Diffusion Module (DICTRA) Example Macros

Thermo-Calc Version 2019b

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

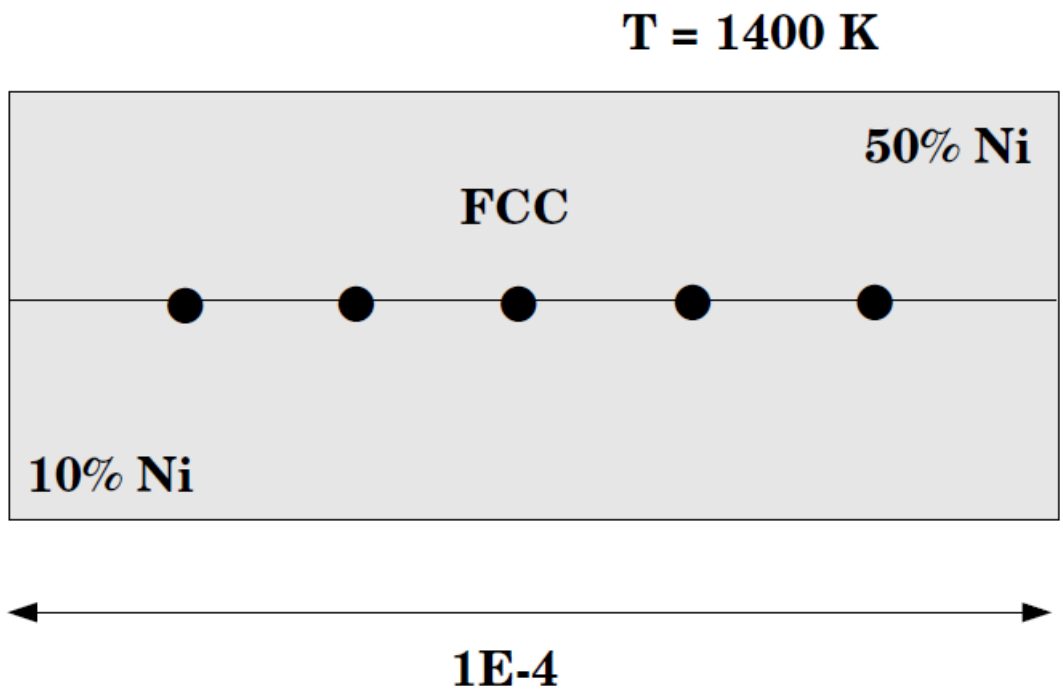
Diffusion in complex phases. Diffusion in iron oxide (FeO) This example shows the oxidation of an iron sample and the consequent growth of an oxide layer.

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

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 Software  (build 20130) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri May 24 17:06:15 2019


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-
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SYS:SYS:SYS:SYS:MODULE NAME: THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.1

 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  v9.1
 TCFE8   =  Steels/Fe-Alloys  v8.1
 FROST1  =  FROST database v1.0
 TCFE7   =  Steels/Fe-Alloys  v7.0
 TCFE6   =  Steels/Fe-Alloys  v6.2
 TCFE5   =  Steels/Fe-Alloys  v5.0
 TCFE4   =  Steels/Fe-Alloys  v4.1
 TCFE3   =  Steels/Fe-Alloys  v3.1
 TCFE2   =  Steels/Fe-Alloys  v2.1
 TCFE1   =  Steels/Fe-Alloys  v1.0
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 NI25    =  NI25 Database
 TCNI8   =  Ni-Alloys  v8.2
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 TCNI5   =  Ni-Alloys  v5.1
 TCNI4   =  Ni-Alloys  v4.0
 TCNI1   =  Ni-Alloys  v1.3
 TCAL6   =  Al-Alloys  v6.0
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 TCAL4   =  Al-Alloys  v4.0
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 TCAL2   =  Al-Alloys  v2.1
 TCAL1   =  Al-Alloys  v1.2
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 TCMG2   =  Mg-Alloys  v2.0
 TCMG1   =  Mg-Alloys  v1.1
 TCTI2   =  Ti-Alloys  v2.1
 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
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 TCSLD1  =  Solder Alloys  v1.1
 TCSI1   =  Ultrapure Silicon  v1.2
 TCMP2   =  Materials Processing  v2.5
 TCES1   =  Combustion/Sintering  v1.1
 TCSC1   =  Super Conductor  v1.0
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 NUMT2   =  Nuclear Materials  v2.1
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 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 v2.1
 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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 USER    =  User defined Database

DATABASE NAME /TCFE9/: Current database: Iron Demo Database v2.1

 VA                      /-  DEFINED
TDB_FEDEMO:
TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO:ELEMENTS: FE                      NI  DEFINED
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 PHASES .......
 PARAMETERS ...
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 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'
  '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

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 TCFE8   =  Steels/Fe-Alloys  v8.1
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 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
 TCSLD1  =  Solder Alloys  v1.1
 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
 TCNF2   =  Nuclear Fuels  v2.1b
 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 v2.1
 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  v1.0
 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>
```

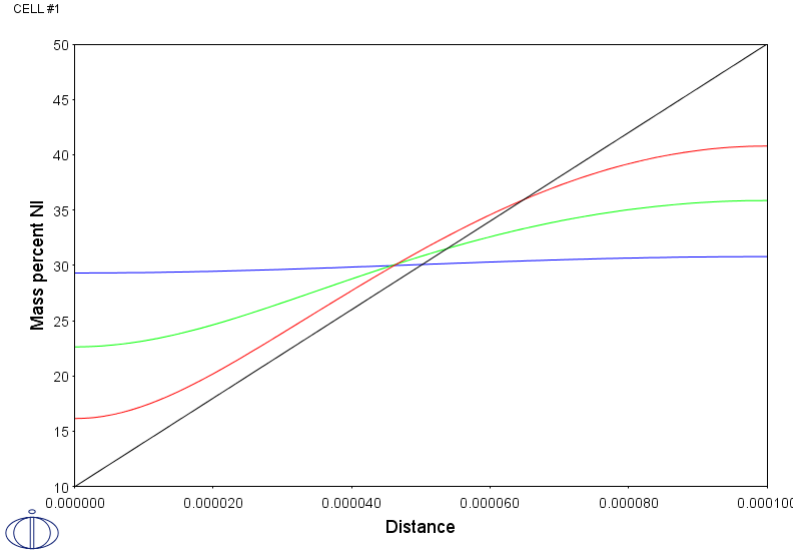
exa1-run

```
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
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
 U-FRACTION IN SYSTEM:  FE = .709680136600384  NI = .290319863399616
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 U-FRACTION IN SYSTEM:  FE = .709680136600384  NI = .290319863399616
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .709680136600384  NI = .290319863399616
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.10010000E-03 DT =  0.10000000E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .709680136600384  NI = .290319863399616
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.40010010     DT =  0.40000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .709680136600384  NI = .290319863399616
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   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                    1 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 = .709680136600385  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 = .709680136600384  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 = .709680136600384  NI = .290319863399616
 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 = .709680136600384  NI = .290319863399616
 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 = .709680136600384  NI = .290319863399616
 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 = .709680136600383  NI = .290319863399616
 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 = .709680136600385  NI = .290319863399616
 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 = .290319863399615
 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 = .709680136600385  NI = .290319863399615
 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 = .290319863399614
 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 = .709680136600386  NI = .290319863399614
 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:
```

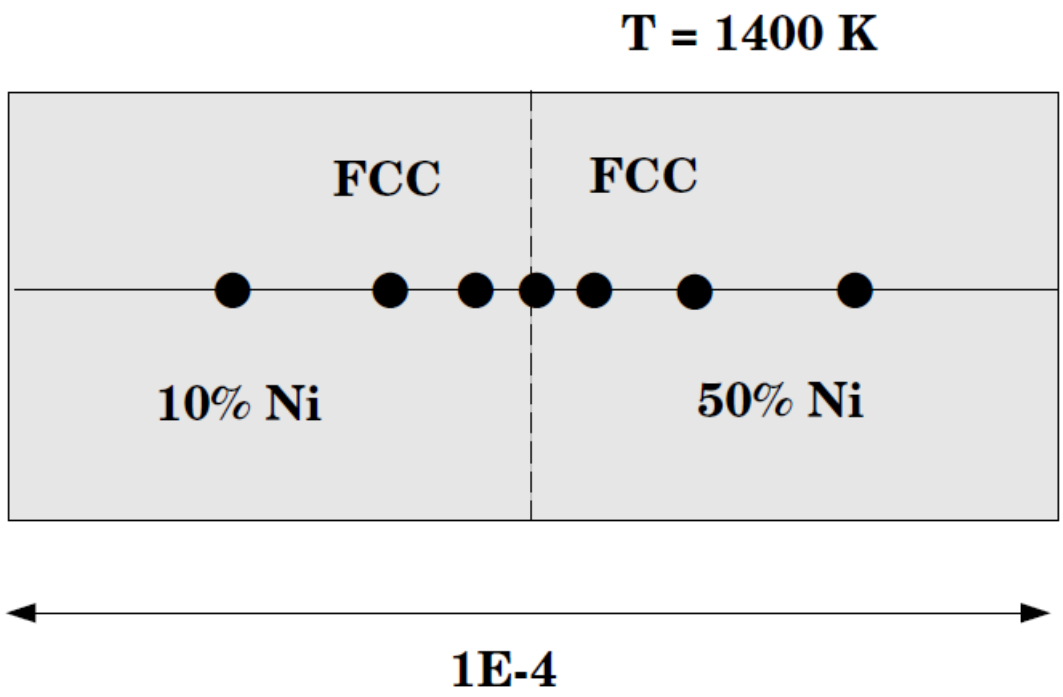



```
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: --OK---
POST-1:
```

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 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 20130) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri May 24 17:06:15 2019


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  v9.1

 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 v2.1

 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                  CBCC_A12
 CUB_A13                  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'
  '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  v9.1
 TCFE8   =  Steels/Fe-Alloys  v8.1
 FROST1  =  FROST database v1.0
 TCFE7   =  Steels/Fe-Alloys  v7.0
 TCFE6   =  Steels/Fe-Alloys  v6.2
 TCFE5   =  Steels/Fe-Alloys  v5.0
 TCFE4   =  Steels/Fe-Alloys  v4.1
 TCFE3   =  Steels/Fe-Alloys  v3.1
 TCFE2   =  Steels/Fe-Alloys  v2.1
 TCFE1   =  Steels/Fe-Alloys  v1.0
 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  v2.1
 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
 TCSLD1  =  Solder Alloys  v1.1
 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
 TCNF2   =  Nuclear Fuels  v2.1b
 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 v2.1
 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  v1.0
 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
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   ... the command in full is COMPUTE_EQUILIBRIUM
   ... the command in full is COMPUTE_EQUILIBRIUM
DIC>
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>   ... the command in full is SAVE_WORKSPACES
DIC>
DIC>   ... the command in full is SET_INTERACTIVE
 --OK---
DIC>
```
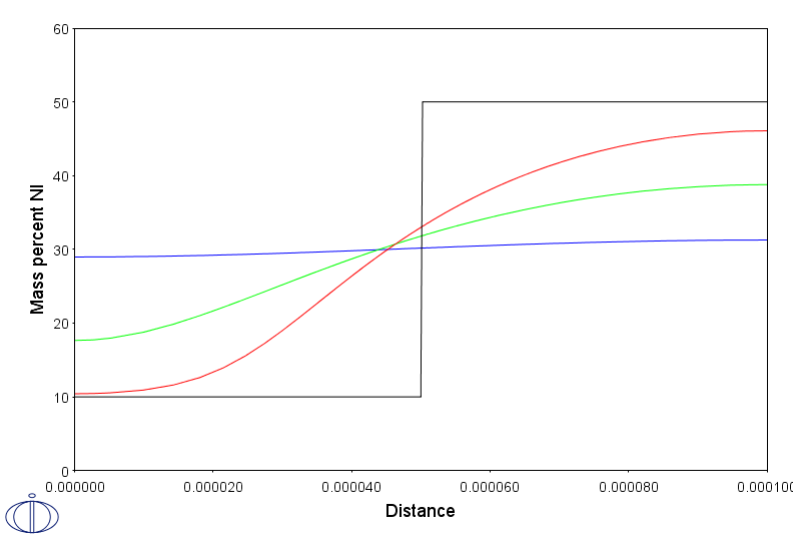

exa2a-run

```
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
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
   ... the command in full is SET_NUMERICAL_LIMITS
 U-FRACTION IN SYSTEM:  FE = .70888824540617  NI = .29111175459383
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 U-FRACTION IN SYSTEM:  FE = .70888824540617  NI = .29111175459383
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  2  GRIDPOINT(S) ADDED   TO   CELL #1   REGION: AUSTENITE
 TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .708888245406169  NI = .29111175459383
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.10010000E-03 DT =  0.10000000E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .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 =   10.408313     DT =   10.008213     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 =   30.424739     DT =   20.016426     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 =   70.457590     DT =   40.032851     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 =   150.52329     DT =   80.065703     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 =   310.65470     DT =   160.13141     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 =   630.91751     DT =   320.26281     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 =   1271.4431     DT =   640.52562     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 =   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 = .70888824540617  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 = .70888824540617  NI = .29111175459383
 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 = .70888824540617  NI = .29111175459383
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    1 seconds
 TIME =   40984.032     DT =   20496.820     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 =   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 = .708888245406168  NI = .291111754593832
 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 = .708888245406168  NI = .291111754593832
 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 = .708888245406168  NI = .291111754593831
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   463964.95     DT =   100000.00     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .708888245406168  NI = .291111754593832
 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 = .708888245406169  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 = .708888245406168  NI = .291111754593832
 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 = .708888245406168  NI = .291111754593832
 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 = .708888245406172  NI = .291111754593828
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 = .291111754593828
TOTAL SIZE OF SYSTEM:  1E-04 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME    0.0000000
DELETING TIME-RECORD FOR TIME   0.10000000E-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>AboutMACRO "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
```

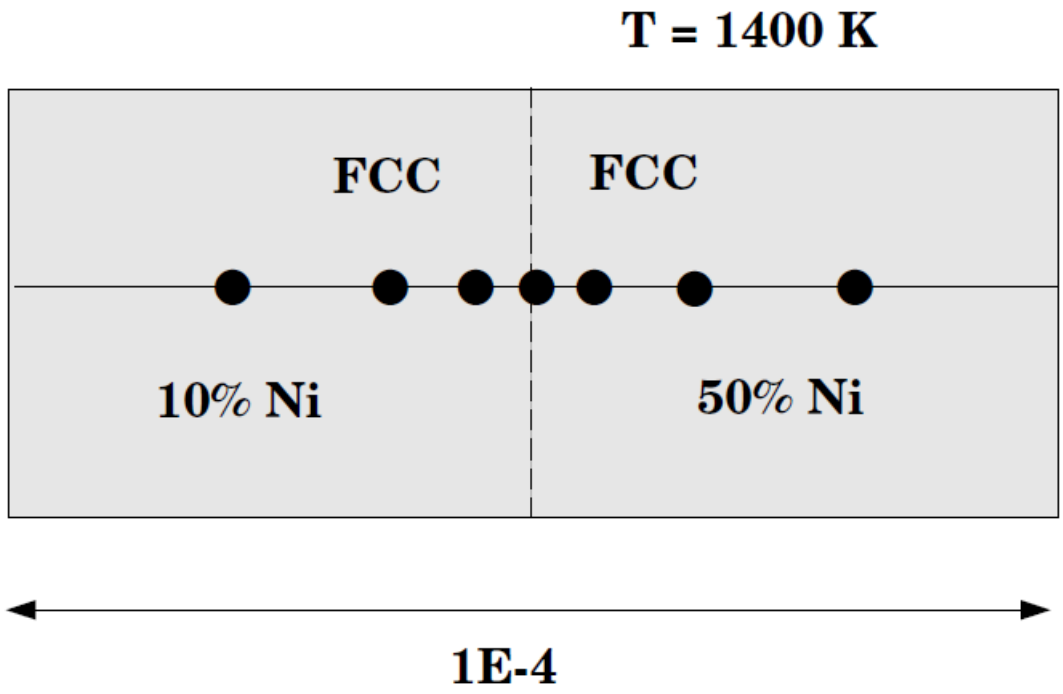



```
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1:   ... the command in full is SET_INTERACTIVE_MODE
 --OK---
POST-1:
```

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
 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 20130) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri May 24 17:06:15 2019


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  v9.1

 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 v2.1

 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                  CBCC_A12
 CUB_A13                 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'
  '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:   ... the command in full is APPEND_DATABASE
 Use one of these databases

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

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 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
 TCSLD1  =  Solder Alloys  v1.1
 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
 TCNF2   =  Nuclear Fuels  v2.1b
 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 v2.1
 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  v1.0
 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
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   ... the command in full is COMPUTE_EQUILIBRIUM
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DIC>
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 /AUTO/:
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -> 1): /AUTO/:MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/: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>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                    1 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

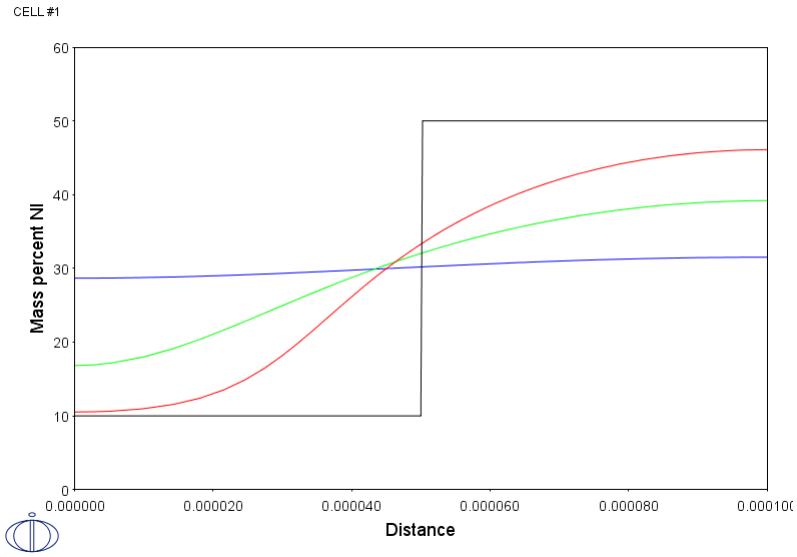
 KEEPING TIME-RECORD FOR TIME    963885.37
 AND FOR TIME                    1000000.0
 WORKSPACE RECLAIMED

 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
```



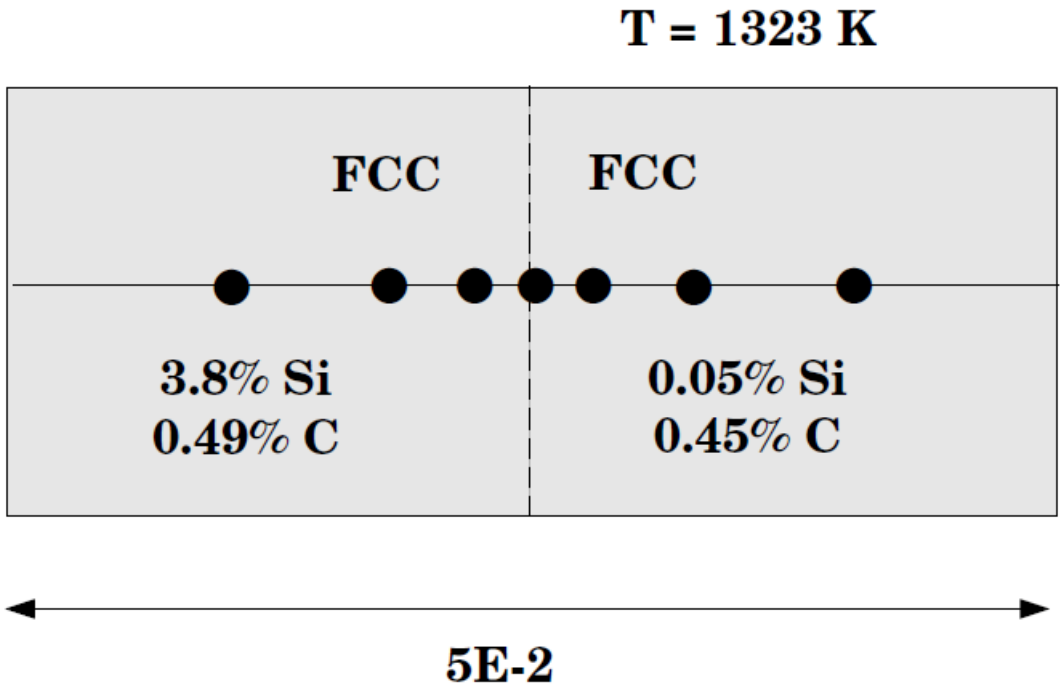

```
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1:   ... the command in full is SET_INTERACTIVE_MODE
 --OK---
POST-1:
```

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

```
About
 Software  (build 20130) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri May 24 17:06:15 2019


SYS:SYS:MACRO "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  v9.1

 VA                       /-  DEFINED
 L12_FCC                  B2_BCC                   DICTRA_FCC_A1
   REJECTED
TDB_TCFE9:
TDB_TCFE9:TDB_TCFE9:TDB_TCFE9:TDB_TCFE9:TDB_TCFE9: FE                       SI                       C
   DEFINED
TDB_TCFE9: GAS:G                    LIQUID:L                 BCC_A2
 FCC_A1                   HCP_A3                   CBCC_A12
 CUB_A13                  DIAMOND_FCC_A4           GRAPHITE
 CEMENTITE                M23C6                    M7C3
 M5C2                     KSI_CARBIDE              FE4N_LP1
 FECN_CHI                 LAVES_PHASE_C14          M3SI
 CR3SI                    FE2SI                    FESI2_H
 FESI2_L                  MSI                      M5SI3
 AL4C3                    FE8SI2C                  SIC
 AL5FE4                   MP_B31                   M2P_C22
 M2O3C:I  REJECTED
TDB_TCFE9: FCC_A1  RESTORED
TDB_TCFE9: 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, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
  'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
  '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'
 -OK-
TDB_TCFE9:
TDB_TCFE9:TDB_TCFE9:TDB_TCFE9:TDB_TCFE9: Current database: Steels/Fe-Alloys Mobility  v4.0

 VA  DEFINED
 B2_BCC  REJECTED
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
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
 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                    1 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                    0 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                    1 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                    0 seconds
 TIME =   1360867.5     DT =   680443.91     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351122812752  FE = .96291921367461
                        SI = .03708078632539
```

```
TOTAL SIZE OF SYSTEM:  .05 [m]
 CPU time used in timestep                    1 seconds
TIME =   2721755.3     DT =   1360887.8     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0215351122812751  FE = .96291921367461
                       SI = .03708078632539
TOTAL SIZE OF SYSTEM:  .05 [m]
 CPU time used in timestep                    0 seconds
TIME =   5443530.9     DT =   2721775.6     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0215351122811045  FE = .96291921367461
                       SI = .03708078632539
TOTAL SIZE OF SYSTEM:  .05 [m]
 CPU time used in timestep                    0 seconds
TIME =   10887082.     DT =   5443551.3     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0215351122807841  FE = .96291921367461
                       SI = .03708078632539
TOTAL SIZE OF SYSTEM:  .05 [m]
 CPU time used in timestep                    0 seconds
TIME =   21774185.     DT =   10887103.     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0215351122805241  FE = .96291921367461
                       SI = .03708078632539
TOTAL SIZE OF SYSTEM:  .05 [m]
 CPU time used in timestep                    1 seconds
TIME =   43548390.     DT =   21774205.     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0215351122804155  FE = .96291921367461
                       SI = .03708078632539
TOTAL SIZE OF SYSTEM:  .05 [m]
 CPU time used in timestep                    0 seconds
TIME =   87096800.     DT =   43548410.     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0215351122803582  FE = .96291921367461
                       SI = .03708078632539
TOTAL SIZE OF SYSTEM:  .05 [m]
 CPU time used in timestep                    0 seconds
TIME =  0.17419362E+09 DT =   87096820.     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0215351122803557  FE = .96291921367461
                       SI = .03708078632539
TOTAL SIZE OF SYSTEM:  .05 [m]
 CPU time used in timestep                    0 seconds
TIME =  0.34838726E+09 DT =  0.17419364E+09 SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0215351122804245  FE = .96291921367461
                       SI = .03708078632539
TOTAL SIZE OF SYSTEM:  .05 [m]
 CPU time used in timestep                    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                    1 seconds
TIME =  0.23935491E+10 DT =  0.10000000E+10 SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .021535112280747  FE = .96291921367461
                       SI = .03708078632539
TOTAL SIZE OF SYSTEM:  .05 [m]
 CPU time used in timestep                    0 seconds
TIME =  0.33935491E+10 DT =  0.10000000E+10 SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0215351122809185  FE = .96291921367461
                       SI = .03708078632539
TOTAL SIZE OF SYSTEM:  .05 [m]
 CPU time used in timestep                    0 seconds
TIME =  0.43935491E+10 DT =  0.10000000E+10 SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0215351122812697  FE = .96291921367461
                       SI = .03708078632539
TOTAL SIZE OF SYSTEM:  .05 [m]
 CPU time used in timestep                    0 seconds
TIME =  0.53935491E+10 DT =  0.10000000E+10 SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0215351122817882  FE = .96291921367461
                       SI = .0370807863253899
TOTAL SIZE OF SYSTEM:  .05 [m]
 CPU time used in timestep                    0 seconds
TIME =  0.63935491E+10 DT =  0.10000000E+10 SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0215351122822708  FE = .96291921367461
                       SI = .03708078632539
TOTAL SIZE OF SYSTEM:  .05 [m]
 CPU time used in timestep                    1 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

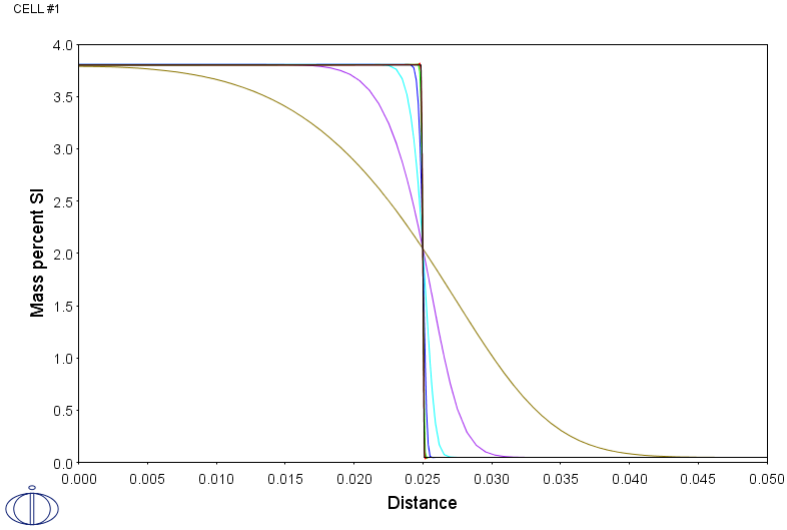
 TIMESTEP AT    0.100000000E+11 SELECTED

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

exa3-plot

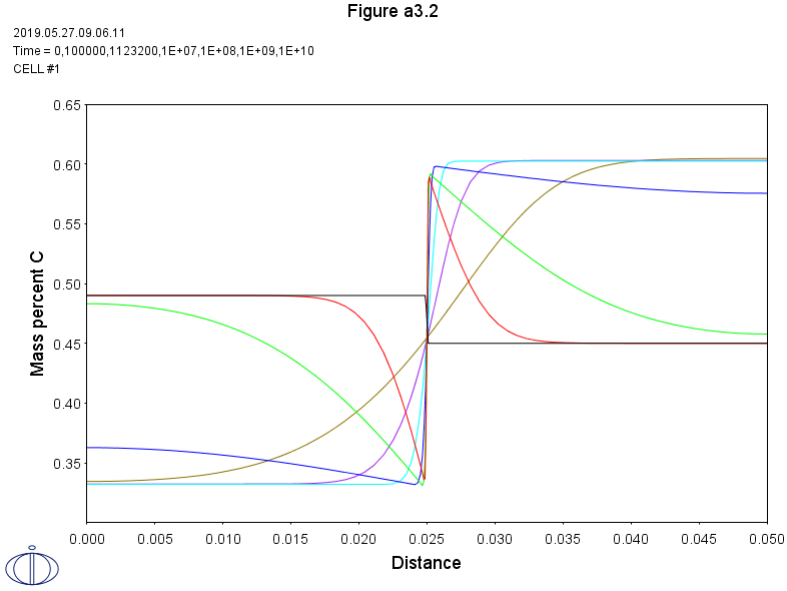
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa3\plot.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  1.00000E+10
DIC> OK
DIC>
DIC>DIC>DIC>DIC>  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:POST-1: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

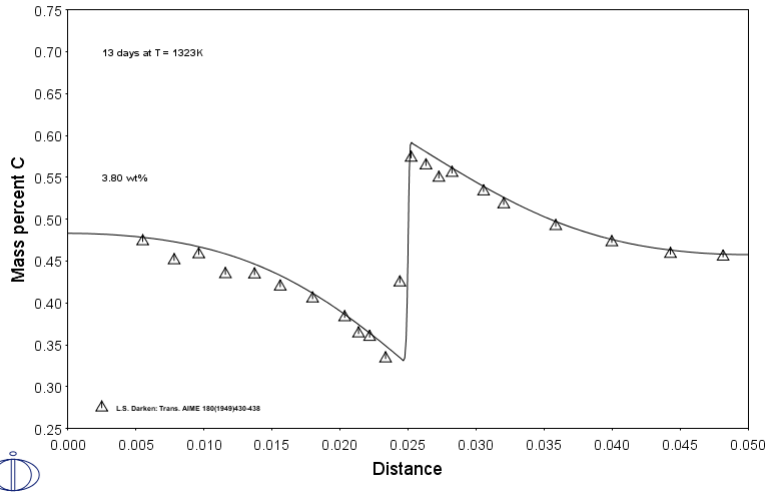
Figure a3.2




```
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

2019.05.27.09.06.12
Time = 1123200
CELL #1

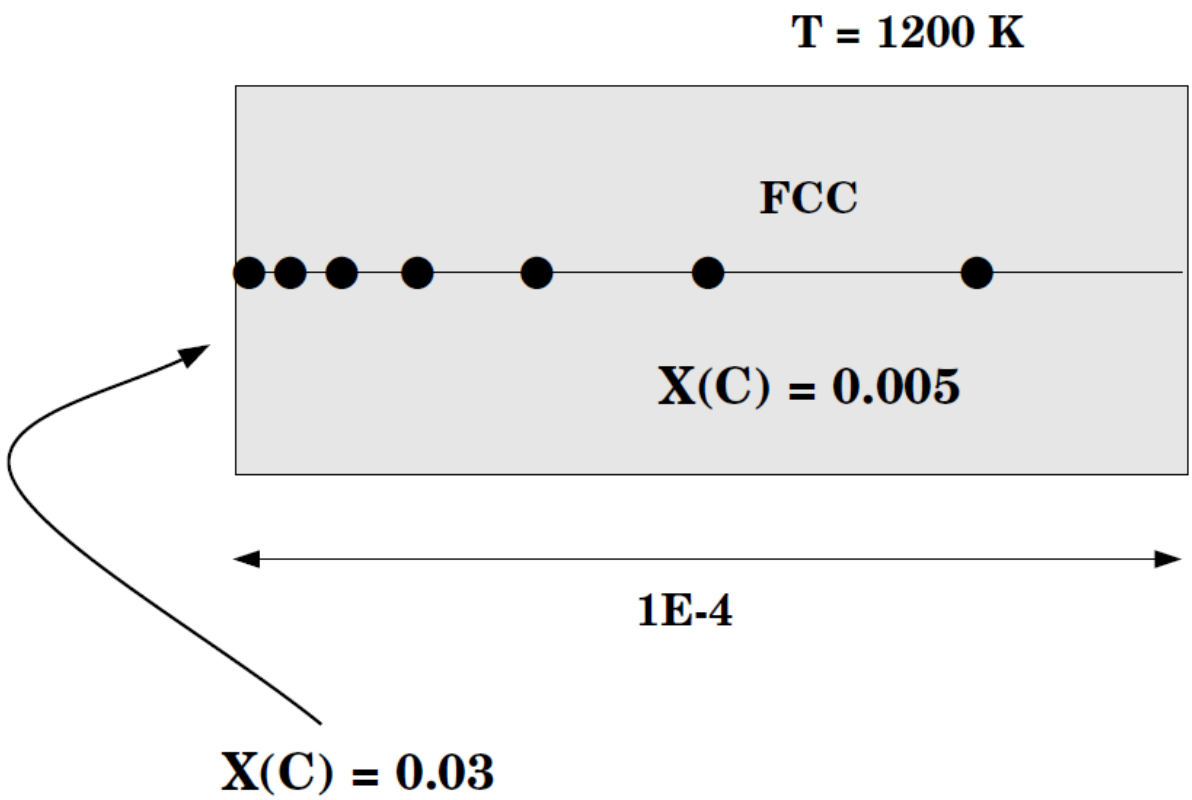



```
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1: --OK---
POST-1:
```

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 Software  (build 20130) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri May 24 17:06:15 2019


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  v9.1

 VA                      /-  DEFINED
 L12_FCC                 B2_BCC                  DICTRA_FCC_A1
   REJECTED
TDB_TCFE9: Current database: Iron Demo Database v2.1

 VA                      /-  DEFINED
TDB_FEDEMO: FE                       C  DEFINED
TDB_FEDEMO: GAS:G                    LIQUID:L                BCC_A2
 CBCC_A12                CEMENTITE               CUB_A13
 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'
  '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
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
 U-FRACTION IN SYSTEM:  C = .0050251256281407  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 U-FRACTION IN SYSTEM:  C = .0050251256281407  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .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                    1 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 = .00508603865206296  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 = .00519741865567008  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 = .00640343298842194  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 = .00697433052866847  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 = .0088773625729356  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 = .00972196664325364  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   40.486185     DT =   10.000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .010436351986536  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

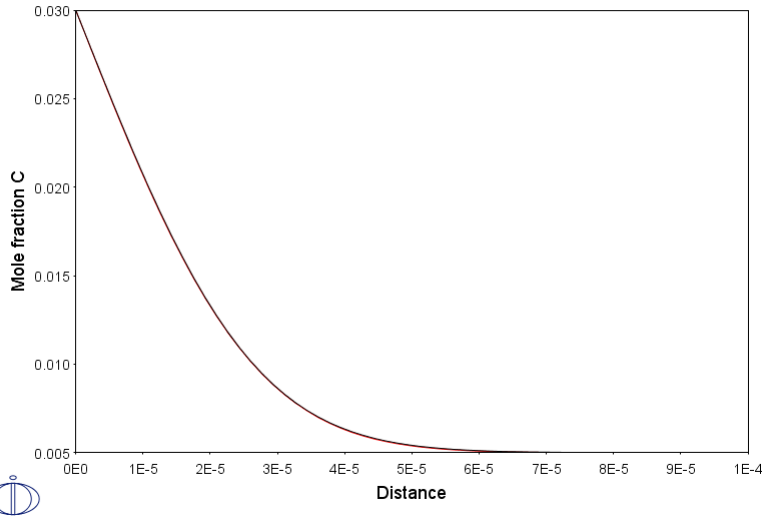
 TIMESTEP AT     100.000000     SELECTED

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

exa4-plot

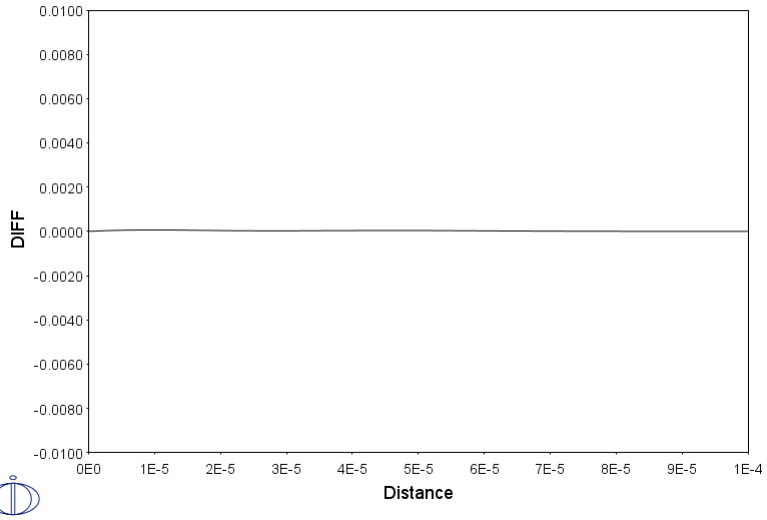
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa4\plot.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  1.00000E+02
DIC> OK
DIC>
DIC>DIC>DIC>DIC>  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:POST-1:POST-1:POST-1:  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:
```

2019.05.27.09.09.26
Time = 25
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:
```

2019.05.27.09.09.27
Time = 25
CELL #1

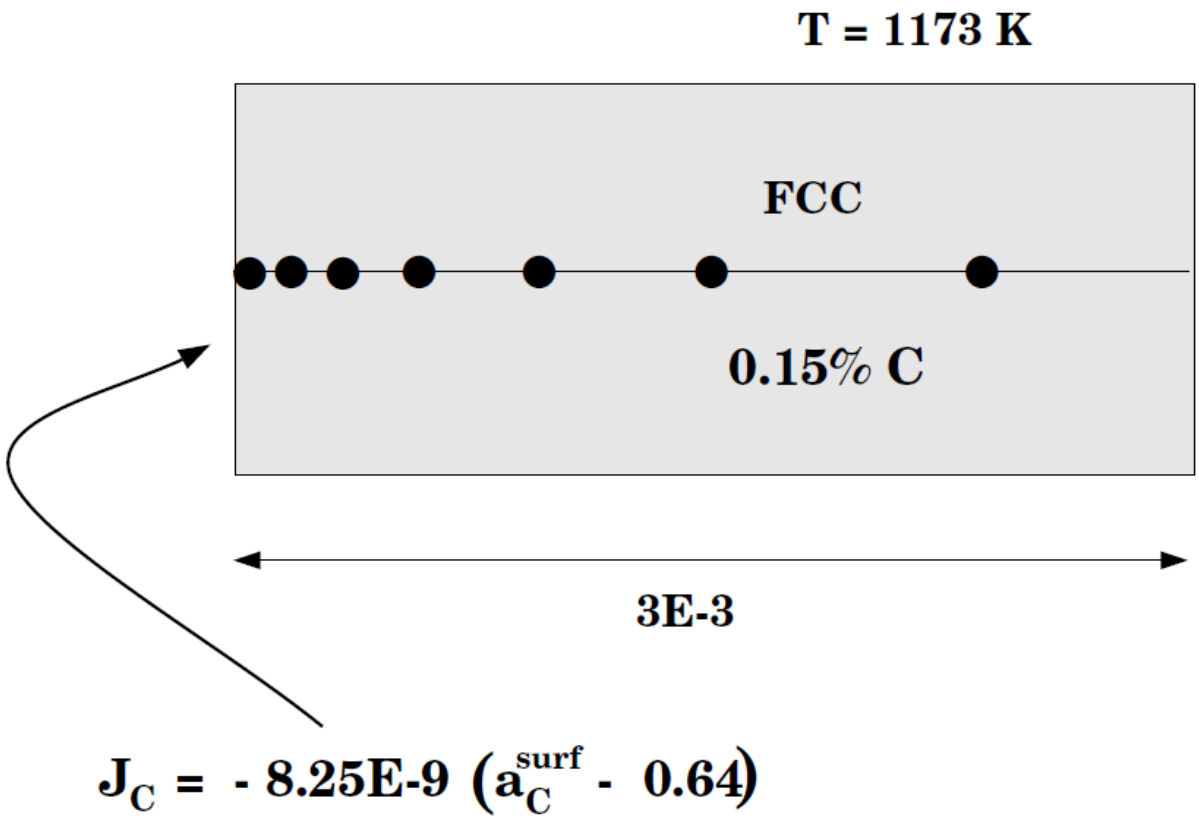



```
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: --OK---
POST-1:
```

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 Software  (build 20130) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri May 24 17:06:15 2019


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  v9.1

 VA                       /-  DEFINED
 L12_FCC                  B2_BCC                  DICTRA_FCC_A1
   REJECTED
TDB_TCFE9: Current database: Iron Demo Database v2.1

 VA                       /-  DEFINED
TDB_FEDEMO: FE                       C  DEFINED
TDB_FEDEMO: GAS:G                    LIQUID:L                BCC_A2
 CBCC_A12                 CEMENTITE               CUB_A13
 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'
  '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  v9.1
 TCFE8   =  Steels/Fe-Alloys  v8.1
 FROST1  =  FROST database v1.0
 TCFE7   =  Steels/Fe-Alloys  v7.0
 TCFE6   =  Steels/Fe-Alloys  v6.2
 TCFE5   =  Steels/Fe-Alloys  v5.0
 TCFE4   =  Steels/Fe-Alloys  v4.1
 TCFE3   =  Steels/Fe-Alloys  v3.1
 TCFE2   =  Steels/Fe-Alloys  v2.1
 TCFE1   =  Steels/Fe-Alloys  v1.0
 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  v2.1
 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
 TCSLD1  =  Solder Alloys  v1.1
 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
 TCNF2   =  Nuclear Fuels  v2.1b
 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 v2.1
 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  v1.0
 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>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC>DIC
DIC>GLOBAL OR BOUNDARY CONDITION /GLOBAL/:BOUNDARY /LOWER/:CONDITION TYPE /CLOSED_SYSTEM/: ENTER THE EXPRESSION AS:
                                 N
   J  V = f (variables)*(ACTIVITY -g (variables))
    k  m   k                     k  k
 FLUX OF FCC_A1,C
LOW TIME LIMIT /0/:f(T,P,TIME)=HIGH TIME LIMIT /*/:ANY MORE RANGES /N/:N /1/:LOW TIME LIMIT /0/:g(T,P,TIME)=HIGH TIME LIMIT /*/:ANY MORE RANGES
DIC>DIC>DIC>DIC>END TIME FOR INTEGRATION /.1/:AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /1800/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>DIC>DIC>DIC>DIC>
DIC> --OK---
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
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
 U-FRACTION IN SYSTEM:  C = .00698495916383109  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
 U-FRACTION IN SYSTEM:  C = .00698495916383109  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
 TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698495916398349  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    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 = .00698495917479988  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 = .00698495918922067  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 = .00698495921806012  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 = .00698495927573318  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 = .00698495939106305  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1 seconds
 TIME =  0.30057903E-03 DT =  0.15142250E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698495962167719  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 = .0069849600827771  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 = .00698496100461466  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 = .00698496284726692  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.48432541E-02 DT =  0.24227600E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698496652968262  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 = .0069849885766828  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 = .00698501789240893  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 = .00698507634097206  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 = .00698519272377667  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 = .00698542404641376  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 = .00698588265674895  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 = .00698678864751834  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 = .00698856957978376  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 = .0069987699663246  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1 seconds
 TIME =   19.847248     DT =   9.9236250     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00701160601590709  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
```

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TIME =   39.694498     DT =   19.847250     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00703569376361482  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 = .00707989462116304  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 = .0071587475710991  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 = .00729474138750384  FE = 1
TOTAL SIZE OF SYSTEM:  .003 [m]
 CPU time used in timestep                    0 seconds
TIME =   635.11200     DT =   317.55600     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00752054375503605  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 = .00788106518443607  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 = .00843611780537584  FE = 1
TOTAL SIZE OF SYSTEM:  .003 [m]
 CPU time used in timestep                    1 seconds
TIME =   4340.4480     DT =   1800.0000     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00904710226999973  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 = .00955134567261045  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 = .0099911367576522  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 = .0103863764716773  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 = .0107484090267344  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 = .0110844421240384  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 = .0113993948509771  FE = 1
TOTAL SIZE OF SYSTEM:  .003 [m]
 CPU time used in timestep                    0 seconds
TIME =   16940.448     DT =   1800.0000     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0116968050295615  FE = 1
TOTAL SIZE OF SYSTEM:  .003 [m]
 CPU time used in timestep                    1 seconds
TIME =   18000.000     DT =   1059.5520     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0118647499013382  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>
```
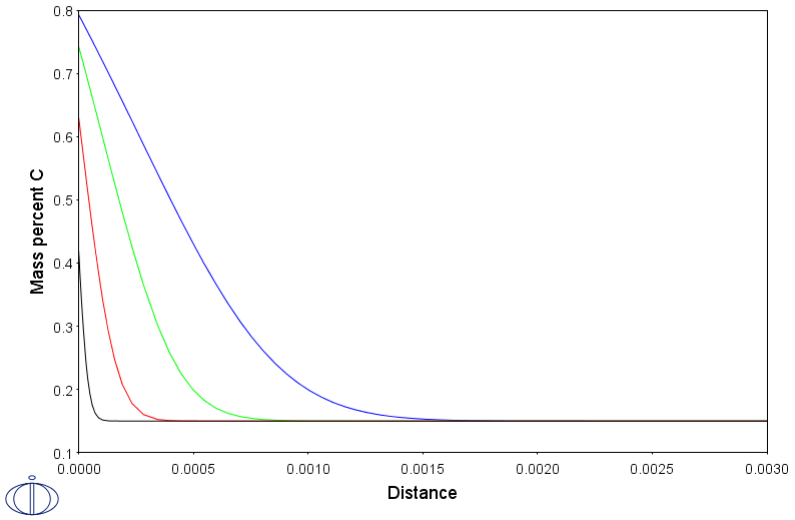
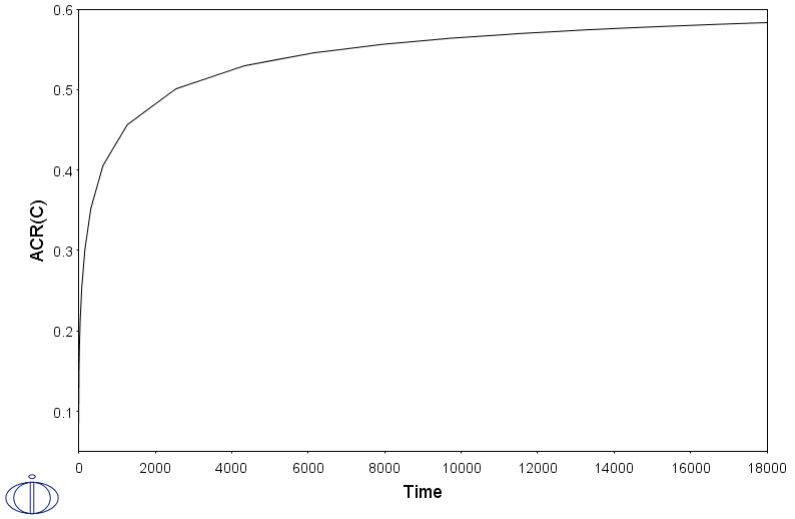

exa5-plot

```
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:
```

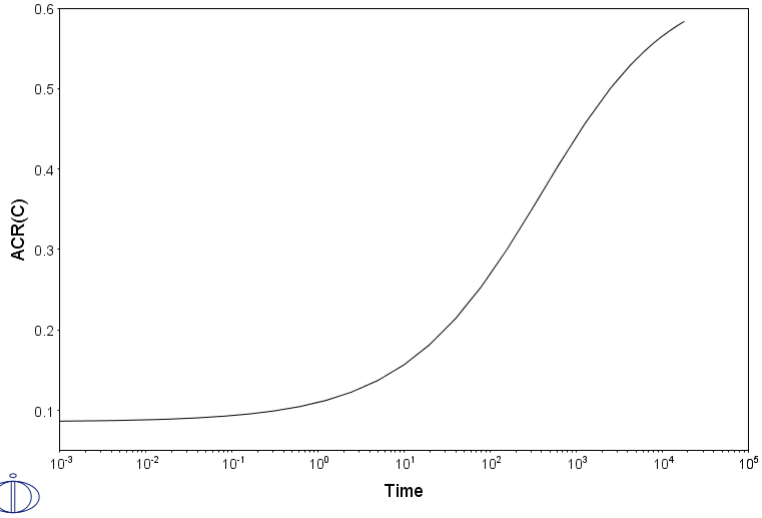



```
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:
POST-1:  INFO: Time is set as independent variable
POST-1:
POST-1:CONDITION /TIME/:INTERFACE :POST-1:
POST-1:
POST-1:POST-1:            OST-1:POST-1:
POST-1:
```



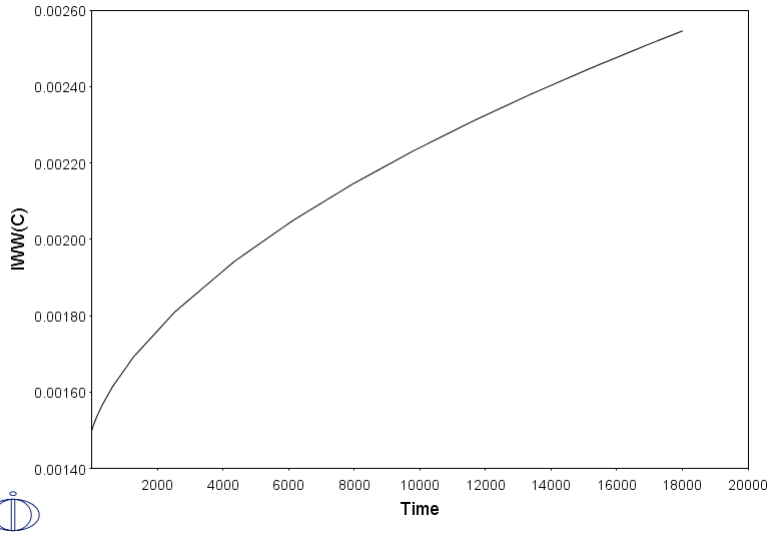

```
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1:POST-1:POST-1:POST-1:AXIS (X, Y OR Z) :AXIS TYPE /LINEAR/:POST-1:
POST-1:POST-1:
POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```

2019.05.27.09.12.45
"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:
```

2019.05.27.09.12.45
CELL #1

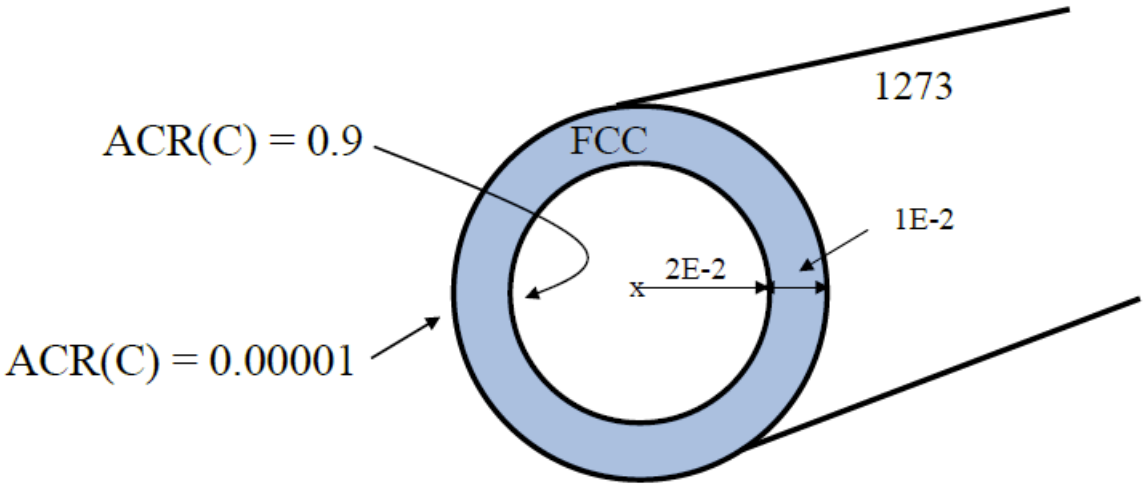



```
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1:
POST-1: --OK---
POST-1:
```

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 Software  (build 20130) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri May 24 17:06:15 2019


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  v9.1

 VA                       /-  DEFINED
 L12_FCC                  B2_BCC                  DICTRA_FCC_A1
   REJECTED
TDB_TCFE9:
TDB_TCFE9:TDB_TCFE9:TDB_TCFE9:TDB_TCFE9:TDB_TCFE9: FE                       SI                       MN
 C  DEFINED
TDB_TCFE9: GAS:G                    LIQUID:L                BCC_A2
 FCC_A1                   HCP_A3                  CBCC_A12
 CUB_A13                  DIAMOND_FCC_A4          GRAPHITE
 CEMENTITE                M23C6                   M7C3
 M5C2                     KSI_CARBIDE             FE4N_LP1
 FECN_CHI                 LAVES_PHASE_C14         M3SI
 MN9SI2                   MN11SI19                MN6SI
 G_PHASE                  CR3SI                   FE2SI
 FESI2_H                  FESI2_L                 MSI
 M5SI3                    AL4C3                   FE8SI2C
 SIC                      MN5SIC                  CUZN_EPSILON
 AL5FE4                   MP_B31                  M2P_C22
 FLUORITE_C1:I            ZRO2_TETR:I             M2O3C:I
 M2O3H:I  REJECTED
TDB_TCFE9: FCC_A1                   GRAPHITE  RESTORED
TDB_TCFE9: 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'
  'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121-127; Molar
      volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
  'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
  'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, CALPHAD, 34, 279
      -85(2010); Mn-C'
  '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'
  'W. Zheng, J. Alloys Compd., 632 (2015) 661-675'
  'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, CALPHAD,
      submitted, 2011; Fe-Mn-C'
  'J. Miettinen and B. Hallstedt, CALPHAD, 22 (1998) 231-256; Fe-Si and Fe
      -Si-C'
  'A. Forsberg and J. Agren, J. Phase Equilib., 14 (1993) 354-363; Fe-Mn-Si'
 -OK-
TDB_TCFE9:
TDB_TCFE9:TDB_TCFE9:TDB_TCFE9:TDB_TCFE9: Use one of these databases

 TCFE9   =  Steels/Fe-Alloys  v9.1
 TCFE8   =  Steels/Fe-Alloys  v8.1
 FROST1  =  FROST database v1.0
 TCFE7   =  Steels/Fe-Alloys  v7.0
 TCFE6   =  Steels/Fe-Alloys  v6.2
 TCFE5   =  Steels/Fe-Alloys  v5.0
 TCFE4   =  Steels/Fe-Alloys  v4.1
 TCFE3   =  Steels/Fe-Alloys  v3.1
 TCFE2   =  Steels/Fe-Alloys  v2.1
 TCFE1   =  Steels/Fe-Alloys  v1.0
 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  v2.1
 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
 TCSLD1  =  Solder Alloys  v1.1
 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
 TCNF2   =  Nuclear Fuels  v2.1b
 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 v2.1
 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  v1.0
 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 /TCFE9/: Current database: Steels/Fe-Alloys Mobility  v4.0

 VA  DEFINED
 B2_BCC  REJECTED
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'
  'Y. Liu, L. Zhang, et al. CALPHAD 33(2009)614-23; Fe-Mn-C (fcc)'
  'M. Yin, et al. (2010) unpublished work.'
  'W. Zheng, et al., J. Alloys and Compounds, 632 (2015) 661-675; Fe-Mn-Si
      (fcc)'
  '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>
```

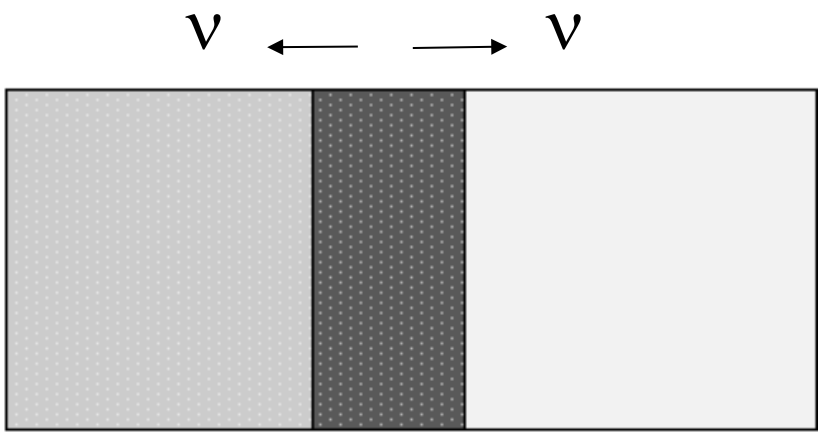
exa6-run

```
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
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
 U-FRACTION IN SYSTEM:  C = .00115488575879621  FE = .490055682684517
                        MN = .00302988813183617  SI = .00691442924890042
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
 U-FRACTION IN SYSTEM:  C = .00115488575879621  FE = .490055682684517
                        MN = .00302988813183617  SI = .00691442924890042
 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 = .00116822817821891  FE = .490055682684517
                        MN = .00302988813183616  SI = .00691442924890042
 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 = .00116829188694328  FE = .490055682684517
                        MN = .00302988813183617  SI = .00691442924890042
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                     1 seconds
 TIME =   3.0557610     DT =   3.0556609     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00118959189435653  FE = .490055682684521
                        MN = .00302988813183664  SI = .00691442924889593
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                     0 seconds
 TIME =   9.1670828     DT =   6.1113218     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00121111672154579  FE = .490055682684524
                        MN = .00302988813183702  SI = .00691442924889251
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                     0 seconds
 TIME =   21.389726     DT =   12.222644     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00123890626455181  FE = .490055682684528
                        MN = .00302988813183746  SI = .00691442924888853
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                     0 seconds
 TIME =   45.835013     DT =   24.445287     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00127670303015352  FE = .490055682684532
                        MN = .00302988813183798  SI = .00691442924888392
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                     1 seconds
 TIME =   94.725588     DT =   48.890574     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00132921753226138  FE = .490055682684536
                        MN = .00302988813183855  SI = .00691442924887889
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                     0 seconds
 TIME =   192.50674     DT =   97.781148     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00140291029963708  FE = .49005568268454
                        MN = .00302988813318391  SI = .00691442924887446
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                     0 seconds
 TIME =   388.06903     DT =   195.56230     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00150683893865951  FE = .490055682684541
                        MN = .00302988813183934  SI = .00691442924887331
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                     1 seconds
 TIME =   779.19363     DT =   391.12459     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00165382101622263  FE = .490055682684533
                        MN = .00302988813183862  SI = .00691442924888217
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                     0 seconds
 TIME =   1561.4428     DT =   782.24919     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00186208912002594  FE = .49005568268452
                        MN = .00302988813183734  SI = .00691442924889648
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                     0 seconds
 TIME =   3125.9412     DT =   1564.4984     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00215763950853838  FE = .490055682684545
                        MN = .00302988813184034  SI = .00691442924886802
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                     1 seconds
 TIME =   6254.9379     DT =   3128.9967     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00257762247234064  FE = .490055682684614
                        MN = .00302988813184873  SI = .00691442924879132
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                     0 seconds
 TIME =   12512.931     DT =   6257.9935     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00317612553687888  FE = .490055682684701
                        MN = .00302988813186053  SI = .00691442924869196
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                     0 seconds
 TIME =   25028.918     DT =   12515.987     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00403212708748458  FE = .490055682684788
                        MN = .00302988813187388  SI = .00691442924859186
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                     1 seconds
 TIME =   50060.892     DT =   25031.974     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0052618594638577  FE = .490055682684867
                        MN = .00302988813188714  SI = .00691442924849985
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                     0 seconds
 TIME =   100124.84     DT =   50063.948     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00703878462392718  FE = .490055682684956
                        MN = .00302988813189985  SI = .00691442924839736
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                     1 seconds
 TIME =   200252.74     DT =   100127.90     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .009614681352058  FE = .490055682685084
                        MN = .00302988813319146  SI = .00691442924825484
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                     1 seconds
 TIME =   400508.53     DT =   200255.79     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0130388550839739  FE = .490055682685343
```

```
                      MN = .00302988813194448  SI = .00691442924796635
TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
 CPU time used in timestep                    0 seconds
TIME =   801020.11     DT =   400511.58     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0158154519815359  FE = .490055682685939
                      MN = .00302988813201556  SI = .00691442924729885
TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
 CPU time used in timestep                    1 seconds
TIME =   1602043.3     DT =   801023.17     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0165165842674943  FE = .490055682687091
                      MN = .00302988813214933  SI = .00691442924601361
TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
 CPU time used in timestep                    0 seconds
TIME =   3071117.5     DT =   1469074.2     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0165253458723482  FE = .490055682689399
                      MN = .00302988813240263  SI = .00691442924345169
TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
 CPU time used in timestep                    1 seconds
TIME =   5521426.5     DT =   2450309.1     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0165254570895418  FE = .490055682693946
                      MN = .00302988813287881  SI = .00691442923842824
TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
 CPU time used in timestep                    0 seconds
TIME =   9715746.1     DT =   4194319.5     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0165253215591162  FE = .490055682703382
                      MN = .00302988813383215  SI = .00691442922803932
TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
 CPU time used in timestep                    1 seconds
TIME =   17813876.     DT =   8098130.0     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0165250052909423  FE = .490055682726195
                      MN = .00302988813607049  SI = .00691442920298777
TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
 CPU time used in timestep                    1 seconds
TIME =   34010136.     DT =   16196260.     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0165246276464089  FE = .490055682784398
                      MN = .00302988814169422  SI = .00691442913916064
TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
 CPU time used in timestep                    0 seconds
TIME =   66402656.     DT =   32392520.     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0165243580713333  FE = .490055682920989
                      MN = .00302988815540702  SI = .00691442898885753
TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
 CPU time used in timestep                    1 seconds
TIME =  0.13118770E+09 DT =   64785040.     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0165244582014699  FE = .490055683192306
                      MN = .00302988818558275  SI = .00691442868736455
TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
 CPU time used in timestep                    1 seconds
TIME =  0.23061023E+09 DT =   99422537.     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0165263917143568  FE = .490055683555767
                      MN = .00302988823056496  SI = .00691442827892098
TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
 CPU time used in timestep                    0 seconds
TIME =  0.33012543E+09 DT =   99515198.     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .016530326785165  FE = .49005568386721
                      MN = .00302988827178368  SI = .0069144279262599
TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
 CPU time used in timestep                    1 seconds
TIME =  0.42970616E+09 DT =   99580728.     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0165336326908906  FE = .490055684142115
                      MN = .00302988830951066  SI = .00691442761362775
TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
 CPU time used in timestep                    1 seconds
TIME =  0.52934108E+09 DT =   99634921.     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0165366300962669  FE = .490055684390274
                      MN = .00302988834435611  SI = .00691442733062355
TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
 CPU time used in timestep                    0 seconds
TIME =  0.62902222E+09 DT =   99681143.     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .016539438424926  FE = .490055684617852
                      MN = .00302988837682077  SI = .00691442707058051
TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
 CPU time used in timestep                    1 seconds
TIME =  0.72874408E+09 DT =   99721854.     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0165421143527826  FE = .490055684829008
                      MN = .00302988840729343  SI = .0069144268289518
TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
 CPU time used in timestep                    1 seconds
TIME =  0.82850228E+09 DT =   99758206.     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0165446894756965  FE = .490055685026688
                      MN = .00302988843607474  SI = .00691442660249089
TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
 CPU time used in timestep                    0 seconds
TIME =  0.92829328E+09 DT =   99791002.     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0165471833610473  FE = .490055685213062
                      MN = .00302988846340022  SI = .00691442638879089
TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
 CPU time used in timestep                    1 seconds
TIME =  0.98979354E+09 DT =   61500257.     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0165498694311613  FE = .490055685322987
                      MN = .00302988847959189  SI = .00691442626267451
TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
 CPU time used in timestep                    1 seconds
TIME =  0.10000000E+10 DT =   10206459.     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0165516055116156  FE = .490055685340902
                      MN = .00302988848223566  SI = .0069144262421159
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    3.0557610
DELETING TIME-RECORD FOR TIME    9.1670828
DELETING TIME-RECORD FOR TIME    21.389726
DELETING TIME-RECORD FOR TIME    45.835013
DELETING TIME-RECORD FOR TIME    94.725588
DELETING TIME-RECORD FOR TIME    192.50674
DELETING TIME-RECORD FOR TIME    388.06903
DELETING TIME-RECORD FOR TIME    779.19363
DELETING TIME-RECORD FOR TIME    1561.4428
DELETING TIME-RECORD FOR TIME    3125.9412
DELETING TIME-RECORD FOR TIME    6254.9379
DELETING TIME-RECORD FOR TIME    12512.931
DELETING TIME-RECORD FOR TIME    25028.918
```

```
 DELETING TIME-RECORD FOR TIME    50060.892
 DELETING TIME-RECORD FOR TIME    100124.84
 DELETING TIME-RECORD FOR TIME    200252.74
 DELETING TIME-RECORD FOR TIME    400508.53
 DELETING TIME-RECORD FOR TIME    801020.11
 DELETING TIME-RECORD FOR TIME    1602043.3
 DELETING TIME-RECORD FOR TIME    3071117.5
 DELETING TIME-RECORD FOR TIME    5521426.5
 DELETING TIME-RECORD FOR TIME    9715746.1
 DELETING TIME-RECORD FOR TIME    17813876.
 DELETING TIME-RECORD FOR TIME    34010136.
 DELETING TIME-RECORD FOR TIME    66402656.
 DELETING TIME-RECORD FOR TIME   0.13118770E+09
 DELETING TIME-RECORD FOR TIME   0.23061023E+09
 DELETING TIME-RECORD FOR TIME   0.33012543E+09
 DELETING TIME-RECORD FOR TIME   0.42970616E+09
 DELETING TIME-RECORD FOR TIME   0.52934108E+09
 DELETING TIME-RECORD FOR TIME   0.62902222E+09
 DELETING TIME-RECORD FOR TIME   0.72874408E+09
 DELETING TIME-RECORD FOR TIME   0.82850228E+09
 DELETING TIME-RECORD FOR TIME   0.92829328E+09

 KEEPING TIME-RECORD FOR TIME   0.98979354E+09
 AND FOR TIME                   0.10000000E+10
 WORKSPACE RECLAIMED

 TIMESTEP AT    0.100000000E+10 SELECTED

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

Moving Boundary Problems

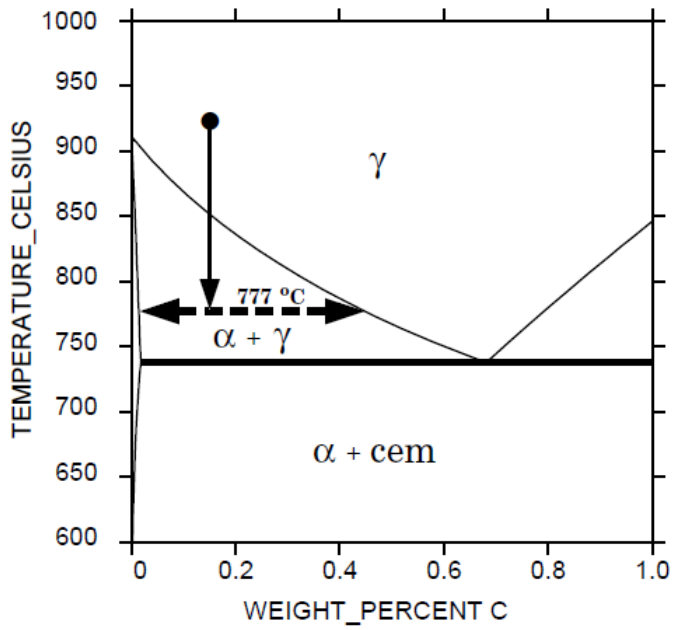


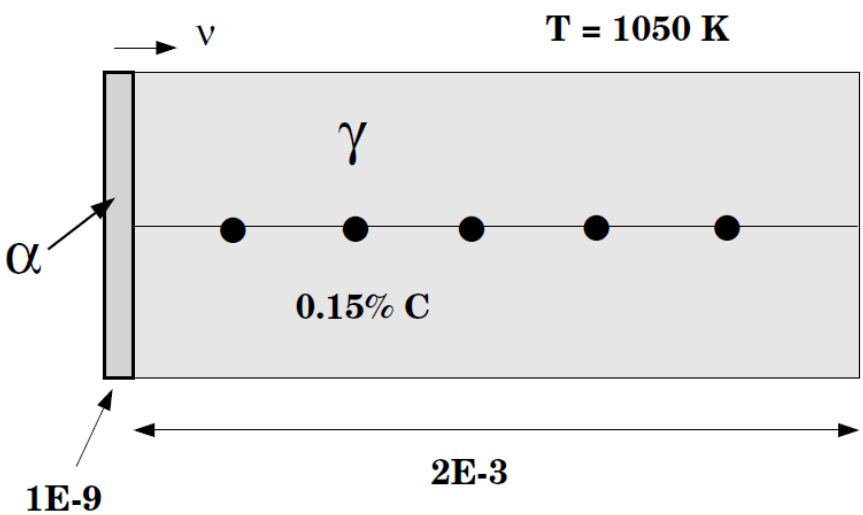
Example exb1a

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



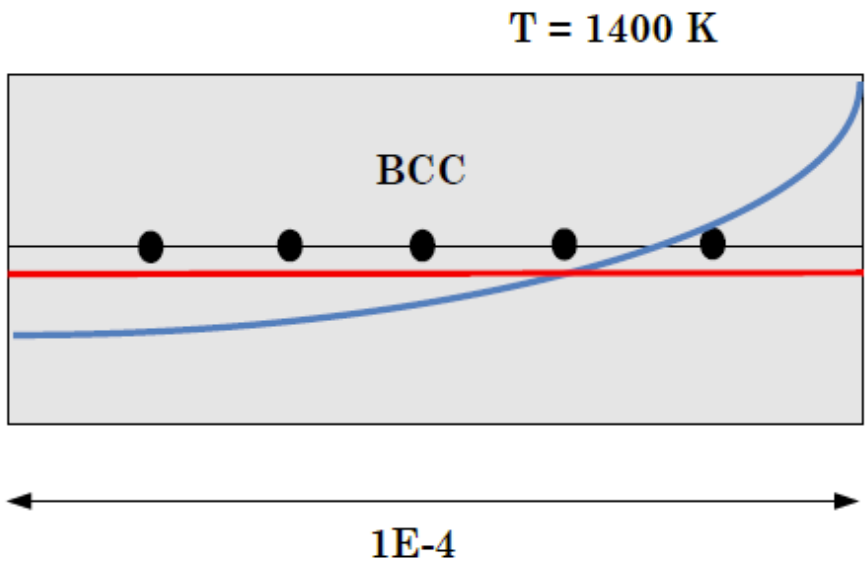


Example exa7

Homogenization heat-treatment

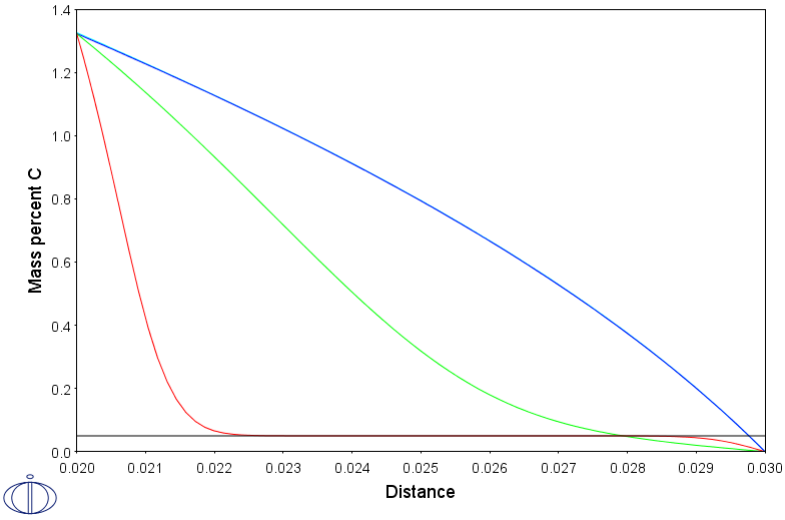
(Initial profile imported from Scheil simulation)

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.

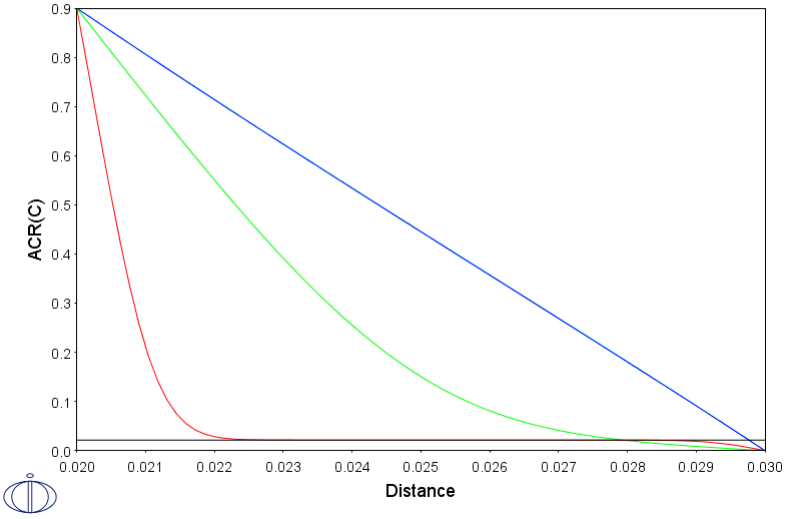


exa6-plot

```
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:
```

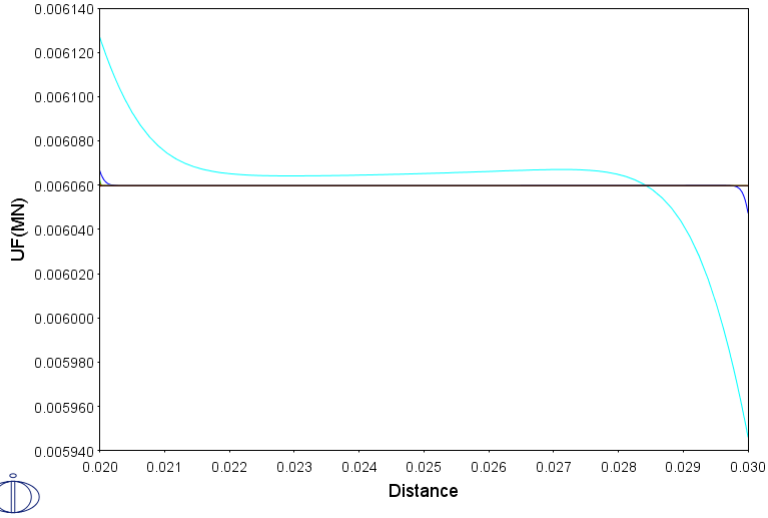



```
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:POST-1:
POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```



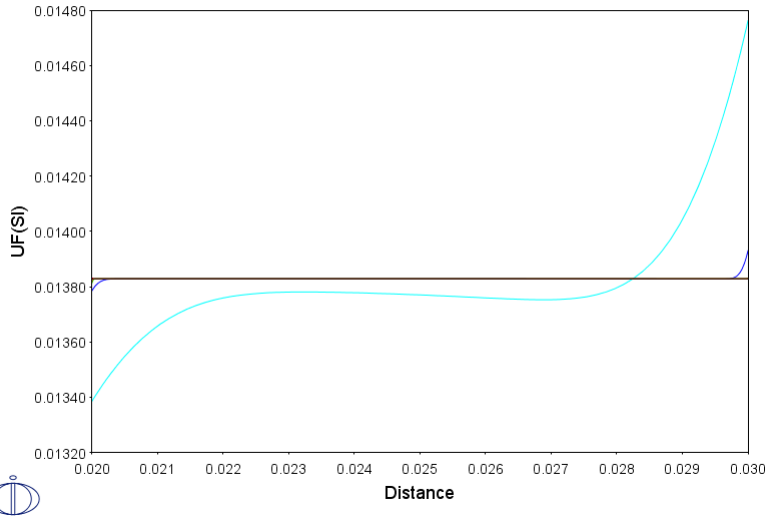

```
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:
POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```

2019.05.27.09.16.27
Time = 0,10000,200000,1E+07,1E+09
CELL #1



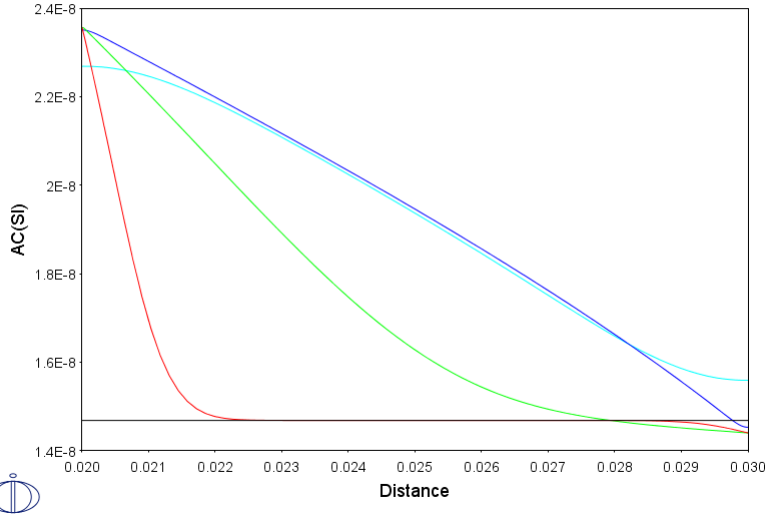

```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1:POST-1:
POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```

2019.05.27.09.16.28
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:
```

2019.05.27.09.16.31
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:
```

exa7-setup

```
About Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri May 24 17:06:15 2019


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  v9.1

 VA                       /-  DEFINED
 L12_FCC                  B2_BCC                  DICTRA_FCC_A1
   REJECTED
TDB_TCFE9: Current database: Iron Demo Database v2.1

 VA                       /-  DEFINED
TDB_FEDEMO: FE                      CR                      NI
 MN  DEFINED
TDB_FEDEMO: LIQUID:L                BCC_A2                  CBCC_A12
 CHI_A12                  CUB_A13                 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, 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>
```

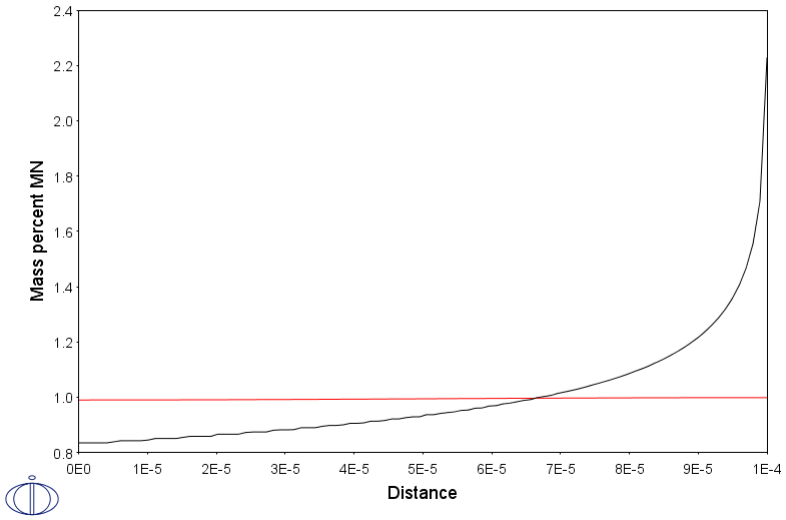
exa7-run

```
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> DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
 U-FRACTION IN SYSTEM:  CR = .180420497424242  FE = .796498787878788
                        MN = .00999016878282828  NI = .0130905459141414
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 U-FRACTION IN SYSTEM:  CR = .180420497424242  FE = .796498787878788
                        MN = .00999016878282828  NI = .0130905459141414
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .180420497424242  FE = .796498787878788
                        MN = .00999016878282828  NI = .0130905459141415
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     0 seconds
 TIME =  0.10010000E-03 DT =  0.10000000E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .180420497424242  FE = .796498787878788
                        MN = .00999016878282828  NI = .0130905459141416
 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 = .00999016878282789  NI = .0130905459141419
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     1 seconds
 TIME =   1.2570517     DT =  0.83796774     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 =   2.9329872     DT =   1.6759355     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .180420497424243  FE = .796498787878789
                        MN = .00999016878282889  NI = .0130905459141398
 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 = .0130905459140888
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     1 seconds
 TIME =   12.988600     DT =   6.7037419     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .180420497424302  FE = .796498787878888
                        MN = .0099901687828762  NI = .013090545913934
 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 = .00999016878290129  NI = .0130905459139196
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     0 seconds
 TIME =   53.211052     DT =   26.814968     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .180420497424435  FE = .796498787878771
                        MN = .00999016878299363  NI = .0130905459138003
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     1 seconds
 TIME =   106.84099     DT =   53.629935     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .180420497424575  FE = .796498787878386
                        MN = .0099901687833697  NI = .0130905459136693
 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 = .7964987878782
                        MN = .00999016878339536  NI = .0130905459139729
 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 = .796498787877758
                        MN = .00999016878350906  NI = .0130905459146428
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     0 seconds
 TIME =   788.62060     DT =   360.00000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .180420497424078  FE = .796498787877897
                        MN = .00999016878346263  NI = .0130905459145626
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     1 seconds
 TIME =   1148.6206     DT =   360.00000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .180420497423614  FE = .796498787877391
                        MN = .00999016878332563  NI = .0130905459156699
 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 = .180420497423267  FE = .796498787877031
                        MN = .00999016878317057  NI = .0130905459165314
 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 = .180420497422968  FE = .79649878787523
                        MN = .00999016878344998  NI = .0130905459183519
 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 = .18042049742269  FE = .796498787872687
                        MN = .00999016878399076  NI = .013090545920632
 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 = .180420497422476  FE = .796498787870922
                        MN = .009990168784371  NI = .0130905459222311
 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 = .180420497422319  FE = .796498787869703
                        MN = .00999016878464196  NI = .0130905459233363
 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 = .180420497422207  FE = .796498787868858
                        MN = .00999016878483109  NI = .0130905459241042
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     1 seconds
 TIME =   3600.0000     DT =   291.37940     SUM OF SQUARES =   0.0000000
```

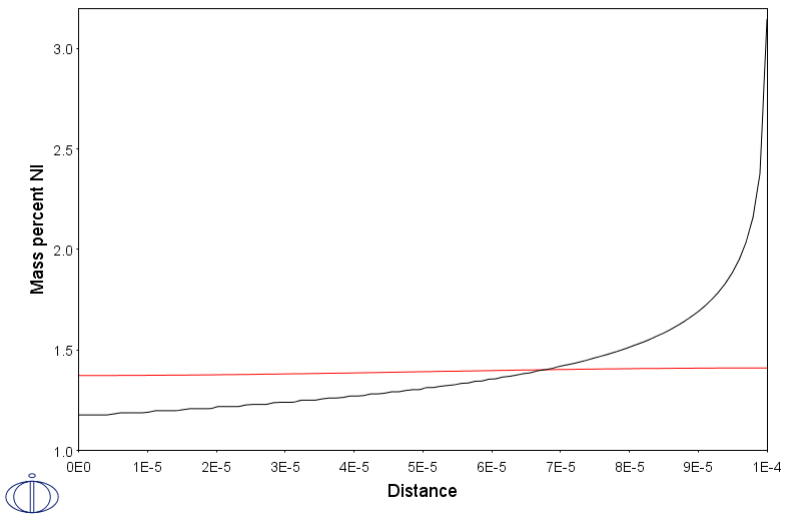
```
 U-FRACTION IN SYSTEM:  CR = .180420497422141  FE = .796498787868433
                        MN = .00999016878491913  NI = .0130905459245072
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 MUST SAVE WORKSPACE ON FILE
 WORKSPACE SAVED ON FILE
 RECLAIMING WORKSPACE
 DELETING TIME-RECORD FOR TIME    0.0000000
 DELETING 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:
```

exb1a-setup

```
About Software  (build 20130) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri May 24 17:06:15 2019


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  v9.1

 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 v2.1

 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
 CBCC_A12                 CEMENTITE               CUB_A13
 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'
  '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  v9.1
 TCFE8   =  Steels/Fe-Alloys  v8.1
 FROST1  =  FROST database v1.0
 TCFE7   =  Steels/Fe-Alloys  v7.0
 TCFE6   =  Steels/Fe-Alloys  v6.2
 TCFE5   =  Steels/Fe-Alloys  v5.0
 TCFE4   =  Steels/Fe-Alloys  v4.1
 TCFE3   =  Steels/Fe-Alloys  v3.1
 TCFE2   =  Steels/Fe-Alloys  v2.1
 TCFE1   =  Steels/Fe-Alloys  v1.0
 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  v2.1
 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
 TCSLD1  =  Solder Alloys  v1.1
 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
 TCNF2   =  Nuclear Fuels  v2.1b
 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 v2.1
 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  v1.0
 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 /AUTO/:
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -> 1): /AUTO/:MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/:
DIC>DIC>DIC>DIC>DIC>
DIC> --OK---
DIC>
```

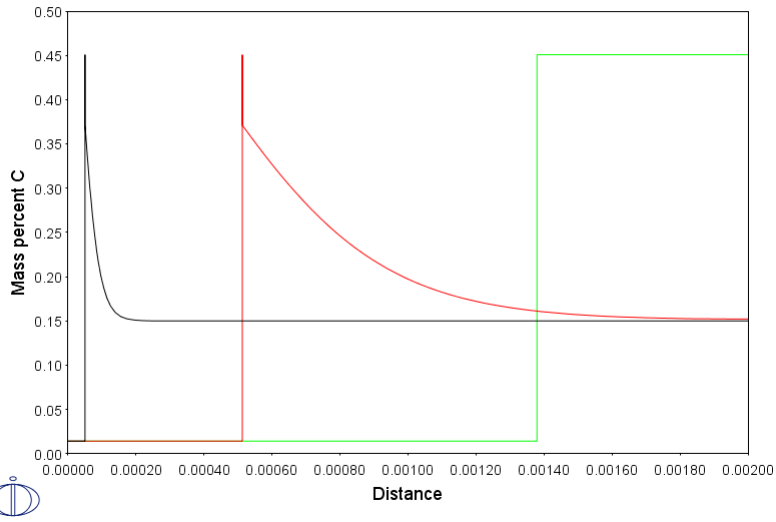
exb1a-run

```
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]
 3.981486698394990E-005        3.982285206223473E-005        1.590380388095982E-012        8.424530635653944E-020       TIME =  0.10000000E-
04 DT =  0.10000000E-04 SUM OF SQUARES =  0.84245306E-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 = .00698495590212103  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]
  13  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUSTENITE

  CPU time used in timestep                     0 seconds
 3.499840028280955E-006        3.500511916382632E-006        1.189257532496498E-007        4.111251341848916E-008        2.962574700552787E-
009        2.530542583416894E-012        1.388067406712368E-016        5.575451655524731E-024       TIME =  0.30000000E-04 DT =  0.20000000E-
04 SUM OF SQUARES =  0.55754517E-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 = .00698495800112135  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]
  CPU time used in timestep                     0 seconds
 8.791374264573459E-008        8.798286033320960E-008        8.685504892276213E-012        8.242919203128171E-016        6.144684543865020E-
024       TIME =  0.70000000E-04 DT =  0.40000000E-04 SUM OF SQUARES =  0.61446845E-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 = .0069849580011213  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]
  CPU time used in timestep                     0 seconds
 3.282053187160803E-006        3.283518226797679E-006        3.522792391228729E-006        1.817585388233140E-007        4.865291987655131E-
008        3.905759626885373E-011        5.263771782924378E-015        6.207194815426254E-022       TIME =  0.15000000E-03 DT =  0.80000000E-
04 SUM OF SQUARES =  0.62071948E-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 = .00698495794642401  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]
  CPU time used in timestep                     0 seconds
  2  GRIDPOINT(S) ADDED   TO   CELL #1   REGION: FERRITE
 4.713654678007882E-007        4.723390786773209E-007        4.587355209156483E-012        4.399467330461789E-017       TIME =  0.31000000E-
03 DT =  0.16000000E-03 SUM OF SQUARES =  0.43994673E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.51923334E-04 AND   0.51923334E-04
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.48655891E-07
 U-FRACTION IN SYSTEM:  C = .0069849538645405  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]
  CPU time used in timestep                     0 seconds
 4.378612640324225E-006        4.381488089608321E-006        1.153721987225422E-009        2.848526234246943E-013        1.742498106885628E-
020       TIME =  0.63000000E-03 DT =  0.32000000E-03 SUM OF SQUARES =  0.17424981E-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 = .00698494858774079  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]
  CPU time used in timestep                     1 seconds
 2.098301747006823E-006        2.099772516598803E-006        6.174250803578723E-010        1.696082157280840E-013        1.284639359343907E-
020       TIME =  0.12700000E-02 DT =  0.64000000E-03 SUM OF SQUARES =  0.12846394E-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 = .00698494270976014  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]
  CPU time used in timestep                     0 seconds
 9.829104756012783E-007        9.836537893792238E-007        1.102463980687662E-010        4.078680421812497E-014        1.060054323429495E-
021       TIME =  0.25500000E-02 DT =  0.12800000E-02 SUM OF SQUARES =  0.10600543E-20
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.18170713E-04 AND   0.18170713E-04
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.99390661E-07
 U-FRACTION IN SYSTEM:  C = .00698493641830839  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]


output ignored...



... output resumed

 2.559287261379622E-005        2.559723361278892E-005        2.554432986134904E-
017       TIME =  0.57592186E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.25544330E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.36721870E-17 AND  -0.36721870E-17
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.13795053E-02
 U-FRACTION IN SYSTEM:  C = .00698537037857388  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUSTENITE

  CPU time used in timestep                     0 seconds
 7.759613011001443E-010        7.718776685600844E-010        2.897557155238471E-
022       TIME =  0.67592186E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.28975572E-21
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.37353278E-17 AND  -0.37353278E-17
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.13795049E-02
 U-FRACTION IN SYSTEM:  C = .00698537418762714  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUSTENITE

  CPU time used in timestep                     0 seconds
 6.089776106692916E-005        6.089892628128532E-005        2.199667331610092E-
017       TIME =  0.77592186E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.21996673E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.34602674E-16 AND   0.34602674E-16
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.13795084E-02
 U-FRACTION IN SYSTEM:  C = .00698533890198685  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: FERRITE
```

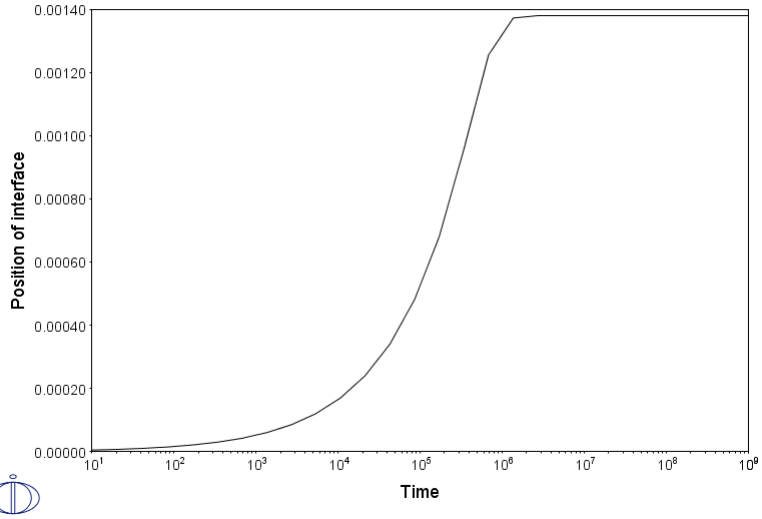
```
  CPU time used in timestep                    0 seconds
 2.588312709279728E-004        2.588535246436656E-004        4.012545367409509E-016        5.033372439653760E-
028       TIME =  0.87592186E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.50333724E-27
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.44973542E-16 AND  -0.44973542E-16
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.13795039E-02
 U-FRACTION IN SYSTEM:  C = .0069853847631887  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUSTENITE

  CPU time used in timestep                    0 seconds
 3.288324475870921E-004        3.288650485046253E-004        2.052295078497241E-
019       TIME =  0.97592186E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.20522951E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.44839647E-16 AND   0.44839647E-16
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.13795084E-02
 U-FRACTION IN SYSTEM:  C = .00698533903852637  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: FERRITE

  CPU time used in timestep                    0 seconds
 1.421385493622018E-004        1.421599195858140E-004        6.435406611488609E-
027       TIME =  0.10000000E+10 DT =   24078140.     SUM OF SQUARES =  0.64354066E-26
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.14514263E-16 AND  -0.14514263E-16
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.13795080E-02
 U-FRACTION IN SYSTEM:  C = .00698534260226762  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:
```

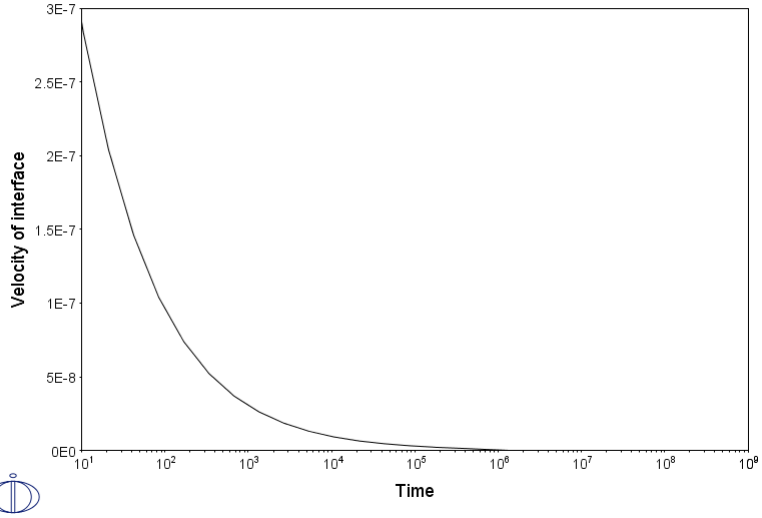



```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1:POST-1:POST-1:POST-1:  INFO: Time is set as independent variable
POST-1:VARIABLE :INTERFACE :UPPER OR LOWER INTERFACE OF REGION AUSTENITE#1 /LOWER/:POST-1:
POST-1:AXIS (X, Y OR Z) :AXIS TYPE /LINEAR/:POST-1:
POST-1:AXIS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

2019.05.27.09.23.10
LOWER INTERFACE OF REGION "AUSTENITE#1"
CELL #1

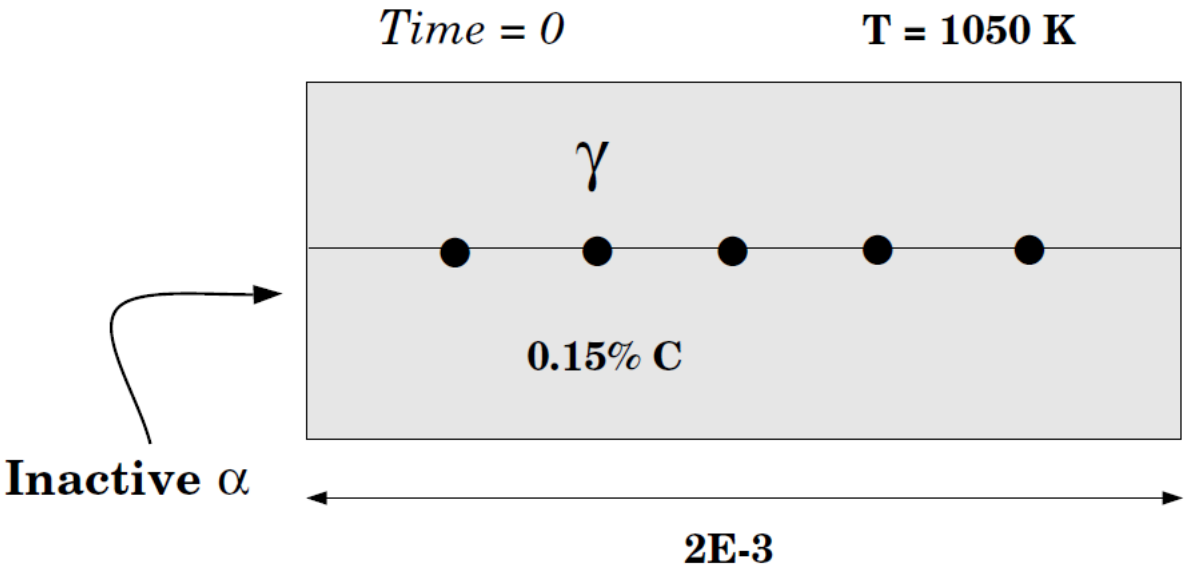


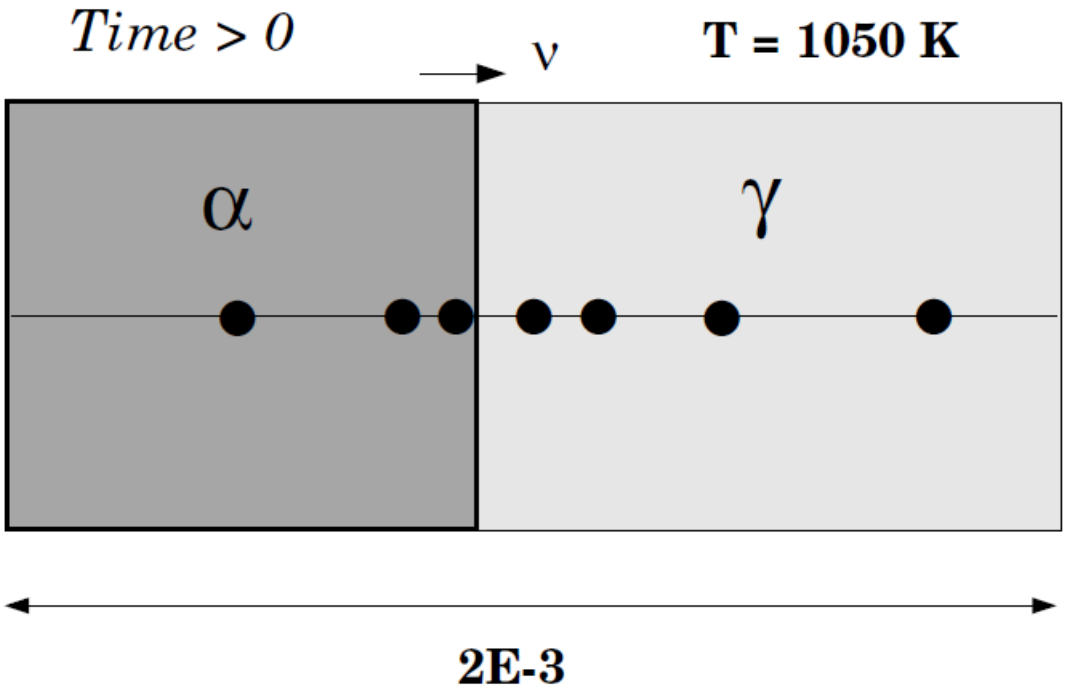

```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: --OK---
POST-1:
```

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 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 20130) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri May 24 17:06:15 2019


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  v9.1

 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 v2.1

 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
 CBCC_A12                 CEMENTITE               CUB_A13
 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'
  '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  v9.1
 TCFE8   =  Steels/Fe-Alloys  v8.1
 FROST1  =  FROST database v1.0
 TCFE7   =  Steels/Fe-Alloys  v7.0
 TCFE6   =  Steels/Fe-Alloys  v6.2
 TCFE5   =  Steels/Fe-Alloys  v5.0
 TCFE4   =  Steels/Fe-Alloys  v4.1
 TCFE3   =  Steels/Fe-Alloys  v3.1
 TCFE2   =  Steels/Fe-Alloys  v2.1
 TCFE1   =  Steels/Fe-Alloys  v1.0
 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  v2.1
 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
 TCSLD1  =  Solder Alloys  v1.1
 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
 TCNF2   =  Nuclear Fuels  v2.1b
 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 v2.1
 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  v1.0
 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 /AUTO/:
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -> 1): /AUTO/:MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/:
DIC>DIC>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>
```

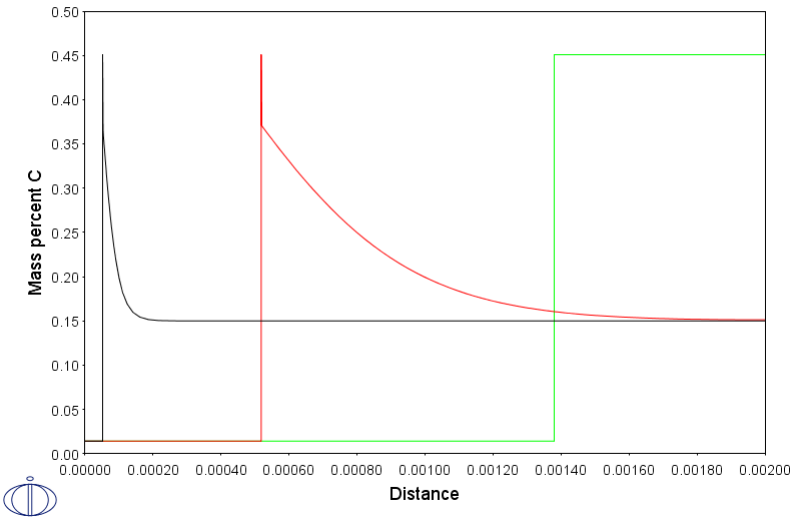
exb1b-run

```
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 = .00698156310125388  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
 U-FRACTION IN SYSTEM:  C = .00698156310125388  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  1  GRIDPOINT(S) ADDED   TO   CELL #1   REGION: R_BCC_A2
 2.641796457622048E-003        2.641820164613264E-003        0.237813344855557        2.896595832944837E-003        2.863309992290608E-
003        2.465854448704384E-003        3.038053031121488E-003        2.558808985711521E-003        2.415833959664912E-
003        2.363564691315323E-003        3.038053031121488E-003        2.415833959664912E-003        2.496303854389706E-
003        2.376837933640112E-003        2.369135026125783E-003        2.366895703947685E-003        2.361896022234620E-
003        2.360225248560526E-003        2.369135026125783E-003        2.361896022234620E-003        2.359389073335120E-
003        2.358662147344551E-003        2.369135026125783E-003        2.359389073335120E-003        2.361278827663708E-
003        2.358761597310680E-003        2.358656989254345E-003        2.358709294280506E-003        2.358624351358417E-
003        2.358591712713206E-003        2.358824313557488E-003        2.358624351358417E-003        2.358620260487213E-
003        2.358624351358417E-003        2.358620260487213E-003        2.358624351358417E-003


     ERROR RETURN FROM NS01A BECAUSE    5 CALLS OF CALFUN FAILED TO IMPROVE THE RESIDUALS
 *** ERROR  1890 IN DCNS01: ERROR RETURN FROM NS01A
 2.641796457622048E-003        2.641796461153495E-003        2.641796457622048E-003        0.237960842559876        2.641796457622048E-
003        2.896598140339542E-003        2.641796461153495E-003        2.641796457622048E-
003        0.237960842559876        2.641796457622048E-003        2.896598140339542E-003        2.641796457622048E-
003        3.037999449281252E-003        2.641796457622048E-003        2.775727731734538E-003        2.641796457622048E-
003        2.558810542864966E-003        2.558810542864966E-003        2.363570352524544E-003        2.363570352524544E-
003        5.737629595390344E-003        2.363570352524544E-003        2.558810542864966E-003        2.363570352612493E-
003        2.363570352524544E-003        3.037999449281252E-003        2.363570352524544E-003        2.415838482500371E-
003        2.363570352524544E-003        2.496264385965409E-003        2.363570352524544E-003        2.376843303864049E-
003        2.363570352524544E-003        2.369098703759602E-003        2.363570352524544E-003        2.366901291996932E-
003        2.363570352524544E-003        2.361901720130741E-003        2.361901720130741E-003        2.358626066836960E-
003        2.358626066836960E-003        2.400615764027539E-003        2.358626066836960E-003

output ignored...



... output resumed

 1.090428334429126E-004        1.785727059260706E-029       TIME =  0.50489327E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.17857271E-28
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.45720055E-15 AND   0.45720055E-15
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13802257E-02
 U-FRACTION IN SYSTEM:  C = .00697801742875898  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  32  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_BCC_A2

  CPU time used in timestep                     1 seconds
 1.286974192565775E-004        1.287181532900188E-004        2.851020269391157E-
019       TIME =  0.60489327E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.28510203E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.10818875E-15 AND  -0.10818875E-15
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13802149E-02
 U-FRACTION IN SYSTEM:  C = .00697812775293031  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUSTENITE

  CPU time used in timestep                     0 seconds
 1.887386805777330E-005        1.887574693328666E-005        9.010674242647424E-
022       TIME =  0.70489327E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.90106742E-21
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.10699087E-15 AND   0.10699087E-15
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13802256E-02
 U-FRACTION IN SYSTEM:  C = .00697801865029116  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  7  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_BCC_A2

  CPU time used in timestep                     0 seconds
 9.093497723430866E-006        9.094787463529474E-006        6.606535085381967E-
030       TIME =  0.80489327E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.66065351E-29
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.43007668E-16 AND  -0.43007668E-16
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13802213E-02
 U-FRACTION IN SYSTEM:  C = .00697806250683863  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUSTENITE

  CPU time used in timestep                     0 seconds
 3.730701913120409E-005        3.731752050993262E-005        1.385500477953649E-
019       TIME =  0.90489327E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.13855005E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.12198899E-16 AND  -0.12198899E-16
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13802200E-02
 U-FRACTION IN SYSTEM:  C = .00697807494651855  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
```

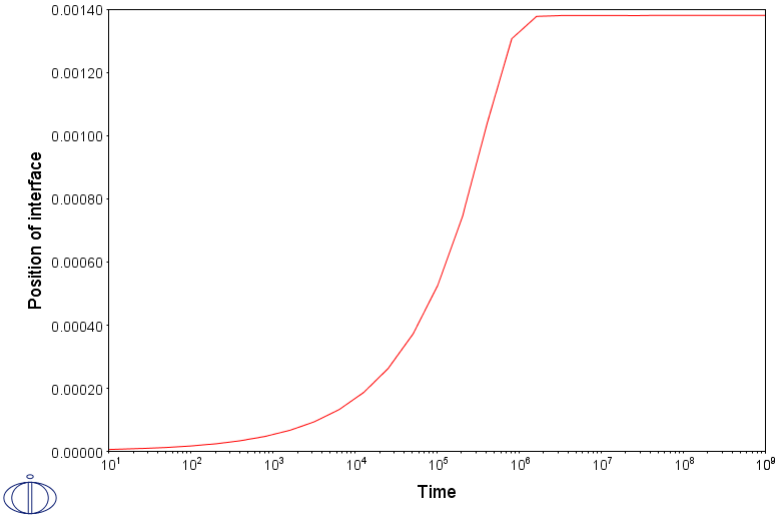
```
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUSTENITE

  CPU time used in timestep                    0 seconds
 9.933775591399644E-005        9.934261615456300E-005        4.125447368830115E-
019       TIME =  0.10000000E+10 DT =   95106731.     SUM OF SQUARES =  0.41254474E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.36914658E-16 AND   0.36914658E-16
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13802236E-02
 U-FRACTION IN SYSTEM:  C = .00697803914523078  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   0.60874920E-05
 DELETING TIME-RECORD FOR TIME   0.18012476E-04
 DELETING TIME-RECORD FOR TIME   0.41862444E-04
 DELETING TIME-RECORD FOR TIME   0.89562380E-04
 DELETING TIME-RECORD FOR TIME   0.18496225E-03
 DELETING TIME-RECORD FOR TIME   0.37576200E-03
 DELETING TIME-RECORD FOR TIME   0.75736149E-03
 DELETING TIME-RECORD FOR TIME   0.15205605E-02
 DELETING TIME-RECORD FOR TIME   0.30469584E-02
 DELETING TIME-RECORD FOR TIME   0.60997543E-02
 DELETING TIME-RECORD FOR TIME   0.12205346E-01
 DELETING TIME-RECORD FOR TIME   0.24416530E-01
 DELETING TIME-RECORD FOR TIME   0.48838897E-01
 DELETING TIME-RECORD FOR TIME   0.97683632E-01
 DELETING TIME-RECORD FOR TIME   0.19537310
 DELETING TIME-RECORD FOR TIME   0.39075204
 DELETING TIME-RECORD FOR TIME   0.78150992
 DELETING TIME-RECORD FOR TIME    1.5630257
 DELETING TIME-RECORD FOR TIME    3.1260572
 DELETING TIME-RECORD FOR TIME    6.2521202
 DELETING TIME-RECORD FOR TIME    12.504246
 DELETING TIME-RECORD FOR TIME    25.008498
 DELETING TIME-RECORD FOR TIME    50.017002
 DELETING TIME-RECORD FOR TIME    100.03401
 DELETING TIME-RECORD FOR TIME    200.06803
 DELETING TIME-RECORD FOR TIME    400.13606
 DELETING TIME-RECORD FOR TIME    800.27213
 DELETING TIME-RECORD FOR TIME    1600.5443
 DELETING TIME-RECORD FOR TIME    3201.0885
 DELETING TIME-RECORD FOR TIME    6402.1770
 DELETING TIME-RECORD FOR TIME    12804.354
 DELETING TIME-RECORD FOR TIME    25608.708
 DELETING TIME-RECORD FOR TIME    51217.416
 DELETING TIME-RECORD FOR TIME    102434.83
 DELETING TIME-RECORD FOR TIME    204869.67
 DELETING TIME-RECORD FOR TIME    409739.33
 DELETING TIME-RECORD FOR TIME    819478.66
 DELETING TIME-RECORD FOR TIME    1638957.3
 DELETING TIME-RECORD FOR TIME    3277914.7
 DELETING TIME-RECORD FOR TIME    6555829.3
 DELETING TIME-RECORD FOR TIME    13111659.
 DELETING TIME-RECORD FOR TIME    26223317.
 DELETING TIME-RECORD FOR TIME    52446634.
 DELETING TIME-RECORD FOR TIME   0.10489327E+09
 DELETING TIME-RECORD FOR TIME   0.20489327E+09
 DELETING TIME-RECORD FOR TIME   0.30489327E+09
 DELETING TIME-RECORD FOR TIME   0.40489327E+09
 DELETING TIME-RECORD FOR TIME   0.50489327E+09
 DELETING TIME-RECORD FOR TIME   0.60489327E+09
 DELETING TIME-RECORD FOR TIME   0.70489327E+09
 DELETING TIME-RECORD FOR TIME   0.80489327E+09

 KEEPING TIME-RECORD FOR TIME   0.90489327E+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:
```

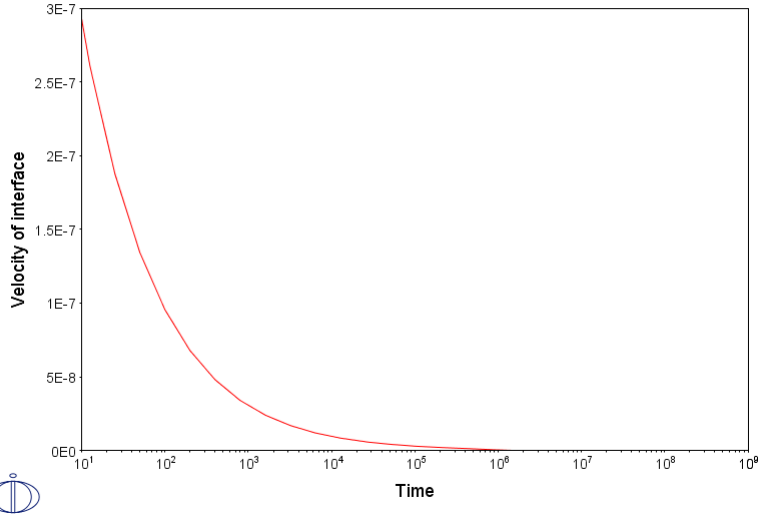



```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1:POST-1:POST-1:POST-1:  INFO: Time is set as independent variable
POST-1:VARIABLE :INTERFACE :UPPER OR LOWER INTERFACE OF REGION AUSTENITE#1 /LOWER/:POST-1:
POST-1:AXIS (X, Y OR Z) :AXIS TYPE /LINEAR/:POST-1:
POST-1:AXIS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

2019.05.27.09.26.30
LOWER INTERFACE OF REGION "AUSTENITE#1"
CELL #1

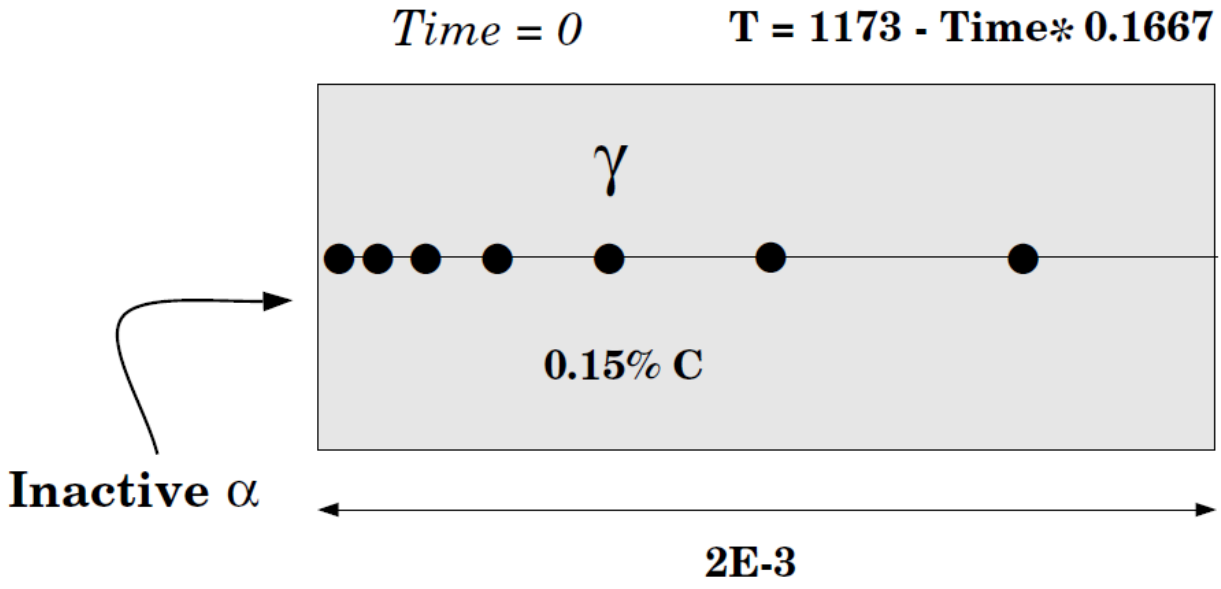


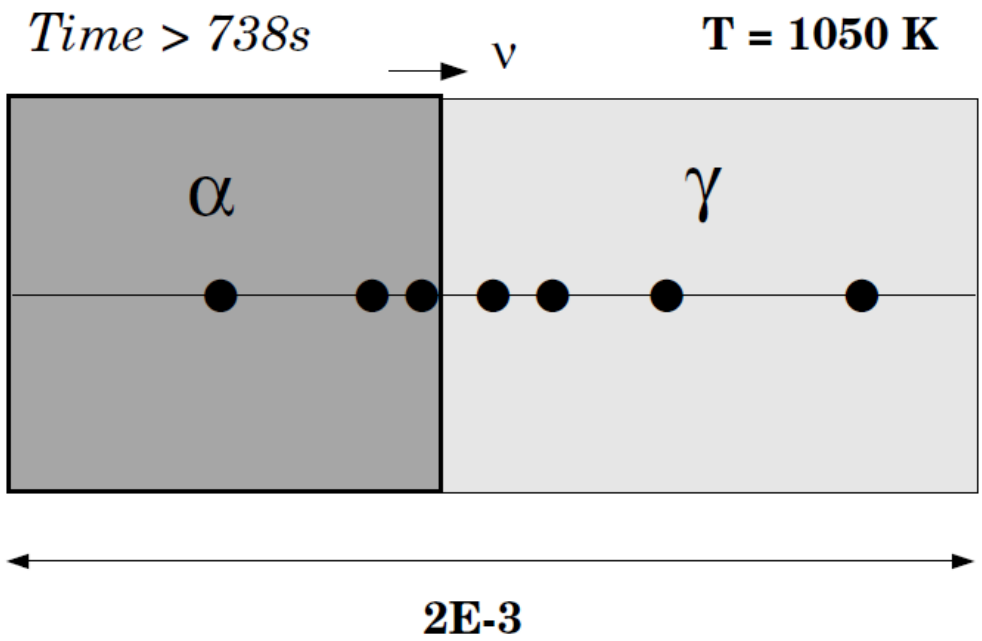

```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: --OK---
POST-1:
```

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 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri May 24 17:06:15 2019


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  v9.1

 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 v2.1

 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
 CBCC_A12                 CEMENTITE               CUB_A13
 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'
  '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  v9.1
 TCFE8   =  Steels/Fe-Alloys  v8.1
 FROST1  =  FROST database v1.0
 TCFE7   =  Steels/Fe-Alloys  v7.0
 TCFE6   =  Steels/Fe-Alloys  v6.2
 TCFE5   =  Steels/Fe-Alloys  v5.0
 TCFE4   =  Steels/Fe-Alloys  v4.1
 TCFE3   =  Steels/Fe-Alloys  v3.1
 TCFE2   =  Steels/Fe-Alloys  v2.1
 TCFE1   =  Steels/Fe-Alloys  v1.0
 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  v2.1
 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
 TCSLD1  =  Solder Alloys  v1.1
 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
 TCNF2   =  Nuclear Fuels  v2.1b
 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 v2.1
 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  v1.0
 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 /AUTO/:
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -> 1): /AUTO/:MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
```

```
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/:
DIC>DIC>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 = .00698495916383108  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
 U-FRACTION IN SYSTEM:  C = .00698495916383108  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 = .00698495916383108  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 = .00698495916383108  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 = .00698495916383108  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 = .00698495916383108  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 = .00698495916383108  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 = .00698495916383108  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 = .00698495916383108  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 = .00698495916383108  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 = .00698495916383108  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 = .00698495916383108  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    1 seconds
 TIME =  0.24205213E-02 DT =  0.12113937E-02 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 =  0.48433087E-02 DT =  0.24227873E-02 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 =  0.96888834E-02 DT =  0.48455747E-02 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 =  0.19380033E-01 DT =  0.96911494E-02 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 =  0.38762332E-01 DT =  0.19382299E-01 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 =  0.77526929E-01 DT =  0.38764598E-01 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 =  0.15505612     DT =  0.77529195E-01 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 =  0.31011451     DT =  0.15505839     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 =  0.62023129     DT =  0.31011678     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698495916383108  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    0 seconds
 TIME =   1.2404649     DT =  0.62023356     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 =   2.4809320     DT =   1.2404671     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 =   4.9618662     DT =   2.4809342     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 =   9.9237347     DT =   4.9618685     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698495916383106  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 = .00698495916383108  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]
```

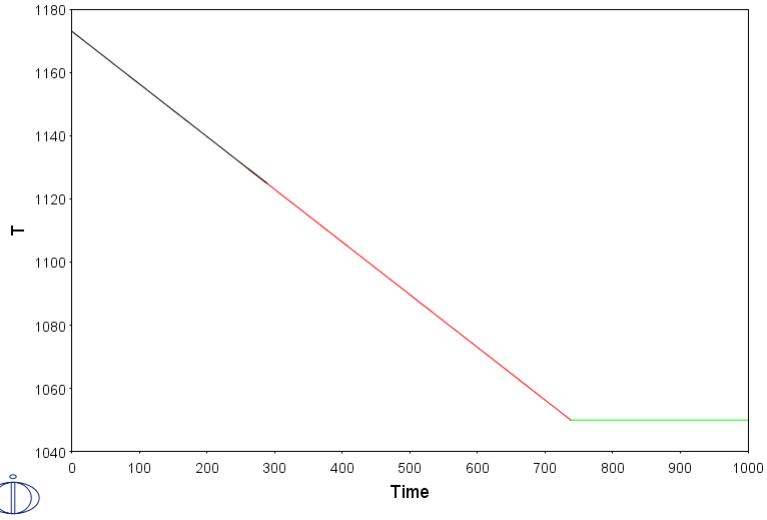
```
  CPU time used in timestep                    0 seconds
 TIME =   76.594946     DT =   36.900000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698495916383112  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    0 seconds
 TIME =   113.49495     DT =   36.900000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698495916383113  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    0 seconds
 TIME =   150.39495     DT =   36.900000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698495916383114  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 = .0069849591638312  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 = .00698495916383122  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]


output ignored...



... output resumed

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

  CPU time used in timestep                    0 seconds
 1.164180598981399E-004        1.164248817227883E-004        1.016769262523636E-
027       TIME =  0.43290458E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.10167693E-26
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.37404245E-16 AND  -0.37404245E-16
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13794256E-02
 U-FRACTION IN SYSTEM:  C = .0069861764105222  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUSTENITE

  CPU time used in timestep                    0 seconds
 3.740945785415924E-003        3.740854335447452E-003        3.366538628372613E-
018       TIME =  0.53290458E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.33665386E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.33655319E-15 AND  -0.33655319E-15
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13793919E-02
 U-FRACTION IN SYSTEM:  C = .00698651960656473  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    0 seconds
 1.584524280521030E-004        1.584693632155386E-004        7.822420331607045E-
022       TIME =  0.63290458E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.78224203E-21
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.28738495E-15 AND   0.28738495E-15
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13794207E-02
 U-FRACTION IN SYSTEM:  C = .00698622654924551  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  32  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_BCC_A2

  CPU time used in timestep                    0 seconds
 4.499234871954129E-005        4.500005467628141E-005        1.856205263385729E-
027       TIME =  0.73290458E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.18562053E-26
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.47252837E-16 AND  -0.47252837E-16
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13794159E-02
 U-FRACTION IN SYSTEM:  C = .00698627473475296  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUSTENITE

  CPU time used in timestep                    0 seconds
 6.192697232299770E-004        6.193167289475208E-004        6.210438802404827E-
019       TIME =  0.83290458E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.62104388E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.75709505E-16 AND   0.75709505E-16
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13794235E-02
 U-FRACTION IN SYSTEM:  C = .00698619753090197  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  8  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_BCC_A2

  CPU time used in timestep                    0 seconds
 7.284639367683529E-006        7.285456215421114E-006        5.898517290944324E-
019       TIME =  0.93290458E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.58985173E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.58143000E-16 AND  -0.58143000E-16
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13794177E-02
 U-FRACTION IN SYSTEM:  C = .00698625682152005  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUSTENITE

  CPU time used in timestep                    0 seconds
 2.855901082007420E-006        2.856293870345931E-006        4.202315144215894E-
021       TIME =  0.10000000E+10 DT =   67095423.     SUM OF SQUARES =  0.42023151E-20
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.25881403E-16 AND   0.25881403E-16
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13794194E-02
 U-FRACTION IN SYSTEM:  C = .00698623911353116  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    769.68675
 DELETING TIME-RECORD FOR TIME    833.06026
 DELETING TIME-RECORD FOR TIME    959.80726
 DELETING TIME-RECORD FOR TIME    1213.3013
 DELETING TIME-RECORD FOR TIME    1720.2893
 DELETING TIME-RECORD FOR TIME    2734.2654
 DELETING TIME-RECORD FOR TIME    4762.2175
 DELETING TIME-RECORD FOR TIME    8818.1218
 DELETING TIME-RECORD FOR TIME    16929.930
 DELETING TIME-RECORD FOR TIME    33153.547
 DELETING TIME-RECORD FOR TIME    65600.781
 DELETING TIME-RECORD FOR TIME    130495.25
 DELETING TIME-RECORD FOR TIME    260284.19
 DELETING TIME-RECORD FOR TIME    519862.06
 DELETING TIME-RECORD FOR TIME    1039017.8
 DELETING TIME-RECORD FOR TIME    2077329.3
 DELETING TIME-RECORD FOR TIME    4153952.3
 DELETING TIME-RECORD FOR TIME    8307198.2
 DELETING TIME-RECORD FOR TIME    16613690.
 DELETING TIME-RECORD FOR TIME    33226674.
 DELETING TIME-RECORD FOR TIME    66452642.
 DELETING TIME-RECORD FOR TIME   0.13290458E+09
 DELETING TIME-RECORD FOR TIME   0.23290458E+09
```

```
 DELETING TIME-RECORD FOR TIME   0.33290458E+09
 DELETING TIME-RECORD FOR TIME   0.43290458E+09
 DELETING TIME-RECORD FOR TIME   0.53290458E+09
 DELETING TIME-RECORD FOR TIME   0.63290458E+09
 DELETING TIME-RECORD FOR TIME   0.73290458E+09
 DELETING TIME-RECORD FOR TIME   0.83290458E+09

 KEEPING TIME-RECORD FOR TIME   0.93290458E+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

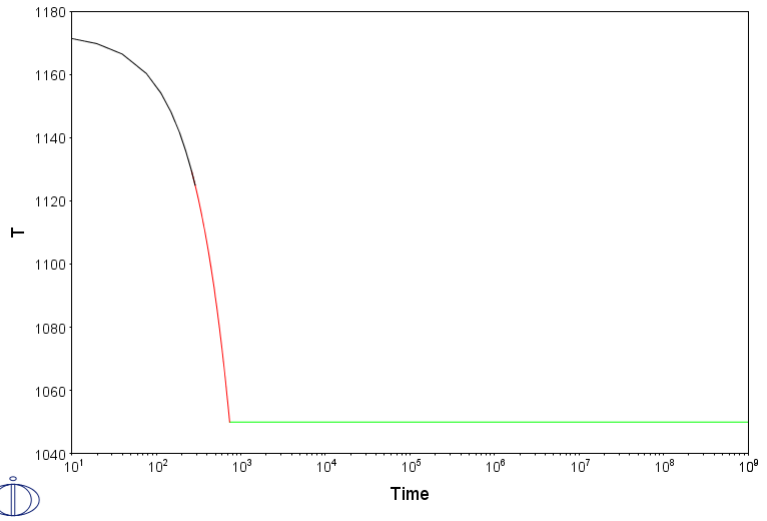
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb1c\plot.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  1.00000E+09
DIC> OK
DIC>
DIC>DIC>DIC>DIC>  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:  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:
```

2019.05.27.09.29.49
LOWER INTERFACE OF REGION "AUSTENITE#1"
CELL #1



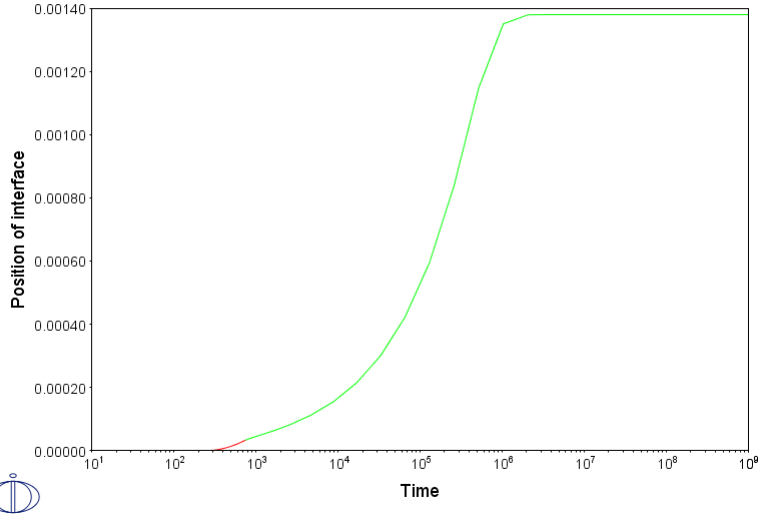

```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:
POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```

2019.05.27.09.29.50
LOWER INTERFACE OF REGION "AUSTENITE#1"
CELL #1



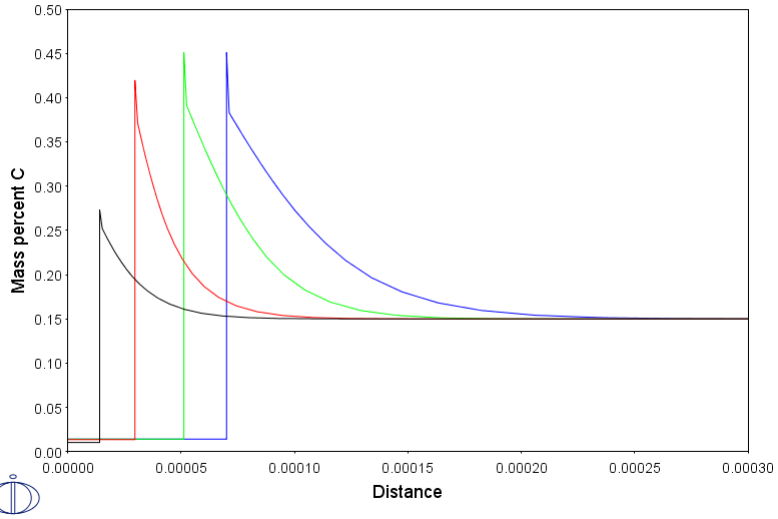

```
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1:POST-1:POST-1:POST-1:AXIS (X, Y OR Z) :VARIABLE :INTERFACE :UPPER OR LOWER INTERFACE OF REGION AUSTENITE#1 /LOWER/:POST-1:
POST-1:
POST-1:POST-1: ORKING ...          OST-1:POST-1:
POST-1:
```

2019.05.27.09.29.51
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:
```

2019.05.27.09.29.51
Time = 500,700,1200,2000
CELL #1

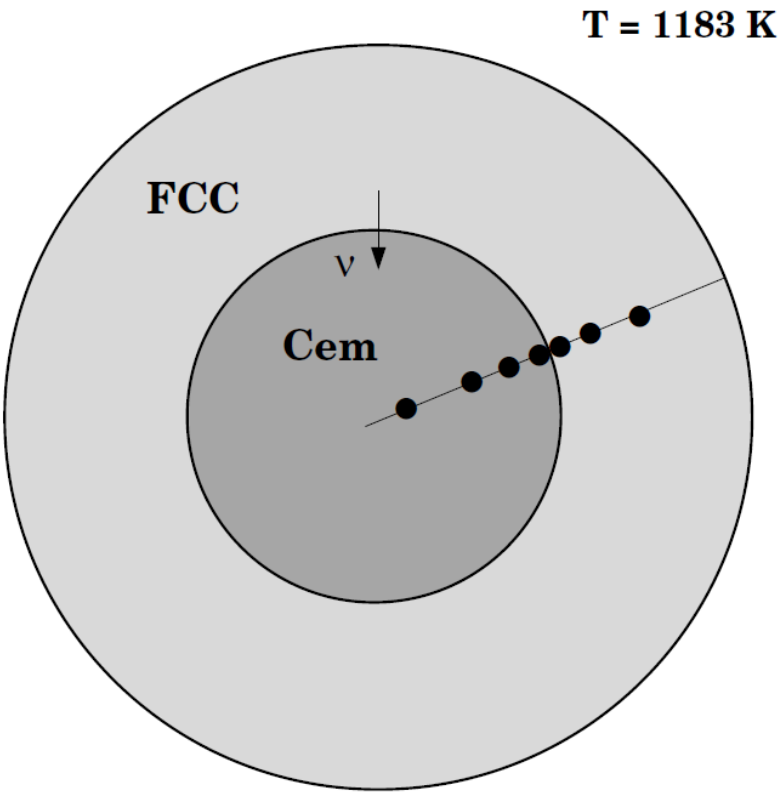



```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1: --OK---
POST-1:
```

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

```
About Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri May 24 17:06:15 2019


SYS:SYS:MACRO "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  v9.1

 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 v2.1

 VA                       /-  DEFINED
TDB_FEDEMO: FE                       CR                      C
   DEFINED
TDB_FEDEMO: GAS:G                    LIQUID:L                BCC_A2
 CBCC_A12                 CEMENTITE               CHI_A12
 CUB_A13                  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 .......
 Creating a new composition set FCC_A1#2
 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'
  '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  v4.0

 VA  DEFINED
 B2_BCC  REJECTED
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 .......
 Creating a new composition set FCC_A1#3
 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:

POLY:POLY:POLY:POLY:POLY:POLY:
POLY:
POLY:POLY:POLY:POLY:
POLY:POLY:POLY:
POLY:POLY:POLY:
POLY:POLY:POLY:
POLY:POLY:POLY:
POLY:POLY:POLY:
POLY:
POLY:POLY:POLY:POLY: 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:
POLY:
```

```
POLY:POLY:POLY:POLY: RMAT=5.3924863E-7
POLY: W(CEMENTITE,CR)=0.12581645
 W(BCC_A2,CR)=4.4332285E-3
 W(BCC_A2,C)=1.510215E-4
POLY:
POLY:POLY:POLY:POLY:
POLY:
POLY:POLY:POLY:POLY: 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

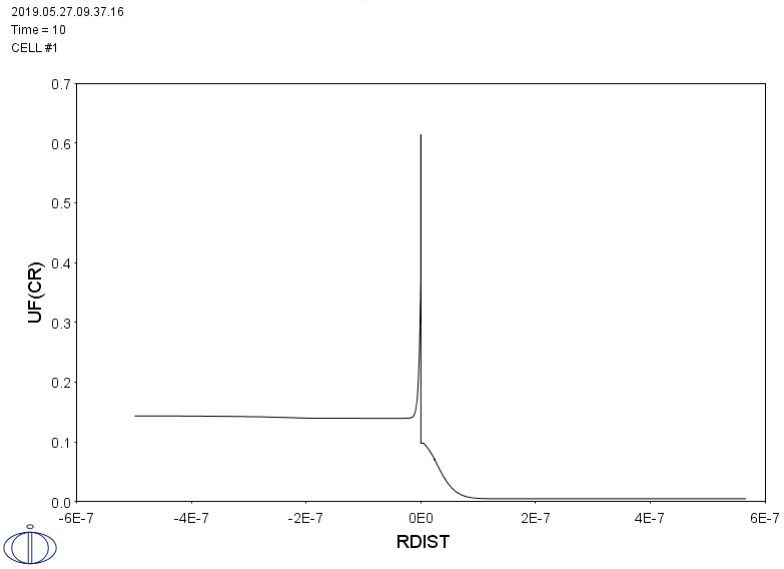
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb2\run.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC> TIME STEP AT TIME  0.00000E+00
 *** ENTERING BCC_A2 AS A DIFFUSION NONE PHASE
DIC> OK
DIC> Region: CARB
 single geometric dense at  0.52550E-06
 0.85084       96
 Region: AUS
 single geometric dense at   0.0000
  1.0072       63
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
  Trying old scheme                      4
 GENERATING STARTING VALUES FOR CELL #  1 INTERFACE #  2
 DETERMINING INITIAL EQUILIBRIUM VALUES
CALCULATING STARTING VALUES:       9   EQUILIBRIUM CALCULATIONS               DONE     6 OUT OF     9
04
 U-FRACTION IN SYSTEM:  C = .0406910188418179  CR = .0214382349908298
                        FE = .978561765139677
 TOTAL SIZE OF SYSTEM:  5.0562655986E-18 [m^3]
 U-FRACTION IN SYSTEM:  C = .0406910188418179  CR = .0214382349908298
                        FE = .978561765139677
 TOTAL SIZE OF SYSTEM:  5.0562655986E-18 [m^3]
 0.175650510569693        0.175691773365777        0.175650565704887        2.957532598255230E-003        7.754437973061249E-
005        5.789560109233930E-006        8.570927947770508E-007        3.747773449112176E-007        3.453239602619964E-
007        1.349945520957791E-007        1.350781378769984E-007        1.346761780035796E-007        1.361219741563121E-
007        1.343486158181300E-007        1.340757896490518E-007        1.335307279083391E-007        1.344901657985585E-
007        1.324431149500731E-007        1.302779707754353E-007        1.259882989101074E-007        1.269270676251932E-
007        1.175749112166747E-007        1.014430318675646E-007        7.217953338804161E-008        7.299680977021324E-
008        2.728135261205191E-008        7.241610562806674E-011        4.089073985024775E-014        7.514686277204363E-
019       TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =  0.75146863E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.39436721E-02 AND  -0.39436721E-02
 POSITION OF INTERFACE CARB / AUS IS   0.52510563E-06
 U-FRACTION IN SYSTEM:  C = .040729015482772  CR = .0214383281162587
                        FE = .978561672014248
 TOTAL SIZE OF SYSTEM:  5.0562655986E-18 [m^3]
  15  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: CARB

  CPU time used in timestep                    1 seconds
 2.248325209321082E-005        2.248775172894383E-005        2.248323619911186E-005        1.887682037244655E-009        1.633889346347317E-
009        1.019554373018429E-009        6.882195667765290E-010        6.885275116618297E-010        2.216754970030033E-
010        6.151372121827326E-014        2.128399910390758E-017       TIME =  0.30000000E-06 DT =  0.20000000E-
06 SUM OF SQUARES =  0.21283999E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.22443437E-04 AND  -0.22443437E-04
 POSITION OF INTERFACE CARB / AUS IS   0.52510114E-06
 U-FRACTION IN SYSTEM:  C = .04072976539935  CR = .0214383291134799
                        FE = .978561671017027
 TOTAL SIZE OF SYSTEM:  5.0562655986E-18 [m^3]
  CPU time used in timestep                    1 seconds
 6.026886170980438E-004        6.026583061711169E-004        6.026723276343818E-004        8.498836168376541E-005        3.515900515891161E-
005        2.728069178681887E-007        4.049298725283639E-010        6.350494380693860E-015        2.881532022611416E-
018       TIME =  0.70000000E-06 DT =  0.40000000E-06 SUM OF SQUARES =  0.28815320E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.46375286E-05 AND  -0.46375286E-05
 POSITION OF INTERFACE CARB / AUS IS   0.52509929E-06
 U-FRACTION IN SYSTEM:  C = .0407315536943019  CR = .0214383294273155
                        FE = .978561670703191
 TOTAL SIZE OF SYSTEM:  5.0562655986E-18 [m^3]
  CPU time used in timestep                    1 seconds
 2.365053654976460E-004        2.365034011183178E-004        2.364987464511019E-004        7.190705399750257E-005        1.444205196201147E-
007        4.667925539517978E-011        2.104125358596133E-014        2.043500290775240E-017       TIME =  0.15000000E-05 DT =  0.80000000E-
06 SUM OF SQUARES =  0.20435003E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.40628788E-05 AND  -0.40628788E-05
 POSITION OF INTERFACE CARB / AUS IS   0.52509604E-06
 U-FRACTION IN SYSTEM:  C = .0407314707249635  CR = .0214383297893152
                        FE = .978561670341192
 TOTAL SIZE OF SYSTEM:  5.0562655986E-18 [m^3]
  CPU time used in timestep                    0 seconds
 3.788611570769321E-005        3.788585986902445E-005        3.788452502271488E-005        1.049980214377798E-005        1.697420016474451E-
008        3.616707217676648E-012        3.087716420676142E-015        2.462505528796002E-018       TIME =  0.31000000E-05 DT =  0.16000000E-
05 SUM OF SQUARES =  0.24625055E-17


output ignored...



... output resumed

 8.133539520648866E-009        2.550182842638402E-009        4.756250712738203E-014        4.112129632478376E-
018       TIME =   8322.3721     DT =   1000.0000     SUM OF SQUARES =  0.41121296E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.10698858E-10 AND  -0.10698858E-10
 POSITION OF INTERFACE CARB / AUS IS   0.24609440E-06
 U-FRACTION IN SYSTEM:  C = .0407634582863258  CR = .021438388813404
                        FE = .978561611317103
 TOTAL SIZE OF SYSTEM:  5.0562655986E-18 [m^3]
  CPU time used in timestep                    1 seconds
 7.781591091064711E-009        7.835851174397842E-009        7.798445151573769E-009        2.587832050303921E-009        8.903124352705346E-
010        5.039280287778270E-015        1.520902674551010E-
017       TIME =   9322.3721     DT =   1000.0000     SUM OF SQUARES =  0.15209027E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.10110966E-10 AND  -0.10110966E-10
 POSITION OF INTERFACE CARB / AUS IS   0.23598343E-06
 U-FRACTION IN SYSTEM:  C = .0407634764146718  CR = .0214383876933364
                        FE = .978561612437171
 TOTAL SIZE OF SYSTEM:  5.0562655986E-18 [m^3]
  CPU time used in timestep                    2 seconds
 9.389971638670603E-007        9.385365564751270E-007        9.381658659024861E-007        7.526530276342791E-008        8.775527090715530E-
013        6.977272844963092E-018       TIME =   10000.000     DT =   677.62792     SUM OF SQUARES =  0.69772728E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.95523048E-11 AND  -0.95523048E-11
 POSITION OF INTERFACE CARB / AUS IS   0.22951052E-06
 U-FRACTION IN SYSTEM:  C = .0407634754631051  CR = .0214383869655506
                        FE = .978561613164957
 TOTAL SIZE OF SYSTEM:  5.0562655986E-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   0.99418841E-04
 DELETING TIME-RECORD FOR TIME   0.17900385E-03
 DELETING TIME-RECORD FOR TIME   0.30071417E-03
 DELETING TIME-RECORD FOR TIME   0.47831765E-03
 DELETING TIME-RECORD FOR TIME   0.72934329E-03
 DELETING TIME-RECORD FOR TIME   0.10758312E-02
 DELETING TIME-RECORD FOR TIME   0.15428938E-02
 DELETING TIME-RECORD FOR TIME   0.21467122E-02
 DELETING TIME-RECORD FOR TIME   0.29017145E-02
 DELETING TIME-RECORD FOR TIME   0.38194470E-02
 DELETING TIME-RECORD FOR TIME   0.49085220E-02
 DELETING TIME-RECORD FOR TIME   0.61737172E-02
 DELETING TIME-RECORD FOR TIME   0.76140704E-02
 DELETING TIME-RECORD FOR TIME   0.92225530E-02
 DELETING TIME-RECORD FOR TIME   0.10986205E-01
 DELETING TIME-RECORD FOR TIME   0.12887621E-01
 DELETING TIME-RECORD FOR TIME   0.14913721E-01
 DELETING TIME-RECORD FOR TIME   0.17051346E-01
 DELETING TIME-RECORD FOR TIME   0.19290988E-01
 DELETING TIME-RECORD FOR TIME   0.21633640E-01
 DELETING TIME-RECORD FOR TIME   0.24076629E-01
 DELETING TIME-RECORD FOR TIME   0.26619724E-01
 DELETING TIME-RECORD FOR TIME   0.29264997E-01
 DELETING TIME-RECORD FOR TIME   0.32010611E-01
 DELETING TIME-RECORD FOR TIME   0.34862598E-01
 DELETING TIME-RECORD FOR TIME   0.37829873E-01
 DELETING TIME-RECORD FOR TIME   0.40921693E-01
 DELETING TIME-RECORD FOR TIME   0.44136483E-01
 DELETING TIME-RECORD FOR TIME   0.47480849E-01
 DELETING TIME-RECORD FOR TIME   0.50961527E-01
 DELETING TIME-RECORD FOR TIME   0.54593384E-01
 DELETING TIME-RECORD FOR TIME   0.58383853E-01
 DELETING TIME-RECORD FOR TIME   0.62357656E-01
 DELETING TIME-RECORD FOR TIME   0.66521873E-01
 DELETING TIME-RECORD FOR TIME   0.68802708E-01
 DELETING TIME-RECORD FOR TIME   0.71497059E-01
 DELETING TIME-RECORD FOR TIME   0.74612522E-01
 DELETING TIME-RECORD FOR TIME   0.78159054E-01
 DELETING TIME-RECORD FOR TIME   0.82115298E-01
 DELETING TIME-RECORD FOR TIME   0.86491020E-01
 DELETING TIME-RECORD FOR TIME   0.91276780E-01
 DELETING TIME-RECORD FOR TIME   0.96473166E-01
 DELETING TIME-RECORD FOR TIME   0.10206052
 DELETING TIME-RECORD FOR TIME   0.10804860
 DELETING TIME-RECORD FOR TIME   0.11445063
 DELETING TIME-RECORD FOR TIME   0.12133071
 DELETING TIME-RECORD FOR TIME   0.12873462
 DELETING TIME-RECORD FOR TIME   0.13674928
 DELETING TIME-RECORD FOR TIME   0.14543690
 DELETING TIME-RECORD FOR TIME   0.15494720
 DELETING TIME-RECORD FOR TIME   0.16561157
 DELETING TIME-RECORD FOR TIME   0.17786478
 DELETING TIME-RECORD FOR TIME   0.19239402
 DELETING TIME-RECORD FOR TIME   0.21034788
 DELETING TIME-RECORD FOR TIME   0.23440524
 DELETING TIME-RECORD FOR TIME   0.27065630
 DELETING TIME-RECORD FOR TIME   0.33538860
 DELETING TIME-RECORD FOR TIME   0.41264653
 DELETING TIME-RECORD FOR TIME   0.50846373
 DELETING TIME-RECORD FOR TIME   0.63474295
 DELETING TIME-RECORD FOR TIME   0.81581357
 DELETING TIME-RECORD FOR TIME   0.91499003
 DELETING TIME-RECORD FOR TIME    1.0985361
 DELETING TIME-RECORD FOR TIME    1.4398814
 DELETING TIME-RECORD FOR TIME    1.6508782
 DELETING TIME-RECORD FOR TIME    2.0594174
 DELETING TIME-RECORD FOR TIME    2.8475124
 DELETING TIME-RECORD FOR TIME    4.3514091
 DELETING TIME-RECORD FOR TIME    7.2050103
 DELETING TIME-RECORD FOR TIME    12.704355
 DELETING TIME-RECORD FOR TIME    23.586122
 DELETING TIME-RECORD FOR TIME    45.349657
 DELETING TIME-RECORD FOR TIME    88.876727
 DELETING TIME-RECORD FOR TIME    175.93087
 DELETING TIME-RECORD FOR TIME    350.03915
 DELETING TIME-RECORD FOR TIME    698.25571
 DELETING TIME-RECORD FOR TIME    1394.6888
 DELETING TIME-RECORD FOR TIME    2322.3721
 DELETING TIME-RECORD FOR TIME    3322.3721
 DELETING TIME-RECORD FOR TIME    4322.3721
 DELETING TIME-RECORD FOR TIME    5322.3721
 DELETING TIME-RECORD FOR TIME    6322.3721
 DELETING TIME-RECORD FOR TIME    7322.3721
 DELETING TIME-RECORD FOR TIME    8322.3721

 KEEPING TIME-RECORD FOR TIME    9322.3721
 AND FOR TIME                    10000.000
 WORKSPACE RECLAIMED

 TIMESTEP AT     10000.0000     SELECTED

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

exb2-plot

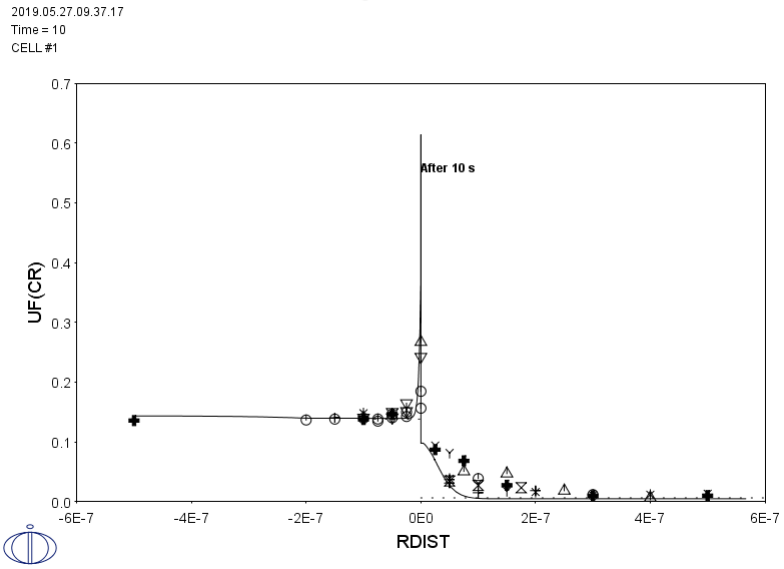
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb2\plot.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  1.00000E+04
 *** ENTERING BCC_A2 AS A DIFFUSION NONE PHASE
DIC> OK
DIC>
DIC>DIC>DIC>DIC>  POST PROCESSOR VERSION   1.7
  Implemented 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:
```

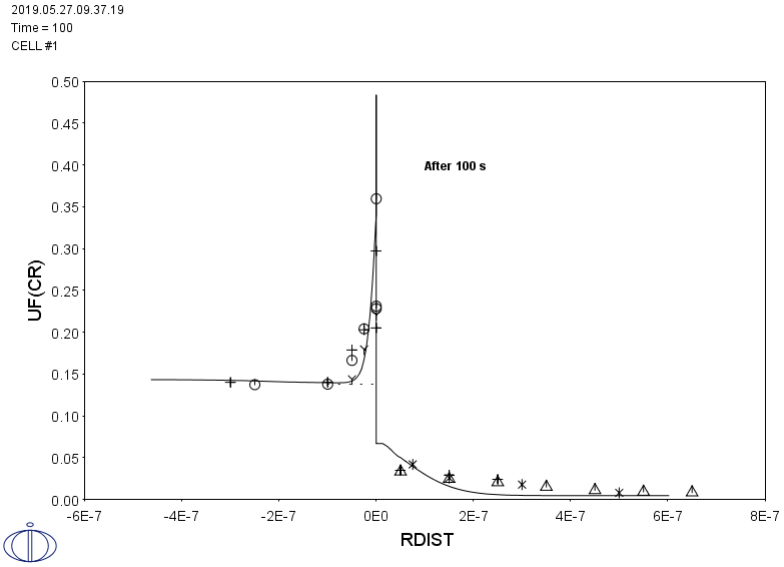
Figure b2.2




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

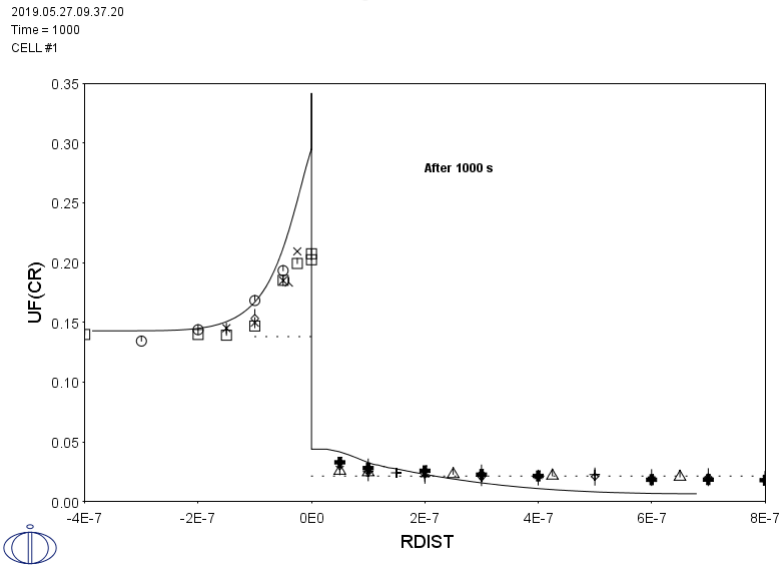
```
POST-1:POST-1:
POST-1:PROLOGUE NUMBER: /0/:DATASET NUMBER(s): /-1/:POST-1:
POST-1:POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```

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:
```

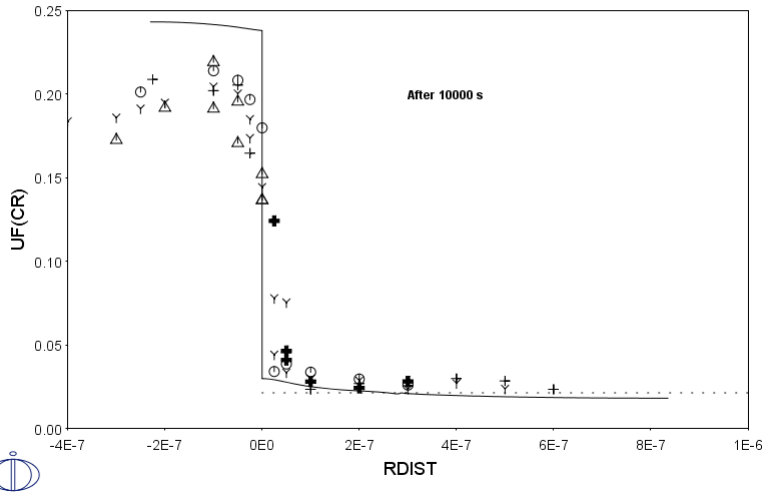
Figure b2.4




```
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

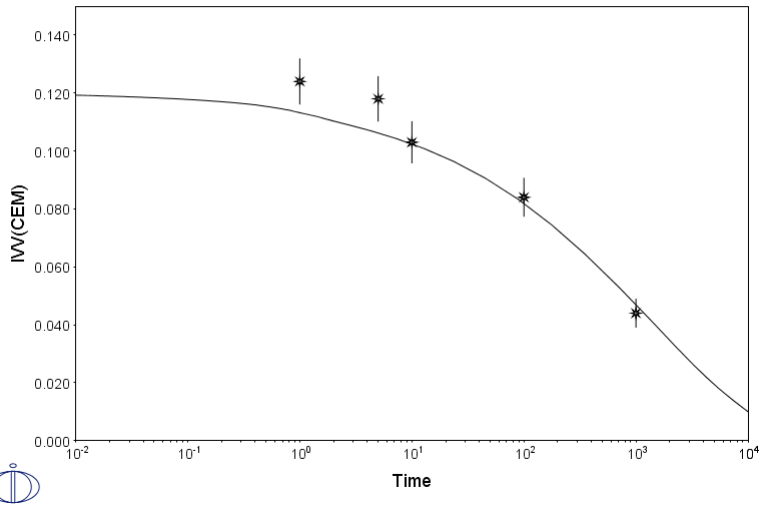
2019.05.27.09.37.21
Time = 10000
CELL #1




```
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:  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

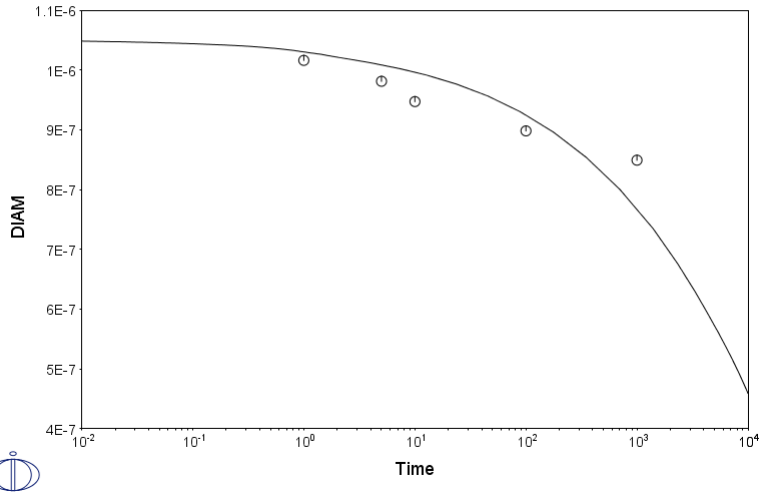
2019.05.27.09.37.23
CELL #1




```
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: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

2019.05.27.09.37.25
UPPER INTERFACE OF REGION "CARB#1"
CELL #1

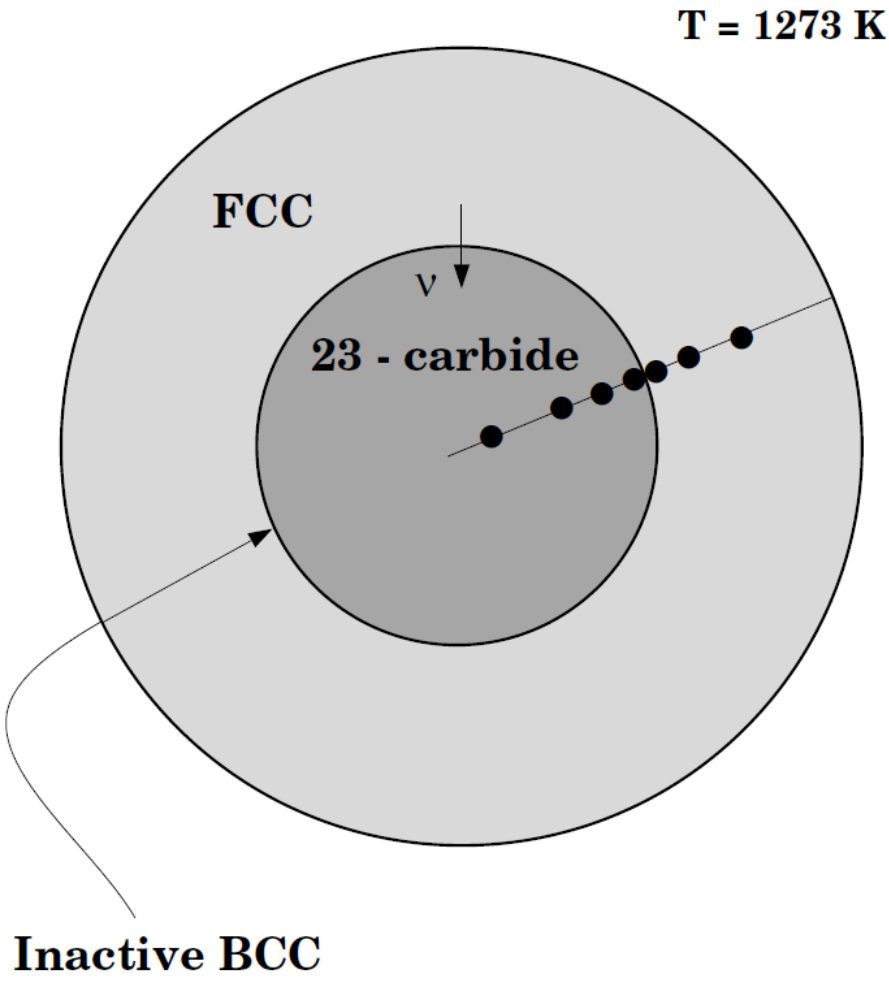



```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: --OK---
POST-1:
```

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 Stockholm, Sweden

 Software  (build 20130) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri May 24 17:06:15 2019


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  v9.1

 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 v2.1

 VA                       /-  DEFINED
TDB_FEDEMO: FE                       C                       CR
   DEFINED
TDB_FEDEMO: GAS:G                    LIQUID:L                BCC_A2
 CBCC_A12                 CEMENTITE               CHI_A12
 CUB_A13                  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 .......
 Creating a new composition set FCC_A1#2
 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'
  '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 .......
 Creating a new composition set FCC_A1#3
 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

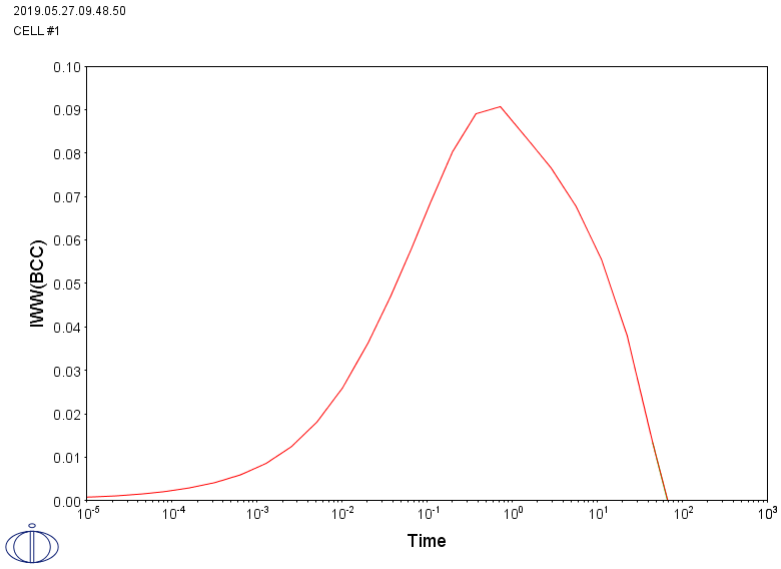
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb3\run.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  0.00000E+00
DIC> OK
DIC>
DIC>DIC>DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> Region: CARBIDE
 single geometric dense at  0.50000E-06
 0.83296       92
 Region: MATRIX
 single geometric dense at   0.0000
  1.0051       62
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
  Trying old scheme                    4
 GENERATING STARTING VALUES FOR CELL #  1 INTERFACE #  2
 DETERMINING INITIAL EQUILIBRIUM VALUES
CALCULATING STARTING VALUES:       9   EQUILIBRIUM CALCULATIONS               DONE     6 OUT OF     9
 U-FRACTION IN SYSTEM:  C = .0278637912207471  CR = .149918318671311
                        FE = .850081681459196
 TOTAL SIZE OF SYSTEM:  4.93068569406E-18 [m^3]
 U-FRACTION IN SYSTEM:  C = .0278637912207471  CR = .149918318671311
                        FE = .850081681459196
 TOTAL SIZE OF SYSTEM:  4.93068569406E-18 [m^3]
 0.565663007975139        0.565797019192573        0.565663812089352        1.015925208844379E-002        3.012654895338431E-
004        4.777345255079571E-005        2.965739035922150E-006        7.215362066507473E-007        8.262638042908063E-
007        4.246506052236764E-008        4.119324775664361E-008        3.974271203580596E-008        4.355497133462941E-
008        3.870625294942815E-008        3.673410109127777E-008        3.294771044651467E-008        3.668595705493653E-
008        2.600355362267187E-008        1.460917535760059E-008        1.658190586440551E-009        4.335933780373599E-
012        1.279149112494073E-015        2.899183993565051E-017       TIME =  0.10000000E-06 DT =  0.10000000E-
06 SUM OF SQUARES =  0.28991840E-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
 1.096405342624390E-004        1.096626445880835E-004        1.096405350851735E-004        5.301312499834021E-008        2.238795340824333E-
008        6.726062378827421E-011        8.232621647244419E-014        3.182681539722668E-019       TIME =  0.30000000E-06 DT =  0.20000000E-
06 SUM OF SQUARES =  0.31826815E-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
 1.217834959633175E-004        1.217822143856248E-004        1.217736602727202E-004        6.952195607601387E-007        2.897692878657929E-
009        5.944752050391817E-012        3.496826716171941E-016        2.033187568885462E-022       TIME =  0.70000000E-06 DT =  0.40000000E-
06 SUM OF SQUARES =  0.20331876E-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                    1 seconds
 6.892011299966989E-006        6.891932131913115E-006        6.890942061812611E-006        6.583124931140831E-007        2.505198161087611E-
010        2.332167041681551E-013        9.589039570194671E-018       TIME =  0.15000000E-05 DT =  0.80000000E-
06 SUM OF SQUARES =  0.95890396E-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 = .027877408342632  CR = .149918501535994
                        FE = .850081498594513
 TOTAL SIZE OF SYSTEM:  4.93068569406E-18 [m^3]
  CPU time used in timestep                    1 seconds
 6.464716136169133E-006        6.468802059546301E-006        6.464210841605345E-006        5.860740495320009E-008        8.516411571958706E-
012

output ignored...



... output resumed

 3.653219923584031E-008        7.718399462613038E-012        6.571235508876515E-
017       TIME =   5409.7865     DT =   800.00000     SUM OF SQUARES =  0.65712355E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.72321094E-12 AND  -0.72321094E-12
 POSITION OF INTERFACE CARBIDE / MATRIX IS   0.39304265E-06
 U-FRACTION IN SYSTEM:  C = .02783525666011  CR = .149831758342062
                        FE = .850168241788446
 TOTAL SIZE OF SYSTEM:  4.93068569406E-18 [m^3]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: MATRIX

  CPU time used in timestep                    1 seconds
 7.263210057522333E-008        7.265277892817326E-008        7.256114672052418E-008        4.642021006825709E-008        3.686083947644681E-
008        1.915274574187503E-008        9.311764372378236E-010        1.638640876373302E-015        4.820682231558121E-
019       TIME =   6209.7865     DT =   800.00000     SUM OF SQUARES =  0.48206822E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.28853856E-12 AND  -0.28853856E-12
 POSITION OF INTERFACE CARBIDE / MATRIX IS   0.39281182E-06
 U-FRACTION IN SYSTEM:  C = .0278352581143596  CR = .14983175883557
                        FE = .850168241294937
 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
 2.499520132276592E-008        2.500003258353834E-008        2.495270397653242E-008        1.653668390058685E-008        1.508810919368310E-
008        1.254278029091032E-008        7.722776870549431E-009        7.724158836869324E-009        1.724009596635087E-
009        4.106457250090244E-015        1.813453714993744E-
020       TIME =   7009.7865     DT =   800.00000     SUM OF SQUARES =  0.18134537E-19
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.39265713E-13 AND  -0.39265713E-13
 POSITION OF INTERFACE CARBIDE / MATRIX IS   0.39278041E-06
 U-FRACTION IN SYSTEM:  C = .0278352606128423  CR = .149831759217731
                        FE = .850168240912775
 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
 8.504364876103371E-009        8.504747418028419E-009        8.478893966596242E-009        5.537461951856428E-009        5.473461826250792E-
```

```
009        5.328277937270323E-009        5.061002982676595E-009        5.062152643021599E-009        4.531082904577822E-
009        3.572404187968678E-009        2.004938613477685E-009        2.004878690006766E-009        2.275751354236961E-
010        9.321907005897389E-018       TIME =   7809.7865     DT =   800.00000     SUM OF SQUARES =  0.93219070E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.10366138E-12 AND   0.10366138E-12
 POSITION OF INTERFACE CARBIDE / MATRIX IS   0.39286334E-06
 U-FRACTION IN SYSTEM:  C = .0278352615864132  CR = .149831759233099
                        FE = .850168240897408
 TOTAL SIZE OF SYSTEM:  4.93068569406E-18 [m^3]
  30  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: CARBIDE

  CPU time used in timestep                     2 seconds
 7.346652370614691E-008        7.346439308130296E-008        7.380091797618705E-008        2.885050004794238E-008        2.846081741609845E-
008        2.735751363320505E-008        2.550268991679218E-008        2.551698106323950E-008        2.177829825648257E-
008        1.539463885896700E-008        5.816092677571175E-009        1.696042488128338E-
016       TIME =   8000.0000     DT =   190.21349     SUM OF SQUARES =  0.16960425E-15
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.41225923E-12 AND   0.41225923E-12
 POSITION OF INTERFACE CARBIDE / MATRIX IS   0.39294175E-06
 U-FRACTION IN SYSTEM:  C = .0278352613285463  CR = .14983175923823
                        FE = .850168240892277
 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    45.316535
 DELETING TIME-RECORD FOR TIME    67.609238
 DELETING TIME-RECORD FOR TIME    67.609248
 DELETING TIME-RECORD FOR TIME    67.609268
 DELETING TIME-RECORD FOR TIME    67.609308
 DELETING TIME-RECORD FOR TIME    67.609388
 DELETING TIME-RECORD FOR TIME    67.609548
 DELETING TIME-RECORD FOR TIME    67.609868
 DELETING TIME-RECORD FOR TIME    67.610508
 DELETING TIME-RECORD FOR TIME    67.611788
 DELETING TIME-RECORD FOR TIME    67.614348
 DELETING TIME-RECORD FOR TIME    67.619468
 DELETING TIME-RECORD FOR TIME    67.629708
 DELETING TIME-RECORD FOR TIME    67.650188
 DELETING TIME-RECORD FOR TIME    67.691148
 DELETING TIME-RECORD FOR TIME    67.773068
 DELETING TIME-RECORD FOR TIME    67.936908
 DELETING TIME-RECORD FOR TIME    68.264588
 DELETING TIME-RECORD FOR TIME    68.919948
 DELETING TIME-RECORD FOR TIME    70.230668
 DELETING TIME-RECORD FOR TIME    72.852108
 DELETING TIME-RECORD FOR TIME    78.094988
 DELETING TIME-RECORD FOR TIME    88.580748
 DELETING TIME-RECORD FOR TIME    109.55227
 DELETING TIME-RECORD FOR TIME    151.49531
 DELETING TIME-RECORD FOR TIME    235.38139
 DELETING TIME-RECORD FOR TIME    403.15355
 DELETING TIME-RECORD FOR TIME    738.69787
 DELETING TIME-RECORD FOR TIME    1409.7865
 DELETING TIME-RECORD FOR TIME    2209.7865
 DELETING TIME-RECORD FOR TIME    3009.7865
 DELETING TIME-RECORD FOR TIME    3809.7865
 DELETING TIME-RECORD FOR TIME    4609.7865
 DELETING TIME-RECORD FOR TIME    5409.7865
 DELETING TIME-RECORD FOR TIME    6209.7865
 DELETING TIME-RECORD FOR TIME    7009.7865

 KEEPING TIME-RECORD FOR TIME    7809.7865
 AND FOR TIME                    8000.0000
 WORKSPACE RECLAIMED

 TIMESTEP AT     8000.00000     SELECTED

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

exb3-plot

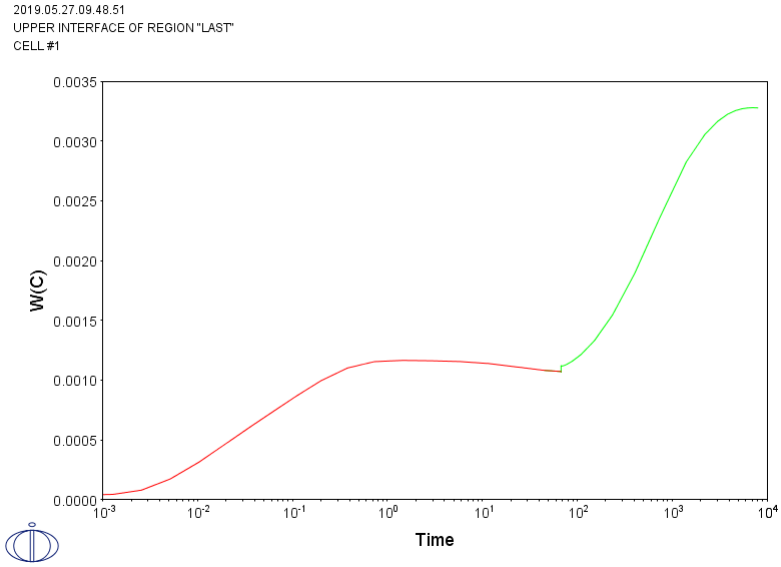
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb3\plot.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  8.00000E+03
DIC> OK
DIC>
DIC>DIC>DIC>DIC>  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:POST-1: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

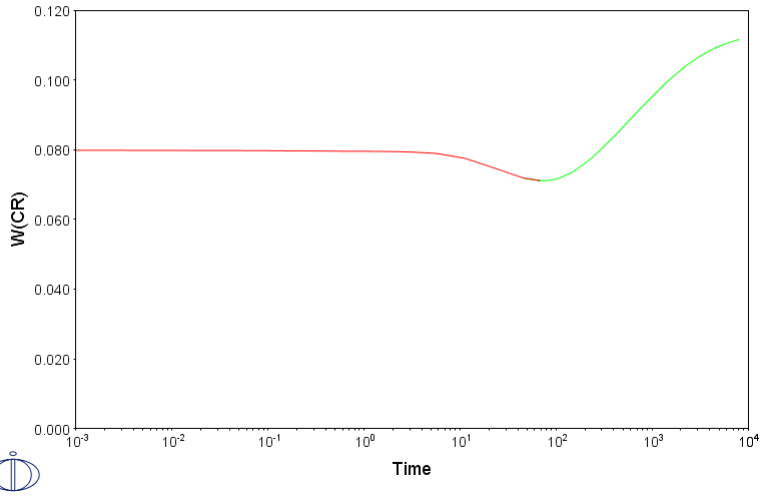
Figure b3.2




```
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

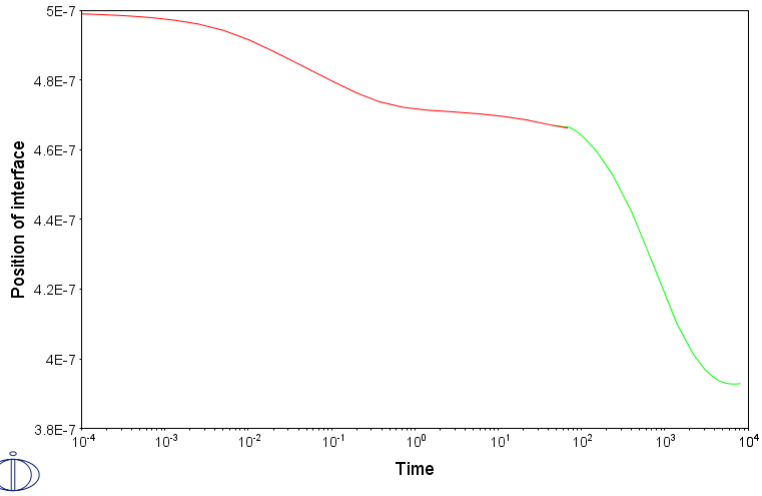
2019.05.27.09.48.52
UPPER INTERFACE OF REGION "LAST"
CELL #1




```
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

2019.05.27.09.48.53
UPPER INTERFACE OF REGION "CARBIDE#1"
CELL #1

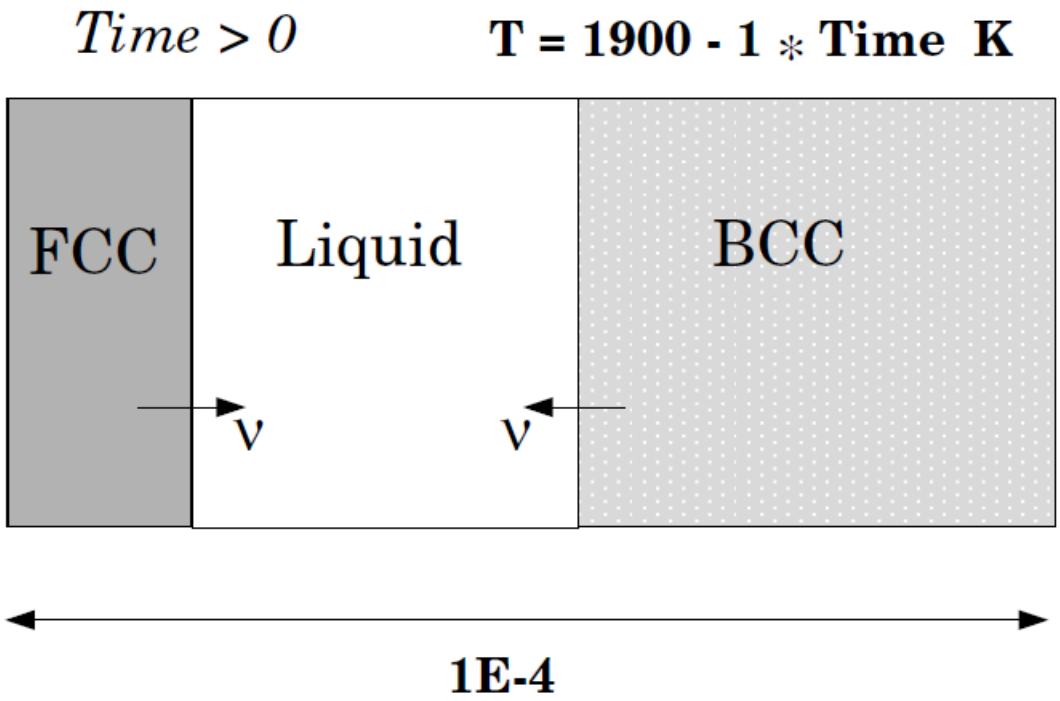



```
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1:
POST-1: --OK---
POST-1:
```

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 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri May 24 17:06:15 2019


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  v9.1

 VA                       /-  DEFINED
 L12_FCC                  B2_BCC                  DICTRA_FCC_A1
   REJECTED
TDB_TCFE9:
TDB_TCFE9:TDB_TCFE9:TDB_TCFE9:
TDB_TCFE9:TDB_TCFE9: FE                      NI                      CR
   DEFINED
TDB_TCFE9:
TDB_TCFE9:TDB_TCFE9: LIQUID:L                BCC_A2                  FCC_A1
 HCP_A3                   CBCC_A12                CUB_A13
 SIGMA                    CHI_A12                 LAVES_PHASE_C14
 CR3SI                    NBNI3                   NI3TI
 CRZN17                   BETA1                   GAMMA
 AL5FE4                   FLUORITE_C1:I           ZRO2_TETR:I
 M2O3C:I                  CENI2                   CENI5
   REJECTED
TDB_TCFE9: FCC_A1                  LIQUID:L                BCC_A2
   RESTORED
TDB_TCFE9:
TDB_TCFE9:TDB_TCFE9: 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, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  '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'
  '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'
  '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_TCFE9:
TDB_TCFE9:TDB_TCFE9:TDB_TCFE9:TDB_TCFE9:TDB_TCFE9: Use one of these databases

 TCFE9   =  Steels/Fe-Alloys  v9.1
 TCFE8   =  Steels/Fe-Alloys  v8.1
 FROST1  =  FROST database v1.0
 TCFE7   =  Steels/Fe-Alloys  v7.0
 TCFE6   =  Steels/Fe-Alloys  v6.2
 TCFE5   =  Steels/Fe-Alloys  v5.0
 TCFE4   =  Steels/Fe-Alloys  v4.1
 TCFE3   =  Steels/Fe-Alloys  v3.1
 TCFE2   =  Steels/Fe-Alloys  v2.1
 TCFE1   =  Steels/Fe-Alloys  v1.0
 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  v2.1
 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
 TCSLD1  =  Solder Alloys  v1.1
 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
 TCNF2   =  Nuclear Fuels  v2.1b
 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 v2.1
 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  v1.0
 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 /TCFE9/: Current database: Steels/Fe-Alloys Mobility  v4.0

 VA  DEFINED
 B2_BCC  REJECTED
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'
  'No assessed or estimated parameters'
  'Estimation by using the modified Sutherland equation from Chen et al.,
      Phil. Magazine 94 (2014) 1552.'
  'L. Zhang et al., Acta Mater., 58(2010)3664.'
 -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/: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>DIC>NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /AUTO/:VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -> 1): /AUTO/:
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/:
DIC>DIC>DIC>DIC>DIC>
DIC> --OK---
DIC>
```

exb4a-run

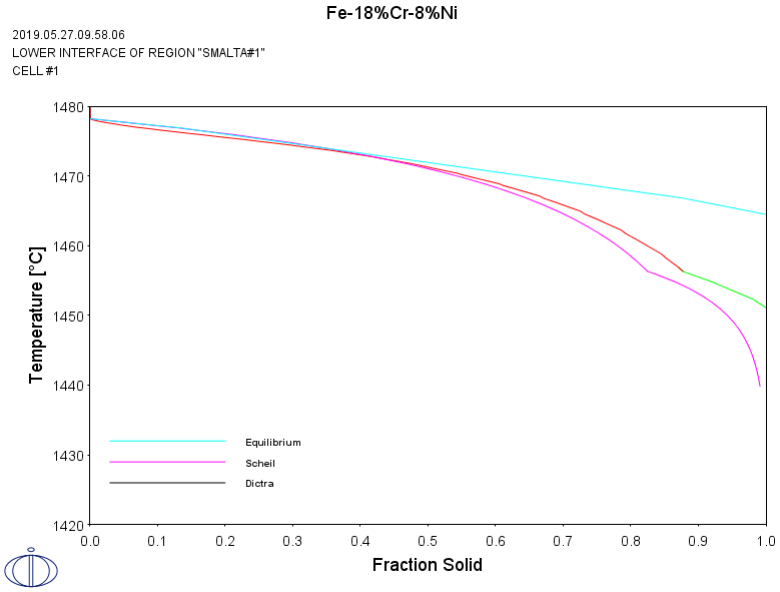
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb4a\run.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  0.00000E+00
DIC> OK
DIC>
DIC>DIC>DIC>DIC> Region: SMALTA
 double geometric
 dense at outer boundaries, coarse at  0.50000E-04
lower part   1.2275       22
upper part  0.81465       22
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
 INFO: TIMESTEP IS CONTROLLED BY INTERFACE POSITION
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.26028659E-05 DT =  0.25028659E-05 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.76085978E-05 DT =  0.50057319E-05 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.17620062E-04 DT =  0.10011464E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.37642989E-04 DT =  0.20022928E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.77688844E-04 DT =  0.40045855E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.15778055E-03 DT =  0.80091710E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    1 seconds
 TIME =  0.31796397E-03 DT =  0.16018342E-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 =  0.63833081E-03 DT =  0.32036684E-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 =  0.12790645E-02 DT =  0.64073368E-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 =  0.25605319E-02 DT =  0.12814674E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.51234666E-02 DT =  0.25629347E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.10249336E-01 DT =  0.51258694E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.20501075E-01 DT =  0.10251739E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.41004553E-01 DT =  0.20503478E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.82011508E-01 DT =  0.41006956E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992484  FE = .73306801121929
                        NI = .0754116207882254
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.16402542     DT =  0.82013911E-01 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 =  0.32805324     DT =  0.16402782     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992487  FE = .733068011219289
                        NI = .075411620788224
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.65610889     DT =  0.32805564     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992488  FE = .733068011219287
```

```
                        NI = .0754116207882257
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   1.3122202     DT =  0.65611129     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992476  FE = .73306801121929
                        NI = .0754116207882343
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   2.6244428     DT =   1.3122226     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992504  FE = .733068011219263
                        NI = .0754116207882327
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   5.2488879     DT =   2.6244452     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992499  FE = .733068011219241
                        NI = .0754116207882606


output ignored...



... output resumed

 U-FRACTION IN SYSTEM:  CR = .191500838087464  FE = .733100607877758
                        NI = .0753985540347778
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    3 seconds
 5.542934412562989E-006        5.543835425129676E-006        5.539195472149345E-006        7.175845934124312E-010        4.399033162823736E-
013        4.451045846363185E-018       TIME =   178.38332     DT =   1.3107200     SUM OF SQUARES =  0.44510458E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.59985781E-07 AND  -0.59985781E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.70798175E-05
 U-FRACTION IN SYSTEM:  CR = .191500838021444  FE = .7331006080149
                        NI = .0753985539636565
 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
 1.087065335790478E-005        1.087060133121829E-005        1.086454143073858E-005        3.773770709865823E-007        3.512326929713329E-
011        3.747192562408119E-016        6.343860977156412E-
021       TIME =   181.00476     DT =   2.6214400     SUM OF SQUARES =  0.63438610E-20
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.43957891E-07 AND  -0.43957891E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.69645846E-05
 U-FRACTION IN SYSTEM:  CR = .191500837939427  FE = .733100608202173
                        NI = .0753985538584004
 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
 7.968409015374515E-006        7.968557781915720E-006        7.965070507085707E-006        9.965449490358049E-007        1.848628663551278E-
007        1.454563530797797E-012        9.973827753369114E-
017       TIME =   186.24764     DT =   5.2428800     SUM OF SQUARES =  0.99738278E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.17721357E-07 AND  -0.17721357E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.68716736E-05
 U-FRACTION IN SYSTEM:  CR = .19150083786292  FE = .733100608442875
                        NI = .075398553694204
 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
 5.760481761915607E-006        5.760635864085793E-006        5.758981435822919E-006        2.368950799971108E-006        1.576724083296975E-
006        3.735114577398261E-007        4.317217146276070E-011        4.720022919121569E-015        6.408695776832642E-
019       TIME =   196.73340     DT =   10.485760     SUM OF SQUARES =  0.64086958E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.21802020E-07 AND   0.21802020E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.71002844E-05
 U-FRACTION IN SYSTEM:  CR = .191500837860463  FE = .733100608488656
                        NI = .0753985536508799
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    4 seconds
 1.322182413050428E-005        1.322203948421540E-005        1.321670093502497E-005        7.855627495168533E-008        2.238376137167841E-
011        5.880588480397629E-017       TIME =   200.00000     DT =   3.2666020     SUM OF SQUARES =  0.58805885E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.13886078E-07 AND   0.13886078E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.71456447E-05
 U-FRACTION IN SYSTEM:  CR = .191500837854575  FE = .733100608517618
                        NI = .0753985536278067
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 MUST SAVE WORKSPACE ON FILE
 WORKSPACE SAVED ON FILE
 RECLAIMING WORKSPACE
 DELETING TIME-RECORD FOR TIME    175.56749
 DELETING TIME-RECORD FOR TIME    175.76189
 DELETING TIME-RECORD FOR TIME    175.76190
 DELETING TIME-RECORD FOR TIME    175.76192
 DELETING TIME-RECORD FOR TIME    175.76196
 DELETING TIME-RECORD FOR TIME    175.76204
 DELETING TIME-RECORD FOR TIME    175.76220
 DELETING TIME-RECORD FOR TIME    175.76252
 DELETING TIME-RECORD FOR TIME    175.76316
 DELETING TIME-RECORD FOR TIME    175.76444
 DELETING TIME-RECORD FOR TIME    175.76700
 DELETING TIME-RECORD FOR TIME    175.77212
 DELETING TIME-RECORD FOR TIME    175.78236
 DELETING TIME-RECORD FOR TIME    175.80284
 DELETING TIME-RECORD FOR TIME    175.84380
 DELETING TIME-RECORD FOR TIME    175.92572
 DELETING TIME-RECORD FOR TIME    176.08956
 DELETING TIME-RECORD FOR TIME    176.41724
 DELETING TIME-RECORD FOR TIME    177.07260
 DELETING TIME-RECORD FOR TIME    178.38332
 DELETING TIME-RECORD FOR TIME    181.00476
 DELETING TIME-RECORD FOR TIME    186.24764

 KEEPING TIME-RECORD FOR TIME    196.73340
 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:
```

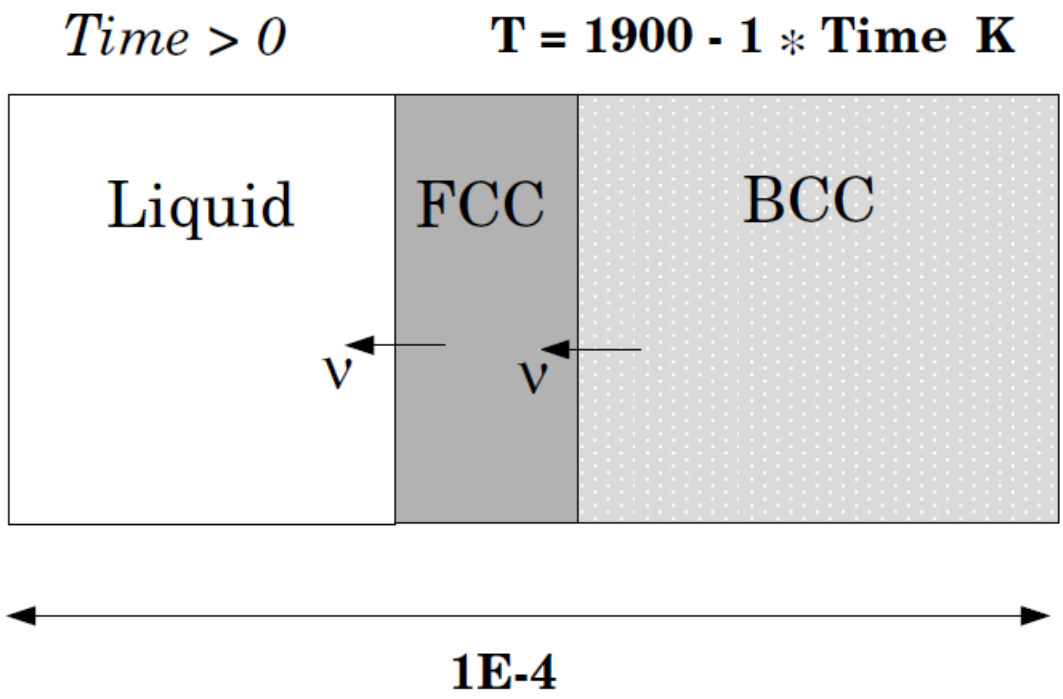



```
POST-1:
POST-1:
POST-1: --OK---
POST-1:
```

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 Software  (build 20130) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri May 24 17:06:15 2019


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  v9.1

 VA                      /-  DEFINED
 L12_FCC                 B2_BCC                  DICTRA_FCC_A1
   REJECTED
TDB_TCFE9:
TDB_TCFE9:TDB_TCFE9: Current database: Iron Demo Database v2.1

 VA                      /-  DEFINED
TDB_FEDEMO:
TDB_FEDEMO:TDB_FEDEMO: FE                      NI                      CR
   DEFINED
TDB_FEDEMO:
TDB_FEDEMO:TDB_FEDEMO: LIQUID:L                BCC_A2                  CBCC_A12
 CHI_A12                 CUB_A13                 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, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  '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'
  '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  v9.1
 TCFE8   =  Steels/Fe-Alloys  v8.1
 FROST1  =  FROST database v1.0
 TCFE7   =  Steels/Fe-Alloys  v7.0
 TCFE6   =  Steels/Fe-Alloys  v6.2
 TCFE5   =  Steels/Fe-Alloys  v5.0
 TCFE4   =  Steels/Fe-Alloys  v4.1
 TCFE3   =  Steels/Fe-Alloys  v3.1
 TCFE2   =  Steels/Fe-Alloys  v2.1
 TCFE1   =  Steels/Fe-Alloys  v1.0
 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  v2.1
 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
 TCSLD1  =  Solder Alloys  v1.1
 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
 TCNF2   =  Nuclear Fuels  v2.1b
 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 v2.1
 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  v1.0
 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  v4.0

 VA  DEFINED
 B2_BCC  REJECTED
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'
  'No assessed or estimated parameters'
  'Estimation by using the modified Sutherland equation from Chen et al.,
      Phil. Magazine 94 (2014) 1552.'
  'L. Zhang et al., Acta Mater., 58(2010)3664.'
 -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/: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 /AUTO/:VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -> 1): /AUTO/:
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/:DIC>DIC>DIC>DIC>
DIC> --OK---
DIC>
```

exb4b-run

```
DIC>About NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "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
 0.93810       83
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
 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 = .733068011219291
                        NI = .0754116207882254
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     0 seconds
 TIME =  0.27420944E-05 DT =  0.26420944E-05 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     0 seconds
 TIME =  0.80262833E-05 DT =  0.52841888E-05 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     1 seconds
 TIME =  0.18594661E-04 DT =  0.10568378E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     0 seconds
 TIME =  0.39731416E-04 DT =  0.21136755E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     0 seconds
 TIME =  0.82004927E-04 DT =  0.42273511E-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 =  0.16655195E-03 DT =  0.84547021E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     0 seconds
 TIME =  0.33564599E-03 DT =  0.16909404E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     0 seconds
 TIME =  0.67383408E-03 DT =  0.33818809E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     0 seconds
 TIME =  0.13502102E-02 DT =  0.67637617E-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 =  0.27029626E-02 DT =  0.13527523E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     0 seconds
 TIME =  0.54084673E-02 DT =  0.27055047E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     0 seconds
 TIME =  0.10819477E-01 DT =  0.54110094E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     0 seconds
 TIME =  0.21641495E-01 DT =  0.10822019E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     0 seconds
 TIME =  0.43285533E-01 DT =  0.21644037E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992484  FE = .73306801121929
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     0 seconds
 TIME =  0.86573608E-01 DT =  0.43288075E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882251
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     0 seconds
 TIME =  0.17314976     DT =  0.86576150E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992484  FE = .733068011219291
                        NI = .0754116207882252
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     0 seconds
 TIME =  0.34630206     DT =  0.17315230     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992488  FE = .733068011219287
                        NI = .0754116207882243
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     0 seconds
 TIME =  0.69260666     DT =  0.34630460     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992494  FE = .733068011219281
                        NI = .075411620788225
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     0 seconds
```

```
 TIME =   1.3852159     DT =  0.69260920     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992487  FE = .733068011219286
                        NI = .0754116207882269
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   2.7704343     DT =   1.3852184     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992471  FE = .733068011219294
                        NI = .0754116207882344
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    1 seconds
 TIME =   5.5408711     DT =   2.7704368     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992456  FE = .733068011219275
                        NI = .0754116207882687
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds


output ignored...



... output resumed

 1.178683541278132E-007        4.704511878359503E-009        3.755110863092210E-009        1.341357104051518E-009        6.780132389577251E-
015        2.989954254900958E-022       TIME =   192.47835     DT =  0.65536000     SUM OF SQUARES =  0.29899543E-21
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.34384332E-07 AND  -0.34384332E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.10512416E-04
 U-FRACTION IN SYSTEM:  CR = .190992128498277  FE = .733624291531083
                        NI = .0753835799706397
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_BCC_A2

  CPU time used in timestep                    4 seconds
 1.271365426222436E-007        1.271989335102665E-007        1.266831333054001E-007        6.715506164339864E-009        5.045844107752260E-
009        2.173897834074366E-009        2.876815352929668E-014        1.038835603228296E-
021       TIME =   193.78907     DT =   1.3107200     SUM OF SQUARES =  0.10388356E-20
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.21224624E-07 AND  -0.21224624E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.10484596E-04
 U-FRACTION IN SYSTEM:  CR = .190992128498074  FE = .733624291531176
                        NI = .0753835799707495
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    3 seconds
 3.673210049787387E-007        3.674203703752205E-007        3.675318455428832E-007        3.422589288687639E-007        3.255311631553288E-
007        2.925075638432603E-007        2.213556831676775E-007        1.125494987610828E-007        1.124791498527678E-
007        3.566343320486406E-009        3.705425989486089E-015        2.253380739898060E-
021       TIME =   196.41051     DT =   2.6214400     SUM OF SQUARES =  0.22533807E-20
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.52820720E-08 AND  -0.52820720E-08
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.10470749E-04
 U-FRACTION IN SYSTEM:  CR = .190992128497841  FE = .733624291531233
                        NI = .0753835799709257
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_BCC_A2

  CPU time used in timestep                    5 seconds
 3.343030111943605E-007        3.343267664895591E-007        3.345156670354546E-007        3.083838877172732E-007        3.032561260821073E-
007        2.931076847460899E-007        2.724485295492416E-007        2.724321055496794E-007        2.340726369525630E-
007        1.654004358274386E-007        6.423404147486290E-008        4.322151027641044E-013        2.030617452674526E-
018       TIME =   200.00000     DT =   3.5894934     SUM OF SQUARES =  0.20306175E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.93527420E-08 AND   0.93527420E-08
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.10504321E-04
 U-FRACTION IN SYSTEM:  CR = .190992128501964  FE = .73362429153093
                        NI = .0753835799671059
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 MUST SAVE WORKSPACE ON FILE
 WORKSPACE SAVED ON FILE
 RECLAIMING WORKSPACE
 DELETING TIME-RECORD FOR TIME    183.93246
 DELETING TIME-RECORD FOR TIME    191.16764
 DELETING TIME-RECORD FOR TIME    191.16765
 DELETING TIME-RECORD FOR TIME    191.16767
 DELETING TIME-RECORD FOR TIME    191.16771
 DELETING TIME-RECORD FOR TIME    191.16779
 DELETING TIME-RECORD FOR TIME    191.16795
 DELETING TIME-RECORD FOR TIME    191.16827
 DELETING TIME-RECORD FOR TIME    191.16891
 DELETING TIME-RECORD FOR TIME    191.17019
 DELETING TIME-RECORD FOR TIME    191.17275
 DELETING TIME-RECORD FOR TIME    191.17787
 DELETING TIME-RECORD FOR TIME    191.18811
 DELETING TIME-RECORD FOR TIME    191.20859
 DELETING TIME-RECORD FOR TIME    191.24955
 DELETING TIME-RECORD FOR TIME    191.33147
 DELETING TIME-RECORD FOR TIME    191.49531
 DELETING TIME-RECORD FOR TIME    191.82299
 DELETING TIME-RECORD FOR TIME    192.47835
 DELETING TIME-RECORD FOR TIME    193.78907

 KEEPING TIME-RECORD FOR TIME    196.41051
 AND FOR TIME                    200.00000
 WORKSPACE RECLAIMED

 TIMESTEP AT     200.000000     SELECTED

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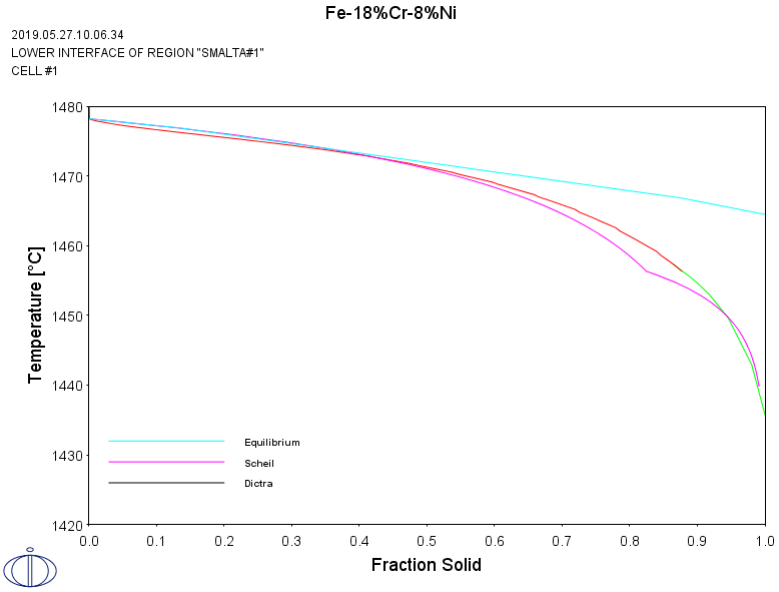

exb4b-plot

```
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:
```

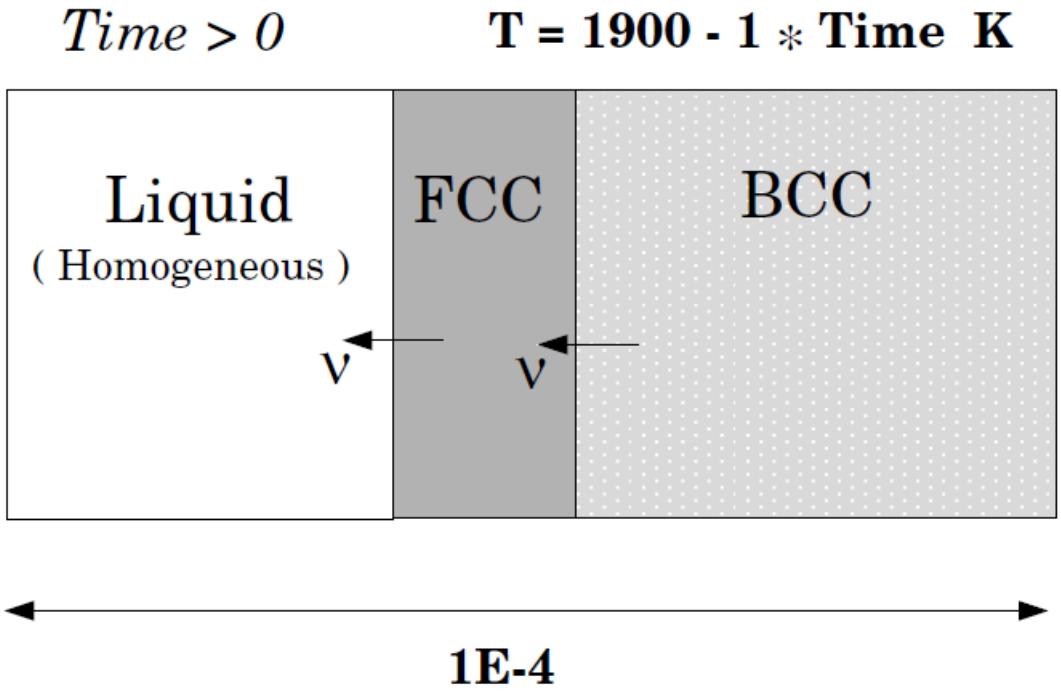



```
POST-1:
POST-1:
POST-1:
POST-1: --OK---
POST-1:
```

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 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri May 24 17:06:15 2019


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  v9.1

 VA                      /-  DEFINED
 L12_FCC                 B2_BCC                  DICTRA_FCC_A1
   REJECTED
TDB_TCFE9:
TDB_TCFE9:TDB_TCFE9:TDB_TCFE9:
TDB_TCFE9:TDB_TCFE9: FE                      NI                      CR
   DEFINED
TDB_TCFE9:
TDB_TCFE9:TDB_TCFE9: LIQUID:L                BCC_A2                  FCC_A1
 HCP_A3                  CBCC_A12                CUB_A13
 SIGMA                   CHI_A12                 LAVES_PHASE_C14
 CR3SI                   NBNI3                   NI3TI
 CRZN17                  BETA1                   GAMMA
 AL5FE4                  FLUORITE_C1:I           ZRO2_TETR:I
 M2O3C:I                 CENI2                   CENI5
   REJECTED
TDB_TCFE9: FCC_A1                  LIQUID:L                BCC_A2
   RESTORED
TDB_TCFE9:
TDB_TCFE9:TDB_TCFE9: 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, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  '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'
  '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'
  '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_TCFE9:
TDB_TCFE9:TDB_TCFE9:TDB_TCFE9:TDB_TCFE9:TDB_TCFE9: Use one of these databases

 TCFE9   =  Steels/Fe-Alloys  v9.1
 TCFE8   =  Steels/Fe-Alloys  v8.1
 FROST1  =  FROST database v1.0
 TCFE7   =  Steels/Fe-Alloys  v7.0
 TCFE6   =  Steels/Fe-Alloys  v6.2
 TCFE5   =  Steels/Fe-Alloys  v5.0
 TCFE4   =  Steels/Fe-Alloys  v4.1
 TCFE3   =  Steels/Fe-Alloys  v3.1
 TCFE2   =  Steels/Fe-Alloys  v2.1
 TCFE1   =  Steels/Fe-Alloys  v1.0
 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  v2.1
 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
 TCSLD1  =  Solder Alloys  v1.1
 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
 TCNF2   =  Nuclear Fuels  v2.1b
 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 v2.1
 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  v1.0
 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 /TCFE9/: Current database: Steels/Fe-Alloys Mobility  v4.0

 VA  DEFINED
 B2_BCC  REJECTED
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'
  'No assessed or estimated parameters'
  'Estimation by using the modified Sutherland equation from Chen et al.,
      Phil. Magazine 94 (2014) 1552.'
  'L. Zhang et al., Acta Mater., 58(2010)3664.'
 -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>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/: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 /AUTO/:VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -> 1): /AUTO/:
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/:DIC>DIC>DIC>DIC>
DIC> --OK---
DIC>
```

exb4c-run

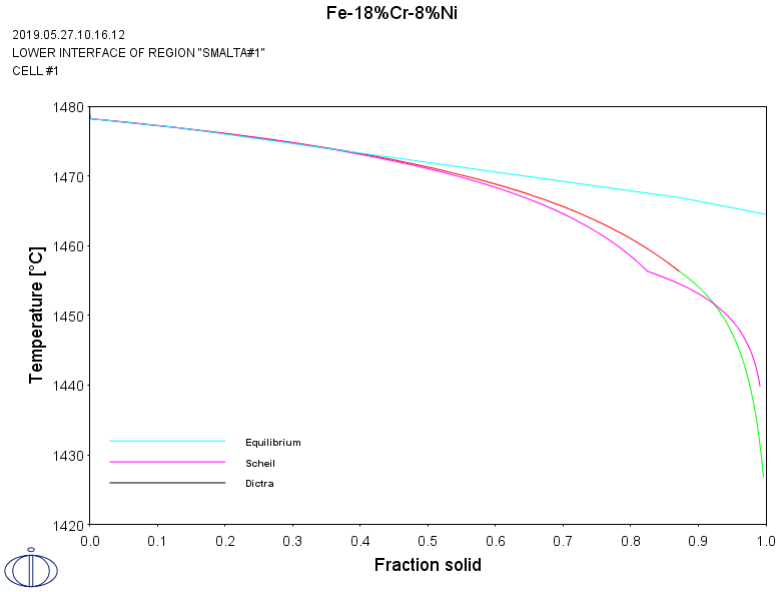
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb4c\run.DCM.test"DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  0.00000E+00
DIC> OK
DIC>
DIC>DIC>DIC>DIC> Region: SMALTA
 single geometric dense at  0.10000E-03
 0.99375       62
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.10773101E-05 DT =  0.97731005E-06 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.30319302E-05 DT =  0.19546201E-05 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.69411704E-05 DT =  0.39092402E-05 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.14759651E-04 DT =  0.78184804E-05 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.30396612E-04 DT =  0.15636961E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.61670533E-04 DT =  0.31273922E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.12421838E-03 DT =  0.62547843E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.24931406E-03 DT =  0.12509569E-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 =  0.49950544E-03 DT =  0.25019137E-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                    1 seconds
 TIME =  0.99988818E-03 DT =  0.50038275E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882253
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.20006537E-02 DT =  0.10007655E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992481  FE = .733068011219294
                        NI = .075411620788225
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.40021847E-02 DT =  0.20015310E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992481  FE = .733068011219294
                        NI = .0754116207882257
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.80052466E-02 DT =  0.40030620E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992479  FE = .733068011219298
                        NI = .0754116207882228
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.16011371E-01 DT =  0.80061239E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992485  FE = .733068011219294
                        NI = .0754116207882214
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.32023618E-01 DT =  0.16012248E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .19152036799249  FE = .733068011219294
                        NI = .0754116207882161
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.64048114E-01 DT =  0.32024496E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992458  FE = .733068011219322
                        NI = .0754116207882198
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.12809711     DT =  0.64048992E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992392  FE = .733068011219407
                        NI = .0754116207882005
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.25619509     DT =  0.12809798     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992345  FE = .733068011219476
                        NI = .0754116207881789
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.51239106     DT =  0.25619597     SUM OF SQUARES =   0.0000000
```

```
 U-FRACTION IN SYSTEM:  CR = .191520367992127  FE = .73306801121947
                        NI = .0754116207884034
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   1.0247830     DT =  0.51239193     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367991479  FE = .73306801122011
                        NI = .0754116207884109
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   2.0247830     DT =   1.0000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367991638  FE = .733068011220196
                        NI = .0754116207881664
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3.0247830     DT =   1.0000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992696  FE = .733068011219081
                        NI = .0754116207882234


output ignored...



... output resumed

 1.694028573359317E-008        3.196543659653224E-009        6.109706428520357E-010        7.797181209086220E-011        1.037668585874810E-
015        5.231822829018067E-016        4.775078455426878E-014        2.579805602936135E-
017       TIME =   199.16001     DT =   1.0000000     SUM OF SQUARES =  0.25798056E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.10042421E-06 AND  -0.10042421E-06
 POSITION OF INTERFACE SMALTA / R_FCC_A1 IS   0.46634213E-06
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.11494119E-07 AND   0.11494119E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.10974305E-04
 U-FRACTION IN SYSTEM:  CR = .191209954446287  FE = .733434883331625
                        NI = .0753551622220873
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  33  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_FCC_A1

  CPU time used in timestep                    6 seconds
 3.726512315235355E-007        3.732097664350338E-007        3.726469226177302E-007        3.726004474515367E-007        3.725375737783300E-
007        2.041286376157335E-008        8.863543709432126E-010        1.769072436724717E-014        6.439442632791217E-
016        4.656904871562189E-014        3.070523271225321E-
016       TIME =   200.00000     DT =  0.83999467     SUM OF SQUARES =  0.30705233E-15
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.85594800E-07 AND  -0.85594800E-07
 POSITION OF INTERFACE SMALTA / R_FCC_A1 IS   0.39444295E-06
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.13575622E-07 AND   0.13575622E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.10985708E-04
 U-FRACTION IN SYSTEM:  CR = .191209946406188  FE = .733434891115933
                        NI = .0753551624778788
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 MUST SAVE WORKSPACE ON FILE
 WORKSPACE SAVED ON FILE
 RECLAIMING WORKSPACE
 DELETING TIME-RECORD FOR TIME    170.32213
 DELETING TIME-RECORD FOR TIME    170.48228
 DELETING TIME-RECORD FOR TIME    170.48228
 DELETING TIME-RECORD FOR TIME    170.48228
 DELETING TIME-RECORD FOR TIME    170.48228
 DELETING TIME-RECORD FOR TIME    170.48229
 DELETING TIME-RECORD FOR TIME    170.48229
 DELETING TIME-RECORD FOR TIME    170.48229
 DELETING TIME-RECORD FOR TIME    170.48230
 DELETING TIME-RECORD FOR TIME    170.48231
 DELETING TIME-RECORD FOR TIME    170.48233
 DELETING TIME-RECORD FOR TIME    170.48239
 DELETING TIME-RECORD FOR TIME    170.48249
 DELETING TIME-RECORD FOR TIME    170.48269
 DELETING TIME-RECORD FOR TIME    170.48310
 DELETING TIME-RECORD FOR TIME    170.48392
 DELETING TIME-RECORD FOR TIME    170.48556
 DELETING TIME-RECORD FOR TIME    170.48884
 DELETING TIME-RECORD FOR TIME    170.49539
 DELETING TIME-RECORD FOR TIME    170.50850
 DELETING TIME-RECORD FOR TIME    170.53471
 DELETING TIME-RECORD FOR TIME    170.58714
 DELETING TIME-RECORD FOR TIME    170.69200
 DELETING TIME-RECORD FOR TIME    170.90171
 DELETING TIME-RECORD FOR TIME    171.32114
 DELETING TIME-RECORD FOR TIME    172.16001
 DELETING TIME-RECORD FOR TIME    173.16001
 DELETING TIME-RECORD FOR TIME    174.16001
 DELETING TIME-RECORD FOR TIME    175.16001
 DELETING TIME-RECORD FOR TIME    176.16001
 DELETING TIME-RECORD FOR TIME    177.16001
 DELETING TIME-RECORD FOR TIME    178.16001
 DELETING TIME-RECORD FOR TIME    179.16001
 DELETING TIME-RECORD FOR TIME    180.16001
 DELETING TIME-RECORD FOR TIME    181.16001
 DELETING TIME-RECORD FOR TIME    182.16001
 DELETING TIME-RECORD FOR TIME    183.16001
 DELETING TIME-RECORD FOR TIME    184.16001
 DELETING TIME-RECORD FOR TIME    185.16001
 DELETING TIME-RECORD FOR TIME    186.16001
 DELETING TIME-RECORD FOR TIME    187.16001
 DELETING TIME-RECORD FOR TIME    188.16001
 DELETING TIME-RECORD FOR TIME    189.16001
 DELETING TIME-RECORD FOR TIME    190.16001
 DELETING TIME-RECORD FOR TIME    191.16001
 DELETING TIME-RECORD FOR TIME    192.16001
 DELETING TIME-RECORD FOR TIME    193.16001
 DELETING TIME-RECORD FOR TIME    194.16001
 DELETING TIME-RECORD FOR TIME    195.16001
 DELETING TIME-RECORD FOR TIME    196.16001
 DELETING TIME-RECORD FOR TIME    197.16001
 DELETING TIME-RECORD FOR TIME    198.16001

 KEEPING TIME-RECORD FOR TIME    199.16001
 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>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:
```

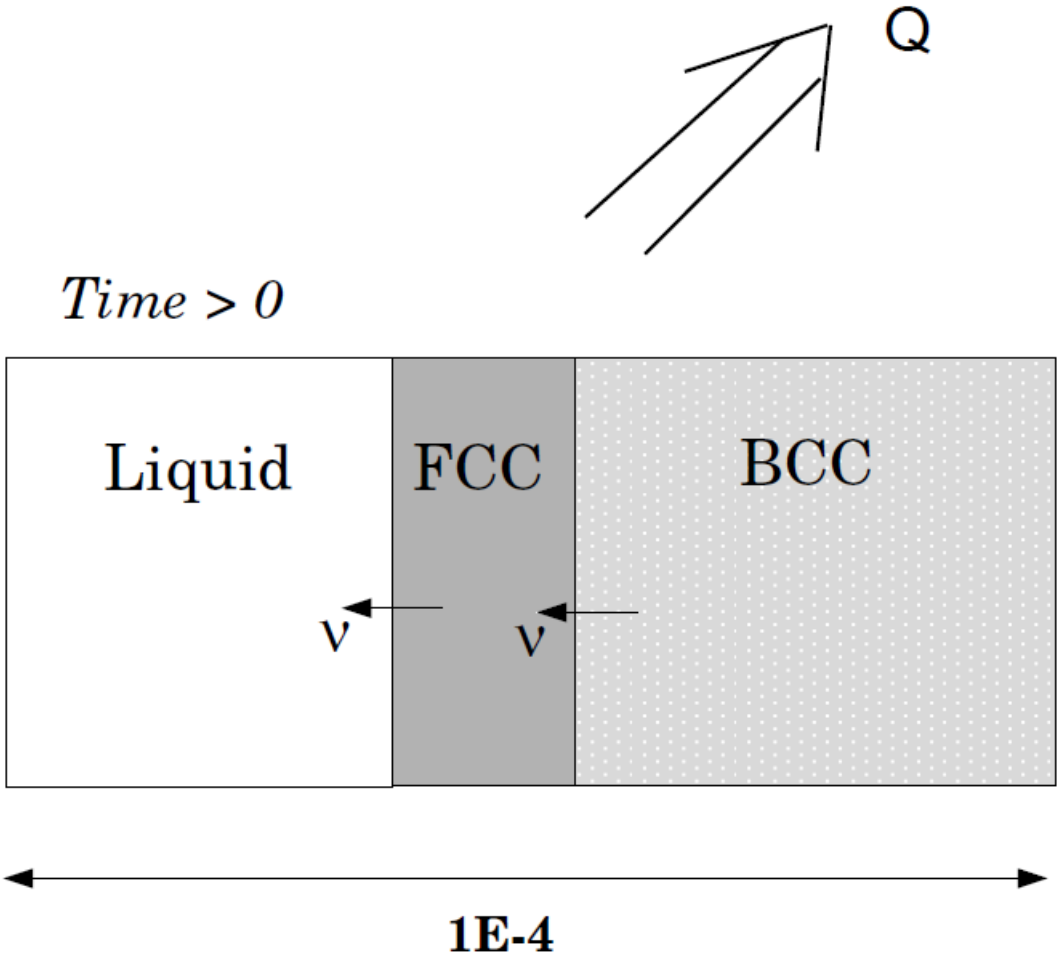



```
POST-1:
POST-1:
POST-1:
POST-1: --OK---
POST-1:
```

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 Software  (build 20130) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri May 24 17:06:15 2019


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  v9.1

 VA                      /-  DEFINED
 L12_FCC                 B2_BCC                  DICTRA_FCC_A1
   REJECTED
TDB_TCFE9:
TDB_TCFE9:TDB_TCFE9: Current database: Iron Demo Database v2.1

 VA                      /-  DEFINED
TDB_FEDEMO:
TDB_FEDEMO:TDB_FEDEMO: FE                      NI                      CR
   DEFINED
TDB_FEDEMO:
TDB_FEDEMO:TDB_FEDEMO: LIQUID:L                BCC_A2                  CBCC_A12
 CHI_A12                 CUB_A13                 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, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  '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'
  '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  v9.1
 TCFE8   =  Steels/Fe-Alloys  v8.1
 FROST1  =  FROST database v1.0
 TCFE7   =  Steels/Fe-Alloys  v7.0
 TCFE6   =  Steels/Fe-Alloys  v6.2
 TCFE5   =  Steels/Fe-Alloys  v5.0
 TCFE4   =  Steels/Fe-Alloys  v4.1
 TCFE3   =  Steels/Fe-Alloys  v3.1
 TCFE2   =  Steels/Fe-Alloys  v2.1
 TCFE1   =  Steels/Fe-Alloys  v1.0
 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  v2.1
 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
 TCSLD1  =  Solder Alloys  v1.1
 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
 TCNF2   =  Nuclear Fuels  v2.1b
 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 v2.1
 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  v1.0
 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/: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 /AUTO/:VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -> 1): /AUTO/:
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/:DIC>DIC>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
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
 TEMPERATURE:   1900.     ENTHALPY:  0.7394E+05
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882254
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 TEMPERATURE:   1900.     ENTHALPY:  0.7394E+05
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882254
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 3.863918610051234E-007        3.864691456616007E-007        3.837208091757153E-016        3.821106605297053E-025       TIME =  0.10000000E-
06 DT =  0.10000000E-06 SUM OF SQUARES =  0.38211066E-24
 TEMPERATURE:   1900.     ENTHALPY:  0.7394E+05
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882254
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 9.508205000173971E-018       TIME =  0.26002472E-05 DT =  0.25002472E-05 SUM OF SQUARES =  0.95082050E-17
 TEMPERATURE:   1900.     ENTHALPY:  0.7394E+05
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 3.803283213789877E-017       TIME =  0.76007416E-05 DT =  0.50004944E-05 SUM OF SQUARES =  0.38032832E-16
 TEMPERATURE:   1900.     ENTHALPY:  0.7394E+05
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882254
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 1.521313188418321E-016        1.521313188418321E-016


     ERROR RETURN FROM NS01A BECAUSE A NEARBY STATIONARY POINT OF F(X) IS PREDICTED
 *** ERROR  1890 IN DCNS01: ERROR RETURN FROM NS01A
 1.521313188418321E-016        1.521313188418321E-016        1.521313188418321E-016        9.309554162466689E-020        1.431856013280617E-
016        3.399417495083793E-017        3.399417495083793E-017        1.089145661025413E-019        1.089145661025413E-
019        1.089145661025413E-019        1.089145661025413E-019        2.673309085540699E-017        1.089153455095704E-
019        1.089153455095704E-019        1.089153455095704E-019        1.089153455095704E-019        1.092199812185641E-
018        1.089145661025413E-019       TIME =  0.17601730E-04 DT =  0.10000989E-04 SUM OF SQUARES =  0.10891457E-18
 TEMPERATURE:   1900.     ENTHALPY:  0.7394E+05
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882254
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 1.666578045201216E-016        1.666578045201216E-016


     ERROR RETURN FROM NS01A BECAUSE A NEARBY STATIONARY POINT OF F(X) IS PREDICTED
 *** ERROR  1890 IN DCNS01: ERROR RETURN FROM NS01A
 1.666578045201216E-016        1.666578045201216E-016        1.666578045201216E-016        1.352478211635110E-012        1.666578045201216E-
016        7.573827019817665E-030        7.573827019817665E-030        7.573827019817665E-030        7.573827019817665E-
030        1.666578045201216E-016        5.562266575976920E-030        5.562266575976920E-030        5.562266575976920E-
030        5.562266575976920E-030        5.562266575976920E-030        5.562266575976920E-030        1.041609024951602E-
017        1.546768164561797E-029       TIME =  0.37603708E-04 DT =  0.20001978E-04 SUM OF SQUARES =  0.15467682E-28
 TEMPERATURE:   1900.     ENTHALPY:  0.7394E+05
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882254
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 6.085250191563469E-016        6.085250191563469E-016


     ERROR RETURN FROM NS01A BECAUSE A NEARBY STATIONARY POINT OF F(X) IS PREDICTED
 *** ERROR  1890 IN DCNS01: ERROR RETURN FROM NS01A
 6.085250191563469E-016        6.085250191563469E-016        6.085250191563469E-016        5.964157854575773E-012

output ignored...



... output resumed

 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.53060193E-05
 TEMPERATURE:   1703.     ENTHALPY:  0.5591E+05
 U-FRACTION IN SYSTEM:  CR = .191426492569575  FE = .733178490650271
                        NI = .0753950167801536
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  6  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_FCC_A1

  CPU time used in timestep                    2 seconds
 1.010611839641213E-007        1.010624112174118E-007        1.010620821966687E-007        1.010407815978725E-007        7.802524850104379E-
009        1.010731516713628E-013        8.491417896581680E-
019       TIME =   197.90144     DT =  0.39375000     SUM OF SQUARES =  0.84914179E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.80357395E-07 AND   0.80357395E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.53376600E-05
 TEMPERATURE:   1702.     ENTHALPY:  0.5587E+05
 U-FRACTION IN SYSTEM:  CR = .19142649256958  FE = .73317849065027
                        NI = .0753950167801494
 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
 5.895191095916032E-007        5.896964303258992E-007        5.902402434406712E-007        5.893737193956263E-007        3.967197178262157E-
007        3.583238933502586E-007        2.901878750191593E-007        2.902122464542427E-007        1.672868017032316E-
007        2.285303868088257E-008        1.345973070721034E-014        6.746593624445023E-
018       TIME =   198.68894     DT =  0.78750000     SUM OF SQUARES =  0.67465936E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.89888651E-07 AND   0.89888651E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.54084473E-05
 TEMPERATURE:   1701.     ENTHALPY:  0.5580E+05
 U-FRACTION IN SYSTEM:  CR = .191426492569597  FE = .733178490650262
                        NI = .0753950167801402
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  26  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_FCC_A1
```

```
  CPU time used in timestep                     3 seconds
 8.992409962562088E-007        8.994672649685910E-007        8.996875978409963E-007        8.989207433122699E-007        7.697281922093334E-
007        6.537207438099848E-007        4.667435970066353E-007        2.098699516454861E-007        9.143767266206913E-
010        4.126082883297032E-014        2.694991653038810E-
019       TIME =   200.00000     DT =   1.3110643     SUM OF SQUARES =  0.26949917E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.10133317E-06 AND   0.10133317E-06
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.55413016E-05
 TEMPERATURE:   1698.     ENTHALPY:  0.5568E+05
 U-FRACTION IN SYSTEM:  CR = .191426492569644  FE = .733178490650235
                        NI = .0753950167801214
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 MUST SAVE WORKSPACE ON FILE
 WORKSPACE SAVED ON FILE
 RECLAIMING WORKSPACE
 DELETING TIME-RECORD FOR TIME    196.67097
 DELETING TIME-RECORD FOR TIME    197.16315
 DELETING TIME-RECORD FOR TIME    197.21237
 DELETING TIME-RECORD FOR TIME    197.31081
 DELETING TIME-RECORD FOR TIME    197.50769
 DELETING TIME-RECORD FOR TIME    197.90144

 KEEPING TIME-RECORD FOR TIME    198.68894
 AND FOR TIME                    200.00000
 WORKSPACE RECLAIMED

 TIMESTEP AT     200.000000     SELECTED

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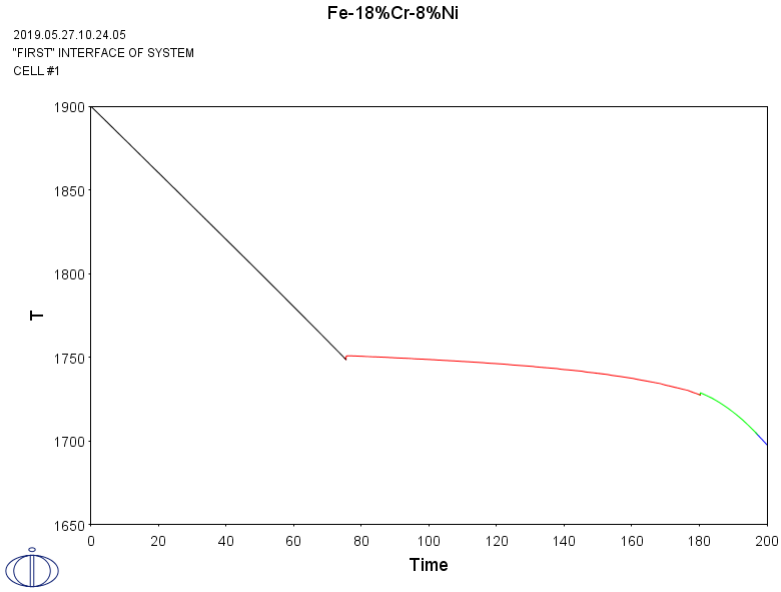
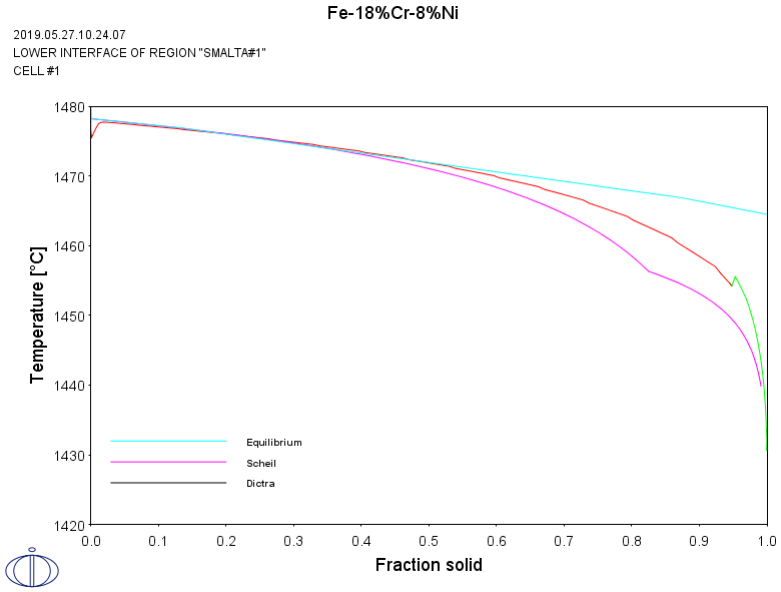

exb4d-plot

```
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:
```

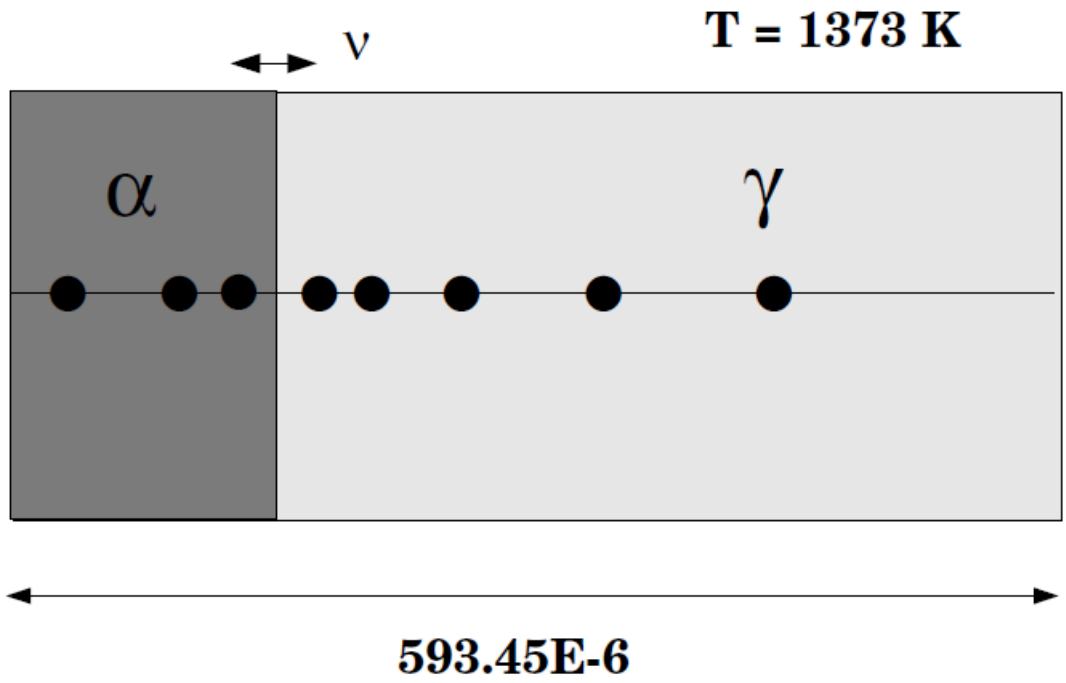



```
POST-1:
POST-1:
POST-1:
POST-1: --OK---
POST-1:
```

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
 Software  (build 20130) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri May 24 17:06:15 2019


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  v9.1

 VA                      /-  DEFINED
 L12_FCC                 B2_BCC                  DICTRA_FCC_A1
   REJECTED
TDB_TCFE9: Current database: Iron Demo Database v2.1

 VA                      /-  DEFINED
TDB_FEDEMO: CR                      FE                      NI
   DEFINED
TDB_FEDEMO: LIQUID:L                BCC_A2                  CBCC_A12
 CHI_A12                 CUB_A13                 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, 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  v9.1
 TCFE8   =  Steels/Fe-Alloys  v8.1
 FROST1  =  FROST database v1.0
 TCFE7   =  Steels/Fe-Alloys  v7.0
 TCFE6   =  Steels/Fe-Alloys  v6.2
 TCFE5   =  Steels/Fe-Alloys  v5.0
 TCFE4   =  Steels/Fe-Alloys  v4.1
 TCFE3   =  Steels/Fe-Alloys  v3.1
 TCFE2   =  Steels/Fe-Alloys  v2.1
 TCFE1   =  Steels/Fe-Alloys  v1.0
 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  v2.1
 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
 TCSLD1  =  Solder Alloys  v1.1
 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
 TCNF2   =  Nuclear Fuels  v2.1b
 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 v2.1
 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  v1.0
 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>
```

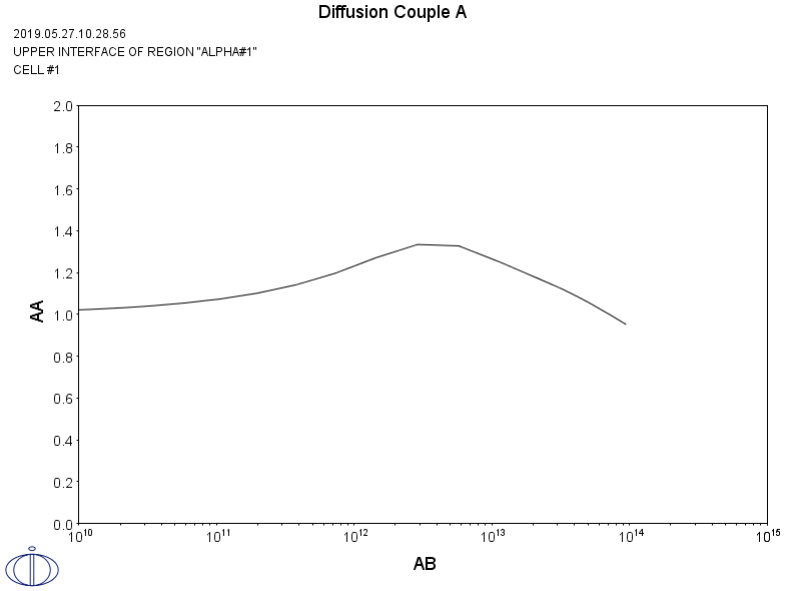
exb5-run

```
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
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
  Trying old scheme                      4
 GENERATING STARTING VALUES FOR CELL #  1 INTERFACE #  2
 DETERMINING INITIAL EQUILIBRIUM VALUES
CALCULATING STARTING VALUES:       9   EQUILIBRIUM CALCULATIONS              *** ERROR  1611 IN QTHISS: TOO MANY ITERATIONS
 Give the command INFO TROUBLE for help
 *** ERROR  1611 IN QTHISS: TOO MANY ITERATIONS
 Give the command INFO TROUBLE for help
 *** ERROR  1611 IN QTHISS: TOO MANY ITERATIONS
 Give the command INFO TROUBLE for help
 DONE     6 OUT OF     9                                                  *** ERROR  1611 IN QTHISS: TOO MANY ITERATIONS
 Give the command INFO TROUBLE for help
 DONE     9 OUT OF     9                                                   try                      2 failed
  try                     3 failed
 DETERMINED ACTIVITIES  ACR(CR) .00275331206673
  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 = .471672082221691
                        NI = .223047485172707
 TOTAL SIZE OF SYSTEM:  5.9345E-04 [m]
 U-FRACTION IN SYSTEM:  CR = .305280432605602  FE = .471672082221691
                        NI = .223047485172707
 TOTAL SIZE OF SYSTEM:  5.9345E-04 [m]
 3.503057562900817E-002        3.503838978395275E-002        3.503070722839279E-002        6.010860846145185E-004        4.996128425546665E-
004        3.843191313070322E-004        2.950449855122880E-004        2.951823956353321E-004        1.282247749685380E-
004        1.515620221804833E-007        2.085128797718068E-009        5.173774480689324E-011        2.514478009075518E-
015        1.078927792050986E-021       TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =  0.10789278E-20
 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 = .223047485341283
 TOTAL SIZE OF SYSTEM:  5.9345E-04 [m]
  26  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: GAMMA

  CPU time used in timestep                     0 seconds
 9.795982825150397E-004        9.797942119370796E-004        9.795987025833710E-004        1.691287126051857E-012        1.336248771807599E-
012        1.296755529211569E-012        1.534999419619486E-012        6.680078205928093E-012        1.211461420685886E-
012        1.208868070220405E-012        1.209218315171875E-012        6.030069838939564E-012        1.204231845954798E-
012        1.202965677883595E-012        1.202807783963411E-012        5.949304410916472E-012        1.202017618606175E-
012        1.201382013720620E-012        1.200629577952038E-012        5.941375547684007E-012        1.199444130951661E-
012        1.197808656202245E-012        1.194411628032861E-012        5.934987281418810E-012        1.188089667415139E-
012        1.175555714094726E-012        1.150437674811740E-012        5.896774062071241E-012        1.102521100096510E-
012        1.012597446905937E-012        8.579124497874131E-013        5.661501504663754E-012        6.016827183657962E-
013        2.433117474811453E-013        1.958377660725463E-014        1.188058497609407E-016       TIME =  0.93355784E-05 DT =  0.92355784E-
05 SUM OF SQUARES =  0.11880585E-15
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.96601180E-05 AND  -0.96601180E-05
 POSITION OF INTERFACE ALPHA / GAMMA IS   0.93465912E-04
 U-FRACTION IN SYSTEM:  CR = .305280432538621  FE = .471672082119084
                        NI = .223047485342295


output ignored...



... output resumed

 5.057252431035297E-009        5.864938687676862E-012        5.504765018181519E-
018       TIME =   2202041.6     DT =   360000.00     SUM OF SQUARES =  0.55047650E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.76089418E-11 AND  -0.76089418E-11
 POSITION OF INTERFACE ALPHA / GAMMA IS   0.95399174E-04
 U-FRACTION IN SYSTEM:  CR = .305280444995874  FE = .471672025910032
                        NI = .223047529094094
 TOTAL SIZE OF SYSTEM:  5.9345E-04 [m]
  7  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: GAMMA

  CPU time used in timestep                     2 seconds
 1.857872772892910E-006        1.860685946350317E-006        1.853239470958732E-006        1.313521846476596E-008        2.825212442383770E-
009        2.753722629056451E-013        5.635284249403554E-
022       TIME =   2562041.6     DT =   360000.00     SUM OF SQUARES =  0.56352842E-21
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.64450403E-11 AND  -0.64450403E-11
 POSITION OF INTERFACE ALPHA / GAMMA IS   0.93078959E-04
 U-FRACTION IN SYSTEM:  CR = .305280445367592  FE = .471672025255687
                        NI = .223047529376722
 TOTAL SIZE OF SYSTEM:  5.9345E-04 [m]
  6  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: GAMMA

  CPU time used in timestep                     3 seconds
 6.448261655697590E-007        6.462435261241559E-007        6.421271632466963E-007        3.404518882331418E-009        6.601888936953931E-
010        3.274513866542853E-015        4.474350280788337E-
023       TIME =   2922041.6     DT =   360000.00     SUM OF SQUARES =  0.44743503E-22
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.58181863E-11 AND  -0.58181863E-11
 POSITION OF INTERFACE ALPHA / GAMMA IS   0.90984412E-04
 U-FRACTION IN SYSTEM:  CR = .305280445545083  FE = .471672025175201
                        NI = .223047529279716
 TOTAL SIZE OF SYSTEM:  5.9345E-04 [m]
  7  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: GAMMA

  CPU time used in timestep                     1 seconds
 3.680530268672295E-007        3.690257870320974E-007        3.660388302394790E-007        1.727327924432970E-009        3.141740127240897E-
010        1.470103456116198E-015        2.833164993243139E-
024       TIME =   3282041.6     DT =   360000.00     SUM OF SQUARES =  0.28331650E-23
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.53569666E-11 AND  -0.53569666E-11
 POSITION OF INTERFACE ALPHA / GAMMA IS   0.89055904E-04
```

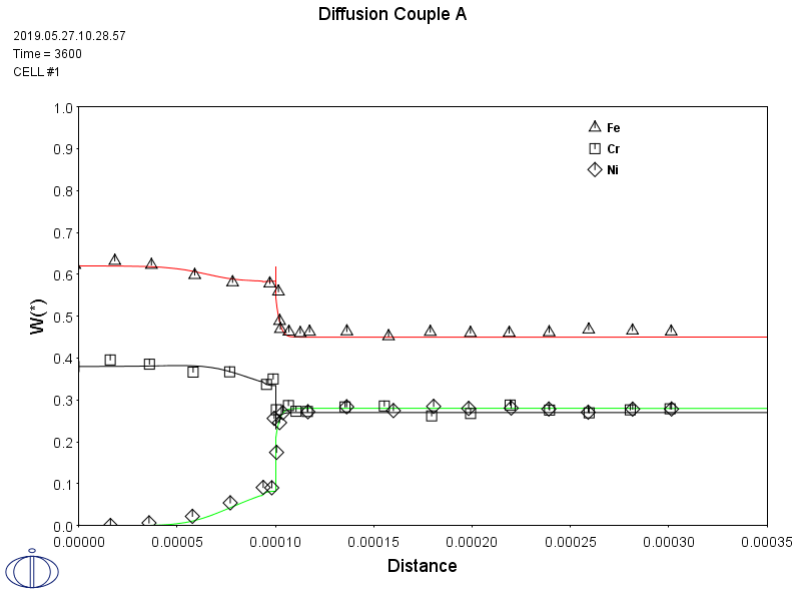
```
 U-FRACTION IN SYSTEM:  CR = .305280446124665  FE = .471672023490968
                        NI = .223047530384366
 TOTAL SIZE OF SYSTEM:  5.9345E-04 [m]
  5  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: GAMMA

  CPU time used in timestep                     2 seconds
 4.272489187836004E-009        4.275024601831475E-009        4.291374343272308E-009        1.879214533709638E-009        8.596279296766209E-
010        4.292646295769693E-016        1.004997860884815E-
024       TIME =   3600000.0     DT =   317958.45     SUM OF SQUARES =  0.10049979E-23
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.49338793E-11 AND  -0.49338793E-11
 POSITION OF INTERFACE ALPHA / GAMMA IS   0.87487135E-04
 U-FRACTION IN SYSTEM:  CR = .305280446376896  FE = .471672022862325
                        NI = .223047530760779
 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    13.853758
 DELETING TIME-RECORD FOR TIME    21.171707
 DELETING TIME-RECORD FOR TIME    35.807604
 DELETING TIME-RECORD FOR TIME    65.079398
 DELETING TIME-RECORD FOR TIME    89.577434
 DELETING TIME-RECORD FOR TIME    138.57351
 DELETING TIME-RECORD FOR TIME    236.56565
 DELETING TIME-RECORD FOR TIME    319.77956
 DELETING TIME-RECORD FOR TIME    486.20738
 DELETING TIME-RECORD FOR TIME    761.28390
 DELETING TIME-RECORD FOR TIME    1232.2085
 DELETING TIME-RECORD FOR TIME    2093.8909
 DELETING TIME-RECORD FOR TIME    3662.3131
 DELETING TIME-RECORD FOR TIME    6799.1575
 DELETING TIME-RECORD FOR TIME    13072.846
 DELETING TIME-RECORD FOR TIME    25620.224
 DELETING TIME-RECORD FOR TIME    50714.979
 DELETING TIME-RECORD FOR TIME    100904.49
 DELETING TIME-RECORD FOR TIME    201283.51
 DELETING TIME-RECORD FOR TIME    402041.55
 DELETING TIME-RECORD FOR TIME    762041.55
 DELETING TIME-RECORD FOR TIME    1122041.6
 DELETING TIME-RECORD FOR TIME    1482041.6
 DELETING TIME-RECORD FOR TIME    1842041.6
 DELETING TIME-RECORD FOR TIME    2202041.6
 DELETING TIME-RECORD FOR TIME    2562041.6
 DELETING TIME-RECORD FOR TIME    2922041.6

 KEEPING TIME-RECORD FOR TIME    3282041.6
 AND FOR TIME                    3600000.0
 WORKSPACE RECLAIMED

 TIMESTEP AT     3600000.00     SELECTED

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

exb5-plot

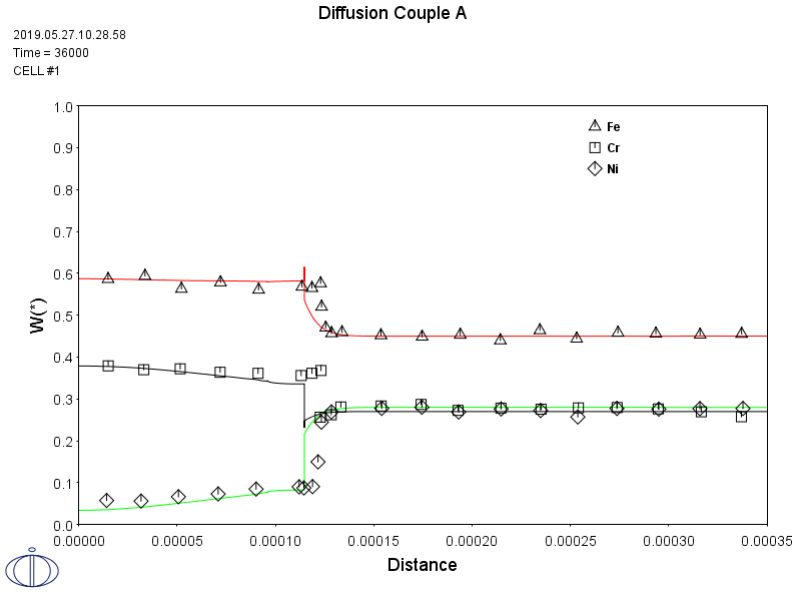
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb5\plot.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  3.60000E+06
DIC> OK
DIC>
DIC>DIC>DIC>DIC>  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1: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



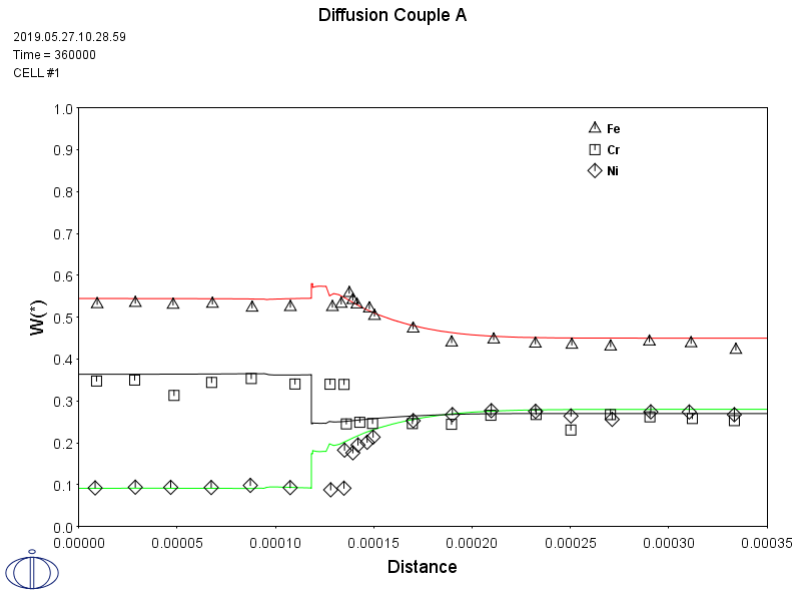

```
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1:POST-1:POST-1:POST-1:  INFO: Distance is set as independent variable
POST-1:POST-1:POST-1:
POST-1:POST-1:POST-1:
POST-1:POST-1:
POST-1:POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```



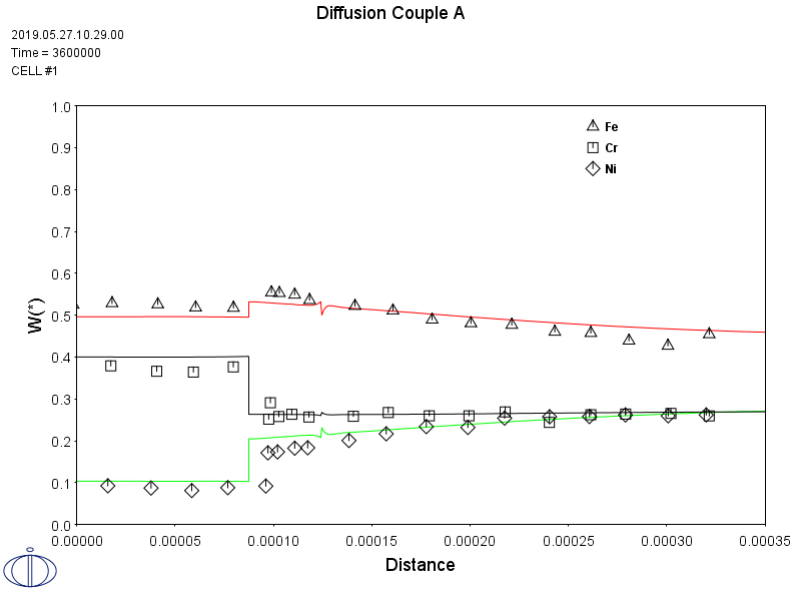

```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1:POST-1:POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```



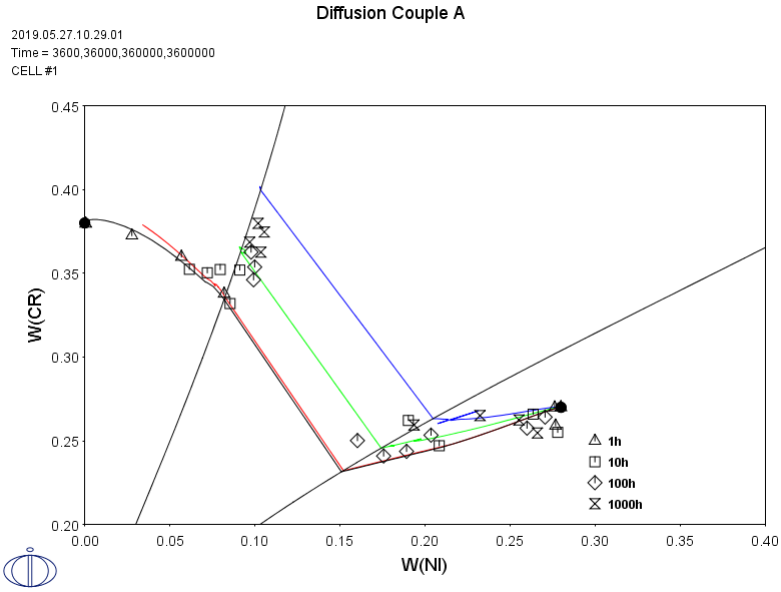

```
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1:POST-1:POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```




```
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:
```

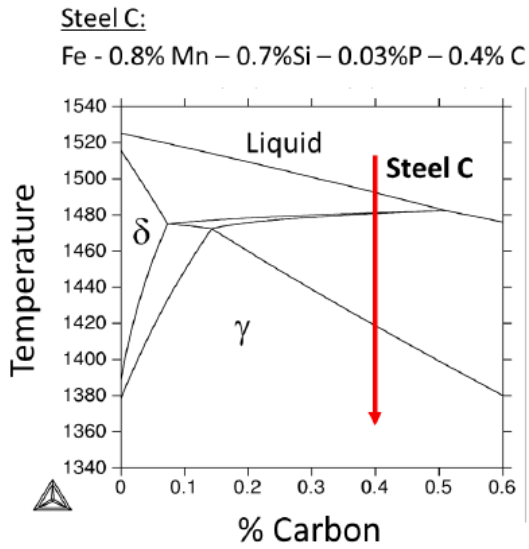


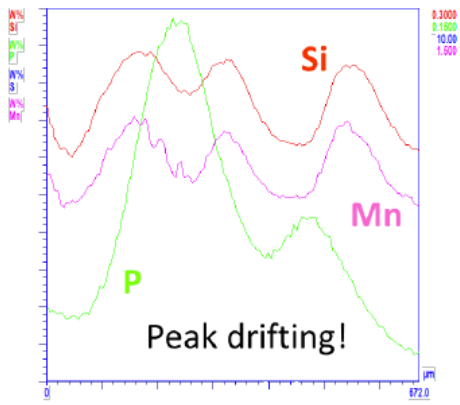

```
POST-1:
POST-1:
POST-1:
POST-1: --OK---
POST-1:
```

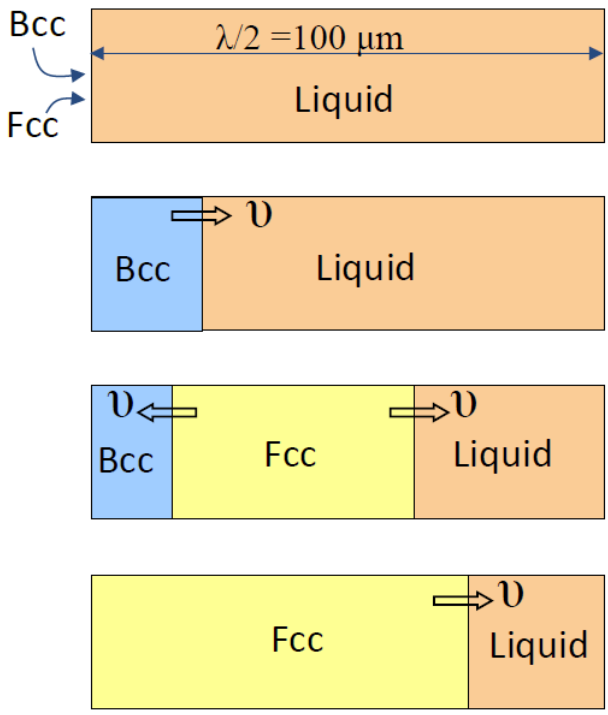
Example exb6

Micro-segregation of phosphorus

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







exb6-setup

```
About
 Software  (build 20130) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri May 24 17:06:15 2019


SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-
Examples\examples\exb6\setup.DCM.test"SYS:SYS:SYS:SYS:SYS: NO SUCH COMMAND, USE HELP
SYS:
SYS:SYS:SYS:SYS: THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.1

 VA                      /-  DEFINED
 L12_FCC                 B2_BCC                  DICTRA_FCC_A1
   REJECTED
TDB_TCFE9:
TDB_TCFE9:TDB_TCFE9:TDB_TCFE9:
TDB_TCFE9:TDB_TCFE9: FE                      C                       SI
 MN                      P  DEFINED
TDB_TCFE9:
TDB_TCFE9:TDB_TCFE9: GAS:G                   LIQUID:L                BCC_A2
 FCC_A1                  HCP_A3                  CBCC_A12
 CUB_A13                 DIAMOND_FCC_A4          RED_P
 WHITE_P                 GRAPHITE                CEMENTITE
 M23C6                   M7C3                    M5C2
 KSI_CARBIDE             FE4N_LP1                FECN_CHI
 LAVES_PHASE_C14         M3SI                    MN9SI2
 MN11SI19                MN6SI                   G_PHASE
 CR3SI                   FE2SI                   FESI2_H
 FESI2_L                 MSI                     M5SI3
 AL4C3                   FE8SI2C                 SIC
 MN5SIC                  CUZN_EPSILON            AL5FE4
 MP_B31                  CU3P_D021               M2P_C22
 M3P_D0E                 MN3P_D0E                FENBP
 FESI4P4                 SIP                     SIP2
 FLUORITE_C1:I           ZRO2_TETR:I             M2O3C:I
 M2O3H:I  REJECTED
TDB_TCFE9: FCC_A1                  LIQUID:L                BCC_A2
   RESTORED
TDB_TCFE9:
TDB_TCFE9:TDB_TCFE9: REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

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      Fe-P-Si'
 -OK-
TDB_TCFE9:
TDB_TCFE9:TDB_TCFE9:TDB_TCFE9:TDB_TCFE9:TDB_TCFE9: Use one of these databases

 TCFE9   =  Steels/Fe-Alloys  v9.1
 TCFE8   =  Steels/Fe-Alloys  v8.1
 FROST1  =  FROST database v1.0
 TCFE7   =  Steels/Fe-Alloys  v7.0
 TCFE6   =  Steels/Fe-Alloys  v6.2
 TCFE5   =  Steels/Fe-Alloys  v5.0
 TCFE4   =  Steels/Fe-Alloys  v4.1
 TCFE3   =  Steels/Fe-Alloys  v3.1
 TCFE2   =  Steels/Fe-Alloys  v2.1
 TCFE1   =  Steels/Fe-Alloys  v1.0
 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  v2.1
 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
 TCSLD1  =  Solder Alloys  v1.1
 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
 TCNF2   =  Nuclear Fuels  v2.1b
 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 v2.1
 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  v1.0
 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 /TCFE9/: Current database: Steels/Fe-Alloys Mobility  v4.0

 VA  DEFINED
 B2_BCC  REJECTED
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
      -Ni'
  'Y. Liu, L. Zhang, et al. CALPHAD 33(2009)614-23; Fe-Mn-C (fcc)'
  'M. Yin, et al. (2010) unpublished work.'
  'W. Zheng, et al., J. Alloys and Compounds, 632 (2015) 661-675; Fe-Mn-Si
      (fcc)'
  'V. V. Mural and P. L. Gruzin, Phys. Met. Metallogr. (English Transl.) 17
      (5) (1964)154.; Impurity diff of P in fcc Fe.'
  'D. Bergner et al., Defect and Diffusion Forum 66-69(1989)409. Impurity
      diffusion of Si in fcc Fe.'
  'B. Jonsson: Z. Metallkunde 85(1994)498-501; C and N diffusion in bcc Cr
      -Fe-Ni'
  'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
      in bcc Fe'
  'S. Deng, et al., CALPHAD, 56 (2017) 230-240.'
  'B. Jonsson: Unpublished research bcc Fe-Si 1994'
  'Assessed from data presented in Landholt-Bornstein, Vol. 26, ed. H.
      Mehrer, springer (1990); Impurity diff of Mn in bcc Fe.'
  'Assessed from data presented in Landholt-Bornstein, Vol. 26, ed. H.
      Mehrer, springer (1990); Impurity diff of P in bcc Fe.'
  'No assessed or estimated parameters'
  'Estimation by using the modified Sutherland equation from Chen et al.,
      Phil. Magazine 94 (2014) 1552.'
  'L. Zhang et al., Acta Mater., 58(2010)3664.'
  'S.Q. Wang et al., Int J Mater Res, 104 (2013) 721-735. '
  'G. Barreau et al., C. R. Acad. Sci. (Paris) C 272(1971)618.; Impurity
      diffusion of Cr in fcc Cu.'
  'Y. Tang et al., CALPHAD, 49(2015)58.'
 -OK-
APP:
APP:APP:APP:APP: NO TIME STEP DEFINED
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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/: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 ? /SI/:COMPOSITION TYPE /MOLE_FRACTION/:PROFILE FOR /C/:PROFILE
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-
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 /AUTO/:VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -> 1): /AUTO/:
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/:
DIC>
DIC>DIC>DIC>DIC>DIC>
DIC> --OK---
DIC>
```

exb6-run

```
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
  1.0649       83
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
 U-FRACTION IN SYSTEM:  C = .0185375871047351  FE = .977481861209078
                        MN = .00810568126669965  P = 5.39133528237327E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 U-FRACTION IN SYSTEM:  C = .0185375871047351  FE = .977481861209078
                        MN = .00810568126669965  P = 5.39133528237327E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .018537587104735  FE = .977481861209078
                        MN = .00810568126669965  P = 5.39133528237327E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.22705714E-05 DT =  0.21705714E-05 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .018537587104735  FE = .977481861209078
                        MN = .00810568126669964  P = 5.39133528237327E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.66117143E-05 DT =  0.43411429E-05 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0185375871047351  FE = .977481861209078
                        MN = .00810568126669965  P = 5.39133528237327E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    1 seconds
 TIME =  0.15294000E-04 DT =  0.86822858E-05 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0185375871047351  FE = .977481861209078
                        MN = .00810568126669964  P = 5.39133528237327E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.32658572E-04 DT =  0.17364572E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .018537587104735  FE = .977481861209078
                        MN = .00810568126669964  P = 5.39133528237327E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.67387715E-04 DT =  0.34729143E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .018537587104735  FE = .977481861209078
                        MN = .00810568126669964  P = 5.39133528237327E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.13684600E-03 DT =  0.69458286E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .018537587104735  FE = .977481861209078
                        MN = .00810568126669965  P = 5.39133528237326E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    1 seconds
 TIME =  0.27576257E-03 DT =  0.13891657E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .018537587104735  FE = .977481861209078
                        MN = .00810568126669965  P = 5.39133528237326E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.55359572E-03 DT =  0.27783314E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .018537587104735  FE = .977481861209078
                        MN = .00810568126669965  P = 5.39133528237326E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.11092620E-02 DT =  0.55566629E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0185375871047351  FE = .977481861209078
                        MN = .00810568126669965  P = 5.39133528237326E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.22205946E-02 DT =  0.11113326E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .018537587104735  FE = .977481861209078
                        MN = .00810568126669965  P = 5.39133528237326E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.44432597E-02 DT =  0.22226652E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .018537587104735  FE = .977481861209078
                        MN = .00810568126669965  P = 5.39133528237326E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    1 seconds
 TIME =  0.88885901E-02 DT =  0.44453303E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0185375871047351  FE = .977481861209078
                        MN = .00810568126669964  P = 5.39133528237326E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.17779251E-01 DT =  0.88906606E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0185375871047351  FE = .977481861209078
                        MN = .00810568126669963  P = 5.39133528237326E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.35560572E-01 DT =  0.17781321E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0185375871047351  FE = .977481861209078
                        MN = .00810568126669964  P = 5.39133528237326E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.71123215E-01 DT =  0.35562643E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .018537587104735  FE = .977481861209078
                        MN = .00810568126669964  P = 5.39133528237328E-04
                        SI = .0138733239959838
```

```
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    1 seconds
 TIME =  0.14224850     DT =  0.71125285E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0185375871047351  FE = .977481861209078
                        MN = .00810568126669966  P = 5.39133528237324E-04
                        SI = .0138733239959837
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.28449907     DT =  0.14225057     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0185375871047352  FE = .977481861209079
                        MN = .00810568126669954  P = 5.39133528237328E-04
                        SI = .0138733239959837
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.56900021     DT =  0.28450114     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0185375871047346  FE = .977481861209079
                        MN = .00810568126669955  P = 5.39133528237295E-04
                        SI = .0138733239959836
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   1.1380025     DT =  0.56900228     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0185375871047344  FE = .97748186120908
                        MN = .00810568126669958  P = 5.39133528237258E-04


output ignored...


... output resumed

 DELETING TIME-RECORD FOR TIME    910.71879
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 DELETING TIME-RECORD FOR TIME    2935.7188
 DELETING TIME-RECORD FOR TIME    2950.7188
 DELETING TIME-RECORD FOR TIME    2965.7188
 DELETING TIME-RECORD FOR TIME    2980.7188

 KEEPING TIME-RECORD FOR TIME    2995.7188
 AND FOR TIME                    3000.0000
 WORKSPACE RECLAIMED

 TIMESTEP AT     3000.00000     SELECTED

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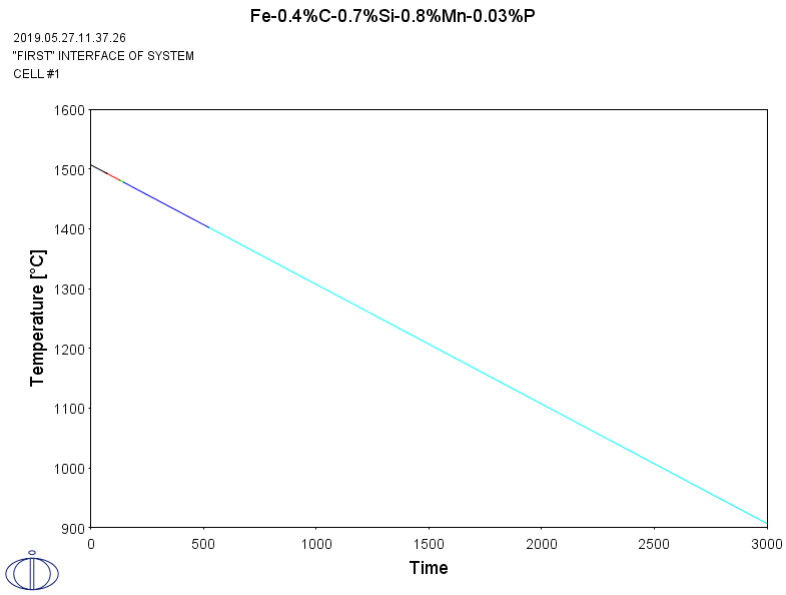
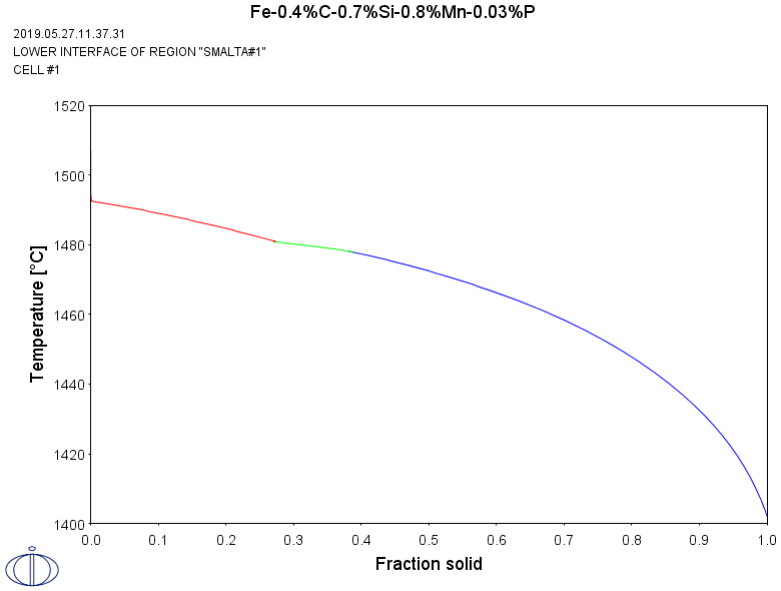

exb6-plot

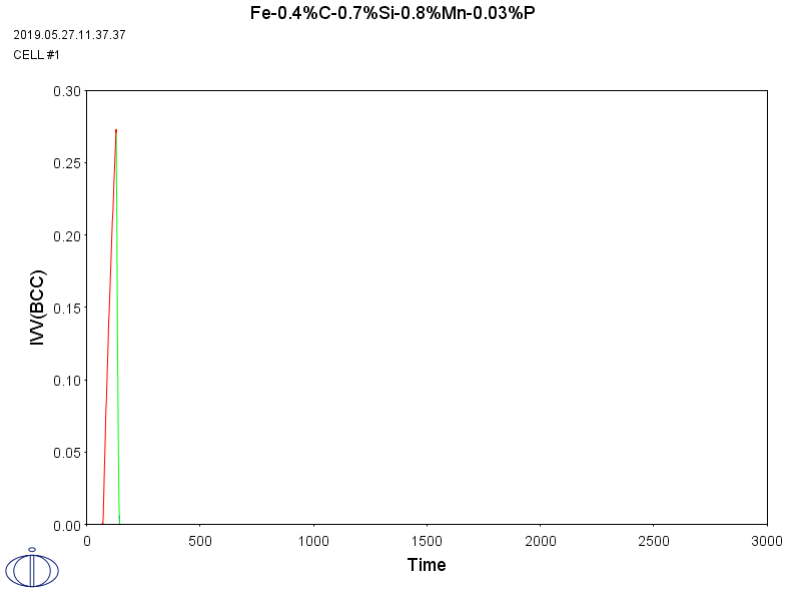
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb6\plot.DCM.test"DIC>
DIC>
DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  3.00000E+03
DIC> OK
DIC>
DIC>DIC>DIC>DIC>  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:POST-1:
POST-1:POST-1:  INFO: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



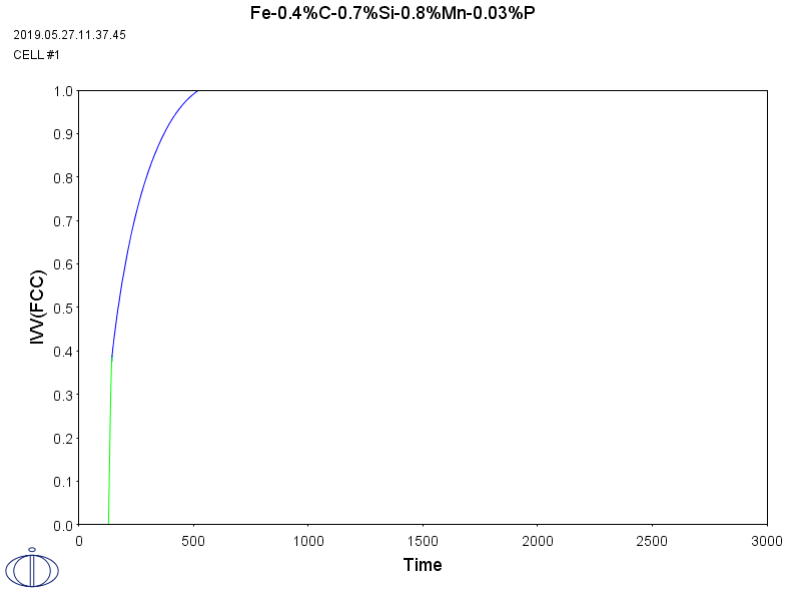

```
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:
POST-1:POST-1:
POST-1:
POST-1:POST-1:
POST-1:
POST-1:
POST-1:POST-1: ORKING ...orking ...          OST-1:POST-1:
POST-1:
```



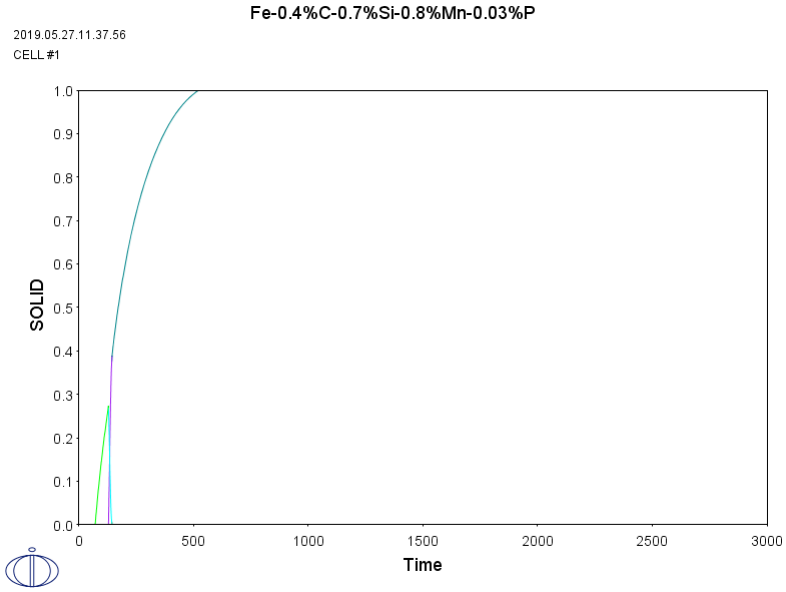

```
POST-1:
POST-1:Hit RETURN to continue
POST-1:POST-1:  INFO: Time is set as independent variable
POST-1:
POST-1:
POST-1:POST-1: ORKING ...orking ...          OST-1:POST-1:
POST-1:
```




```
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:
```

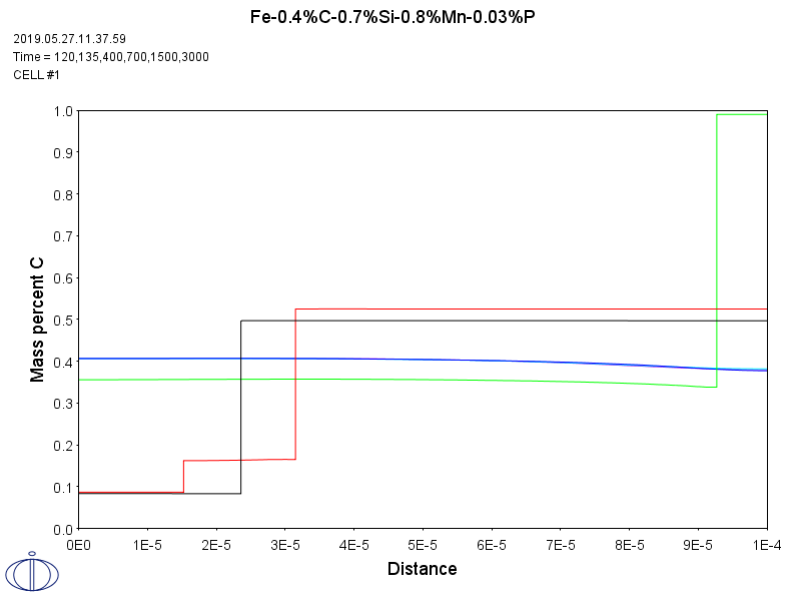



```
POST-1:
POST-1:Hit RETURN to continue
POST-1:Variable(s)POST-1:
POST-1:COLUMN NUMBER /*/:
POST-1:
POST-1:
POST-1:POST-1: ORKING ...orking ...          OST-1:POST-1:
POST-1:
```

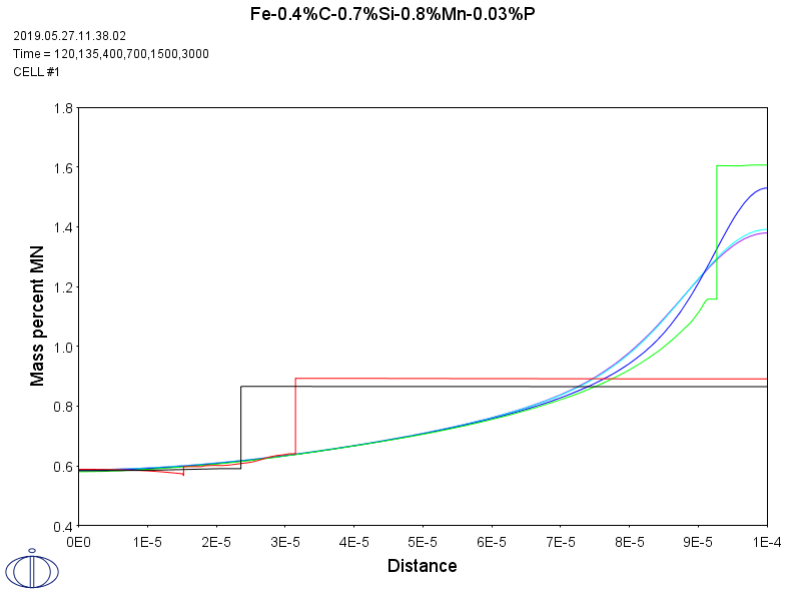



```
POST-1:
```

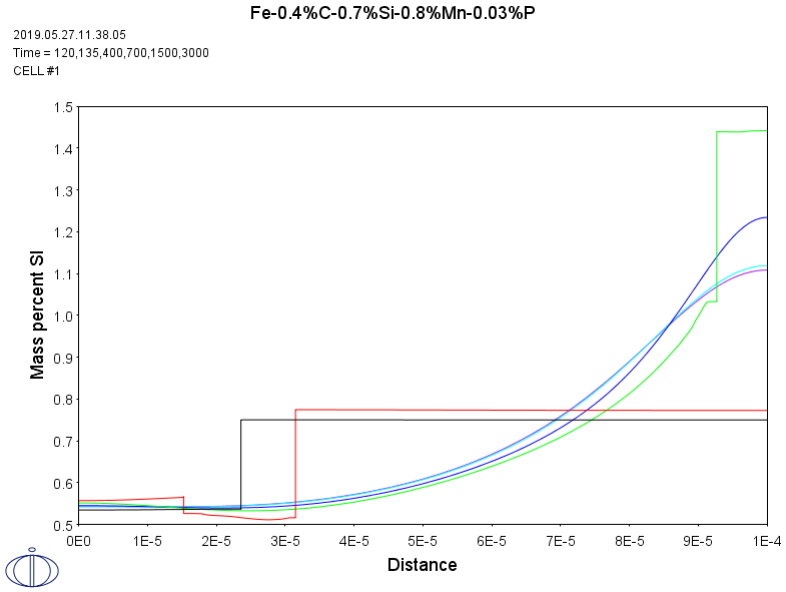
```
POST-1:Hit RETURN to continue
POST-1:POST-1:  INFO: Distance is set as independent variable
POST-1:POST-1:
POST-1:
POST-1:POST-1: ORKING ...orking ...OST-1:POST-1:
POST-1:
```



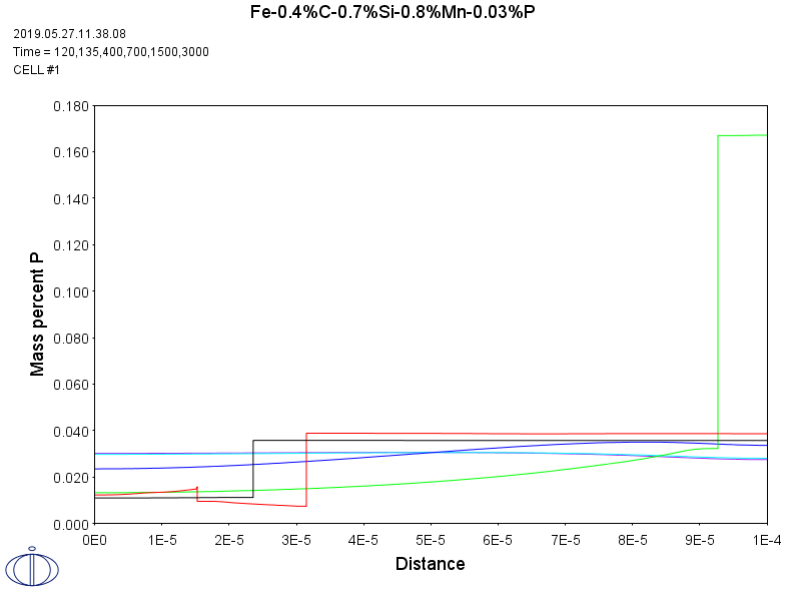

```
POST-1:
POST-1:Hit RETURN to continue
POST-1:POST-1:
POST-1:POST-1: ORKING ...orking ...OST-1:POST-1:
POST-1:
```



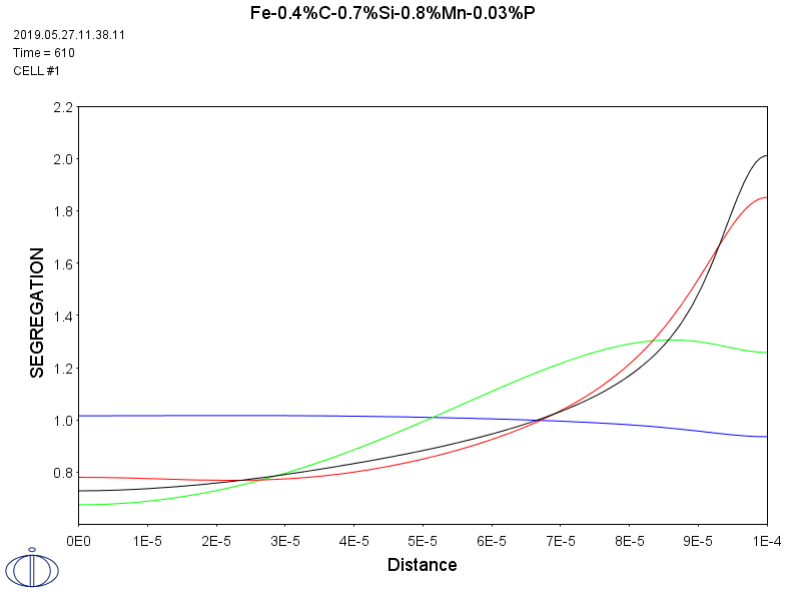

```
POST-1:
POST-1:Hit RETURN to continue
POST-1:POST-1:
POST-1:POST-1: ORKING ...orking ...OST-1:POST-1:
POST-1:
```



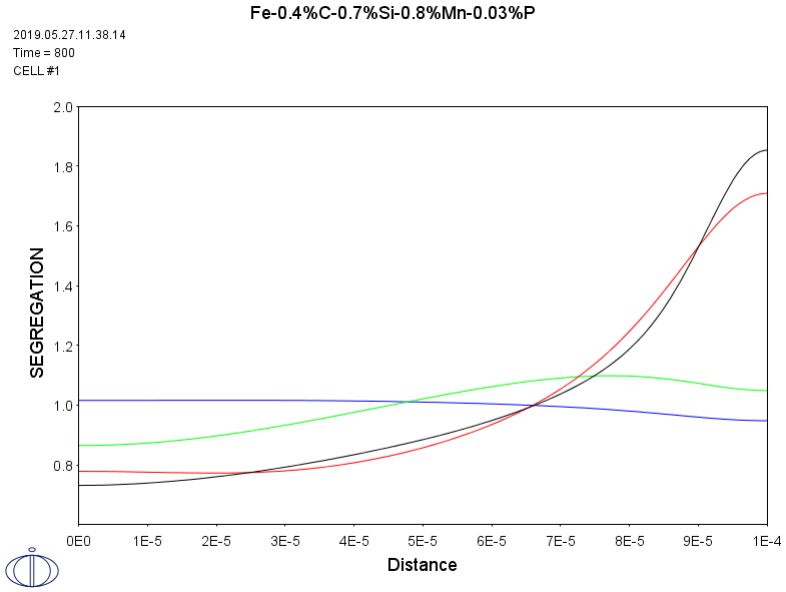

```
POST-1:
POST-1:Hit RETURN to continue
POST-1:POST-1:
POST-1:POST-1: ORKING ...orking ...OST-1:POST-1:
POST-1:
```



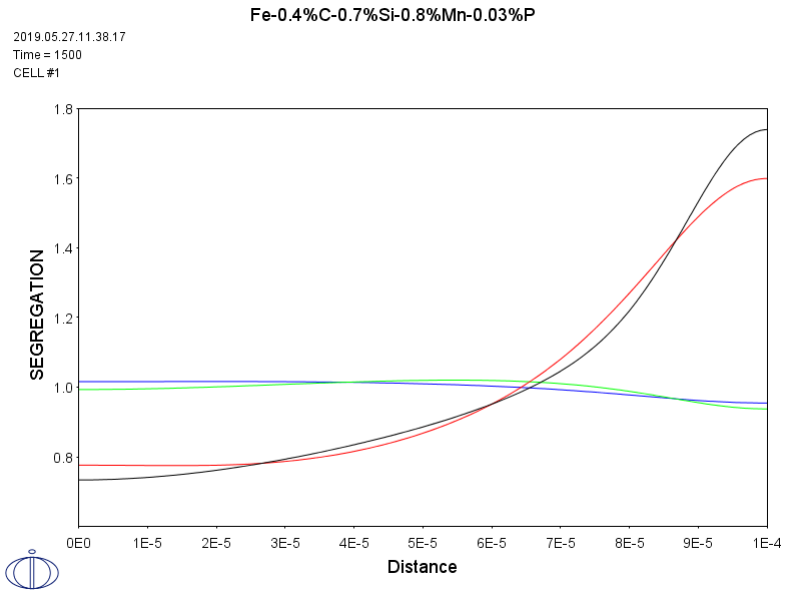

```
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1:FUNCTION:&
POST-1:FUNCTION:&
POST-1:FUNCTION:&
POST-1:FUNCTION:&
POST-1:Variable(s)POST-1:
POST-1:
POST-1:COLUMN NUMBER /*/:
POST-1:
POST-1:
POST-1:POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```




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

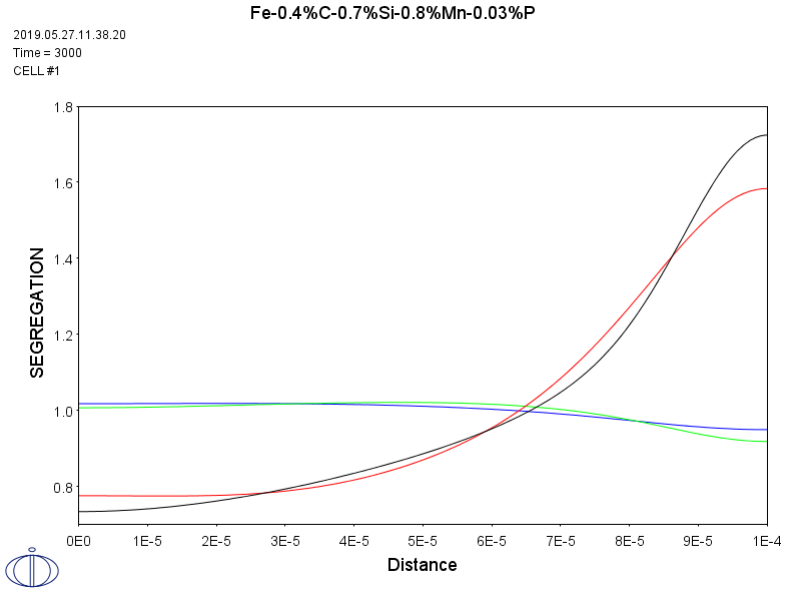



```
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1:POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```




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

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

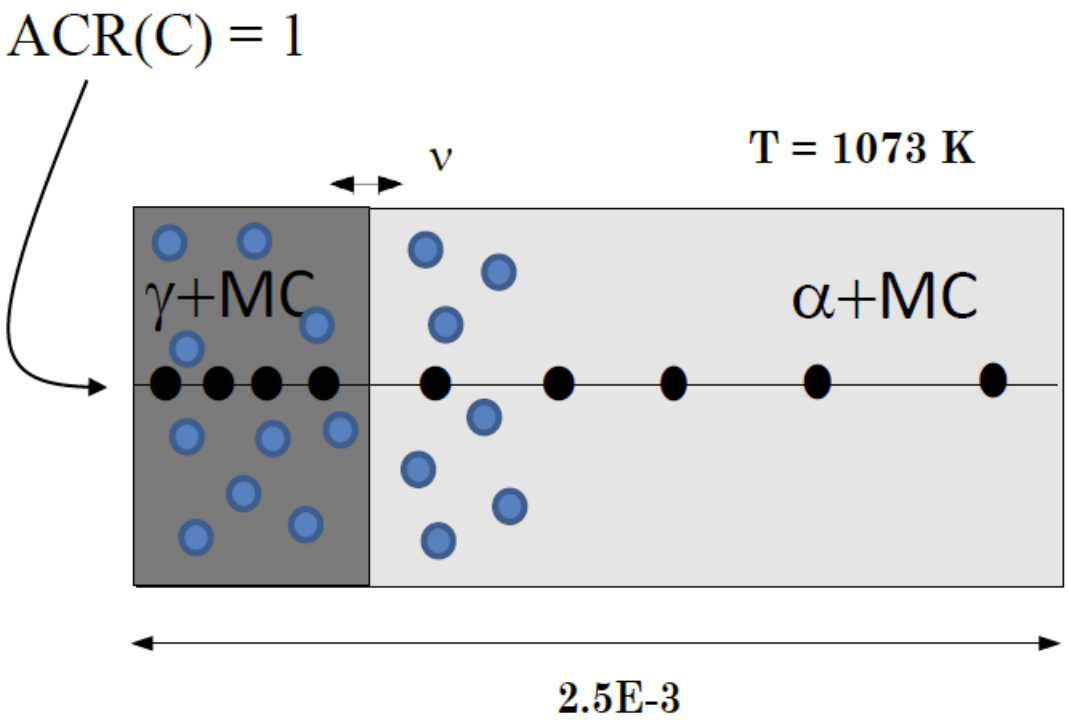



```
POST-1:
POST-1:Hit RETURN to continue
POST-1: --OK---
POST-1:
```

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 License library version: 8.5.1.0017
 Linked: Fri May 24 17:06:15 2019


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  v9.1

 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 tcfe9
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ DEFINE THE SYSTEM TO WORK WITH
TDB_TCFE9: @@
TDB_TCFE9: def-species fe c nb
 FE                      C                       NB
   DEFINED
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ EXCLUDE THE THERMODYNAMIC DATA FOR THE PHASES THAT ARE NOT NEEDED
TDB_TCFE9: @@
TDB_TCFE9: rej ph * all
 GAS:G                   LIQUID:L                BCC_A2
 FCC_A1                  HCP_A3                  CBCC_A12
 CUB_A13                 DIAMOND_FCC_A4          GRAPHITE
 CEMENTITE               M23C6                   M7C3
 M6C                     M5C2                    KSI_CARBIDE
 Z_PHASE                 FE4N_LP1                FECN_CHI
 SIGMA                   MU_PHASE                LAVES_PHASE_C14
 G_PHASE                 CR3SI                   NBNI3
 AL5FE4  REJECTED
TDB_TCFE9: res ph fcc bcc grap
 FCC_A1                  BCC_A2                  GRAPHITE
   RESTORED
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ RETRIEVE DATA FROM THE DATABASE FILE
TDB_TCFE9: @@
TDB_TCFE9: get
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 Creating a new composition set FCC_A1#2
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121-127; Molar
      volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'A. Markstrom, Swerea KIMAB, Sweden; 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'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
  'A.V. Khvan, B. Hallstedt, CALPHAD, 40, 10-15(2013); Fe-Nb, Nb-C, Nb-N, Fe
      -Mn-Nb, Fe-Nb-C, Fe-Nb-N, Nb-C-N, Fe-Mn-Nb-C, Fe-Mn-Nb-N'
  'B.-J. Lee, Metall. Mater. Trans. A, 32A (2001) 2423-39'
  'S. Canderyd, Report IM-2005-109, Stockholm, Sweden; Fe-Nb-C'
  'W. Huang, Z. Metallkd., 6 (1990) 397-404; Fe-Nb-C'
 -OK-
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ NOW APPEND A SSUB DATABASE FROM WHICH WE READ THE THERMODYNAMIC
TDB_TCFE9: @@ DESCRIPTION OF NIOBIUM CARBIDE
TDB_TCFE9: @@
TDB_TCFE9:
TDB_TCFE9: app SSUB6
 Current database: SGTE Substances Database v6.0

 VA  DEFINED
APP: def-sys  fe c nb
 FE                      C                       NB
   DEFINED
APP: rej ph *
 GAS:G                   C0_749NB1_S             C0_877NB1_S
 C0_98NB1_S              C_S                     C_L
 DIAMOND                 C1FE3_S                 C1NB1_S
 C1NB2_S                 C60_S                   FE_S
 FE_S2                   FE_S3                   FE_L
 FE2NB1_S                NB_S                    NB_L
   REJECTED
APP: rest ph c1nb1_s
 C1NB1_S  RESTORED
APP: get
 ELEMENTS .....
```

```
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   C1NB1 I. BARIN 3rd. Edition
      C1NB1
      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 mobfe4
 Current database: Steels/Fe-Alloys Mobility  v4.0

 VA  DEFINED
 B2_BCC  REJECTED
APP: def-sys fe c nb
 FE                      C                       NB
   DEFINED
APP: rej ph * all
 BCC_A2                  CEMENTITE               FCC_A1
 FE4N_LP1                HCP_A3                  LIQUID:L
   REJECTED
APP: res ph fcc bcc
 FCC_A1                  BCC_A2  RESTORED
APP: get
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 Creating a new composition set FCC_A1#3
 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
 INFO: EQUILIBRIUM COMPOSITION AND FRACTION OF SPHEROID PHASES USED AS DEFAULT
DIC>
DIC>
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /AUS/: aus
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC>
DIC> en-ph
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /AUS/: aus
PHASE TYPE /MATRIX/: sph
PHASE NAME: /NONE/: c1nb1_s
 INFO: EQUILIBRIUM COMPOSITION AND FRACTION OF SPHEROID PHASES USED AS DEFAULT
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITIONS OF THE PHASES
DIC> @@
DIC> enter-composition
REGION NAME : /AUS/: ferr
PHASE NAME: /BCC_A2/: bcc
DEPENDENT COMPONENT ? /NB/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: C
TYPE /LINEAR/: lin
VALUE OF FIRST POINT : 1e-3
VALUE OF LAST POINT : /1E-3/: 1e-3
PROFILE FOR /NB/: nb
TYPE /LINEAR/: lin
VALUE OF FIRST POINT : 0.28
VALUE OF LAST POINT : /0.28/: 0.28
DIC>
DIC> en-co
REGION NAME : /AUS/: ferr
PHASE NAME: /BCC_A2/: c1nb1_s
USE EQUILIBRIUM VALUE /Y/: y
DIC>
DIC> enter-composition
REGION NAME : /AUS/: aus
PHASE NAME: /FCC_A1#1/: fcc#1
DEPENDENT COMPONENT ? /NB/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: C
TYPE /LINEAR/: lin
VALUE OF FIRST POINT : 0.89
VALUE OF LAST POINT : /0.89/: 0.89
PROFILE FOR /NB/: nb
TYPE /LINEAR/: lin
VALUE OF FIRST POINT : 0.28
VALUE OF LAST POINT : /0.28/: 0.28
DIC>
DIC> en-co
REGION NAME : /AUS/: aus
PHASE NAME: /FCC_A1#1/: c1nb1_s
USE EQUILIBRIUM VALUE /Y/: y
DIC>
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 32400
AUTOMATIC TIMESTEP CONTROL /YES/: y
MAX TIMESTEP DURING INTEGRATION /3240/: 3240
INITIAL TIMESTEP : /1E-07/: 1e-8
SMALLEST ACCEPTABLE TIMESTEP : /1E-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
 DEGREE OF IMPLICITY SET TO EULER BACKWARD
 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)
  WARNING:C1NB1_S HAS NO VOLUME FRACTION, CREATING ONE
  WARNING:C1NB1_S HAS NO VOLUME FRACTION, CREATING ONE
Starting time-step t0=   0.0000000     dt=  0.10000000E-07
 Error                    408
 Error                    408
Starting time-step t0=  0.48828125E-11 dt=  0.48828125E-11
Starting time-step t0=  0.97656250E-11 dt=  0.97656250E-11
Starting time-step t0=  0.19531250E-10 dt=  0.19531250E-10
Starting time-step t0=  0.39062500E-10 dt=  0.39062500E-10
Starting time-step t0=  0.78125000E-10 dt=  0.78125000E-10
Starting time-step t0=  0.15625000E-09 dt=  0.15625000E-09
Starting time-step t0=  0.31250000E-09 dt=  0.15625000E-09
Starting time-step t0=  0.46875000E-09 dt=  0.31250000E-09
Starting time-step t0=  0.78125000E-09 dt=  0.31250000E-09
Starting time-step t0=  0.10937500E-08 dt=  0.31250000E-09
Starting time-step t0=  0.14062500E-08 dt=  0.31250000E-09
Starting time-step t0=  0.17187500E-08 dt=  0.62500000E-09
Starting time-step t0=  0.23437500E-08 dt=  0.62500000E-09
Starting time-step t0=  0.29687500E-08 dt=  0.12500000E-08
Starting time-step t0=  0.42187500E-08 dt=  0.25000000E-08
Starting time-step t0=  0.67187500E-08 dt=  0.50000000E-08
Starting time-step t0=  0.11718750E-07 dt=  0.10000000E-07
Starting time-step t0=  0.21718750E-07 dt=  0.10000000E-07
Starting time-step t0=  0.31718750E-07 dt=  0.10000000E-07
Starting time-step t0=  0.41718750E-07 dt=  0.10000000E-07
Starting time-step t0=  0.51718750E-07 dt=  0.20000000E-07
Starting time-step t0=  0.71718750E-07 dt=  0.20000000E-07
Starting time-step t0=  0.91718750E-07 dt=  0.20000000E-07
Starting time-step t0=  0.11171875E-06 dt=  0.40000000E-07
Starting time-step t0=  0.15171875E-06 dt=  0.40000000E-07
Starting time-step t0=  0.19171875E-06 dt=  0.80000000E-07
Starting time-step t0=  0.27171875E-06 dt=  0.80000000E-07
Starting time-step t0=  0.35171875E-06 dt=  0.16000000E-06
Starting time-step t0=  0.51171875E-06 dt=  0.32000000E-06
Starting time-step t0=  0.83171875E-06 dt=  0.64000000E-06
Starting time-step t0=  0.14717187E-05 dt=  0.12800000E-05
Starting time-step t0=  0.27517187E-05 dt=  0.25600000E-05
Starting time-step t0=  0.53117187E-05 dt=  0.51200000E-05
Starting time-step t0=  0.10431719E-04 dt=  0.10240000E-04
Starting time-step t0=  0.20671719E-04 dt=  0.20480000E-04
Starting time-step t0=  0.41151719E-04 dt=  0.40960000E-04
Starting time-step t0=  0.82111719E-04 dt=  0.81920000E-04
Starting time-step t0=  0.16403172E-03 dt=  0.16384000E-03
Starting time-step t0=  0.32787172E-03 dt=  0.32768000E-03
Starting time-step t0=  0.65555172E-03 dt=  0.65536000E-03
Starting time-step t0=  0.13109117E-02 dt=  0.13107200E-02
Starting time-step t0=  0.26216317E-02 dt=  0.26214400E-02
Starting time-step t0=  0.52430717E-02 dt=  0.52428800E-02
Starting time-step t0=  0.10485952E-01 dt=  0.10485760E-01
Starting time-step t0=  0.20971712E-01 dt=  0.20971520E-01
Starting time-step t0=  0.41943232E-01 dt=  0.41943040E-01
Starting time-step t0=  0.83886272E-01 dt=  0.41943040E-01
Starting time-step t0=  0.12582931     dt=  0.41943040E-01
Starting time-step t0=  0.16777235     dt=  0.83886080E-01
Starting time-step t0=  0.18874387     dt=  0.20971520E-01
 Error                    408
 Error                    408
Starting time-step t0=  0.18907155     dt=  0.32768000E-03
Starting time-step t0=  0.18939923     dt=  0.32768000E-03
Starting time-step t0=  0.18972691     dt=  0.32768000E-03
Starting time-step t0=  0.19005459     dt=  0.32768000E-03
Starting time-step t0=  0.19038227     dt=  0.32768000E-03
Starting time-step t0=  0.19070995     dt=  0.32768000E-03
Starting time-step t0=  0.19103763     dt=  0.32768000E-03
Starting time-step t0=  0.19136531     dt=  0.32768000E-03
Starting time-step t0=  0.19169299     dt=  0.32768000E-03
Starting time-step t0=  0.19202067     dt=  0.65536000E-03
Starting time-step t0=  0.19267603     dt=  0.65536000E-03
Starting time-step t0=  0.19333139     dt=  0.65536000E-03
Starting time-step t0=  0.19398675     dt=  0.65536000E-03
Starting time-step t0=  0.19464211     dt=  0.65536000E-03
Starting time-step t0=  0.19529747     dt=  0.65536000E-03
Starting time-step t0=  0.19595283     dt=  0.13107200E-02
Starting time-step t0=  0.19726355     dt=  0.13107200E-02
Starting time-step t0=  0.19857427     dt=  0.13107200E-02
Starting time-step t0=  0.19988499     dt=  0.13107200E-02
Starting time-step t0=  0.20119571     dt=  0.13107200E-02
Starting time-step t0=  0.20250643     dt=  0.26214400E-02
```

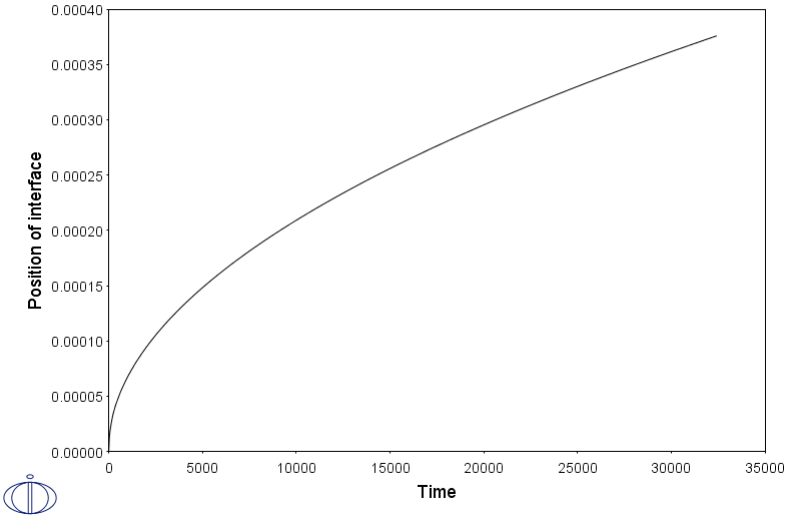
```
Starting time-step t0=  0.20512787     dt=  0.26214400E-02
Starting time-step t0=  0.20774931     dt=  0.52428800E-02
Starting time-step t0=  0.21299219     dt=  0.52428800E-02
Starting time-step t0=  0.21823507     dt=  0.52428800E-02
Starting time-step t0=  0.22347795     dt=  0.10485760E-01
Starting time-step t0=  0.23396371     dt=  0.10485760E-01
Starting time-step t0=  0.24444947     dt=  0.10485760E-01
Starting time-step t0=  0.25493523     dt=  0.10485760E-01
Starting time-step t0=  0.26542099     dt=  0.10485760E-01
Starting time-step t0=  0.27590675     dt=  0.20971520E-01
Starting time-step t0=  0.29687827     dt=  0.20971520E-01
Starting time-step t0=  0.31784979     dt=  0.20971520E-01
Starting time-step t0=  0.33882131     dt=  0.20971520E-01
Starting time-step t0=  0.35979283     dt=  0.20971520E-01
Starting time-step t0=  0.38076435     dt=  0.20971520E-01
Starting time-step t0=  0.40173587     dt=  0.20971520E-01
Starting time-step t0=  0.42270739     dt=  0.20971520E-01
Starting time-step t0=  0.44367891     dt=  0.20971520E-01
Starting time-step t0=  0.46465043     dt=  0.20971520E-01
Starting time-step t0=  0.48562195     dt=  0.20971520E-01
Starting time-step t0=  0.50659347     dt=  0.41943040E-01
Starting time-step t0=  0.54853651     dt=  0.41943040E-01
Starting time-step t0=  0.59047955     dt=  0.41943040E-01
Starting time-step t0=  0.63242259     dt=  0.83886080E-01
Starting time-step t0=  0.71630867     dt=  0.83886080E-01
Starting time-step t0=  0.80019475     dt=  0.83886080E-01
Starting time-step t0=  0.88408083     dt=  0.83886080E-01


output ignored...



... output resumed

 DELETING TIME-RECORD FOR TIME    26681.271
 DELETING TIME-RECORD FOR TIME    26724.221
 DELETING TIME-RECORD FOR TIME    26777.908
 DELETING TIME-RECORD FOR TIME    26842.333
 DELETING TIME-RECORD FOR TIME    26885.282
 DELETING TIME-RECORD FOR TIME    26928.232
 DELETING TIME-RECORD FOR TIME    26971.182
 DELETING TIME-RECORD FOR TIME    27014.131
 DELETING TIME-RECORD FOR TIME    27057.081
 DELETING TIME-RECORD FOR TIME    27100.031
 DELETING TIME-RECORD FOR TIME    27142.980
 DELETING TIME-RECORD FOR TIME    27185.930
 DELETING TIME-RECORD FOR TIME    27228.880
 DELETING TIME-RECORD FOR TIME    27271.829
 DELETING TIME-RECORD FOR TIME    27314.779
 DELETING TIME-RECORD FOR TIME    27357.729
 DELETING TIME-RECORD FOR TIME    27400.678
 DELETING TIME-RECORD FOR TIME    27443.628
 DELETING TIME-RECORD FOR TIME    27486.578
 DELETING TIME-RECORD FOR TIME    27529.527
 DELETING TIME-RECORD FOR TIME    27572.477
 DELETING TIME-RECORD FOR TIME    27615.427
 DELETING TIME-RECORD FOR TIME    27658.376
 DELETING TIME-RECORD FOR TIME    27701.326
 DELETING TIME-RECORD FOR TIME    27744.276
 DELETING TIME-RECORD FOR TIME    27787.225
 DELETING TIME-RECORD FOR TIME    27830.175
 DELETING TIME-RECORD FOR TIME    27873.125
 DELETING TIME-RECORD FOR TIME    27916.074
 DELETING TIME-RECORD FOR TIME    27959.024
 DELETING TIME-RECORD FOR TIME    28001.974
 DELETING TIME-RECORD FOR TIME    28044.923
 DELETING TIME-RECORD FOR TIME    28087.873
 DELETING TIME-RECORD FOR TIME    28130.823
 DELETING TIME-RECORD FOR TIME    28173.772
 DELETING TIME-RECORD FOR TIME    28216.722
 DELETING TIME-RECORD FOR TIME    28259.672
 DELETING TIME-RECORD FOR TIME    28302.621
 DELETING TIME-RECORD FOR TIME    28345.571
 DELETING TIME-RECORD FOR TIME    28388.521
 DELETING TIME-RECORD FOR TIME    28431.470
 DELETING TIME-RECORD FOR TIME    28474.420
 DELETING TIME-RECORD FOR TIME    28517.370
 DELETING TIME-RECORD FOR TIME    28560.319
 DELETING TIME-RECORD FOR TIME    28603.269
 DELETING TIME-RECORD FOR TIME    28646.219
 DELETING TIME-RECORD FOR TIME    28689.168
 DELETING TIME-RECORD FOR TIME    28732.118
 DELETING TIME-RECORD FOR TIME    28775.068
 DELETING TIME-RECORD FOR TIME    28850.230
 DELETING TIME-RECORD FOR TIME    28893.179
 DELETING TIME-RECORD FOR TIME    28957.604
 DELETING TIME-RECORD FOR TIME    29000.554
 DELETING TIME-RECORD FOR TIME    29043.503
 DELETING TIME-RECORD FOR TIME    29086.453
 DELETING TIME-RECORD FOR TIME    29129.403
 DELETING TIME-RECORD FOR TIME    29172.352
 DELETING TIME-RECORD FOR TIME    29215.302
 DELETING TIME-RECORD FOR TIME    29258.252
 DELETING TIME-RECORD FOR TIME    29301.201
 DELETING TIME-RECORD FOR TIME    29344.151
 DELETING TIME-RECORD FOR TIME    29387.101
 DELETING TIME-RECORD FOR TIME    29430.050
 DELETING TIME-RECORD FOR TIME    29473.000
 DELETING TIME-RECORD FOR TIME    29515.950
 DELETING TIME-RECORD FOR TIME    29558.899
 DELETING TIME-RECORD FOR TIME    29623.324
 DELETING TIME-RECORD FOR TIME    29666.274
 DELETING TIME-RECORD FOR TIME    29709.223
 DELETING TIME-RECORD FOR TIME    29752.173
 DELETING TIME-RECORD FOR TIME    29795.123
 DELETING TIME-RECORD FOR TIME    29838.072
 DELETING TIME-RECORD FOR TIME    29881.022
 DELETING TIME-RECORD FOR TIME    29923.972
 DELETING TIME-RECORD FOR TIME    29966.921
 DELETING TIME-RECORD FOR TIME    30009.871
 DELETING TIME-RECORD FOR TIME    30052.821
 DELETING TIME-RECORD FOR TIME    30095.770
 DELETING TIME-RECORD FOR TIME    30138.720
 DELETING TIME-RECORD FOR TIME    30181.670
 DELETING TIME-RECORD FOR TIME    30224.619
```

```
 DELETING TIME-RECORD FOR TIME    30267.569
 DELETING TIME-RECORD FOR TIME    30310.519
 DELETING TIME-RECORD FOR TIME    30353.468
 DELETING TIME-RECORD FOR TIME    30396.418
 DELETING TIME-RECORD FOR TIME    30439.368
 DELETING TIME-RECORD FOR TIME    30482.317
 DELETING TIME-RECORD FOR TIME    30525.267
 DELETING TIME-RECORD FOR TIME    30589.691
 DELETING TIME-RECORD FOR TIME    30632.641
 DELETING TIME-RECORD FOR TIME    30675.591
 DELETING TIME-RECORD FOR TIME    30740.015
 DELETING TIME-RECORD FOR TIME    30782.965
 DELETING TIME-RECORD FOR TIME    30825.915
 DELETING TIME-RECORD FOR TIME    30868.864
 DELETING TIME-RECORD FOR TIME    30933.289
 DELETING TIME-RECORD FOR TIME    30976.239
 DELETING TIME-RECORD FOR TIME    31019.188
 DELETING TIME-RECORD FOR TIME    31062.138
 DELETING TIME-RECORD FOR TIME    31105.088
 DELETING TIME-RECORD FOR TIME    31158.775
 DELETING TIME-RECORD FOR TIME    31201.724
 DELETING TIME-RECORD FOR TIME    31244.674
 DELETING TIME-RECORD FOR TIME    31287.624
 DELETING TIME-RECORD FOR TIME    31330.573
 DELETING TIME-RECORD FOR TIME    31373.523
 DELETING TIME-RECORD FOR TIME    31416.473
 DELETING TIME-RECORD FOR TIME    31459.422
 DELETING TIME-RECORD FOR TIME    31502.372
 DELETING TIME-RECORD FOR TIME    31566.797
 DELETING TIME-RECORD FOR TIME    31609.746
 DELETING TIME-RECORD FOR TIME    31652.696
 DELETING TIME-RECORD FOR TIME    31717.120
 DELETING TIME-RECORD FOR TIME    31760.070
 DELETING TIME-RECORD FOR TIME    31803.020
 DELETING TIME-RECORD FOR TIME    31845.969
 DELETING TIME-RECORD FOR TIME    31888.919
 DELETING TIME-RECORD FOR TIME    31931.869
 DELETING TIME-RECORD FOR TIME    31974.818
 DELETING TIME-RECORD FOR TIME    32017.768
 DELETING TIME-RECORD FOR TIME    32060.718
 DELETING TIME-RECORD FOR TIME    32103.667
 DELETING TIME-RECORD FOR TIME    32146.617
 DELETING TIME-RECORD FOR TIME    32189.567
 DELETING TIME-RECORD FOR TIME    32232.516
 DELETING TIME-RECORD FOR TIME    32275.466
 DELETING TIME-RECORD FOR TIME    32318.416

 KEEPING TIME-RECORD FOR TIME    32361.366
 AND FOR TIME                    32400.000
 WORKSPACE RECLAIMED
 ------------------------------------------------
 INTERPOLATION SCHEME USED THIS FRACTION OF
 THE ALLOCATED MEMORY:    1.00000000000000
 EFFICIENCY FACTOR:    33.2778787632882
 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

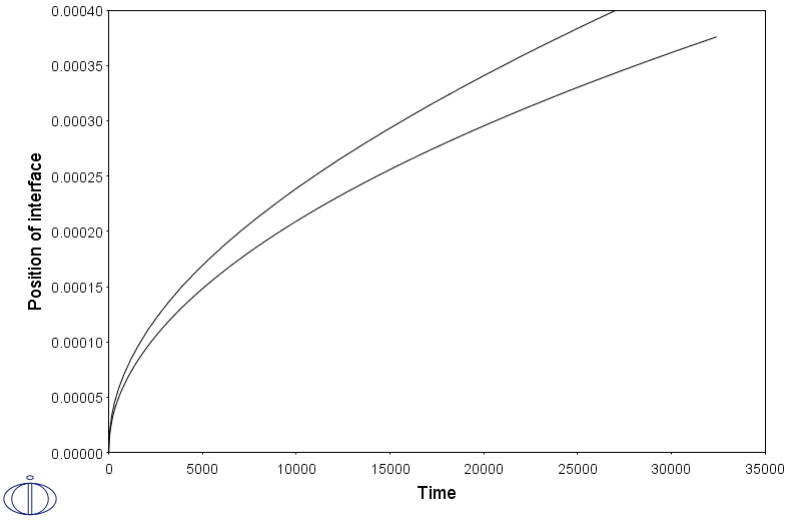
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb7\plot.DCM"DIC>
DIC>
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  3.24000E+04
 *** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
 *** ENTERING C1NB1_S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

2019.05.27.11.50.40
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
```

2019.05.27.11.50.47
UPPER INTERFACE OF REGION "AUS#1"
CELL #1




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

exc1-setup

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

 Software  (build 20130) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri May 24 17:06:15 2019


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  v9.1

 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 v2.1

 VA                      /-  DEFINED
TDB_FEDEMO: def-sys fe c
 FE                      C  DEFINED
TDB_FEDEMO: rej ph * all
 GAS:G                   LIQUID:L                BCC_A2
 CBCC_A12                CEMENTITE               CUB_A13
 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'
  '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 /AUTO/:
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 (AUTO, 0 -> 0.5 -> 1): /AUTO/: 1.0
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/:
DIC-2> @@
DIC-2> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC-2> @@
DIC-2> save exc1 Y
DIC-2>
DIC-2> set-inter
 --OK---
DIC-2>
```

exc1-run

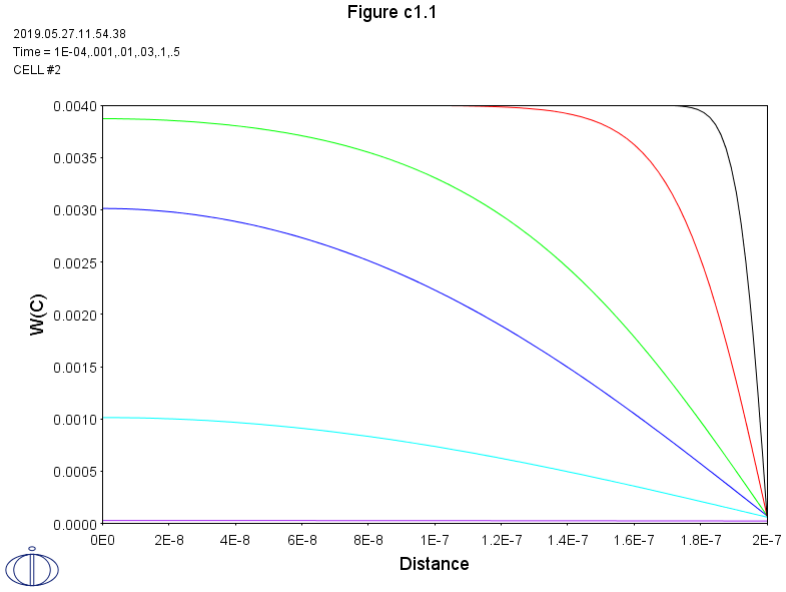
```
DIC-2>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exc1\run.DCM"DIC-2>
DIC-2>
DIC-2> @@ exc1_run.DCM
DIC-2>
DIC-2> @@
DIC-2> @@ READ THE WORKSPACE AND START THE SIMULATION
DIC-2> @@
DIC-2> go d-m
 TIME STEP AT TIME  0.00000E+00
DIC-2> read exc1
 OK
DIC> sim
 Region: 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]
 2.570491440876794E-002        2.570457646506867E-002        1.632468393332992E-002        1.481595185063469E-003        4.374341053626947E-
005        2.088304823750715E-007        2.465148254353641E-011        1.324760532636705E-017       TIME =  0.10000000E-06 DT =  0.10000000E-
06 SUM OF SQUARES =  0.13247605E-16
 U-FRACTION IN SYSTEM:  C = .018673311178092  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    1 seconds
 1.721271285522169E-002        1.721309826251357E-002        1.320114678449893E-003        1.780264096152656E-004        4.883616077889357E-
006        2.701426699389010E-008        4.894446443955106E-012        5.060994963843985E-018       TIME =  0.30000000E-06 DT =  0.20000000E-
06 SUM OF SQUARES =  0.50609950E-17
 U-FRACTION IN SYSTEM:  C = .018673311178317  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    0 seconds
 1.723030673037728E-002        1.722973038976243E-002        6.546665197602261E-004        1.540163278312917E-005        9.847912767787774E-
009        1.575452889984416E-013        1.596354274765439E-021       TIME =  0.70000000E-06 DT =  0.40000000E-
06 SUM OF SQUARES =  0.15963543E-20
 U-FRACTION IN SYSTEM:  C = .0186733111783162  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    1 seconds
 2.046536420972691E-003        2.046359859032466E-003        1.093844175405200E-005        4.894918035805911E-008        1.003356983338762E-
012        9.304057925474044E-020       TIME =  0.15000000E-05 DT =  0.80000000E-06 SUM OF SQUARES =  0.93040579E-19
 U-FRACTION IN SYSTEM:  C = .0186733111783284  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    1 seconds
 1.307886964749793E-003        1.307786277163456E-003        8.937182320576807E-006        4.994501068084317E-008        1.605936733880706E-
012        2.925324017603110E-019       TIME =  0.31000000E-05 DT =  0.16000000E-05 SUM OF SQUARES =  0.29253240E-18
 U-FRACTION IN SYSTEM:  C = .0186733111783716  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    0 seconds
 5.482172962186058E-004        5.481699846889692E-004        2.979476148357670E-006        1.354118196359522E-008        2.862903213068261E-
013        2.781376314686506E-020       TIME =  0.63000000E-05 DT =  0.32000000E-05 SUM OF SQUARES =  0.27813763E-19
 U-FRACTION IN SYSTEM:  C = .0186733111783983  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    1 seconds
 2.615717394236215E-002        2.615484476818396E-002        1.336512898461473E-004        5.745045966578183E-007        1.084421153895432E-
011        8.890690003038978E-019       TIME =  0.12700000E-04 DT =  0.64000000E-05 SUM OF SQUARES =  0.88906900E-18
 U-FRACTION IN SYSTEM:  C = .0186733111784285  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    1 seconds
 1.276911017789708E-002        1.276795521546182E-002        6.327037900285266E-005        2.645587781998716E-007        4.737844545365976E-
012        3.569529504846276E-019       TIME =  0.25500000E-04 DT =  0.12800000E-04 SUM OF SQUARES =  0.35695295E-18
 U-FRACTION IN SYSTEM:  C = .0186733111784667  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    0 seconds
 6.319101225972034E-003        6.318525707101470E-003        3.090594834652315E-005        1.275882700895499E-007        2.220822141360515E-
012        1.611790108715721E-019       TIME =  0.51100000E-04 DT =  0.25600000E-04 SUM OF SQUARES =  0.16117901E-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                    1 seconds
 1.041680260882442E-005        1.044882763652513E-005        2.674275432539641E-011        6.870275122969418E-
017       TIME =  0.19801409     DT =  0.25429002E-01 SUM OF SQUARES =  0.68702751E-16
 U-FRACTION IN SYSTEM:  C = .0186734961934044  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    1 seconds
 2.750911885911548E-005        2.755302230046246E-005        1.960821123207396E-010        2.118986962176743E-015        5.313898432161943E-
028       TIME =  0.22607048     DT =  0.28056387E-01 SUM OF SQUARES =  0.53138984E-27
 U-FRACTION IN SYSTEM:  C = .0186734961934049  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    1 seconds
 5.476254512856389E-005        5.481399792604490E-005        9.963529647110896E-010        3.091448606271068E-014        1.321201479747374E-
023       TIME =  0.25814941     DT =  0.32078937E-01 SUM OF SQUARES =  0.13212015E-22
 U-FRACTION IN SYSTEM:  C = .0186734961934102  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    1 seconds
 1.037340039584005E-004        1.037913251895126E-004        5.851058195306921E-009        4.334114174409202E-013        1.567695673085159E-
021       TIME =  0.29683922     DT =  0.38689804E-01 SUM OF SQUARES =  0.15676957E-20
 U-FRACTION IN SYSTEM:  C = .0186734961934877  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    1 seconds
 1.750218760491141E-004        1.750799684386786E-004        2.677170373600729E-008        4.755116475621694E-012        1.227652656337170E-
019       TIME =  0.34683922     DT =  0.50000000E-01 SUM OF SQUARES =  0.12276527E-18
 U-FRACTION IN SYSTEM:  C = .0186734961943632  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    1 seconds
 1.655026934240656E-005        1.656587674471100E-005        2.353929133586293E-010        5.747655919641521E-015        2.196599640739929E-
024       TIME =  0.39683922     DT =  0.50000000E-01 SUM OF SQUARES =  0.21965996E-23
 U-FRACTION IN SYSTEM:  C = .0186734961943663  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    1 seconds
 2.721459416063167E-006        2.715794025694317E-006        1.265713320098800E-011        3.005845734691372E-
017       TIME =  0.44683922     DT =  0.50000000E-01 SUM OF SQUARES =  0.30058457E-16
 U-FRACTION IN SYSTEM:  C = .0186734961806593  FE = 1
```

```
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    1 seconds
 2.924257073688714E-005        2.922561803641230E-005        1.420288784171981E-009        5.383932618707661E-014        1.098305480479962E-
022        TIME =  0.49683922     DT =  0.50000000E-01 SUM OF SQUARES =  0.10983055E-21
 U-FRACTION IN SYSTEM:  C = .0186734961806328  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    1 seconds
 1.311639930567306E-002        1.311509713863354E-002        1.933615198528166E-005        2.528807186922510E-008        6.842230242383434E-
014        1.059286751789518E-022       TIME =  0.50000000     DT =  0.31607821E-02 SUM OF SQUARES =  0.10592868E-21
 U-FRACTION IN SYSTEM:  C = .0186734961806344  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

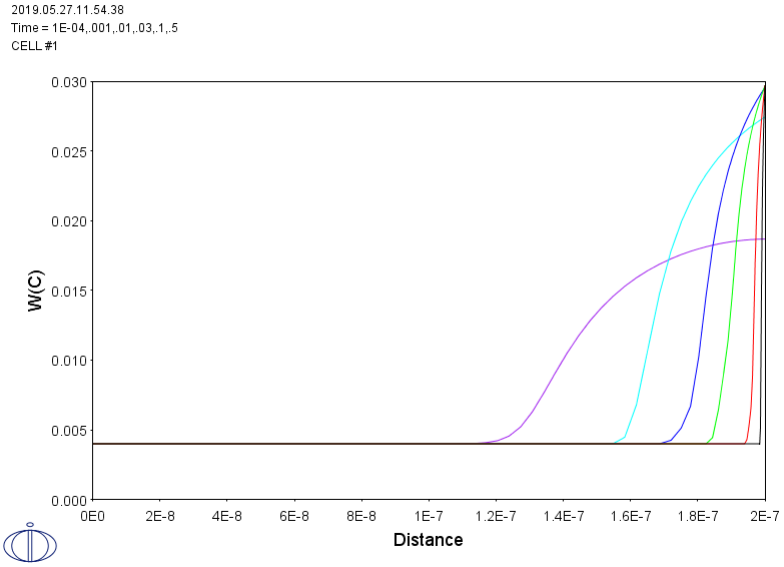
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exc1\plot.DCM"DIC>
DIC>
DIC> @@ exc1_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE c1
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go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



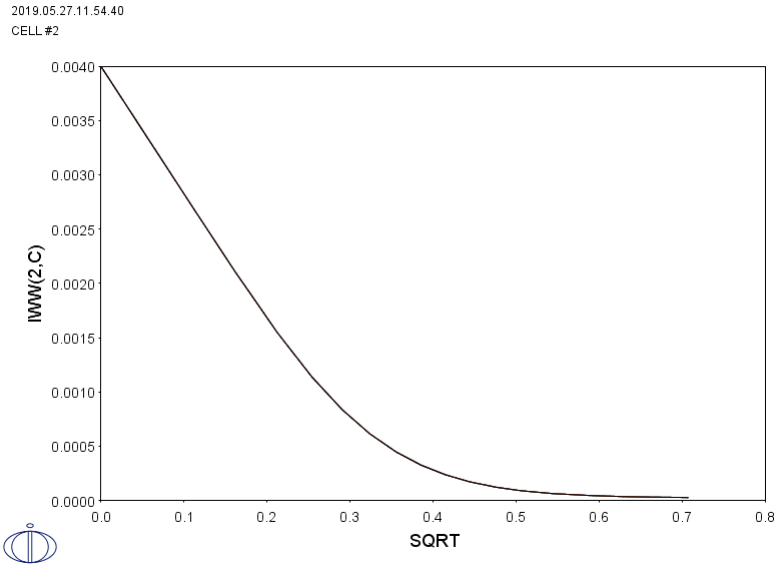

```
POST-2:
POST-2:
POST-2:
POST-2:@?<_hit_return_to_continue_>
POST-2:
POST-2: @@
POST-2: @@ DO THE SAME THING FOR THE AUSTENITE (CELL-1)
POST-2: @@
POST-2: select-cell
Number /NEXT/: 1
 CELL   1 SELECTED
POST-1: set-title Figure c1.2
POST-1: plot
```

Figure c1.2



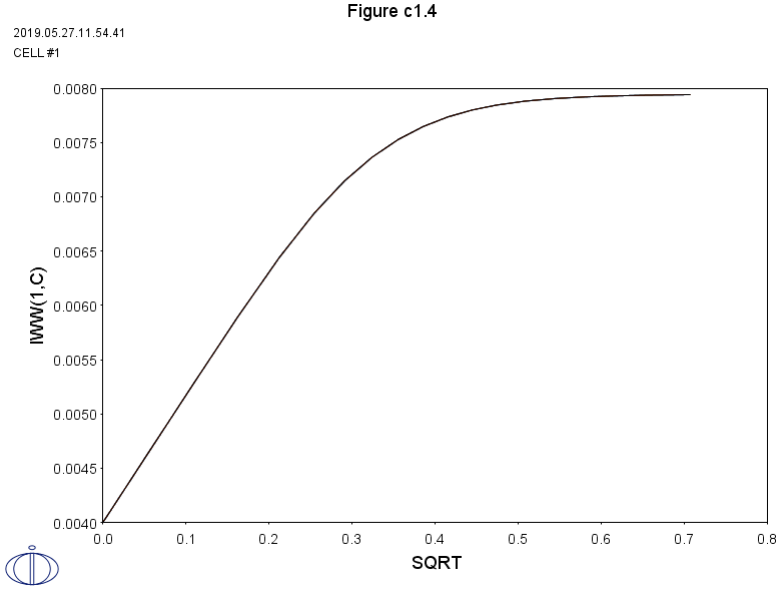

```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: @@
POST-1: @@ PLOT THE AVARAGE WEIGHT FRACTION OF CARBON IN FERRITE VS. SQUARE ROOT
POST-1: @@ OF TIME. START BY DEFINING A "SQUARE-ROOT-OF-TIME" FUNCTION.
POST-1: @@
POST-1: sel-cell 2
 CELL    2 SELECTED
POST-2: enter func 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



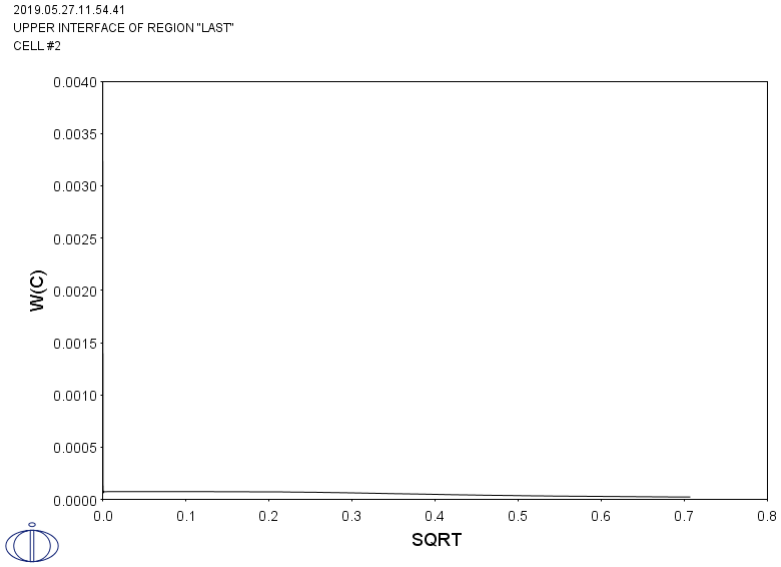

```
POST-2:
POST-2:
POST-2:
POST-2:@?<_hit_return_to_continue_>
POST-2:
POST-2: @@
POST-2: @@ DO THE SAME THING FOR THE AUSTENITE
POST-2: @@
POST-2: sel-cell 1
 CELL    1 SELECTED
POST-1: s-d-a y iww(1,c)
POST-1: set-title Figure c1.4
POST-1: plot
```

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
```

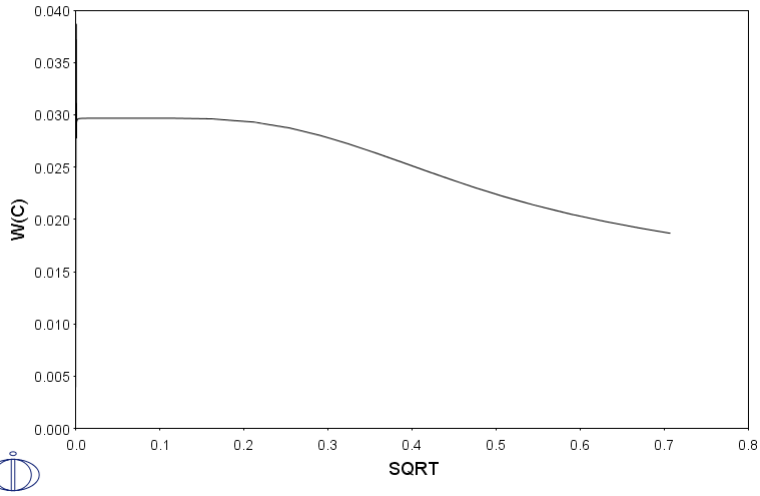
Figure c1.5




```
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

2019.05.27.11.54.42
UPPER INTERFACE OF REGION "LAST"
CELL #1

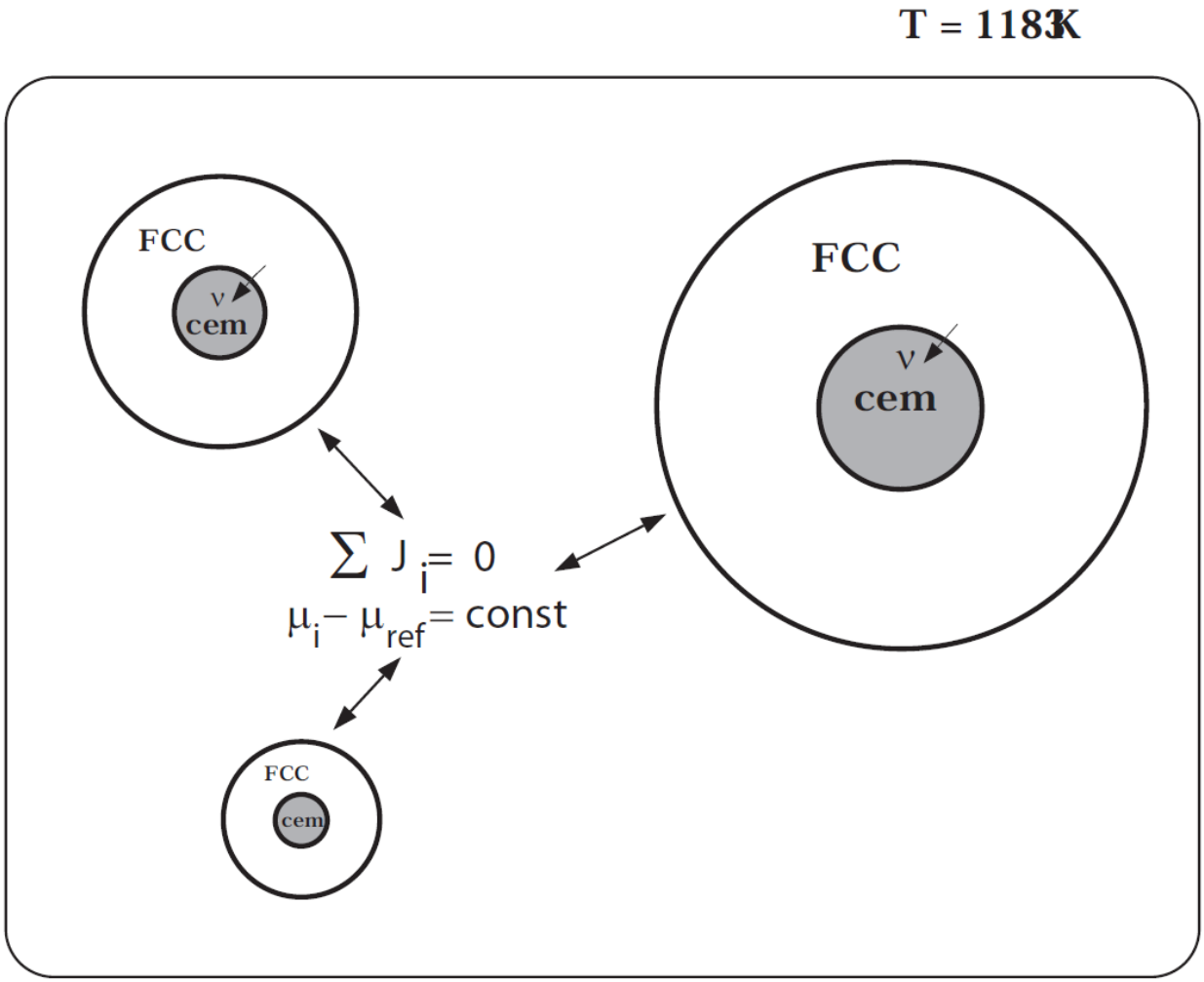



```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: set-inter
 --OK---
POST-1:
```

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 Software  (build 20130) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri May 24 17:06:15 2019


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  v9.1

 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 v2.1

 VA                      /-  DEFINED
TDB_FEDEMO: def-sys fe cr c
 FE                      CR                      C
   DEFINED
TDB_FEDEMO: rej ph * all
 GAS:G                   LIQUID:L                BCC_A2
 CBCC_A12                CEMENTITE               CHI_A12
 CUB_A13                 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 .......
 Creating a new composition set FCC_A1#2
 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'
  '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 mobfe4
 Current database: Steels/Fe-Alloys Mobility  v4.0

 VA  DEFINED
 B2_BCC  REJECTED
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 .......
 Creating a new composition set FCC_A1#3
 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

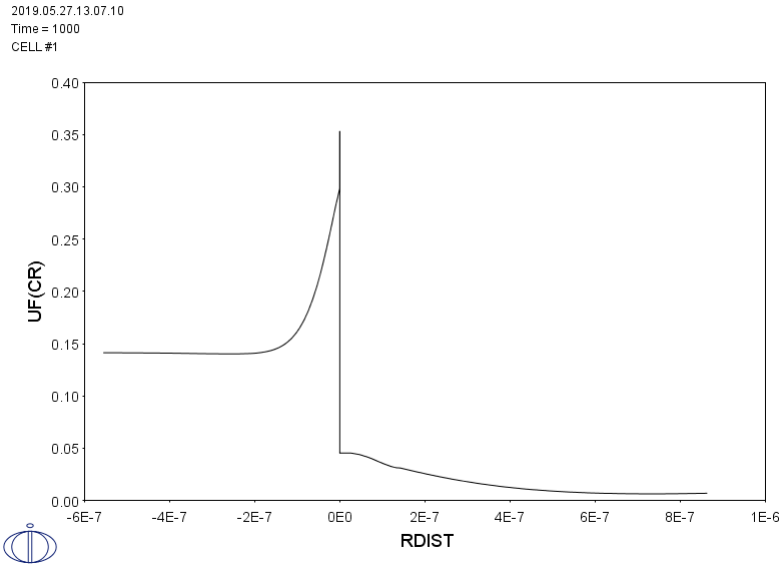
```
DIC-3>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exc2\run.DCM"DIC-3>
DIC-3>
DIC-3> @@ exc2_run.DCM
DIC-3>
DIC-3> @@
DIC-3> @@ READ THE SET UP FROM FILE AND START THE SIMULATION
DIC-3> @@
DIC-3>
DIC-3> go d-m
 TIME STEP AT TIME  0.00000E+00
DIC-3> read exc2
 OK
DIC> 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
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
  Trying old scheme                       4
 GENERATING STARTING VALUES FOR CELL #  1 INTERFACE #  2
 DETERMINING INITIAL EQUILIBRIUM VALUES
CALCULATING STARTING VALUES:       9   EQUILIBRIUM CALCULATIONS               DONE     6 OUT OF     9
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]
 0.549881621022649        0.549917064641369        0.549938978099244        0.549921828506974        0.549881463442408        0.549881396770029
002        3.584789100881467E-004        4.707896218999935E-005        1.368538549944173E-006        9.616968061761579E-
006        1.052143983683236E-006        9.010518128287986E-007        8.267746917998884E-007        8.321573840471592E-
007        8.024773010550435E-007        8.036126148447211E-007        7.984608479711728E-007        8.050009080731271E-
007        8.000667876559454E-007        7.984620140422961E-007        7.984782243516489E-007        8.003049929398167E-
007        8.048504050345887E-007        8.013658008984975E-007        7.869048260317326E-007        7.845298608572306E-
007        7.828052493112217E-007        7.795100507772101E-007        7.765420050224403E-007        7.772966895163242E-
007        7.719168100491267E-007        7.729228850492248E-007        7.669031199806729E-007        7.600329286498509E-
007        7.604611933906988E-007        7.600341337146238E-007        7.600503467624317E-007        7.525562577114374E-
007        7.561970194060387E-007        7.540768031268558E-007        7.401555177047882E-007        7.236762721530465E-
007        7.065875830777363E-007        6.785553056600359E-007        6.488672001393395E-007        6.495030274909185E-
007        5.991860194423810E-007        6.000961681833830E-007        5.458302373915301E-007        4.547576410749867E-
007        4.549588583203923E-007        4.547588547543342E-007        4.547750672790243E-007        3.591727466713041E-
007        3.588608050279693E-007        3.590808309830802E-007        5.291229247137280E-007        4.381093704977365E-
007        3.219088008831952E-007

output ignored...



... output resumed

  CPU time used in timestep                    9 seconds
 5.620617336968824E-003        5.620617476466289E-003        5.620617420614695E-003        5.620576836122061E-003        5.620556418586897E-
003        5.620362325768683E-003        5.619738558010859E-003        7.742065618344161E-005        1.342697952648981E-
007        4.548597652562482E-011        3.675730676182928E-015        8.943291431172318E-
019       TIME =   7809.6319     DT =   1000.0000     SUM OF SQUARES =  0.89432914E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.11246971E-10 AND  -0.11246971E-10
 POSITION OF INTERFACE CARB / AUS IS   0.41766604E-06
 CELL # 3 VELOCITY AT INTERFACE # 2 IS  -0.12055399E-10 AND  -0.12055399E-10
 POSITION OF INTERFACE CARB / AUS IS   0.24051172E-06
 U-FRACTION IN SYSTEM:  C = .0407685558940953  CR = .0215929304894515
                        FE = .978407069641056
 TOTAL SIZE OF SYSTEM:  2.90023192349E-17 [m^3]
  2  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUS

  CPU time used in timestep                    9 seconds
 7.934070180199346E-003        7.934070267768944E-003        7.934070201679940E-003        7.934027720875647E-003        7.934008399195485E-
003        7.933759761924527E-003        7.932997935777421E-003        1.064629110156520E-004        1.767216323431270E-
007        6.741104548963670E-011        8.805225893782716E-015        2.224081054706568E-
018       TIME =   8809.6319     DT =   1000.0000     SUM OF SQUARES =  0.22240811E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.10004238E-10 AND  -0.10004238E-10
 POSITION OF INTERFACE CARB / AUS IS   0.40766181E-06
 CELL # 3 VELOCITY AT INTERFACE # 2 IS  -0.11461673E-10 AND  -0.11461673E-10
 POSITION OF INTERFACE CARB / AUS IS   0.22905005E-06
 U-FRACTION IN SYSTEM:  C = .0407686055478557  CR = .021592730595975
                        FE = .978407269534532
 TOTAL SIZE OF SYSTEM:  2.90023192349E-17 [m^3]
  CPU time used in timestep                    8 seconds
 1.006117053767977E-002        1.006117059828544E-002        1.006117053014299E-002        1.006113162210481E-002        1.006111613944877E-
002        1.006081554118568E-002        1.005993345397135E-002        1.098010324181776E-004        2.139986226301289E-
007        1.112284935060296E-010        1.882723558612200E-014        7.981962950289253E-
018       TIME =   9809.6319     DT =   1000.0000     SUM OF SQUARES =  0.79819630E-17
```

```
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.90231061E-11 AND  -0.90231061E-11
 POSITION OF INTERFACE CARB / AUS IS   0.39863870E-06
 CELL # 3 VELOCITY AT INTERFACE # 2 IS  -0.11230264E-10 AND  -0.11230264E-10
 POSITION OF INTERFACE CARB / AUS IS   0.21781978E-06
 U-FRACTION IN SYSTEM:  C = .0407686379562253  CR = .0215925869931017
                        FE = .978407413137406
 TOTAL SIZE OF SYSTEM:  2.90023192349E-17 [m^3]
  CPU time used in timestep                    9 seconds
 1.779065602583954E-003        1.779065716154161E-003        1.779065833851167E-003        1.779003561073671E-003        1.778978860370710E-
003        1.778989503224045E-003        1.778950376217402E-003        4.689939976276202E-004        1.296551249947344E-
005        1.326262689860154E-008        2.092185778554777E-012        1.623060235038117E-
016       TIME =   10000.000     DT =   190.36806     SUM OF SQUARES =  0.16230602E-15
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.74915741E-11 AND  -0.74915741E-11
 POSITION OF INTERFACE CARB / AUS IS   0.39721254E-06
 CELL # 3 VELOCITY AT INTERFACE # 2 IS  -0.86402698E-11 AND  -0.86402698E-11
 POSITION OF INTERFACE CARB / AUS IS   0.21617495E-06
 U-FRACTION IN SYSTEM:  C = .0407686583482657  CR = .0215925539047019
                        FE = .978407446225805
 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

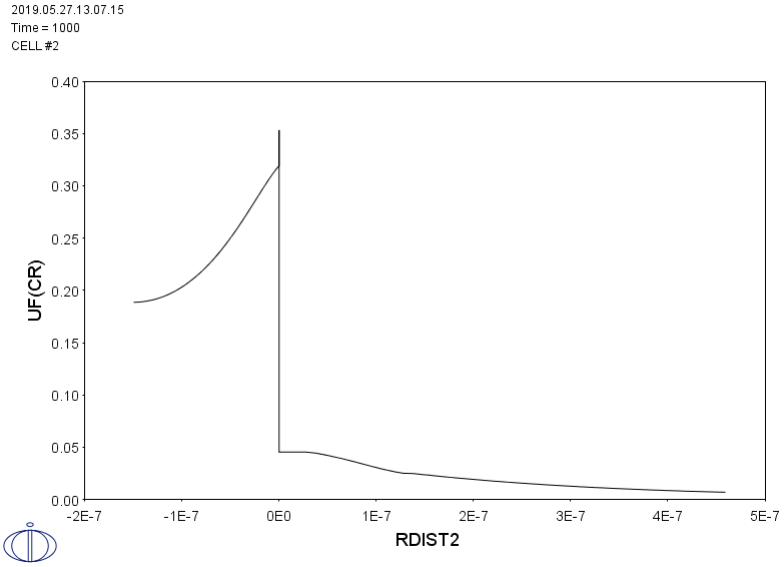
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exc2\plot.DCM"DIC>
DIC>
DIC> @@ exc2_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE c2
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go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



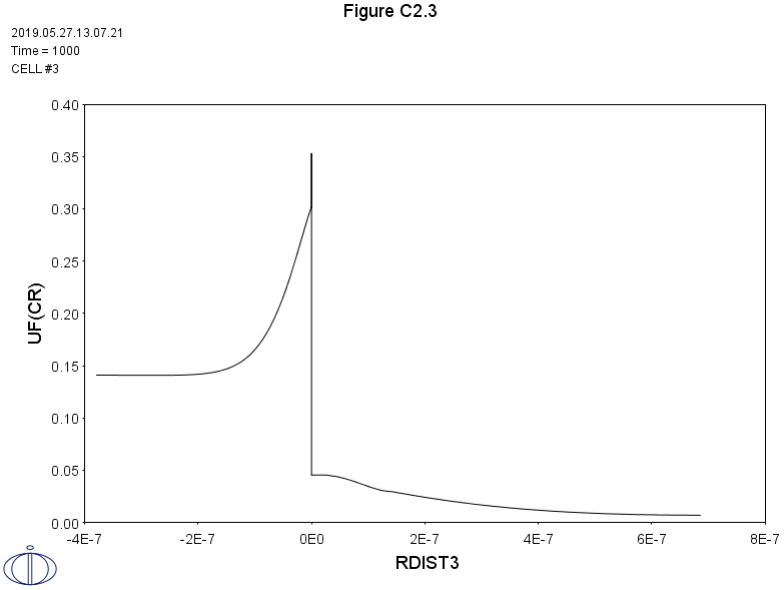

```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: @@
POST-1: @@ SELECT CELL 2
POST-1: @@
POST-1: select-cell
Number /NEXT/: 2
 CELL   2 SELECTED
POST-2:
POST-2: enter-symb
Function or table /FUNCTION/: func
NAME: rdist2
FUNCTION: gd-poi(carb,u);
POST-2:
POST-2: s-d-a x rdist2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

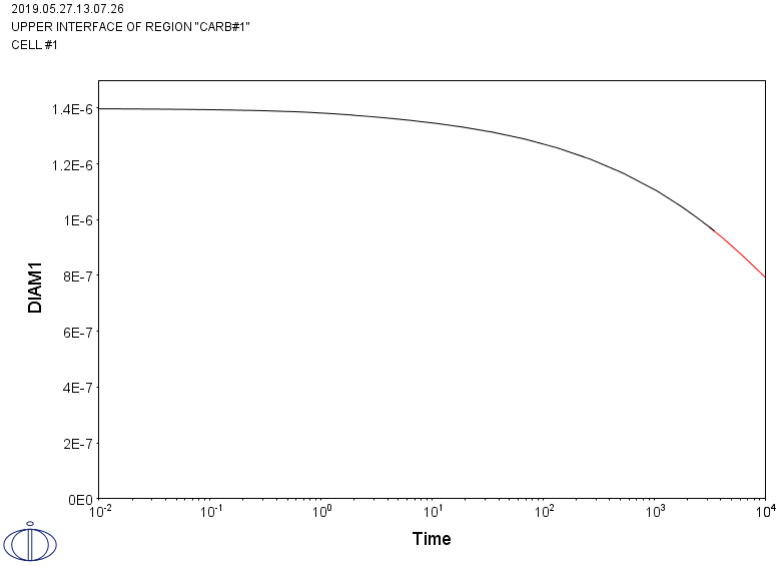
Figure C2.3




```
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:
```

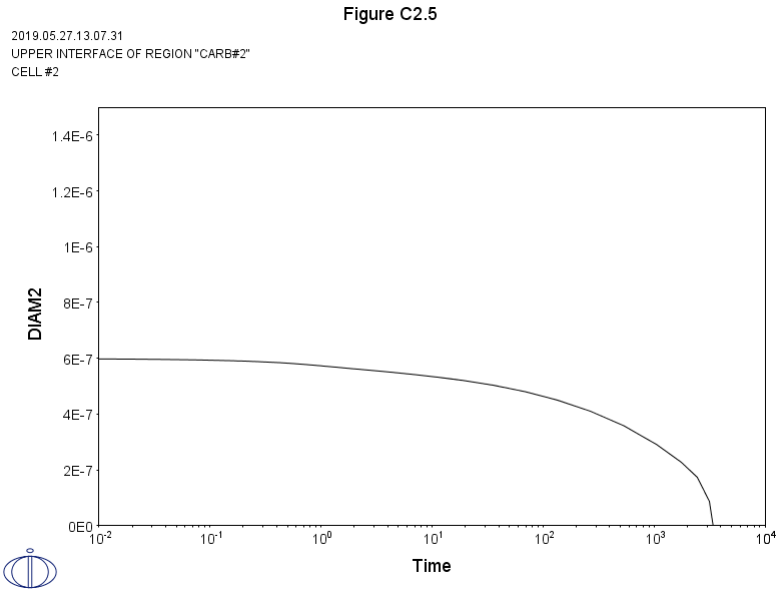
```
POST-1: s-p-c interf carb upp
POST-1:
POST-1: app n
POST-1: set-title Figure C2.4
POST-1: plot
```

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
```

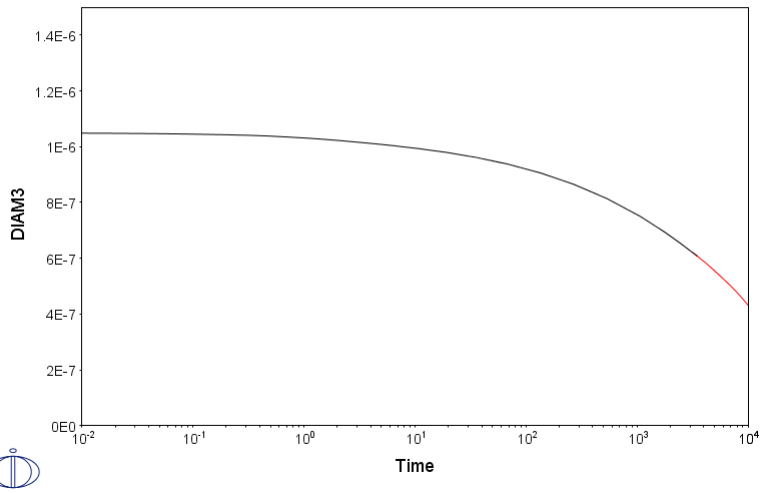
Figure C2.5




```
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

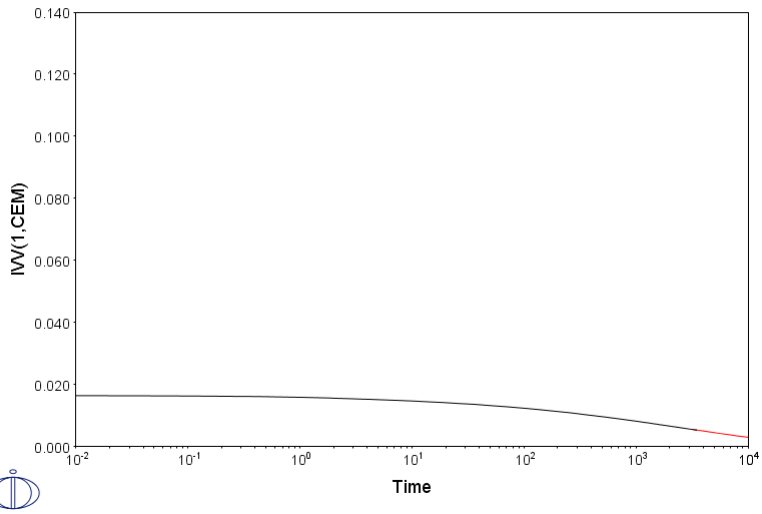
2019.05.27.13.07.37
UPPER INTERFACE OF REGION "CARB#3"
CELL #3




```
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
```

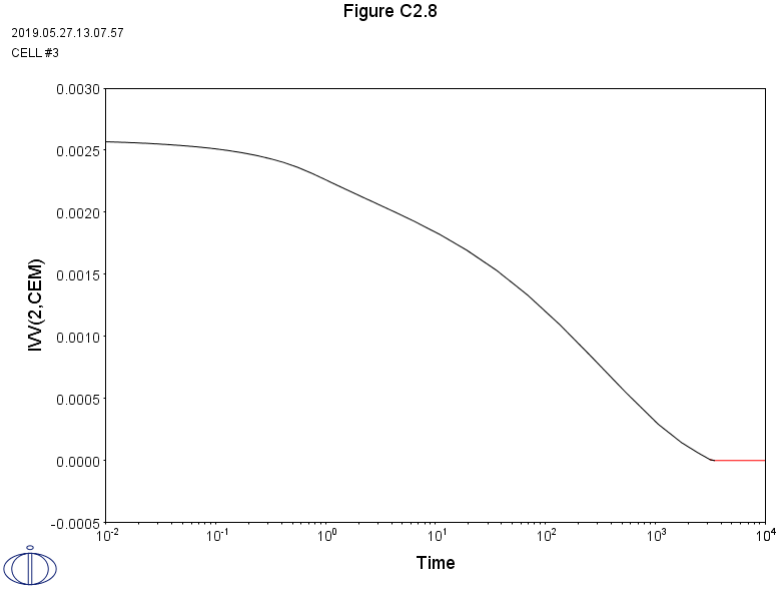
Figure C2.7

2019.05.27.13.07.46
CELL #3



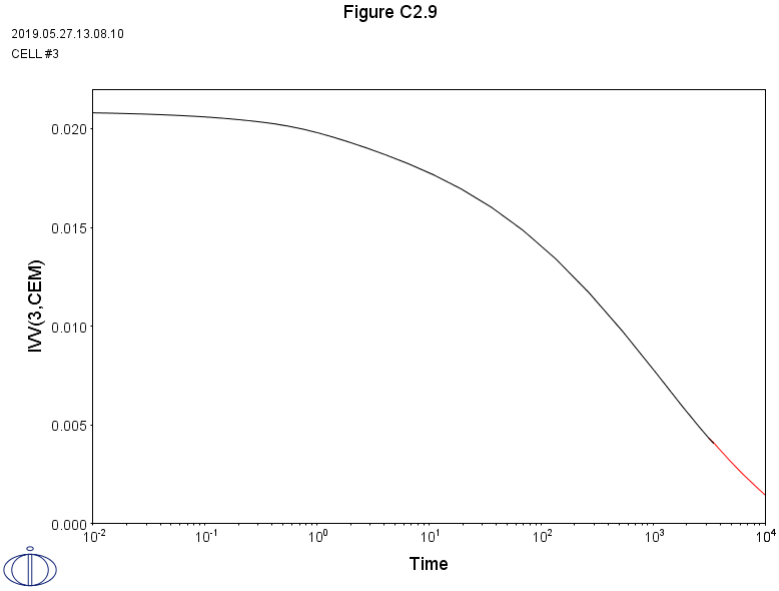

```
POST-3:
POST-3:
POST-3:
POST-3:
POST-3:@?<_hit_return_to_continue_>
POST-3:
POST-3: @@
POST-3: @@ CELL 2
POST-3: @@
POST-3: s-d-a y ivv(2,cem)
POST-3:
POST-3: set-title Figure C2.8
POST-3: plot
```

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
```

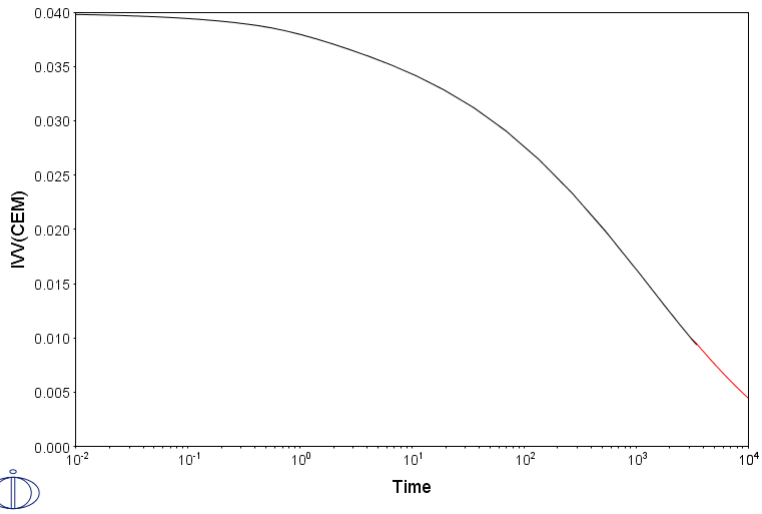
Figure C2.9




```
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
```

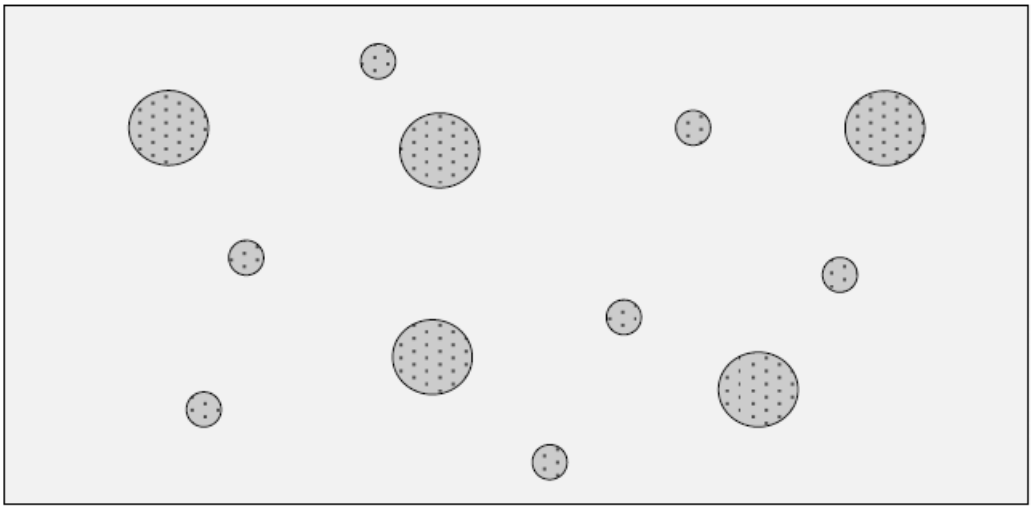
Figure C2.10

2019.05.27.13.08.22
CELL #3

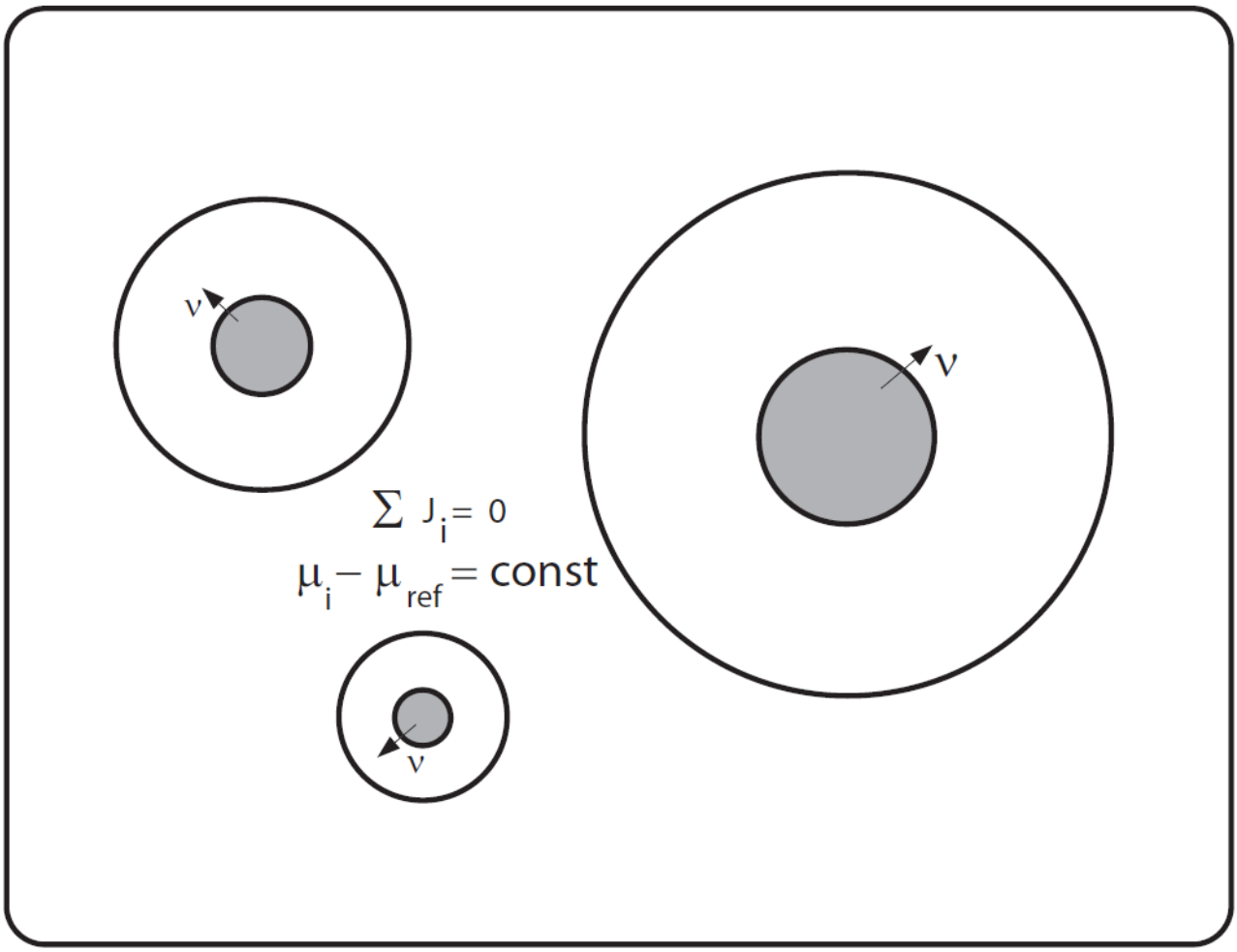



```
POST-3:
POST-3:
POST-3:
POST-3:
POST-3:@?<_hit_return_to_continue_>
POST-3:
POST-3: set-inter
 --OK---
POST-3:
```

Diffusion in Dispersed Systems



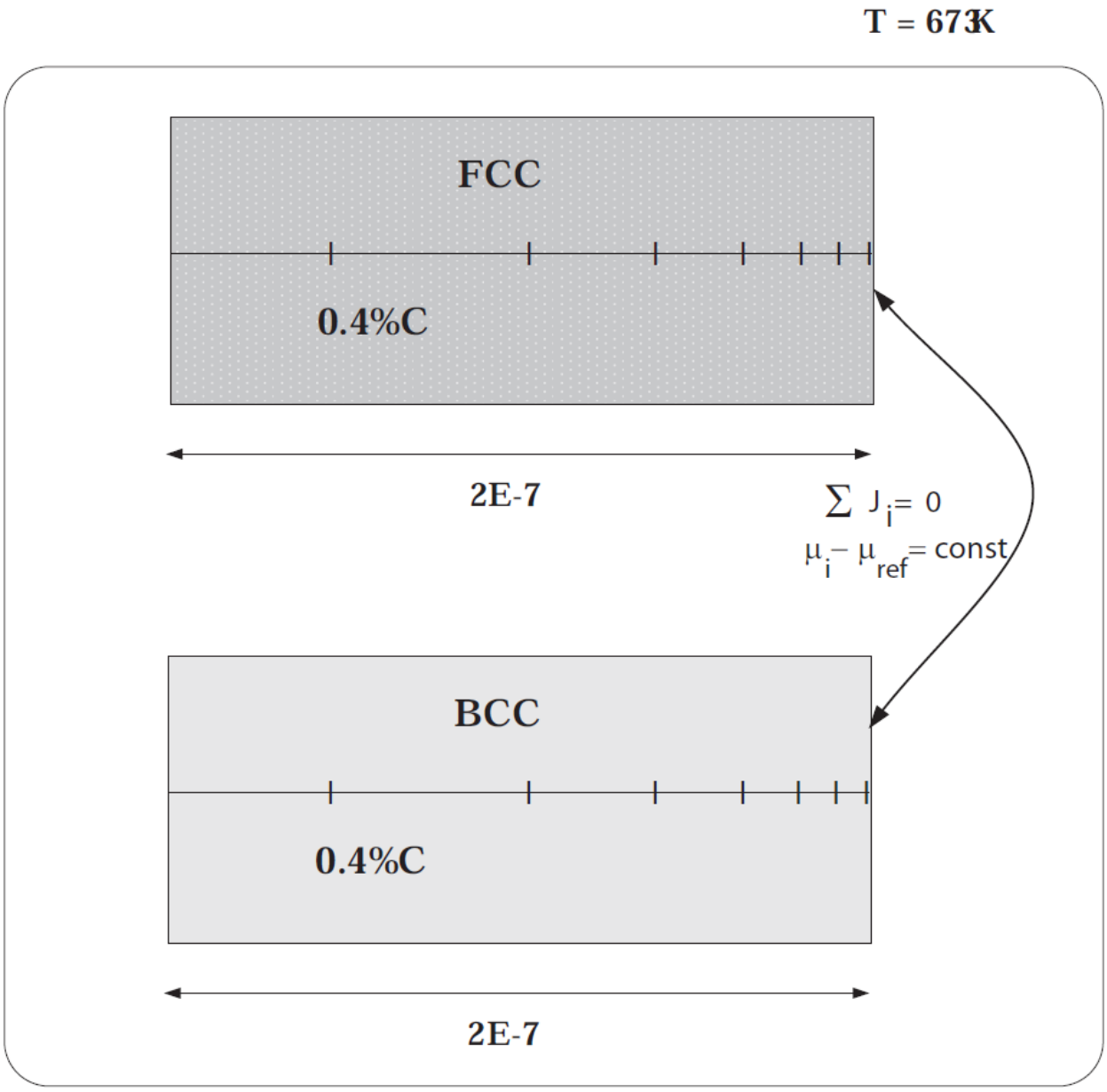
Cell Calculations



Example exc1

'Carbon cannon' in α/γ Fe-C system: Two-cell calculation

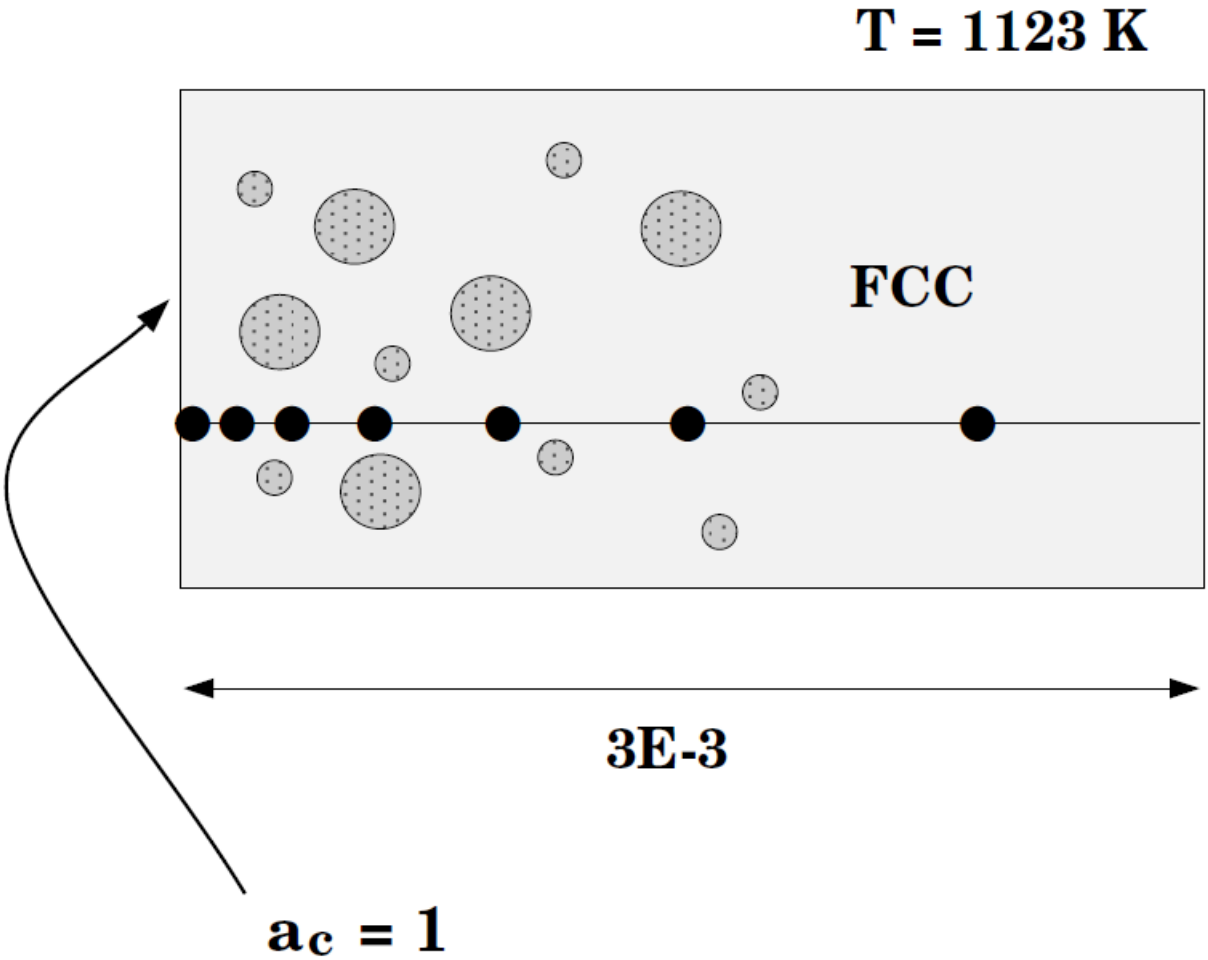
This example simulates what happens to a ferrite plate that has inherited the carbon content of its parent austenite. The ferrite plate formed is embedded in an austenite matrix. This setup corresponds to a proposed mechanism for formation of Widmannstätten ferrite or for the ferrite phase of the bainite 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.



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 Software  (build 20130) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri May 24 17:06:15 2019


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  v9.1

 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 fedemo
 Current database: Iron Demo Database v2.1

 VA                      /-  DEFINED
TDB_FEDEMO: def-sys ni cr c
 NI                      CR                      C
   DEFINED
TDB_FEDEMO: rej ph * all
 GAS:G                   LIQUID:L                BCC_A2
 CBCC_A12                CEMENTITE               CHI_A12
 CUB_A13                 DIAMOND_FCC_A4          FCC_A1
 GRAPHITE                HCP_A3                  KSI_CARBIDE
 LAVES_PHASE_C14         M23C6                   M3C2
 M7C3                    SIGMA  REJECTED
TDB_FEDEMO: res ph fcc,m7c3,m3c2,grap
 FCC_A1                  M7C3                    M3C2
 GRAPHITE  RESTORED
TDB_FEDEMO: get
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 Creating a new composition set FCC_A1#2
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'J. Bratberg, Z. Metallkd., 96 (2005) 335-344; Fe-Cr-Mo-C'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'A. Markstrom, Swerea KIMAB, Sweden; 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. 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'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, 2016; FCC Fe-Cr-C and C-Cr-Ni'
  'NPL, Unpublished work (1989); C-Cr-Ni'
  'A. Dinsdale and T. Chart, MTDS NPL, Unpublished work (1986); CR -NI'
  'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121 -127; Molar
      volumes'
  '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'
  'A. Fernandez Guillermet and G. Grimvall,J. Phys. Chem. Solids, 1992, 53,
      105-125; Molar volumes'
 -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 ni c cr
 NI                      C                       CR
   DEFINED
APP: rej ph * all
 BCC_A2                  FCC_A1  REJECTED
APP: res ph fcc,m7c3,m3c2,grap
 *** M7C3 INPUT IGNORED
 *** M3C2 INPUT IGNORED
 *** GRAP INPUT IGNORED
 FCC_A1  RESTORED
APP: get
 ELEMENTS .....
 SPECIES ......
```

```
 PHASES .......
 Creating a new composition set FCC_A1#3
 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
 INFO: EQUILIBRIUM COMPOSITION AND FRACTION OF SPHEROID PHASES USED AS DEFAULT
DIC>
DIC> @@
DIC> @@ ENTER A STOICHOMETRIC SPHEROIDAL PHASE IN THE REGION
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /AUS/: aus
PHASE TYPE /MATRIX/: sph
PHASE NAME: /NONE/: m3c2
 INFO: EQUILIBRIUM COMPOSITION AND FRACTION OF SPHEROID PHASES USED AS DEFAULT
DIC>
DIC>
DIC> @@
DIC> @@ ENTER A START COMPOSITION FOR THE SPHEROIDAL PHASES
DIC> @@
DIC> enter-composition
REGION NAME : /AUS/: aus
PHASE NAME: /FCC_A1#1/: m7c3
USE EQUILIBRIUM VALUE /Y/: Y
DIC> enter-composition
REGION NAME : /AUS/: aus
PHASE NAME: /FCC_A1#1/: m3c2
USE EQUILIBRIUM VALUE /Y/: Y
DIC>
DIC> @@
DIC> @@ SET THE BOUNDARY CONDITION
DIC> @@
DIC> set-cond
GLOBAL OR BOUNDARY CONDITION /GLOBAL/: boundary
BOUNDARY /LOWER/: lower
CONDITION TYPE /CLOSED_SYSTEM/: mixed
Dependent substitutional element:NI
Dependent interstitial element:VA
TYPE OF CONDITION FOR COMPONENT C /ZERO_FLUX/: activity
LOW TIME LIMIT /0/: 0
ACR(C)(TIME)= 1;
HIGH TIME LIMIT /*/: *
```

```
ANY MORE RANGES /N/: N
TYPE OF CONDITION FOR COMPONENT CR /ZERO_FLUX/: zero-flux
DIC>
DIC> @@
DIC> @@ ENTER THE LABYRINTH FACTOR
DIC> @@
DIC> enter-lab
REGION NAME : aus
f(T,P,VOLFR,X)= volfr**2;
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME. REMEMBER TO BE CAREFUL WITH THE
DIC> @@ TIMESTEP WHEN THERE ARE SPHEROIDAL PHASES PRESENT. IN THIS CASE
DIC> @@ THE TIMESTEP IS NOT ALLOWED TO BE LARGER THAN 1800s.
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 3600000
AUTOMATIC TIMESTEP CONTROL /YES/: YES
MAX TIMESTEP DURING INTEGRATION /360000/: 1800
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC> @@
DIC> @@ IN ORDER SO SAVE SOME SPACE ON THE DISK THE RESULT IS STORED
DIC> @@ SELECTIVELY. OTHERWISE THE STORE-RESULT-FILE FROM THIS EXAMPLE
DIC> @@ WOULD BE VERY LARGE.
DIC> @@
DIC> set-simulation-condition
NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /AUTO/:
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/: 99
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -> 1): /AUTO/:
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/:
DIC>
DIC> @@ BY DEFAULT THE "HOMOGENIZATION MODEL" IS USED WHEN MULTIPLE PHASES
DIC> @@ ARE ENTERED IN A SINGLE REGION. FOR THIS EXAMPLE THE HOMOGENIZATION
DIC> @@ MODEL IS DISABLED.
DIC> ho n
 HOMOGENIZATION DISABLED
DIC>
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exd1 y
DIC>
DIC> set-inter
 --OK---
DIC>
```

exd1a-run

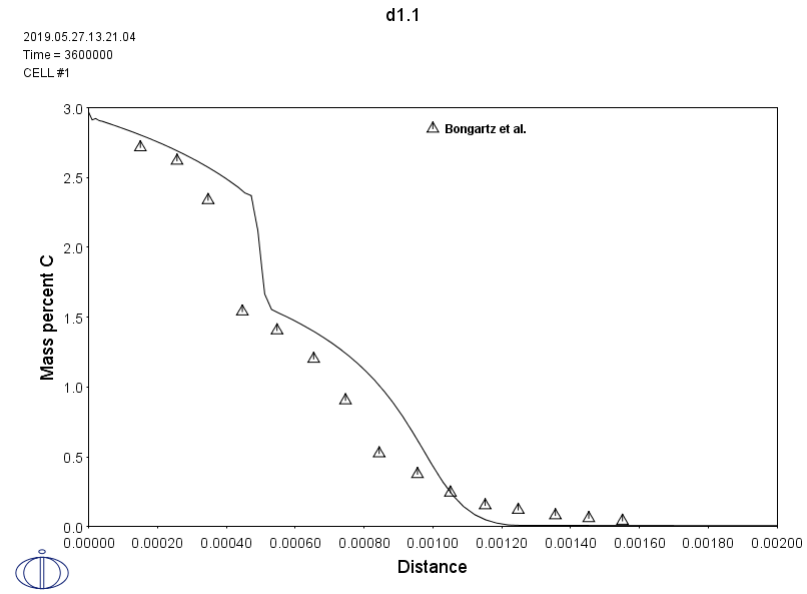
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exd1a\run.DCM"DIC>
DIC>
DIC> @@ exd1_run.DCM
DIC>
DIC> @@
DIC> @@ READ THE SETUP FILE AND START THE SIMULATION
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  0.00000E+00
 *** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
 *** ENTERING M3C2 AS A DIFFUSION NONE PHASE
 *** ENTERING M7C3 AS A DIFFUSION NONE PHASE
DIC> read exd1
 OK
DIC> sim
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
 U-FRACTION IN SYSTEM:  C = 4.73399450059566E-06  CR = .273386452547573
                        NI = .726613547452427
 TOTAL SIZE OF SYSTEM:  .003 [m]
  WARNING:M7C3 HAS NO VOLUME FRACTION, CREATING ONE
  WARNING:M3C2 HAS NO VOLUME FRACTION, CREATING ONE
 U-FRACTION IN SYSTEM:  C = 4.73399450059565E-06  CR = .273386452547573
                        NI = .726613547452427
 TOTAL SIZE OF SYSTEM:  .003 [m]
 TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = 8.32233829951643E-05  CR = .273386452547572
                        NI = .726613547452428
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                     0 seconds
 TIME =  0.10010000E-03 DT =  0.10000000E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = 1.14491977930615E-04  CR = .273386452547544
                        NI = .726613547452456
 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 = 1.34397531949353E-04  CR = .273386452541228
                        NI = .726613547458772
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                     1 seconds
 TIME =   61.226617     DT =   60.826517     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = 1.73234190866322E-04  CR = .273386451404805
                        NI = .726613548595195
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                     0 seconds
 TIME =   136.73132     DT =   75.504702     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = 2.15195361346141E-04  CR = .273386450378639
                        NI = .726613549621361
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                     0 seconds
 TIME =   246.77986     DT =   110.04854     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = 2.65132773423414E-04  CR = .273386449367934
                        NI = .726613550632066
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                     0 seconds
 TIME =   417.73078     DT =   170.95092     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = 3.26703519714753E-04  CR = .273386448427441
                        NI = .72661355157256
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                     0 seconds
 TIME =   700.87762     DT =   283.14684     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = 4.0385218367726E-04  CR = .273386447458974
                        NI = .726613552541025
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                     0 seconds
 TIME =   1196.7621     DT =   495.88443     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = 5.03958315341E-04  CR = .273386446322885
                        NI = .726613553677115
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                     1 seconds
 TIME =   2136.4660     DT =   939.70399     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = 6.43012086810243E-04  CR = .273386444988437
                        NI = .726613555011563
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                     0 seconds
 TIME =   3936.4660     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = 8.38519749163091E-04  CR = .273386443511134
                        NI = .726613556488866
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                     0 seconds
 TIME =   5736.4660     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00101736970332151  CR = .273386442681225
                        NI = .726613557318775
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                     0 seconds
 TIME =   7536.4660     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00118296902880159  CR = .273386442066142
                        NI = .726613557933858
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                     1 seconds
 TIME =   9336.4660     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00133879540957737  CR = .273386441011294
                        NI = .726613558988706
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                     0 seconds
 TIME =   11136.466     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00148538430057559  CR = .27338643927903
                        NI = .72661356072097
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                     0 seconds
 TIME =   12936.466     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00162329996141556  CR = .273386436825667
                        NI = .726613563174333
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                     0 seconds
 TIME =   14736.466     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00175666371078122  CR = .273386434544898
                        NI = .726613565455102
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                     1 seconds
 TIME =   16509.560     DT =   1773.0939     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0018841969867604  CR = .273386432317815
                        NI = .726613567682185
```

```
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   18202.529     DT =   1692.9692     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00200374370728574  CR = .273386430131716
                        NI = .726613569868284
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   19871.496     DT =   1668.9668     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00212043403493915  CR = .273386427985689
                        NI = .726613572014311
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   21585.287     DT =   1713.7913     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00223651041851038  CR = .273386426227076
                        NI = .726613573772924
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1 seconds
 TIME =   23385.287     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00235302551823153  CR = .273386424970865
                        NI = .726613575029135
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   25185.287     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00246605263454349  CR = .273386424047238


output ignored...



... output resumed

  CPU time used in timestep                    1 seconds
 TIME =   3563985.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0314537983526268  CR = .273386325210633
                        NI = .726613674789367
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3565785.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .031461732903015  CR = .273386325190176
                        NI = .726613674809824
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3567585.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0314696650642583  CR = .273386325169501
                        NI = .726613674830499
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3569385.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0314775948480469  CR = .273386325148609
                        NI = .726613674851391
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1 seconds
 TIME =   3571185.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0314855222664732  CR = .2733863251275
                        NI = .7266136748725
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3572985.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0314934473320118  CR = .273386325106173
                        NI = .726613674893827
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3574785.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0315013700574986  CR = .273386325084628
                        NI = .726613674915372
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3576585.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0315092904561122  CR = .273386325062865
                        NI = .726613674937135
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1 seconds
 TIME =   3578385.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .031517208541354  CR = .273386325040884
                        NI = .726613674959116
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3580185.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0315251243270302  CR = .273386325018685
                        NI = .726613674981315
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3581985.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0315330378272334  CR = .273386324996267
                        NI = .726613675003733
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3583785.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0315409490563254  CR = .273386324973631
                        NI = .726613675026369
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1 seconds
 TIME =   3585585.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0315488580289196  CR = .273386324950775
                        NI = .726613675049225
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3587385.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0315567647598653  CR = .273386324927701
                        NI = .726613675072299
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3589185.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0315646692642311  CR = .273386324904407
                        NI = .726613675095593
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3590985.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0315725715572894  CR = .273386324880894
                        NI = .726613675119106
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1 seconds
 TIME =   3592785.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .031580471654502  CR = .273386324857161
                        NI = .726613675142839
```

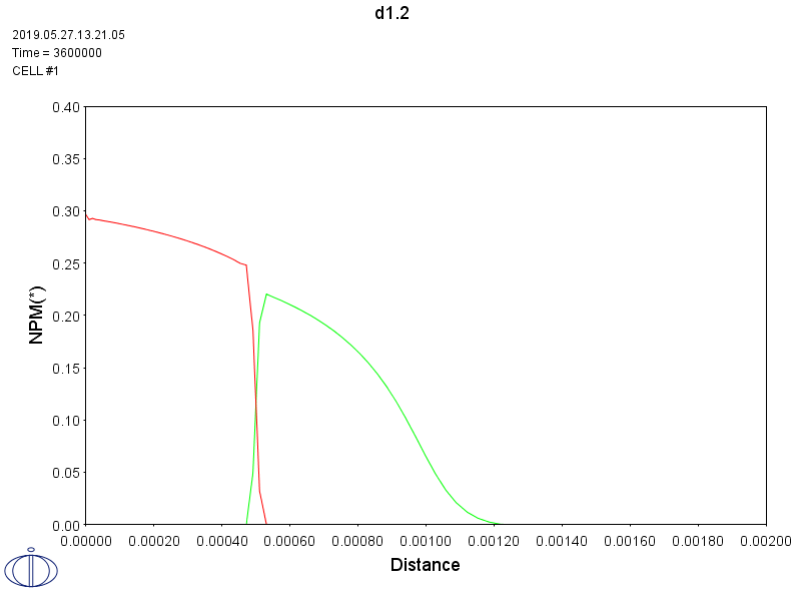
```
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3594585.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0315883695715049  CR = .273386324833209
                        NI = .726613675166791
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3596385.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .031596265324095  CR = .273386324809036
                        NI = .726613675190964
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3598185.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0316041589282162  CR = .273386324784643
                        NI = .726613675215357
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1 seconds
 TIME =   3599985.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0316120503999464  CR = .27338632476003
                        NI = .72661367523997
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3600000.0     DT =   14.712794     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .031612115745499  CR = .273386324759819
                        NI = .726613675240181
 TOTAL SIZE OF SYSTEM:  .003 [m]
 MUST SAVE WORKSPACE ON FILE
 WORKSPACE SAVED ON FILE
 RECLAIMING WORKSPACE
 DELETING TIME-RECORD FOR TIME    0.0000000
 DELETING TIME-RECORD FOR TIME   0.10000000E-06
 DELETING TIME-RECORD FOR TIME   0.10010000E-03
 DELETING TIME-RECORD FOR TIME    163785.29
 DELETING TIME-RECORD FOR TIME    341985.29
 DELETING TIME-RECORD FOR TIME    520185.29
 DELETING TIME-RECORD FOR TIME    698385.29
 DELETING TIME-RECORD FOR TIME    876585.29
 DELETING TIME-RECORD FOR TIME    1054785.3
 DELETING TIME-RECORD FOR TIME    1232985.3
 DELETING TIME-RECORD FOR TIME    1411185.3
 DELETING TIME-RECORD FOR TIME    1589385.3
 DELETING TIME-RECORD FOR TIME    1767585.3
 DELETING TIME-RECORD FOR TIME    1945785.3
 DELETING TIME-RECORD FOR TIME    2123985.3
 DELETING TIME-RECORD FOR TIME    2302185.3
 DELETING TIME-RECORD FOR TIME    2480385.3
 DELETING TIME-RECORD FOR TIME    2658585.3
 DELETING TIME-RECORD FOR TIME    2836785.3
 DELETING TIME-RECORD FOR TIME    3014985.3
 DELETING TIME-RECORD FOR TIME    3193185.3
 DELETING TIME-RECORD FOR TIME    3371385.3
 DELETING TIME-RECORD FOR TIME    3549585.3
 DELETING TIME-RECORD FOR TIME    3596385.3
 DELETING TIME-RECORD FOR TIME    3598185.3

 KEEPING TIME-RECORD FOR TIME    3599985.3
 AND FOR TIME                    3600000.0
 WORKSPACE RECLAIMED

 TIMESTEP AT     3600000.00     SELECTED

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

exd1a-plot

```
DIC>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
```

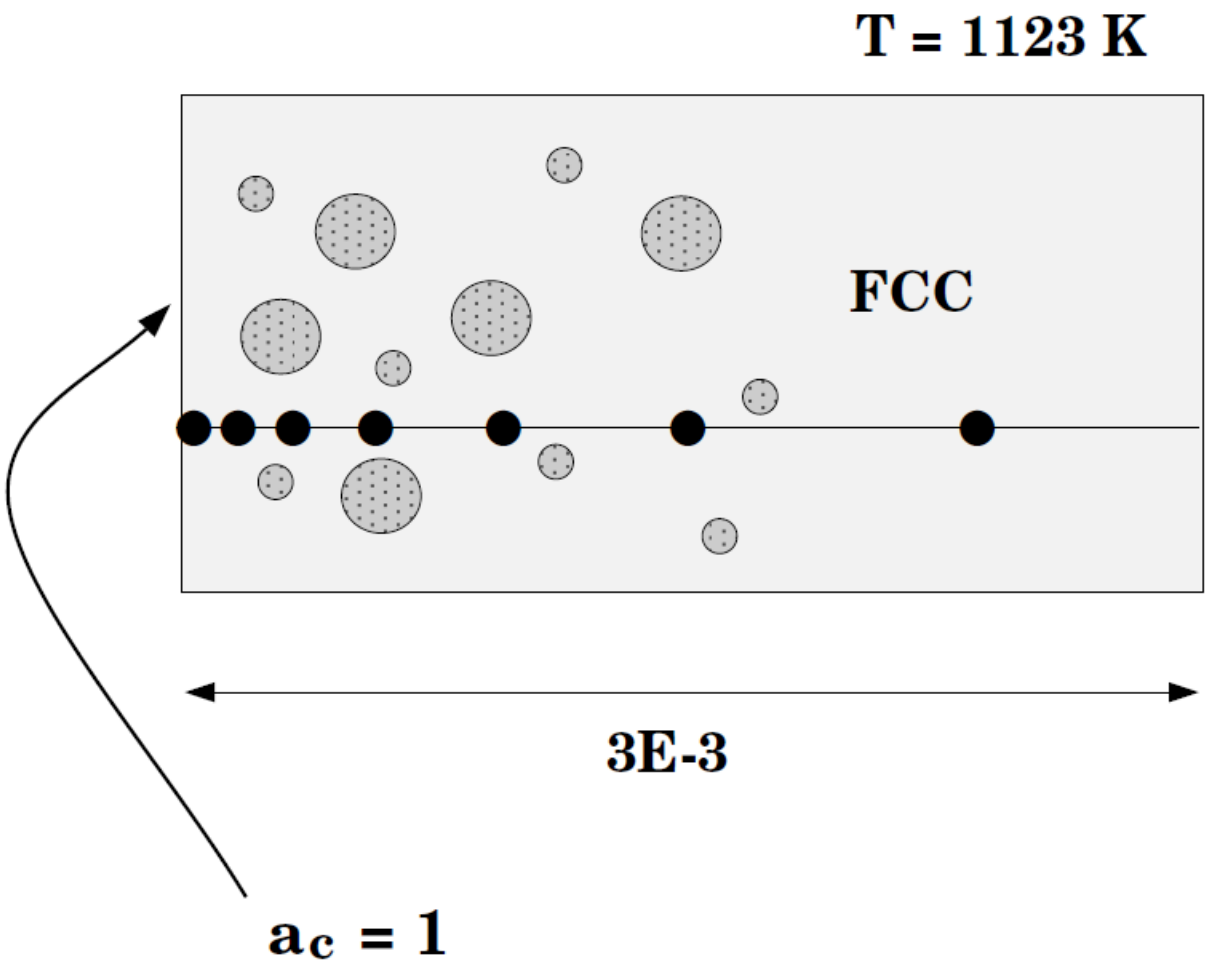



```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: set-inter
 --OK---
POST-1:
```

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
 Software  (build 20130) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri May 24 17:06:15 2019


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  v9.1

 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 fedemo
 Current database: Iron Demo Database v2.1

 VA                      /-  DEFINED
TDB_FEDEMO: def-sys ni cr c
 NI                      CR                      C
   DEFINED
TDB_FEDEMO: rej ph * all
 GAS:G                   LIQUID:L                BCC_A2
 CBCC_A12                CEMENTITE               CHI_A12
 CUB_A13                 DIAMOND_FCC_A4          FCC_A1
 GRAPHITE                HCP_A3                  KSI_CARBIDE
 LAVES_PHASE_C14         M23C6                   M3C2
 M7C3                    SIGMA  REJECTED
TDB_FEDEMO: res ph fcc,m7c3,m3c2,grap
 FCC_A1                  M7C3                    M3C2
 GRAPHITE  RESTORED
TDB_FEDEMO: get
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 Creating a new composition set FCC_A1#2
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'J. Bratberg, Z. Metallkd., 96 (2005) 335-344; Fe-Cr-Mo-C'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'A. Markstrom, Swerea KIMAB, Sweden; 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. 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'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, 2016; FCC Fe-Cr-C and C-Cr-Ni'
  'NPL, Unpublished work (1989); C-Cr-Ni'
  'A. Dinsdale and T. Chart, MTDS NPL, Unpublished work (1986); CR -NI'
  'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121 -127; Molar
      volumes'
  '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'
  'A. Fernandez Guillermet and G. Grimvall,J. Phys. Chem. Solids, 1992, 53,
      105-125; Molar volumes'
 -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 ni c cr
 NI                      C                       CR
   DEFINED
APP: rej ph * all
 BCC_A2                  FCC_A1  REJECTED
APP: res ph fcc,m7c3,m3c2,grap
 *** M7C3 INPUT IGNORED
 *** M3C2 INPUT IGNORED
 *** GRAP INPUT IGNORED
 FCC_A1  RESTORED
APP: get
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 Creating a new composition set FCC_A1#3
```

```
 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
 INFO: EQUILIBRIUM COMPOSITION AND FRACTION OF SPHEROID PHASES USED AS DEFAULT
DIC>
DIC> @@
DIC> @@ ENTER A STOICHOMETRIC SPHEROIDAL PHASE IN THE REGION
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /AUS/: aus
PHASE TYPE /MATRIX/: sph
PHASE NAME: /NONE/: m3c2
 INFO: EQUILIBRIUM COMPOSITION AND FRACTION OF SPHEROID PHASES USED AS DEFAULT
DIC>
DIC>
DIC> @@
DIC> @@ ENTER A START COMPOSITION FOR THE SPHEROIDAL PHASES
DIC> @@
DIC> enter-composition
REGION NAME : /AUS/: aus
PHASE NAME: /FCC_A1#1/: m7c3
USE EQUILIBRIUM VALUE /Y/: Y
DIC> enter-composition
REGION NAME : /AUS/: aus
PHASE NAME: /FCC_A1#1/: m3c2
USE EQUILIBRIUM VALUE /Y/: Y
DIC>
DIC> @@
DIC> @@ SET THE BOUNDARY CONDITION
DIC> @@
DIC> set-cond
GLOBAL OR BOUNDARY CONDITION /GLOBAL/: boundary
BOUNDARY /LOWER/: lower
CONDITION TYPE /CLOSED_SYSTEM/: mixed
Dependent substitutional element:NI
Dependent interstitial element:VA
TYPE OF CONDITION FOR COMPONENT C /ZERO_FLUX/: activity
LOW TIME LIMIT /0/: 0
ACR(C)(TIME)= 1;
HIGH TIME LIMIT /*/: *
ANY MORE RANGES /N/: N
TYPE OF CONDITION FOR COMPONENT CR /ZERO_FLUX/: zero-flux
```

```
DIC>
DIC> @@
DIC> @@ SELECT THE HOMOGENIZATION FUNCTION
DIC> @@
DIC> enter-homo
ENTER HOMOGENIZATION FUNCTION # /5/: 8
 SELECTED FUNCTION IS LABYRINTH FACTOR f**2 WITH PRESCRIBED MATRIX PHASE
PHASE NAME: fcc#1
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME. REMEMBER TO BE CAREFUL WITH THE
DIC> @@ TIMESTEP WHEN SPHEROIDAL PHASES ARE PRESENT. IN THIS CASE
DIC> @@ THE TIMESTEP IS NOT ALLOWED TO BE LARGER THAN 1800s.
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 3600000
AUTOMATIC TIMESTEP CONTROL /YES/: YES
MAX TIMESTEP DURING INTEGRATION /360000/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC> @@
DIC> @@ TO SAVE SOME SPACE ON THE DISK THE RESULTS ARE STORED SELECTIVELY,
DIC> @@ OTHERWISE THE STORE-RESULT-FILE FROM THIS EXAMPLE WOULD BE
DIC> @@ VERY LARGE.
DIC> @@
DIC> set-simulation-condition
NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /AUTO/:
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/: 99
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -> 1): /AUTO/:
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/:
DIC>
DIC> @@
DIC> @@ SAVE THE SETUP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exd1 y
DIC>
DIC> set-inter
 --OK---
DIC>
```

exd1b-run

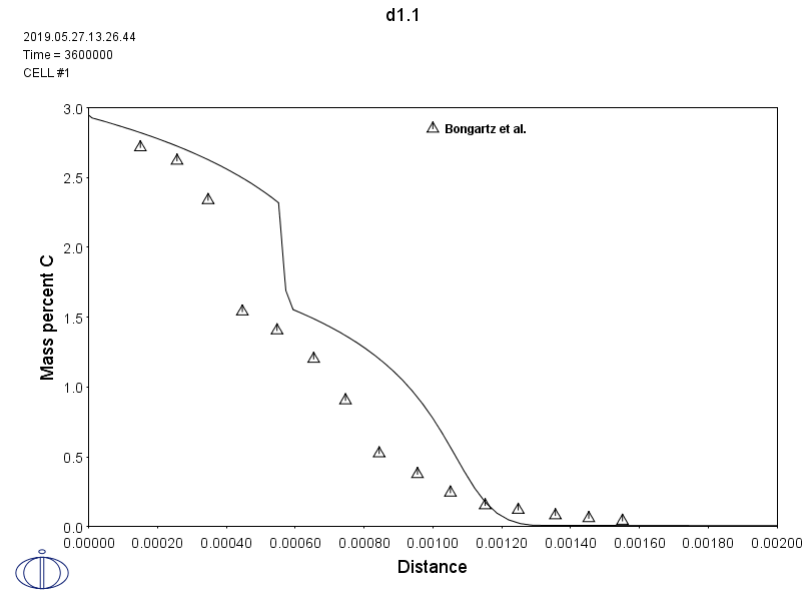
```
DIC>AboutDIC>DIC>MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exd1b\run.DCM"DIC>
DIC>
DIC> @@ exd1_run.DCM
DIC>
DIC> @@
DIC> @@ READ THE SETUP FILE AND START THE SIMULATION
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  0.00000E+00
 *** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
 *** ENTERING M3C2 AS A DIFFUSION NONE PHASE
 *** ENTERING M7C3 AS A DIFFUSION NONE PHASE
DIC> read exd1
 OK
DIC> sim
 DEGREE OF IMPLICITY SET TO EULER BACKWARD
 STARTING SIMULATION USING HOMOGENIZATION MODEL
 ----------------------------------------------
 INFO: PHASE WITH LIMITED SOLUBILITY OF ELEMENT(S) EXIST
 A FALLBACK PHASE ZZDICTRA_GHOST WILL BE DEFINED
 ALONG WITH THE FOLLOWING PARAMETERS:
 G(ZZDICTRA_GHOST,C;0)-H298(GRAPHITE,C;0)
 G(ZZDICTRA_GHOST,CR;0)-H298(BCC_A2,CR;0)
 G(ZZDICTRA_GHOST,NI;0)-H298(FCC_A1,NI;0)
 L(ZZDICTRA_GHOST,C,CR;0)
 L(ZZDICTRA_GHOST,C,NI;0)
 L(ZZDICTRA_GHOST,CR,NI;0)
  WARNING:M7C3 HAS NO VOLUME FRACTION, CREATING ONE
  WARNING:M3C2 HAS NO VOLUME FRACTION, CREATING ONE
Starting time-step t0=   0.0000000     dt=  0.10000000E-06
Starting time-step t0=  0.10000000E-06 dt=  0.20000000E-06
Starting time-step t0=  0.30000000E-06 dt=  0.40000000E-06
Starting time-step t0=  0.70000000E-06 dt=  0.80000000E-06
Starting time-step t0=  0.15000000E-05 dt=  0.16000000E-05
Starting time-step t0=  0.31000000E-05 dt=  0.32000000E-05
Starting time-step t0=  0.63000000E-05 dt=  0.64000000E-05
Starting time-step t0=  0.12700000E-04 dt=  0.12800000E-04
Starting time-step t0=  0.25500000E-04 dt=  0.25600000E-04
Starting time-step t0=  0.51100000E-04 dt=  0.51200000E-04
Starting time-step t0=  0.10230000E-03 dt=  0.10240000E-03
Starting time-step t0=  0.20470000E-03 dt=  0.20480000E-03
Starting time-step t0=  0.40950000E-03 dt=  0.40960000E-03
Starting time-step t0=  0.81910000E-03 dt=  0.81920000E-03
Starting time-step t0=  0.16383000E-02 dt=  0.16384000E-02
Starting time-step t0=  0.32767000E-02 dt=  0.32768000E-02
Starting time-step t0=  0.65535000E-02 dt=  0.65536000E-02
Starting time-step t0=  0.13107100E-01 dt=  0.13107200E-01
Starting time-step t0=  0.26214300E-01 dt=  0.26214400E-01
Starting time-step t0=  0.52428700E-01 dt=  0.52428800E-01
Starting time-step t0=  0.10485750     dt=  0.52428800E-01
Starting time-step t0=  0.15728630     dt=  0.52428800E-01
Starting time-step t0=  0.20971510     dt=  0.52428800E-01
Starting time-step t0=  0.26214390     dt=  0.52428800E-01
Starting time-step t0=  0.31457270     dt=  0.52428800E-01
Starting time-step t0=  0.36700150     dt=  0.10485760
Starting time-step t0=  0.47185910     dt=  0.20971520
Starting time-step t0=  0.68157430     dt=  0.41943040
Starting time-step t0=   1.1010047     dt=  0.41943040
Starting time-step t0=   1.5204351     dt=  0.83886080
Starting time-step t0=   2.3592959     dt=  0.83886080
Starting time-step t0=   3.1981567     dt=  0.83886080
Starting time-step t0=   4.0370175     dt=  0.83886080
Starting time-step t0=   4.8758783     dt=  0.83886080
Starting time-step t0=   5.7147391     dt=  0.83886080
Starting time-step t0=   6.5535999     dt=  0.83886080
Starting time-step t0=   7.3924607     dt=  0.83886080
Starting time-step t0=   8.2313215     dt=  0.83886080
Starting time-step t0=   9.0701823     dt=  0.83886080
Starting time-step t0=   9.9090431     dt=  0.83886080
Starting time-step t0=   10.747904     dt=  0.83886080
Starting time-step t0=   11.586765     dt=  0.83886080
Starting time-step t0=   12.425625     dt=  0.83886080
Starting time-step t0=   13.264486     dt=  0.83886080
Starting time-step t0=   14.103347     dt=  0.83886080
Starting time-step t0=   14.942208     dt=  0.83886080
Starting time-step t0=   15.781069     dt=  0.83886080
Starting time-step t0=   16.619929     dt=  0.83886080
Starting time-step t0=   17.458790     dt=  0.83886080
Starting time-step t0=   18.297651     dt=  0.83886080
Starting time-step t0=   19.136512     dt=  0.83886080
Starting time-step t0=   19.975373     dt=  0.83886080
Starting time-step t0=   20.814233     dt=  0.83886080
Starting time-step t0=   21.653094     dt=  0.83886080
Starting time-step t0=   22.491955     dt=  0.83886080
Starting time-step t0=   23.330816     dt=  0.83886080
Starting time-step t0=   24.169677     dt=  0.83886080
Starting time-step t0=   25.008537     dt=  0.83886080
Starting time-step t0=   25.847398     dt=  0.83886080
Starting time-step t0=   26.686259     dt=  0.83886080
Starting time-step t0=   27.525120     dt=  0.83886080
Starting time-step t0=   28.363981     dt=  0.83886080
Starting time-step t0=   29.202841     dt=  0.83886080
Starting time-step t0=   30.041702     dt=  0.83886080
Starting time-step t0=   30.880563     dt=  0.83886080
Starting time-step t0=   31.719424     dt=  0.83886080
Starting time-step t0=   32.558285     dt=  0.83886080
Starting time-step t0=   33.397145     dt=  0.83886080
Starting time-step t0=   34.236006     dt=  0.83886080
Starting time-step t0=   35.074867     dt=  0.83886080
Starting time-step t0=   35.913728     dt=  0.83886080
Starting time-step t0=   36.752589     dt=  0.83886080
Starting time-step t0=   37.591449     dt=  0.83886080
Starting time-step t0=   38.430310     dt=   1.6777216
Starting time-step t0=   40.108032     dt=   1.6777216
Starting time-step t0=   41.785753     dt=   1.6777216
Starting time-step t0=   43.463475     dt=   1.6777216
Starting time-step t0=   45.141197     dt=   1.6777216
Starting time-step t0=   46.818918     dt=   1.6777216
Starting time-step t0=   48.496640     dt=   1.6777216
Starting time-step t0=   50.174361     dt=   1.6777216
Starting time-step t0=   51.852083     dt=   1.6777216
Starting time-step t0=   53.529805     dt=   1.6777216
```

```
Starting time-step t0=   55.207526     dt=   1.6777216
Starting time-step t0=   56.885248     dt=   1.6777216
Starting time-step t0=   58.562969     dt=   1.6777216
Starting time-step t0=   60.240691     dt=   1.6777216
Starting time-step t0=   61.918413     dt=   1.6777216
Starting time-step t0=   63.596134     dt=   1.6777216
Starting time-step t0=   65.273856     dt=   1.6777216
Starting time-step t0=   66.951577     dt=   1.6777216
Starting time-step t0=   68.629299     dt=   1.6777216
Starting time-step t0=   70.307021     dt=   1.6777216
Starting time-step t0=   71.984742     dt=   1.6777216
Starting time-step t0=   73.662464     dt=   1.6777216
Starting time-step t0=   75.340185     dt=   1.6777216
Starting time-step t0=   77.017907     dt=   3.3554432
Starting time-step t0=   80.373350     dt=   3.3554432
Starting time-step t0=   83.728793     dt=   3.3554432
Starting time-step t0=   87.084237     dt=   3.3554432
Starting time-step t0=   90.439680     dt=   3.3554432
Starting time-step t0=   93.795123     dt=   3.3554432
Starting time-step t0=   97.150566     dt=   3.3554432
Starting time-step t0=   100.50601     dt=   3.3554432
Starting time-step t0=   103.86145     dt=   3.3554432


output ignored...



... output resumed

 DELETING TIME-RECORD FOR TIME    2273980.3
 DELETING TIME-RECORD FOR TIME    2280852.3
 DELETING TIME-RECORD FOR TIME    2287724.2
 DELETING TIME-RECORD FOR TIME    2294596.2
 DELETING TIME-RECORD FOR TIME    2301468.1
 DELETING TIME-RECORD FOR TIME    2308340.1
 DELETING TIME-RECORD FOR TIME    2315212.0
 DELETING TIME-RECORD FOR TIME    2322084.0
 DELETING TIME-RECORD FOR TIME    2328955.9
 DELETING TIME-RECORD FOR TIME    2335827.9
 DELETING TIME-RECORD FOR TIME    2342699.8
 DELETING TIME-RECORD FOR TIME    2349571.8
 DELETING TIME-RECORD FOR TIME    2356443.7
 DELETING TIME-RECORD FOR TIME    2363315.7
 DELETING TIME-RECORD FOR TIME    2370187.6
 DELETING TIME-RECORD FOR TIME    2377059.6
 DELETING TIME-RECORD FOR TIME    2383931.5
 DELETING TIME-RECORD FOR TIME    2390803.5
 DELETING TIME-RECORD FOR TIME    2397675.4
 DELETING TIME-RECORD FOR TIME    2404547.3
 DELETING TIME-RECORD FOR TIME    2411419.3
 DELETING TIME-RECORD FOR TIME    2418291.2
 DELETING TIME-RECORD FOR TIME    2425163.2
 DELETING TIME-RECORD FOR TIME    2432035.1
 DELETING TIME-RECORD FOR TIME    2438907.1
 DELETING TIME-RECORD FOR TIME    2445779.0
 DELETING TIME-RECORD FOR TIME    2452651.0
 DELETING TIME-RECORD FOR TIME    2459522.9
 DELETING TIME-RECORD FOR TIME    2466394.9
 DELETING TIME-RECORD FOR TIME    2473266.8
 DELETING TIME-RECORD FOR TIME    2480138.8
 DELETING TIME-RECORD FOR TIME    2487010.7
 DELETING TIME-RECORD FOR TIME    2493882.7
 DELETING TIME-RECORD FOR TIME    2500754.6
 DELETING TIME-RECORD FOR TIME    2507626.6
 DELETING TIME-RECORD FOR TIME    2514498.5
 DELETING TIME-RECORD FOR TIME    2521370.5
 DELETING TIME-RECORD FOR TIME    2528242.4
 DELETING TIME-RECORD FOR TIME    2535114.4
 DELETING TIME-RECORD FOR TIME    2541986.3
 DELETING TIME-RECORD FOR TIME    2548858.3
 DELETING TIME-RECORD FOR TIME    2555730.2
 DELETING TIME-RECORD FOR TIME    2562602.1
 DELETING TIME-RECORD FOR TIME    2569474.1
 DELETING TIME-RECORD FOR TIME    2576346.0
 DELETING TIME-RECORD FOR TIME    2583218.0
 DELETING TIME-RECORD FOR TIME    2593525.9
 DELETING TIME-RECORD FOR TIME    2600397.9
 DELETING TIME-RECORD FOR TIME    2607269.8
 DELETING TIME-RECORD FOR TIME    2614141.8
 DELETING TIME-RECORD FOR TIME    2621013.7
 DELETING TIME-RECORD FOR TIME    2627885.6
 DELETING TIME-RECORD FOR TIME    2634757.6
 DELETING TIME-RECORD FOR TIME    2641629.5
 DELETING TIME-RECORD FOR TIME    2648501.5
 DELETING TIME-RECORD FOR TIME    2655373.4
 DELETING TIME-RECORD FOR TIME    2662245.4
 DELETING TIME-RECORD FOR TIME    2669117.3
 DELETING TIME-RECORD FOR TIME    2675989.3
 DELETING TIME-RECORD FOR TIME    2682861.2
 DELETING TIME-RECORD FOR TIME    2689733.2
 DELETING TIME-RECORD FOR TIME    2696605.1
 DELETING TIME-RECORD FOR TIME    2703477.1
 DELETING TIME-RECORD FOR TIME    2710349.0
 DELETING TIME-RECORD FOR TIME    2717221.0
 DELETING TIME-RECORD FOR TIME    2724092.9
 DELETING TIME-RECORD FOR TIME    2730964.9
 DELETING TIME-RECORD FOR TIME    2737836.8
 DELETING TIME-RECORD FOR TIME    2744708.8
 DELETING TIME-RECORD FOR TIME    2758452.7
 DELETING TIME-RECORD FOR TIME    2772196.6
 DELETING TIME-RECORD FOR TIME    2785940.4
 DELETING TIME-RECORD FOR TIME    2799684.3
 DELETING TIME-RECORD FOR TIME    2813428.2
 DELETING TIME-RECORD FOR TIME    2827172.1
 DELETING TIME-RECORD FOR TIME    2840916.0
 DELETING TIME-RECORD FOR TIME    2854659.9
 DELETING TIME-RECORD FOR TIME    2868403.8
 DELETING TIME-RECORD FOR TIME    2875275.8
 DELETING TIME-RECORD FOR TIME    2882147.7
 DELETING TIME-RECORD FOR TIME    2895891.6
 DELETING TIME-RECORD FOR TIME    2909635.5
 DELETING TIME-RECORD FOR TIME    2923379.4
 DELETING TIME-RECORD FOR TIME    2937123.3
 DELETING TIME-RECORD FOR TIME    2950867.2
 DELETING TIME-RECORD FOR TIME    2964611.1
```

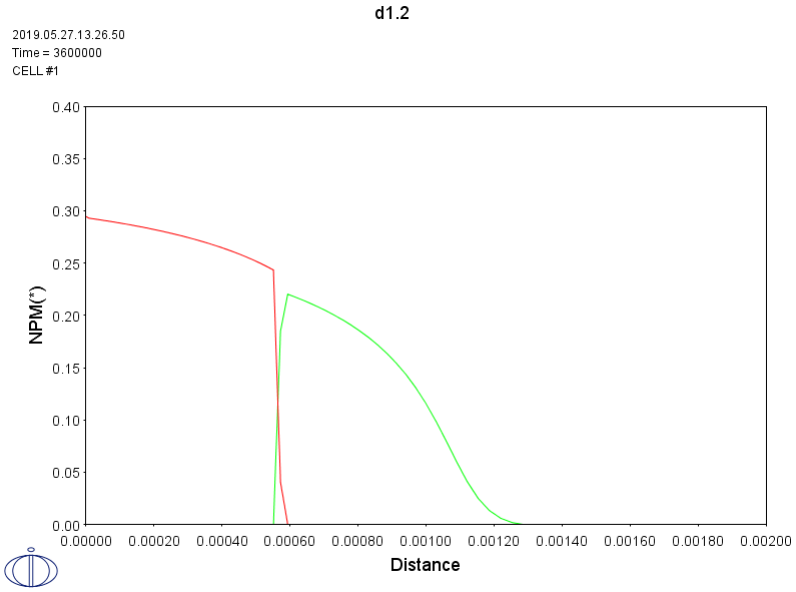
```
 DELETING TIME-RECORD FOR TIME    2978355.0
 DELETING TIME-RECORD FOR TIME    2992098.9
 DELETING TIME-RECORD FOR TIME    3005842.8
 DELETING TIME-RECORD FOR TIME    3019586.7
 DELETING TIME-RECORD FOR TIME    3033330.6
 DELETING TIME-RECORD FOR TIME    3047074.5
 DELETING TIME-RECORD FOR TIME    3060818.4
 DELETING TIME-RECORD FOR TIME    3074562.2
 DELETING TIME-RECORD FOR TIME    3088306.1
 DELETING TIME-RECORD FOR TIME    3102050.0
 DELETING TIME-RECORD FOR TIME    3115793.9
 DELETING TIME-RECORD FOR TIME    3129537.8
 DELETING TIME-RECORD FOR TIME    3143281.7
 DELETING TIME-RECORD FOR TIME    3157025.6
 DELETING TIME-RECORD FOR TIME    3170769.5
 DELETING TIME-RECORD FOR TIME    3184513.4
 DELETING TIME-RECORD FOR TIME    3198257.3
 DELETING TIME-RECORD FOR TIME    3212001.2
 DELETING TIME-RECORD FOR TIME    3225745.1
 DELETING TIME-RECORD FOR TIME    3239489.0
 DELETING TIME-RECORD FOR TIME    3253232.9
 DELETING TIME-RECORD FOR TIME    3266976.8
 DELETING TIME-RECORD FOR TIME    3280720.7
 DELETING TIME-RECORD FOR TIME    3294464.6
 DELETING TIME-RECORD FOR TIME    3308208.5
 DELETING TIME-RECORD FOR TIME    3321952.4
 DELETING TIME-RECORD FOR TIME    3335696.3
 DELETING TIME-RECORD FOR TIME    3349440.2
 DELETING TIME-RECORD FOR TIME    3363184.1
 DELETING TIME-RECORD FOR TIME    3376927.9
 DELETING TIME-RECORD FOR TIME    3390671.8
 DELETING TIME-RECORD FOR TIME    3404415.7
 DELETING TIME-RECORD FOR TIME    3418159.6
 DELETING TIME-RECORD FOR TIME    3431903.5
 DELETING TIME-RECORD FOR TIME    3445647.4
 DELETING TIME-RECORD FOR TIME    3459391.3
 DELETING TIME-RECORD FOR TIME    3473135.2
 DELETING TIME-RECORD FOR TIME    3486879.1
 DELETING TIME-RECORD FOR TIME    3500623.0
 DELETING TIME-RECORD FOR TIME    3514366.9
 DELETING TIME-RECORD FOR TIME    3528110.8
 DELETING TIME-RECORD FOR TIME    3541854.7
 DELETING TIME-RECORD FOR TIME    3555598.6
 DELETING TIME-RECORD FOR TIME    3562470.5
 DELETING TIME-RECORD FOR TIME    3572778.5

 KEEPING TIME-RECORD FOR TIME    3586522.3
 AND FOR TIME                    3600000.0
 WORKSPACE RECLAIMED
 ------------------------------------------------
 INTERPOLATION SCHEME USED THIS FRACTION OF
 THE ALLOCATED MEMORY:    1.00000000000000
 EFFICIENCY FACTOR:    64.9774292801857
 ------------------------------------------------
 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
```



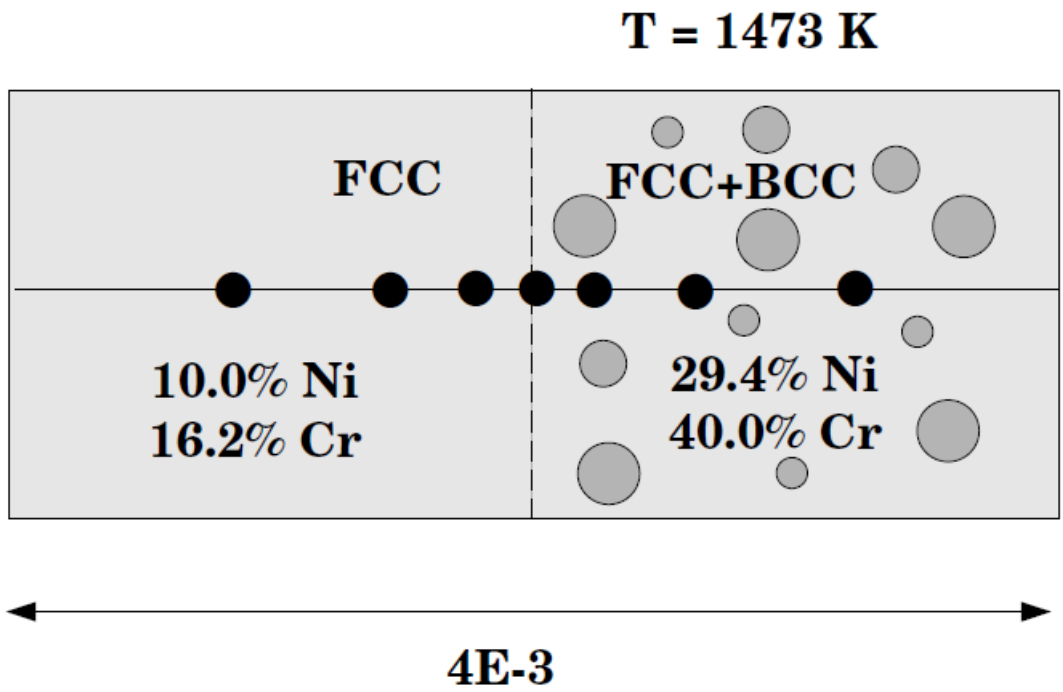

```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: set-inter
 --OK---
POST-1:
```

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 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri May 24 17:06:15 2019


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  v9.1

 VA                      /-  DEFINED
 L12_FCC                 B2_BCC                  DICTRA_FCC_A1
   REJECTED
TDB_TCFE9: sw fedemo
 Current database: Iron Demo Database v2.1

 VA                      /-  DEFINED
TDB_FEDEMO: def-sys fe ni cr
 FE                      NI                      CR
   DEFINED
TDB_FEDEMO: rej ph * all
 LIQUID:L                BCC_A2                  CBCC_A12
 CHI_A12                 CUB_A13                 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, 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
 INFO: EQUILIBRIUM COMPOSITION AND FRACTION OF SPHEROID PHASES USED AS DEFAULT
DIC>
DIC> @@
DIC> @@ ENTER A COMPOSITION FOR THE SPHEROIDAL PHASE
DIC> @@ USE THE EQUILIBRIUM VALUE
DIC> @@
DIC> enter-composition
REGION NAME : /FER/: fer
PHASE NAME: /FCC_A1/: bcc
USE EQUILIBRIUM VALUE /Y/: y
DIC>
DIC>
DIC> @@
DIC> @@ ENTER A LABYRINTH FACTOR
DIC> @@ IN THIS CASE THE LOW DIFFUSIVITY PHASE IS THE MATRIX AND THE
DIC> @@ "EFFECTIVE" DIFFUSIVITY IN THE AUSTENITE+FERRITE TWO-PHASE
DIC> @@ REGION IS EXPECTED TO BE HIGHER THAN THE DIFFUSIVITY IN THE
DIC> @@ AUSTENITE.
DIC> enter-lab
REGION NAME : fer
f(T,P,VOLFR,X)= 1+3*(1-volfr)/volfr;
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME AND OTHER SIMULATION PARAMETERS
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 720000
AUTOMATIC TIMESTEP CONTROL /YES/: YES
MAX TIMESTEP DURING INTEGRATION /72000/: 5000
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC> set-simulation-condition
NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /AUTO/:
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/: 99
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -> 1): /AUTO/:
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/:
DIC> @@ BY DEFAULT THE "HOMOGENIZATION MODEL" IS USED WHEN MULTIPLE PHASES
DIC> @@ ARE ENTERED IN A SINGLE REGION. THE HOMOGENIZATION MODEL NEEDS TO BE
DIC> @@ DISABLED FOR THIS EXAMPLE.
DIC> ho n
 HOMOGENIZATION DISABLED
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
```

```
DIC>
DIC> save exd2 y
DIC>
DIC> set-inter
 --OK---
DIC>
```

exd2a-run

```
DIC>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
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
 U-FRACTION IN SYSTEM:  CR = .297842647391913  FE = .517227320517284
                        NI = .184930032090802
 TOTAL SIZE OF SYSTEM:  .004 [m]
  WARNING:BCC_A2 HAS NO VOLUME FRACTION, CREATING ONE
 U-FRACTION IN SYSTEM:  CR = .297842647391913  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 = .184930032042605
 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 = .517227251840506
                        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 = .297847760270075  FE = .517216317308819
                        NI = .184935922421106
 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 = .297849615184743  FE = .517212946633451
                        NI = .184937438181806
 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 = .297850550731974  FE = .517211426818697
                        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 = .29785111900064  FE = .517210569323811
                        NI = .184938311675549
 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 = .297851494954334  FE = .517210020163942
                        NI = .184938484881724
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                     1 seconds
 TIME =   13721.379     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297851732113689  FE = .517209740277054
                        NI = .184938527609257
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                     0 seconds
 TIME =   18721.379     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297851883453508  FE = .517209584045533
                        NI = .184938532500958
 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 = .297851977657557  FE = .517209483265973
                        NI = .184938539076471
 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 = .297852029985828  FE = .517209412426189
                        NI = .184938557587982
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                     1 seconds
 TIME =   33721.379     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852049766012  FE = .517209361691076
                        NI = .184938588542912
 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 = .29785204501547  FE = .517209326359909
                        NI = .184938628624622
 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 = .297852052300693  FE = .517209299378173
                        NI = .184938648321134
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                     0 seconds
 TIME =   48721.379     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852064900642  FE = .517209276184262
                        NI = .184938658915095
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                     1 seconds
 TIME =   53721.379     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852069935261  FE = .517209260646724
                        NI = .184938669418015
 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 = .297852077632326  FE = .517209244116553
```

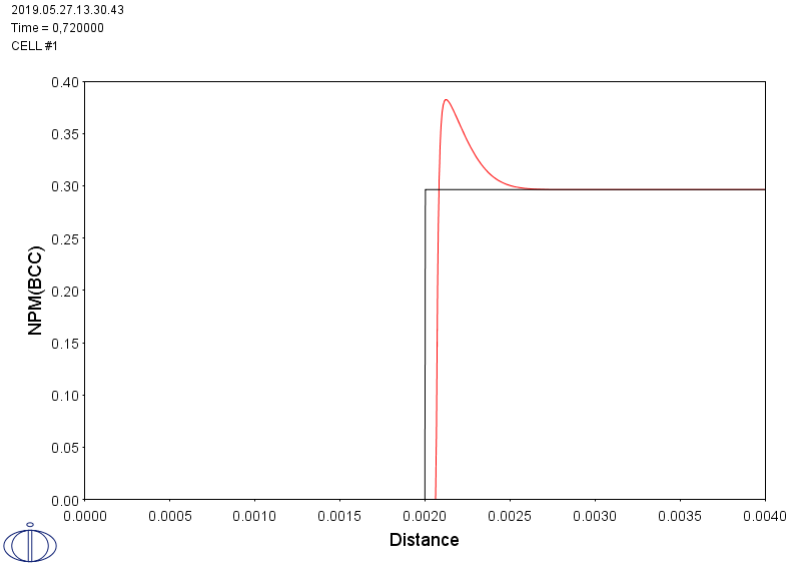
```
                        NI = .184938678251121
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0 seconds
 TIME =   63721.379     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .29785208730734  FE = .517209229697543
                        NI = .184938682995118
 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 = .297852092166834  FE = .517209219702969
                        NI = .184938688130197
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    1 seconds
 TIME =   73721.379     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .29785209023546  FE = .517209210713441
                        NI = .184938699051099
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0 seconds
 TIME =   78721.379     DT =   5000.0000     SUM OF SQUARES =   0.0000000


output ignored...



... output resumed

 U-FRACTION IN SYSTEM:  CR = .297852035243634  FE = .517209097316277
                        NI = .184938867440089
 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 = .297852040343918  FE = .51720909582834
                        NI = .184938863827742
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    1 seconds
 TIME =   613721.38     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852046756562  FE = .517209094403527
                        NI = .184938858839911
 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 = .297852053277546  FE = .51720909326319
                        NI = .184938853459265
 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 = .297852059288763  FE = .517209092514195
                        NI = .184938848197042
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0 seconds
 TIME =   628721.38     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852064436495  FE = .517209092217949
                        NI = .184938843345555
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    1 seconds
 TIME =   633721.38     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852068500945  FE = .517209092415531
                        NI = .184938839083524
 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 = .297852071392548  FE = .51720909308393
                        NI = .184938835523521
 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 = .297852073681694  FE = .517209091807033
                        NI = .184938834511273
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    1 seconds
 TIME =   648721.38     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852074518781  FE = .517209091190446
                        NI = .184938834290772
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0 seconds
 TIME =   653721.38     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852073880059  FE = .517209091158174
                        NI = .184938834961767
 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 = .297852071737295  FE = .517209091673231
                        NI = .184938836589474
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    1 seconds
 TIME =   663721.38     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852068061709  FE = .517209092719061
                        NI = .18493883921923
 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 = .297852062825048  FE = .517209094290038
                        NI = .184938842884914
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0 seconds
 TIME =   673721.38     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852056000144  FE = .51720909638732
                        NI = .184938847612535
 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 = .297852047560721  FE = .517209099016377
                        NI = .184938853422903
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    1 seconds
 TIME =   683721.38     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852037481161  FE = .517209102185645
                        NI = .184938860333194
 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 = .29785203172092  FE = .517209104528002
                        NI = .184938863751078
 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 = .297852035107032  FE = .517209102778462
                        NI = .184938862114506
 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 = .297852041265683  FE = .517209100862437
                        NI = .18493885787188
 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 = .297852048239016  FE = .517209099115002
                        NI = .184938852645982
 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 = .297852055131711  FE = .517209097666818
                        NI = .184938847201471
 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 = .297852061470741  FE = .517209096580471
                        NI = .184938841948787
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    1 seconds
 TIME =   718721.38     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852066979961  FE = .517209095891388
                        NI = .184938837128651
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0 seconds
 TIME =   720000.00     DT =   1278.6211     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852071767321  FE = .517209095429353
                        NI = .184938832803325
 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

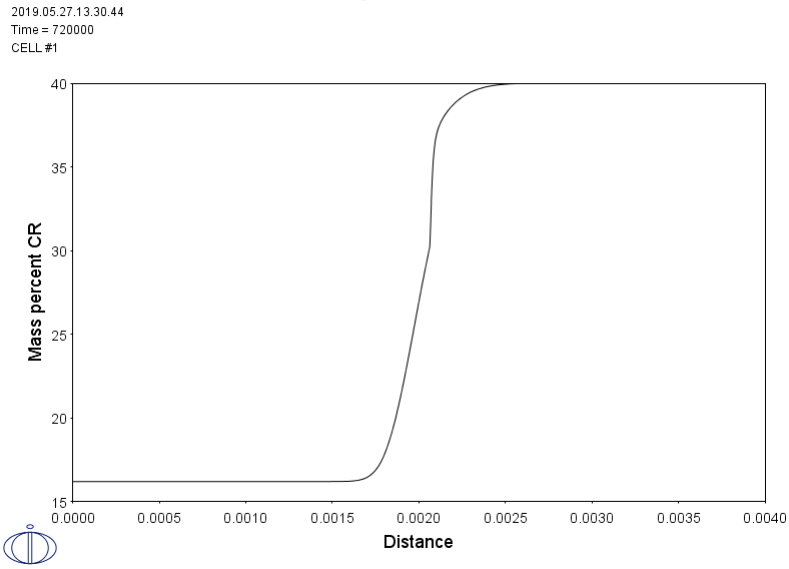
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exd2a\plot.DCM"DIC>
DIC>
DIC> @@ exd2_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE D2
DIC> @@
DIC> @@ ENTER THE DICTRA MODULE AND SPECIFY THE STORE-RESULT FILE
DIC> @@
DIC>
DIC> go d-m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



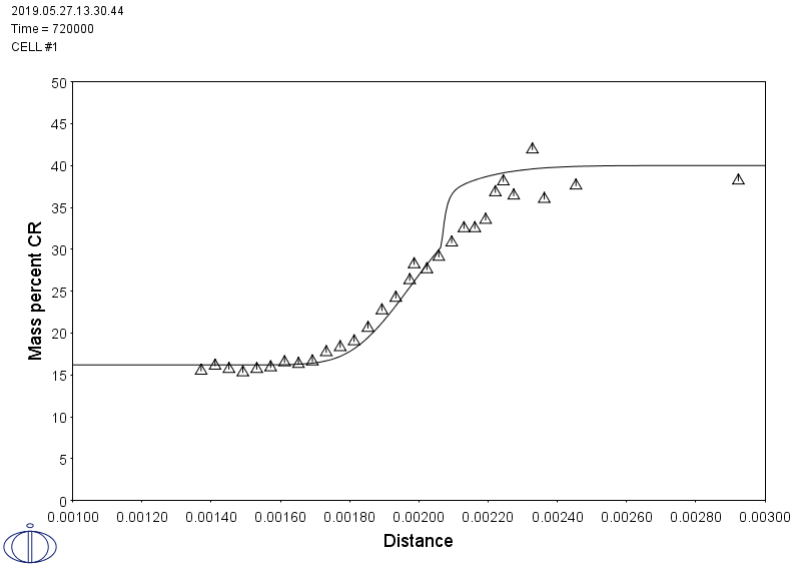

```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1: @@
POST-1: @@ NOW PLOT HOW THE AVERAGE Cr-CONCENTRATION VARIES WITH DISTANCE
POST-1: @@
POST-1: s-d-a y w-p cr
POST-1: s-p-c time last
POST-1: set-tit Figure D2.2
POST-1: plot
```

Figure D2.2



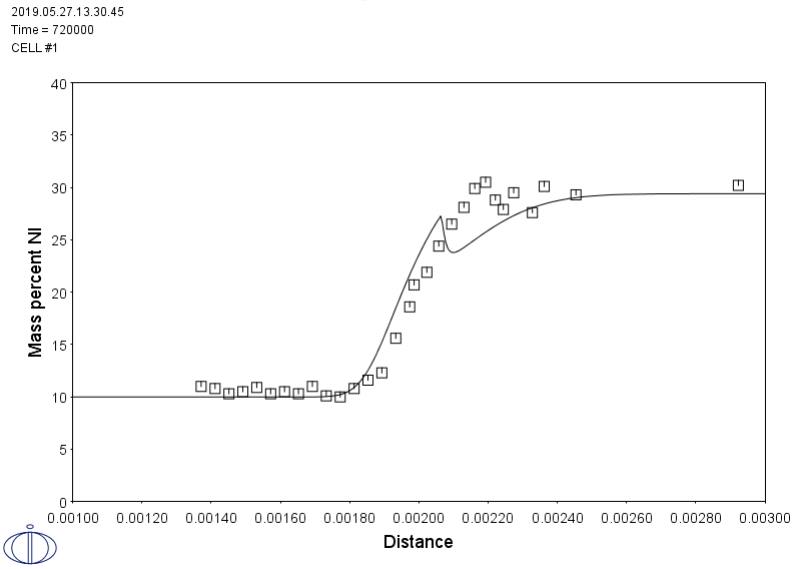
```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1: @@
POST-1: @@ NOW SELECT A BETTER SCALING AND APPEND THE EXPERIMENTAL DATA
POST-1: @@
POST-1:
POST-1: app y exd2.exp
PROLOGUE NUMBER: /0/: 1
DATASET NUMBER(s): /-1/: 4
POST-1:
POST-1: s-s-s y n 0 50
POST-1: s-s-s x n 10e-4 30e-4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

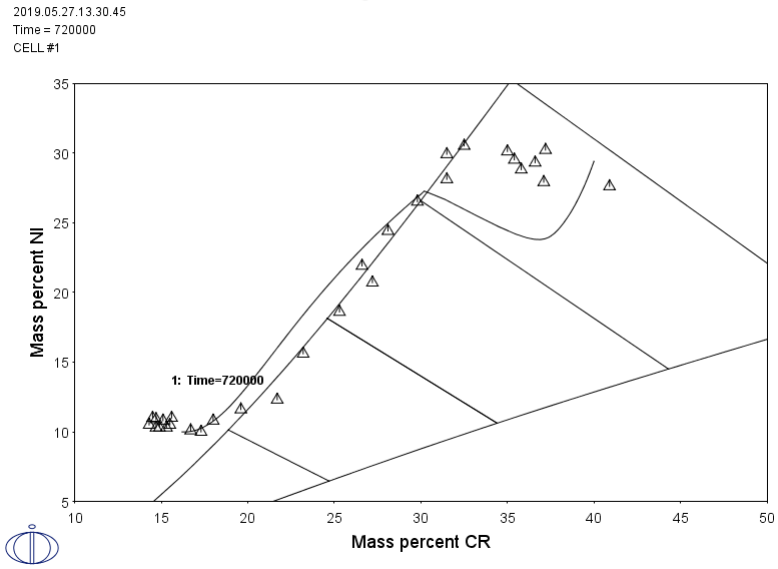
Figure D2.4




```
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



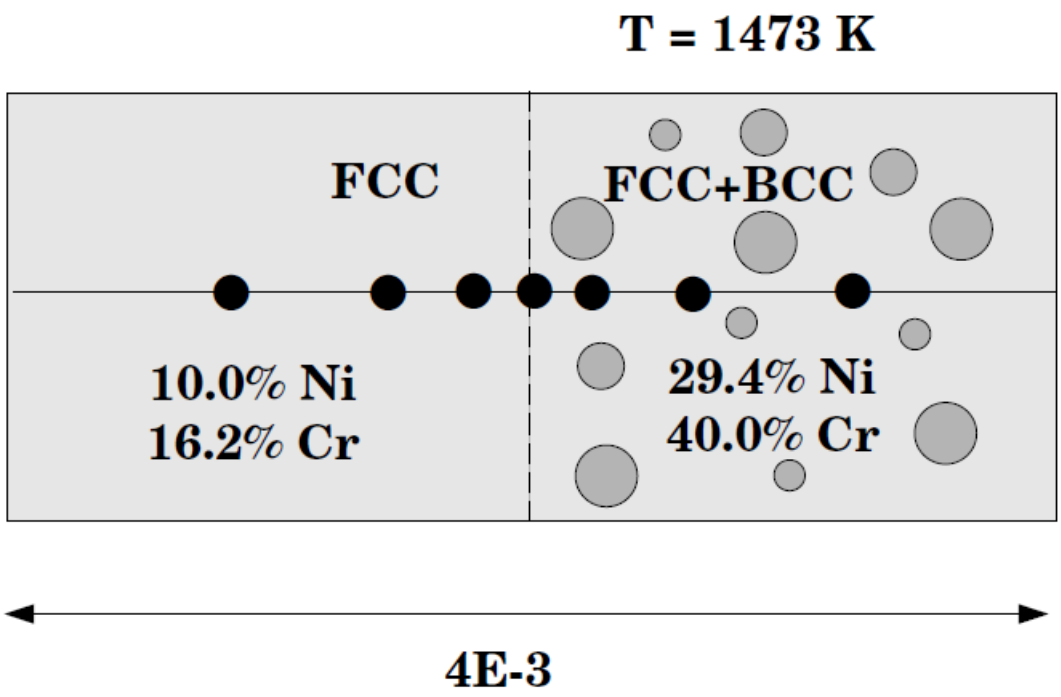

```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1: set-interactive
 --OK---
POST-1:
```

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
 Software  (build 20130) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri May 24 17:06:15 2019


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  v9.1

 VA                      /-  DEFINED
 L12_FCC                 B2_BCC                  DICTRA_FCC_A1
   REJECTED
TDB_TCFE9: sw fedemo
 Current database: Iron Demo Database v2.1

 VA                      /-  DEFINED
TDB_FEDEMO: def-sys fe ni cr
 FE                      NI                      CR
   DEFINED
TDB_FEDEMO: rej ph * all
 LIQUID:L                BCC_A2                  CBCC_A12
 CHI_A12                 CUB_A13                 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, 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
 INFO: EQUILIBRIUM COMPOSITION AND FRACTION OF SPHEROID PHASES USED AS DEFAULT
DIC>
DIC> @@
DIC> @@ ENTER THE COMPOSITION FOR THE SPHEROIDAL PHASE
DIC> @@ USE THE EQUILIBRIUM VALUE
DIC> @@
DIC> enter-composition
REGION NAME : /FER/: fer
PHASE NAME: /FCC_A1/: bcc
USE EQUILIBRIUM VALUE /Y/: y
DIC>
DIC> @@ SELECT A HOMOGENIZATION FUNCTION
DIC> @@ IN THIS CASE THE LOWER HASHIN-SHTRIKMAN BOUND
DIC> en-ho 1
 SELECTED FUNCTION IS HASHIN-SHTRIKMAN BOUND: GENERAL LOWER
DIC>
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME AND OTHER SIMULATION PARAMETERS
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 720000
AUTOMATIC TIMESTEP CONTROL /YES/: YES
MAX TIMESTEP DURING INTEGRATION /72000/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC> set-simulation-condition
NS01A PRINT CONTROL : /0/: 0
FLUX CORRECTION FACTOR : /1/: 1
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/: 2
CHECK INTERFACE POSITION /AUTO/: n
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/: act
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/: y
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/: 99
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -> 1): /AUTO/: 1
MAX TIMESTEP CHANGE PER TIMESTEP : /2/: 2
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/: n
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/: y
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/: n
DIC>
DIC>
DIC> @@
DIC> @@ SAVE THE SETUP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC>
DIC> save exd2 y
DIC>
DIC> set-inter
 --OK---
DIC>
```

exd2b-run

```
DIC>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
 ----------------------------------------------
  WARNING:BCC_A2 HAS NO VOLUME FRACTION, CREATING ONE
Starting time-step t0=   0.0000000     dt=  0.10000000E-06
Starting time-step t0=  0.10000000E-06 dt=  0.20000000E-06
Starting time-step t0=  0.30000000E-06 dt=  0.40000000E-06
Starting time-step t0=  0.70000000E-06 dt=  0.80000000E-06
Starting time-step t0=  0.15000000E-05 dt=  0.16000000E-05
Starting time-step t0=  0.31000000E-05 dt=  0.32000000E-05
Starting time-step t0=  0.63000000E-05 dt=  0.64000000E-05
Starting time-step t0=  0.12700000E-04 dt=  0.12800000E-04
Starting time-step t0=  0.25500000E-04 dt=  0.25600000E-04
Starting time-step t0=  0.51100000E-04 dt=  0.51200000E-04
Starting time-step t0=  0.10230000E-03 dt=  0.10240000E-03
Starting time-step t0=  0.20470000E-03 dt=  0.20480000E-03
Starting time-step t0=  0.40950000E-03 dt=  0.40960000E-03
Starting time-step t0=  0.81910000E-03 dt=  0.81920000E-03
Starting time-step t0=  0.16383000E-02 dt=  0.16384000E-02
Starting time-step t0=  0.32767000E-02 dt=  0.32768000E-02
Starting time-step t0=  0.65535000E-02 dt=  0.65536000E-02
Starting time-step t0=  0.13107100E-01 dt=  0.13107200E-01
Starting time-step t0=  0.26214300E-01 dt=  0.26214400E-01
Starting time-step t0=  0.52428700E-01 dt=  0.52428800E-01
Starting time-step t0=  0.10485750     dt=  0.10485760
Starting time-step t0=  0.20971510     dt=  0.20971520
Starting time-step t0=  0.41943030     dt=  0.41943040
Starting time-step t0=  0.83886070     dt=  0.83886080
Starting time-step t0=   1.6777215     dt=   1.6777216
Starting time-step t0=   3.3554431     dt=   3.3554432
Starting time-step t0=   6.7108863     dt=   6.7108864
Starting time-step t0=   13.421773     dt=   13.421773
Starting time-step t0=   26.843545     dt=   26.843546
Starting time-step t0=   53.687091     dt=   26.843546
Starting time-step t0=   80.530637     dt=   26.843546
Starting time-step t0=   107.37418     dt=   26.843546
Starting time-step t0=   134.21773     dt=   26.843546
Starting time-step t0=   161.06127     dt=   26.843546
Starting time-step t0=   187.90482     dt=   26.843546
Starting time-step t0=   214.74836     dt=   53.687091
Starting time-step t0=   268.43546     dt=   53.687091
Starting time-step t0=   322.12255     dt=   53.687091
Starting time-step t0=   375.80964     dt=   53.687091
Starting time-step t0=   429.49673     dt=   53.687091
Starting time-step t0=   483.18382     dt=   53.687091
Starting time-step t0=   536.87091     dt=   53.687091
Starting time-step t0=   590.55800     dt=   107.37418
Starting time-step t0=   697.93219     dt=   107.37418
Starting time-step t0=   805.30637     dt=   107.37418
Starting time-step t0=   912.68055     dt=   107.37418
Starting time-step t0=   1020.0547     dt=   107.37418
Starting time-step t0=   1127.4289     dt=   214.74836
Starting time-step t0=   1342.1773     dt=   214.74836
Starting time-step t0=   1556.9256     dt=   214.74836
Starting time-step t0=   1771.6740     dt=   214.74836
Starting time-step t0=   1986.4224     dt=   214.74836
Starting time-step t0=   2201.1707     dt=   214.74836
Starting time-step t0=   2415.9191     dt=   214.74836
Starting time-step t0=   2630.6675     dt=   429.49673
Starting time-step t0=   3060.1642     dt=   429.49673
Starting time-step t0=   3489.6609     dt=   429.49673
Starting time-step t0=   3919.1577     dt=   429.49673
Starting time-step t0=   4348.6544     dt=   429.49673
Starting time-step t0=   4778.1511     dt=   429.49673
Starting time-step t0=   5207.6478     dt=   429.49673
Starting time-step t0=   5637.1446     dt=   858.99346
Starting time-step t0=   6496.1380     dt=   858.99346
Starting time-step t0=   7355.1315     dt=   858.99346
Starting time-step t0=   8214.1250     dt=   858.99346
Starting time-step t0=   9073.1184     dt=   858.99346
Starting time-step t0=   9932.1119     dt=   858.99346
Starting time-step t0=   10791.105     dt=   858.99346
Starting time-step t0=   11650.099     dt=   1717.9869
Starting time-step t0=   13368.086     dt=   1717.9869
Starting time-step t0=   15086.073     dt=   1717.9869
Starting time-step t0=   16804.060     dt=   1717.9869
Starting time-step t0=   18522.046     dt=   1717.9869
Starting time-step t0=   20240.033     dt=   1717.9869
Starting time-step t0=   21958.020     dt=   3435.9738
Starting time-step t0=   25393.994     dt=   3435.9738
Starting time-step t0=   28829.968     dt=   3435.9738
Starting time-step t0=   30547.955     dt=   3435.9738
Starting time-step t0=   33983.929     dt=   3435.9738
Starting time-step t0=   37419.903     dt=   3435.9738
Starting time-step t0=   40855.876     dt=   3435.9738
Starting time-step t0=   44291.850     dt=   6871.9477
Starting time-step t0=   51163.798     dt=   6871.9477
Starting time-step t0=   58035.746     dt=   6871.9477
Starting time-step t0=   64907.693     dt=   6871.9477
Starting time-step t0=   71779.641     dt=   6871.9477
Starting time-step t0=   78651.589     dt=   6871.9477
Starting time-step t0=   85523.536     dt=   6871.9477
Starting time-step t0=   88959.510     dt=   6871.9477
Starting time-step t0=   95831.458     dt=   13743.895
Starting time-step t0=   109575.35     dt=   13743.895
Starting time-step t0=   116447.30     dt=   13743.895
```

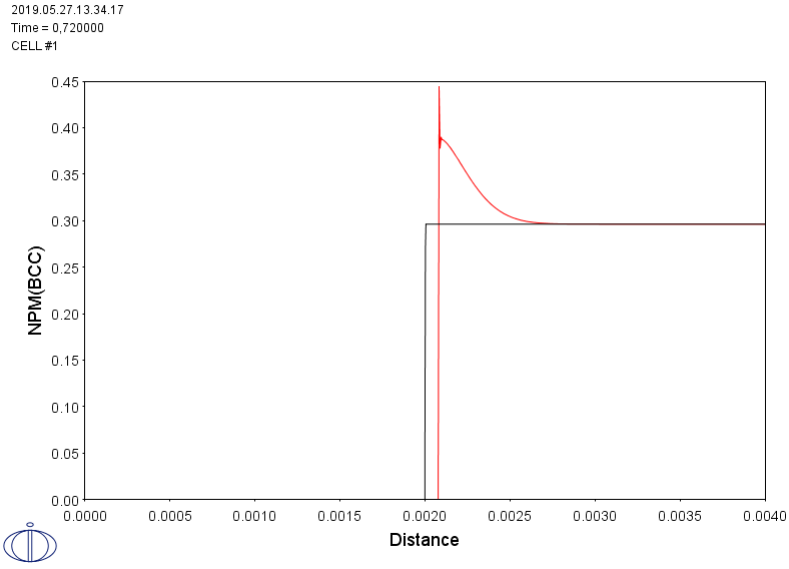
```
Starting time-step t0=   130191.20     dt=   13743.895
Starting time-step t0=   143935.09     dt=   13743.895
Starting time-step t0=   147371.07     dt=   6871.9477
Starting time-step t0=   150807.04     dt=   3435.9738
Starting time-step t0=   154243.01     dt=   6871.9477
Starting time-step t0=   161114.96     dt=   13743.895
Starting time-step t0=   174858.86     dt=   13743.895
Starting time-step t0=   188602.75     dt=   27487.791
Starting time-step t0=   216090.54     dt=   27487.791
Starting time-step t0=   229834.44     dt=   13743.895
Starting time-step t0=   243578.33     dt=   27487.791
Starting time-step t0=   271066.12     dt=   27487.791
Starting time-step t0=   277938.07     dt=   13743.895
Starting time-step t0=   291681.97     dt=   27487.791
Starting time-step t0=   319169.76     dt=   27487.791
Starting time-step t0=   346657.55     dt=   27487.791
Starting time-step t0=   374145.34     dt=   27487.791
Starting time-step t0=   387889.23     dt=   27487.791
Starting time-step t0=   394761.18     dt=   13743.895
Starting time-step t0=   408505.08     dt=   13743.895
Starting time-step t0=   422248.97     dt=   27487.791
Starting time-step t0=   449736.76     dt=   27487.791
Starting time-step t0=   463480.66     dt=   27487.791
Starting time-step t0=   470352.61     dt=   6871.9477
Starting time-step t0=   477224.55     dt=   13743.895
Starting time-step t0=   490968.45     dt=   27487.791
Starting time-step t0=   518456.24     dt=   27487.791
Starting time-step t0=   532200.14     dt=   27487.791
Starting time-step t0=   545944.03     dt=   27487.791
Starting time-step t0=   573431.82     dt=   27487.791
Starting time-step t0=   600919.61     dt=   54975.581
Starting time-step t0=   628407.40     dt=   27487.791
Starting time-step t0=   642151.30     dt=   13743.895
Starting time-step t0=   655895.19     dt=   27487.791
Starting time-step t0=   683382.98     dt=   36617.016
 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:    36.7764948453608
 ------------------------------------------------
 DEALLOCATING
 ------------------------------------------------

 TIMESTEP AT     720000.000     SELECTED

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

exd2b-plot

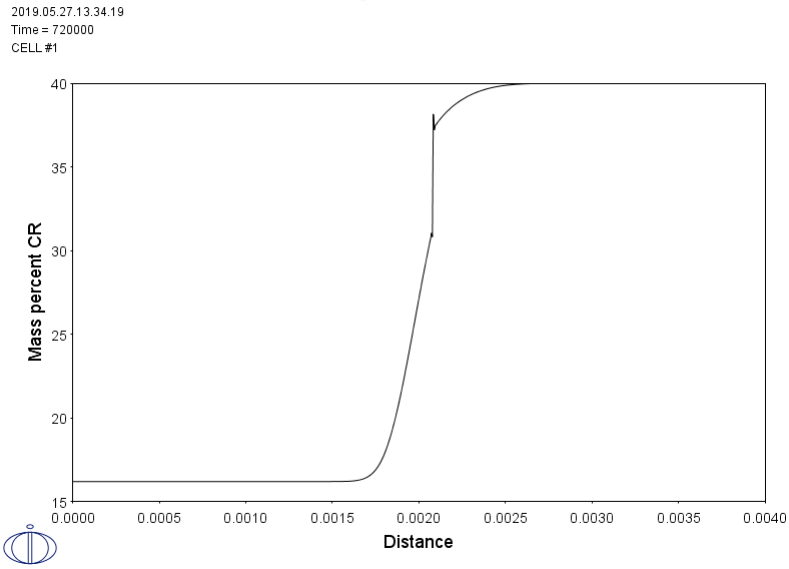
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exd2b\plot.DCM"DIC>
DIC>
DIC> @@ exd2_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE D2
DIC> @@
DIC> @@ ENTER THE DICTRA MODULE AND SPECIFY THE STORE-RESULT FILE
DIC> @@
DIC>
DIC> go d-m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



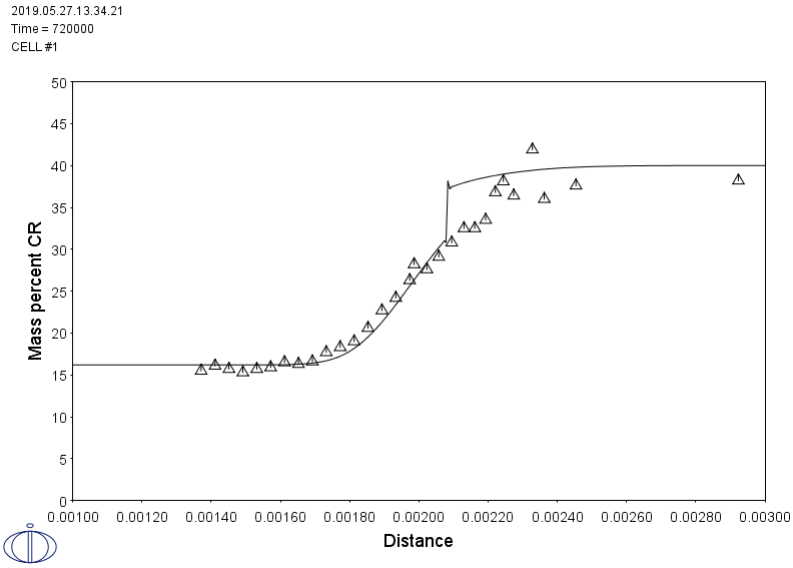

```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1: @@
POST-1: @@ LET US NOW PLOT HOW THE AVERAGE CR-CONCENTRATION VARIES WITH DISTANCE
POST-1: @@
POST-1: s-d-a y w-p cr
POST-1: s-p-c time last
POST-1: set-tit Figure D2.2
POST-1: plot
```

Figure D2.2



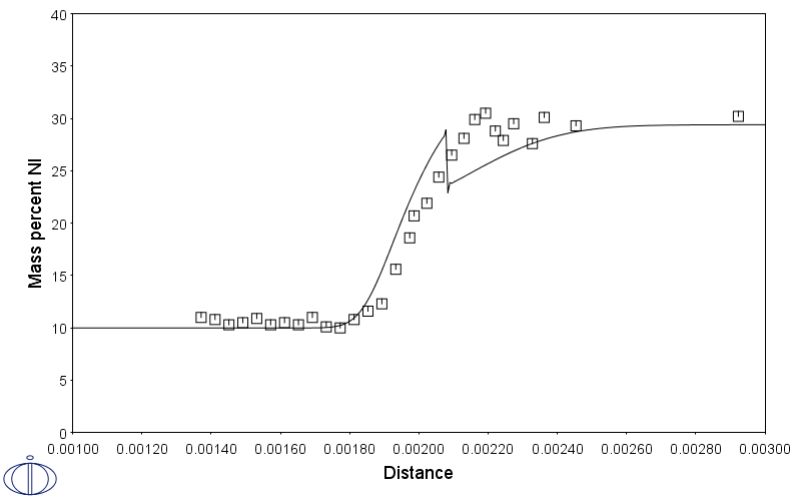
```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1: @@
POST-1: @@ WE SELECT A BETTER SCALING AND APPEND EXPERIMENTAL DATA
POST-1: @@
POST-1:
POST-1: app y exd2.exp
PROLOGUE NUMBER: /0/: 1
DATASET NUMBER(s): /-1/: 4
POST-1:
POST-1: s-s-s y n 0 50
POST-1: s-s-s x n 10e-4 30e-4
POST-1: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

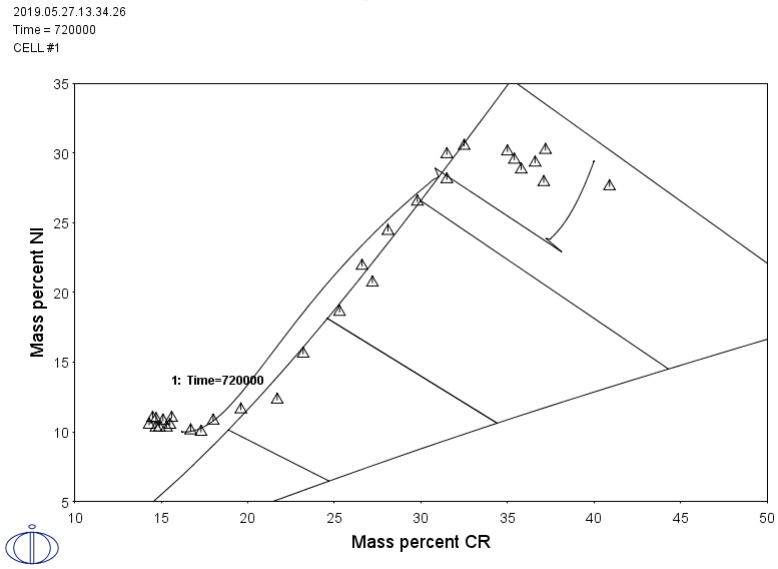
Figure D2.4




```
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

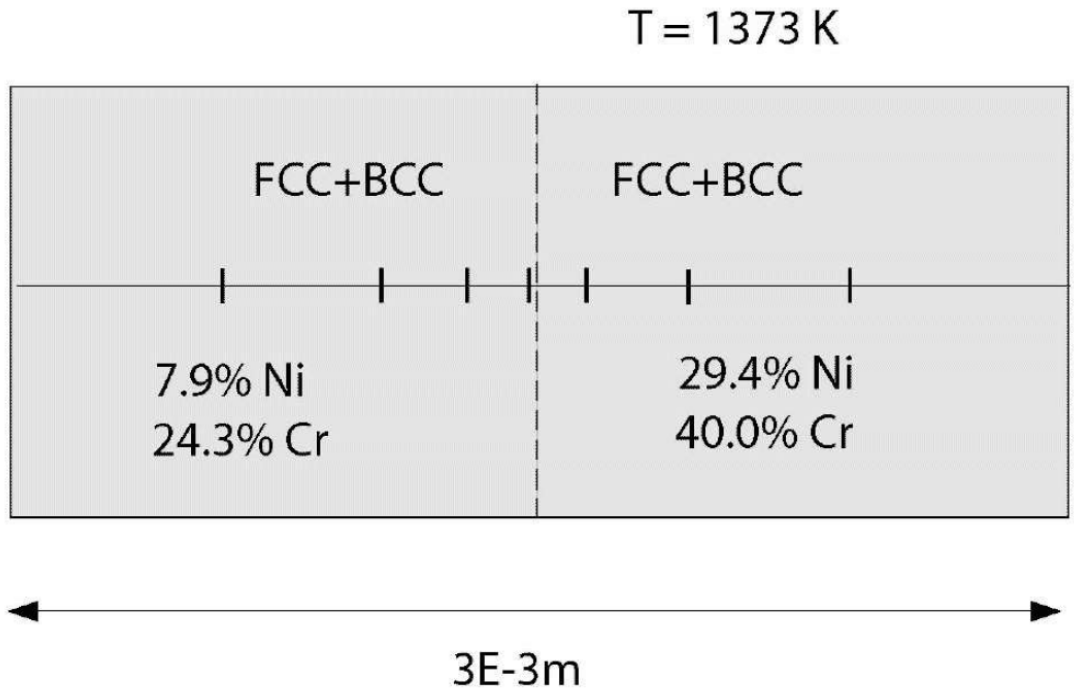



```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1: set-interactive
 --OK---
POST-1:
```

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 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 20130) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri May 24 17:06:15 2019


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:SYS: NO SUCH COMMAND, USE HELP
SYS:
SYS:SYS:
SYS:
SYS: THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.1

 VA                      /-  DEFINED
 L12_FCC                 B2_BCC                  DICTRA_FCC_A1
   REJECTED
TDB_TCFE9: Current database: Iron Demo Database v2.1

 VA                      /-  DEFINED
TDB_FEDEMO: FE                      CR                      NI
   DEFINED
TDB_FEDEMO: LIQUID:L                BCC_A2                  CBCC_A12
 CHI_A12                 CUB_A13                 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, 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/: INFO: EQUILIBRIUM COMPOSITION AND FRACTION
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 /A
999) /YES/:DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -
> 1): /AUTO/:MAX TIMESTEP CHANGE PER TIMESTEP : /2/:USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:ALWAYS CALCULATE STIFFNES MATR
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>
```

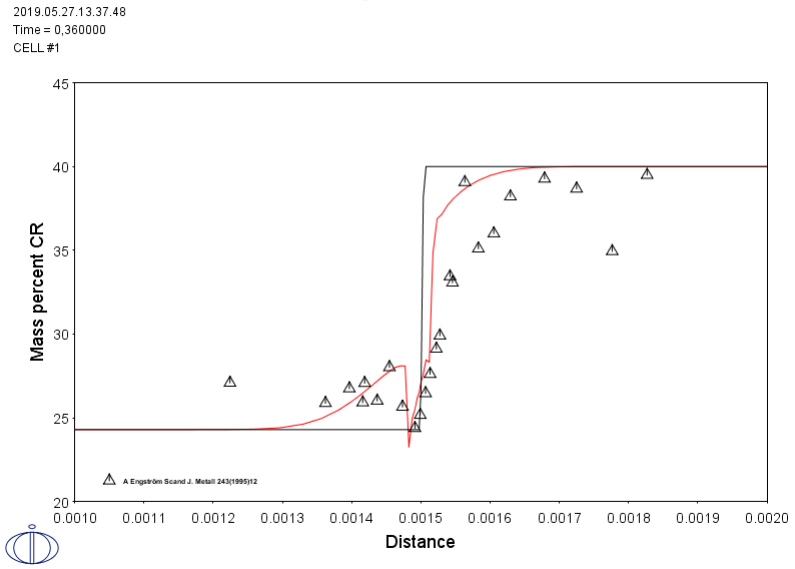
exd3-run

```
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
 ----------------------------------------------
  WARNING:BCC_A2 HAS NO VOLUME FRACTION, CREATING ONE
Starting time-step t0=   0.0000000     dt=   1.0000000
Starting time-step t0=   1.0000000     dt=   2.0000000
Starting time-step t0=   3.0000000     dt=   4.0000000
Starting time-step t0=   7.0000000     dt=   8.0000000
Starting time-step t0=   15.000000     dt=   16.000000
Starting time-step t0=   31.000000     dt=   32.000000
Starting time-step t0=   63.000000     dt=   64.000000
Starting time-step t0=   127.00000     dt=   128.00000
Starting time-step t0=   255.00000     dt=   256.00000
Starting time-step t0=   511.00000     dt=   256.00000
Starting time-step t0=   767.00000     dt=   256.00000
Starting time-step t0=   1023.0000     dt=   512.00000
Starting time-step t0=   1535.0000     dt=   512.00000
Starting time-step t0=   2047.0000     dt=   1024.0000
Starting time-step t0=   3071.0000     dt=   1024.0000
Starting time-step t0=   4095.0000     dt=   2048.0000
Starting time-step t0=   6143.0000     dt=   2048.0000
Starting time-step t0=   8191.0000     dt=   2048.0000
Starting time-step t0=   10239.000     dt=   2048.0000
Starting time-step t0=   12287.000     dt=   4096.0000
Starting time-step t0=   16383.000     dt=   8192.0000
Starting time-step t0=   24575.000     dt=   8192.0000
Starting time-step t0=   32767.000     dt=   8192.0000
Starting time-step t0=   40959.000     dt=   8192.0000
Starting time-step t0=   49151.000     dt=   16384.000
Starting time-step t0=   65535.000     dt=   16384.000
Starting time-step t0=   81919.000     dt=   16384.000
Starting time-step t0=   98303.000     dt=   16384.000
Starting time-step t0=   114687.00     dt=   16384.000
Starting time-step t0=   131071.00     dt=   16384.000
Starting time-step t0=   147455.00     dt=   16384.000
Starting time-step t0=   163839.00     dt=   16384.000
Starting time-step t0=   180223.00     dt=   16384.000
Starting time-step t0=   196607.00     dt=   16384.000
Starting time-step t0=   212991.00     dt=   16384.000
Starting time-step t0=   229375.00     dt=   16384.000
Starting time-step t0=   245759.00     dt=   16384.000
Starting time-step t0=   262143.00     dt=   16384.000
Starting time-step t0=   278527.00     dt=   16384.000
Starting time-step t0=   294911.00     dt=   16384.000
Starting time-step t0=   311295.00     dt=   16384.000
Starting time-step t0=   327679.00     dt=   16384.000
Starting time-step t0=   344063.00     dt=   15937.000
 MUST SAVE WORKSPACE ON FILE
 WORKSPACE SAVED ON FILE
 RECLAIMING WORKSPACE
 DELETING TIME-RECORD FOR TIME    0.0000000
 DELETING TIME-RECORD FOR TIME    1.0000000
 DELETING TIME-RECORD FOR TIME    511.00000
 DELETING TIME-RECORD FOR TIME    1023.0000
 DELETING TIME-RECORD FOR TIME    1535.0000
 DELETING TIME-RECORD FOR TIME    2047.0000
 DELETING TIME-RECORD FOR TIME    3071.0000
 DELETING TIME-RECORD FOR TIME    4095.0000
 DELETING TIME-RECORD FOR TIME    6143.0000
 DELETING TIME-RECORD FOR TIME    8191.0000
 DELETING TIME-RECORD FOR TIME    10239.000
 DELETING TIME-RECORD FOR TIME    12287.000
 DELETING TIME-RECORD FOR TIME    16383.000
 DELETING TIME-RECORD FOR TIME    24575.000
 DELETING TIME-RECORD FOR TIME    32767.000
 DELETING TIME-RECORD FOR TIME    40959.000
 DELETING TIME-RECORD FOR TIME    49151.000
 DELETING TIME-RECORD FOR TIME    65535.000
 DELETING TIME-RECORD FOR TIME    81919.000
 DELETING TIME-RECORD FOR TIME    98303.000
 DELETING TIME-RECORD FOR TIME    114687.00
 DELETING TIME-RECORD FOR TIME    131071.00
 DELETING TIME-RECORD FOR TIME    147455.00
 DELETING TIME-RECORD FOR TIME    163839.00
 DELETING TIME-RECORD FOR TIME    180223.00
 DELETING TIME-RECORD FOR TIME    196607.00
 DELETING TIME-RECORD FOR TIME    212991.00
 DELETING TIME-RECORD FOR TIME    229375.00
 DELETING TIME-RECORD FOR TIME    245759.00
 DELETING TIME-RECORD FOR TIME    262143.00
 DELETING TIME-RECORD FOR TIME    278527.00
 DELETING TIME-RECORD FOR TIME    294911.00
 DELETING TIME-RECORD FOR TIME    311295.00
 DELETING TIME-RECORD FOR TIME    327679.00

 KEEPING TIME-RECORD FOR TIME    344063.00
 AND FOR TIME                    360000.00
 WORKSPACE RECLAIMED
 ------------------------------------------------
 INTERPOLATION SCHEME USED THIS FRACTION OF
 THE ALLOCATED MEMORY:   0.762615825611626
 EFFICIENCY FACTOR:    7.09082167832168
 ------------------------------------------------
 DEALLOCATING
 ------------------------------------------------

 TIMESTEP AT     360000.000     SELECTED

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

exd3-plot

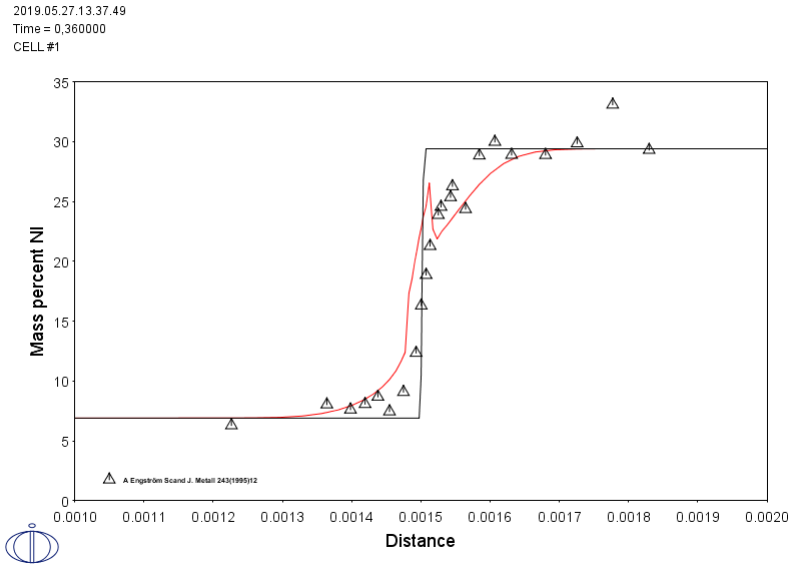
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exd3\plot.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>DIC>DIC>
DIC> TIME STEP AT TIME  3.60000E+05
DIC> OK
DIC>
DIC>DIC>DIC>DIC>  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:
POST-1:POST-1:POST-1:POST-1: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



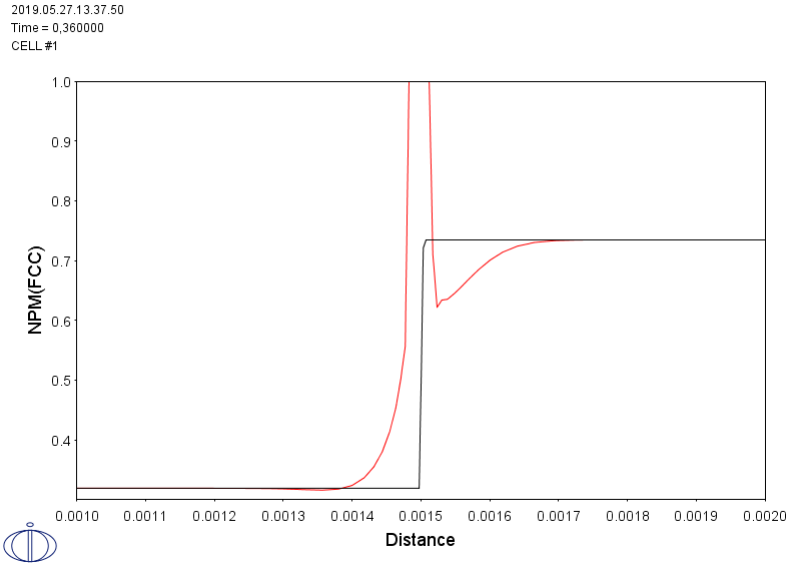

```
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:POST-1:POST-1:
POST-1:POST-1:
POST-1:POST-1:
POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```

Figure D3.2



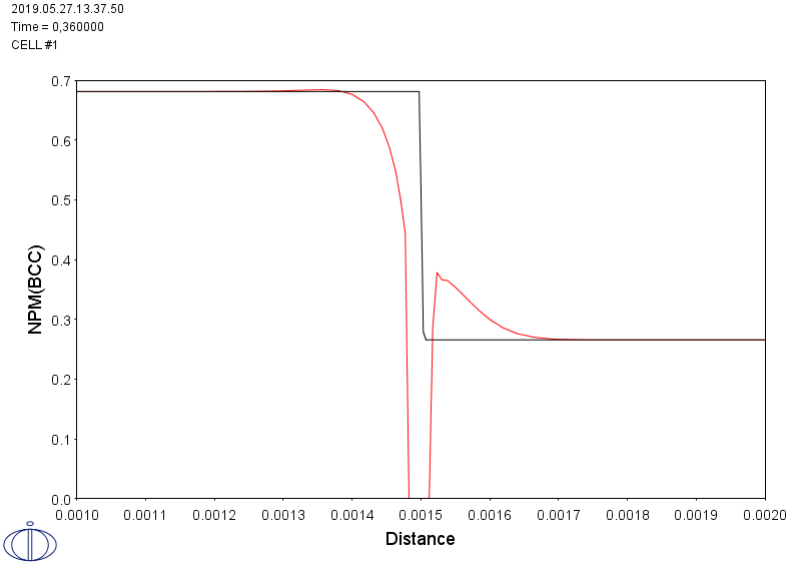

```
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:POST-1:POST-1:POST-1:POST-1:POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```

Figure D3.3



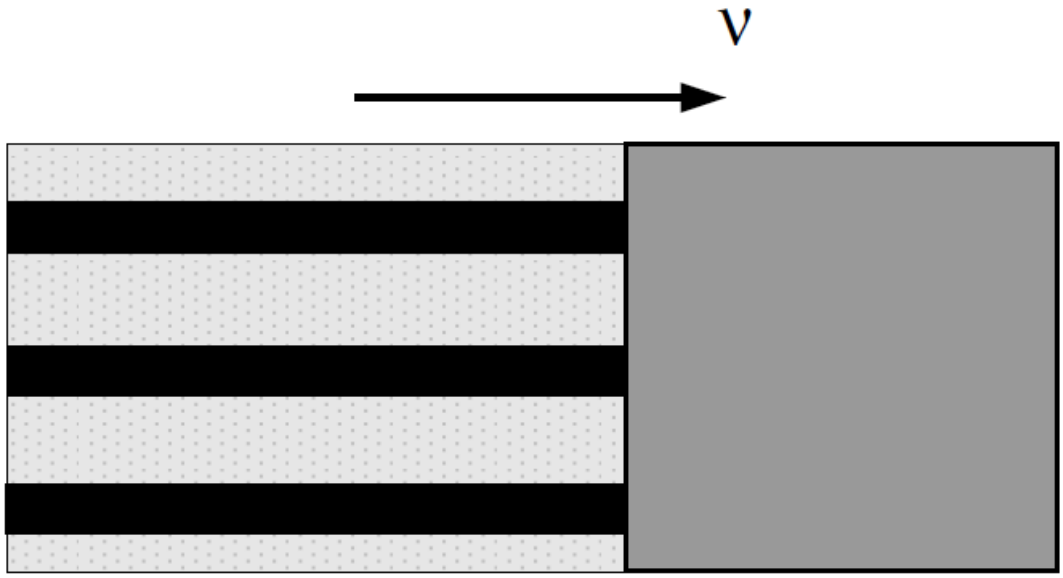

```
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:POST-1:POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```

Figure D3.4




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

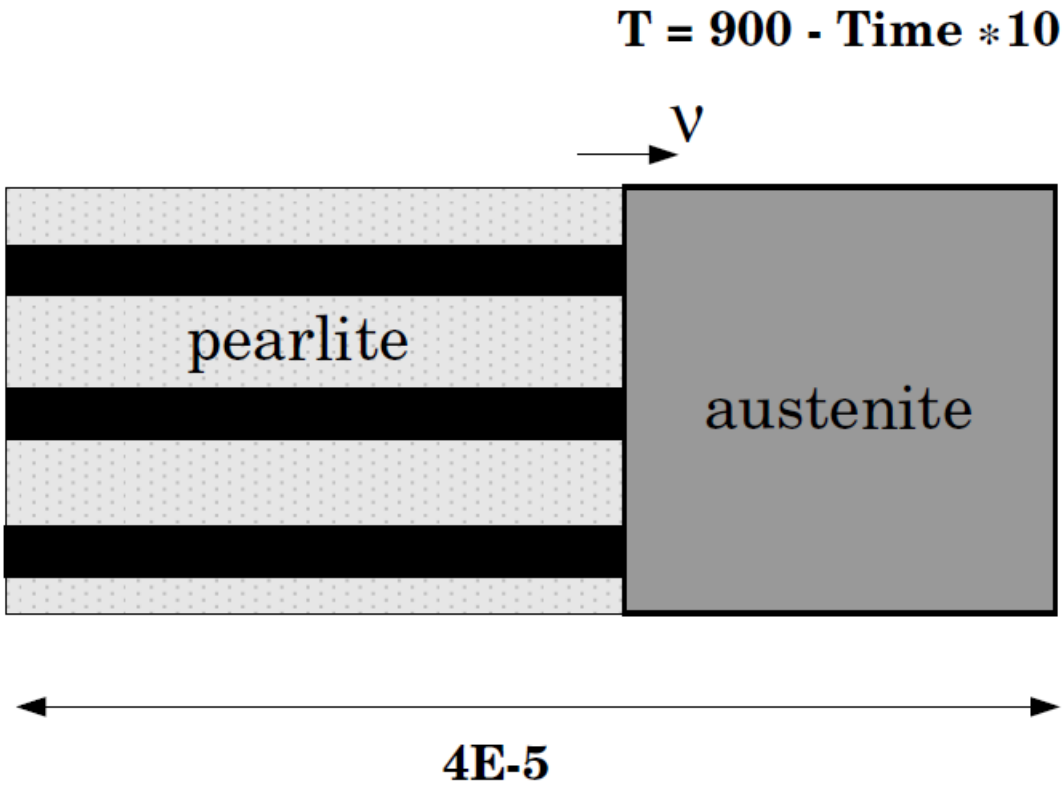
Cooperative Growth



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 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 20130) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri May 24 17:06:15 2019


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  v9.1

 VA                       /-  DEFINED
 L12_FCC                  B2_BCC                  DICTRA_FCC_A1
   REJECTED
TDB_TCFE9: Current database: Iron Demo Database v2.1

 VA                       /-  DEFINED
TDB_FEDEMO:
TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO: FE                       C                        MN
   DEFINED
TDB_FEDEMO:
TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO: GAS:G                    LIQUID:L                 BCC_A2
 CBCC_A12                 CEMENTITE                CUB_A13
 DIAMOND_FCC_A4           FCC_A1                   GRAPHITE
 HCP_A3                   KSI_CARBIDE              LAVES_PHASE_C14
 M23C6                    M5C2                     M7C3
   REJECTED
TDB_FEDEMO: FCC_A1                   BCC_A2                   CEMENTITE
   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'
  'W. Huang, Metall. Trans. A, 21A (1990) 2115-2123; TRITA-MAC 411 (Rev
      1989); C-FE-MN'
  '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'
  'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, CALPHAD,
      submitted, 2011; Fe-Mn-C'
  'W. Huang, CALPHAD, 13 (1989) 243-252; TRITA-MAC 388 (rev 1989); FE-MN'
  'B. Hallstedt, D. Djurovic, J. von Appen, R. Dronskowski, A. Dick, F.
      Koermann, T. Hickel, J. Neugebauer, CALPHAD, 34, 129 -33(2010); Fe-C'
  'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, CALPHAD, 34, 279
      -85(2010); Mn-C'
  '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'
  '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: Steels/Fe-Alloys Mobility  v4.0

 VA  DEFINED
 B2_BCC  REJECTED
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'
  'Y. Liu, L. Zhang, et al. CALPHAD 33(2009)614-23; Fe-Mn-C (fcc)'
  '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'
  'S. Deng, et al., CALPHAD, 56 (2017) 230-240.'
  '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>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>
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> DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
  Trying old scheme                        4
 U-FRACTION IN SYSTEM:  C = .0233843320030518  FE = .990707670399293
                        MN = .0092923297312127
 TOTAL SIZE OF SYSTEM:  2.68092626329E-13 [m^3]
 U-FRACTION IN SYSTEM:  C = .0233843320030518  FE = .990707670399293
                        MN = .0092923297312127
 TOTAL SIZE OF SYSTEM:  2.68092626329E-13 [m^3]
  17  GRIDPOINT(S) ADDED   TO   CELL #1   REGION: AUSTENITE
 TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =   0.0000000
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.77961766E-05 AND   0.77961766E-05
 POSITION OF INTERFACE PEARLITE / AUSTENITE IS   0.50077962E-09
 U-FRACTION IN SYSTEM:  C = .0233843320030518  FE = .990707670399294
                        MN = .00929232973121272
 TOTAL SIZE OF SYSTEM:  2.68092626329E-13 [m^3]
  10  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUSTENITE

  CPU time used in timestep                    1 seconds
  4  GRIDPOINT(S) ADDED   TO   CELL #1   REGION: AUSTENITE
 TIME =  0.10010000E-03 DT =  0.10000000E-03 SUM OF SQUARES =   0.0000000
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.77964173E-05 AND   0.77964173E-05
 POSITION OF INTERFACE PEARLITE / AUSTENITE IS   0.12804214E-08
 U-FRACTION IN SYSTEM:  C = .0233843320030518  FE = .990707670399294
                        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 =  0.13027597E-02 DT =  0.12026597E-02 SUM OF SQUARES =   0.0000000
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.77993126E-05 AND   0.77993126E-05
 POSITION OF INTERFACE PEARLITE / AUSTENITE IS   0.10660340E-07
 U-FRACTION IN SYSTEM:  C = .0233843320030518  FE = .990707670399294
                        MN = .0092923297312127
 TOTAL SIZE OF SYSTEM:  2.68092626329E-13 [m^3]
  CPU time used in timestep                    0 seconds
  2 GRIDPOINT(S) REMOVED FROM CELL#  1 REGION #  1
 TIME =  0.37080790E-02 DT =  0.24053193E-02 SUM OF SQUARES =   0.0000000
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.78051044E-05 AND   0.78051044E-05
 POSITION OF INTERFACE PEARLITE / AUSTENITE IS   0.29434109E-07
 U-FRACTION IN SYSTEM:  C = .0233843320030518  FE = .990707670399294
                        MN = .00929232973121269
 TOTAL SIZE OF SYSTEM:  2.68092626329E-13 [m^3]
  CPU time used in timestep                    0 seconds
  1 GRIDPOINT(S) REMOVED FROM CELL#  1 REGION #  1
 TIME =  0.85187176E-02 DT =  0.48106387E-02 SUM OF SQUARES =   0.0000000
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.78166927E-05 AND   0.78166927E-05
 POSITION OF INTERFACE PEARLITE / AUSTENITE IS   0.67037393E-07
 U-FRACTION IN SYSTEM:  C = .0233843320030517  FE = .990707670399294
                        MN = .00929232973121269
 TOTAL SIZE OF SYSTEM:  2.68092626329E-13 [m^3]
  CPU time used in timestep                    0 seconds
  1 GRIDPOINT(S) REMOVED FROM CELL#  1 REGION #  1
 TIME =  0.18139995E-01 DT =  0.96212773E-02 SUM OF SQUARES =   0.0000000
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.78398880E-05 AND   0.78398880E-05
 POSITION OF INTERFACE PEARLITE / AUSTENITE IS   0.14246713E-06
 U-FRACTION IN SYSTEM:  C = .0233843320030517  FE = .990707670399295
                        MN = .00929232973121268
 TOTAL SIZE OF SYSTEM:  2.68092626329E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =  0.37382550E-01 DT =  0.19242555E-01 SUM OF SQUARES =   0.0000000
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.78863534E-05 AND   0.78863534E-05
 POSITION OF INTERFACE PEARLITE / AUSTENITE IS   0.29422072E-06
 U-FRACTION IN SYSTEM:  C = .0233843320030517  FE = .990707670399295
                        MN = .00929232973121267
 TOTAL SIZE OF SYSTEM:  2.68092626329E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =  0.75867659E-01 DT =  0.38485109E-01 SUM OF SQUARES =   0.0000000
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.79795809E-05 AND   0.79795809E-05
 POSITION OF INTERFACE PEARLITE / AUSTENITE IS   0.60131576E-06
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399294
                        MN = .00929232973121267
 TOTAL SIZE OF SYSTEM:  2.68092626329E-13 [m^3]
  CPU time used in timestep                    0 seconds
  1 GRIDPOINT(S) REMOVED FROM CELL#  1 REGION #  1
 TIME =  0.15283788     DT =  0.76970219E-01 SUM OF SQUARES =   0.0000000
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.81672056E-05 AND   0.81672056E-05
 POSITION OF INTERFACE PEARLITE / AUSTENITE IS   0.12299474E-05
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399294
                        MN = .00929232973121266
 TOTAL SIZE OF SYSTEM:  2.68092626329E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =  0.25283788     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.84132409E-05 AND   0.84132409E-05
 POSITION OF INTERFACE PEARLITE / AUSTENITE IS   0.20712715E-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 =  0.35283788     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.86617616E-05 AND   0.86617616E-05
 POSITION OF INTERFACE PEARLITE / AUSTENITE IS   0.29374476E-05
 U-FRACTION IN SYSTEM:  C = .0233843320030515  FE = .990707670399294
                        MN = .00929232973121271
 TOTAL SIZE OF SYSTEM:  2.68092626329E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =  0.45283788     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.89126768E-05 AND   0.89126768E-05
 POSITION OF INTERFACE PEARLITE / AUSTENITE IS   0.38287153E-05
 U-FRACTION IN SYSTEM:  C = .0233843320030515  FE = .990707670399294
                        MN = .00929232973121281
 TOTAL SIZE OF SYSTEM:  2.68092626329E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =  0.55283788     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.91658949E-05 AND   0.91658949E-05
```

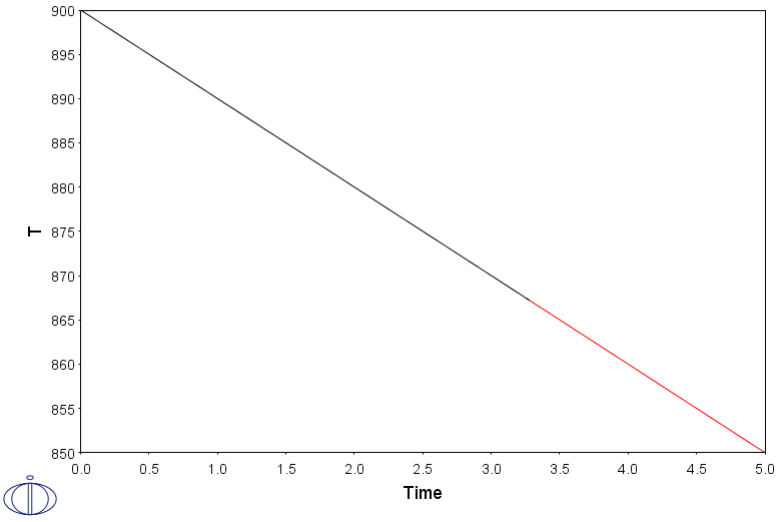
```
 POSITION OF INTERFACE PEARLITE / AUSTENITE IS   0.47453048E-05
 U-FRACTION IN SYSTEM:  C = .0233843320030514  FE = .990707670399294
                        MN = .00929232973121301
 TOTAL SIZE OF SYSTEM:  2.68092626329E-13 [m^3]
  CPU time used in timestep                    0 seconds
  1 GRIDPOINT(S) REMOVED FROM CELL#  1 REGION #  1
 TIME =  0.65283788     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.94213234E-05 AND   0.94213234E-05
 POSITION OF INTERFACE PEARLITE / AUSTENITE IS   0.56874371E-05
 U-FRACTION IN SYSTEM:  C = .0233843320030514  FE = .990707670399294
                        MN = .00929232973121338
 TOTAL SIZE OF SYSTEM:  2.68092626329E-13 [m^3]


output ignored...



... output resumed

 DELETING TIME-RECORD FOR TIME    3.1528379

 KEEPING TIME-RECORD FOR TIME    3.2528379
 AND FOR TIME                    3.2743223
 WORKSPACE RECLAIMED
  INFO: CELL   1 REGION AUSTENITE   DELETED
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399329
                        MN = .00929232973117855
 TOTAL SIZE OF SYSTEM:  2.68126144219E-13 [m^3]
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399329
                        MN = .00929232973117855
 TOTAL SIZE OF SYSTEM:  2.68126144219E-13 [m^3]
 TIME =   3.2743323     DT =  0.10000000E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399329
                        MN = .00929232973117855
 TOTAL SIZE OF SYSTEM:  2.68126144219E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   3.2843323     DT =  0.10000000E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399329
                        MN = .00929232973117855
 TOTAL SIZE OF SYSTEM:  2.68126144219E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   3.3843323     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399329
                        MN = .00929232973117855
 TOTAL SIZE OF SYSTEM:  2.68126144219E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   3.4843323     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399329
                        MN = .00929232973117855
 TOTAL SIZE OF SYSTEM:  2.68126144219E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   3.5843323     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399329
                        MN = .00929232973117855
 TOTAL SIZE OF SYSTEM:  2.68126144219E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   3.6843323     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399329
                        MN = .00929232973117855
 TOTAL SIZE OF SYSTEM:  2.68126144219E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   3.7843323     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399329
                        MN = .00929232973117855
 TOTAL SIZE OF SYSTEM:  2.68126144219E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   3.8843323     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399329
                        MN = .00929232973117855
 TOTAL SIZE OF SYSTEM:  2.68126144219E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   3.9843323     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399329
                        MN = .00929232973117855
 TOTAL SIZE OF SYSTEM:  2.68126144219E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   4.0843323     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399329
                        MN = .00929232973117855
 TOTAL SIZE OF SYSTEM:  2.68126144219E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   4.1843323     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399329
                        MN = .00929232973117855
 TOTAL SIZE OF SYSTEM:  2.68126144219E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   4.2843323     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399329
                        MN = .00929232973117855
 TOTAL SIZE OF SYSTEM:  2.68126144219E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   4.3843323     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399329
                        MN = .00929232973117855
 TOTAL SIZE OF SYSTEM:  2.68126144219E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   4.4843323     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399329
                        MN = .00929232973117855
 TOTAL SIZE OF SYSTEM:  2.68126144219E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   4.5843323     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399329
                        MN = .00929232973117855
 TOTAL SIZE OF SYSTEM:  2.68126144219E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   4.6843323     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399329
                        MN = .00929232973117855
 TOTAL SIZE OF SYSTEM:  2.68126144219E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   4.7843323     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399329
                        MN = .00929232973117855
 TOTAL SIZE OF SYSTEM:  2.68126144219E-13 [m^3]
```

```
 CPU time used in timestep                    0 seconds
TIME =   4.8843323     DT =  0.10000000     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399329
                       MN = .00929232973117855
TOTAL SIZE OF SYSTEM:  2.68126144219E-13 [m^3]
 CPU time used in timestep                    0 seconds
TIME =   4.9843323     DT =  0.10000000     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399329
                       MN = .00929232973117855
TOTAL SIZE OF SYSTEM:  2.68126144219E-13 [m^3]
 CPU time used in timestep                    0 seconds
TIME =   5.0000000     DT =  0.15667748E-01 SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399329
                       MN = .00929232973117855
TOTAL SIZE OF SYSTEM:  2.68126144219E-13 [m^3]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME    3.2528379
DELETING TIME-RECORD FOR TIME    3.2743223
DELETING TIME-RECORD FOR TIME    3.2743323
DELETING TIME-RECORD FOR TIME    3.2843323
DELETING TIME-RECORD FOR TIME    3.3843323
DELETING TIME-RECORD FOR TIME    3.4843323
DELETING TIME-RECORD FOR TIME    3.5843323
DELETING TIME-RECORD FOR TIME    3.6843323
DELETING TIME-RECORD FOR TIME    3.7843323
DELETING TIME-RECORD FOR TIME    3.8843323
DELETING TIME-RECORD FOR TIME    3.9843323
DELETING TIME-RECORD FOR TIME    4.0843323
DELETING TIME-RECORD FOR TIME    4.1843323
DELETING TIME-RECORD FOR TIME    4.2843323
DELETING TIME-RECORD FOR TIME    4.3843323
DELETING TIME-RECORD FOR TIME    4.4843323
DELETING TIME-RECORD FOR TIME    4.5843323
DELETING TIME-RECORD FOR TIME    4.6843323
DELETING TIME-RECORD FOR TIME    4.7843323
DELETING TIME-RECORD FOR TIME    4.8843323

KEEPING TIME-RECORD FOR TIME    4.9843323
AND FOR TIME                    5.0000000
WORKSPACE RECLAIMED

TIMESTEP AT     5.00000000     SELECTED

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

exe1-plot

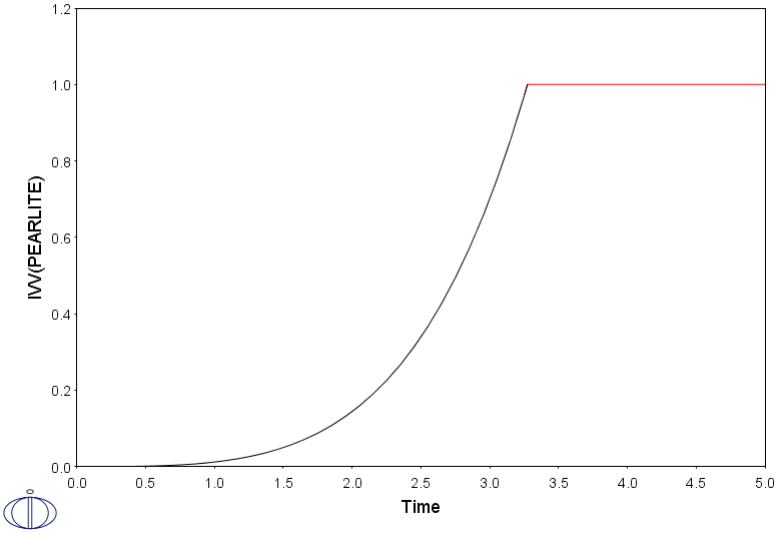
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exe1\plot.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  5.00000E+00
DIC> OK
DIC>
DIC>DIC>DIC>DIC>  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:POST-1:POST-1:POST-1: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

2019.05.27.13.41.08
"FIRST" INTERFACE OF SYSTEM
CELL #1



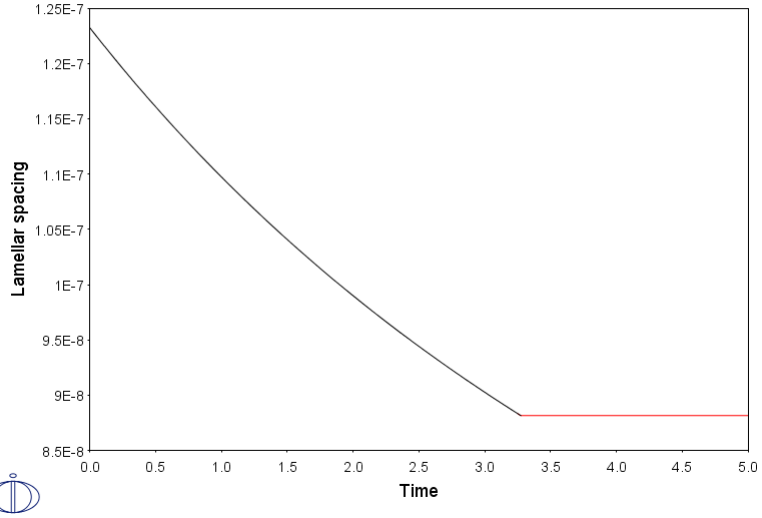

```
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:
POST-1:
POST-1:POST-1: ORKING ...          OST-1:POST-1:
POST-1:
```

2019.05.27.13.41.09
CELL #1



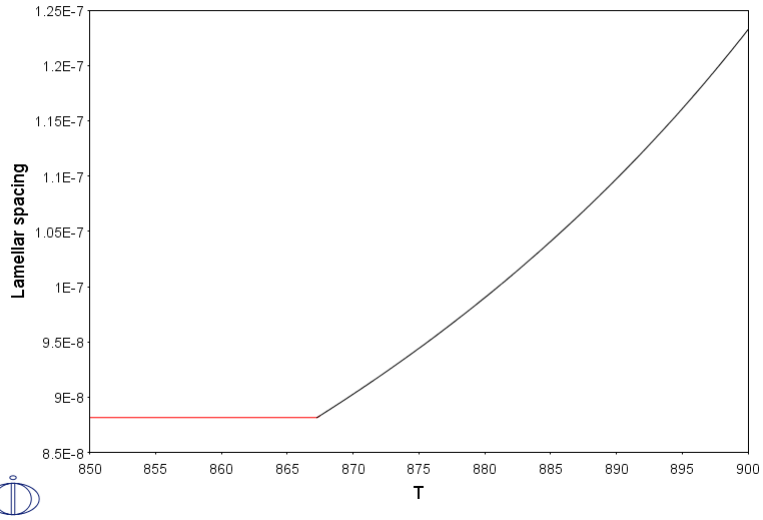

```
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1:POST-1:POST-1:POST-1:AXIS (X, Y OR Z) :VARIABLE :IN REGION: /*/:POST-1:
POST-1:CONDITION /INTEGRAL/:INTERFACE :UPPER OR LOWER INTERFACE OF REGION PEARLITE#1 /LOWER/:POST-1:
POST-1:
POST-1:POST-1: ORKING ...          OST-1:POST-1: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

2019.05.27.13.41.10
UPPER INTERFACE OF REGION "PEARLITE#1"
CELL #1



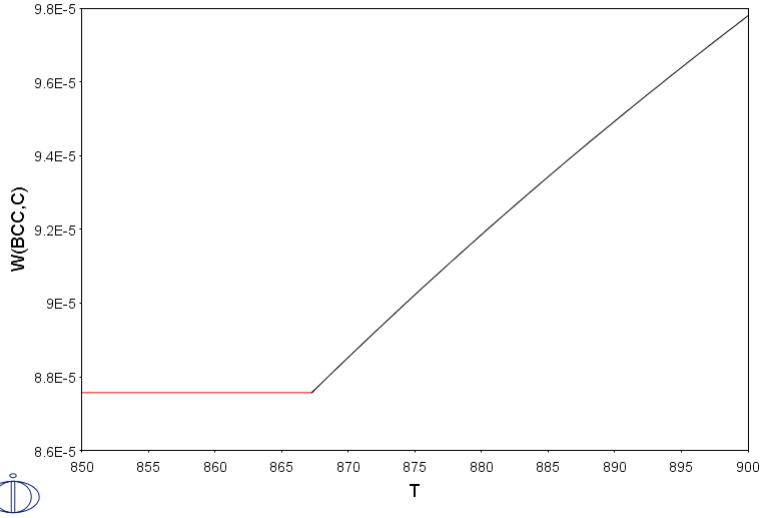

```
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:
POST-1:POST-1:
POST-1:
POST-1:POST-1: ORKING ...          OST-1:POST-1:
POST-1:
```

2019.05.27.13.41.10
UPPER INTERFACE OF REGION "PEARLITE#1"
CELL #1



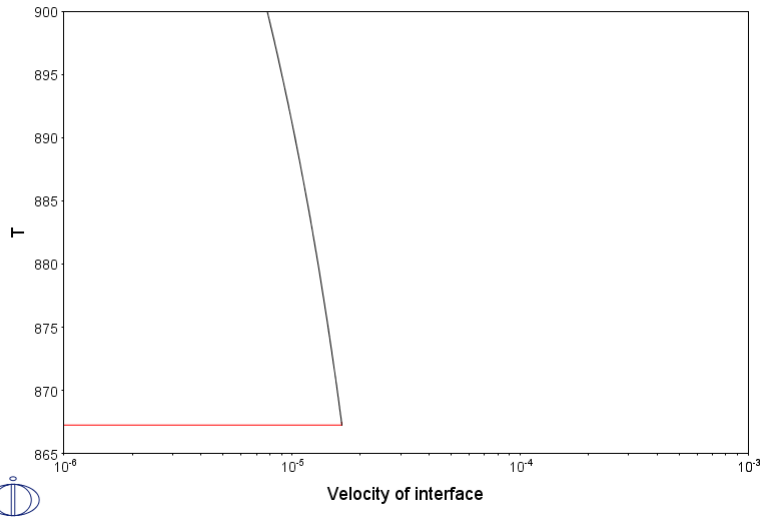

```
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:
POST-1:
POST-1:
POST-1:POST-1: ORKING ...          OST-1:POST-1:
POST-1:
```

2019.05.27.13.41.11
UPPER INTERFACE OF REGION "PEARLITE#1"
CELL #1



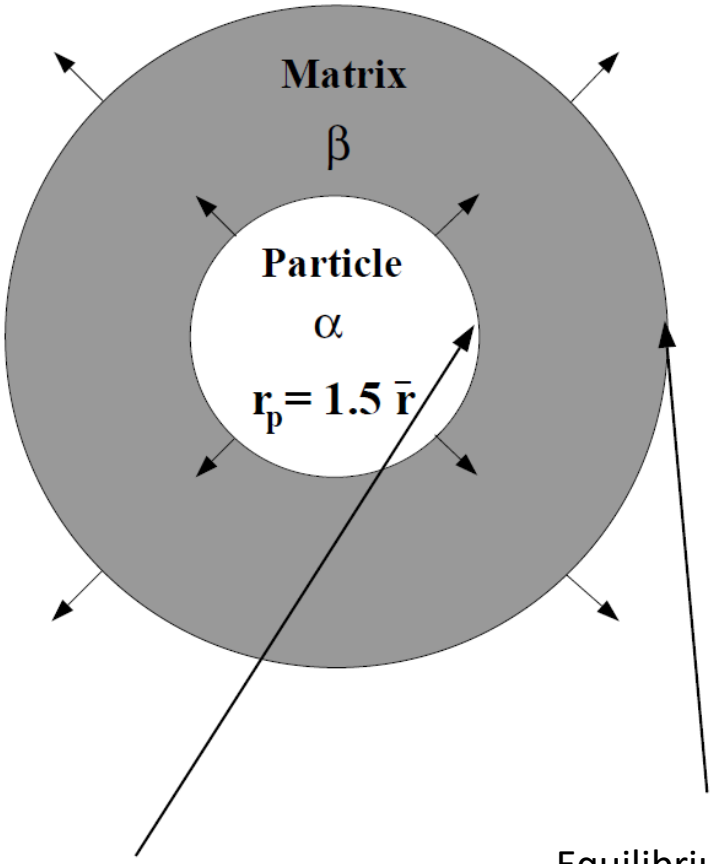

```
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:INTERFACE :UPPER OR LOWER INTERFACE OF REGION PEARLITE#1 /LOWER/:POST-1:POST-1:POST-1:
POST-1:
POST-1:POST-1: ORKING ...          OST-1:POST-1:
POST-1:
```

2019.05.27.13.41.12
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

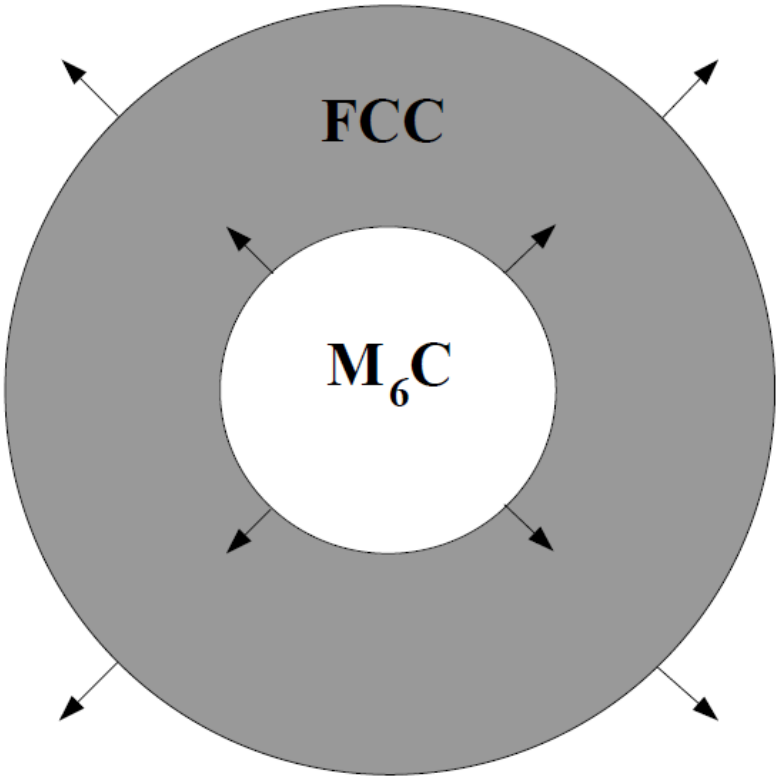
Equilibrium as defined by the average composition in the system.

$\frac{2\sigma V_m}{r_p}$ 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 20130) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri May 24 17:06:15 2019


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  v9.1

 VA                      /-  DEFINED
 L12_FCC                 B2_BCC                  DICTRA_FCC_A1
   REJECTED
TDB_TCFE9:TDB_TCFE9: FE                      MO                      C
   DEFINED
TDB_TCFE9: GAS:G                    LIQUID:L                BCC_A2
 FCC_A1                  HCP_A3                  CBCC_A12
 CUB_A13                 DIAMOND_FCC_A4          GRAPHITE
 CEMENTITE               M23C6                   M7C3
 M6C                     M5C2                    M3C2
 MC_ETA                  MC_SHP                  KSI_CARBIDE
 Z_PHASE                 FE4N_LP1                FECN_CHI
 SIGMA                   MU_PHASE                P_PHASE
 R_PHASE                 CHI_A12                 LAVES_PHASE_C14
 AL5FE4                  M2O3C:I  REJECTED
TDB_TCFE9: FCC_A1                    M6C  RESTORED
TDB_TCFE9: 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, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
  'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
  'J-O. Andersson, CALPHAD, 12 (1988) 1-8; TRITA 0317 (1986); C-MO'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  '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'
  'S. Nagakura, Transactions of the Iron and Steel Institute of Japan, 8
      (1968) 265-294; Molar volumes'
  'I.K. Kupalova, V.I. Pavlova, High Speed Steels: Physical Properties,
      Prop. Data Updat. 2 (1988) 67-78; Molar volumes'
 -OK-
TDB_TCFE9:
TDB_TCFE9:TDB_TCFE9:TDB_TCFE9:TDB_TCFE9: Use one of these databases

 TCFE9   =  Steels/Fe-Alloys  v9.1
 TCFE8   =  Steels/Fe-Alloys  v8.1
 FROST1  =  FROST database v1.0
 TCFE7   =  Steels/Fe-Alloys  v7.0
 TCFE6   =  Steels/Fe-Alloys  v6.2
 TCFE5   =  Steels/Fe-Alloys  v5.0
 TCFE4   =  Steels/Fe-Alloys  v4.1
 TCFE3   =  Steels/Fe-Alloys  v3.1
 TCFE2   =  Steels/Fe-Alloys  v2.1
 TCFE1   =  Steels/Fe-Alloys  v1.0
 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  v2.1
 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
 TCSLD1  =  Solder Alloys  v1.1
 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
 TCNF2   =  Nuclear Fuels  v2.1b
 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 v2.1
 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  v1.0
 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 /TCFE9/: Current database: Steels/Fe-Alloys Mobility  v4.0

 VA  DEFINED
 B2_BCC  REJECTED
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'
  'Y. Liu et al., Calphad 34(2010)253-262; fcc Cu-Fe.'
  'W. Zheng, et al., Metall Mater Trans, 48 (2017) 536-550; Fe-Mn-Mo (fcc
      and bcc)'
 -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>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

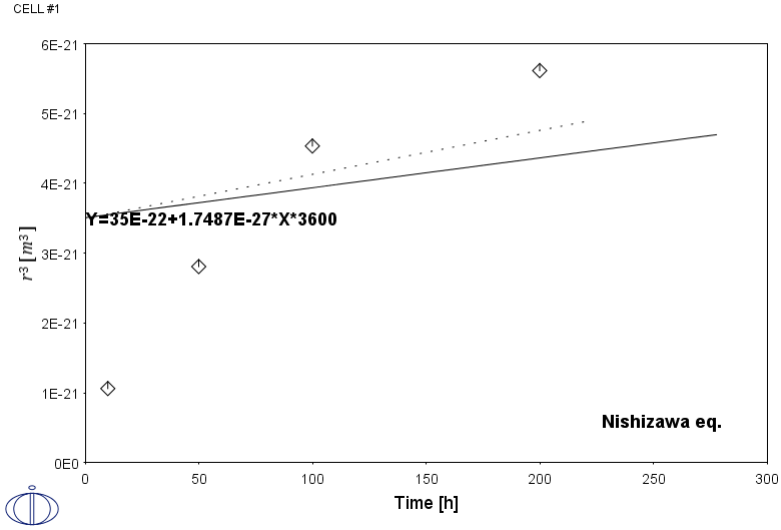
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exf1\run.DCM.test"DIC>DIC>
DIC>DIC>DIC>DIC>
DIC> TIME STEP AT TIME  0.00000E+00
 *** ENTERING M6C AS A DIFFUSION NONE PHASE
DIC> OK
DIC> Region: PART
 single geometric dense at  0.22800E-06
 0.80000       64
 Region: AUS
 single geometric dense at   0.0000
  1.0060       63
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
  Trying old scheme                 4
 GENERATING STARTING VALUES FOR CELL #  1 INTERFACE #  2
 DETERMINING INITIAL EQUILIBRIUM VALUES
CALCULATING STARTING VALUES:       9   EQUILIBRIUM CALCULATIONS               DONE     6 OUT OF     9
 U-FRACTION IN SYSTEM:  C = .0190652843033664  FE = .970761291162784
                        MO = .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]
 0.610222970497625        0.610391048253349        0.610222911134897        2.564830791805986E-002        2.191933775056683E-
003        1.266865136539016E-004        1.096501637402910E-003        1.278319034980207E-004        4.432656423657809E-
007        1.566395384770823E-009        1.947833797566236E-009        3.659995990186460E-009        1.418022159108813E-
009        1.309139560626615E-009        1.103984995435807E-009        3.800021122231109E-009        7.446660768169544E-
010        2.344009328983523E-010        1.080152657431134E-013        1.867048992018644E-018       TIME =  0.10000000E-06 DT =  0.10000000E-
06 SUM OF SQUARES =  0.18670490E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.50349408E-05 AND  -0.50349408E-05
 POSITION OF INTERFACE PART / AUS IS   0.22799950E-06
 U-FRACTION IN SYSTEM:  C = .0190659317665348  FE = .97075948763499
                        MO = .0292405124955171
 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
 5.960103084512673E-005        5.961330246326774E-005        5.959458011837933E-005        3.934421762395374E-007        1.790920453097894E-
012        8.025964155192889E-020       SWITCHING ACTIVITIES FOR INTERFACE #2, CELL #1
 FROM: C  TO: MO
 TIME =  0.25446964E-05 DT =  0.24446964E-05 SUM OF SQUARES =  0.80259642E-19
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.39293667E-08 AND  -0.39293667E-08
 POSITION OF INTERFACE PART / AUS IS   0.22799949E-06
 U-FRACTION IN SYSTEM:  C = .0190664790756638  FE = .970759484159471
                        MO = .029240515971036
 TOTAL SIZE OF SYSTEM:  1.32375709311E-18 [m^3]
  CPU time used in timestep                     0 seconds
 2.515158577242374E-008        2.515761986903607E-008        2.499573880413570E-008        2.005534167482623E-008        1.975331982786994E-
008        1.917061732580525E-008        1.798309026836323E-008        1.798198226700991E-008        1.576453665210291E-
008        1.173116060015417E-008        5.468961700099629E-009        5.475062089199896E-009        2.640250387782055E-
011        1.077657407940353E-019       TIME =  0.74340891E-05 DT =  0.48893927E-05 SUM OF SQUARES =  0.10776574E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.56129636E-09 AND  -0.56129636E-09
 POSITION OF INTERFACE PART / AUS IS   0.22799948E-06
 U-FRACTION IN SYSTEM:  C = .0190671017629171  FE = .970759483986866
                        MO = .0292405161436416
 TOTAL SIZE OF SYSTEM:  1.32375704531E-18 [m^3]
  CPU time used in timestep                     1 seconds
 4.333438082333519E-010        4.334345192117615E-010        4.419215184528116E-010        4.026611769322621E-010        4.018893331119746E-
010        4.003483961313763E-010        3.972574071925327E-010        3.977091064626878E-010        3.911287926551470E-
010        3.789974355040575E-010        3.553242197488224E-010        3.559796445304182E-010        3.102532490708667E-
010        2.292896944027144E-010        1.040111351283042E-010        1.045003417932500E-010        9.690622034980271E-
014        4.717320715952978E-024       TIME =  0.17212874E-04 DT =  0.97787854E-05 SUM OF SQUARES =  0.47173207E-23
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.11440105E-09 AND  -0.11440105E-09
 POSITION OF INTERFACE PART / AUS IS   0.22799948E-06
 U-FRACTION IN SYSTEM:  C = .0190679130516543  FE = .970759484521661
                        MO = .0292405156088452
 TOTAL SIZE OF SYSTEM:  1.32375702582E-18 [m^3]
  CPU time used in timestep                     0 seconds
 2.078097505783963E-011        2.078435613986830E-011        2.355548441512695E-011        1.450907171683003E-011        1.448890247199484E-
011        1.444815490174228E-011        1.436727711948279E-011        1.460833291638921E-011        1.420576096044696E-
011        1.388590156999237E-011        1.325668990489150E-011

output ignored...



... output resumed

 1.830839512261248E-011        2.171297166715594E-011        9.341086471467834E-013        1.185646269228700E-013        1.157311355779890E-
022       TIME =   667998.25     DT =   100000.00     SUM OF SQUARES =  0.11573114E-21
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.22669488E-13 AND   0.22669488E-13
 POSITION OF INTERFACE PART / AUS IS   0.24398484E-06
 U-FRACTION IN SYSTEM:  C = .0195561971882076  FE = .970692497669243
                        MO = .0293075024612628
 TOTAL SIZE OF SYSTEM:  1.62216577705E-18 [m^3]
  29  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: PART
  29  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUS

  CPU time used in timestep                     0 seconds
 8.463229172580973E-012        8.732923770518564E-012        1.106305683610398E-011        1.671261429107251E-012        8.083192020157945E-
013        2.031410141915157E-015        4.685010844754274E-
025       TIME =   767998.25     DT =   100000.00     SUM OF SQUARES =  0.46850108E-24
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.22252996E-13 AND   0.22252996E-13
 POSITION OF INTERFACE PART / AUS IS   0.24621014E-06
 U-FRACTION IN SYSTEM:  C = .0195587075255283  FE = .970694293020122
                        MO = .0293057071103846
 TOTAL SIZE OF SYSTEM:  1.66695743696E-18 [m^3]
  16  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: PART
  16  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUS

  CPU time used in timestep                     1 seconds
 4.716189846859196E-012        4.737893940446968E-012        6.250071114960049E-012        2.547264425603688E-012        1.906488082888713E-
012        8.178987489178293E-013        4.566429376922698E-
022       TIME =   867998.25     DT =   100000.00     SUM OF SQUARES =  0.45664294E-21
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.21855116E-13 AND   0.21855116E-13
 POSITION OF INTERFACE PART / AUS IS   0.24839565E-06
 U-FRACTION IN SYSTEM:  C = .0195611435099224  FE = .970696048456854
                        MO = .0293039516736528
 TOTAL SIZE OF SYSTEM:  1.71174343902E-18 [m^3]
  25  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: PART
  25  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUS

  CPU time used in timestep                     0 seconds
```

```
 3.963242814704096E-012        3.789984523496892E-012        4.665295368988863E-012        3.497963738126882E-012        3.136690146229866E-
012        2.396321553550503E-012        1.082065622076279E-012        1.796678880501578E-015        5.677791012762993E-
025       TIME =   967998.25     DT =   100000.00     SUM OF SQUARES =  0.56777910E-24
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.21474553E-13 AND   0.21474553E-13
 POSITION OF INTERFACE PART / AUS IS   0.25054311E-06
 U-FRACTION IN SYSTEM:  C = .0195635100799648  FE = .970697758696435
                        MO = .0293022414340725
 TOTAL SIZE OF SYSTEM:  1.75652397337E-18 [m^3]
  13  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: PART
  13  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUS

  CPU time used in timestep                    1 seconds
 3.163580376870747E-010        3.128551237604002E-010        3.018312579563825E-010        3.724165852379791E-011        1.354265497009896E-
011        1.037003584921101E-019       TIME =   1000000.0     DT =   32001.746     SUM OF SQUARES =  0.10370036E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.21247167E-13 AND   0.21247167E-13
 POSITION OF INTERFACE PART / AUS IS   0.25122306E-06
 U-FRACTION IN SYSTEM:  C = .0195660575765657  FE = .970698831747602
                        MO = .0293011683829052
 TOTAL SIZE OF SYSTEM:  1.77086385838E-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   0.25446964E-05
 DELETING TIME-RECORD FOR TIME   0.74340891E-05
 DELETING TIME-RECORD FOR TIME   0.17212874E-04
 DELETING TIME-RECORD FOR TIME   0.36770445E-04
 DELETING TIME-RECORD FOR TIME   0.75885587E-04
 DELETING TIME-RECORD FOR TIME   0.15411587E-03
 DELETING TIME-RECORD FOR TIME   0.31057644E-03
 DELETING TIME-RECORD FOR TIME   0.62349757E-03
 DELETING TIME-RECORD FOR TIME   0.12493398E-02
 DELETING TIME-RECORD FOR TIME   0.25010244E-02
 DELETING TIME-RECORD FOR TIME   0.50043934E-02
 DELETING TIME-RECORD FOR TIME   0.10011132E-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   0.16021328
 DELETING TIME-RECORD FOR TIME   0.32042890
 DELETING TIME-RECORD FOR TIME   0.64086014
 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    82.030395
 DELETING TIME-RECORD FOR TIME    164.06079
 DELETING TIME-RECORD FOR TIME    328.12159
 DELETING TIME-RECORD FOR TIME    656.24318
 DELETING TIME-RECORD FOR TIME    1312.4864
 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    41999.564
 DELETING TIME-RECORD FOR TIME    83999.127
 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

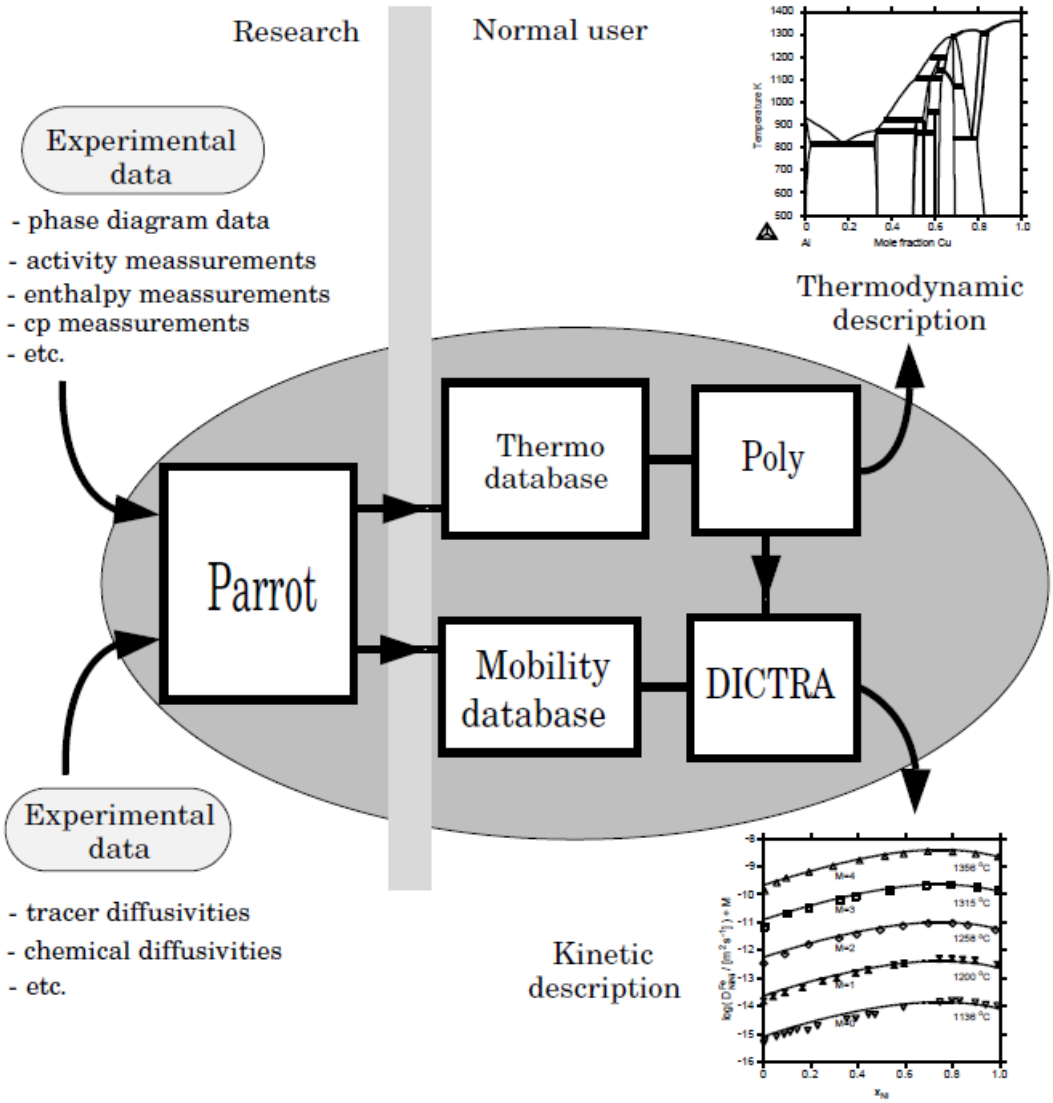
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exf1\plot.DCM.test"DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  1.00000E+06
 *** ENTERING M6C AS A DIFFUSION NONE PHASE
DIC> OK
DIC>
DIC>DIC>DIC>DIC>  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn 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:
```

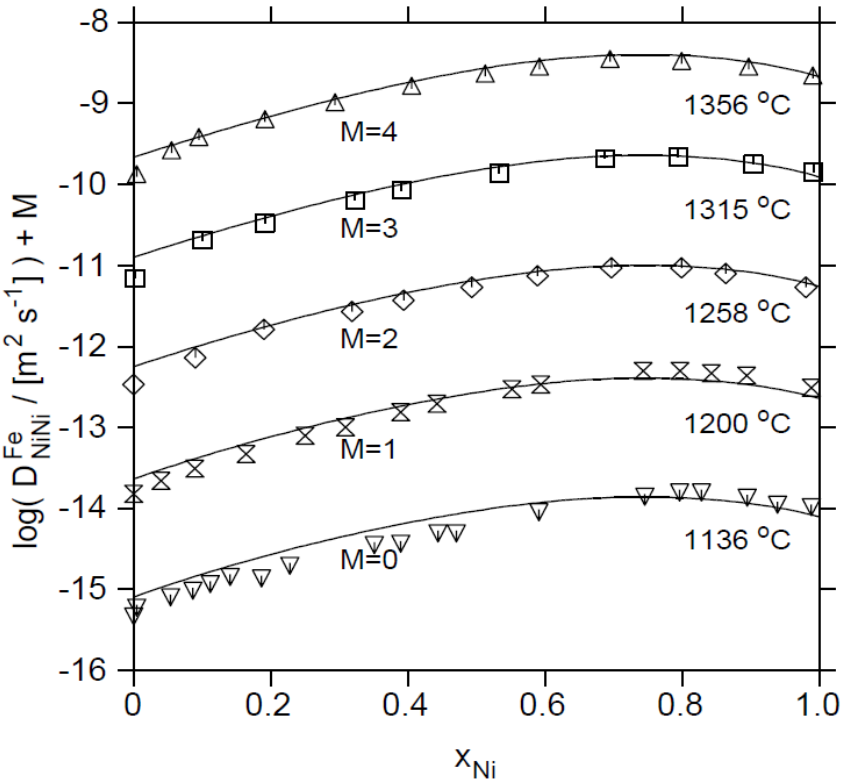
Kinetic Data



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

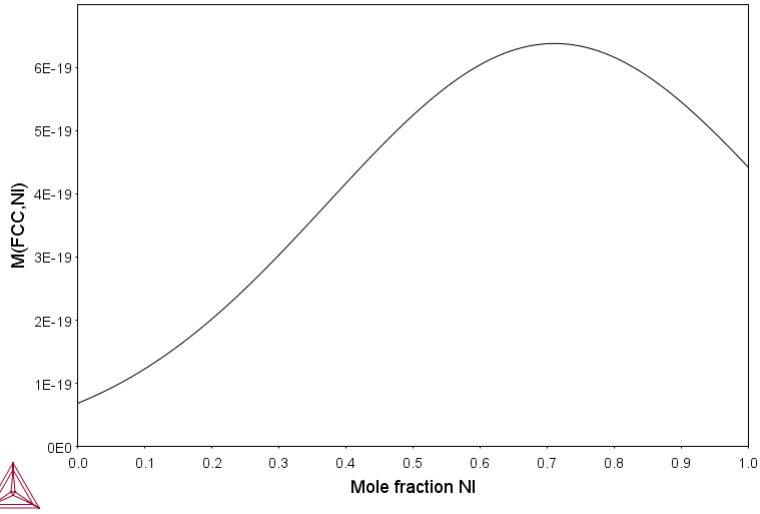
```
About Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 20130) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri May 24 17:06:15 2019


SYS:SYS:MACRO "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  v9.1

 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 v2.1

 VA                       /-  DEFINED
TDB_FEDEMO:
TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO: FE                       NI  DEFINED
TDB_FEDEMO:
TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO:TDB_FEDEMO: LIQUID:L                 BCC_A2                  CBCC_A12
 CUB_A13                  FCC_A1                  HCP_A3
 LAVES_PHASE_C14  REJECTED
TDB_FEDEMO: FCC_A1  RESTORED
TDB_FEDEMO:
TDB_FEDEMO: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'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  '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: Use one of these databases

 TCFE9   =  Steels/Fe-Alloys  v9.1
 TCFE8   =  Steels/Fe-Alloys  v8.1
 FROST1  =  FROST database v1.0
 TCFE7   =  Steels/Fe-Alloys  v7.0
 TCFE6   =  Steels/Fe-Alloys  v6.2
 TCFE5   =  Steels/Fe-Alloys  v5.0
 TCFE4   =  Steels/Fe-Alloys  v4.1
 TCFE3   =  Steels/Fe-Alloys  v3.1
 TCFE2   =  Steels/Fe-Alloys  v2.1
 TCFE1   =  Steels/Fe-Alloys  v1.0
 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  v2.1
 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
 TCSLD1  =  Solder Alloys  v1.1
 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
 TCNF2   =  Nuclear Fuels  v2.1b
 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 v2.1
 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  v1.0
 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                      NI  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'
  '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>OUTPUT TO SCREEN OR FILE /SCREEN/:
PHASE NAME :DEPENDENT COMPONENT ? /NI/:CONCENTRATION OF NI IN U-
FRACTION /1/:Pressure /100000/:Temperature /298.15/:OPTION ( dlpbmx0ez or * ) /D/:
  Dkj (reduced n=FE)
  k / j NI
  NI   +3.83335E-15
   L0kj = Uk*Mvak IF (kES) ELSE Uk*Yva*Mvak
  k / j   FE             NI
  FE    +9.0901E-20
  NI                   +9.0901E-20


  Volume =   1.000000000000000E-005

DIC>
DIC>
DIC>@?<Hit_return_to_continue>
DIC>
DIC>DIC>DIC>DIC>POLY:POLY: 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:

POLY:Axis number: /1/:Condition /NONE/:Min value /0/:Max value /1/:Increment /.025/:POLY:
POLY: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:
POLY:POLY:POLY:POLY:  POLY-3 POSTPROCESSOR VERSION 3.2
POST:
POST:
POST:
```

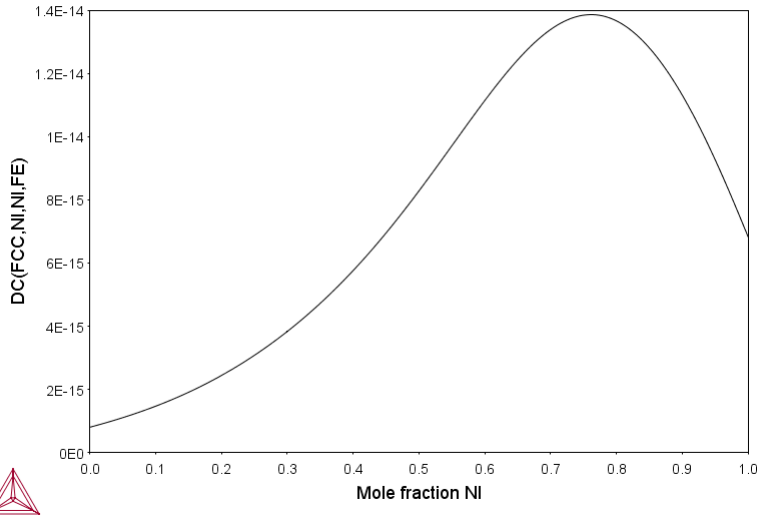
```
POST:POST:POST:POST:POST:POST:
POST:
POST:POST:POST:POST:
POST:
```

2019.05.27.13.46.19
MFEDEMO: FE, NI
T=1409, P=1.01325E5, N=1



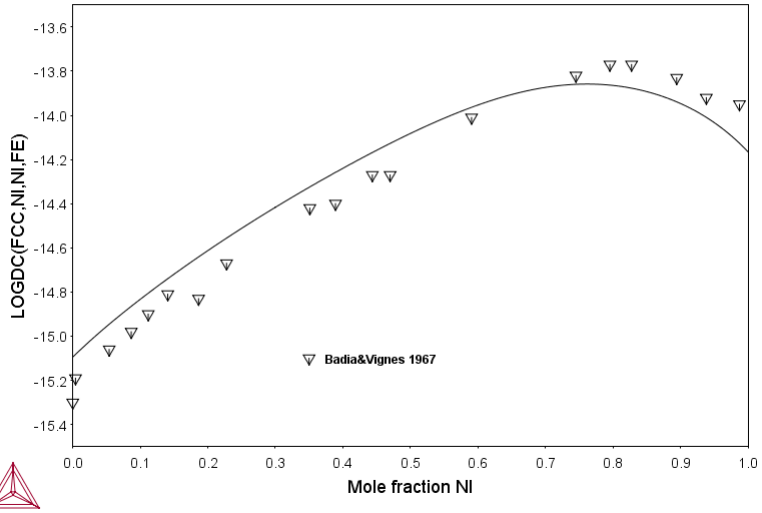

```
POST:
POST:
POST:
POST:@?<Hit_return_to_continue>
POST:
POST:POST:POST:POST:POST:
POST:
POST:POST:POST:POST:
POST:
```

2019.05.27.13.46.19
MFEDEMO: 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:
```

2019.05.27.13.46.20
MFEDEMO: FE, NI
T=1409, P=1.01325E5, N=1

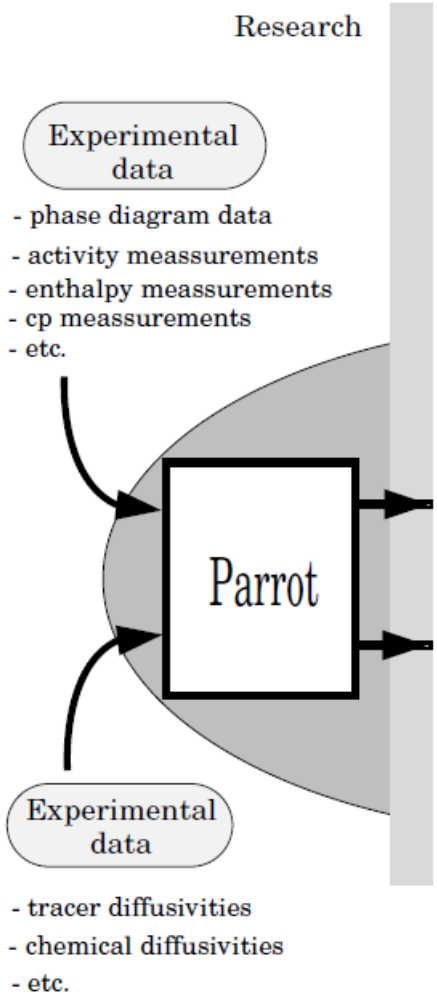



```
POST:
POST:
POST:@?<Hit_return_to_continue>
POST:
POST:POST:
```

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 Software  (build 20130) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri May 24 17:06:15 2019


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:SYS:SYS:SYS:
SYS:SYS:SYS:SYS: THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.1

 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: 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: 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
```

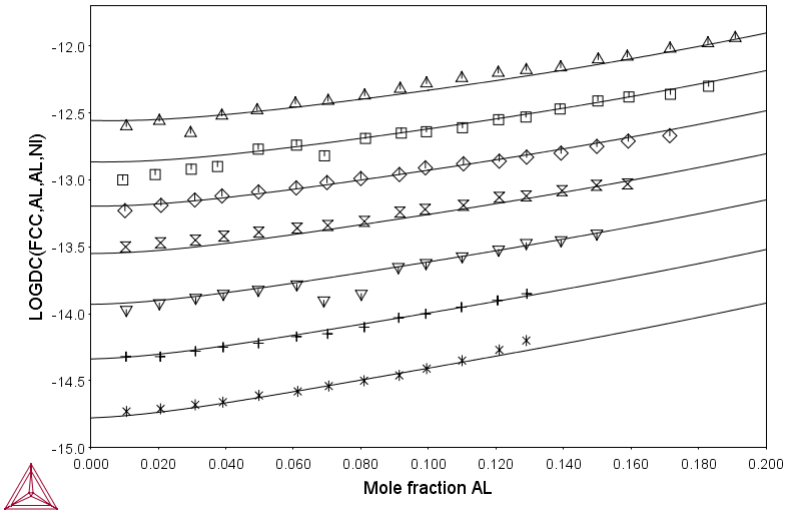
```
80 LOGDC(F...,AL,NI)=-13.19      -13.22      0.10     -2.6230E-02 -0.2623
81 LOGDC(F...,AL,NI)=-13.13      -13.17      0.10     -4.3098E-02 -0.4310
82 LOGDC(F...,AL,NI)=-13.12      -13.14      0.10     -1.9773E-02 -0.1977
83 LOGDC(F...,AL,NI)=-13.08      -13.09      0.10     -1.4457E-02 -0.1446
84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

POLY:POLY: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:POLY:POLY:POLY:POLY: 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:POLY: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:POLY: 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:POLY: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
```

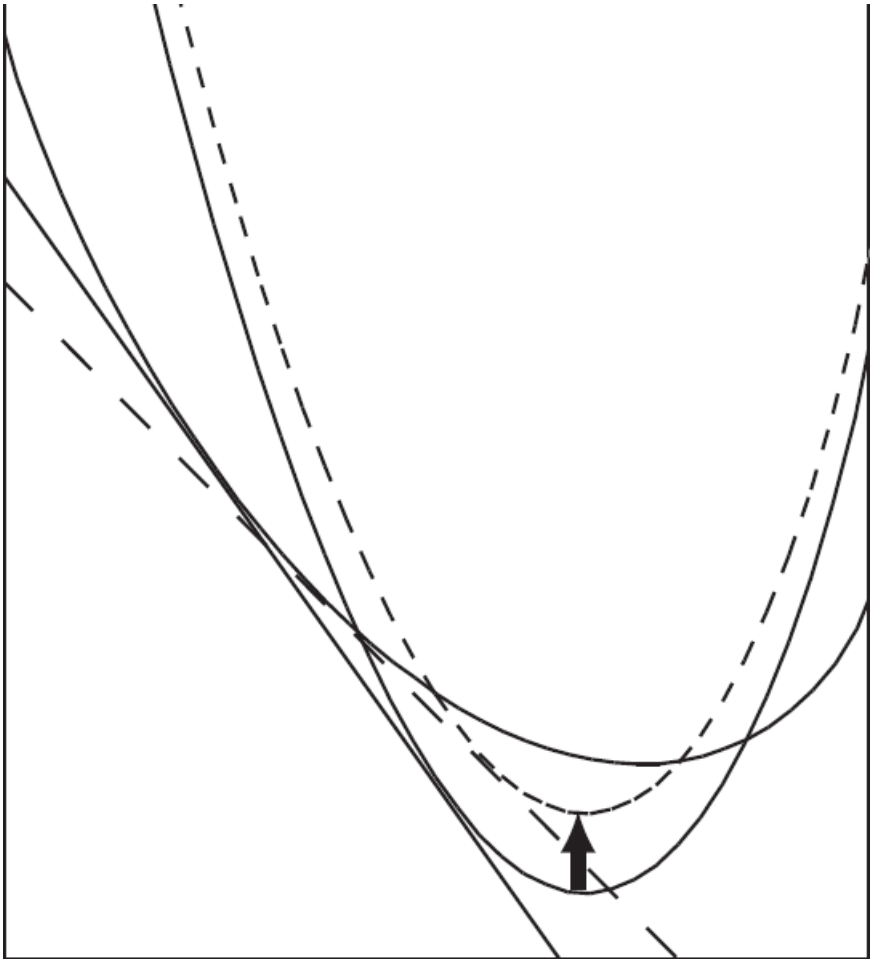
```
 Global test at  4.20000E-02 .... OK
 Global test at  3.20000E-02 .... OK
 Global test at  2.20000E-02 .... OK
 Global test at  1.20000E-02 .... OK
 Global test at  2.00000E-03 .... OK
 Terminating at   0.100000E-03
 Calculated   103 equilibria
 *** Buffer saved on file: C:\Users\developer\Documents\RESULT_002.POLY3
POLY:POLY: 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:POLY: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:POLY: 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:POLY: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:POLY: 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:POLY: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:POLY: 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:POLY: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:POLY:POLY:POLY:POLY:  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:
```

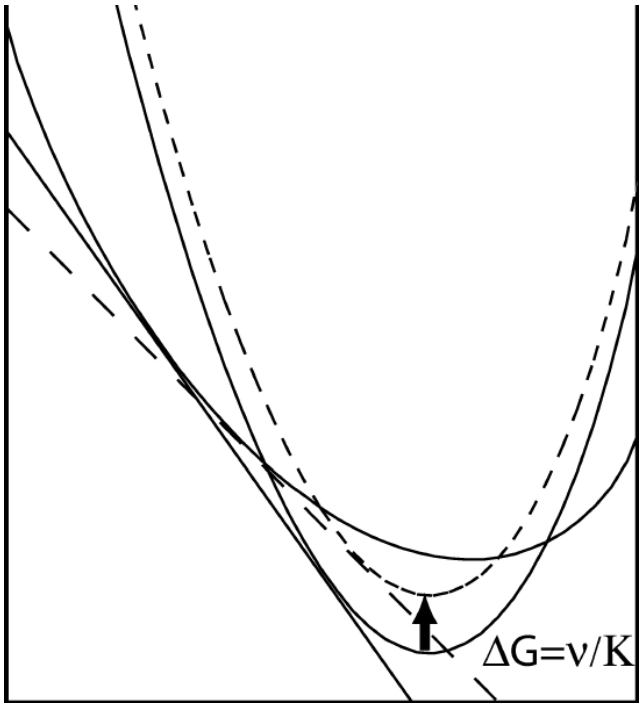
Deviation From Local Equilibrium



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 Software  (build 20130) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri May 24 17:06:15 2019


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  v9.1

 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 v2.1

 VA                       /-  DEFINED
TDB_FEDEMO: FE                       C  DEFINED
TDB_FEDEMO: GAS:G                    LIQUID:L                BCC_A2
 CBCC_A12                 CEMENTITE               CUB_A13
 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'
  '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

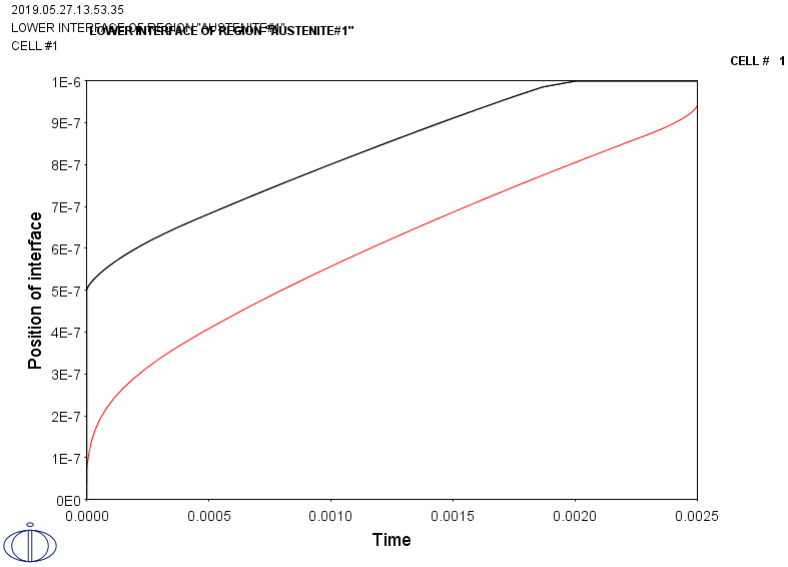
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exh1\run.DCM.test"DIC>
DIC>
DIC>DIC>DIC>DIC>
DIC> TIME STEP AT TIME  0.00000E+00
DIC>
DIC> OK
DIC>
DIC>DIC>DIC>DIC>END TIME FOR INTEGRATION /.1/:AUTOMATIC TIMESTEP CONTROL /YES/:MAX TIMESTEP DURING INTEGRATION /2.5E-04/:
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
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
  Trying old scheme                       3
 U-FRACTION IN SYSTEM:  C = 8.8825328568563E-04  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-06 [m]
 U-FRACTION IN SYSTEM:  C = 8.8825328568563E-04  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-06 [m]
 2.137709938545117E-004        2.137625593784731E-004        13.8289493075457        2.120998910989481E-004        2.112667987368479E-
004        2.108508673097270E-004        2.106430552846505E-004        2.104353457185482E-004        2.101948159747293E-
004        2.097141691148264E-004        2.087545259060967E-004        2.068418415330113E-004        2.030428809643886E-
004        1.955505925372636E-004        1.809885465233079E-004        1.535545778568047E-004        1.054471339695762E-
004        3.627421997801256E-005         13.8289493975683        3.615700625668437E-005        3.609847052764370E-
005        3.606922044603054E-005        3.605459985093341E-005        3.603998221969593E-005        3.602477832953839E-
005        3.599438017219486E-005        3.593362234919143E-005        3.581226067032396E-005        3.557015318069909E-
005        3.508840167395374E-005        3.413475255057607E-005        3.226686986425067E-005        2.868876673322590E-
005        2.216320943769695E-005        1.163469071283029E-005         7.48347169303506        1.161266679204479E-
005        1.160166265598601E-005        1.159616254402650E-005        1.159341297706724E-005        1.159066373617003E-
005        1.158790564696634E-005        1.158239045322414E-005        1.157136400401342E-005        1.154932685894056E-
005        1.150531558187507E-005        1.141754508040302E-005        1.124301228790148E-005        1.089797954462179E-
005        1.022404542521614E-005        1.490118236986448E-002        1.019021766640512E-005        1.017332480757794E-
005        1.016488363329335E-005        1.016066435994746E-005        1.015644596244697E-005        1.015204955140657E-
005        1.014325958456044E-005        1.012569107177291E-005        1.009059972974884E-005        1.002059978000648E-
005        9.881330817733185E-006        4.762707304410066E-006        4.438312986653563E-003        2.058831466677496E-
006        2.181365186740473E-007        6.215863454363136E-009        1.005966933715624E-011        2.807707685834128E-
008        1.740878115116929E-015        2.916483858733431E-008        3.123141534652535E-019       TIME =  0.10000000E-06 DT =  0.10000000E-
06 SUM OF SQUARES =  0.31231415E-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 = 9.00101592836941E-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
 2.884385690560541E-004        2.884962732781007E-004        6.725395559763418E-012        2.964586457296539E-012        7.238230803264643E-
013        1.865556888535795E-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 = 9.00450100183248E-04  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-06 [m]
  CPU time used in timestep                     0 seconds
 6.614507143838177E-006

output ignored...



... output resumed

 8.723042581764741E-023       TIME =  0.24974221E-02 DT =  0.18903328E-05 SUM OF SQUARES =  0.87230426E-22
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.83033507E-03 AND   0.83033507E-03
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.93676959E-06
 U-FRACTION IN SYSTEM:  C = 8.98900765332414E-04  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-06 [m]
  CPU time used in timestep                     0 seconds
 7.855335891908584E-008        7.845462688193365E-008        2.895741352396423E-010        1.377394974932415E-012        3.299199757771801E-
017       TIME =  0.24986191E-02 DT =  0.11969967E-05 SUM OF SQUARES =  0.32991998E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.95215868E-03 AND   0.95215868E-03
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.93790932E-06
 U-FRACTION IN SYSTEM:  C = 8.98953471320335E-04  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-06 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: FERRITE

  CPU time used in timestep                     1 seconds
 1.224785093490384E-007        1.223255533698191E-007        2.395876491183955E-010        6.518552140022120E-013        4.308845465113762E-
018       TIME =  0.24993550E-02 DT =  0.73586310E-06 SUM OF SQUARES =  0.43088455E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.10897996E-02 AND   0.10897996E-02
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.93871126E-06
 U-FRACTION IN SYSTEM:  C = 8.98994461255808E-04  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-06 [m]
  CPU time used in timestep                     0 seconds
 3.060409488024728E-007        3.057363397219153E-007        3.253002600302852E-010        5.404637980843020E-013        1.316152837296719E-
018       TIME =  0.24997404E-02 DT =  0.38538383E-06 SUM OF SQUARES =  0.13161528E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.12900929E-02 AND   0.12900929E-02
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.93920844E-06
 U-FRACTION IN SYSTEM:  C = 8.99052140183798E-04  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-06 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: FERRITE

  CPU time used in timestep                     1 seconds
 3.534169165519616E-007        3.530044163655197E-007        1.634713104061553E-010        8.223310409455192E-014        2.121724965302169E-
020       TIME =  0.24999375E-02 DT =  0.19709686E-06 SUM OF SQUARES =  0.21217250E-19
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.14857381E-02 AND   0.14857381E-02
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.93950128E-06
 U-FRACTION IN SYSTEM:  C = 8.99110503818547E-04  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-06 [m]
  CPU time used in timestep                     0 seconds
 1.382372414161934E-006        1.381369908229288E-006        1.794190027287522E-010        9.492447257334572E-015        3.810267507248266E-
022       TIME =  0.25000000E-02 DT =  0.62514884E-07 SUM OF SQUARES =  0.38102675E-21
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.18529421E-02 AND   0.18529421E-02
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.93961711E-06
 U-FRACTION IN SYSTEM:  C = 8.99171783958494E-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   0.28565341E-05
 DELETING TIME-RECORD FOR TIME   0.52015356E-05
 DELETING TIME-RECORD FOR TIME   0.98915386E-05
 DELETING TIME-RECORD FOR TIME   0.19271545E-04
 DELETING TIME-RECORD FOR TIME   0.33687181E-04
 DELETING TIME-RECORD FOR TIME   0.53417477E-04
 DELETING TIME-RECORD FOR TIME   0.78654360E-04
 DELETING TIME-RECORD FOR TIME   0.10952899E-03
 DELETING TIME-RECORD FOR TIME   0.14613094E-03
 DELETING TIME-RECORD FOR TIME   0.18853082E-03
 DELETING TIME-RECORD FOR TIME   0.23679896E-03
 DELETING TIME-RECORD FOR TIME   0.29104871E-03
 DELETING TIME-RECORD FOR TIME   0.35145425E-03
 DELETING TIME-RECORD FOR TIME   0.41823582E-03
 DELETING TIME-RECORD FOR TIME   0.48723339E-03
 DELETING TIME-RECORD FOR TIME   0.55628739E-03
 DELETING TIME-RECORD FOR TIME   0.62546249E-03
 DELETING TIME-RECORD FOR TIME   0.69481220E-03
 DELETING TIME-RECORD FOR TIME   0.76438013E-03
 DELETING TIME-RECORD FOR TIME   0.83419603E-03
 DELETING TIME-RECORD FOR TIME   0.90425851E-03
 DELETING TIME-RECORD FOR TIME   0.97473727E-03
 DELETING TIME-RECORD FOR TIME   0.10456577E-02
 DELETING TIME-RECORD FOR TIME   0.11169997E-02
 DELETING TIME-RECORD FOR TIME   0.11887868E-02
 DELETING TIME-RECORD FOR TIME   0.12609691E-02
 DELETING TIME-RECORD FOR TIME   0.13331752E-02
 DELETING TIME-RECORD FOR TIME   0.14056137E-02
 DELETING TIME-RECORD FOR TIME   0.14782827E-02
 DELETING TIME-RECORD FOR TIME   0.15511176E-02
 DELETING TIME-RECORD FOR TIME   0.16239995E-02
 DELETING TIME-RECORD FOR TIME   0.16973710E-02
 DELETING TIME-RECORD FOR TIME   0.17714237E-02
 DELETING TIME-RECORD FOR TIME   0.18459454E-02
 DELETING TIME-RECORD FOR TIME   0.19208359E-02
 DELETING TIME-RECORD FOR TIME   0.19960899E-02
 DELETING TIME-RECORD FOR TIME   0.20715733E-02
 DELETING TIME-RECORD FOR TIME   0.21477958E-02
 DELETING TIME-RECORD FOR TIME   0.22245451E-02
 DELETING TIME-RECORD FOR TIME   0.23020845E-02
 DELETING TIME-RECORD FOR TIME   0.23637496E-02
 DELETING TIME-RECORD FOR TIME   0.24066139E-02
 DELETING TIME-RECORD FOR TIME   0.24364991E-02
 DELETING TIME-RECORD FOR TIME   0.24572378E-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

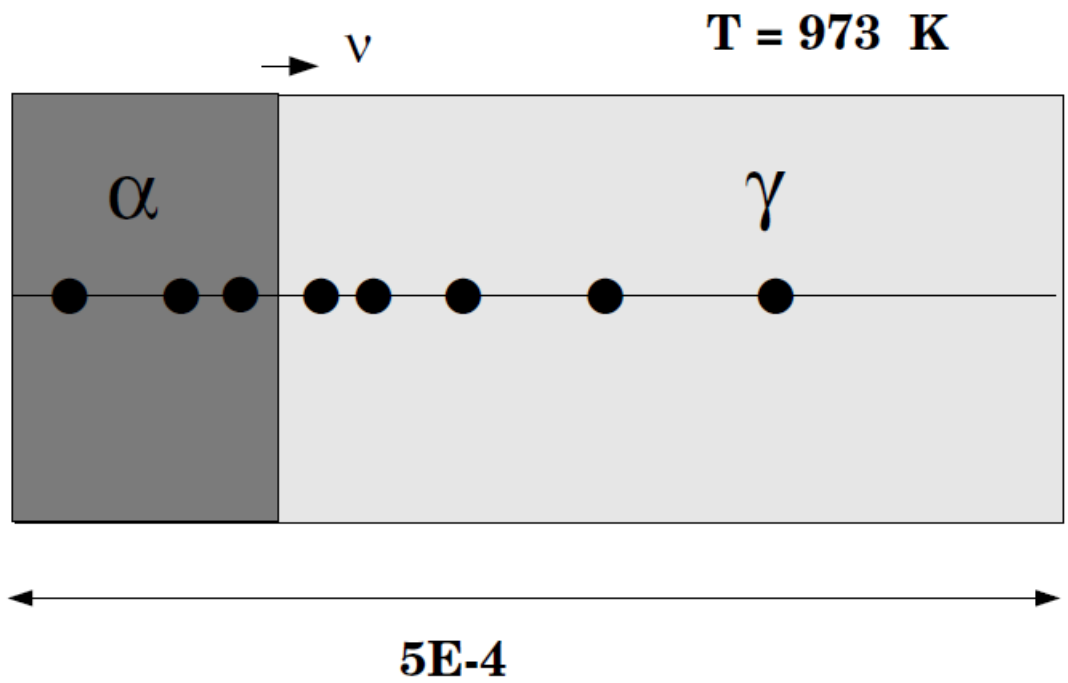



```
POST-1:
POST-1:
POST-1: --OK---
POST-1:
```

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 Software  (build 20130) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri May 24 17:06:15 2019


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  v9.1

 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 v2.1

 VA                      /-  DEFINED
TDB_FEDEMO: FE                       NI                      C
   DEFINED
TDB_FEDEMO: GAS:G                    LIQUID:L                BCC_A2
 CBCC_A12                CEMENTITE               CUB_A13
 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'
  '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>
```

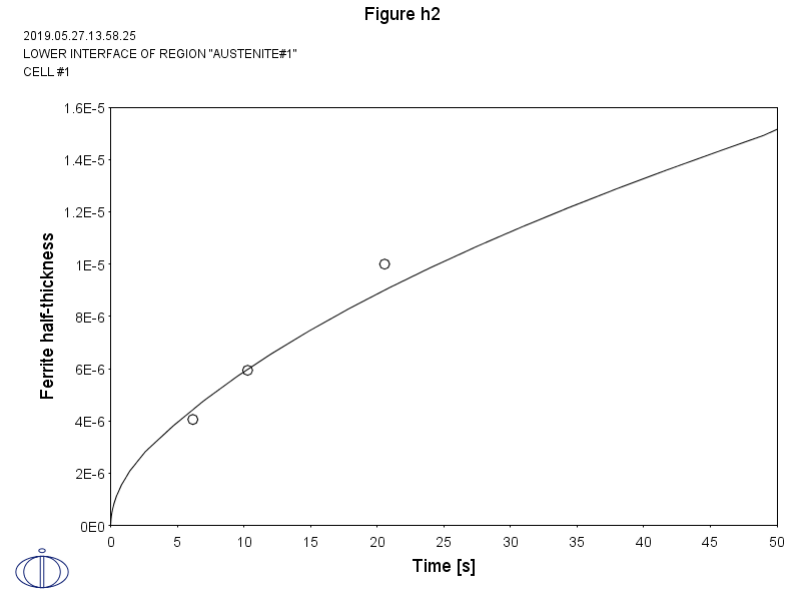
exh2-run

```
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
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
  Trying old scheme                    4
 GENERATING STARTING VALUES FOR CELL #  1 INTERFACE #  2
 DETERMINING INITIAL EQUILIBRIUM VALUES
CALCULATING STARTING VALUES:       9   EQUILIBRIUM CALCULATIONS               DONE     6 OUT OF     9
 U-FRACTION IN SYSTEM:  C = .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]
  13403.6958745532         13403.6958745560         13396.6824657606         181.652814770086         1.24966113910028         3.83383221700482
003        1.422760417512304E-005        4.522016845669663E-007        2.881067182217709E-014       TIME =  0.10000000E-06 DT =  0.10000000E-
06 SUM OF SQUARES =  0.28810672E-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 = .00412273714809207  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
  13162.2365643669         13162.2365643854         13155.2460353462         172.785449886281         1.16154706429747         4.1445216513136
003        1.903424670850253E-003        2.796483852397174E-006        4.535465491428548E-007        1.548523224829952E-
009        7.179391642484034E-013       TIME =  0.20000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =  0.71793916E-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 = .00412273399769255  FE = .980742621143594
                        NI = .0192573788564064
 TOTAL SIZE OF SYSTEM:  5.0001E-05 [m]
  CPU time used in timestep                    2 seconds
  12924.7969674950         12924.7969674949         12917.8299122851         164.371511427609         1.07976154526347         5.304375562747494
002        1.617763337362580E-004        1.560231860701586E-007        1.263010253836241E-003        6.062350394755839E-
016       TIME =  0.35656740E-06 DT =  0.15656740E-06 SUM OF SQUARES =  0.60623504E-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 = .00412273399769264  FE = .980742621143593
                        NI = .0192573788564064
 TOTAL SIZE OF SYSTEM:  5.0001E-05 [m]
  CPU time used in timestep                    1 seconds
  12691.3220847414         12691.3220847404         12684.3790790120         156.386669255908         1.00388574886515         1.360047886719004
004        1.392594367896651E-006        9.264887113131991E-009        1.340641618517111E-003        4.330244192718537E-
018       TIME =  0.63794974E-06 DT =  0.28138234E-06 SUM OF SQUARES =  0.43302442E-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 = .00412273399769142  FE = .980742621143593


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 = .00412855131241422  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
  6134.60951334942         6134.60951335030         6128.88995331836         24.2689880423745         6.413322468570902E-
002        8.380048789282951E-004        3.990461406660846E-006        5.061492706426717E-011        1.608627859978953E-
003        2.562274922307538E-020       TIME =   41.718584     DT =   3.7168197     SUM OF SQUARES =  0.25622749E-19
 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 = .00412892447598121  FE = .980742621143594
                        NI = .0192573788564066
 TOTAL SIZE OF SYSTEM:  5.0001E-05 [m]
  14  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: FERRITE

  CPU time used in timestep                    3 seconds
  6019.29790049884         6019.29790050192         6013.61359254715         23.1752711368688         5.988603848637142E-
002        6.191104424660428E-004        3.230252466322621E-006        5.179323336504226E-011        1.618147722970193E-
003        1.037615717682425E-020       TIME =   45.525738     DT =   3.8071537     SUM OF SQUARES =  0.10376157E-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 = .004129270238027  FE = .980742621143593
                        NI = .0192573788564066
 TOTAL SIZE OF SYSTEM:  5.0001E-05 [m]
  15  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: FERRITE

  CPU time used in timestep                    2 seconds
  5906.07319970362         5906.07319970446         5900.42420052854         22.1323479632572         5.592492896851547E-
002        1.888924537845122E-003        1.151756008875738E-006        1.342517986229366E-010        1.162543875065609E-
003        2.594038402071405E-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 = .00412980312100442  FE = .980742621143593
                        NI = .0192573788564066
 TOTAL SIZE OF SYSTEM:  5.0001E-05 [m]
  12  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: FERRITE
```

```
  CPU time used in timestep                    3 seconds
  5794.90030702523         5794.90030702527         5789.28666554335         21.1377742970635        5.223027658161766E-
002        1.429845900093700E-002        3.466078227164368E-005        1.478441800509203E-007        1.640219088335622E-
003        7.325988053684877E-018       TIME =   50.000000     DT =  0.99808402     SUM OF SQUARES =  0.73259881E-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 = .00413094813368368  FE = .980742621143593
                        NI = .0192573788564066
 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   0.42048762E-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:
```



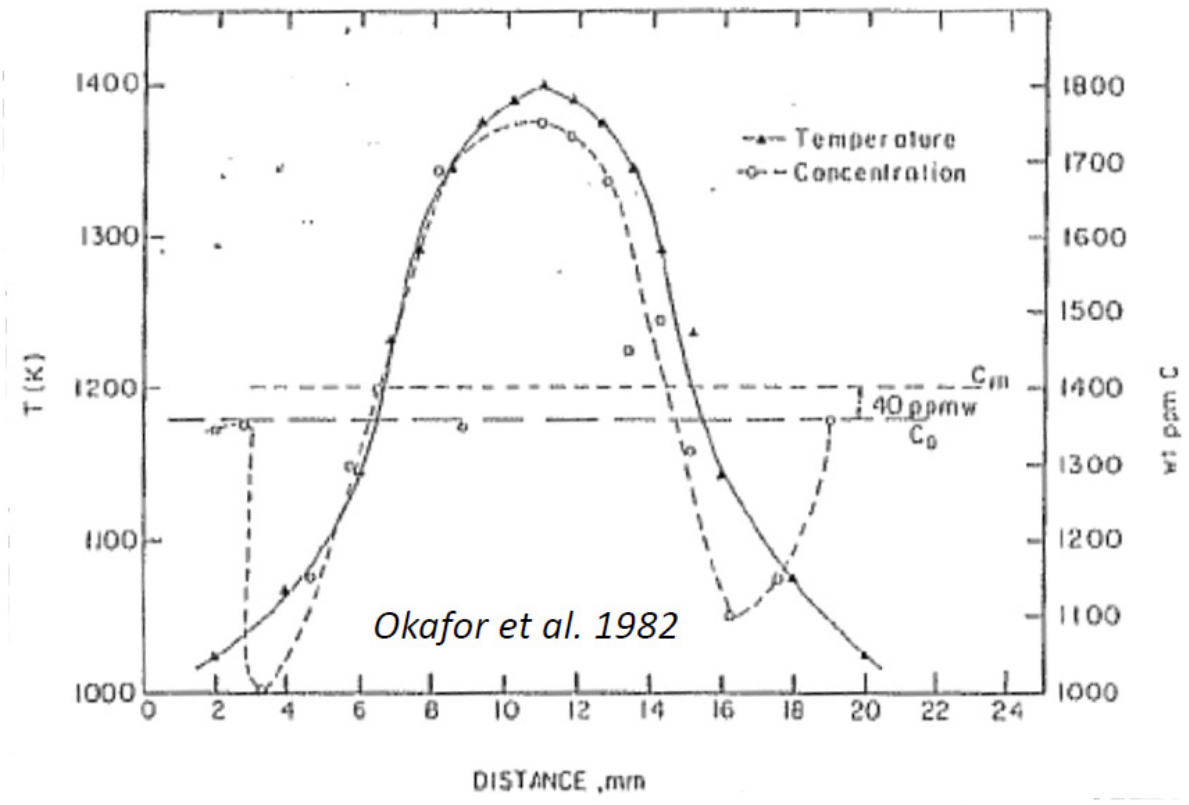

```
POST-1:
POST-1:
POST-1:
POST-1: --OK---
POST-1:
```

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 Software  (build 20130) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri May 24 17:06:15 2019


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  v9.1

 VA                       /-  DEFINED
 L12_FCC                  B2_BCC                  DICTRA_FCC_A1
   REJECTED
TDB_TCFE9: Current database: Iron Demo Database v2.1

 VA                       /-  DEFINED
TDB_FEDEMO: FE                       NI                      C
   DEFINED
TDB_FEDEMO: GAS:G                    LIQUID:L                BCC_A2
 CBCC_A12                 CEMENTITE               CUB_A13
 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'
  '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>
```

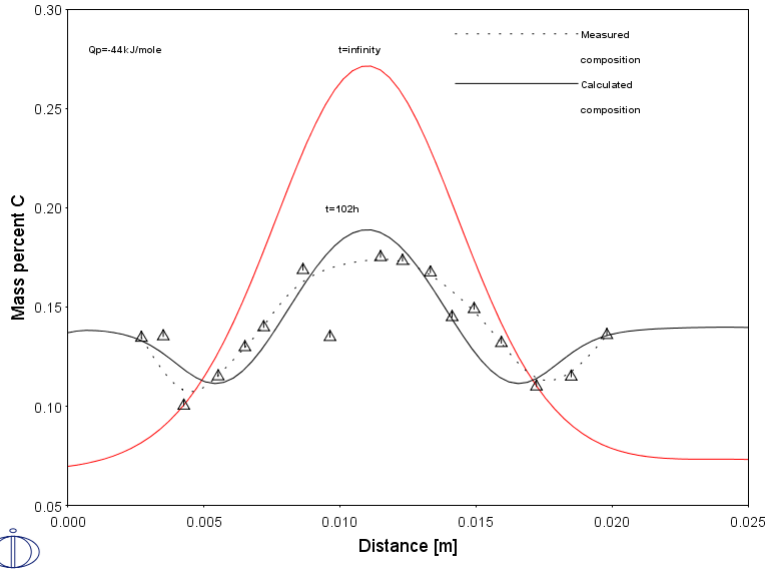
exh3-run

```
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
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
 U-FRACTION IN SYSTEM:  C = .00662305741857946  FE = .68534915460493
                        NI = .31465084539507
 TOTAL SIZE OF SYSTEM:  .025 [m]
 U-FRACTION IN SYSTEM:  C = .00662305741857946  FE = .68534915460493
                        NI = .31465084539507
 TOTAL SIZE OF SYSTEM:  .025 [m]
 TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741857946  FE = .68534915460493
                        NI = .31465084539507
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.10010000E-03 DT =  0.10000000E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741857946  FE = .68534915460493
                        NI = .31465084539507
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.40010010     DT =  0.40000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741857946  FE = .68534915460493
                        NI = .31465084539507
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    1 seconds
 TIME =   1600.4001     DT =   1600.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0066230574185794  FE = .68534915460493
                        NI = .31465084539507
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    0 seconds
 TIME =   75752.427     DT =   74152.027     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741850888  FE = .68534915460493
                        NI = .31465084539507
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    1 seconds
 TIME =   224056.48     DT =   148304.05     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741822249  FE = .685349154604931
                        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 = .00662305741822202  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 = .00662305741822177  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 = .00662305741819811  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 = .00662305741817961  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 = .00662305741818964  FE = .68534915460493
                        NI = .314650845395069
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    1 seconds
 TIME =   10079984.     DT =   2480649.1     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741819595  FE = .68534915460493
                        NI = .31465084539507
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    0 seconds
 TIME =   12348045.     DT =   2268061.6     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741819968  FE = .68534915460493
                        NI = .31465084539507
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    1 seconds
 TIME =   14506749.     DT =   2158703.9     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741820226  FE = .68534915460493
                        NI = .31465084539507
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    0 seconds
 TIME =   16599481.     DT =   2092732.2     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741820466  FE = .68534915460493
                        NI = .31465084539507
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    1 seconds
 TIME =   18648923.     DT =   2049441.3     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741790974  FE = .68534915460493
                        NI = .31465084539507
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    1 seconds
 TIME =   20668354.     DT =   2019431.3     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741737902  FE = .68534915460493
                        NI = .31465084539507
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    0 seconds
 TIME =   22666114.     DT =   1997759.7     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0066230574169279  FE = .68534915460493
                        NI = .31465084539507
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    1 seconds
 TIME =   24647703.     DT =   1981589.3     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741653883  FE = .68534915460493
                        NI = .31465084539507
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                    0 seconds
 TIME =   26616876.     DT =   1969173.4     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741620075  FE = .68534915460493
```

```
                        NI = .31465084539507
TOTAL SIZE OF SYSTEM:  .025 [m]
 CPU time used in timestep                    1 seconds
TIME =   28576276.     DT =   1959399.6     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00662305741590579  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 = .00662305741564762  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 = .00662305741542133  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 = .00662305741522093  FE = .68534915460493
                        NI = .31465084539507
TOTAL SIZE OF SYSTEM:  .025 [m]
 CPU time used in timestep                    1 seconds
TIME =   36347704.     DT =   1935131.5     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00662305741504477  FE = .68534915460493
                        NI = .31465084539507
TOTAL SIZE OF SYSTEM:  .025 [m]
 CPU time used in timestep                    0 seconds
TIME =   38278937.     DT =   1931233.7     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00662305741488849  FE = .68534915460493
                        NI = .31465084539507
TOTAL SIZE OF SYSTEM:  .025 [m]
 CPU time used in timestep                    1 seconds
TIME =   40206807.     DT =   1927869.8     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00662305741475141  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 = .00662305741462873  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 = .00662305741451915  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 = .00662305741442087  FE = .68534915460493
                        NI = .31465084539507
TOTAL SIZE OF SYSTEM:  .025 [m]
 CPU time used in timestep                    0 seconds
TIME =   47614300.     DT =   1640007.6     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00662305741435106  FE = .68534915460493
                        NI = .31465084539507
TOTAL SIZE OF SYSTEM:  .025 [m]
 CPU time used in timestep                    1 seconds
TIME =   48910464.     DT =   1296163.5     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0066230574143058  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 = .00662305741428373  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 = .00662305741428332  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>
```

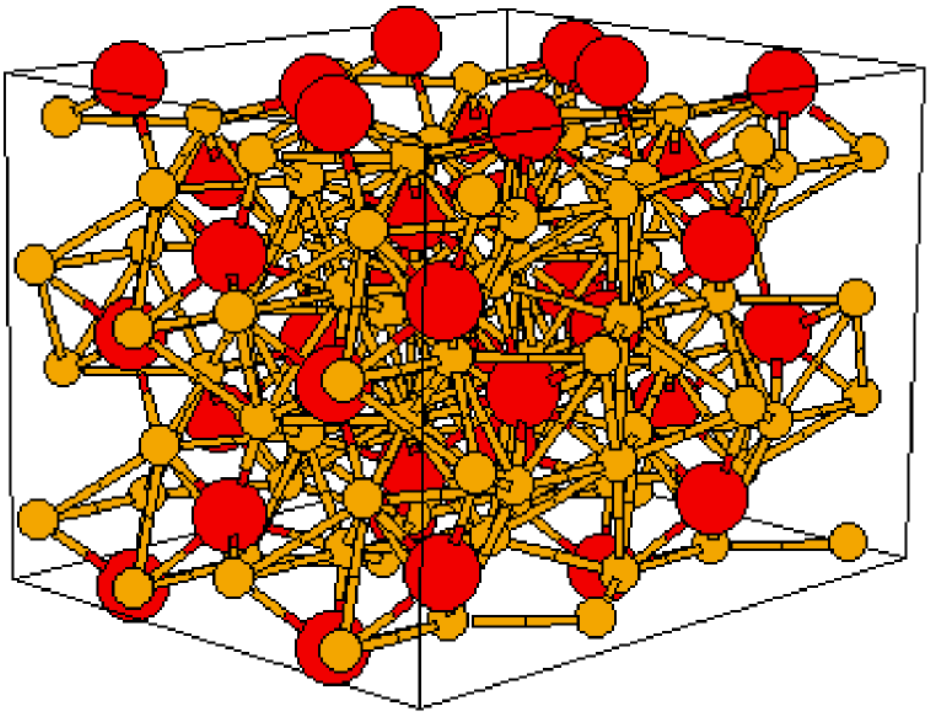
exh3-plot

```
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:
```

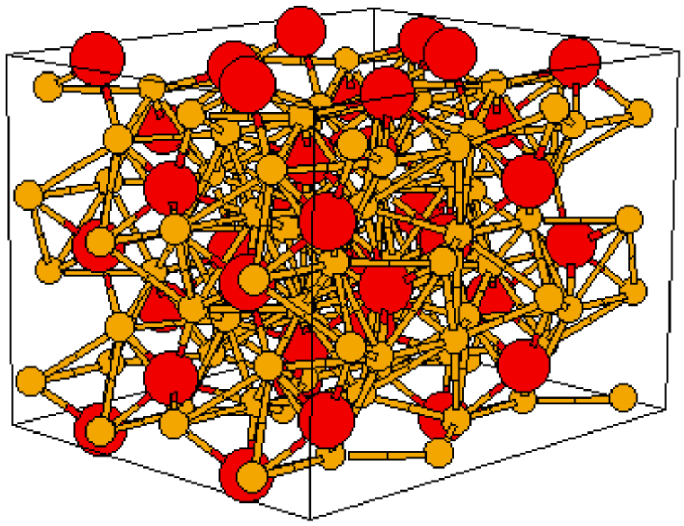
Diffusion in Complex Phases



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 Software  (build 20130) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri May 24 17:06:15 2019


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  v9.1

 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/:DIC>
DIC>REGION NAME : /BETA/:PHASE NAME: /B2_ORD/:DEPENDENT COMPONENT ? /NI/:COMPOSITION TYPE /MOLE_FRACTION/:PROFILE FOR /AL/:TYPE /LINEAR/:Functi
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>
```

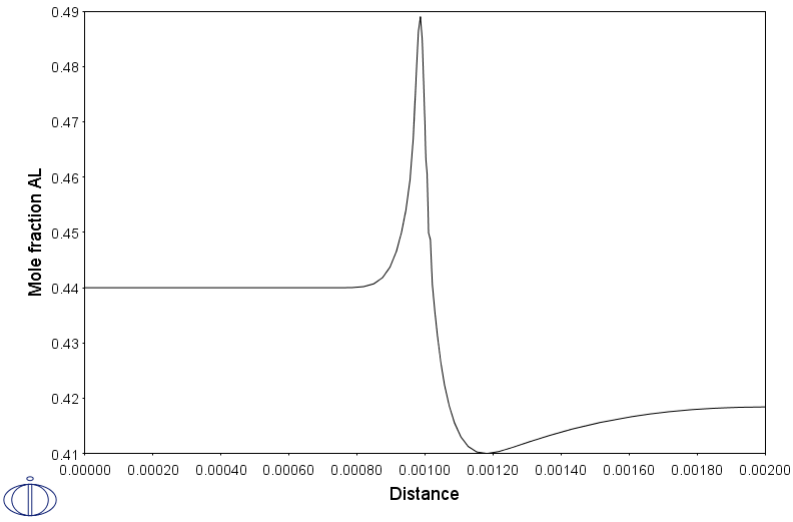
exi1-run

```
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> DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
 INFO: FORCED STARTING VALUES TURNED ON
 U-FRACTION IN SYSTEM:  AL = .429499345639258  FE = .290517917020317
                        NI = .279982737340425
 TOTAL SIZE OF SYSTEM:  .002 [m]
 U-FRACTION IN SYSTEM:  AL = .429499345639258  FE = .290517917020317
                        NI = .279982737340425
 TOTAL SIZE OF SYSTEM:  .002 [m]
  6  GRIDPOINT(S) ADDED   TO   CELL #1   REGION: BETA
 TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  AL = .429499345639258  FE = .290517917020317
                        NI = .279982737340425
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    1 seconds
 TIME =  0.10010000E-03 DT =  0.10000000E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  AL = .429499345639258  FE = .290517917020317
                        NI = .279982737340425
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.40010010     DT =  0.40000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  AL = .429499345639258  FE = .290517917020317
                        NI = .279982737340425
 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 = .290517917020327
                        NI = .279982737340426
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    2 seconds
 TIME =   1538.4655     DT =   1025.3769     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  AL = .429499345639233  FE = .290517917020342
                        NI = .279982737340425
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    1 seconds
 TIME =   3589.2193     DT =   2050.7538     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  AL = .429499345639231  FE = .290517917020345
                        NI = .279982737340424
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    2 seconds
 TIME =   7690.7270     DT =   4101.5077     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  AL = .429499345639227  FE = .290517917020346
                        NI = .279982737340427
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    2 seconds
 TIME =   15893.742     DT =   8203.0154     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  AL = .429499345639233  FE = .290517917020342
                        NI = .279982737340426
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    2 seconds
 TIME =   32299.773     DT =   16406.031     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  AL = .42949934563921  FE = .290517917020363
                        NI = .279982737340427
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    3 seconds
 TIME =   65111.835     DT =   32812.062     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  AL = .429499345639174  FE = .290517917020383
                        NI = .279982737340444
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    3 seconds
 TIME =   99671.835     DT =   34560.000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  AL = .429499345639088  FE = .290517917020497
                        NI = .279982737340415
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    3 seconds
 TIME =   134231.83     DT =   34560.000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  AL = .429499345639131  FE = .290517917020483
                        NI = .279982737340386
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    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                    3 seconds
 TIME =   203351.83     DT =   34560.000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  AL = .429499345639157  FE = .290517917020456
                        NI = .279982737340387
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    3 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 = .429499345639152  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                    3 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
```

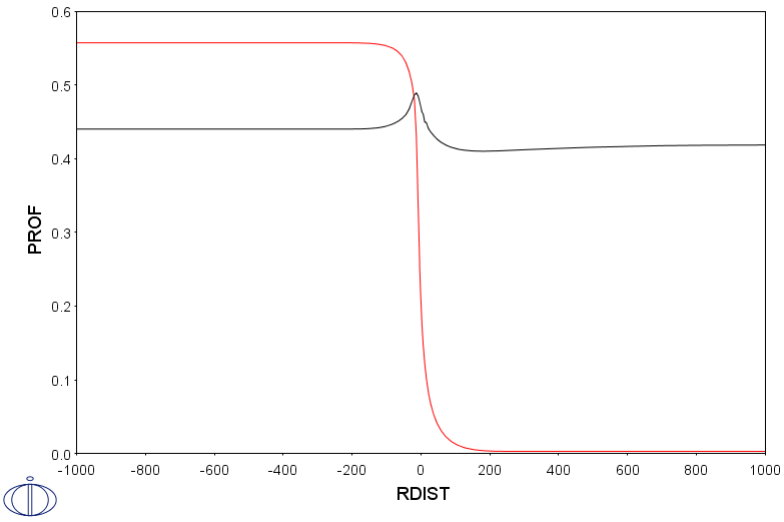
```
 RECLAIMING WORKSPACE
 DELETING TIME-RECORD FOR TIME    0.0000000
 DELETING TIME-RECORD FOR TIME   0.10000000E-06
 DELETING TIME-RECORD FOR TIME   0.10010000E-03
 DELETING TIME-RECORD FOR TIME   0.40010010
 DELETING TIME-RECORD FOR TIME    513.08856
 DELETING TIME-RECORD FOR TIME    1538.4655
 DELETING 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:
```

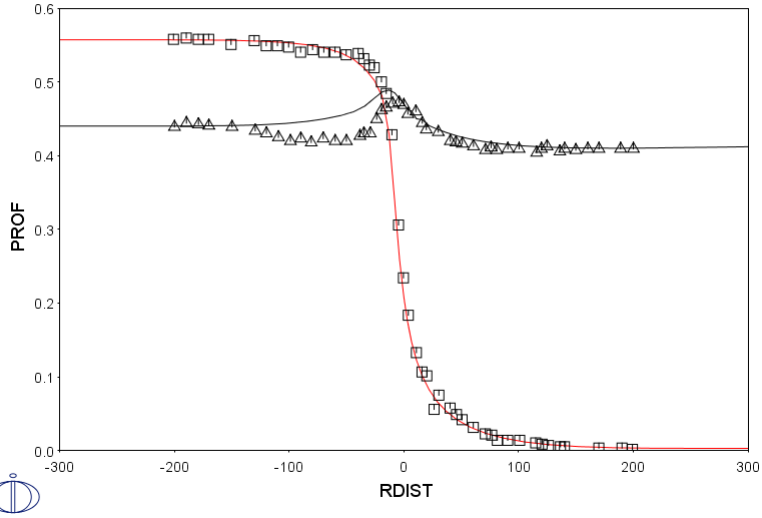



```
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1:Variable(s)POST-1:
POST-1:FUNCTION:&
POST-1:COLUMN NUMBER /*/:POST-1:
POST-1:POST-1:
POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```




```
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:
```

2019.05.27.14.05.45
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 License library version: 8.5.1.0017
 Linked: Fri May 24 17:06:15 2019


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: NO SUCH COMMAND, USE HELP
SYS:
SYS:SYS:SYS:SYS: THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v9.1

 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 v2.1

 VA                      /-  DEFINED
TDB_FEDEMO: FE                       C  DEFINED
TDB_FEDEMO: GAS:G                    LIQUID:L                BCC_A2
 CBCC_A12                CEMENTITE               CUB_A13
 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'
  '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 ....
 -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

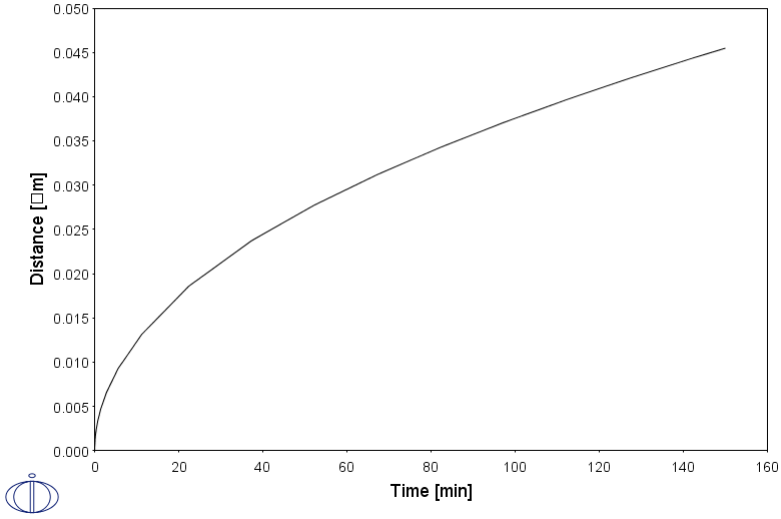
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exi2\run.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  0.00000E+00
 *** ENTERING FCC_A1 AS A DIFFUSION NONE PHASE
 *** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
DIC> OK
DIC>
DIC>DIC>DIC>DIC> 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
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
  Trying old scheme                    3
 U-FRACTION IN SYSTEM:  C = 4.6598005784384E-05  FE = 1
 TOTAL SIZE OF SYSTEM:  3.300001E-06 [m]
 U-FRACTION IN SYSTEM:  C = 4.6598005784384E-05  FE = 1
 TOTAL SIZE OF SYSTEM:  3.300001E-06 [m]
 0.111094107740055        0.111116327660160        1.168933545216859E-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        1.986016682715919E-006        8.572114928361613E-023       TIME =  0.25999666E-05 DT =  0.24999666E-
05 SUM OF SQUARES =  0.85721149E-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
 9.632817666617065E-007        9.640732404059803E-007        1.172366770910728E-025       TIME =  0.75998999E-05 DT =  0.49999333E-
05 SUM OF SQUARES =  0.11723668E-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
 5.520598281694916E-007        5.525040595645642E-007        1.253055714807193E-026       TIME =  0.17599767E-04 DT =  0.99998666E-
05 SUM OF SQUARES =  0.12530557E-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
 3.294904029768015E-007        3.297431202244252E-007        1.291814049659919E-026       TIME =  0.37599500E-04 DT =  0.19999733E-
04 SUM OF SQUARES =  0.12918140E-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
 1.842051604943190E-007        1.843420424821420E-007        2.901742677796220E-025       TIME =  0.77598966E-04 DT =  0.39999466E-
04 SUM OF SQUARES =  0.29017427E-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 = 4.69308608646657E-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
 9.778279834848840E-008        9.785422396897427E-008        3.091773286515432E-026       TIME =  0.15759790E-03 DT =  0.79998933E-
04 SUM OF SQUARES =  0.30917733E-25
 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 = 4.7107484088289E-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
 5.038045609672919E-006        5.041694025204943E-006        1.149093623281428E-023       TIME =  0.31759576E-03 DT =  0.15999787E-
03 SUM OF SQUARES =  0.11490936E-22
 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 = 4.7358254999821E-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
 2.556050636887337E-006        2.557893896114751E-006        8.879277635978856E-025       TIME =  0.63759149E-03 DT =  0.31999573E-
03 SUM OF SQUARES =  0.88792776E-24
 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 = 4.7713574122212E-05  FE = 1


output ignored...



... output resumed

 3.075207767610041E-027       TIME =   3142.1594     DT =   900.00000     SUM OF SQUARES =  0.30752078E-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 = .00283057618776024  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
 3.512901236539970E-008        3.518395504735430E-008        9.542674894918838E-
029       TIME =   4042.1594     DT =   900.00000     SUM OF SQUARES =  0.95426749E-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 = .00317904137490605  FE = 1
 TOTAL SIZE OF SYSTEM:  3.300001E-06 [m]
  9  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: CARB

  CPU time used in timestep                    1 seconds
 1.337273691048750E-008        1.340171249758079E-008        1.437553403147849E-
026       TIME =   4942.1594     DT =   900.00000     SUM OF SQUARES =  0.14375534E-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 = .00348899893656021  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
 6.238597393008355E-009        6.256204153067999E-009        5.998642887288550E-
030       TIME =   5842.1594     DT =   900.00000     SUM OF SQUARES =  0.59986429E-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 = .00377121604704145  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
 3.280281446639082E-009        3.291907996115809E-009        1.422606785007092E-
030       TIME =   6742.1594     DT =   900.00000     SUM OF SQUARES =  0.14226068E-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 = .00403216870914539  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
 1.864873576940722E-007        1.872981046291128E-007        1.371690940742892E-
029       TIME =   7642.1594     DT =   900.00000     SUM OF SQUARES =  0.13716909E-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 = .00427612481768385  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
 1.118941665839780E-007        1.124814013292195E-007        9.793401915457704E-
030       TIME =   8542.1594     DT =   900.00000     SUM OF SQUARES =  0.97934019E-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 = .00450607892012216  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
 6.975845439367061E-008        7.019562005406918E-008        7.713352436536418E-
030       TIME =   9000.0000     DT =   457.84063     SUM OF SQUARES =  0.77133524E-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 = .00461705531635742  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

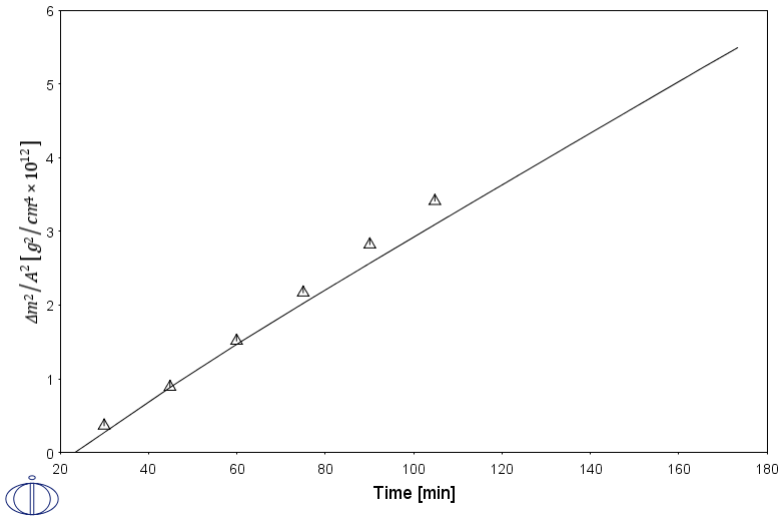
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exi2\plot.DCM.test"DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  9.00000E+03
 *** ENTERING FCC_A1 AS A DIFFUSION NONE PHASE
 *** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
DIC>
DIC>
DIC> OK
DIC>
DIC>
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:
```

2019.05.27.14.09.00
"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:
```

2019.05.27.14.09.01
"FIRST" INTERFACE OF SYSTEM
CELL #1

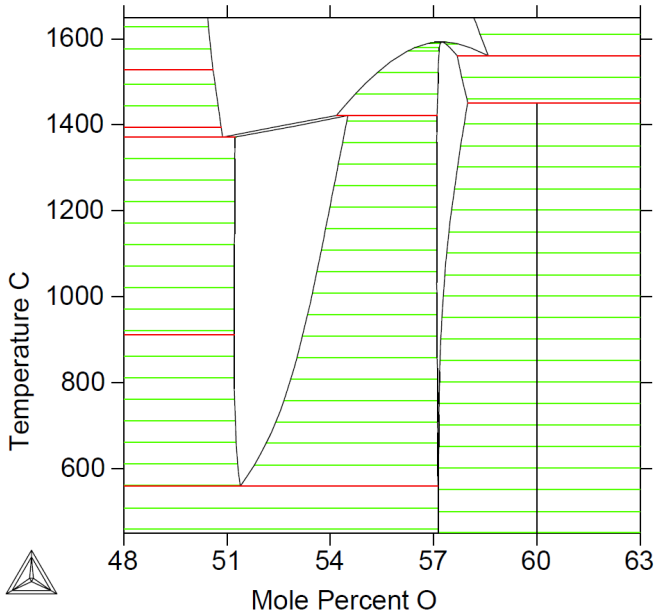



```
POST-1:
POST-1:
POST-1: --OK---
POST-1:
```

Example i3b

Diffusion in iron oxide (FeO) with grain boundary contribution

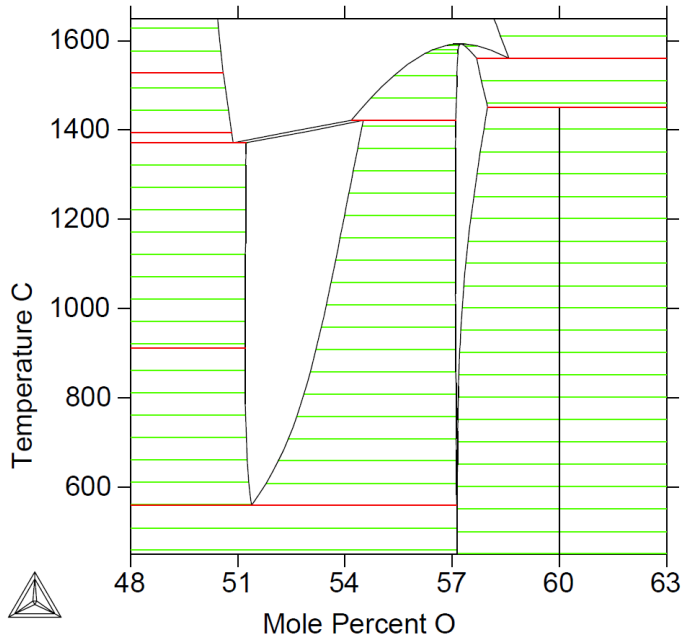
Oxidation of iron sample and consequent growth of an oxide layer using the grain boundary diffusion contribution model.



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 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri May 24 17:06:15 2019


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  v9.1

 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 ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317 -425'
  'M. Kowalski and P.J. Spencer, Calphad, 19 (1995), 229-243; Cr-O, Fe-O and
      Ni-O'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
      Molar volumes'
  'B. Sundman, J. Phase Equil., 12 (1991), 127-140; Fe-O'
 -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 ....
 -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>
```

exi3a-run

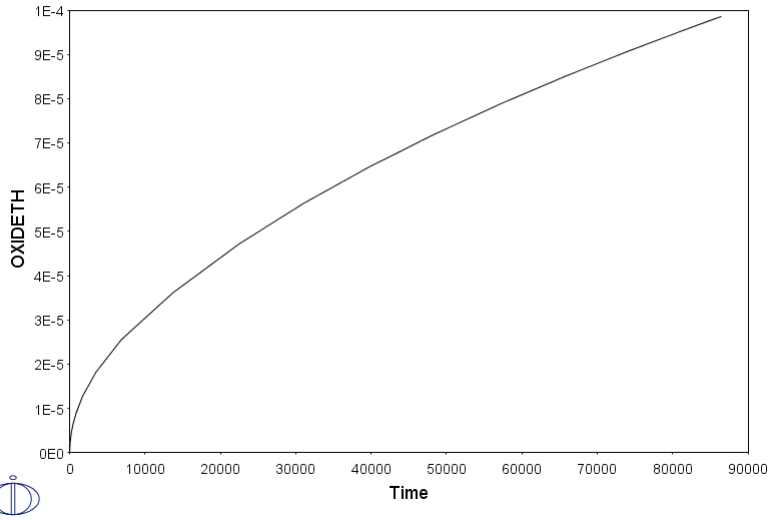
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exi3a\run.DCM.test"DIC>
DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  0.00000E+00
DIC> OK
DIC>
DIC>DIC>DIC>DIC> Region: FER
 single geometric dense at  0.50000E-02
 0.87701       95
 Region: SP
 double 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]
 0.347387301620389        0.347386528700301        0.347386701355537        4.618089872590951E-002        6.656544255012604E-
023       TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =  0.66565443E-22
 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 = 3.44025119032269E-08
 TOTAL SIZE OF SYSTEM:  .00499999012734 [m]
  9  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: FER

  CPU time used in timestep                    1 seconds
 1.507552605981734E-005        1.507739146458280E-005        1.507822847278430E-005        2.226308397553746E-007        5.019252732530892E-
032       TIME =  0.30000000E-06 DT =  0.20000000E-06 SUM OF SQUARES =  0.50192527E-31
 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 = 4.25594164341045E-08
 TOTAL SIZE OF SYSTEM:  .00499999013842 [m]
  CPU time used in timestep                    1 seconds
 1.398975101884493E-008        1.397926494986202E-008        1.395940586749686E-008        3.137487097463036E-011        3.385423730368188E-
036       TIME =  0.70000000E-06 DT =  0.40000000E-06 SUM OF SQUARES =  0.33854237E-35
 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 = 5.98849352760284E-08
 TOTAL SIZE OF SYSTEM:  .00499999016539 [m]
  CPU time used in timestep                    0 seconds
 5.609742547736858E-007        5.611284846397880E-007        5.611264634683927E-007        2.444637656461759E-010        1.543482857347205E-
033       TIME =  0.15000000E-05 DT =  0.80000000E-06 SUM OF SQUARES =  0.15434829E-32
 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 = 8.12308039073763E-08
 TOTAL SIZE OF SYSTEM:  .00499999019739 [m]
  23  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    0 seconds
 8.108701238861243E-006        8.112502967034163E-006        8.112138099431511E-006        1.121067579181819E-008        2.140565808892579E-
032       TIME =  0.31000000E-05 DT =  0.16000000E-05 SUM OF SQUARES =  0.21405658E-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 = 1.13822384430487E-07
 TOTAL SIZE OF SYSTEM:  .00499999024711 [m]
  35  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    1 seconds
 8.100481734460367E-006        8.103302413600414E-006        8.103162850520866E-006        7.195354229709166E-009        1.458658714794128E-
031       TIME =  0.63000000E-05 DT =  0.32000000E-05 SUM OF SQUARES =  0.14586587E-30
 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 = 1.58802706768075E-07
 TOTAL SIZE OF SYSTEM:  .00499999031513 [m]
  28  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    0 seconds
 3.178061987530644E-006        3.179295506989282E-006        3.179211108795882E-006        3.565487607380151E-009        6.761236618924053E-
032       TIME =  0.12700000E-04 DT =  0.64000000E-05 SUM OF SQUARES =  0.67612366E-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 = .995601423066387  O = .0143132204530815
 TOTAL SIZE OF SYSTEM:  .005021600735 [m]
  23  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    1 seconds
 2.789556771575429E-007        2.794057583822531E-007        2.793655766630949E-007        3.800585454837353E-010        2.411174012406676E-
033       TIME =   56943.895     DT =   8640.0000     SUM OF SQUARES =  0.24111740E-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 = .995194725257641  O = .0156544064678654
 TOTAL SIZE OF SYSTEM:  .00502363765793 [m]
  8  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP
```

```
  CPU time used in timestep                    0 seconds
 1.595105700155058E-007        1.598217866208553E-007        1.597953811124363E-007        2.020602965724977E-010        1.145025537248974E-
033       TIME =   65583.895     DT =   8640.0000     SUM OF SQUARES =  0.11450255E-32
 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 = .994817249745987  O = .0168979971924892
 TOTAL SIZE OF SYSTEM:  .0050255321232 [m]
  7  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    0 seconds
 9.568367496895681E-008        9.590684461689169E-008        9.588874680435883E-008        1.147888044286007E-010        6.018531076210112E-
036       TIME =   74223.895     DT =   8640.0000     SUM OF SQUARES =  0.60185311E-35
 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 = .99446375481309  O = .0180617615442488
 TOTAL SIZE OF SYSTEM:  .00502730918328 [m]
  10  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    0 seconds
 5.962030964014512E-008        5.978502104198708E-008        5.977212462770474E-008        6.869420013219069E-011        3.190573786775886E-
033       TIME =   82863.895     DT =   8640.0000     SUM OF SQUARES =  0.31905738E-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 = .994130359456913  O = .0191587681410927
 TOTAL SIZE OF SYSTEM:  .00502898750134 [m]
  8  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    1 seconds
 9.162180973662354E-009        9.108164932083602E-009        9.224421743951149E-009        1.011580317218201E-011        3.385423730368188E-
034       TIME =   86400.000     DT =   3536.1047     SUM OF SQUARES =  0.33854237E-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 = .994008758985554  O = .0195911680902242
 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

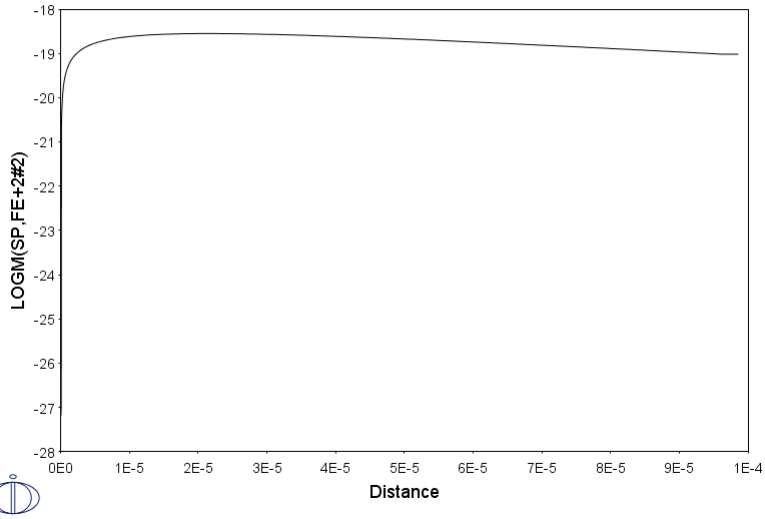
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exi3a\plot.DCM.test"DIC>
DIC>DIC>
DIC>DIC>DIC>DIC>
DIC>DIC>DIC>DIC> TIME STEP AT TIME  8.64000E+04
DIC> OK
DIC>
DIC>DIC>DIC>DIC>  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:POST-1:POST-1:POST-1:FUNCTION:&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

2019.05.27.14.12.30
UPPER INTERFACE OF REGION "SP#1"
CELL #1



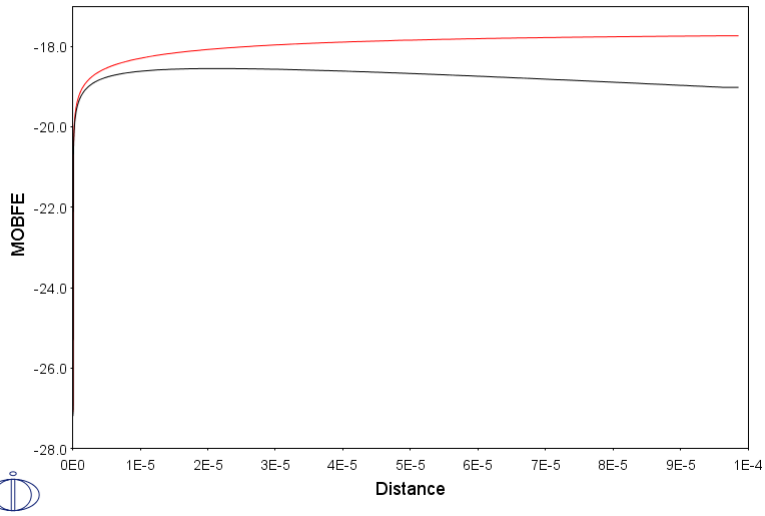

```
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:
POST-1:POST-1:POST-1:POST-1:  INFO: Distance is set as independent variable
POST-1:
POST-1:POST-1:
POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```

2019.05.27.14.12.31
Time = 86400
CELL #1



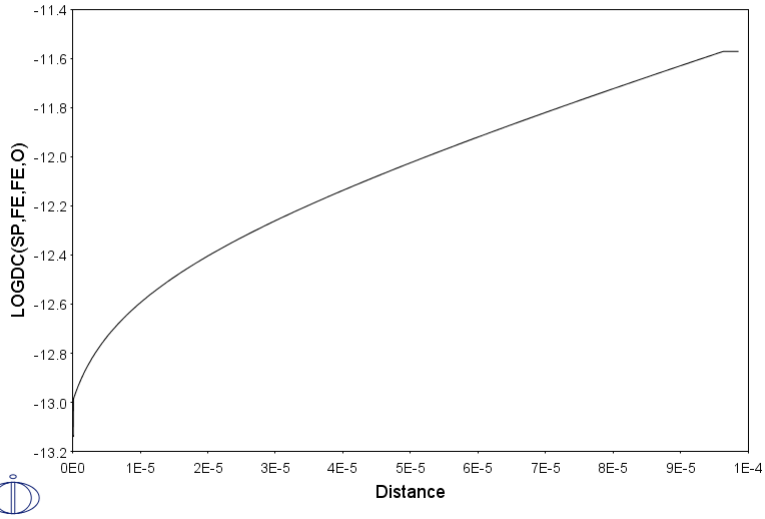

```
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1:POST-1:POST-1:POST-1:POST-1:Variable(s)POST-1:
POST-1:COLUMN NUMBER /*/:
POST-1:
POST-1:
POST-1:POST-1:POST-1:POST-1:
POST-1:
```

2019.05.27.14.12.32
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:
```

2019.05.27.14.12.34
Time = 86400
CELL #1




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

exi3b-setup

```
About Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Fri May 24 17:06:15 2019


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  v9.1

 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 ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317 -425'
  'M. Kowalski and P.J. Spencer, Calphad, 19 (1995), 229-243; Cr-O, Fe-O and
      Ni-O'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
      Molar volumes'
  'B. Sundman, J. Phase Equil., 12 (1991), 127-140; Fe-O'
 -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 ....
 -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> --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
 0.87701       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 = 2.69779084025034E-08
 TOTAL SIZE OF SYSTEM:  .00499999011352 [m]
  9  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 = 4.97800698647711E-08
 TOTAL SIZE OF SYSTEM:  .00499999015258 [m]
  CPU time used in timestep                    1 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 = 6.90668859329386E-08
 TOTAL SIZE OF SYSTEM:  .00499999017858 [m]
  CPU time used in timestep                    0 seconds
 1.134920301888734E-007        1.135894804039261E-007        1.135506444176019E-007        5.608707817274067E-010        5.589428618385944E-
033       TIME =  0.15000000E-05 DT =  0.80000000E-06 SUM OF SQUARES =  0.55894286E-32
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.14432292E-03 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49999897E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.20898651E-03 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.49999902E-02
 U-FRACTION IN SYSTEM:  FE = 0.99999996836327  O = 1.02507650482238E-07
 TOTAL SIZE OF SYSTEM:  .00499999023031 [m]
  8  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    1 seconds
 4.495117154993389E-007        4.496453319495406E-007        4.496431998391493E-007        2.514741666006164E-010        2.513206922058051E-
034       TIME =  0.31000000E-05 DT =  0.16000000E-05 SUM OF SQUARES =  0.25132069E-33
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.94208025E-04 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49999896E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.13424763E-03 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.49999903E-02
 U-FRACTION IN SYSTEM:  FE = 0.99999995509026  O = 1.4547196415591E-07
 TOTAL SIZE OF SYSTEM:  .00499999029437 [m]
  32  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    1 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 = 2.07573864745155E-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 = .0189442387175316
 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 = .0206594865694811
 TOTAL SIZE OF SYSTEM:  .00503121911345 [m]
  9  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP
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  CPU time used in timestep                    1 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 = .0222444823738337
 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 = .0237257189756388
 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 = .0251191391110372
 TOTAL SIZE OF SYSTEM:  .00503804716129 [m]
  7  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    1 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 = .0256664807147801
 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
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 DELETING TIME-RECORD FOR TIME    6.7108863
 DELETING TIME-RECORD FOR TIME    13.421773
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 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>
```
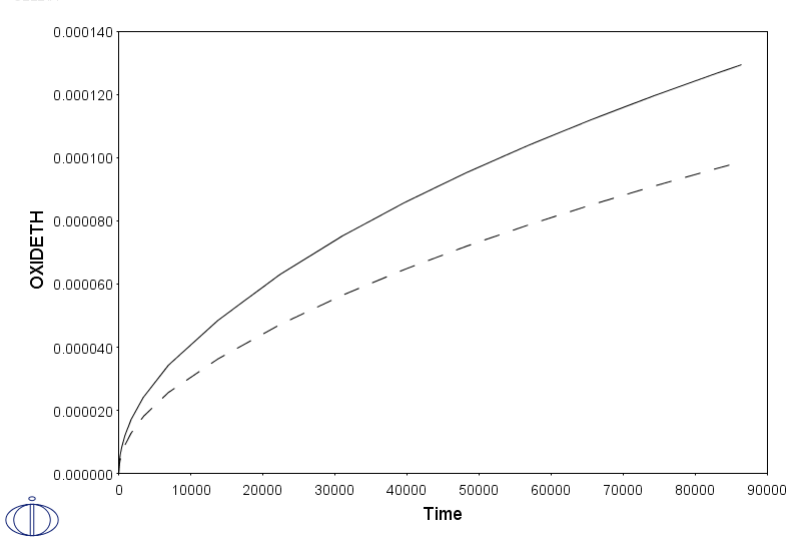

exi3b-plot

```
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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