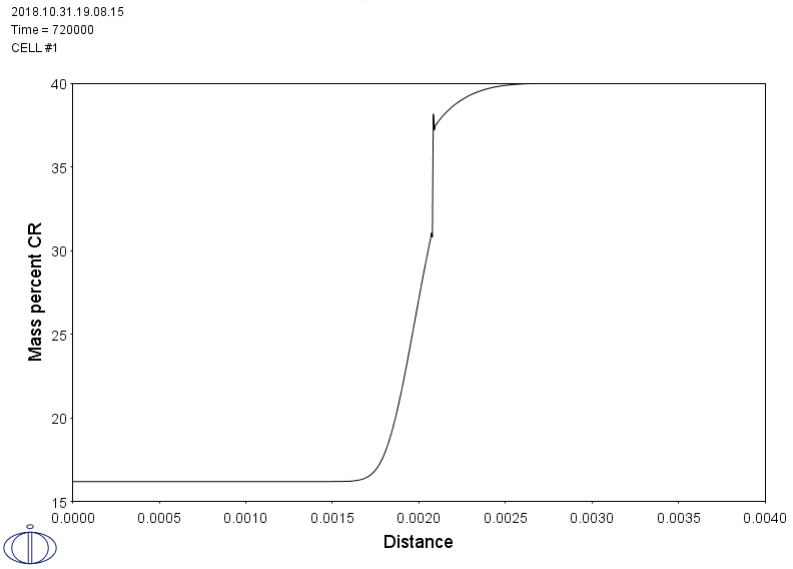
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exd2b\plot.DCM"DIC>
DIC>
DIC> @@ exd2_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE D2
DIC> @@
DIC> @@ ENTER THE DICTRA MODULE AND SPECIFY THE STORE-RESULT FILE
DIC> @@
DIC>
DIC> go d-m
 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: plot
```

Figure D2.1



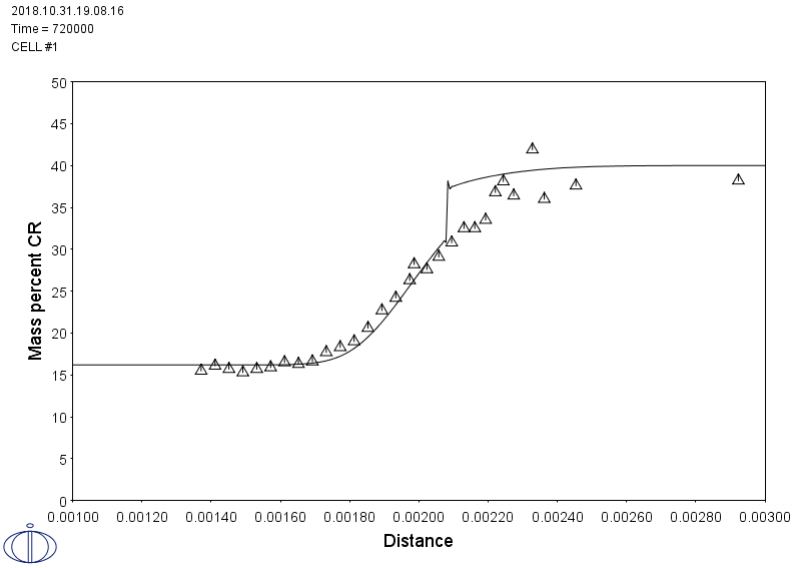

```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1: @@
POST-1: @@ LET US NOW PLOT HOW THE AVERAGE CR-CONCENTRATION VARIES WITH DISTANCE
POST-1: @@
POST-1: s-d-a y w-p cr
POST-1: s-p-c time last
POST-1: set-tit Figure D2.2
POST-1: plot
```

Figure D2.2



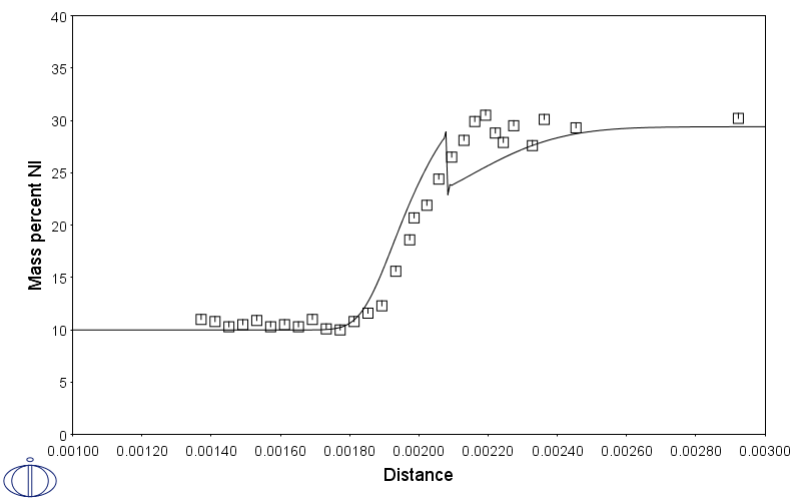
```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1: @@
POST-1: @@ WE SELECT A BETTER SCALING AND APPEND EXPERIMENTAL DATA
POST-1: @@
POST-1:
POST-1: app y exd2.exp
PROLOGUE NUMBER: /0/: 1
DATASET NUMBER(s): /-1/: 4
POST-1:
POST-1: s-s-s y n 0 50
POST-1: s-s-s x n 10e-4 30e-4
POST-1: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

Figure D2.3




```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1: @@
POST-1: @@ NOW WE DO THE SAME FOR NICKEL
POST-1: @@
POST-1:
POST-1: s-d-a y w-p ni
POST-1:
POST-1: app y exd2.exp
PROLOGUE NUMBER: /1/: 1
DATASET NUMBER(s): /-1/: 5
POST-1:
POST-1: s-s-s x n 10e-4 30e-4
POST-1: s-s-s y n 0 40
POST-1:
POST-1: set-tit Figure D2.4
POST-1: plot
```

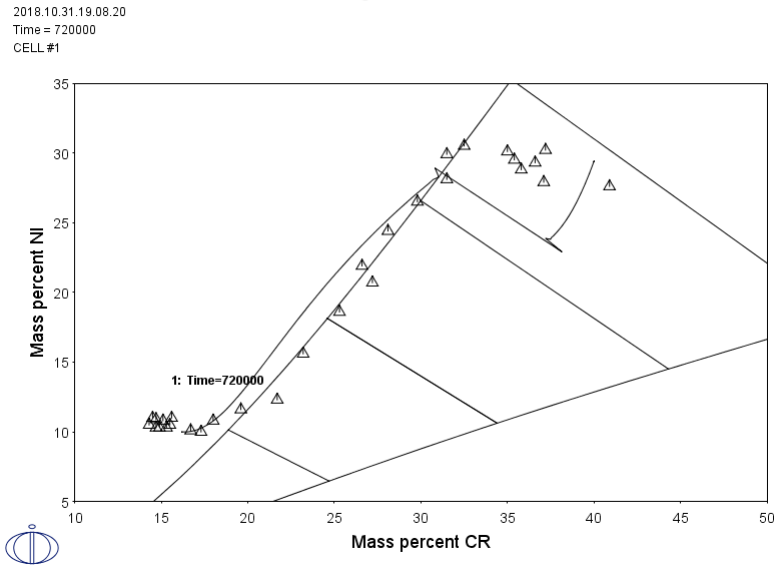
Figure D2.4




```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1: @@
POST-1: @@ LET US PLOT THE DIFFUSION PATH FOR THE COUPLE
POST-1: @@ WE APPEND THE TERNARY PHASE-DIAGRAM CALCULATED IN THERMO-CALC
POST-1: @@ AND THE EXPERIMENTAL DATA
POST-1: @@
POST-1: s-d-a x w-p cr
POST-1: s-d-a y w-p ni
```

```
POST-1: s-i-v dis gl
POST-1: s-p-c time last
POST-1:
POST-1: app y exd2.exp
PROLOGUE NUMBER: /1/: 1
DATASET NUMBER(s): /-1/: 6 7 8
POST-1:
POST-1: s-s-s x n 10 50
POST-1: s-s-s y n 5 35
POST-1:
POST-1: set-tit Figure D2.5
POST-1: plot
```

Figure D2.5

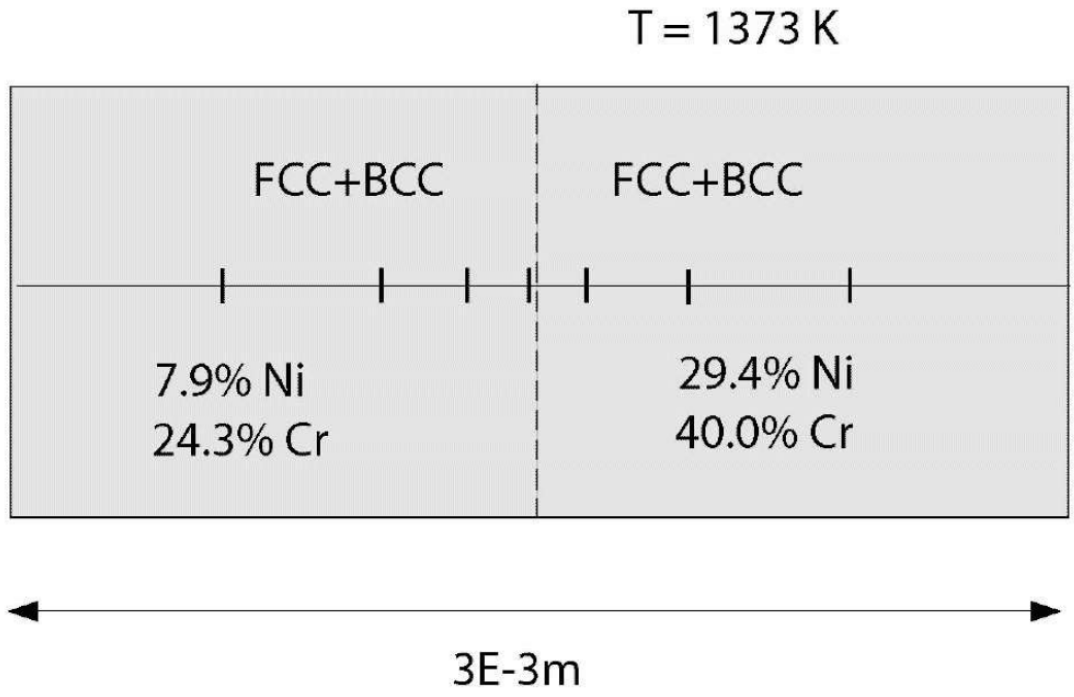



```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1: set-interactive
 --OK---
POST-1:
```

Example exd3

Diffusion couple of Fe-Ni-Cr alloys: Homogenization Model

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



exd3-setup

```
About Linked: Wed Oct 31 13:18:51 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exd3\setup.DCM.test"SYS: NO SUCH COMMAND, USE HELP
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: NO SUCH COMMAND, USE HELP
SYS:
SYS:SYS:
SYS:
SYS: THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

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

 VA                      /-  DEFINED
TDB_FEDEMO: FE                      CR                      NI
   DEFINED
TDB_FEDEMO: LIQUID:L                BCC_A2                  CHI_A12
 FCC_A1                  HCP_A3                  LAVES_PHASE_C14
 SIGMA  REJECTED
TDB_FEDEMO: BCC_A2                  FCC_A1  RESTORED
TDB_FEDEMO: 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: Current database: Fe-Alloys Mobility demo database v2.0

 VA  DEFINED
APP: FE                     CR                      NI
   DEFINED
APP: BCC_A2                 FCC_A1  REJECTED
APP: BCC_A2                 FCC_A1  RESTORED
APP: 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: NO TIME STEP DEFINED
DIC>
DIC>DIC>
DIC>DIC>
DIC>REGION NAME :DIC>
DIC>REGION NAME : /FECRNI/:WIDTH OF REGION /1/:TYPE /LINEAR/:NUMBER OF POINTS /50/:VALUE OF R IN THE GEOMETRICAL SERIE FOR LOWER PART OF REGION
DIC>ACTIVE OR INACTIVE PHASE /ACTIVE/:REGION NAME : /FECRNI/:PHASE TYPE /MATRIX/:PHASE NAME: /NONE/:DIC>
DIC>ACTIVE OR INACTIVE PHASE /ACTIVE/:REGION NAME : /FECRNI/:PHASE TYPE /MATRIX/:PHASE NAME: /NONE/:DIC>
DIC>REGION NAME : /FECRNI/:PHASE NAME: /FCC_A1/:DEPENDENT COMPONENT ? /NI/:COMPOSITION TYPE /MOLE_FRACTION/:PROFILE FOR /CR/:TYPE /LINEAR/:PROF
DIC>REGION NAME : /FECRNI/:PHASE NAME: /FCC_A1/:USE EQUILIBRIUM VALUE /Y/:DIC>
DIC>END TIME FOR INTEGRATION /.1/:AUTOMATIC TIMESTEP CONTROL /YES/:MAX TIMESTEP DURING INTEGRATION /36000/:INITIAL TIMESTEP : /1E-
07/:SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:DIC>
DIC>DIC>DIC>NS01A PRINT CONTROL : /0/:FLUX CORRECTION FACTOR : /1/:NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/:CHECK INTERFACE POSITION /N
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 I
DIC>
DIC>DIC>DIC>DIC>DIC>DIC> INFO: HOMOGENIZATION MODEL ENABLED
DIC>
DIC>DIC>DIC>DIC>DIC>ENTER HOMOGENIZATION FUNCTION # /5/: SELECTED FUNCTION IS HASHIN-SHTRIKMAN BOUND: GENERAL LOWER
DIC>
DIC>
DIC>
DIC>DIC>
DIC>
DIC> --OK---
DIC>
```

exd3-run

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exd3\run.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC> TIME STEP AT TIME  0.00000E+00
DIC> OK
DIC>
DIC> 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
```

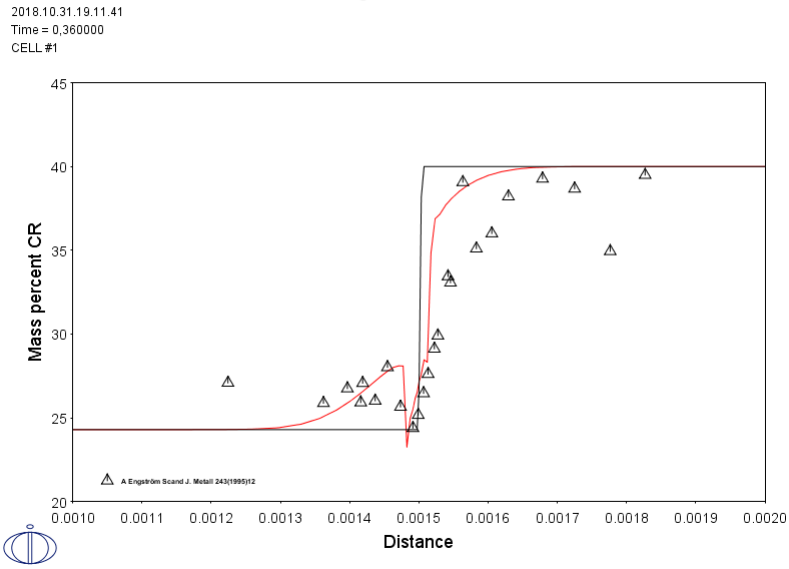
```
 Stage 1
Iteration #   1 sum residual **2:    24933.971
Iteration #   2 sum residual **2:    200.02314
Iteration #   3 sum residual **2:    2.7825925
Iteration #   4 sum residual **2:   0.14360047E-02
 Stage 2
Iteration #   1 sum residual **2:    6.6165731
Iteration #   2 sum residual **2:   0.11349870E-02
 Stage 3
Iteration #   1 sum residual **2:   0.25821584
 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=   255.00000     dt=   256.00000
 ----------------------------------
 Saving results
 ----------------------------------
Starting time-step t0=   511.00000     dt=   256.00000
 Stage 1
Iteration #   1 sum residual **2:    9231.4950
Iteration #   2 sum residual **2:    64.272931


output ignored...



... output resumed

 ----------------------------------
Starting time-step t0=   311295.00     dt=   16384.000
 Stage 1
 Evaluating Jacobian
Iteration #   1 sum residual **2:    5.0898694
Iteration #   2 sum residual **2:   0.71445933E-02
 Stage 2
Iteration #   1 sum residual **2:    5973.7468
Iteration #   2 sum residual **2:    1266.0153
Iteration #   3 sum residual **2:    266.12130
Iteration #   4 sum residual **2:    54.514791
Iteration #   5 sum residual **2:    10.336129
Iteration #   6 sum residual **2:    1.4125894
 Stage 3
Iteration #   1 sum residual **2:    18280.914
Iteration #   2 sum residual **2:    3875.4682
Iteration #   3 sum residual **2:    819.02890
Iteration #   4 sum residual **2:    171.30972
Iteration #   5 sum residual **2:    34.571630
Iteration #   6 sum residual **2:    6.2737270
Iteration #   7 sum residual **2:   0.63432703
 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:    172038.56
Iteration #   2 sum residual **2:    23347.303
Iteration #   3 sum residual **2:    6988.3767
Iteration #   4 sum residual **2:    541.49215
Iteration #   5 sum residual **2:    100.67335
Iteration #   6 sum residual **2:   0.32806993E-01
 Stage 2
Iteration #   1 sum residual **2:    10572.788
Iteration #   2 sum residual **2:    2930.2846
Iteration #   3 sum residual **2:    841.76464
Iteration #   4 sum residual **2:    232.17498
Iteration #   5 sum residual **2:    64.453470
Iteration #   6 sum residual **2:    16.244452
Iteration #   7 sum residual **2:    3.5425304
Iteration #   8 sum residual **2:   0.31899649
 Stage 3
Iteration #   1 sum residual **2:    21243.982
Iteration #   2 sum residual **2:    4572.8347
Iteration #   3 sum residual **2:    1021.0873
Iteration #   4 sum residual **2:    248.94267
Iteration #   5 sum residual **2:    70.003766
Iteration #   6 sum residual **2:    18.319866
Iteration #   7 sum residual **2:    4.1285597
Iteration #   8 sum residual **2:   0.40410875
 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:    10895.615
Iteration #   2 sum residual **2:    147.99196
Iteration #   3 sum residual **2:    1.3598369
Iteration #   4 sum residual **2:   0.92740667E-02
 Stage 2
Iteration #   1 sum residual **2:    7309.2430
Iteration #   2 sum residual **2:    1630.0224
Iteration #   3 sum residual **2:    366.56792
Iteration #   4 sum residual **2:    82.126825
Iteration #   5 sum residual **2:    18.510341
Iteration #   6 sum residual **2:    3.9591069
Iteration #   7 sum residual **2:   0.37088338
 Stage 3
Iteration #   1 sum residual **2:    22379.730
Iteration #   2 sum residual **2:    4976.6759
Iteration #   3 sum residual **2:    1104.5575
Iteration #   4 sum residual **2:    243.20826
Iteration #   5 sum residual **2:    52.287927
Iteration #   6 sum residual **2:    10.410362
Iteration #   7 sum residual **2:    1.5409812
 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:    1.00000000000000
 EFFICIENCY FACTOR:    7.09082167832168
 ------------------------------------------------
 DEALLOCATING
 ------------------------------------------------

 TIMESTEP AT     360000.000     SELECTED

DIC>
DIC>
DIC> --OK---
DIC>
```

exd3-plot

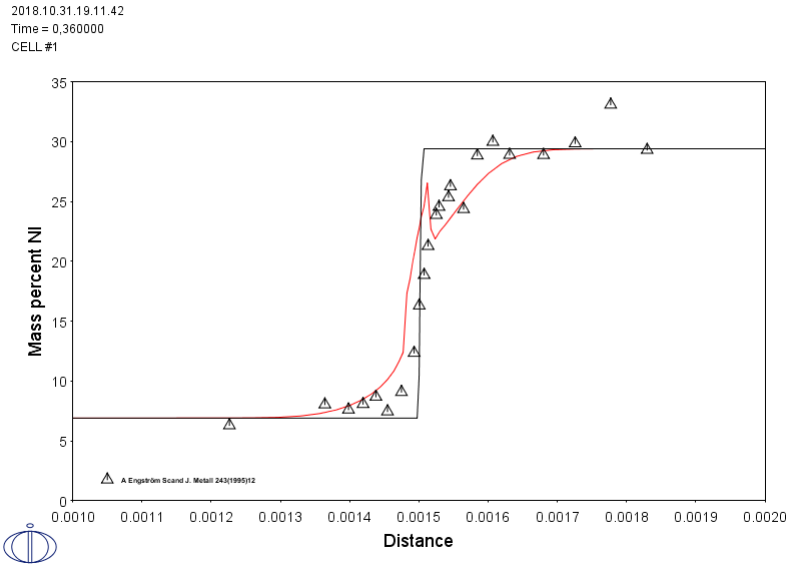
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exd3\plot.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>DIC>DIC>
DIC> TIME STEP AT TIME  3.60000E+05
DIC> OK
DIC>
DIC>DIC>DIC>DIC>  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:
POST-1:POST-1:POST-1:POST-1:  INFO: Distance is set as independent variable
POST-1:POST-1:POST-1:POST-1:
POST-1:POST-1:
POST-1:POST-1:
POST-1:POST-1:
POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```

Figure D3.1



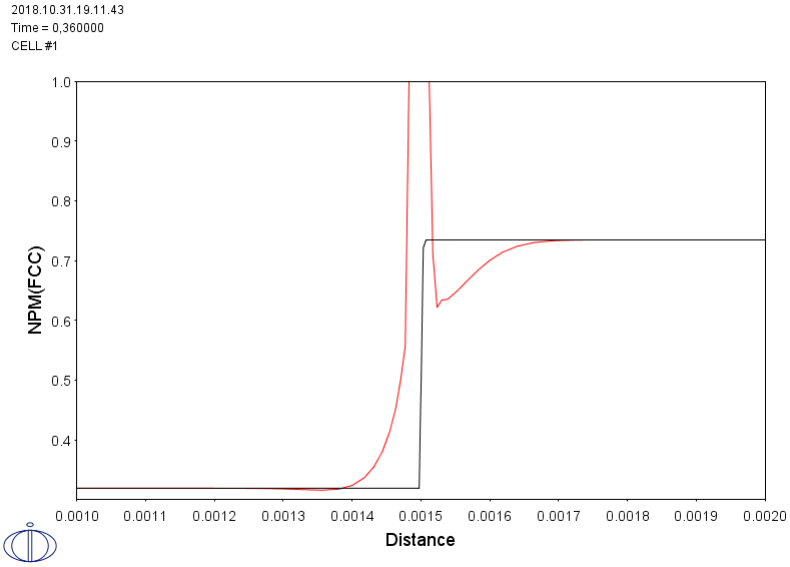

```
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:POST-1:POST-1:
POST-1:POST-1:
POST-1:POST-1:
POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```

Figure D3.2



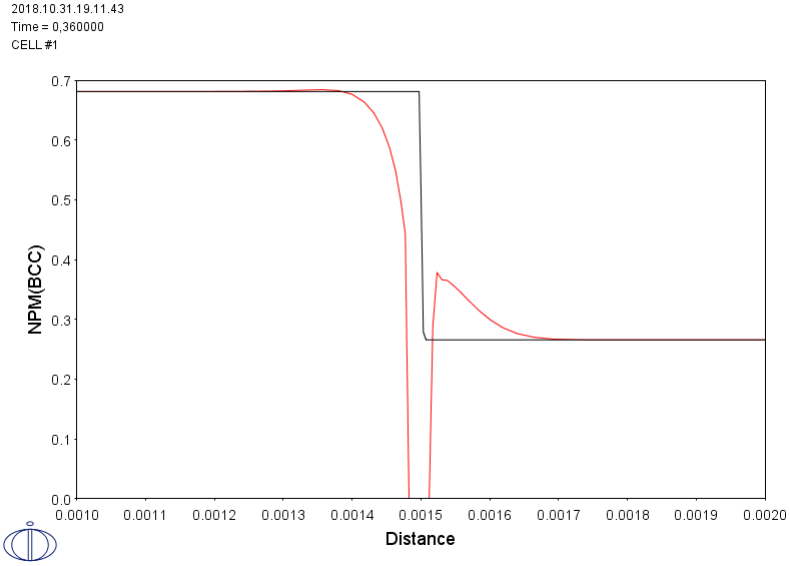

```
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```

Figure D3.3



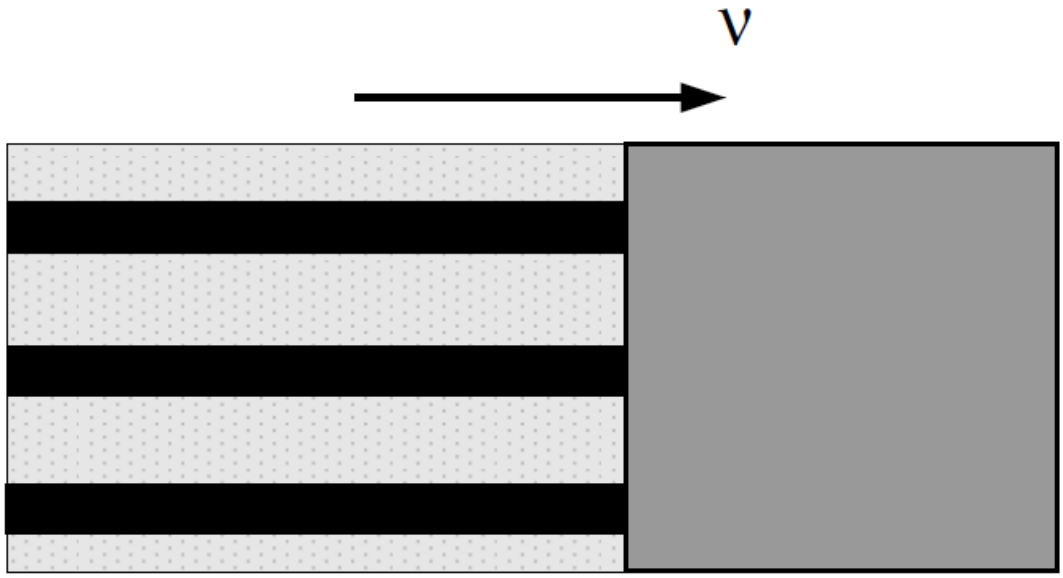

```
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:POST-1:POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```

Figure D3.4




```
POST-1:
POST-1:
POST-1: --OK---
POST-1:
```

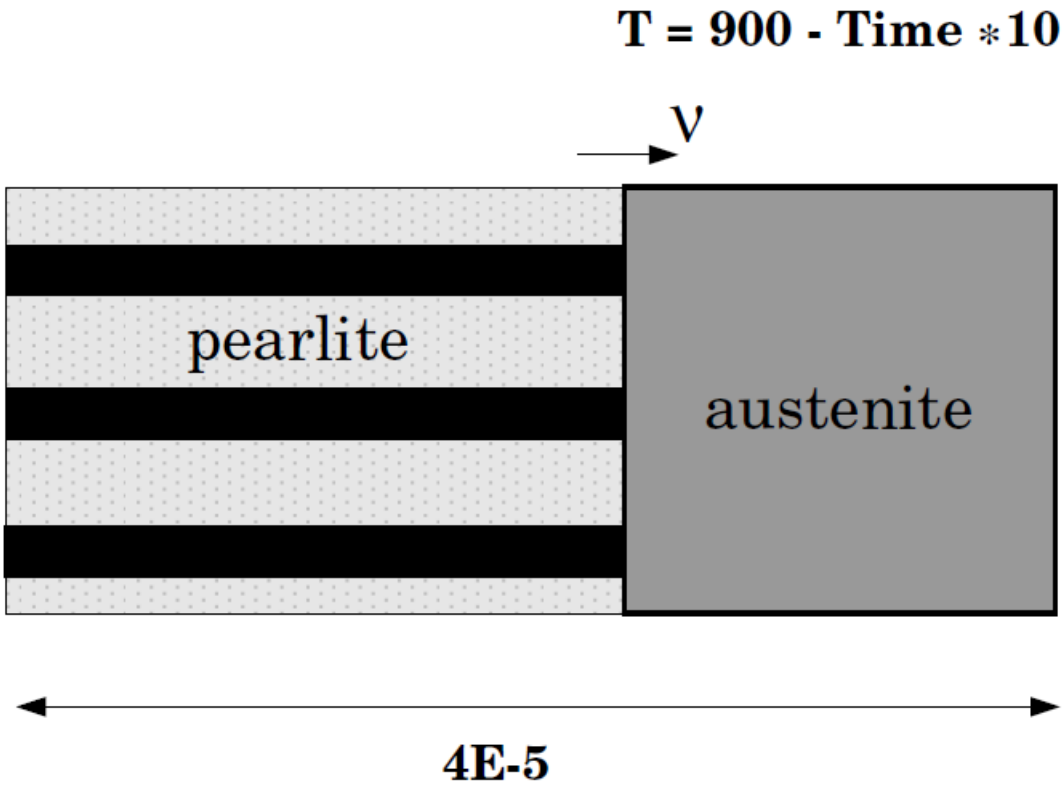
Cooperative Growth



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
SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exe1\setup.DCM.test"SYS: NO SUCH COMMAND, USE HELP
SYS:SYS:SYS:SYS: NO SUCH COMMAND, USE HELP
SYS:
SYS:SYS:
SYS:
SYS:SYS:SYS:SYS: THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

 VA                      /-  DEFINED
 L12_FCC                 B2_BCC                  DICTRA_FCC_A1
   REJECTED
TDB_TCFE9: 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:TDB_TCFE7:TDB_TCFE7: FE                      C                       MN
   DEFINED
TDB_TCFE7:
TDB_TCFE7:TDB_TCFE7:TDB_TCFE7:TDB_TCFE7: 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: FCC_A1                  BCC_A2                  CEMENTITE
   RESTORED
TDB_TCFE7:
TDB_TCFE7:TDB_TCFE7:TDB_TCFE7:TDB_TCFE7: 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:TDB_TCFE7:TDB_TCFE7: Current database: Steels/Fe-Alloys Mobility  v2.0
   TCS Steel Mobility Database Version 2.0 from 2011-12-09.

 VA  DEFINED
APP: FE                      C                       MN
   DEFINED
APP: BCC_A2                  CEMENTITE               FCC_A1
 FE4N_LP1                HCP_A3                  LIQUID:L
   REJECTED
APP: BCC_A2                  FCC_A1                  CEMENTITE
   RESTORED
APP: 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:APP:APP:APP: NO TIME STEP DEFINED
DIC>
DIC>DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>ACTIVE OR INACTIVE PHASE /ACTIVE/:REGION NAME : /PEARLITE/:PHASE TYPE /
 Enter name of "ALPHA" phase /BCC_A2/: Enter name of "BETA" phase /CEMENTITE/: Enter name of "GAMMA" phase /FCC_A1/: Enter "ALPHA"/"BETA" surfa
LOW TIME LIMIT /0/: Surface tension(T,P,TIME)=HIGH TIME LIMIT /*/:ANY MORE RANGES /N/: Enter "ALPHA"/"GAMMA" surface tension
LOW TIME LIMIT /0/: Surface tension(T,P,TIME)=HIGH TIME LIMIT /*/:ANY MORE RANGES /N/: Enter "BETA"/"GAMMA" surface tension
LOW TIME LIMIT /0/: Surface tension(T,P,TIME)=HIGH TIME LIMIT /*/:ANY MORE RANGES /N/: Optimum growth condition factor /2/: Name of dependent e
   Growth model (VOLUME/BOUNDARY/KIRKALDY) for element C /BOUNDARY/:     DF(C) = /value/AUTOMATIC/MIXED/:   Growth model (VOLUME/BOUNDARY/KIRKA
DIC>DIC>DIC>DIC>REGION NAME : /PEARLITE/:DIC>
DIC>DIC>DIC>DIC>DIC>ATTACH TO REGION NAMED /PEARLITE/:
ATTACHED TO THE RIGHT OF PEARLITE /YES/:
DIC>DIC>DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>DIC>DIC>DIC>
DIC>
DIC>
DIC>DIC>DIC>DIC>DIC>REGION NAME : /AUSTENITE/:PHASE NAME: /FCC_A1/:DEPENDENT COMPONENT ? /MN/:COMPOSITION TYPE /MOLE_FRACTION/: PROFILE FOR MN
TYPE /LINEAR/: PROFILE FOR C
TYPE /LINEAR/:DIC>
```

```
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>END TIME FOR INTEGRATION /.1/:AUTOMATIC TIMESTEP CONTROL /YES/:MAX TIMESTEP DURING INTEGRATION /.5/:INITIAL TIMESTEP : /1E-
07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>DIC>DIC>DIC>
DIC> --OK---
DIC>
```

exe1-run

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exe1\run.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  0.00000E+00
DIC>
DIC>DIC>DIC>DIC> OK
DIC>
DIC>DIC>DIC>DIC>  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                    1 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]
  CPU time used in timestep                    0 seconds
 TIME =  0.55282298     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.89841460E-05 AND   0.89841460E-05
 POSITION OF INTERFACE PEARLITE / AUSTENITE IS   0.46523734E-05
```

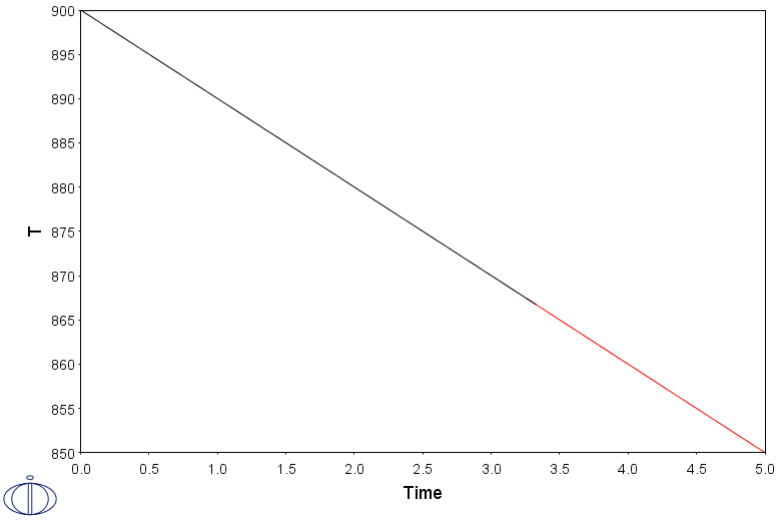
```
 U-FRACTION IN SYSTEM:  C = .0233843320030515  FE = .990707670399294
                        MN = .00929232973121289
 TOTAL SIZE OF SYSTEM:  2.68092626329E-13 [m^3]
  CPU time used in timestep                    0 seconds
  1 GRIDPOINT(S) REMOVED FROM CELL#  1 REGION #  1
 TIME =  0.65282298     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.92333273E-05 AND   0.92333273E-05
 POSITION OF INTERFACE PEARLITE / AUSTENITE IS   0.55757062E-05
 U-FRACTION IN SYSTEM:  C = .0233843320030514  FE = .990707670399294
                        MN = .00929232973121313
 TOTAL SIZE OF SYSTEM:  2.68092626329E-13 [m^3]
  CPU time used in timestep                    0 seconds


output ignored...



... output resumed

 DELETING TIME-RECORD FOR TIME    2.5528230
 DELETING TIME-RECORD FOR TIME    2.6528230
 DELETING TIME-RECORD FOR TIME    2.7528230
 DELETING TIME-RECORD FOR TIME    2.8528230
 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>DIC>DIC>
DIC> --OK---
DIC>
```

exe1-plot

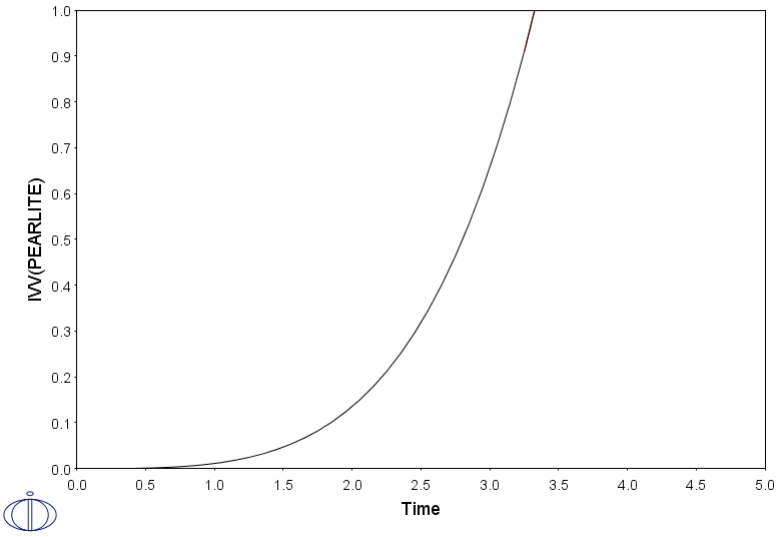
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exe1\plot.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  5.00000E+00
DIC> OK
DIC>
DIC>DIC>DIC>DIC>  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:POST-1:POST-1:POST-1:  INFO: Time is set as independent variable
POST-1:POST-1:POST-1:
POST-1:
POST-1:POST-1: ORKING ...          OST-1:POST-1:
POST-1:
```

2018.10.31.19.15.04
"FIRST" INTERFACE OF SYSTEM
CELL #1



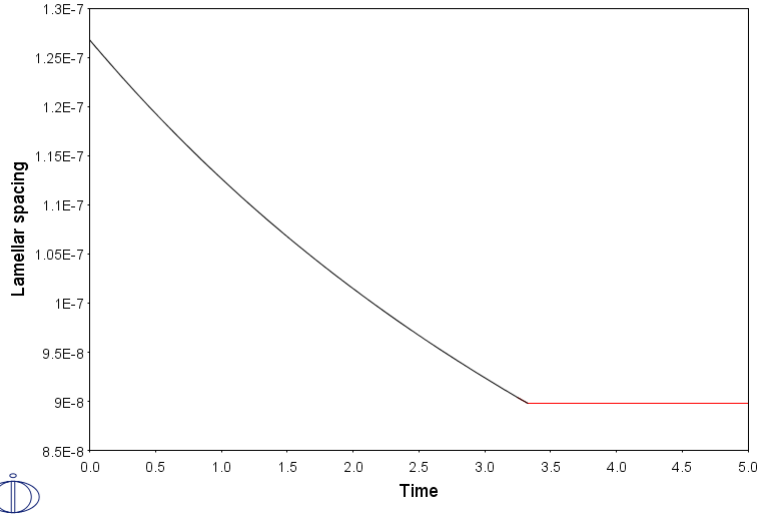

```
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:
POST-1:
POST-1:POST-1: ORKING ...          OST-1:POST-1:
POST-1:
```

2018.10.31.19.15.05
CELL #1



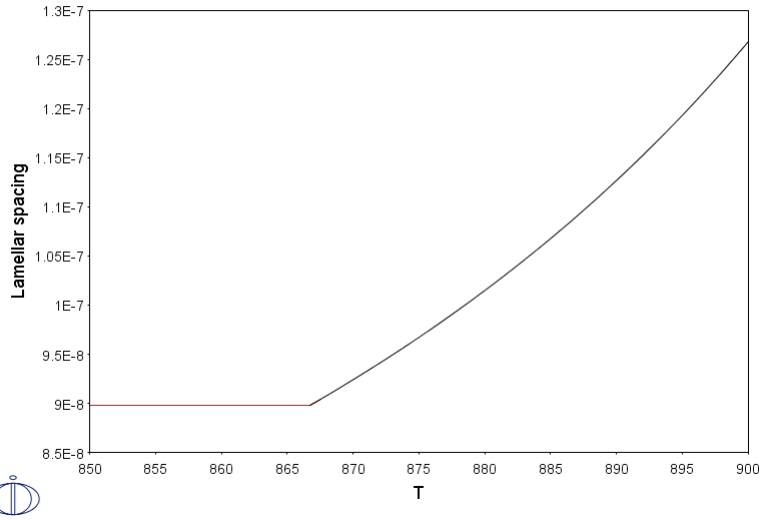

```
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1:POST-1:POST-1:POST-1:AXIS (X, Y OR Z) :VARIABLE :IN REGION: /*/:POST-1:
POST-1:CONDITION /INTEGRAL/:INTERFACE :UPPER OR LOWER INTERFACE OF REGION PEARLITE#1 /LOWER/:POST-1:
POST-1:
POST-1:POST-1: ORKING ...          OST-1:POST-1:
POST-1:
```

2018.10.31.19.15.05
UPPER INTERFACE OF REGION "PEARLITE#1"
CELL #1



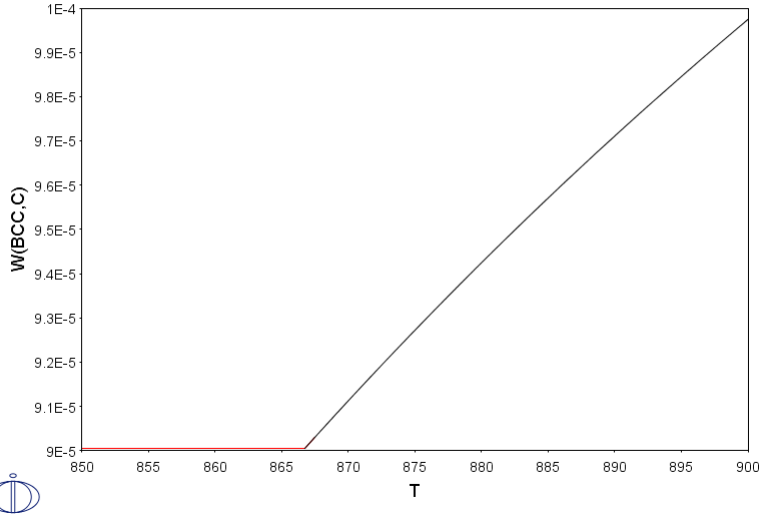

```
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:
POST-1:POST-1:
POST-1:
POST-1:POST-1: ORKING ...          OST-1:POST-1:
POST-1:
```

2018.10.31.19.15.06
UPPER INTERFACE OF REGION "PEARLITE#1"
CELL #1



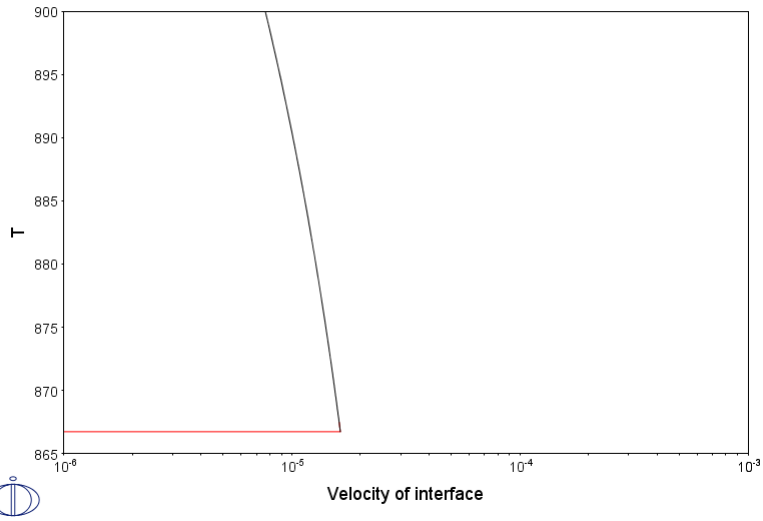

```
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:
POST-1:
POST-1:
POST-1:POST-1: ORKING ...          OST-1:POST-1:
POST-1:
```

2018.10.31.19.15.06
UPPER INTERFACE OF REGION "PEARLITE#1"
CELL #1



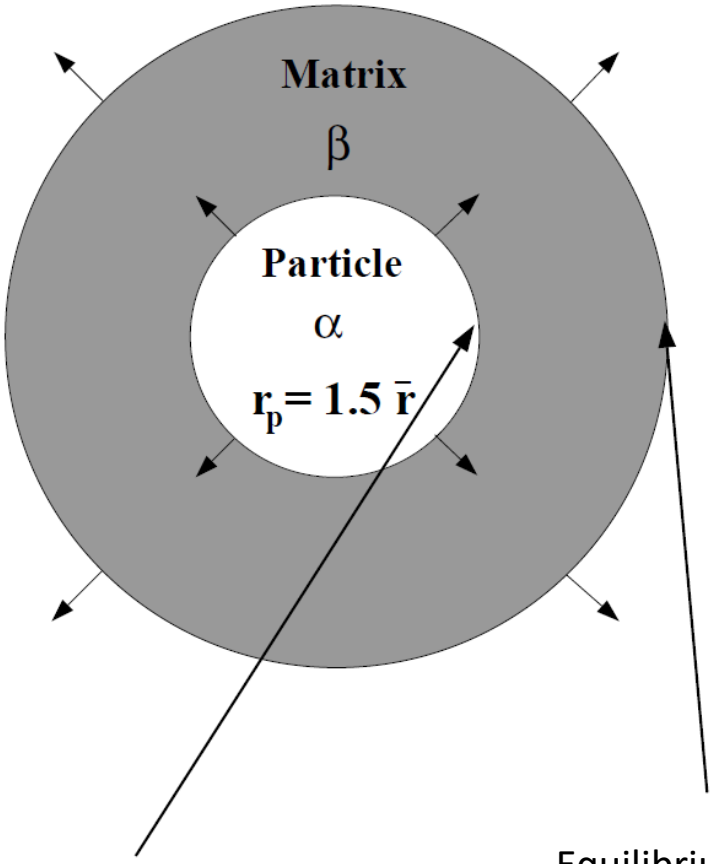

```
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:INTERFACE :UPPER OR LOWER INTERFACE OF REGION PEARLITE#1 /LOWER/:POST-1:POST-1:POST-1:
POST-1:
POST-1:POST-1: ORKING ...          OST-1:POST-1:
POST-1:
```

2018.10.31.19.15.07
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: --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

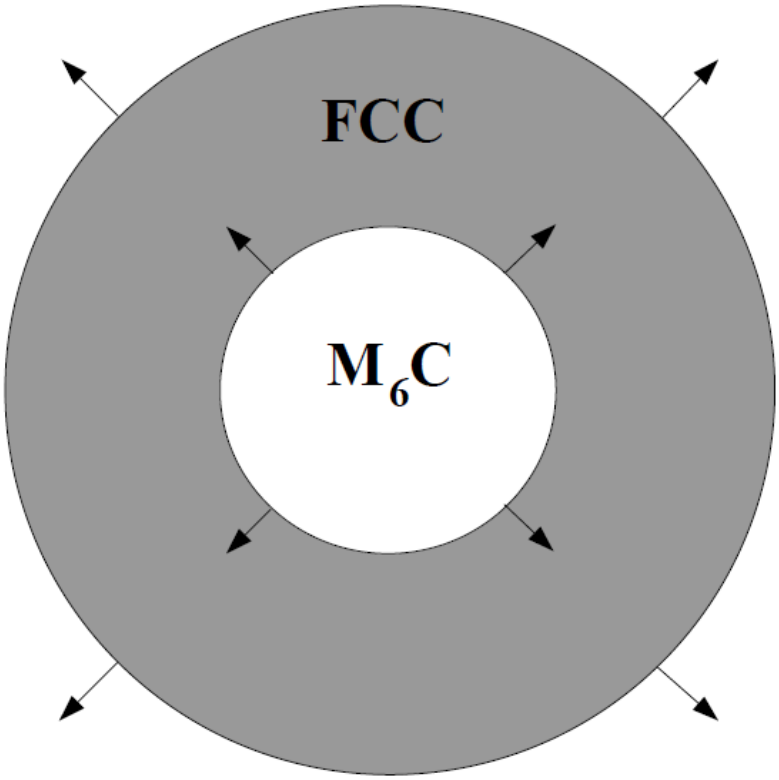
Equilibrium as defined by the average composition in the system.

$\frac{2\sigma V_m}{r_p}$ 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
 Software  (build 17825) 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: Wed Oct 31 13:18:51 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-
Examples\examples\exf1\setup.DCM.test"SYS:SYS:SYS:SYS:SYS:SYS: NO SUCH COMMAND, USE HELP
SYS:SYS:SYS:SYS: THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

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

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
TDB_TCFE7: FE                      MO                      C
   DEFINED
TDB_TCFE7: 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: FCC_A1                  M6C  RESTORED
TDB_TCFE7: 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:TDB_TCFE7:TDB_TCFE7: Use one of these databases

 TCFE9   =  Steels/Fe-Alloys  v9.0
 TCFE8   =  Steels/Fe-Alloys  v8.1
 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
 FEDAT   =  TCS/TT Steels Database v1.0
 TCNI9   =  Ni-Alloys  v9.0
 NI25    =  NI25 Database
 TCNI8   =  Ni-Alloys  v8.2
 TCNI7   =  Ni-Alloys  v7.2
 TCNI6   =  Ni-Alloys  v6.1
 TCNI5   =  Ni-Alloys  v5.1
 TCNI4   =  Ni-Alloys  v4.0
 TCNI1   =  Ni-Alloys  v1.3
 TCAL6   =  Al-Alloys  v6.0
 TCAL5   =  Al-Alloys  v5.1
 TCAL4   =  Al-Alloys  v4.0
 TCAL3   =  Al-Alloys  v3.0
 TCAL2   =  Al-Alloys  v2.1
 TCAL1   =  Al-Alloys  v1.2
 TCMG5   =  Mg-Alloys  v5.1
 TCMG4   =  Mg-Alloys  v4.0
 TCMG3   =  Mg-Alloys  v3.0
 TCMG2   =  Mg-Alloys  v2.0
 TCMG1   =  Mg-Alloys  v1.1
 TCTI2   =  Ti-Alloys  v2.0
 TCTI1   =  Ti-Alloys  v1.0
 TCCU2   =  Cu-Alloys  v2.0
 TCCU1   =  Cu-Alloys  v1.0
 TCCC1   =  Cemented carbide  v1.0
 TCHEA3  =  High Entropy Alloy  v3.1
 TCHEA2  =  High Entropy Alloy  v2.1.1
 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
 TCOX9   =  Metal Oxide Solutions  v9.0 SNAPSHOT
 TCOX8   =  Metal Oxide Solutions  v8.0
 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  v2.7
 AQS2    =  TGG Aqueous Solution Database v2.6
 GCE2    =  TGG Geochemical/Environmental TDB v2.3
 FEDEMO  =  Iron Demo Database v2.0
 ALDEMO  =  Aluminum Demo Database v3.0
 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  v1.1
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBNI5  =  Ni-Alloys Mobility  v5.0
 MOBNI4  =  Ni-Alloys Mobility  v4.1
 MOBNI3  =  Ni-Alloys Mobility  v3.2
 MOBNI2  =  Ni-Alloys Mobility  v2.4
 MOBNI1  =  Ni-Alloys Mobility  v1.9
 MOBAL5  =  Al-Alloys Mobility  v5.0
 MOBAL4  =  Al-Alloys Mobility  v4.0
 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
 MOBHEA1 =  High Entropy Alloys Mobility  v1.0
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBSLD1 =  Solder-Alloys Mobility  v1.1
 MOBTI3  =  Ti-Alloys Mobility  v3.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v2.0
 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/: Current database: Steels/Fe-Alloys Mobility  v2.0
   TCS Steel Mobility Database Version 2.0 from 2011-12-09.

 VA  DEFINED
APP: FE                      MO                      C
   DEFINED
APP: BCC_A2                  CEMENTITE               FCC_A1
 FE4N_LP1                HCP_A3                  LIQUID:L
   REJECTED
APP: *** M6C INPUT IGNORED
 FCC_A1  RESTORED
APP: 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:APP:APP: NO TIME STEP DEFINED
 *** ENTERING M6C AS A DIFFUSION NONE PHASE
DIC>
DIC>DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>REGION NAME :DIC>ATTACH TO REGION NAMED /PART/:
ATTACHED TO THE RIGHT OF PART /YES/:
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>REGION NAME : /PART/:WIDTH OF REGION /1/:TYPE /LINEAR/:DIC>
DIC>REGION NAME : /AUS/:WIDTH OF REGION /1/:TYPE /LINEAR/:DIC>
DIC>DIC>DIC>DIC>DIC>
DIC>DIC>
DIC>
DIC>DIC>DIC>DIC>REGION NAME : /PART/:PHASE NAME: /M6C/:DEPENDENT COMPONENT ? /MO/:COMPOSITION TYPE /MOLE_FRACTION/:PROFILE FOR /MO/:DIC>
```

```
DIC>REGION NAME : /AUS/:PHASE NAME: /FCC_A1/:DEPENDENT COMPONENT ? /MO/:COMPOSITION TYPE /MOLE_FRACTION/:PROFILE FOR /C/:PROFILE FOR /MO/:DIC>
DIC>
DIC>DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC> ENTERED FUNCTION :2*.7*.71*7/6/X FOR CELL #1
DIC>
DIC>
DIC>DIC>DIC>DIC>DIC>
DIC>
DIC>DIC>DIC>DIC>AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /100000/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>DIC>DIC>DIC>DIC>
DIC> --OK---
DIC>
```

exf1-run

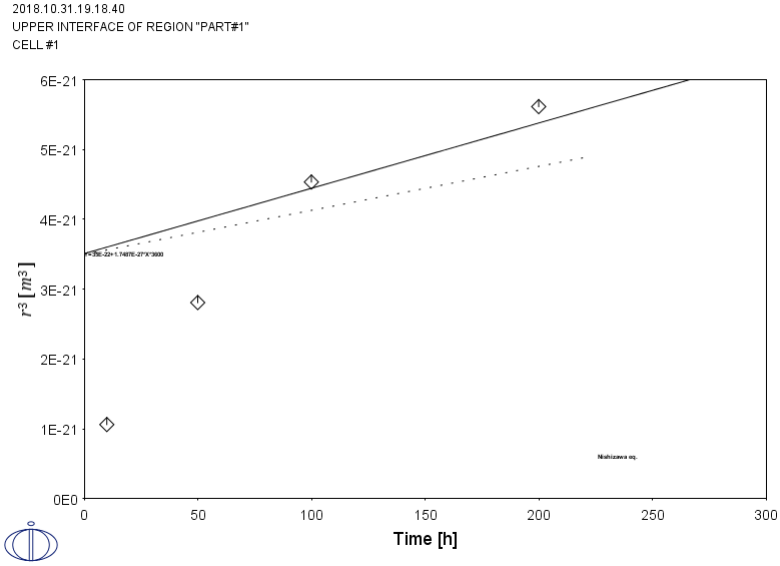
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exf1\run.DCM.test"DIC>DIC>
DIC>DIC>DIC>DIC>
DIC> TIME STEP AT TIME  0.00000E+00
 *** ENTERING M6C AS A DIFFUSION NONE PHASE
DIC> OK
DIC> Region: PART
 single geometric dense at  0.22800E-06
 0.80000       64
 Region: AUS
 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        1.449313509448919E-011        1.447263620894437E-
011        1.443123428591732E-011        1.434904974185966E-011        1.459015585153180E-011        1.418494697541381E-
011        1.386000271529504E-011        1.322099436552274E-011        1.347571674184001E-011

output ignored...



... output resumed

  26  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUS

  CPU time used in timestep                     0 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                     1 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                     0 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                     1 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> --OK---
DIC>
```

exf1-plot

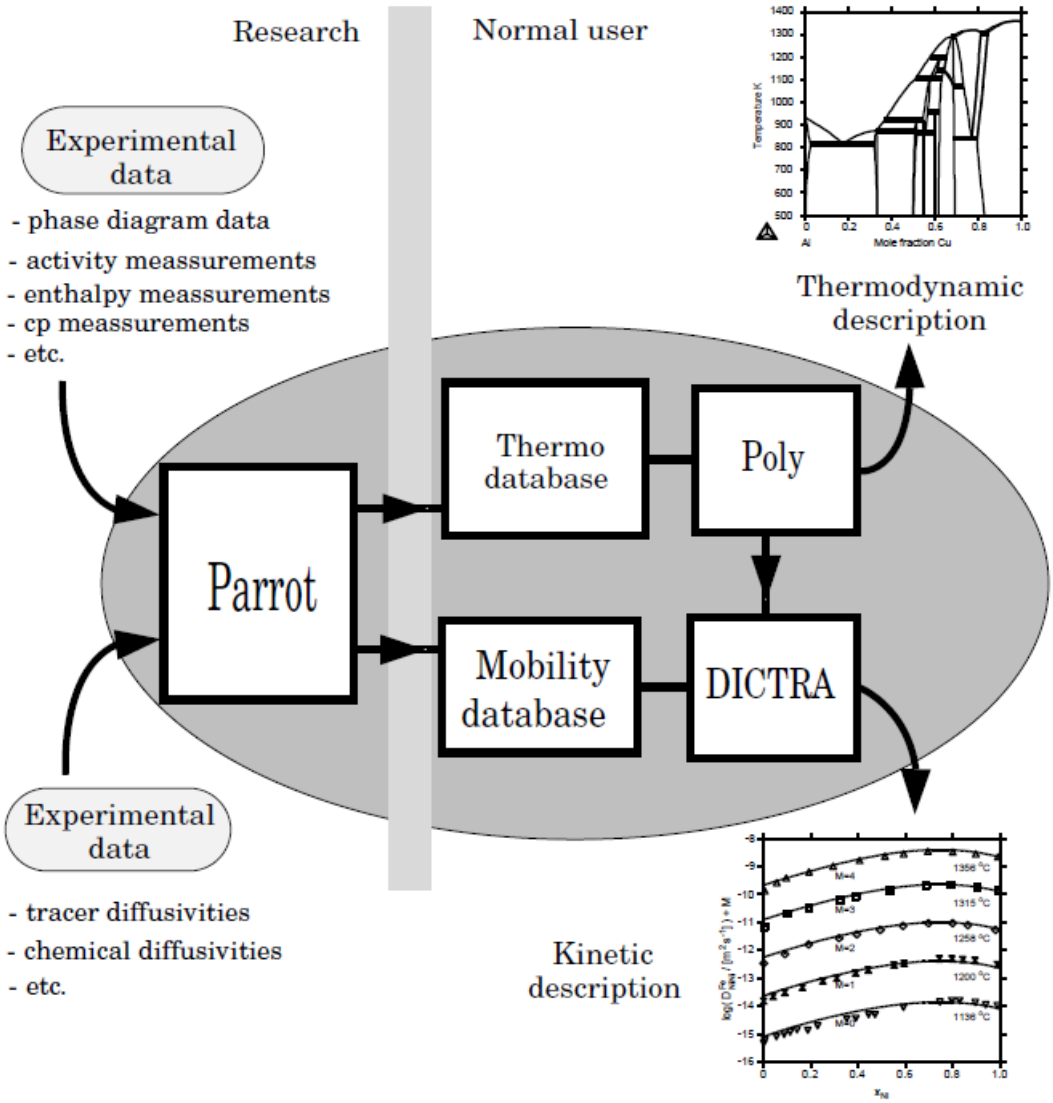
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exf1\plot.DCM.test"DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  1.00000E+06
 *** ENTERING M6C AS A DIFFUSION NONE PHASE
DIC> OK
DIC>
DIC>DIC>DIC>DIC>  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:INTERFACE :POST-1:
POST-1:
POST-1:AXIS TEXT :POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:
POST-1:
POST-1:AXIS TEXT :POST-1:
POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:
POST-1:PROLOGUE NUMBER: /0/:DATASET NUMBER(s): /-1/:POST-1:
POST-1:POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:
POST-1:
POST-1:POST-1:            OST-1:POST-1:
POST-1:
```

Figure f1.1




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

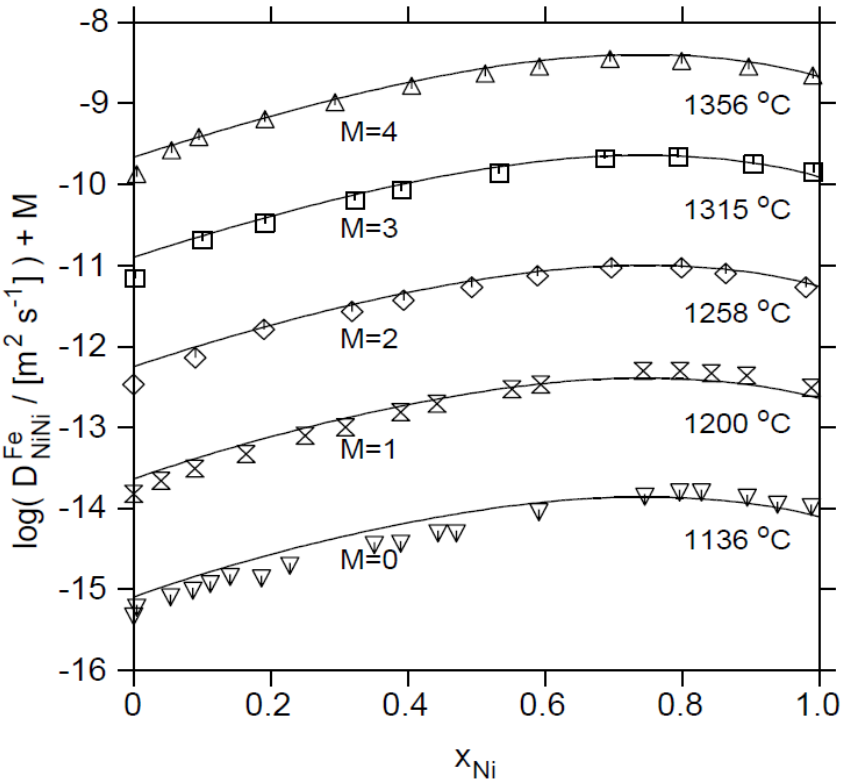
Kinetic Data



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.



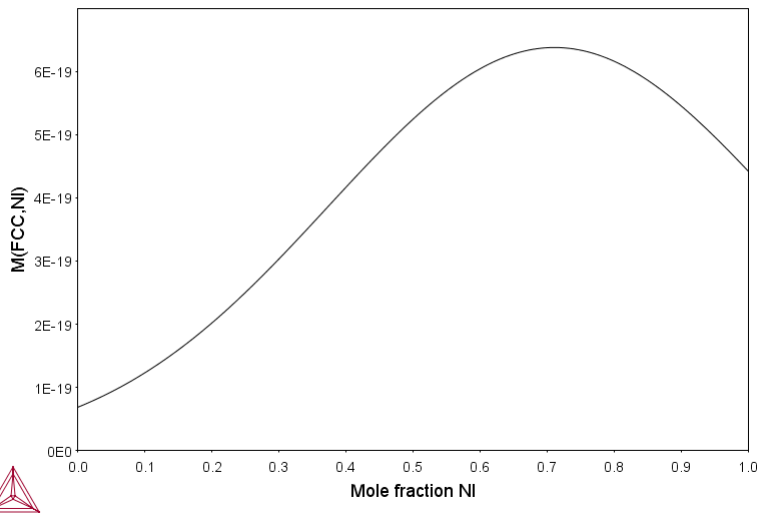
exg1-setup

```
AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-
Examples\examples\exg1\setup.DCM.test"SYS:SYS:SYS:SYS:SYS:SYS: NO SUCH COMMAND, USE HELP
SYS:
SYS:SYS:
SYS:SYS:SYS:SYS: 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:TDB_TCFE9:TDB_TCFE9: 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:TDB_TCFE7:TDB_TCFE7: FE                      NI  DEFINED
TDB_TCFE7:
TDB_TCFE7:TDB_TCFE7:TDB_TCFE7:TDB_TCFE7: LIQUID:L                BCC_A2                  FCC_A1
 HCP_A3                   A1_KAPPA                KAPPA
 LAVES_PHASE_C14          NBNI3                   NI3TI
   REJECTED
TDB_TCFE7: FCC_A1  RESTORED
TDB_TCFE7:
TDB_TCFE7:TDB_TCFE7:TDB_TCFE7:TDB_TCFE7: 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:TDB_TCFE7:TDB_TCFE7:TDB_TCFE7: Use one of these databases

 TCFE9   =  Steels/Fe-Alloys  v9.0
 TCFE8   =  Steels/Fe-Alloys  v8.1
 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
 FEDAT   =  TCS/TT Steels Database v1.0
 TCNI9   =  Ni-Alloys  v9.0
 NI25    =  NI25 Database
 TCNI8   =  Ni-Alloys  v8.2
 TCNI7   =  Ni-Alloys  v7.2
 TCNI6   =  Ni-Alloys  v6.1
 TCNI5   =  Ni-Alloys  v5.1
 TCNI4   =  Ni-Alloys  v4.0
 TCNI1   =  Ni-Alloys  v1.3
 TCAL6   =  Al-Alloys  v6.0
 TCAL5   =  Al-Alloys  v5.1
 TCAL4   =  Al-Alloys  v4.0
 TCAL3   =  Al-Alloys  v3.0
 TCAL2   =  Al-Alloys  v2.1
 TCAL1   =  Al-Alloys  v1.2
 TCMG5   =  Mg-Alloys  v5.1
 TCMG4   =  Mg-Alloys  v4.0
 TCMG3   =  Mg-Alloys  v3.0
 TCMG2   =  Mg-Alloys  v2.0
 TCMG1   =  Mg-Alloys  v1.1
 TCTI2   =  Ti-Alloys  v2.0
 TCTI1   =  Ti-Alloys  v1.0
 TCCU2   =  Cu-Alloys  v2.0
 TCCU1   =  Cu-Alloys  v1.0
 TCCC1   =  Cemented carbide  v1.0
 TCHEA3  =  High Entropy Alloy  v3.1
 TCHEA2  =  High Entropy Alloy  v2.1.1
 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
 TCOX9   =  Metal Oxide Solutions  v9.0 SNAPSHOT
 TCOX8   =  Metal Oxide Solutions  v8.0
 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  v2.7
 AQS2    =  TGG Aqueous Solution Database v2.6
 GCE2    =  TGG Geochemical/Environmental TDB v2.3
 FEDEMO  =  Iron Demo Database v2.0
 ALDEMO  =  Aluminum Demo Database v3.0
 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  v1.1
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBNI5  =  Ni-Alloys Mobility  v5.0
 MOBNI4  =  Ni-Alloys Mobility  v4.1
 MOBNI3  =  Ni-Alloys Mobility  v3.2
 MOBNI2  =  Ni-Alloys Mobility  v2.4
 MOBNI1  =  Ni-Alloys Mobility  v1.9
 MOBAL5  =  Al-Alloys Mobility  v5.0
 MOBAL4  =  Al-Alloys Mobility  v4.0
 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
 MOBHEA1 =  High Entropy Alloys Mobility  v1.0
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBSLD1 =  Solder-Alloys Mobility  v1.1
 MOBTI3  =  Ti-Alloys Mobility  v3.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v2.0
 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/: Current database: Steels/Fe-Alloys Mobility  v2.0
   TCS Steel Mobility Database Version 2.0 from 2011-12-09.

 VA  DEFINED
APP: FE                      NI  DEFINED
APP: BCC_A2                  FCC_A1                  HCP_A3
 LIQUID:L  REJECTED
APP: FCC_A1  RESTORED
APP: 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:APP:APP: NO TIME STEP DEFINED
DIC>
DIC>DIC>DIC>DIC> Sorry, LIST-DATA disabled for this database
DIC>
DIC>
DIC>
DIC>@?<Hit_return_to_continue>
DIC>
DIC>DIC>DIC>DIC> AMBIGUOUS COMMAND, USE HELP
DIC>
DIC> NO SUCH COMMAND, USE HELP
DIC> NO SUCH COMMAND, USE HELP
DIC> NO SUCH COMMAND, USE HELP
DIC> NO SUCH COMMAND, USE HELP
DIC> NO SUCH COMMAND, USE HELP
DIC> NO SUCH COMMAND, USE HELP
DIC>
DIC>
DIC>@?<Hit_return_to_continue>
DIC>
DIC>DIC>DIC>DIC>POLY_3:POLY_3: 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:Axis number: /1/:Condition /NONE/:Min value /0/:Max value /1/:Increment /.025/:POLY_3:
POLY_3:Option? /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
```

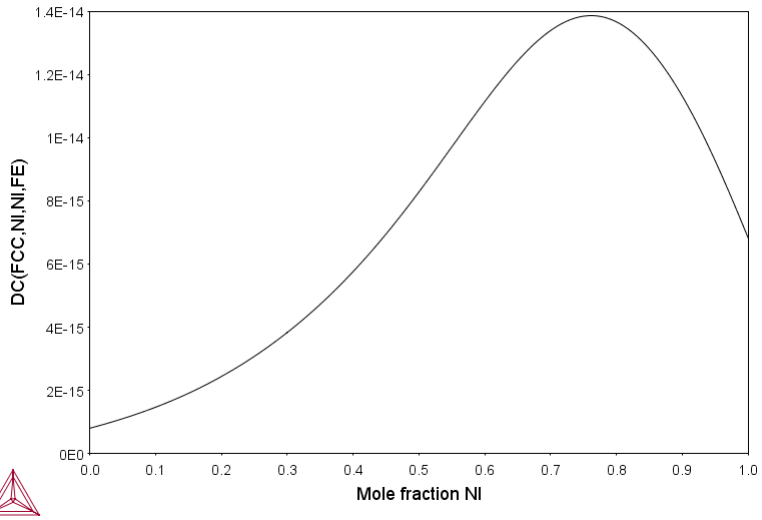
```
 Global test at  3.38000E-01 .... OK
 Global test at  3.48000E-01 .... OK
 Global test at  3.58000E-01 .... OK
 Global test at  3.68000E-01 .... OK
 Global test at  3.78000E-01 .... OK
 Global test at  3.88000E-01 .... OK
 Global test at  3.98000E-01 .... OK
 Global test at  4.08000E-01 .... OK
 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:POLY_3:POLY_3:  POLY-3 POSTPROCESSOR VERSION 3.2
POST:
POST:
POST:
POST:POST:POST:POST:POST:POST:
POST:
POST:POST:POST:POST:
POST:
```

2018.10.31.19.20.11
MOBFE2: FE, NI
T=1409, P=1.01325E5, N=1



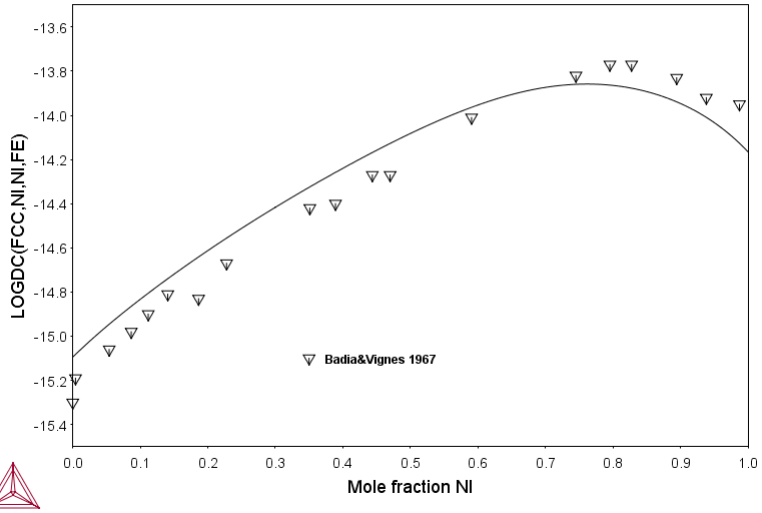

```
POST:
POST:
POST:
POST:@?<Hit_return_to_continue>
POST:
POST:POST:POST:POST:POST:
POST:
POST:POST:POST:POST:
POST:
```

2018.10.31.19.20.11
MOBFE2: FE, NI
T=1409, P=1.01325E5, N=1




```
POST:
POST:
POST:@?<Hit_return_to_continue>
POST:
POST:POST:POST:POST:POST:
POST:PROLOGUE NUMBER: /0/:DATASET NUMBER(s): /-1/:POST:
POST:POST:
POST:
POST:POST:POST:POST:
POST:
```

2018.10.31.19.20.12
MOBFE2: FE, NI
T=1409, P=1.01325E5, N=1

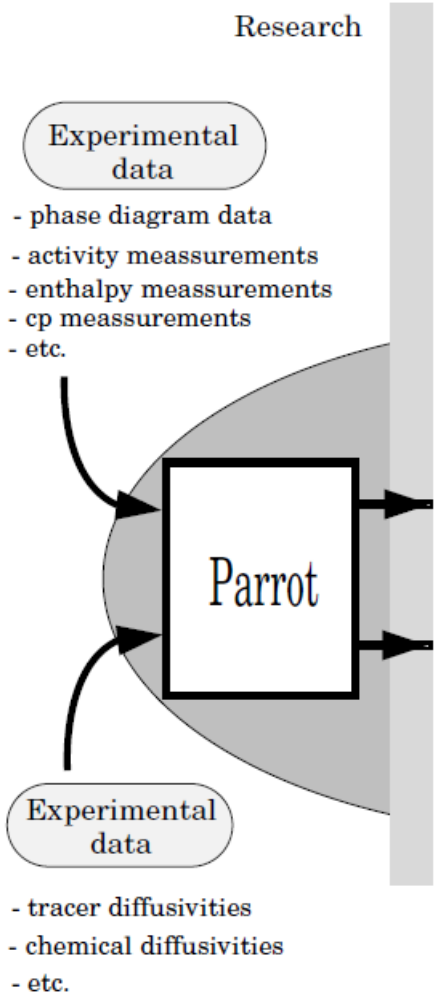



```
POST:
POST:
POST:@?<Hit_return_to_continue>
POST:
POST:POST:
```

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
SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exg2\setup.DCM.test"SYS: NO SUCH COMMAND, USE HELP
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: NO SUCH COMMAND, USE HELP
SYS:
SYS:SYS:
SYS:SYS:SYS:SYS: THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

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

 VA  DEFINED
TDB_USER:ELEMENTS: AL                       NI  DEFINED
TDB_USER: LIQUID                  B2_BCC                  BCC_A2
 FCC_A1                   GAMMA_PRIME  REJECTED
TDB_USER: FCC_A1  RESTORED
TDB_USER: ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....
 -OK-
TDB_USER:
TDB_USER:TDB_USER:TDB_USER:TDB_USER:TDB_USER: Current database: Alloys Mobility  v2.7

 VA  DEFINED
 GAS:G  REJECTED
APP:ELEMENTS: AL                       NI  DEFINED
APP: BCC_A2                   FCC_A1                  M4N
 HCP_A3                   LIQUID:L  REJECTED
APP: FCC_A1  RESTORED
APP: 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:APP:APP:APP:APP:APP:APP:APP: 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: NO TIME STEP DEFINED
DIC>
DIC>DIC>PARAMETER: MQ(FCC_A1&AL#1,AL:VA;0)
DIC>
DIC>DIC>PARAMETER: MQ(FCC_A1&AL#1,NI:VA;0)
DIC>
DIC>DIC>PARAMETER: MQ(FCC_A1&AL#1,AL,NI:VA;0)
DIC>
DIC>DIC>PARAMETER: MQ(FCC_A1&NI#1,AL:VA;0)
DIC>
DIC>DIC>PARAMETER: MQ(FCC_A1&NI#1,NI:VA;0)
DIC>
DIC>DIC>PARAMETER: MQ(FCC_A1&NI#1,AL,NI:VA;0)
DIC>
DIC>DIC>DIC>DIC> PARROT  VERSION 5.3d RUNNING ON PC/WINDOWS NT
PARROT:PARROT:
PARROT: --OK---
PARROT:
```

exg2-run

```
PARROT:AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exg2\run.DCM.test"PARROT:PARROT:
PARROT:PARROT:PARROT:PARROT:
PARROT:PARROT:PARROT:PARROT: PARROT  VERSION 5.3d RUNNING ON PC/WINDOWS NT
PARROT:PARROT:
PARROT:
PARROT:PARROT:PARROT:PARROT: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
```

```
 C-S PH FCC=ENT 1
 S-C T=1573,N=1,P=P0
 S-C X(AL)=.1828
 EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-11.98:.1
 CREATE_NEW 0029,1
 C-S PH FCC=ENT 1
 S-C T=1573,N=1,P=P0
 S-C X(AL)=.1909
 EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-11.94:.1


 TABLE_HEAD 30
 CREATE_NEW 0030,1
 C-S PH FCC=ENT 1
 S-C T=1523,N=1,P=P0


output ignored...



... output resumed

    6.29664191E-01    6.29664191E-01    6.29664191E-01
 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
```

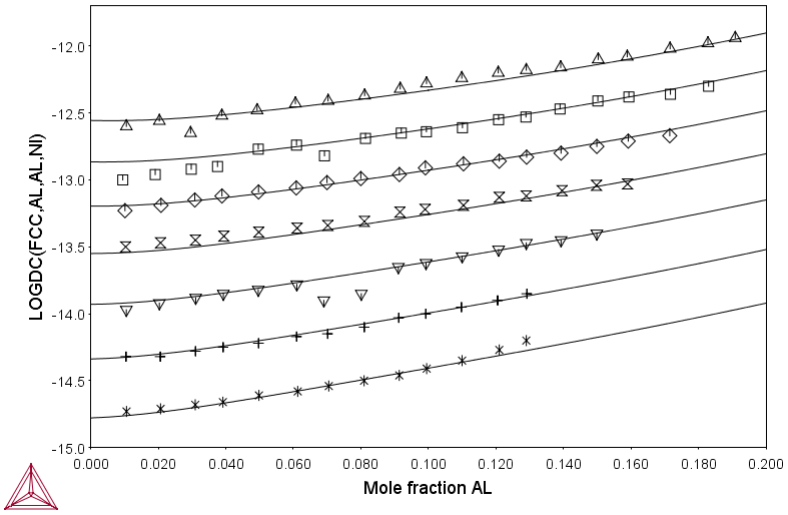
```
80 LOGDC(F...,AL,NI)=-13.19      -13.22      0.10     -2.6230E-02 -0.2623
81 LOGDC(F...,AL,NI)=-13.13      -13.17      0.10     -4.3098E-02 -0.4310
82 LOGDC(F...,AL,NI)=-13.12      -13.14      0.10     -1.9773E-02 -0.1977
83 LOGDC(F...,AL,NI)=-13.08      -13.09      0.10     -1.4457E-02 -0.1446
84 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: --OK---
PARROT:
```

exg2-plot

```
PARROT:AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exg2\plot.DCM.test"PARROT:PARROT:
PARROT:PARROT:PARROT:PARROT:PARROT:PARROT:
PARROT:PARROT:PARROT:PARROT:PARROT: PARROT  VERSION 5.3d RUNNING ON PC/WINDOWS NT
PARROT:PARROT:
PARROT:PARROT:PARROT:PARROT:POLY_3:POLY_3:POLY_3: 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:

POLY_3:POLY_3: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:POLY_3:POLY_3:POLY_3: 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: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: 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: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
```

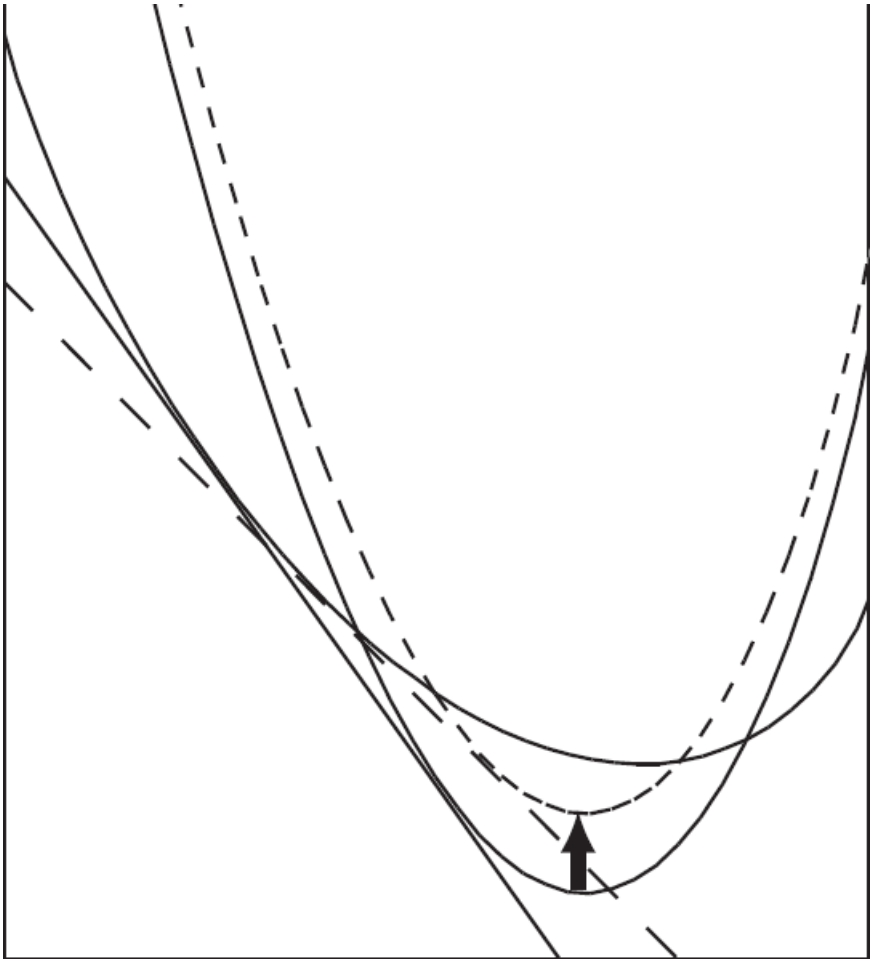
```
 Global test at  4.20000E-02 .... OK
 Global test at  3.20000E-02 .... OK
 Global test at  2.20000E-02 .... OK
 Global test at  1.20000E-02 .... OK
 Global test at  2.00000E-03 .... OK
 Terminating at   0.100000E-03
 Calculated   103 equilibria
 *** Buffer saved on file: C:\Users\developer\Documents\RESULT_002.POLY3
POLY_3:POLY_3: 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: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: 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: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: 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: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: 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: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:POLY_3:POLY_3:POLY_3:  POLY-3 POSTPROCESSOR VERSION 3.2
POST:
POST:POST:POST:
POST:PROLOGUE NUMBER: /0/:DATASET NUMBER(s): /-1/:POST:
POST:
POST: COMMAND NOT SUPPORTED IN THIS PLOT DRIVER
POST:POST: COMMAND NOT SUPPORTED IN THIS PLOT DRIVER
POST:
POST:POST:POST:POST:
POST:
```




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

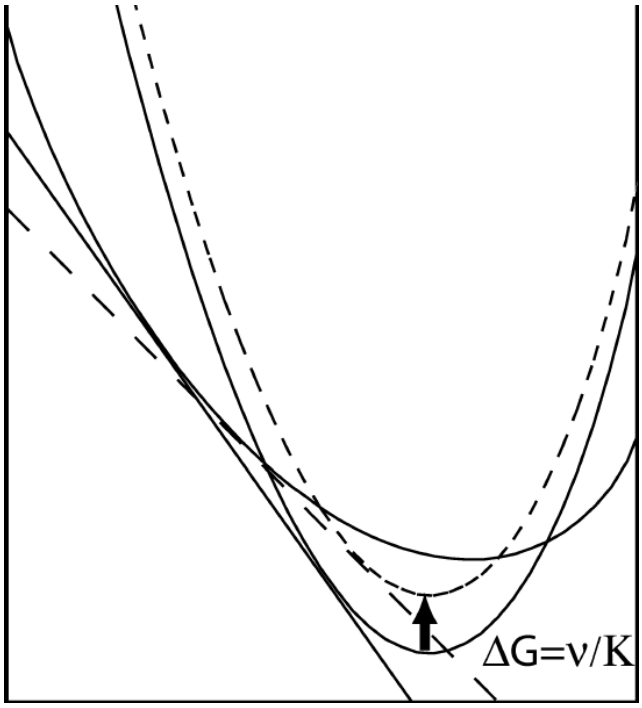
Deviation From Local Equilibrium



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 Stockholm, Sweden

 Software  (build 17825) 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: Wed Oct 31 13:18:51 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-
Examples\examples\exh1\setup.DCM.test"SYS:SYS:SYS:SYS:SYS:SYS:SYS: NO SUCH COMMAND, USE HELP
SYS:
SYS:SYS:SYS:SYS: 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:TDB_TCFE9:TDB_TCFE9: Current database: Iron Demo Database v2.0

 VA                       /-  DEFINED
TDB_FEDEMO: FE                       C  DEFINED
TDB_FEDEMO: 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: BCC_A2                   FCC_A1  RESTORED
TDB_FEDEMO: 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:TDB_FEDEMO:TDB_FEDEMO: Current database: Fe-Alloys Mobility demo database v2.0

 VA  DEFINED
APP: FE                       C  DEFINED
APP: BCC_A2                   FCC_A1  REJECTED
APP: BCC_A2                   FCC_A1  RESTORED
APP: 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:APP:APP: NO TIME STEP DEFINED
DIC>
DIC>DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>DIC>DIC>REGION NAME :DIC>
DIC>REGION NAME :ATTACH TO REGION NAMED /FERRITE/:
ATTACHED TO THE RIGHT OF FERRITE /YES/:
DIC>
DIC>DIC>DIC>DIC>REGION NAME : /FERRITE/:WIDTH OF REGION /1/:TYPE /LINEAR/:DIC>
DIC>WIDTH OF REGION /1/:TYPE /LINEAR/:DIC>
DIC>DIC>DIC>DIC>ACTIVE OR INACTIVE PHASE /ACTIVE/:REGION NAME : /FERRITE/:PHASE TYPE /MATRIX/:PHASE NAME: /NONE/:DIC>
DIC>ACTIVE OR INACTIVE PHASE /ACTIVE/:REGION NAME : /AUSTENITE/:PHASE TYPE /MATRIX/:PHASE NAME: /NONE/:DIC>
DIC>
DIC>
DIC>DIC>DIC>DIC>REGION NAME : /FERRITE/:PHASE NAME: /BCC_A2/:COMPOSITION TYPE /MOLE_FRACTION/:PROFILE FOR /C/:TYPE /LINEAR/:VALUE OF FIRST POIN
2/:DIC>
DIC>DIC>DIC>DIC>REGION NAME : /AUSTENITE/:PHASE NAME: /FCC_A1/:COMPOSITION TYPE /MOLE_FRACTION/:PROFILE FOR /C/:TYPE /LINEAR/:VALUE OF FIRST PO
2/:DIC>
DIC>DIC>DIC>DIC>DIC>
DIC> --OK---
DIC>
```

exh1-run

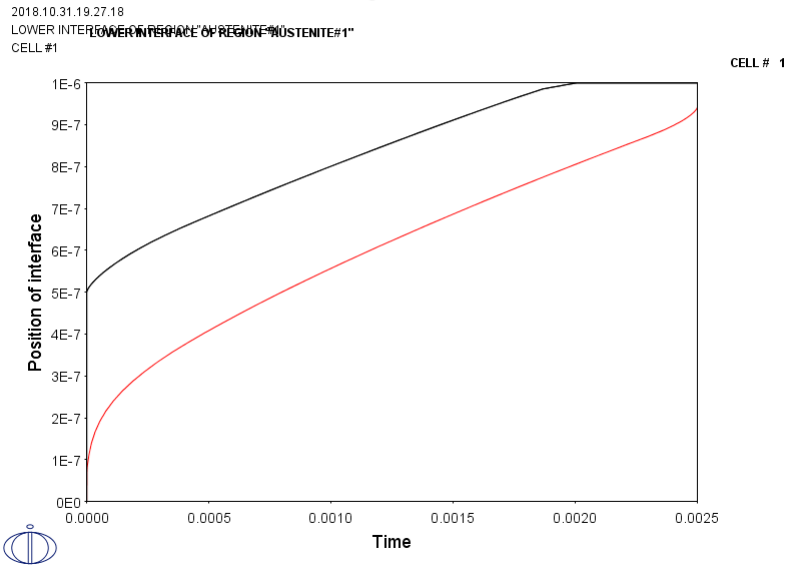
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exh1\run.DCM.test"DIC>
DIC>
DIC>DIC>DIC>DIC>
DIC> TIME STEP AT TIME  0.00000E+00
DIC>
DIC> OK
DIC>
DIC>DIC>DIC>DIC>END TIME FOR INTEGRATION /.1/:AUTOMATIC TIMESTEP CONTROL /YES/:MAX TIMESTEP DURING INTEGRATION /2.5E-04/:
INITIAL TIMESTEP : /1E-07/:SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:DIC>
DIC>
DIC>DIC>DIC>DIC> 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
 2.884385690570846E-004        2.884962732791314E-004        6.725395552062010E-012        2.964586453906864E-012        7.238230795034652E-
013        1.865556879603171E-017       TIME =  0.30000000E-06 DT =  0.20000000E-06 SUM OF SQUARES =  0.18655569E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.33805889E-02 AND   0.33805889E-02
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.50128675E-06
 U-FRACTION IN SYSTEM:  C = 9.00450100185133E-04  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-06 [m]
  CPU time used in timestep                    0 seconds
 6.614507143291235E-006        6.616493774939203E-006

output ignored...



... output resumed

 8.718550390928004E-023       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                    1 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 = 8.9905213314465E-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
 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> --OK---
DIC>
```

exh1-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exh1\plot.DCM.test"DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  2.50000E-03
DIC>
DIC> OK
DIC>
DIC>DIC>DIC>DIC>  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:POST-1:POST-1:POST-1: COMMAND NOT SUPPORTED IN THIS PLOT DRIVER
POST-1:
POST-1:POST-1:POST-1:POST-1:  INFO: Time is set as independent variable
POST-1:POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:POST-1: ORKING ...          OST-1:POST-1:
POST-1:
```

Figure h1

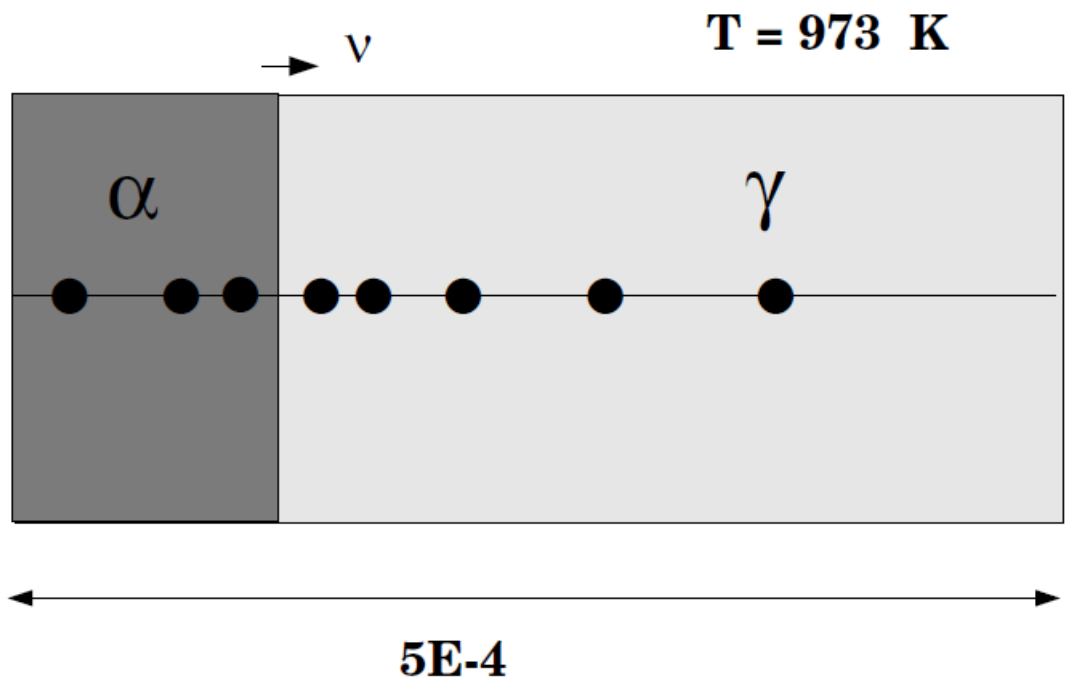



```
POST-1:
POST-1:
POST-1: --OK---
POST-1:
```

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

```
About Stockholm, Sweden

 Software  (build 17825) 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: Wed Oct 31 13:18:51 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-
Examples\examples\exh2\setup.DCM.test"SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: NO SUCH COMMAND, USE HELP
SYS:
SYS:SYS:SYS:SYS: 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:TDB_TCFE9:TDB_TCFE9: Current database: Iron Demo Database v2.0

 VA                       /-  DEFINED
TDB_FEDEMO: FE                       NI                      C
   DEFINED
TDB_FEDEMO: 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: BCC_A2                   FCC_A1  RESTORED
TDB_FEDEMO: 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:TDB_FEDEMO:TDB_FEDEMO: Current database: Fe-Alloys Mobility demo database v2.0

 VA  DEFINED
APP: FE                      NI                      C
   DEFINED
APP: BCC_A2                  FCC_A1  REJECTED
APP: BCC_A2                  FCC_A1  RESTORED
APP: 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:APP:APP: NO TIME STEP DEFINED
DIC>
DIC>DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>DIC>DIC>REGION NAME :DIC>
DIC>REGION NAME :ATTACH TO REGION NAMED /FERRITE/:
ATTACHED TO THE RIGHT OF FERRITE /YES/:
DIC>
DIC>DIC>DIC>DIC>REGION NAME : /FERRITE/:WIDTH OF REGION /1/:TYPE /LINEAR/:DIC>
DIC>WIDTH OF REGION /1/:TYPE /LINEAR/:DIC>
DIC>DIC>DIC>DIC>ACTIVE OR INACTIVE PHASE /ACTIVE/:REGION NAME : /FERRITE/:PHASE TYPE /MATRIX/:PHASE NAME: /NONE/:DIC>
DIC>ACTIVE OR INACTIVE PHASE /ACTIVE/:REGION NAME : /AUSTENITE/:PHASE TYPE /MATRIX/:PHASE NAME: /NONE/:DIC>
DIC>
DIC>
DIC>DIC>DIC>DIC>REGION NAME : /FERRITE/:PHASE NAME: /BCC_A2/:DEPENDENT COMPONENT ? /NI/:COMPOSITION TYPE /MOLE_FRACTION/:PROFILE FOR /C/:TYPE /
2/:PROFILE FOR /NI/:TYPE /LINEAR/:VALUE OF FIRST POINT :VALUE OF LAST POINT : /2.02/:DIC>
DIC>DIC>DIC>DIC>REGION NAME : /AUSTENITE/:PHASE NAME: /FCC_A1/:DEPENDENT COMPONENT ? /NI/:COMPOSITION TYPE /MOLE_FRACTION/:PROFILE FOR /C/:TYPE
2/:PROFILE FOR /NI/:TYPE /LINEAR/:VALUE OF FIRST POINT :VALUE OF LAST POINT : /2.02/:DIC>
DIC>
DIC>DIC>DIC>DIC>DIC>
DIC> --OK---
DIC>
```

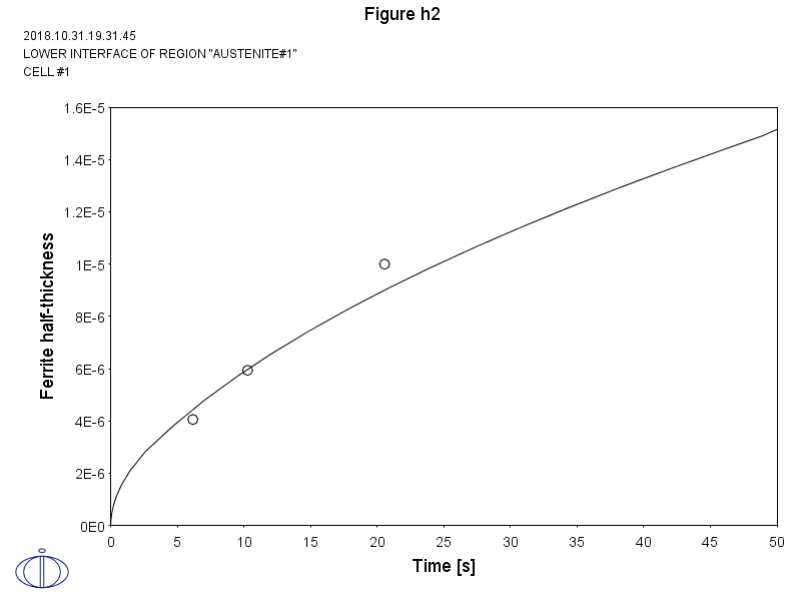
exh2-run

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exh2\run.DCM.test"DIC>
DIC>
DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>
DIC> TIME STEP AT TIME  0.00000E+00
DIC>
DIC> OK
DIC>
DIC>DIC>DIC>DIC>DIC>
DIC>
DIC>
DIC>DIC>DIC>DIC>ENABLE PARAEQ : /NO/:U-FRACTION OF COMPONENT FE /AUTO/:U-FRACTION OF COMPONENT NI /AUTO/:DIC>
DIC>DIC>DIC>DIC> 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        1.179394106722943E-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         5.30437602525244E
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
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.16241126E-02 AND   0.16241126E-02
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.35538743E-08
 U-FRACTION IN SYSTEM:  C = .00412273399769269  FE = .980742621143593
                        NI = .0192573788564064
 TOTAL SIZE OF SYSTEM:  5.0001E-05 [m]
  CPU time used in timestep                     1 seconds
  12691.3220847414         12691.3220847421         12684.3790790055         156.386666039620         1.00388579193494         1.36004850614605E
004        1.392593887067853E-006        9.264877308344736E-009        1.340641619582741E-003        4.391018806454902E-
018       TIME =  0.63794974E-06 DT =  0.28138234E-06 SUM OF SQUARES =  0.43910188E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.10447653E-02 AND   0.10447653E-02
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.38478528E-08
 U-FRACTION IN SYSTEM:  C = .00412273399769148  FE = .980742621143594
                        NI = .0192573788564064


output ignored...



... output resumed

 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.19993048E-06 AND   0.19993048E-06
 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                     2 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> --OK---
DIC>
```

exh2-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exh2\plot.DCM.test"DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  5.00000E+01
DIC>
DIC> OK
DIC>
DIC>DIC>DIC>DIC>  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:  INFO: Time is set as independent variable
POST-1:POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:
POST-1:POST-1:POST-1:POST-1:AXIS (X, Y OR Z) :AUTOMATIC AXIS TEXT  (Y OR N) /N/:AXIS TEXT :POST-1:
POST-1:AXIS (X, Y OR Z) :AUTOMATIC AXIS TEXT  (Y OR N) /N/:AXIS TEXT :POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:POST-1:            OST-1:POST-1:
POST-1:
```



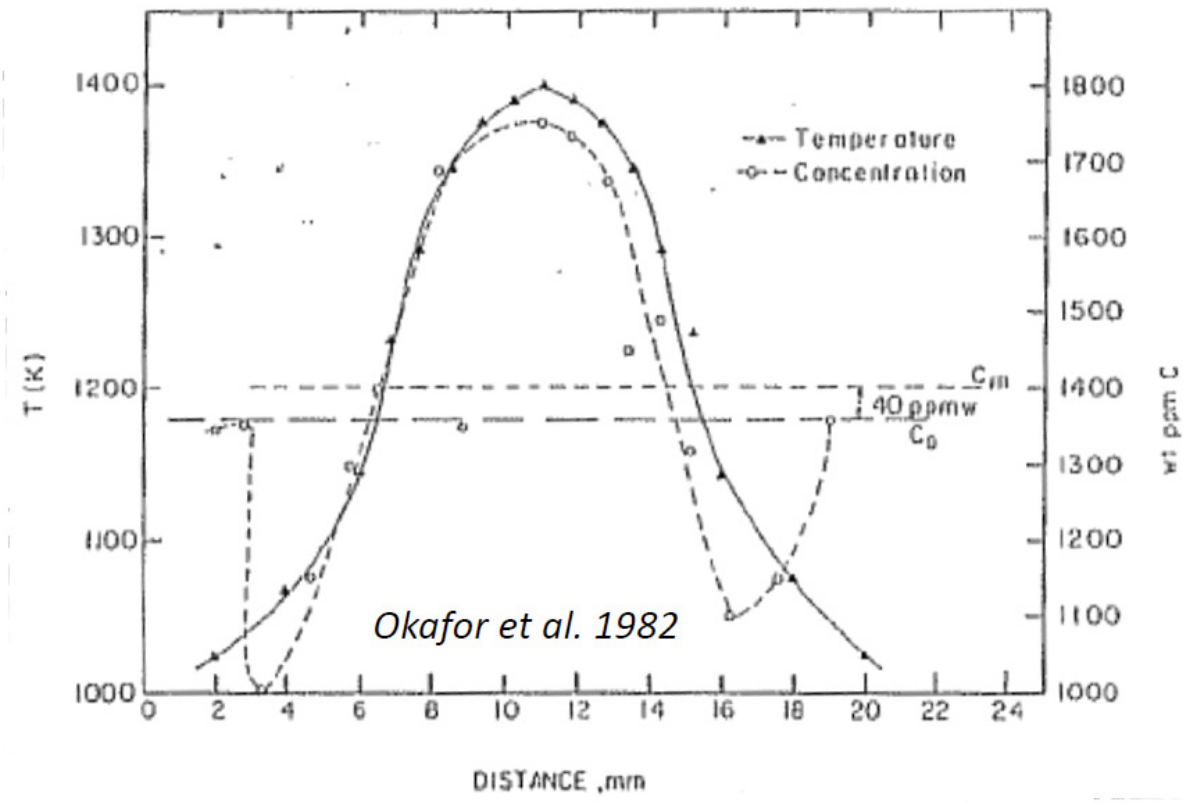

```
POST-1:
POST-1:
POST-1:
POST-1: --OK---
POST-1:
```

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

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 17825) 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: Wed Oct 31 13:18:51 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-
Examples\examples\exh3\setup.DCM.test"SYS:SYS:SYS:SYS:SYS:SYS: NO SUCH COMMAND, USE HELP
SYS:
SYS: THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

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

 VA                       /-  DEFINED
TDB_FEDEMO: FE                       NI                      C
   DEFINED
TDB_FEDEMO: 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: FCC_A1                   GRAPHITE  RESTORED
TDB_FEDEMO: 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: Current database: Fe-Alloys Mobility demo database v2.0

 VA  DEFINED
APP: FE                      NI                      C
   DEFINED
APP: BCC_A2                  FCC_A1  REJECTED
APP: FCC_A1  RESTORED
APP: 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: NO TIME STEP DEFINED
 *** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
DIC>
DIC>DIC>DIC>
DIC>DIC>
DIC>DIC>
DIC>DIC>
DIC>DIC>
DIC>PROFILE FOR /C/:PROFILE FOR /NI/:DIC>
DIC>DIC>
DIC>DIC>HEAT TRANSFER PARAMETER FOR PHASE:ELEMENT:PARAMETER /0/:DIC>
DIC>
DIC>DIC>
DIC> --OK---
DIC>
```

exh3-run

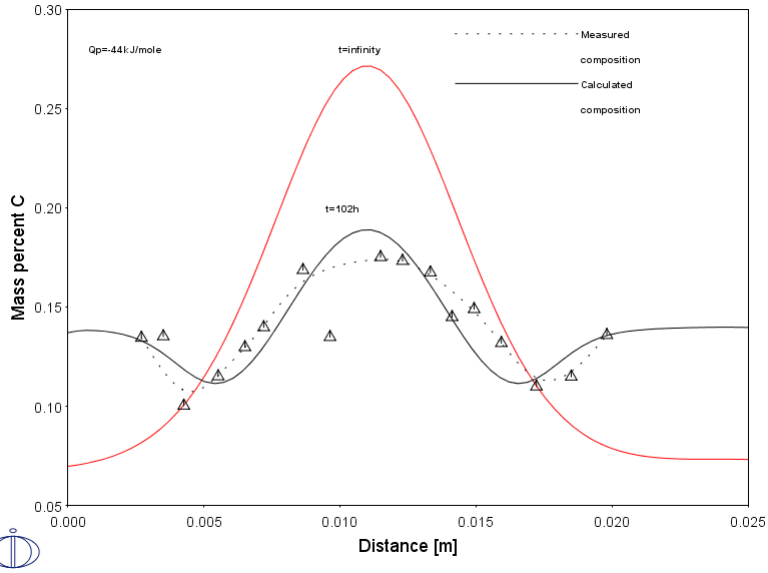
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exh3\run.DCM.test"DIC>
DIC> TIME STEP AT TIME  0.00000E+00
 *** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
DIC>
DIC> OK
DIC>
DIC> Region: AUS
 linear grid   75
 U-FRACTION IN SYSTEM:  C = .00662305741857947  FE = .68534915460493
                        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                    1 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                    0 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                    1 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                    0 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                    1 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                    0 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                    1 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                    0 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                    1 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                    0 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                    1 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                    0 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                    1 seconds
 TIME =   26616876.     DT =   1969173.4     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0066230574162012  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                    0 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                    1 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                    0 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                    1 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                    0 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                    1 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 = .68534915460493
                       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> --OK---
```

DIC>

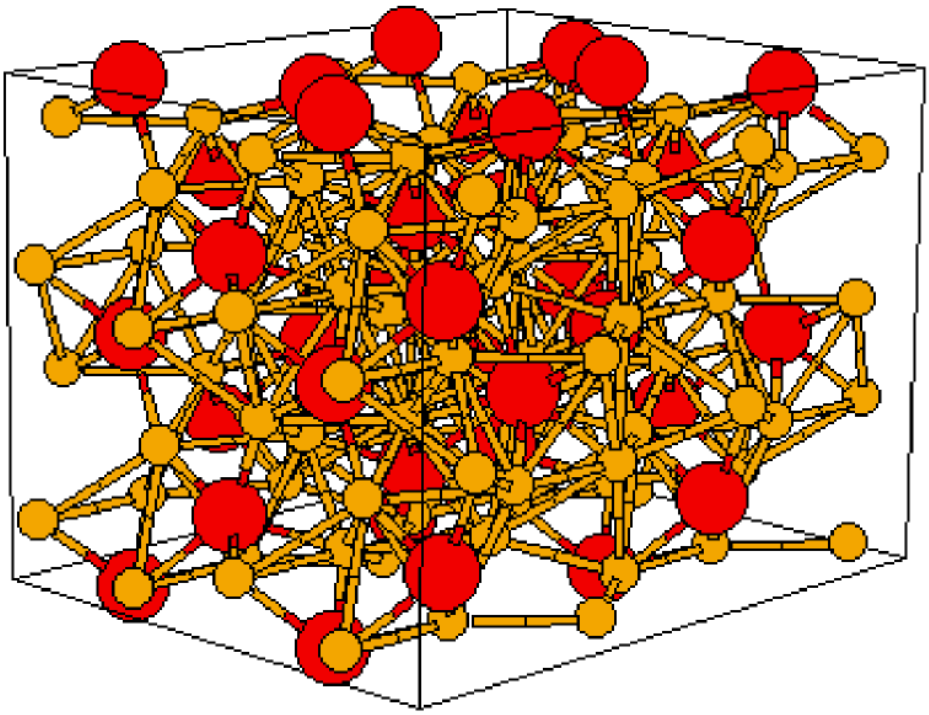
exh3-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exh3\plot.DCM.test"DIC> TIME STEP AT TIME  5.00000E+07
 *** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
DIC>
DIC>
DIC> OK
DIC>
DIC>  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:  INFO: Distance is set as independent variable
POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:
POST-1:AUTOMATIC AXIS TEXT  (Y OR N) /N/:AXIS TEXT :POST-1:
POST-1:AUTOMATIC AXIS TEXT  (Y OR N) /N/:AXIS TEXT :POST-1:
POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```




```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1: --OK---
POST-1:
```

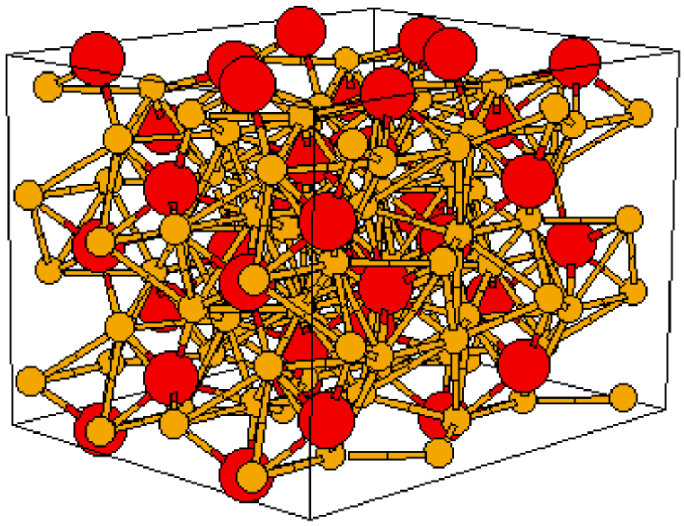
Diffusion in Complex Phases



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: Wed Oct 31 13:18:51 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-
Examples\examples\exi1\setup.DCM.test"SYS:SYS:SYS:SYS:SYS:SYS:SYS: NO SUCH COMMAND, USE HELP
SYS:
SYS:SYS:
SYS:
SYS: THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.0

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

 VA  DEFINED
TDB_USER: FE                      AL                      NI
   DEFINED
TDB_USER: B2_BCC                  BCC_DIS                 B2_ORD
   REJECTED
TDB_USER: BCC_DIS                 B2_ORD  RESTORED
TDB_USER: ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....
 INFO: Forcing option USE_POLY3 for complex phase B2_ORD
 -OK-
TDB_USER: NO TIME STEP DEFINED
DIC>DIC>
DIC>DIC>
DIC>WIDTH OF REGION /1/:TYPE /LINEAR/:NUMBER OF POINTS /50/:VALUE OF R IN THE GEOMETRICAL SERIE FOR LOWER PART OF REGION:VALUE OF R IN THE GEOM
DIC>ACTIVE OR INACTIVE PHASE /ACTIVE/:REGION NAME : /BETA/:PHASE TYPE /MATRIX/:PHASE NAME: /NONE/: INFO: PHASE HAS DISORDERED CONTRIBUTION
 FORCED STARTING VALUES ARE ENABLED
DIC>
DIC>REGION NAME : /BETA/:PHASE NAME: /B2_ORD/:DEPENDENT COMPONENT ? /NI/:COMPOSITION TYPE /MOLE_FRACTION/:PROFILE FOR /AL/:TYPE /LINEAR/:Functi
 Automatic start values will be set
 Forcing automatic start values
 Automatic start values will be set
 Forcing automatic start values
 Automatic start values will be set
 Forcing automatic start values
```

```
 Forcing automatic start values
 Automatic start values will be set
 Forcing automatic start values
 Automatic start values will be set
 Forcing automatic start values
 Automatic start values will be set
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 Forcing automatic start values
 Automatic start values will be set
 Forcing automatic start values
 Automatic start values will be set
 Forcing automatic start values
 Automatic start values will be set
DIC>
DIC>END TIME FOR INTEGRATION /.1/:AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /34560/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>AUTOMATIC STARTING VALUES FOR PHASE COMPOSITIONS /YES/:START VALUES FOR PHASES IN REGION BETA
PHASE: B2_ORD
MAJOR CONSTITUENTS IN PHASE B2_ORD:DIC>
DIC>
DIC>
DIC>
DIC>
DIC>DIC>
DIC> --OK---
DIC>
```
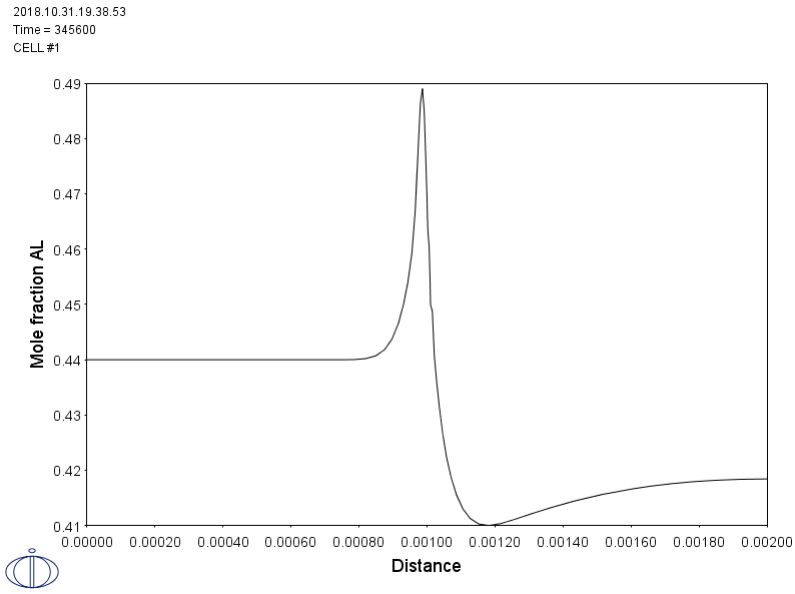

exi1-run

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exi1\run.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  0.00000E+00
DIC> OK
DIC>
DIC>DIC>DIC>DIC> 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                    0 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                    2 seconds
 TIME =   1538.4655     DT =   1025.3769     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  AL = .429499345639233  FE = .290517917020342
                        NI = .279982737340425
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    1 seconds
 TIME =   3589.2193     DT =   2050.7538     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  AL = .429499345639231  FE = .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                    1 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                    2 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
```

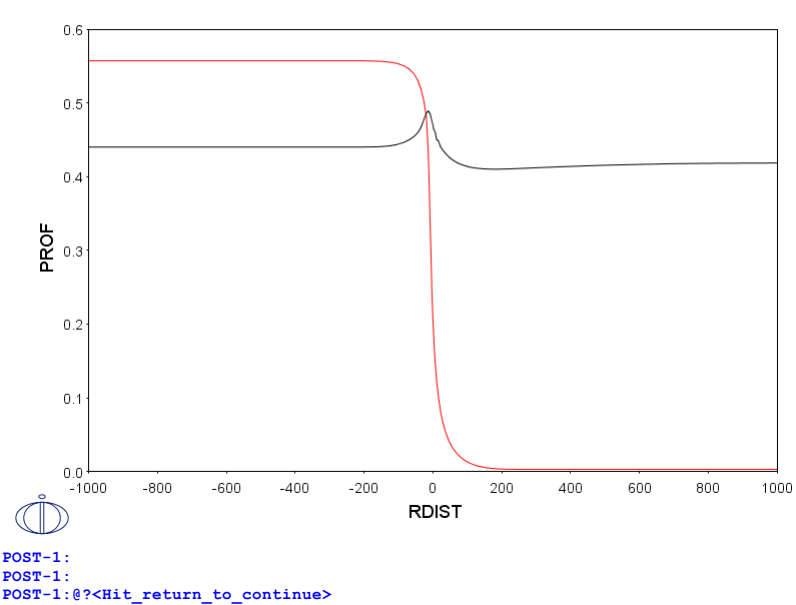
```
 DELETING TIME-RECORD FOR TIME   0.10000000E-06
 DELETING TIME-RECORD FOR TIME   0.10010000E-03
 DELETING TIME-RECORD FOR TIME   0.40010010
 DELETING TIME-RECORD FOR TIME    513.08856
 DELETING TIME-RECORD FOR TIME    1538.4655
 DELETING TIME-RECORD FOR TIME    3589.2193
 DELETING TIME-RECORD FOR 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> --OK---
DIC>
```

exi1-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exi1\plot.DCM.test"DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  3.45600E+05
DIC> OK
DIC>
DIC>DIC>DIC>DIC>  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:  INFO: Distance is set as independent variable
POST-1:
POST-1:POST-1:
POST-1:POST-1:
POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```

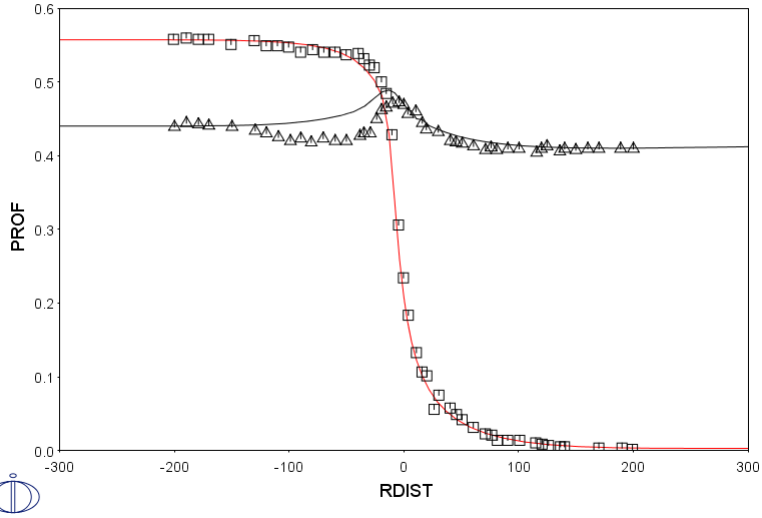



```
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1:Variable(s)POST-1:
POST-1:FUNCTION:&
POST-1:COLUMN NUMBER /*/:POST-1:
POST-1:POST-1:
POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```




```
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1:PROLOGUE NUMBER: /0/:DATASET NUMBER(s): /-1/:POST-1:
POST-1:POST-1:
POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```

2018.10.31.19.38.54
Time = 345600
CELL #1




```
POST-1:
POST-1:
POST-1: --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
 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 17825) 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: Wed Oct 31 13:18:51 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-
Examples\examples\exi2\setup.DCM.test"SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: NO SUCH COMMAND, USE HELP
SYS:
SYS:SYS:SYS:SYS: 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:TDB_TCFE9:TDB_TCFE9: Current database: Iron Demo Database v2.0

 VA                       /-  DEFINED
TDB_FEDEMO: FE                       C  DEFINED
TDB_FEDEMO: 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: BCC_A2                   FCC_A1                  CEMENTITE
 GRAPHITE  RESTORED
TDB_FEDEMO: 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:TDB_FEDEMO:TDB_FEDEMO: Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

 VA  DEFINED
TDB_APP: FE                       C  DEFINED
TDB_APP: BCC_A2                   CEMENTITE  REJECTED
TDB_APP: *** FCC INPUT IGNORED
 BCC_A2                   CEMENTITE  RESTORED
TDB_APP: 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:TDB_APP: NO TIME STEP DEFINED
 *** ENTERING FCC_A1 AS A DIFFUSION NONE PHASE
 *** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>REGION NAME :DIC>
DIC>REGION NAME :ATTACH TO REGION NAMED /FER/:
ATTACHED TO THE RIGHT OF FER /YES/:
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>REGION NAME : /FER/:WIDTH OF REGION /1/:TYPE /LINEAR/:DIC>
DIC>DIC>DIC>DIC>DIC>REGION NAME : /CARB/:WIDTH OF REGION /1/:TYPE /LINEAR/:DIC>
DIC>
DIC>DIC>DIC>DIC>  COMPOSITION RECORD FOR STOICHIOMETRIC PHASE CEMENTITE IN REGION CARB CREATED
DIC>DIC>
DIC>DIC>DIC>DIC>REGION NAME : /FER/:PHASE NAME: /CEMENTITE/:DIC>
DIC>REGION NAME : /FER/:PHASE NAME: /BCC_A2/:COMPOSITION TYPE /MOLE_FRACTION/:PROFILE FOR /C/:DIC>
DIC>CONDITION TYPE /CLOSED_SYSTEM/:Dependent substitutional element:FE
Dependent interstitial element:VA
LOW TIME LIMIT /0/:ACR(C)(TIME)=HIGH TIME LIMIT /*/:ANY MORE RANGES /N/:DIC>
DIC>
DIC>
DIC>DIC>DIC>DIC>END TIME FOR INTEGRATION /.1/:AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /900/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>DIC>DIC>DIC>DIC>
DIC> --OK---
DIC>
```

exi2-run

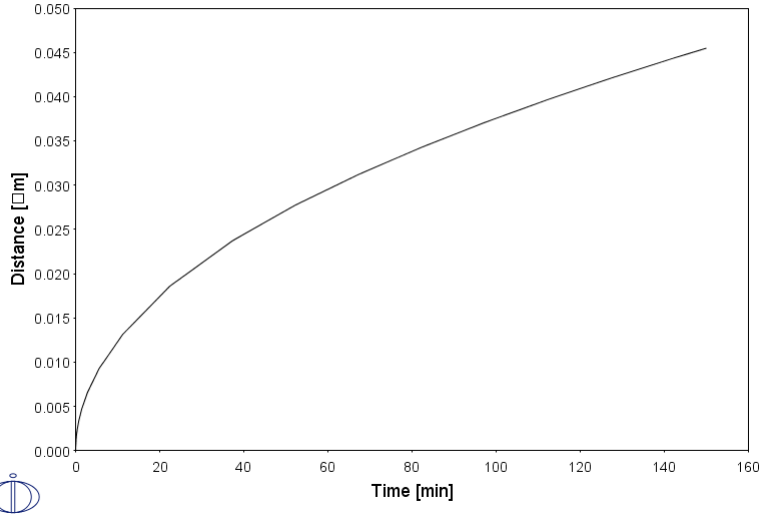
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exi2\run.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  0.00000E+00
 *** ENTERING FCC_A1 AS A DIFFUSION NONE PHASE
 *** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
DIC> OK
DIC>
DIC>DIC>DIC>DIC> 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]
  24  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: CARB

  CPU time used in timestep                    0 seconds
 2.556050647385387E-006        2.557893906616863E-006        2.321065696136770E-024       TIME =  0.63759149E-03 DT =  0.31999573E-
03 SUM OF SQUARES =  0.23210657E-23
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.12495496E-07 AND  -0.12495496E-07
 POSITION OF INTERFACE FER / CARB IS   0.32999873E-05
 U-FRACTION IN SYSTEM:  C = 4.77135741222547E-05  FE = 1
 TOTAL SIZE OF SYSTEM:  3.300001E-06 [m]


output ignored...



... output resumed

 3.022550110094207E-027       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                    0 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> --OK---
DIC>
```

exi2-plot

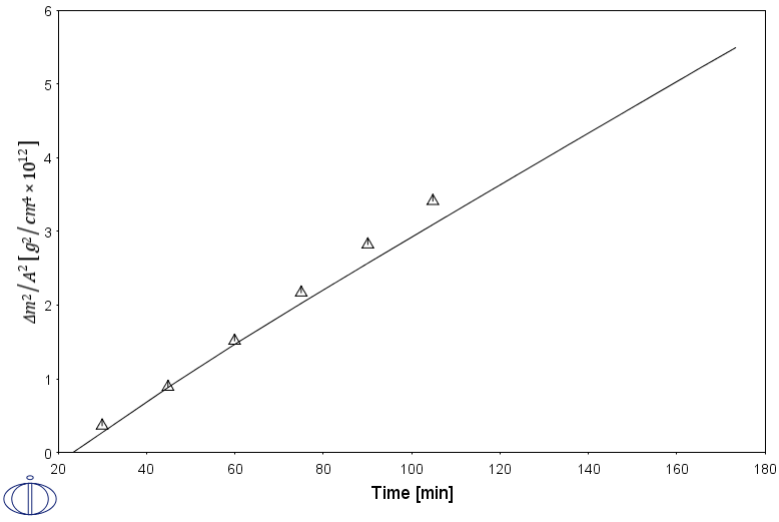
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exi2\plot.DCM.test"DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  9.00000E+03
 *** ENTERING FCC_A1 AS A DIFFUSION NONE PHASE
 *** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
DIC>
DIC>
DIC> OK
DIC>
DIC>
DIC>DIC>DIC>DIC>  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:FUNCTION:POST-1:
POST-1:FUNCTION:POST-1:
POST-1:POST-1:POST-1:
POST-1:POST-1:
POST-1:POST-1:POST-1:
POST-1:
POST-1:POST-1:            OST-1:POST-1:
POST-1:
```

2018.10.31.19.42.10
"FIRST" INTERFACE OF SYSTEM
CELL #1




```
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1:
POST-1:POST-1:POST-1:POST-1:FUNCTION:POST-1:
POST-1:POST-1:POST-1:POST-1:FUNCTION:POST-1:
POST-1:
POST-1:POST-1:POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:
POST-1:
POST-1:POST-1:POST-1:
POST-1:
POST-1:POST-1:            OST-1:POST-1:
POST-1:
```

2018.10.31.19.42.10
"FIRST" INTERFACE OF SYSTEM
CELL #1

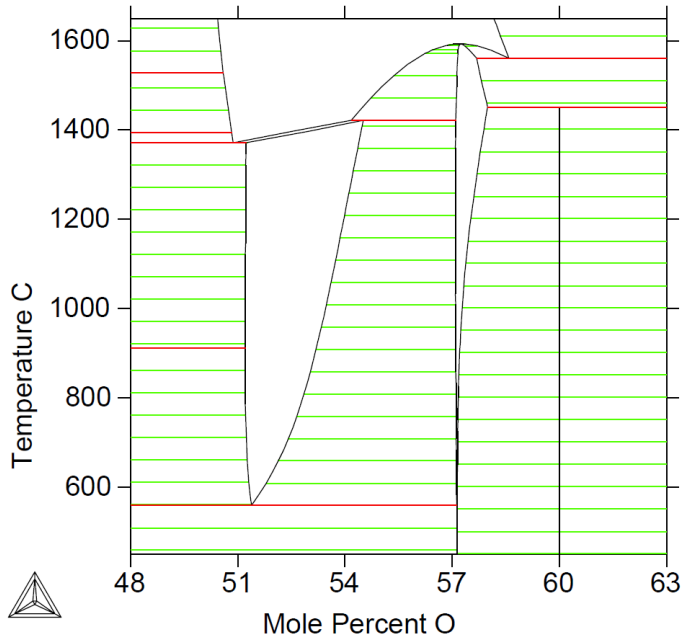



```
POST-1:
POST-1:
POST-1: --OK---
POST-1:
```

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

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 17825) 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: Wed Oct 31 13:18:51 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-
Examples\examples\exi3a\setup.DCM.test"SYS:SYS:SYS:SYS:SYS:SYS: NO SUCH COMMAND, USE HELP
SYS:
SYS:SYS:
SYS:SYS:SYS:SYS: 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:TDB_TCFE9:TDB_TCFE9: Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

 VA                      /-  DEFINED
TDB_USER: FE                     O  DEFINED
TDB_USER: /-                     VA                      FE
 O                       FE+2                    FE+3
 FE+4                    FE2O3                   FEO
 FEO3/2                  O-2                     O2
   REJECTED
TDB_USER: FE                     FE+2                    FE+3
 O                       O2                      O-2
 VA  RESTORED
TDB_USER: GAS:G                  BCC_A2                  SPINEL:I
   REJECTED
TDB_USER: BCC_A2                 SPINEL:I                GAS:G
   RESTORED
TDB_USER:
TDB_USER: 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:TDB_USER:TDB_USER: Current database: User defined Database
         test database

 VA                      /-                      O
   DEFINED
TDB_APP: FE  DEFINED
TDB_APP: /-                      VA                      FE
 O                       FE+2                    FE+3
 FE2O3                   FEO                     FEO3/2
 O-2                     O2  REJECTED
TDB_APP: FE                      FE+2                    FE+3
 O                       O2                      O-2
 VA  RESTORED
TDB_APP: SPINEL:I                GAS:G                   BCC_A2
   REJECTED
TDB_APP: BCC_A2                  SPINEL:I                GAS:G
   RESTORED
TDB_APP:
TDB_APP: ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 *** ERROR  2018 IN DESHPH: DIFFUSION DATA NOT POSSIBLE FOR GAS PHASE
 *** ERROR  2018 IN DESHPH: DIFFUSION DATA NOT POSSIBLE FOR GAS PHASE
 FUNCTIONS ....

 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:TDB_APP:TDB_APP: NO TIME STEP DEFINED
DIC>
DIC>
DIC>DIC>DIC>DIC>DIC>
DIC>
DIC>DIC>DIC>DIC>DIC>
DIC>
DIC>DIC>DIC>DIC>DIC>DIC>
DIC>
DIC>DIC>DIC>DIC>DIC>DIC>
DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>DIC>DIC>
DIC>
DIC>DIC>DIC>DIC>PROFILE FOR /O/:DIC>
DIC>
DIC>DIC>DIC>DIC>  this is a phase with charged species
  with more than 2 sublattices
PROFILE FOR /FE/:DIC>
DIC>
DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>TYPE OF CONDITION FOR COMPONENT FE /ZERO_FLUX/:TYPE OF CONDITION FOR COMPONENT O /ZERO_FLUX/:LOW TIME LIMIT
DIC>
DIC>DIC>DIC>DIC> STARTING VALUES WILL BE TAKEN FROM PROFILES
DIC>
DIC>
DIC>DIC>DIC>DIC>SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>DIC>DIC>DIC>DIC> RELEASING OLD STARTING VALUES
DIC>
DIC>
DIC>DIC>DIC>DIC>DIC>
DIC> --OK---
DIC>
```

exi3a-run

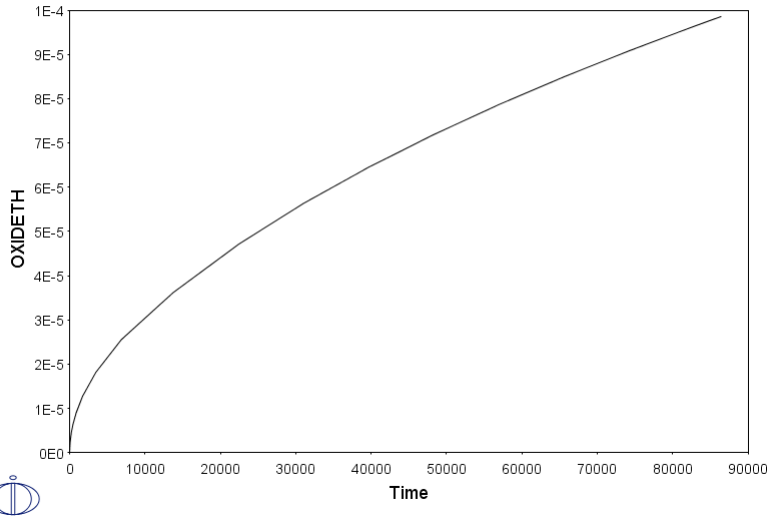
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exi3a\run.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  0.00000E+00
DIC> OK
DIC>
DIC>DIC>DIC>DIC> Region: FER
 single geometric dense at  0.50000E-02
 0.87386       95
 Region: SP
 double 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                    1 seconds
 1.507552605990936E-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                    0 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                    1 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]
  28  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    0 seconds
 3.178061987677804E-006        3.179295507136431E-006        3.179211108943127E-006        3.565487603550355E-009        1.330132983661661E-
032       TIME =  0.12700000E-04 DT =  0.64000000E-05 SUM OF SQUARES =  0.13301330E-31
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.35192806E-04 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49999893E-02


output ignored...



... output resumed

 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.59777883E-09 AND    0.0000000
 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                    0 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                    1 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> --OK---
DIC>
```

exi3a-plot

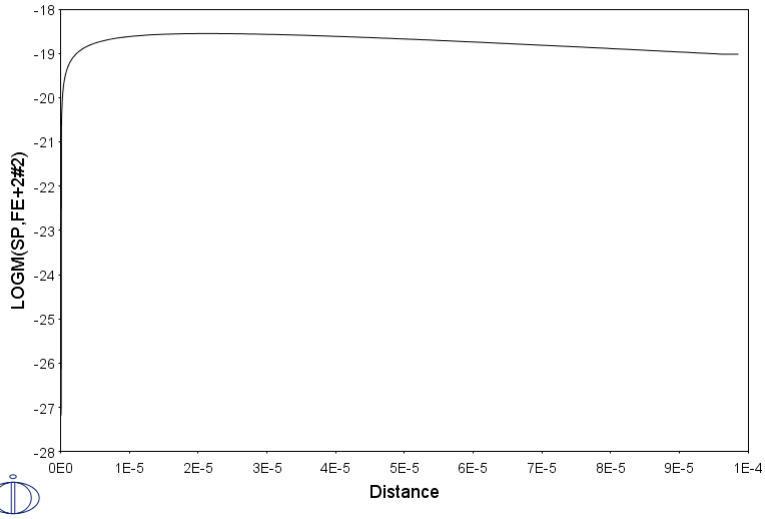
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exi3a\plot.DCM.test"DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  8.64000E+04
DIC> OK
DIC>
DIC>DIC>DIC>DIC>  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:POST-1:POST-1:POST-1:FUNCTION:&
POST-1:POST-1:POST-1:POST-1:POST-1:
POST-1:POST-1:POST-1:POST-1:  INFO: Time is set as independent variable
POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:
POST-1:
POST-1:POST-1:            OST-1:POST-1:
POST-1:
```

2018.10.31.19.45.36
UPPER INTERFACE OF REGION "SP#1"
CELL #1



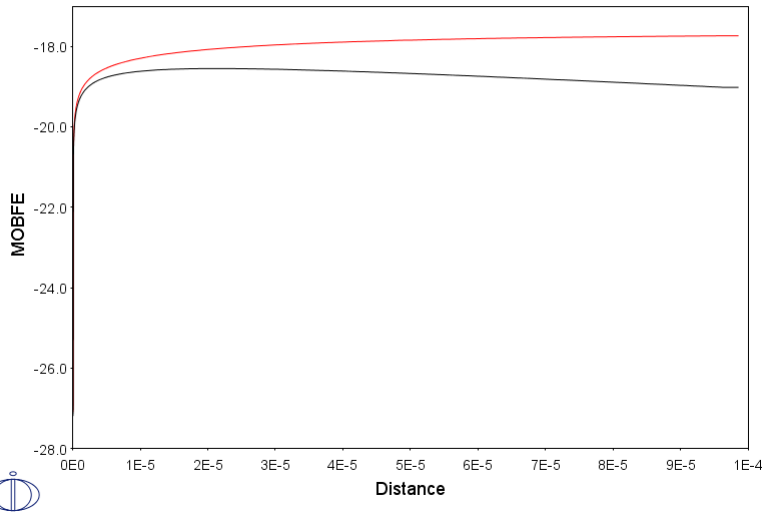

```
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:
POST-1:POST-1:POST-1:POST-1:  INFO: Distance is set as independent variable
POST-1:
POST-1:POST-1:
POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```

2018.10.31.19.45.37
Time = 86400
CELL #1



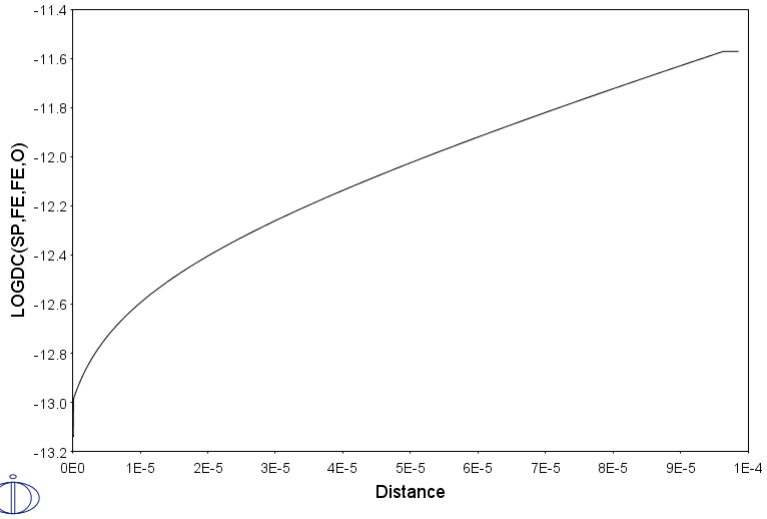

```
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:Variable(s)POST-1:
POST-1:COLUMN NUMBER /*/:
POST-1:
POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```

2018.10.31.19.45.38
Time = 86400
CELL #1




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

2018.10.31.19.45.40
Time = 86400
CELL #1

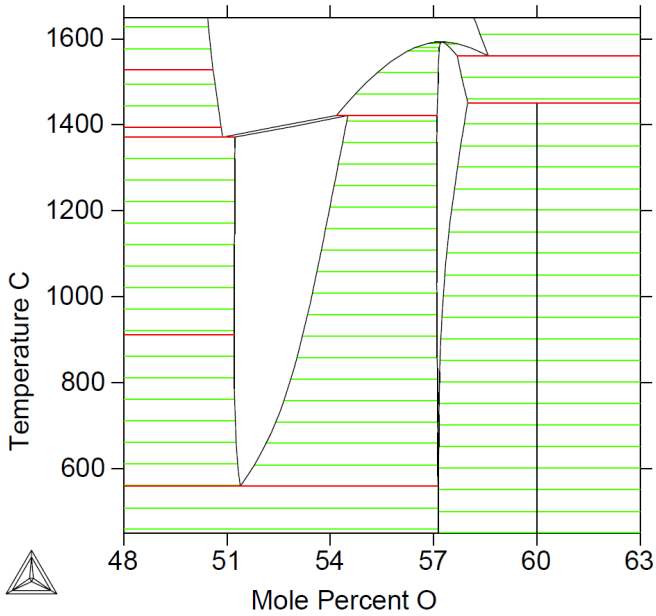



```
POST-1:
POST-1:
POST-1: --OK---
POST-1:
```

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 License library version: 8.5.1.0017
 Linked: Wed Oct 31 13:18:51 2018


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-
Examples\examples\exi3b\setup.DCM.test"SYS:SYS:SYS:SYS:SYS:SYS:SYS: NO SUCH COMMAND, USE HELP
SYS:
SYS:SYS:
SYS:SYS:SYS:SYS: 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:TDB_TCFE9:TDB_TCFE9: Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

 VA                       /-  DEFINED
TDB_USER: FE                      O  DEFINED
TDB_USER: /-                      VA                      FE
 O                        FE+2                    FE+3
 FE+4                     FE2O3                   FEO
 FEO3/2                   O-2                     O2
   REJECTED
TDB_USER: FE                      FE+2                    FE+3
 O                        O2                      O-2
 VA  RESTORED
TDB_USER: GAS:G                   BCC_A2                  SPINEL:I
   REJECTED
TDB_USER: BCC_A2                  SPINEL:I                GAS:G
   RESTORED
TDB_USER:
TDB_USER: 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:TDB_USER:TDB_USER: Current database: User defined Database
         test database
```

```
 VA                      /-                      O
   DEFINED
TDB_APP: FE  DEFINED
TDB_APP: /-                      VA                      FE
 O                       FE+2                    FE+3
 FE2O3                   FEO                     FEO3/2
 O-2                     O2  REJECTED
TDB_APP: FE                      FE+2                    FE+3
 O                       O2                      O-2
 VA  RESTORED
TDB_APP: SPINEL:I                GAS:G                   BCC_A2
   REJECTED
TDB_APP: BCC_A2                  SPINEL:I                GAS:G
   RESTORED
TDB_APP:
TDB_APP: ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 *** ERROR  2018 IN DESHPH: DIFFUSION DATA NOT POSSIBLE FOR GAS PHASE
 *** ERROR  2018 IN DESHPH: DIFFUSION DATA NOT POSSIBLE FOR GAS PHASE
 FUNCTIONS ....

 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:TDB_APP:TDB_APP: NO TIME STEP DEFINED
DIC>
DIC>
DIC>DIC>DIC>DIC>DIC>
DIC>
DIC>DIC>DIC>DIC>DIC>
DIC>
DIC>DIC>DIC>DIC>DIC>DIC>
DIC>
DIC>DIC>DIC>DIC>DIC>DIC>
DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC>DIC>DIC>
DIC>
DIC>DIC>DIC>DIC>PROFILE FOR /O/:DIC>
DIC>
DIC>DIC>DIC>DIC>  this is a phase with charged species
  with more than 2 sublattices
PROFILE FOR /FE/:DIC>
DIC>
DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>TYPE OF CONDITION FOR COMPONENT FE /ZERO_FLUX/:TYPE OF CONDITION FOR COMPONENT O /ZERO_FLUX/:LOW TIME LIMIT
DIC>
DIC>DIC>DIC>DIC> STARTING VALUES WILL BE TAKEN FROM PROFILES
DIC>
DIC>
DIC>DIC>DIC>DIC>SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>DIC>DIC>DIC>DIC> RELEASING OLD STARTING VALUES
DIC>
DIC>
DIC>DIC>REGION NAME : /SP/:PHASE NAME: /SPINEL/:Enable model for grainboundary contribution to diffusion /YES/:Grainboundary thickness /5E-
10/:Grainsize(T,P,TIME)=Bulkdiffusion activation energy multiplier /.5/:Enable model for dislocation contribution to diffusion /YES/:DIC>
DIC>
DIC>
DIC>DIC>DIC>DIC>DIC>
DIC>
DIC>
DIC> --OK---
DIC>
```

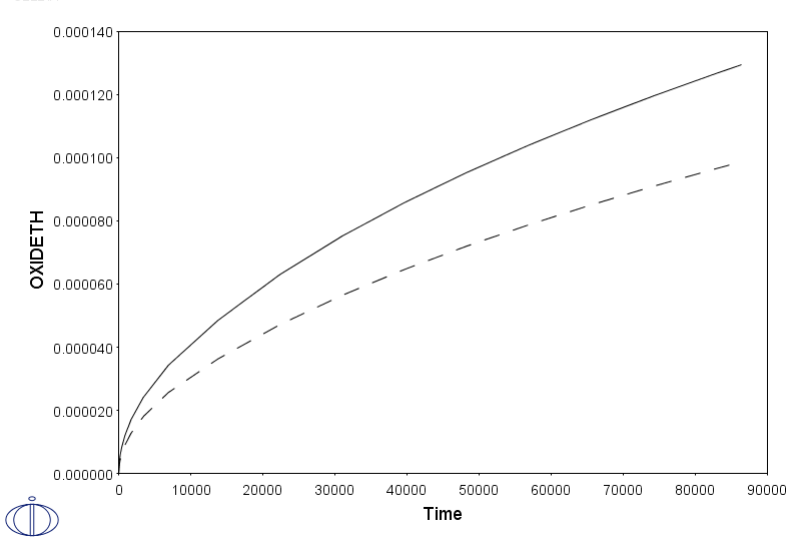
exi3b-run

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exi3b\run.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  0.00000E+00
DIC> OK
DIC>
DIC>DIC>DIC>DIC> 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                    1 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                    0 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]
  35  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    1 seconds
 6.846436546859467E-006        6.848924860330321E-006        6.848774655972661E-006        7.322138692691440E-009        3.845675848093666E-
031       TIME =  0.12700000E-04 DT =  0.64000000E-05 SUM OF SQUARES =  0.38456758E-30
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.47490676E-04 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49999891E-02


output ignored...



... output resumed

 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.77035589E-09 AND    0.0000000
 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> --OK---
DIC>
```

exi3b-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exi3b\plot.DCM.test"DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  8.64000E+04
DIC> OK
DIC>
DIC>DIC>DIC>DIC>  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:POST-1:POST-1:POST-1:FUNCTION:&
POST-1:POST-1:POST-1:POST-1:POST-1:
POST-1:POST-1:POST-1:POST-1:  INFO: Time is set as independent variable
POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:
POST-1:POST-1:
POST-1:
POST-1:POST-1:            OST-1:POST-1:
POST-1:
```




```
POST-1:
POST-1:
POST-1: --OK---
POST-1:
```

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