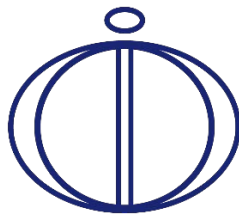


Diffusion Module (DICTRA) Example Macros

Thermo-Calc Version 2018b



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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. Kikuchi: Acta Metall.Mater. 41 (1993), pp.2045-2059.

[exb6](#)

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

[exb7](#)

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.

[exc1a](#)

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.

[exc1b](#)

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.

[exc2a](#)

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.

[exc2b](#)

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.

[exc3](#)

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

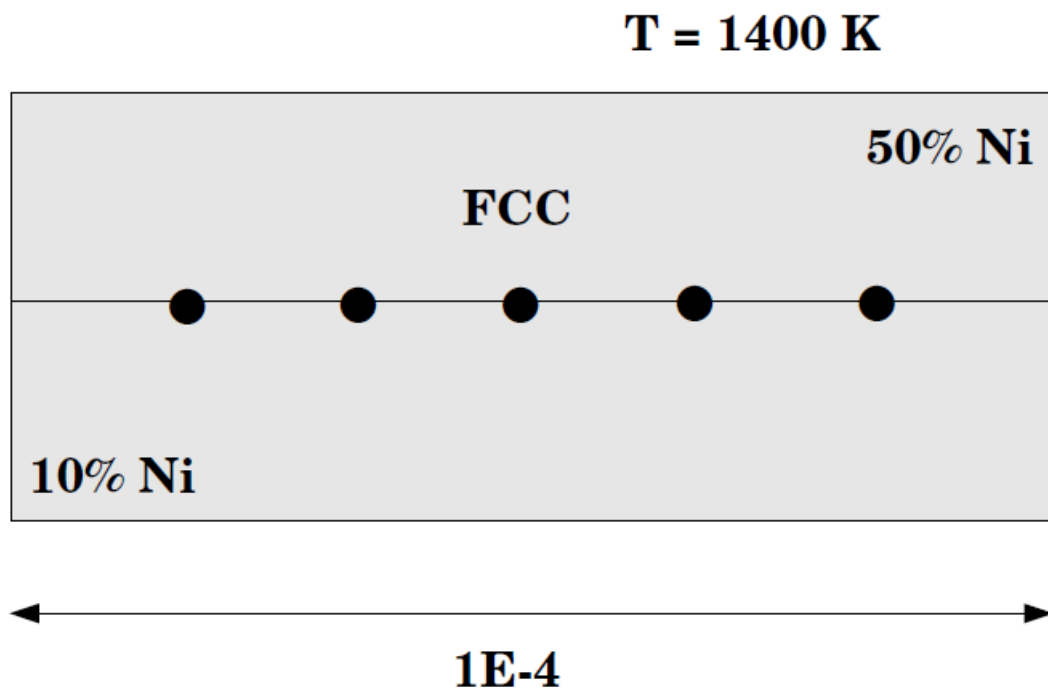




Example exa1

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

exal-setup

About Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

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

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

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

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

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

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

```
SYS: -----  
NO SUCH COMMAND, USE HELP
```

```
SYS:
```

```
SYS: @@
```

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

```
SYS: @@
```

```
SYS: goto_module
```

```
MODULE NAME: data
```

```
THERMODYNAMIC DATABASE module
```

```
Current database: Steels/Fe-Alloys v9.0
```

```
VA          /- DEFINED  
L12_FCC      B2_BCC          DICTRA_FCC_A1  
REJECTED
```

```
TDB_TCFE9:
```

```
TDB_TCFE9: @@
```

```
TDB_TCFE9: @@ USE THERMODYNAMIC DATABASE TO RETRIEVE DATA
```

```
TDB_TCFE9: @@
```

```
TDB_TCFE9: switch_database
```

```
Use one of these databases
```

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



```

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

```

```

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

```

```

VA /- DEFINED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ DEFINE THE SYSTEM TO WORK WITH
TDB_FEDEMO: @@
TDB_FEDEMO: define_system
ELEMENTS: fe ni
FE NI DEFINED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ EXCLUDE THE THERMODYNAMIC DATA FOR THE PHASES THAT ARE NOT NEEDED
TDB_FEDEMO: @@
TDB_FEDEMO: reject
ELEMENTS, SPECIES, PHASES, CONSTITUENT OR SYSTEM: /PHASES/: phase
PHASES: *
LIQUID:L BCC_A2 FCC_A1
HCP_A3 LAVES_PHASE_C14 REJECTED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ RESTORE THE THERMODYNAMIC DATA FOR THE FCC PHASE
TDB_FEDEMO: @@
TDB_FEDEMO: restore
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /ELEMENTS/: phase
PHASES: fcc
FCC_A1 RESTORED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ RETRIEVE DATA FROM THE DATABASE FILE
TDB_FEDEMO: @@
TDB_FEDEMO: get_data
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

```

List of references for assessed data

```

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

```

```

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

```

```

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

```

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

DATABASE NAME /FEDEMO/: mfedemo

Current database: Fe-Alloys Mobility demo database v2.0

VA DEFINED

APP: define_system

ELEMENTS: fe ni

FE

NI DEFINED

```

APP: reject
ELEMENTS, SPECIES, PHASES, CONSTITUENT OR SYSTEM: /PHASES/: phase
PHASES: *
  BCC_A2                      FCC_A1  REJECTED
APP:
APP: restore
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /ELEMENTS/: phase
PHASES: fcc
  FCC_A1  RESTORED
APP:
APP: get_data
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

List of references for assessed data

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

GLOBAL OR BOUNDARY CONDITION /GLOBAL/: global
VARIABLE : T
LOW TIME LIMIT /0/: 0
T(TIME,X)= 1400;
HIGH TIME LIMIT /*/: *
ANY MORE RANGES /N/: N
DIC>
DIC> @@
DIC> @@ START BY ENTERING A REGION
DIC> @@
DIC> enter_region
REGION NAME : austenite
DIC>
DIC> @@
DIC> @@ ENTER A GRID INTO THE REGION
DIC> @@
DIC> @@ FOR SIMPLICITY, AN EQUIDISTANT GRID IS USED
DIC> @@
DIC> enter_grid_coordinates
REGION NAME : /AUSTENITE/: austenite
WIDTH OF REGION /1/: 1e-4
TYPE /LINEAR/: AUTO
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE active PHASE INTO THE REGION
DIC> @@
DIC> enter_phase_in_region
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /AUSTENITE/: austenite
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC> @@
DIC> @@ ENTER AN INITIAL Ni COMPOSITION INTO THE PHASE. A LINEAR
DIC> @@ VARIATION IN THE REGION IS ASSUMED.
DIC> @@
DIC> enter_compositions
REGION NAME : /AUSTENITE/: austenite
PHASE NAME: /FCC_A1/: fcc#1
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: weight_percent
PROFILE FOR /NI/: ni
TYPE /LINEAR/: linear
VALUE OF FIRST POINT : 10
VALUE OF LAST POINT : /10/: 50
DIC>
DIC> @@
DIC> @@ THE BOUNDARY CONDITION IS A CLOSED SYSTEM AS WE DO NOT SPECIFY
DIC> @@ ANYTHING ELSE
DIC> @@
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set_simulation_time
END TIME FOR INTEGRATION /.1/: 1E6
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /100000/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO FILE AND EXIT
DIC> @@
DIC> save_workspaces exal Y
DIC>
DIC> set_interactive
--OK--
DIC>

```

exal-run

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exal\run.DCM"DIC>
DIC>
DIC> @@ exal_run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING EXAMPLE a1
DIC> @@
DIC> goto_module
MODULE NAME: dictra_monitor
TIME STEP AT TIME 0.000000E+00
DIC>
DIC> read_workspaces exal
OK
DIC>
DIC> @@
DIC> @@ Start the simulation
DIC> @@
DIC> simulate_reaction
Region: AUSTENITE
linear grid 75
U-FRACTION IN SYSTEM: FE = .709680136600384 NI = .290319863399616
TOTAL SIZE OF SYSTEM: 1E-04 [m]
U-FRACTION IN SYSTEM: FE = .709680136600384 NI = .290319863399616
TOTAL SIZE OF SYSTEM: 1E-04 [m]
TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680136600384 NI = .290319863399616
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.10010000E-03 DT = 0.10000000E-03 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680136600384 NI = .290319863399616
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.40010010 DT = 0.40000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680136600384 NI = .290319863399616
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 241.69569 DT = 241.29559 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680136600384 NI = .290319863399616
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 724.28686 DT = 482.59117 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680136600384 NI = .290319863399616
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 1689.4692 DT = 965.18235 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680136600384 NI = .290319863399616
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 3619.8339 DT = 1930.3647 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680136600384 NI = .290319863399616
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 7480.5633 DT = 3860.7294 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680136600384 NI = .290319863399616
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 15202.022 DT = 7721.4588 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680136600384 NI = .290319863399616
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 30644.940 DT = 15442.918 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680136600384 NI = .290319863399616
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 61530.775 DT = 30885.835 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680136600384 NI = .290319863399616
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 123302.44 DT = 61771.670 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680136600385 NI = .290319863399616
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 223302.44 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680136600385 NI = .290319863399615
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 323302.44 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680136600386 NI = .290319863399613
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 423302.44 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680136600386 NI = .290319863399614
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 523302.44 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680136600386 NI = .290319863399614
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 623302.44 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680136600386 NI = .290319863399614
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 723302.44 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680136600386 NI = .290319863399614
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 823302.44 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680136600386 NI = .290319863399614
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 923302.44 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680136600386 NI = .290319863399615
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 1 seconds
TIME = 1000000.0 DT = 76697.555 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .709680136600385 NI = .290319863399615
TOTAL SIZE OF SYSTEM: 1E-04 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 0.0000000
DELETING TIME-RECORD FOR TIME 0.10000000E-06
```

```
DELETING TIME-RECORD FOR TIME 0.10010000E-03
DELETING TIME-RECORD FOR TIME 0.40010010
DELETING TIME-RECORD FOR TIME 241.69569
DELETING TIME-RECORD FOR TIME 724.28686
DELETING TIME-RECORD FOR TIME 1689.4692
DELETING TIME-RECORD FOR TIME 3619.8339
DELETING TIME-RECORD FOR TIME 7480.5633
DELETING TIME-RECORD FOR TIME 15202.022
DELETING TIME-RECORD FOR TIME 30644.940
DELETING TIME-RECORD FOR TIME 61530.775
DELETING TIME-RECORD FOR TIME 123302.44
DELETING TIME-RECORD FOR TIME 223302.44
DELETING TIME-RECORD FOR TIME 323302.44
DELETING TIME-RECORD FOR TIME 423302.44
DELETING TIME-RECORD FOR TIME 523302.44
DELETING TIME-RECORD FOR TIME 623302.44
DELETING TIME-RECORD FOR TIME 723302.44
DELETING TIME-RECORD FOR TIME 823302.44
```

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

```
TIMESTEP AT 1000000.00 SELECTED
```

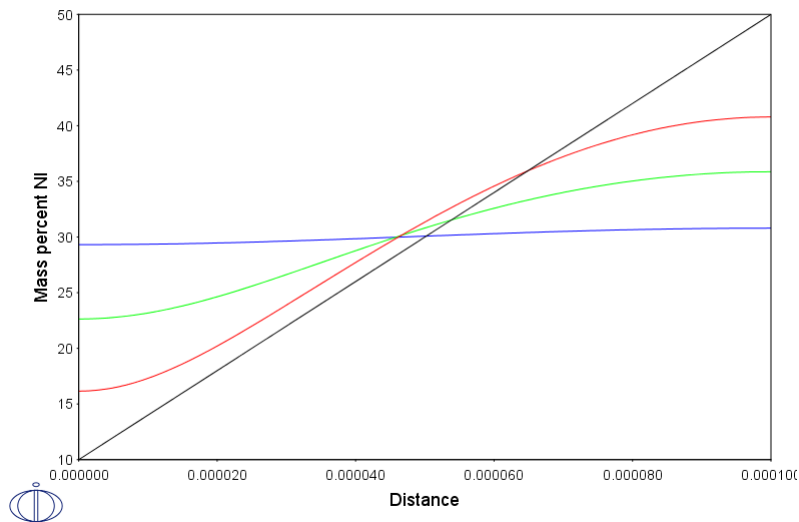
```
DIC>
DIC> @@
DIC> @@ THE SIMULATION IS FINISHED
DIC> @@
DIC>
DIC> set_interactive
--OK--
DIC>
```

exal-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exal\plot.DCM"DIC>
DIC>
DIC> @@ exal_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE a1
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> goto_module
MODULE NAME: dictra_monitor
TIME STEP AT TIME 1.00000E+06
DIC> read_workspaces exal
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post_processor

POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
```

```
POST-1:
POST-1:
POST-1: @@
POST-1: @@ PLOT SOME CONCENTRATION PROFILES
POST-1: @@
POST-1: set_diagram_axis
AXIS (X, Y OR Z) : x
VARIABLE : distance
INFO: Distance is set as independent variable
DISTANCE : /GLOBAL/: global
POST-1:
POST-1: set_diagram_axis
AXIS (X, Y OR Z) : y
VARIABLE : weight-percent
FOR COMPONENT : ni
POST-1:
POST-1: set_plot_condition
CONDITION /TIME/: time
VALUE(S) /LAST/: 0 1e5 3e5 1e6
POST-1:
POST-1: plot_diagram
2018.02.18.18.26.44
Time = 0,100000,300000,1000000
CELL #1
```



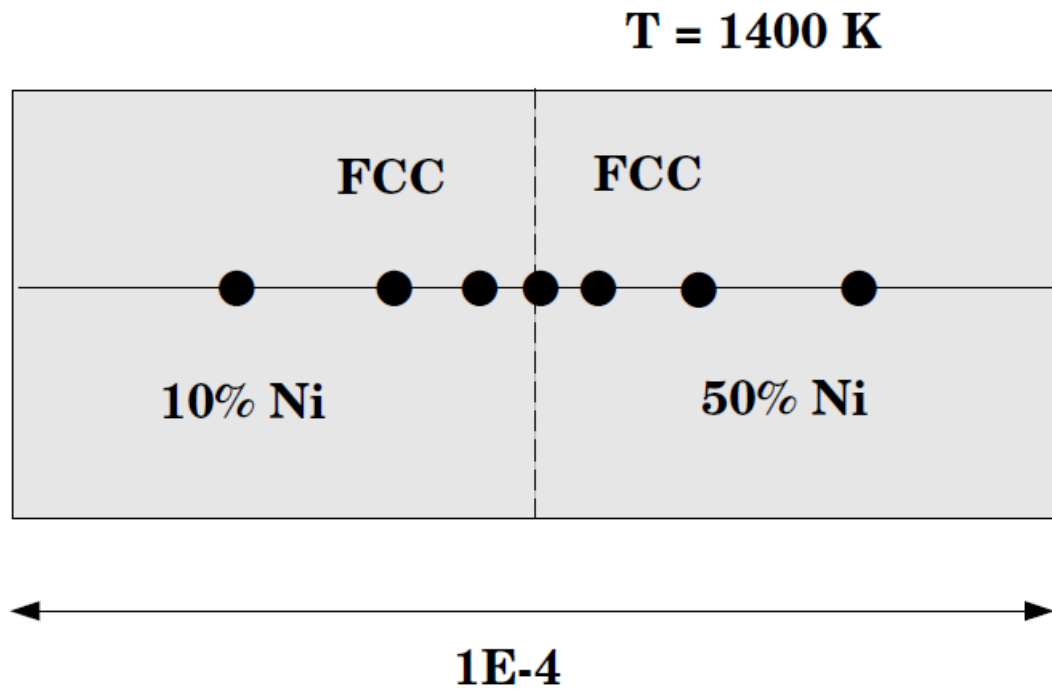
```
POST-1:
POST-1:
POST-1:
POST-1: @?<Hit_return_to_continue>
POST-1:
POST-1: set_interactive
--OK--
POST-1:
```



Example exa2a

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

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



exa2a-setup

About simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

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

```
SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa2a\setup.DCM" @@
```

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

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

```
SYS: @@ A Ni rich and a Ni lean alloy are put together and initially
```

```
SYS: @@ there is a step profile.
```

```
SYS: -----  
NO SUCH COMMAND, USE HELP
```

```
SYS:
```

```
SYS: @@ exa2a_setup.DCM
```

```
SYS:
```

```
SYS: @@
```

```
SYS: @@ IN exa1 ALL THE COMMANDS WERE WRITTEN IN FULL BUT NOW ABBREVIATED
```

```
SYS: @@ COMMANDS ARE USED
```

```
SYS: @@
```

```
SYS:
```

```
SYS: @@
```

```
SYS: @@ FIRST DEFINE A LOG-FILE FOR THIS EXAMPLE
```

```
SYS: @@
```

```
SYS: set_log_file setup
```

```
Heading:
```

```
SYS: @@
```

```
SYS: @@ NOW GO TO THE DATABASE MODULE
```

```
SYS: @@
```

```
SYS: go da
```

```
... the command in full is GOTO_MODULE
```

```
THERMODYNAMIC DATABASE module
```

```
Current database: Steels/Fe-Alloys v9.0
```

```
VA                /-  DEFINED  
LI12_FCC          B2_BCC                DICTRA_FCC_A1  
REJECTED
```

```
TDB_TCFE9:
```

```
TDB_TCFE9: @@
```

```
TDB_TCFE9: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA
```

```
TDB_TCFE9: @@
```

```
TDB_TCFE9: sw FEDEMO
```

```
... the command in full is SWITCH_DATABASE
```

```
Current database: Iron Demo Database v2.0
```

```
VA                /-  DEFINED
```

```
TDB_FEDEMO:
```

```
TDB_FEDEMO: @@
```

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

```
TDB_FEDEMO: @@
```

```
TDB_FEDEMO: def-system fe ni
```

```
... the command in full is DEFINE_SYSTEM
```

```
FE                NI  DEFINED
```

```
TDB_FEDEMO:
```

```
TDB_FEDEMO: @@
```

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

```
TDB_FEDEMO: @@
```

```
TDB_FEDEMO: rej ph * all
```

```
... the command in full is REJECT
```

```
LIQUID:L          BCC_A2                FCC_A1  
HCP_A3            LAVES_PHASE_C14  REJECTED
```

```
TDB_FEDEMO: res ph fcc
```

```
... the command in full is RESTORE
```

```
FCC_A1  RESTORED
```

```
TDB_FEDEMO:
```

```
TDB_FEDEMO: @@
```

```
TDB_FEDEMO: @@ RETRIEVE DATA FROM THE DATABASE FILE
```

```
TDB_FEDEMO: @@
```

```
TDB_FEDEMO: get
```

```
... the command in full is GET_DATA
```

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

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

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

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

```
... the command in full is AMEND_PHASE_DESCRIPTION
```

```
PARAMETERS ...
```

```
FUNCTIONS ...
```

```
List of references for assessed data
```

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

```
TDB_FEDEMO:
```

```
TDB_FEDEMO: @@
```

```
TDB_FEDEMO: @@ MOBILITY/DIFFUSIVITY DATA ARE STORED IN A SEPARATE DATABASE FILE.
```

```
TDB_FEDEMO: @@ SWITCH TO THE MOBILITY DATABASE TO RETRIEVE DATA
```

```
TDB_FEDEMO: @@
```

```
TDB_FEDEMO: app
```

```
... the command in full is APPEND_DATABASE
```

```
Use one of these databases
```

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



```

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

```

```

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

```

```

VA DEFINED
APP: def-sys fe ni
... the command in full is DEFINE_SYSTEM
FE NI DEFINED
APP: rej ph * all
... the command in full is REJECT
BCC_A2 FCC_A1 REJECTED

```

[illegible]

[illegible]

exa2a-run

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa2a\run.DCM"DIC>
DIC>
DIC> @@ exa2a_run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING EXAMPLE a2a
DIC> @@
DIC>
DIC> @@
DIC> @@ LET US DEFINE A LOG-FILE FOR THIS EXAMPLE
DIC> @@
DIC> @@set-log-file run
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA MONITOR AN READ SETUP FROM FILE
DIC> @@
DIC> go d-m
... the command in full is GOTO_MODULE
TIME STEP AT TIME 0.00000E+00
DIC>
DIC> read exa2a
... the command in full is READ_WORKSPACES
... the command in full is DEFINE_COMPONENTS
... the command in full is SELECT_EQUILIBRIUM
OK
DIC>
DIC> @@
DIC> @@ START THE SIMULATION
DIC> @@
DIC> simulate
... the command in full is SIMULATE_REACTION
... the command in full is SET_NUMERICAL_LIMITS
U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
2 GRIDPOINT(S) ADDED TO CELL #1 REGION: AUSTENITE
TIME = 0.1000000E-06 DT = 0.1000000E-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 = 0.1001000E-03 DT = 0.1000000E-03 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.40010010 DT = 0.40000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 10.408313 DT = 10.008213 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 30.424739 DT = 20.016426 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 70.457590 DT = 40.032851 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 150.52329 DT = 80.065703 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 310.65470 DT = 160.13141 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .291111754593831
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 630.91751 DT = 320.26281 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 1271.4431 DT = 640.52562 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 2552.4944 DT = 1281.0512 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 5114.5969 DT = 2562.1025 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 10238.802 DT = 5124.2050 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .291111754593831
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 20487.212 DT = 10248.410 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .291111754593831
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 40984.032 DT = 20496.820 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 81977.671 DT = 40993.640 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 163964.95 DT = 81987.280 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .291111754593831
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 263964.95 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 363964.95 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406171 NI = .291111754593829
```

```

TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 463964.95 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 563964.95 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406168 NI = .291111754593831
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 663964.95 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 763964.95 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .291111754593831
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 863964.95 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .291111754593831
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 1 seconds
TIME = 963964.95 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406171 NI = .291111754593829
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 1000000.0 DT = 36035.049 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406172 NI = .291111754593829
TOTAL SIZE OF SYSTEM: 1E-04 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 0.0000000
DELETING TIME-RECORD FOR TIME 0.10000000E-06
DELETING TIME-RECORD FOR TIME 0.10010000E-03
DELETING TIME-RECORD FOR TIME 0.40010010
DELETING TIME-RECORD FOR TIME 10.408313
DELETING TIME-RECORD FOR TIME 30.424739
DELETING TIME-RECORD FOR TIME 70.457590
DELETING TIME-RECORD FOR TIME 150.52329
DELETING TIME-RECORD FOR TIME 310.65470
DELETING TIME-RECORD FOR TIME 630.91751
DELETING TIME-RECORD FOR TIME 1271.4431
DELETING TIME-RECORD FOR TIME 2552.4944
DELETING TIME-RECORD FOR TIME 5114.5969
DELETING TIME-RECORD FOR TIME 10238.802
DELETING TIME-RECORD FOR TIME 20487.212
DELETING TIME-RECORD FOR TIME 40984.032
DELETING TIME-RECORD FOR TIME 81977.671
DELETING TIME-RECORD FOR TIME 163964.95
DELETING TIME-RECORD FOR TIME 263964.95
DELETING TIME-RECORD FOR TIME 363964.95
DELETING TIME-RECORD FOR TIME 463964.95
DELETING TIME-RECORD FOR TIME 563964.95
DELETING TIME-RECORD FOR TIME 663964.95
DELETING TIME-RECORD FOR TIME 763964.95
DELETING TIME-RECORD FOR TIME 863964.95

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

TIMESTEP AT 1000000.00 SELECTED

```

```

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

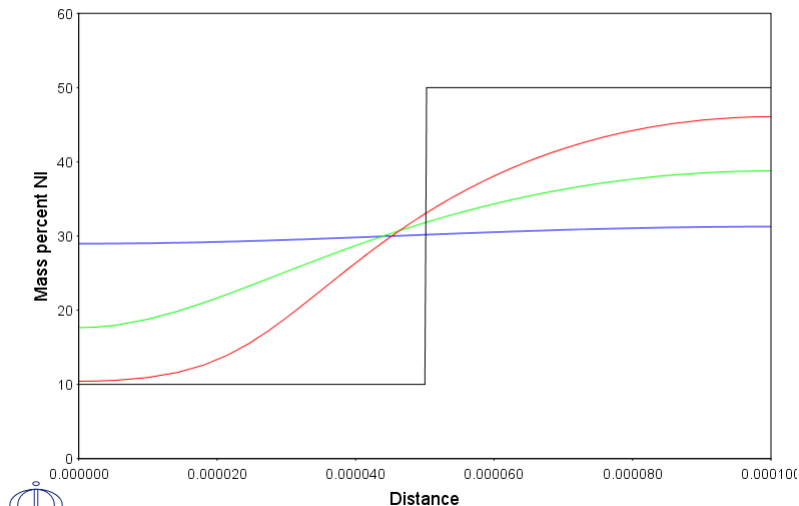
```

exa2a-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa2a\plot.DCM"DIC>
DIC>
DIC> @@ exa2a_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE a2a
DIC> @@
DIC>
DIC> @@
DIC> @@ LET US DEFINE A LOG-FILE FOR THIS EXAMPLE
DIC> @@
DIC> set-log-file plot
    AMBIGUOUS COMMAND, USE HELP
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
    ... the command in full is GOTO_MODULE
    TIME STEP AT TIME  1.00000E+06
DIC>
DIC> read exa2a
    ... the command in full is READ_WORKSPACES
    ... the command in full is DEFINE_COMPONENTS
    ... the command in full is SELECT_EQUILIBRIUM
    OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
    ... the command in full is POST_PROCESSOR

    POST PROCESSOR VERSION  1.7
    Implemented by Bjorn Jonsson

POST-1:
POST-1:
POST-1: @@
POST-1: @@ PLOT SOME NI-CONCENTRATION PROFILES
POST-1: @@
POST-1: s-d-a
    ... the command in full is SET_DIAGRAM_AXIS
AXIS (X, Y OR Z) : x
VARIABLE : dist
    INFO: Distance is set as independent variable
    ... the command in full is SET_INDEPENDENT_VARIABLE
DISTANCE : /GLOBAL/: glo
POST-1:
POST-1: s-d-a
    ... the command in full is SET_DIAGRAM_AXIS
AXIS (X, Y OR Z) : y
VARIABLE : weight-percent
FOR COMPONENT : ni
POST-1:
POST-1: s-p-c
    ... the command in full is SET_PLOT_CONDITION
CONDITION /TIME/: time
VALUE(S) /LAST/: 0 1e5 3e5 1e6
POST-1:
POST-1: @@
POST-1: @@ SET SCALING ON Y-AXIS BEFORE PLOTTING
POST-1: @@
POST-1: s-s-s
    ... the command in full is SET_SCALING_STATUS
AXIS (X, Y OR Z) : y
AUTOMATIC SCALING (Y OR N) /N/: n
MIN VALUE : 0
MAX VALUE : 60
POST-1:
POST-1: plot
    ... the command in full is PLOT_DIAGRAM
    2018.02.18.18.29.45
    Time=0.100000,3000000,1000000
    CELL #1
```



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

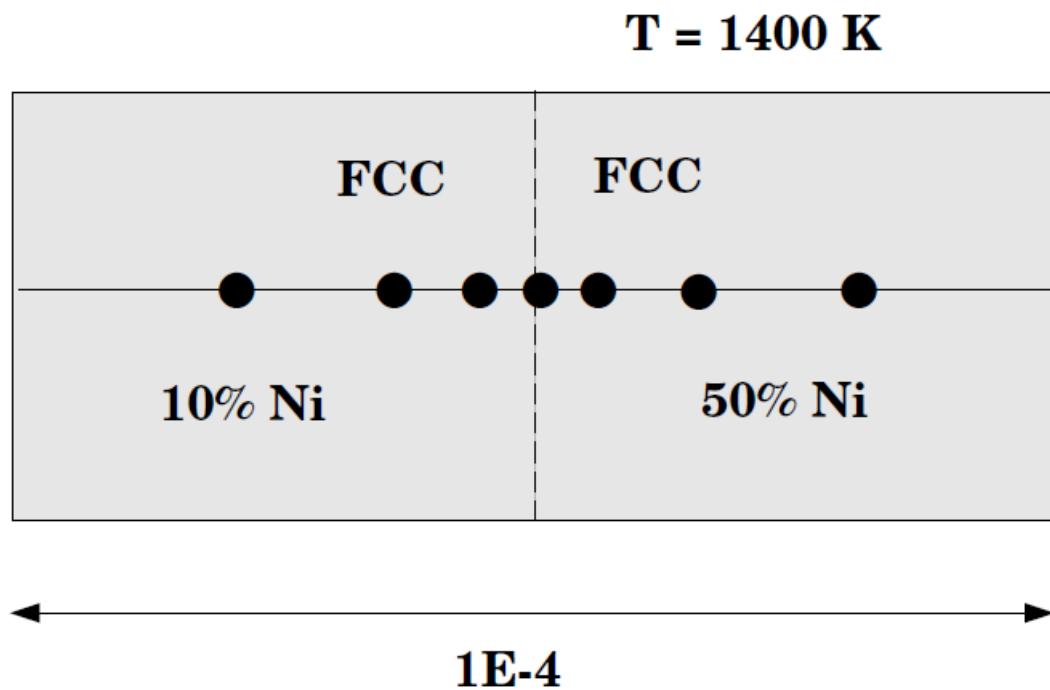
```
POST-1:
POST-1: set-inter
... the command in full is SET_INTERACTIVE_MODE
--OK--
POST-1:
```




Example exa2b

Homogenization of a binary Fe-Ni alloy

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



exa2b-setup

About

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

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

```
SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa2b\setup.DCM" @@
```

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

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

```
SYS: @@ This example is identical to a2a but instead it uses implicit time
```

```
SYS: @@ integration instead of the trapezoidal method for solving the PDEs.
```

```
SYS: -----  
NO SUCH COMMAND, USE HELP
```

```
SYS:
```

```
SYS: @@ exa2b_setup.DCM
```

```
SYS:
```

```
SYS: @@
```

```
SYS: @@ FIRST DEFINE A LOG-FILE FOR THIS EXAMPLE
```

```
SYS: @@
```

```
SYS: set_log_file setup
```

```
Heading:
```

```
SYS: @@
```

```
SYS: @@ THEN GO TO THE DATABASE MODULE
```

```
SYS: @@
```

```
SYS: go da
```

```
... the command in full is GOTO_MODULE
```

```
THERMODYNAMIC DATABASE module
```

```
Current database: Steels/Fe-Alloys v9.0
```

```
VA          /-  DEFINED  
LI2_FCC      B2_BCC          DICTRA_FCC_A1  
REJECTED
```

```
TDB_TCFE9:
```

```
TDB_TCFE9: @@
```

```
TDB_TCFE9: @@ USE THE TCFE DATABASE FOR THERMODYNAMIC DATA
```

```
TDB_TCFE9: @@
```

```
TDB_TCFE9: sw tcfe7
```

```
... the command in full is SWITCH_DATABASE
```

```
Current database: Steels/Fe-Alloys v7.0
```

```
VA  DEFINED  
LI2_FCC      B2_BCC      B2_VACANCY  
HIGH_SIGMA   DICTRA_FCC_A1  REJECTED
```

```
TDB_TCFE7:
```

```
TDB_TCFE7: @@
```

```
TDB_TCFE7: @@ DEFINE THE SYSTEM TO WORK WITH
```

```
TDB_TCFE7: @@
```

```
TDB_TCFE7: def-system fe ni
```

```
... the command in full is DEFINE_SYSTEM
```

```
FE          NI  DEFINED
```

```
TDB_TCFE7:
```

```
TDB_TCFE7: @@
```

```
TDB_TCFE7: @@ EXCLUDE THE THERMODYNAMIC DATA FOR THE PHASES THAT ARE NOT NEEDED
```

```
TDB_TCFE7: @@
```

```
TDB_TCFE7: rej ph * all
```

```
... the command in full is REJECT
```

```
LIQUID:L      BCC_A2      FCC_A1  
HCP_A3        A1_KAPPA    KAPPA  
LAVES_PHASE_C14  NBNI3     NI3TI  
REJECTED
```

```
TDB_TCFE7: res ph fcc
```

```
... the command in full is RESTORE
```

```
FCC_A1  RESTORED
```

```
TDB_TCFE7:
```

```
TDB_TCFE7: @@
```

```
TDB_TCFE7: @@ RETRIEVE DATA FROM THE DATABASE FILE
```

```
TDB_TCFE7: @@
```

```
TDB_TCFE7: get
```

```
... the command in full is GET_DATA
```

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

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

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

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

```
... the command in full is AMEND_PHASE_DESCRIPTION
```

```
PARAMETERS ...
```

```
FUNCTIONS ...
```

```
List of references for assessed data
```

```
'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'
```

```
'A. Dinsdale, T. Chart, MTDS NPL, unpublished work (1986); FE-NI'
```

```
'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
```

```
  Molar volumes'
```

```
'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
```

```
-OK-
```

```
TDB_TCFE7:
```

```
TDB_TCFE7: @@
```

```
TDB_TCFE7: @@ MOBILITY/DIFFUSIVITY DATA ARE STORED IN A SEPARATE DATABASE FILE.
```

```
TDB_TCFE7: @@ SWITCH TO THE MOBILITY DATABASE TO RETRIEVE DATA.
```

```
TDB_TCFE7: @@
```

```
TDB_TCFE7: app
```

```
... the command in full is APPEND_DATABASE
```

```
Use one of these databases
```

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

```

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

```

DATABASE NAME /TCFE7/: mobfe2

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

VA DEFINED

APP: def-sys fe ni

... the command in full is DEFINE_SYSTEM

FE NI DEFINED

APP: rej ph * all

... the command in full is REJECT

BCC_A2 FCC_A1 HCP_A3

LIQUID:L REJECTED

APP: res ph fcc

[illegible]

[illegible]

```
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 1E6
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /100000/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO FILE AND EXIT
DIC> @@
DIC> save exa2b Y
... the command in full is SAVE_WORKSPACES
DIC>
DIC> set-inter
... the command in full is SET_INTERACTIVE
--OK--
DIC>
```

exa2b-run

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa2b\run.DCM"DIC>
DIC>
DIC> @@ exa2b_run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING EXAMPLE a2b
DIC> @@
DIC>
DIC> @@
DIC> @@ LET US DEFINE A LOG-FILE FOR THIS EXAMPLE
DIC> @@
DIC> set-log-file run
    AMBIGUOUS COMMAND, USE HELP
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA MONITOR AN READ SETUP FROM FILE
DIC> @@
DIC> go d-m
    ... the command in full is GOTO_MODULE
    TIME STEP AT TIME 0.00000E+00
DIC> read exa2b
    ... the command in full is READ_WORKSPACES
    ... the command in full is DEFINE_COMPONENTS
    ... the command in full is SELECT_EQUILIBRIUM
    OK
DIC>
DIC> @@
DIC> @@ Start the simulation
DIC> @@
DIC> simulate
    ... the command in full is SIMULATE_REACTION
    ... the command in full is SET_NUMERICAL_LIMITS
U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
    2 GRIDPOINT(S) ADDED TO CELL #1 REGION: AUSTENITE
TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
    CPU time used in timestep 0 seconds
TIME = 0.10010000E-03 DT = 0.10000000E-03 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
    CPU time used in timestep 0 seconds
TIME = 0.40010010 DT = 0.40000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
    CPU time used in timestep 0 seconds
TIME = 10.403455 DT = 10.003355 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
    CPU time used in timestep 0 seconds
TIME = 30.410165 DT = 20.006710 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
    CPU time used in timestep 0 seconds
TIME = 70.423585 DT = 40.013420 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
    CPU time used in timestep 0 seconds
TIME = 150.45043 DT = 80.026840 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
    CPU time used in timestep 0 seconds
TIME = 310.50411 DT = 160.05368 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
    CPU time used in timestep 0 seconds
TIME = 630.61147 DT = 320.10736 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
    CPU time used in timestep 0 seconds
TIME = 1270.8262 DT = 640.21472 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
    CPU time used in timestep 0 seconds
TIME = 2551.2556 DT = 1280.4294 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
    CPU time used in timestep 0 seconds
TIME = 5112.1145 DT = 2560.8589 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
    CPU time used in timestep 0 seconds
TIME = 10233.832 DT = 5121.7178 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406169 NI = .291111754593831
TOTAL SIZE OF SYSTEM: 1E-04 [m]
    CPU time used in timestep 0 seconds
TIME = 20477.268 DT = 10243.436 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
    CPU time used in timestep 0 seconds
TIME = 40964.139 DT = 20486.871 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
    CPU time used in timestep 0 seconds
TIME = 81937.881 DT = 40973.742 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .70888824540617 NI = .29111175459383
TOTAL SIZE OF SYSTEM: 1E-04 [m]
    CPU time used in timestep 0 seconds
TIME = 163885.37 DT = 81947.484 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406167 NI = .291111754593833
TOTAL SIZE OF SYSTEM: 1E-04 [m]
    CPU time used in timestep 0 seconds
TIME = 263885.37 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406165 NI = .291111754593835
TOTAL SIZE OF SYSTEM: 1E-04 [m]
    CPU time used in timestep 0 seconds
TIME = 363885.37 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406164 NI = .291111754593836
```

```

TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 463885.37 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406165 NI = .291111754593835
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 563885.37 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406162 NI = .291111754593838
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 663885.37 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406158 NI = .291111754593842
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 763885.37 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406157 NI = .291111754593843
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 863885.37 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406157 NI = .291111754593843
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 963885.37 DT = 100000.00 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406154 NI = .291111754593846
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 1000000.0 DT = 36114.635 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: FE = .708888245406156 NI = .291111754593844
TOTAL SIZE OF SYSTEM: 1E-04 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 0.0000000
DELETING TIME-RECORD FOR TIME 0.100000000E-06
DELETING TIME-RECORD FOR TIME 0.100100000E-03
DELETING TIME-RECORD FOR TIME 0.40010010
DELETING TIME-RECORD FOR TIME 10.403455
DELETING TIME-RECORD FOR TIME 30.410165
DELETING TIME-RECORD FOR TIME 70.423585
DELETING TIME-RECORD FOR TIME 150.45043
DELETING TIME-RECORD FOR TIME 310.50411
DELETING TIME-RECORD FOR TIME 630.61147
DELETING TIME-RECORD FOR TIME 1270.8262
DELETING TIME-RECORD FOR TIME 2551.2556
DELETING TIME-RECORD FOR TIME 5112.1145
DELETING TIME-RECORD FOR TIME 10233.832
DELETING TIME-RECORD FOR TIME 20477.268
DELETING TIME-RECORD FOR TIME 40964.139
DELETING TIME-RECORD FOR TIME 81937.881
DELETING TIME-RECORD FOR TIME 163885.37
DELETING TIME-RECORD FOR TIME 263885.37
DELETING TIME-RECORD FOR TIME 363885.37
DELETING TIME-RECORD FOR TIME 463885.37
DELETING TIME-RECORD FOR TIME 563885.37
DELETING TIME-RECORD FOR TIME 663885.37
DELETING TIME-RECORD FOR TIME 763885.37
DELETING TIME-RECORD FOR TIME 863885.37

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

TIMESTEP AT 1000000.00 SELECTED

```

```

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

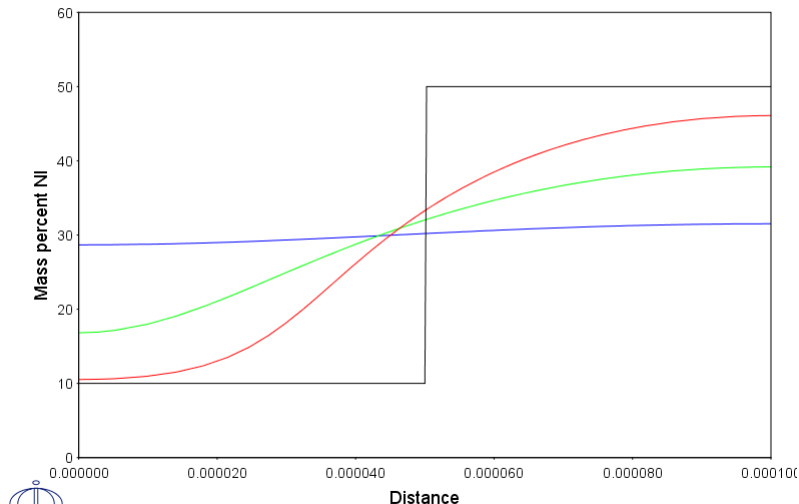
```


exa2b-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa2b\plot.DCM"DIC>
DIC>
DIC> @@ exa2b_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE a2b
DIC> @@
DIC>
DIC> @@
DIC> @@ LET US DEFINE A LOG-FILE FOR THIS EXAMPLE
DIC> @@
DIC> set-log-file plot
    AMBIGUOUS COMMAND, USE HELP
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
    ... the command in full is GOTO_MODULE
    TIME STEP AT TIME 1.00000E+06
DIC> read exa2b
    ... the command in full is READ_WORKSPACES
    ... the command in full is DEFINE_COMPONENTS
    ... the command in full is SELECT_EQUILIBRIUM
    OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
    ... the command in full is POST_PROCESSOR

    POST PROCESSOR VERSION 1.7
    Implemented by Bjorn Jonsson

POST-1:
POST-1:
POST-1: @@
POST-1: @@ PLOT SOME CONCENTRATION PROFILES
POST-1: @@
POST-1: s-d-a
    ... the command in full is SET_DIAGRAM_AXIS
    AXIS (X, Y OR Z) : x
    VARIABLE : dist
    INFO: Distance is set as independent variable
    ... the command in full is SET_INDEPENDENT_VARIABLE
    DISTANCE : /GLOBAL/: glo
POST-1:
POST-1: s-d-a
    ... the command in full is SET_DIAGRAM_AXIS
    AXIS (X, Y OR Z) : y
    VARIABLE : w-p
    FOR COMPONENT : ni
POST-1:
POST-1: s-p-c
    ... the command in full is SET_PLOT_CONDITION
    CONDITION /TIME/: time
    VALUE(S) /LAST/: 0 1e5 3e5 1e6
POST-1:
POST-1: @@
POST-1: @@ SET SCALING ON Y-AXIS BEFORE PLOTTING
POST-1: @@
POST-1: s-s-s
    ... the command in full is SET_SCALING_STATUS
    AXIS (X, Y OR Z) : y
    AUTOMATIC SCALING (Y OR N) /N/: n
    MIN VALUE : 0
    MAX VALUE : 60
POST-1:
POST-1: plot
    ... the command in full is PLOT_DIAGRAM
    2018.02.18.18.32.49
    Time=0,100000,300000,1000000
    CELL #1
```



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

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

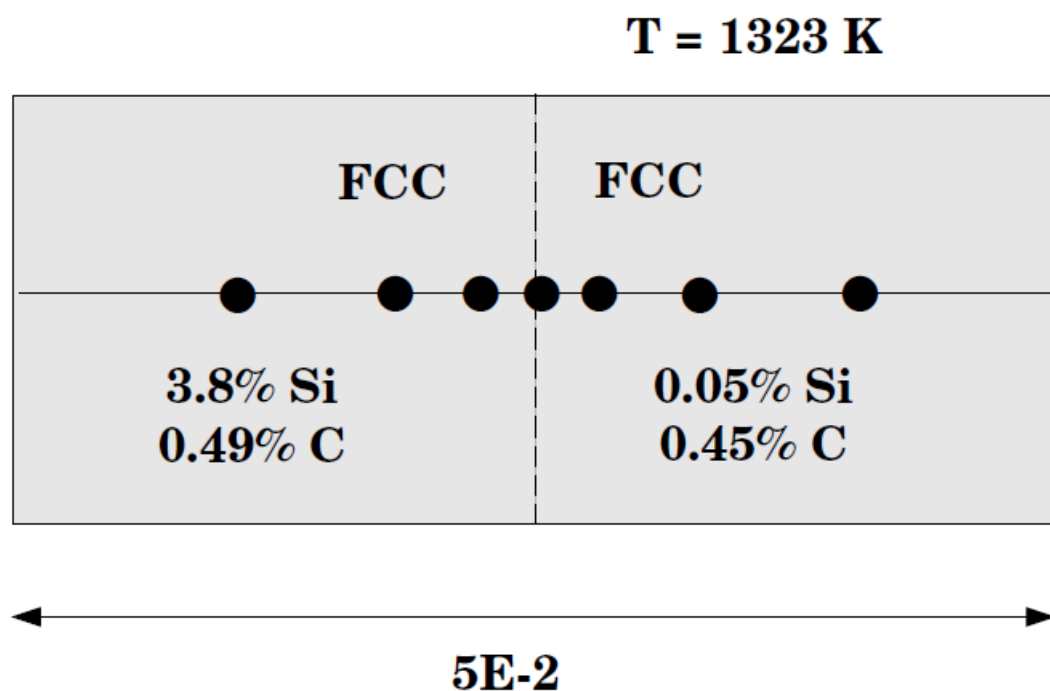


Example exa3

Uphill diffusion in an Fe-Si-C alloy

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

In this example, two pieces of austenite (3.80 wt%Si, 0.49 wt%C) and (0.05 wt%Si, 0.45 wt%C) are put together and are subsequently annealed at 1050 C for 13 days. As both pieces are austenite they must be entered into the same region. This is done by giving the compositions of Si and C in each gridpoint individually. These data are then stored on file.



exa3-setup

AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa3\setup.DCM" @@

SYS: @@ One-phase problem.

SYS: @@ Uphill diffusion in an Fe-Si-C alloy

SYS: @@ This is an example to simulate uphill diffusion in a ternary single

SYS: @@ phase austenite matrix due to the classical Darken experiment published

SYS: @@ by L.S. Darken: Trans. Aime, v.180 (1949), pp. 430-438.

SYS: @@

SYS: @@ In this example two pieces of austenite (3.80 wt%Si, 0.49 wt%C) and

SYS: @@ (0.05 wt%Si, 0.45 wt%C) are put together and are subsequently annealed

SYS: @@ at 1050C for 13 days. As both pieces are austenite they must be entered

SYS: @@ into the same region. This is done by individually giving the compositions

SYS: @@ of Si and C in each grid point. These data are then stored to file.

SYS: -----

NO SUCH COMMAND, USE HELP

SYS:

SYS: @@ darken_setup.DCM

SYS:

SYS: @@

SYS: @@ Note that LOG-FILES used previously in examples a2a and a2b are

SYS: @@ no longer used.

SYS: @@

SYS:

SYS: @@

SYS: @@ RETRIEVE DATA FROM THE DATABASE

SYS: @@

SYS: go da

THERMODYNAMIC DATABASE module

Current database: Steels/Fe-Alloys v9.0

VA /- DEFINED

L12_FCC B2_BCC DICTRA_FCC_A1

REJECTED

TDB_TCFE9:

TDB_TCFE9: @@

TDB_TCFE9: @@ USE A TCFE DATABASE FOR THE THERMODYNAMIC DATA

TDB_TCFE9: @@

TDB_TCFE9: sw tcfe7

Current database: Steels/Fe-Alloys v7.0

VA DEFINED

L12_FCC B2_BCC B2_VACANCY

HIGH_SIGMA DICTRA_FCC_A1 REJECTED

TDB_TCFE7: def-sys fe si c

FE SI C

DEFINED

TDB_TCFE7: rej ph * all

GAS:G LIQUID:L BCC_A2

FCC_A1 HCP_A3 DIAMOND_FCC_A4

GRAPHITE CEMENTITE M23C6

M7C3 M5C2 KSI_CARBIDE

Al_KAPPA KAPPA FE4N_LP1

FECH_CHI LAVES_PHASE_C14 M3SI

CR3SI FE2SI MSI

M5SI3 AL4C3 FE8SI2C

SIC REJECTED

TDB_TCFE7: res ph fcc

FCC_A1 RESTORED

TDB_TCFE7: get

REINITIATING GES

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

FUNCTIONS

List of references for assessed data

'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'

'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C

-FE'

'J. Lacaze and B. Sundman, Metall. Mater. Trans. A, 22A (1991), 2211-2223;

Fe-Si and Fe-Si-C'

'J. Miettinen and B. Hallstedt, Calphad, 22 (1998), 231-256; Fe-Si and Fe

-Si-C'

'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;

Molar volumes'

'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'

'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'

-OK-

TDB_TCFE7:

TDB_TCFE7: @@

TDB_TCFE7: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE MOBILITY DATA

TDB_TCFE7: @@

TDB_TCFE7: app mobfe2

Current database: Steels/Fe-Alloys Mobility v2.0

TCS Steel Mobility Database Version 2.0 from 2011-12-09.

VA DEFINED

APP: def-sys fe si c

FE SI C

DEFINED

APP: rej ph * all

BCC_A2 CEMENTITE FCC_A1

FE4N_LP1 HCP_A3 LIQUID:L

REJECTED

APP: res ph fcc

FCC_A1 RESTORED

APP: get

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

FUNCTIONS

List of references for assessed data

'This parameter has not been assessed'

'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'

'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe

-Ni'

```

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

DIC>
DIC> @@
DIC> @@ ENTER THE REGION austenite
DIC> @@
DIC> enter-region
REGION NAME : austenite
DIC>
DIC> @@
DIC> @@ ENTER THE GRID
DIC> @@ NOTE THAT GRID POINT DISTANCES ARE SMALLEST AROUND THE MIDDLE
DIC> @@
DIC> enter-grid
REGION NAME : /AUSTENITE/: austenite
WIDTH OF REGION /1/: 50E-3
TYPE /LINEAR/: AUTO
DIC>
DIC> @@
DIC> @@ ENTER THE PHASE INTO A REGION (BOTH PIECES ARE AUSTENITIC)
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /AUSTENITE/: austenite
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC> @@
DIC> @@ ENTER COMPOSITIONS INTO THE PHASE
DIC> @@
DIC> enter-composition
REGION NAME : /AUSTENITE/: austenite
PHASE NAME: /FCC_A1/: fcc#1
DEPENDENT COMPONENT ? /SI/: FE
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: C func 0.49-0.04*hs(x-25e-3);
PROFILE FOR /SI/: SI func 3.80-3.75*hs(x-25e-3);
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME AND OTHER SIMULATION PARAMETERS
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 1e10
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /1E+09/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC> save exa3 Y
DIC>
DIC> set-inter
--OK--
DIC>

```

exa3-run

DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa3\run.DCM"DIC>

DIC>

DIC> @@ darken_run.DCM

DIC>

DIC> @@

DIC> @@ ENTER THE DICTRA MONITOR

DIC> @@

DIC> go d-m

TIME STEP AT TIME 0.00000E+00

DIC>

DIC> @@

DIC> @@ READ SETUP FROM FILE AND START SIMULATION

DIC> @@

DIC> read exa3

OK

DIC>

DIC> sim

Region: AUSTENITE

double geometric

coarse at outer boundaries dense at 0.25047E-01

lower part 0.80000 22

upper part 1.2500 22

U-FRACTION IN SYSTEM: C = .0215351122808224 FE = .96291921367461

SI = .0370807863253901

TOTAL SIZE OF SYSTEM: .05 [m]

U-FRACTION IN SYSTEM: C = .0215351122808224 FE = .96291921367461

SI = .0370807863253901

TOTAL SIZE OF SYSTEM: .05 [m]

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

U-FRACTION IN SYSTEM: C = .0215351122808224 FE = .96291921367461

SI = .0370807863253901

TOTAL SIZE OF SYSTEM: .05 [m]

CPU time used in timestep 0 seconds

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

U-FRACTION IN SYSTEM: C = .0215351122808224 FE = .96291921367461

SI = .0370807863253901

TOTAL SIZE OF SYSTEM: .05 [m]

CPU time used in timestep 0 seconds

TIME = 0.40010010 DT = 0.40000000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .0215351122808224 FE = .96291921367461

SI = .0370807863253901

TOTAL SIZE OF SYSTEM: .05 [m]

CPU time used in timestep 0 seconds

TIME = 21.165600 DT = 20.765500 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .0215351122808224 FE = .96291921367461

SI = .0370807863253901

TOTAL SIZE OF SYSTEM: .05 [m]

CPU time used in timestep 0 seconds

TIME = 62.696601 DT = 41.531000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .0215351122808224 FE = .96291921367461

SI = .0370807863253901

TOTAL SIZE OF SYSTEM: .05 [m]

CPU time used in timestep 0 seconds

TIME = 145.75860 DT = 83.062001 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .0215351122808224 FE = .96291921367461

SI = .0370807863253901

TOTAL SIZE OF SYSTEM: .05 [m]

CPU time used in timestep 0 seconds

TIME = 311.88260 DT = 166.12400 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .0215351122808223 FE = .96291921367461

SI = .0370807863253901

TOTAL SIZE OF SYSTEM: .05 [m]

CPU time used in timestep 0 seconds

TIME = 644.13060 DT = 332.24800 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .0215351122808223 FE = .96291921367461

SI = .0370807863253901

TOTAL SIZE OF SYSTEM: .05 [m]

CPU time used in timestep 0 seconds

TIME = 1308.6266 DT = 664.49600 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .0215351122808225 FE = .96291921367461

SI = .0370807863253901

TOTAL SIZE OF SYSTEM: .05 [m]

CPU time used in timestep 0 seconds

TIME = 2637.6186 DT = 1328.9920 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .021535112280823 FE = .96291921367461

SI = .0370807863253901

TOTAL SIZE OF SYSTEM: .05 [m]

CPU time used in timestep 1 seconds

TIME = 5295.6026 DT = 2657.9840 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .0215351122808237 FE = .96291921367461

SI = .0370807863253901

TOTAL SIZE OF SYSTEM: .05 [m]

CPU time used in timestep 0 seconds

TIME = 10611.571 DT = 5315.9680 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .0215351122808241 FE = .96291921367461

SI = .0370807863253901

TOTAL SIZE OF SYSTEM: .05 [m]

CPU time used in timestep 0 seconds

TIME = 21243.507 DT = 10631.936 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .0215351122808231 FE = .96291921367461

SI = .0370807863253901

TOTAL SIZE OF SYSTEM: .05 [m]

CPU time used in timestep 0 seconds

TIME = 42507.379 DT = 21263.872 SUM OF SQUARES = 0.0000000

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

```

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

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

```
TIMESTEP AT      0.10000000E+11 SELECTED
```

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


exa3-plot

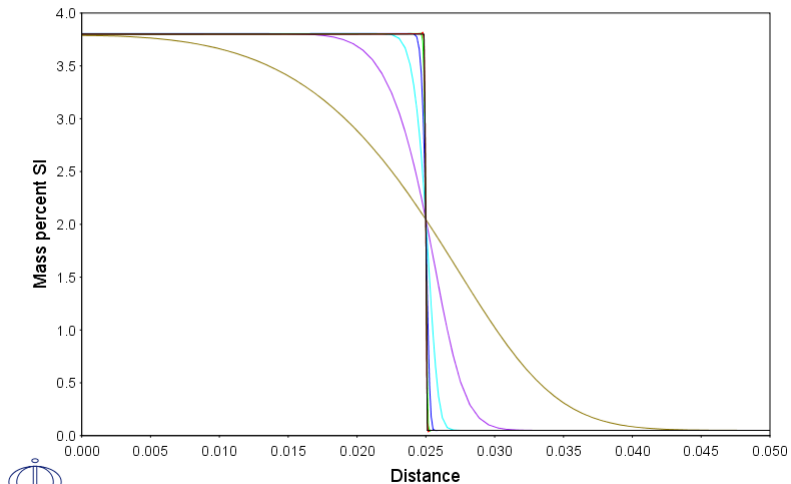
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa3\plot.DCM"DIC>
DIC>
DIC> @@ darken_plot.DCM
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA MODULE AND SPECIFY THE STORE-RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 1.00000E+10
DIC> read exa3
OK
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA POST PROCESSOR
DIC> @@
DIC> post
```

POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson

```
POST-1:
POST-1: @@
POST-1: @@ PLOT THE CONCENTRATION PROFILE FOR Si AT TIMES 0, 1E5, 1123200, 1E7,
POST-1: @@ 1E8, 1E9 AND 1E10 S
POST-1: @@
POST-1: @@ SET DISTANCE IN SYSTEM AS X-AXIS, WEIGHT-% SI ON Y-AXIS AND SPECIFY
POST-1: @@ FOR WHICH SIMULATION TIMES TO PLOT THE PROFILES.
POST-1: @@
POST-1: set-diagram-axis x distance global
INFO: Distance is set as independent variable
POST-1: set-diagram-axis y weight-percent si
POST-1: set-plot-condition time 0 1E5 1123200 1e7 1E8 1E9 1E10
POST-1:
POST-1: @@
POST-1: @@ PLOT THE DIAGRAM
POST-1: @@
POST-1: set-title
TITLE : Figure a3.1
POST-1:
POST-1: plot
```

Figure a3.1

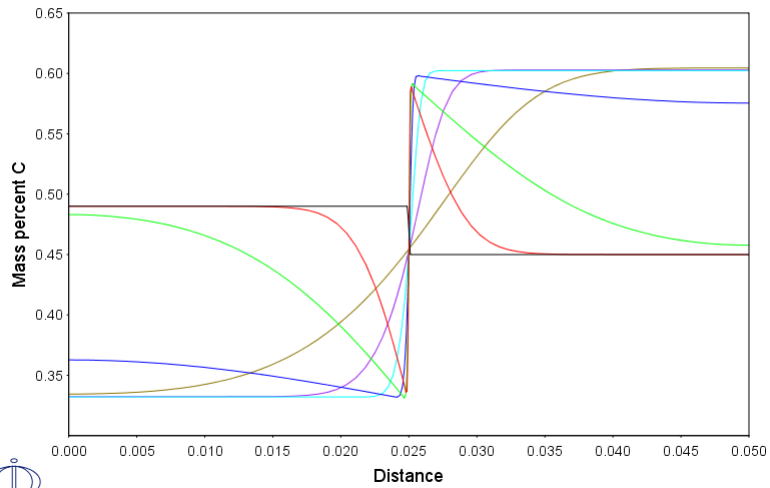
2018.02.18.18.35.55
Time=0,100000,1123200,1E+07,1E+08,1E+09,1E+10
CELL#1



```
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1: @@
POST-1: @@ PLOT THE CONCENTRATION PROFILES FOR C
POST-1: @@
POST-1: @@ WE ONLY NEED TO CHANGE THE Y-AXIS
POST-1: @@
POST-1: set-diagram-axis y w-p c
POST-1: set-title Figure a3.2
POST-1: plot
```

Figure a3.2

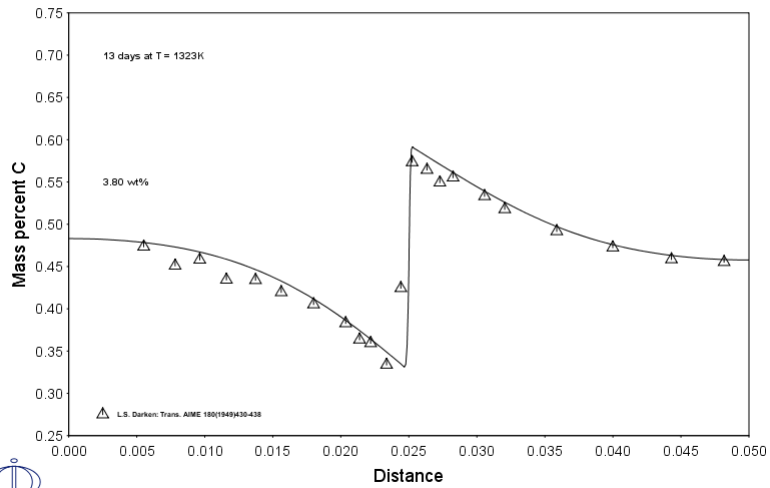
2018.02.18.18.35.55
 Time = 0,100000,1123200,1E+07,1E+08,1E+09,1E+10
 CELL #1



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

Figure a3.3

2018.02.18.18.35.56
 Time = 1123200
 CELL #1



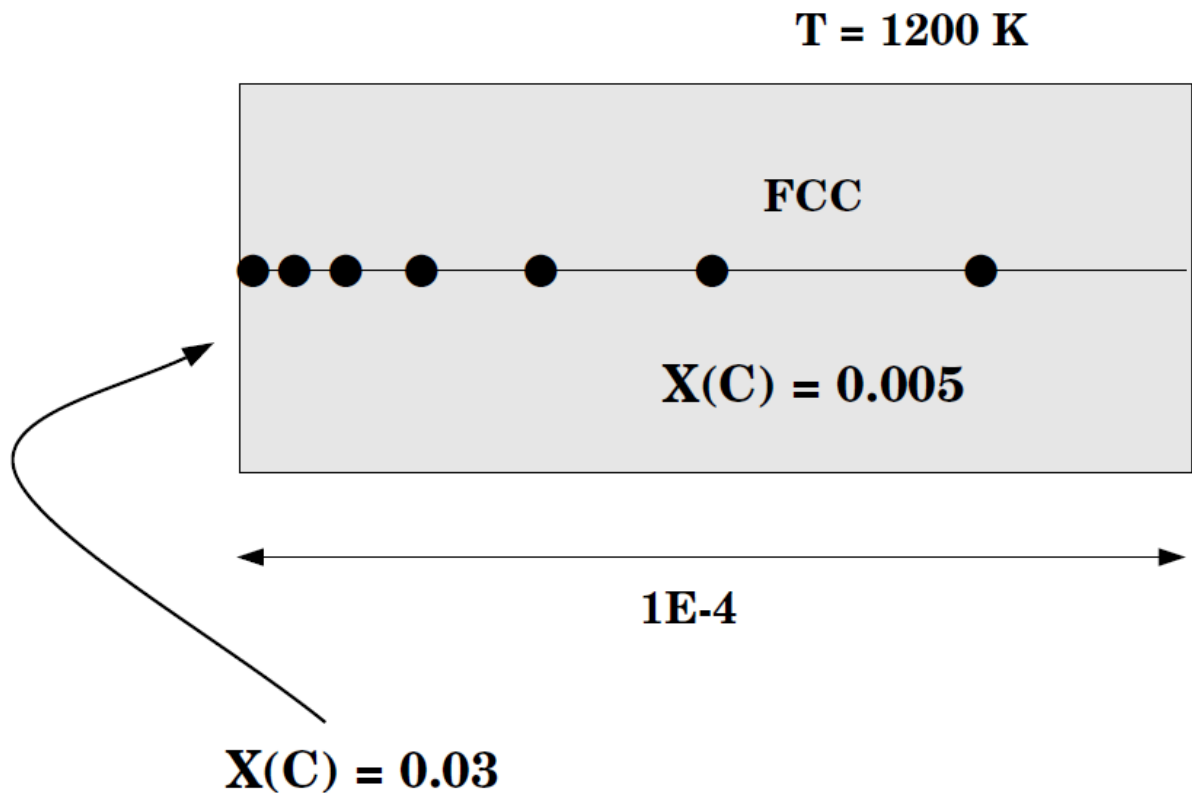
```
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1: set-inter
--OK--
POST-1:
```



Example exa4

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

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



exa4-setup

About Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

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

SYS: **SYS:** **MACRO** "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa4\setup.DCM" @@

SYS: @@ One-phase problem.

SYS: @@ Carburization of binary Fe-C alloy: Comparison to an analytical erf solution

SYS: @@ This is a simple binary simulation with a single phase region.

SYS: @@ The numerical simulation is compared with an analytical erf solution.

SYS: @@ For this reason a special database erf.tdb is created where the

SYS: @@ diffusion coefficient is set to a concentration independent value.

SYS: -----

NO SUCH COMMAND, USE HELP

SYS:

SYS: @@ exa4_setup.DCM

SYS:

SYS:

SYS: @@

SYS: @@ READ THE DATA FROM THE DATABASES

SYS: @@

SYS: go da

THERMODYNAMIC DATABASE module

Current database: Steels/Fe-Alloys v9.0

VA /- DEFINED

L12_FCC B2_BCC DICTRA_FCC_A1

REJECTED

TDB_TCFE9: sw FEDEMO

Current database: Iron Demo Database v2.0

VA /- DEFINED

TDB_FEDEMO: def-system fe,c

FE C DEFINED

TDB_FEDEMO: rej-ph *

GAS:G LIQUID:L BCC_A2

CEMENTITE DIAMOND_FCC_A4 FCC_A1

GRAPHITE HCP_A3 KSI_CARBIDE

LAVES_PHASE_C14 M23C6 M5C2

M7C3 REJECTED

TDB_FEDEMO: rest-ph fcc

FCC_A1 RESTORED

TDB_FEDEMO: get

REINITIATING GES

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

FUNCTIONS

List of references for assessed data

'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-Fe'

'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'

'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'

'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar

volumes'

'X.-G. Lu, M. Selleby, B. Sundman, CALPHAD, 29 (2005) 49-55; Fe P-T diagram'

'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'

-OK-

TDB_FEDEMO:

TDB_FEDEMO: append user exa4.TDB

Current database: User defined Database

This database does not support the DATABASE_INFORMATION command

VA DEFINED

TDB_APP: def-system fe,c

FE C DEFINED

TDB_APP: rej-ph *

FCC_A1 REJECTED

TDB_APP: rest-ph fcc

FCC_A1 RESTORED

TDB_APP: get

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

FUNCTIONS

-OK-

TDB_APP:

TDB_APP: @@

TDB_APP: @@ GO TO THE DICTRA MODULE AND SET UP THE SYSTEM

TDB_APP: @@

TDB_APP: go d-m

NO TIME STEP DEFINED

DIC>

DIC> @@

DIC> @@ ENTER GLOBAL CONDITION T

DIC> @@

DIC> set-cond glob T 0 1200; * N

DIC>

DIC> @@

DIC> @@ ENTER THE REGION steel

DIC> @@

DIC> enter-region

REGION NAME : steel

DIC>

DIC> @@

DIC> @@ ENTER THE GRID

DIC> @@ CARBON ENTERS THE SYSTEM FROM THE LOWER BOUNDARY AND CONSEQUENTLY

DIC> @@ MORE POINTS ARE REQUIRED AT THAT BOUNDARY. THIS IS WHY A GEOMETRIC

DIC> @@ GRID IS USED.

DIC> @@

DIC> enter-grid

REGION NAME : /STEEL/: steel

```

WIDTH OF REGION /1/: 1E-4
TYPE /LINEAR/: AUTO
DIC>
DIC> @@
DIC> @@ ENTER THE PHASE INTO THE REGION
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /STEEL/: steel
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITION IN THE FCC PHASE
DIC> @@
DIC> enter-composition
REGION NAME : /STEEL/: steel
PHASE NAME: /FCC_A1/: fcc#1
COMPOSITION TYPE /MOLE_FRACTION/: mole-fraction
PROFILE FOR /C/: c
TYPE /LINEAR/: linear
VALUE OF FIRST POINT : 0.005
VALUE OF LAST POINT : /5E-3/: 0.005
DIC>
DIC>
DIC> @@
DIC> @@ SET A FIXED COMPOSITION AS THE BOUNDARY VALUE
DIC> @@
DIC> set-condition

GLOBAL OR BOUNDARY CONDITION /GLOBAL/: boundary
BOUNDARY /LOWER/: lower
CONDITION TYPE /CLOSED_SYSTEM/: state-variable-value
State variable expression #1 : /N=1/: n=1
State variable expression #2 : x(c)=0.03
DIC>
DIC>
DIC> @@
DIC> @@ SET A SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 100
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /10/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC>
DIC> save exa4 Y
DIC>
DIC> set-inter
--OK--
DIC>

```

exa4-run

DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa4\run.DCM"DIC>

DIC>

DIC> @@ exa4_run.DCM

DIC>

DIC> @@

DIC> @@ FILE FOR RUNNING EXAMPLE a4

DIC> @@

DIC>

DIC> @@

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

DIC> @@

DIC> go d-m

TIME STEP AT TIME 0.00000E+00

DIC> read exa4

OK

DIC>

DIC> @@

DIC> @@ START THE SIMULATION

DIC> @@

DIC> sim

Region: STEEL
single geometric dense at 0.0000
1.1388 96
U-FRACTION IN SYSTEM: C = .0050251256281407 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
U-FRACTION IN SYSTEM: C = .0050251256281407 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.00000000
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 = 0.00000000
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 = 0.00000000
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 = 0.00000000
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 = 0.00000000
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 = 0.00000000
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 = 0.00000000
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 = 0.00000000
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 = 0.00000000
U-FRACTION IN SYSTEM: C = .00504664654067874 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.12776521E-02 DT = 0.64002611E-03 SUM OF SQUARES = 0.00000000
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 = 0.00000000
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 = 0.00000000
U-FRACTION IN SYSTEM: C = .00508603865206295 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.10238018E-01 DT = 0.51202089E-02 SUM OF SQUARES = 0.00000000
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 = 0.00000000
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 = 0.00000000
U-FRACTION IN SYSTEM: C = .00519741865567009 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.81920942E-01 DT = 0.40961671E-01 SUM OF SQUARES = 0.00000000
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 = 0.00000000
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 = 0.00000000
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 = 0.00000000
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 = 0.00000000
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 = 0.00000000
U-FRACTION IN SYSTEM: C = .00640343298842195 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 5.2430915 DT = 2.6215470 SUM OF SQUARES = 0.00000000

```

U-FRACTION IN SYSTEM: C = .00697433052866846 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 10.486185 DT = 5.2430939 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00778159421638381 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 20.486185 DT = 10.000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00887736257293559 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 30.486185 DT = 10.000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00972196664325365 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 40.486185 DT = 10.000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0104363519865359 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 50.486185 DT = 10.000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0110669328932657 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 60.486185 DT = 10.000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0116377078880251 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 70.486185 DT = 10.000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0121630223717782 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 80.486185 DT = 10.000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0126522650845277 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 90.486185 DT = 10.000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0131119785059757 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 100.00000 DT = 9.5138146 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .013526298212787 FE = 1
TOTAL SIZE OF SYSTEM: 1E-04 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 0.0000000
DELETING TIME-RECORD FOR TIME 0.10000000E-06
DELETING TIME-RECORD FOR TIME 0.26001020E-05
DELETING TIME-RECORD FOR TIME 0.76003060E-05
DELETING TIME-RECORD FOR TIME 0.17600714E-04
DELETING TIME-RECORD FOR TIME 0.37601530E-04
DELETING TIME-RECORD FOR TIME 0.77603162E-04
DELETING TIME-RECORD FOR TIME 0.15760643E-03
DELETING TIME-RECORD FOR TIME 0.31761295E-03
DELETING TIME-RECORD FOR TIME 0.63762601E-03
DELETING TIME-RECORD FOR TIME 0.12776521E-02
DELETING TIME-RECORD FOR TIME 0.25577043E-02
DELETING TIME-RECORD FOR TIME 0.51178088E-02
DELETING TIME-RECORD FOR TIME 0.10238018E-01
DELETING TIME-RECORD FOR TIME 0.20478435E-01
DELETING TIME-RECORD FOR TIME 0.40959271E-01
DELETING TIME-RECORD FOR TIME 0.81920942E-01
DELETING TIME-RECORD FOR TIME 0.16384428
DELETING TIME-RECORD FOR TIME 0.32769097
DELETING TIME-RECORD FOR TIME 0.65538434
DELETING TIME-RECORD FOR TIME 1.3107711
DELETING TIME-RECORD FOR TIME 2.6215446
DELETING TIME-RECORD FOR TIME 5.2430915
DELETING TIME-RECORD FOR TIME 10.486185
DELETING TIME-RECORD FOR TIME 20.486185
DELETING TIME-RECORD FOR TIME 30.486185
DELETING TIME-RECORD FOR TIME 40.486185
DELETING TIME-RECORD FOR TIME 50.486185
DELETING TIME-RECORD FOR TIME 60.486185
DELETING TIME-RECORD FOR TIME 70.486185
DELETING TIME-RECORD FOR TIME 80.486185

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

TIMESTEP AT 100.000000 SELECTED

```

```

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

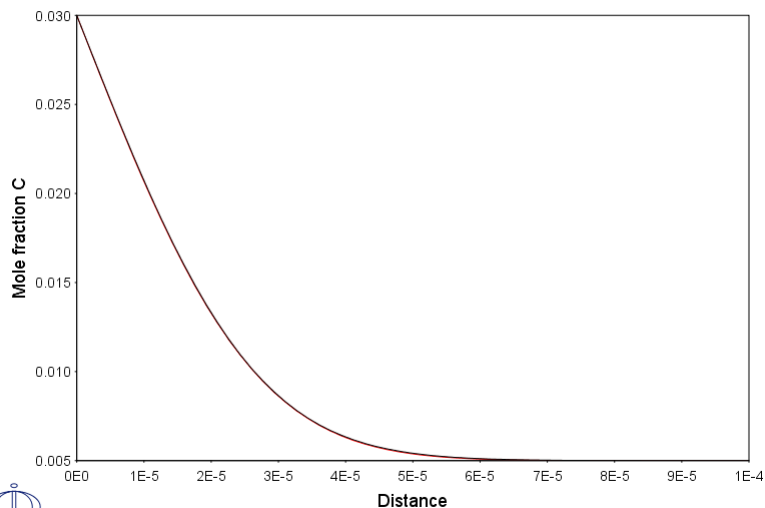
```

exa4-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa4\plot.DCM"DIC>
DIC>
DIC> @@ exa4_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE exa4
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 1.00000E+02
DIC> read exa4
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
```

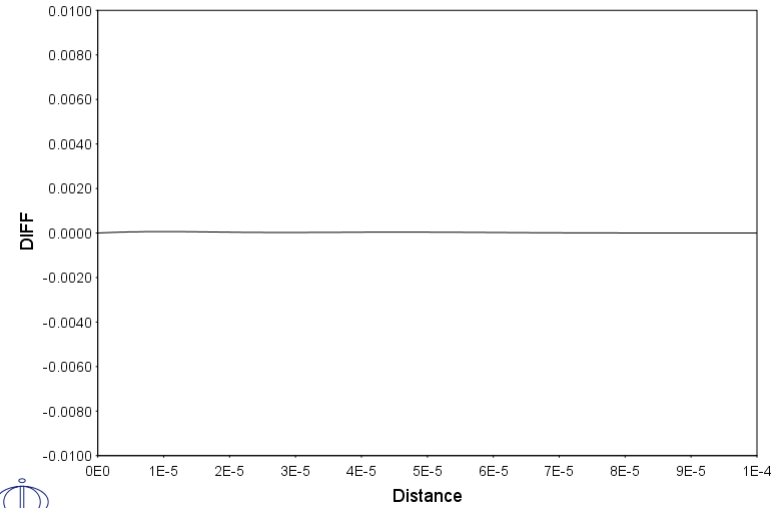
```
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
```

```
POST-1:
POST-1: @@
POST-1: @@ PLOT A COMPOSITION PROFILE
POST-1: @@
POST-1: s-d-a x distance global
INFO: Distance is set as independent variable
POST-1: s-d-a y x(c)
POST-1: s-p-c time 25
POST-1:
POST-1: @@
POST-1: @@ ENTER THE ANALYTICAL SOLUTION, CALLED ERF SOL
POST-1: @@
POST-1: enter-symbol
Function or table /FUNCTION/: function
NAME: erfsol
FUNCTION: 0.03-0.025*erf(gd/sqrt(4*dc(fcc,c,c,fe)*25));
POST-1:
POST-1: @@
POST-1: @@ COMPARE THE ANALYTICAL AND NUMERICAL SOLUTIONS
POST-1: @@
POST-1: enter-symbol
Function or table /FUNCTION/: table
NAME: aaa
Variable(s) x(c) erfsol
POST-1:
POST-1: s-d-a y aaa
COLUMN NUMBER /*/: 1 2
POST-1:
POST-1: set-axis-text
AXIS (X, Y OR Z) : y
AUTOMATIC AXIS TEXT (Y OR N) /N/: n
AXIS TEXT : Mole fraction C
POST-1:
POST-1: plot
2018.02.18.18.38.56
Time = 25
CELL #1
```



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


2018.02.18.18.38.56
Time = 25
CELL #1



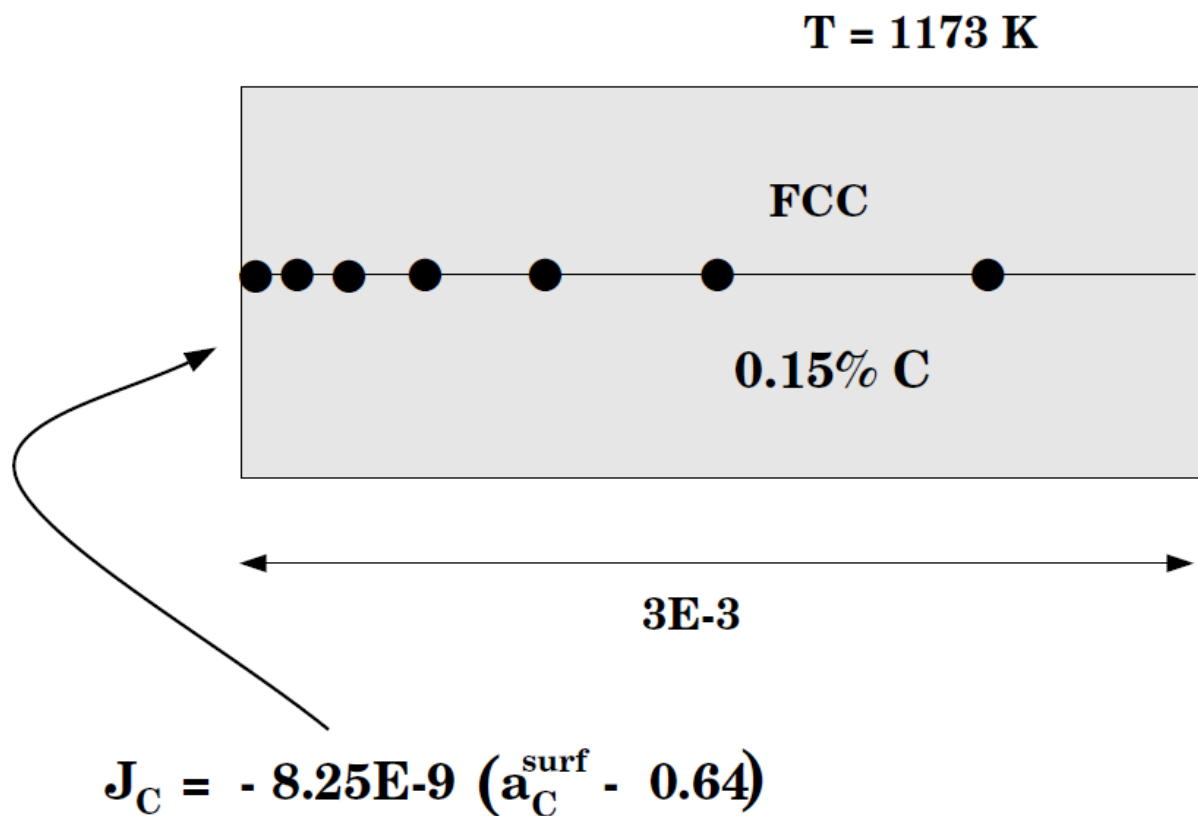
POST-1:
POST-1:
POST-1:
POST-1: @?<Hit_return_to_continue>
POST-1:
POST-1: set-interactive
--OK--
POST-1:



Example exa5

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

A mixture of 40% N₂ and 60% cracked methanol is used as carrier gas. The carburizing "carbon potential" in the gas is 0.85 wt%.



exa5-setup

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

```
SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa5\setup.DCM"SYS: ?@@
NO SUCH COMMAND, USE HELP
SYS: @@ One-phase problem.
SYS: @@ Carburation of a binary Fe-0.15 wt% C alloy.
SYS: @@ A mixture of 40% N2 and 60% cracked methanol is used as carrier gas.
SYS: @@ The carburizing "carbon potential" in the gas is 0.85 wt%.
SYS: @@ A surface reaction controls the flux of C at the surface.
SYS: -----
NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exa5_setup.DCM
SYS:
SYS: @@
SYS: @@ GO TO THE DATABASES AND READ THE THERMODYNAMIC AND KINETIC DATA
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Current database: Steels/Fe-Alloys v9.0

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

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

List of references for assessed data

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

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

```

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

```

DATABASE NAME /FEDEMO/: mfedemo

Current database: Fe-Alloys Mobility demo database v2.0

```

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

```

List of references for assessed data

```

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

```

-OK-

APP:@?

APP: @@

APP: @@ GO TO THE DICTRA MONITOR TO SET UP THE INITIAL STATE OF THE SPECIMEN

APP: @@

APP: go d-m

NO TIME STEP DEFINED

*** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE

DIC>

DIC> set-cond glob T 0 1173; * N

DIC>

DIC> @@

DIC> @@ SELECT A REFERENCE STATE FOR THE C ACTIVITY

DIC> @@

DIC> set-ref-state

Component: c

Reference state: graph

Temperature */: *

Pressure /100000/: 1e5

DIC>

DIC> @@

DIC> @@ ENTER A REGION, GRID, PHASE AND COMPOSITION

DIC> @@

```

DIC> enter-region
REGION NAME : steel
DIC>
DIC> enter-grid
REGION NAME : /STEEL/: steel
WIDTH OF REGION /1/: 3E-3
TYPE /LINEAR/: AUTO
DIC>
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /STEEL/: steel
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC> enter-composition
REGION NAME : /STEEL/: steel
PHASE NAME: /FCC_A1/: fcc#1
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: c
TYPE /LINEAR/: lin
VALUE OF FIRST POINT : 0.15
VALUE OF LAST POINT : /0.15/: 0.15
DIC>
DIC> @@
DIC> @@ NOW SET THE BOUNDARY CONDITIONS. WE ARE ONLY INTERESTED IN THE
DIC> @@ SURFACE REGION, FOR EXAMPLE IT IS SUFFICIENT TO SET CONDITIONS AT THE
DIC> @@ LOWER BOUNDARY.
DIC> @@
DIC>
DIC> @@
DIC> @@ Specify the activity flux function which controls the uptake of C.
DIC> @@
DIC> @@ The functions f and g and the parameter N has to be specified.
DIC> @@          k          k
DIC> @@
DIC> @@          N
DIC> @@ J V = f (variables)*(ACTIVITY -g (variables))      (1)
DIC> @@          k m k          k k
DIC> @@
DIC> @@ f and g in equation 1 is the mass-transfer coefficient and
DIC> @@          k          k
DIC> @@ the activity of k in the gas, respectively. ACTIVITY in eq. 1 means
DIC> @@ the actual activity of species k at the surface.
DIC> @@
DIC>
DIC> @@
DIC> @@ The main carburizing reaction for our atmosphere is:
DIC> @@
DIC> @@ CO + H  ->  C + H O      (I)
DIC> @@      2  <-  -      2
DIC> @@
DIC> @@ Following Sproge and Ågren (J. Heat Treating, v6, no 1, 1988 pp. 9-19)
DIC> @@ we calculate the mass-transfer coefficient for carbon, f in
DIC> @@ eq. 1 above by means of eq. 3, 4 and 12 in Sproge and Ågren's paper.
DIC> @@
DIC> @@
DIC> @@          A * K * P * sqrt( P )
DIC> @@          I   CO      H
DIC> @@          2
DIC> @@ f = ----- / gamma      (2)
DIC> @@          a + B * K * P * sqrt( P )
DIC> @@          C   I   CO      H
DIC> @@          2
DIC> @@
DIC> @@ K is the equilibrium constant for reaction (I)
DIC> @@ I
DIC> @@
DIC> @@ A and B are constants defined in Sproge and Ågren's paper. gamma
DIC> @@ is the activity coefficient for carbon in the steel.
DIC> @@
DIC> @@ Assume a constant value for P * sqrt( P ) = 0.14
DIC> @@          CO      H
DIC> @@          2
DIC> @@ The carbon activity in the gas is controlled by the partial
DIC> @@ pressure of water as can be understood from reaction (I).
DIC> @@
DIC> @@ Assume that the carbon activity, a of the gas is 0.64
DIC> @@          C
DIC> @@ which corresponds to a carburizing "carbon potential" of 0.85 wt%.
DIC> @@
DIC> @@ In this way we may calculate f to 8.25E-9 mol/s.
DIC> @@
DIC>
DIC> set-cond

GLOBAL OR BOUNDARY CONDITION /GLOBAL/: bound
BOUNDARY /LOWER/: lower
CONDITION TYPE /CLOSED_SYSTEM/: activity_flux_function
ENTER THE EXPRESSION AS:

          N
          J V = f (variables)*(ACTIVITY -g (variables))
          k m k          k k
          FLUX OF FCC_A1,C
LOW TIME LIMIT /0/: 0
f(T,P,TIME)= -8.25E-9;
HIGH TIME LIMIT /*/: *
ANY MORE RANGES /N/: N
N /1/: 1
LOW TIME LIMIT /0/: 0
g(T,P,TIME)= 0.64;
HIGH TIME LIMIT /*/: *
ANY MORE RANGES /N/: N
DIC>
DIC> @@
DIC> @@ SPECIFY A SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 18000
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /1800/:

```

```
INITIAL TIMESTEP : /1E-07/:  
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:  
DIC>  
DIC> @@  
DIC> @@ SAVE THE SET UP TO FILE  
DIC> @@  
DIC> Save exa5 Y  
DIC>  
DIC> set-inter  
--OK--  
DIC>
```

exa5-run

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa5\run.DCM"DIC>
DIC>
DIC> @@ exa5_run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING EXAMPLE a5
DIC> @@
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 0.00000E+00
*** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
DIC> read exa5
OK
DIC>
DIC> @@
DIC> @@ Start the simulation
DIC> @@
DIC> sim
Region: STEEL
single geometric dense at 0.0000
1.2176 101
U-FRACTION IN SYSTEM: C = .00698495916383109 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
U-FRACTION IN SYSTEM: C = .00698495916383109 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698495916398349 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 0.24659766E-05 DT = 0.23659766E-05 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698495916758908 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 0.71979297E-05 DT = 0.47319532E-05 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698495917479989 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 0.16661836E-04 DT = 0.94639063E-05 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698495918922068 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 0.35589649E-04 DT = 0.18927813E-04 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698495921806013 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 0.73445274E-04 DT = 0.37855625E-04 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698495927573319 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 0.14915652E-03 DT = 0.75711250E-04 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698495939106306 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 0.30057903E-03 DT = 0.15142250E-03 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0069849596216772 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 0.60342403E-03 DT = 0.30284500E-03 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698496008277711 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 0.12091140E-02 DT = 0.60569000E-03 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698496100461467 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 0.24204940E-02 DT = 0.12113800E-02 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698496284726693 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 0.48432541E-02 DT = 0.24227600E-02 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698496652968263 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 0.96887741E-02 DT = 0.48455200E-02 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698497388635673 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 0.19379814E-01 DT = 0.96910401E-02 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698498857668281 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 0.38761894E-01 DT = 0.19382080E-01 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698501789240894 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 0.77526054E-01 DT = 0.38764160E-01 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698507634097207 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 0.15505437 DT = 0.77528320E-01 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698519272377669 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 0.31011102 DT = 0.15505664 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698542404641377 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 0.62022430 DT = 0.31011328 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698588265674896 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 1.2404509 DT = 0.62022656 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698678864751836 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 1 seconds
TIME = 2.4809040 DT = 1.2404531 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698856957978377 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
```

```

TIME = 4.9618102 DT = 2.4809063 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0069920463860113 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 9.9236228 DT = 4.9618125 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00699876996632461 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 19.847248 DT = 9.9236250 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0070116060159071 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 39.694498 DT = 19.847250 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00703569376361486 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 79.388998 DT = 39.694500 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00707989462116314 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 158.77800 DT = 79.389000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00715874757109928 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 317.55600 DT = 158.77800 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00729474138750415 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 635.11200 DT = 317.55600 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00752054375503615 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 1270.2240 DT = 635.11200 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00788106518443645 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 2540.4480 DT = 1270.2240 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00843611780537184 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 4340.4480 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .009047102269993 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 6140.4480 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00955134567260647 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 7940.4480 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00999113675765163 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 1 seconds
TIME = 9740.4480 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0103863764716823 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 11540.448 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0107484090267409 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 13340.448 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0110844421240477 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 15140.448 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0113993948509805 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 16940.448 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0116968050295665 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 18000.000 DT = 1059.5520 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0118647499013449 FE = 1
TOTAL SIZE OF SYSTEM: .003 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 0.0000000
DELETING TIME-RECORD FOR TIME 0.10000000E-06
DELETING TIME-RECORD FOR TIME 0.24659766E-05
DELETING TIME-RECORD FOR TIME 0.71979297E-05
DELETING TIME-RECORD FOR TIME 0.16661836E-04
DELETING TIME-RECORD FOR TIME 0.35589649E-04
DELETING TIME-RECORD FOR TIME 0.73445274E-04
DELETING TIME-RECORD FOR TIME 0.14915652E-03
DELETING TIME-RECORD FOR TIME 0.30057903E-03
DELETING TIME-RECORD FOR TIME 0.60342403E-03
DELETING TIME-RECORD FOR TIME 0.12091140E-02
DELETING TIME-RECORD FOR TIME 0.24204940E-02
DELETING TIME-RECORD FOR TIME 0.48432541E-02
DELETING TIME-RECORD FOR TIME 0.96887741E-02
DELETING TIME-RECORD FOR TIME 0.19379814E-01
DELETING TIME-RECORD FOR TIME 0.38761894E-01
DELETING TIME-RECORD FOR TIME 0.77526054E-01
DELETING TIME-RECORD FOR TIME 0.15505437
DELETING TIME-RECORD FOR TIME 0.31011102
DELETING TIME-RECORD FOR TIME 0.62022430
DELETING TIME-RECORD FOR TIME 1.2404509
DELETING TIME-RECORD FOR TIME 2.4809040
DELETING TIME-RECORD FOR TIME 4.9618102
DELETING TIME-RECORD FOR TIME 9.9236228
DELETING TIME-RECORD FOR TIME 19.847248
DELETING TIME-RECORD FOR TIME 39.694498
DELETING TIME-RECORD FOR TIME 79.388998
DELETING TIME-RECORD FOR TIME 158.77800
DELETING TIME-RECORD FOR TIME 317.55600
DELETING TIME-RECORD FOR TIME 635.11200
DELETING TIME-RECORD FOR TIME 1270.2240
DELETING TIME-RECORD FOR TIME 2540.4480
DELETING TIME-RECORD FOR TIME 4340.4480
DELETING TIME-RECORD FOR TIME 6140.4480
DELETING TIME-RECORD FOR TIME 7940.4480
DELETING TIME-RECORD FOR TIME 9740.4480
DELETING TIME-RECORD FOR TIME 11540.448
DELETING TIME-RECORD FOR TIME 13340.448

```


DELETING TIME-RECORD FOR TIME 15140.448

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

TIMESTEP AT 18000.0000 SELECTED

DIC>

DIC> set-inter

--OK--

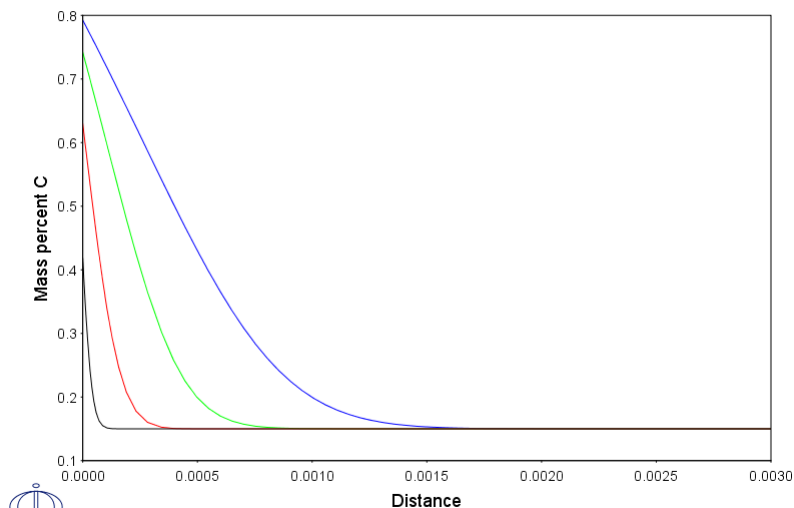
DIC>

exa5-plot

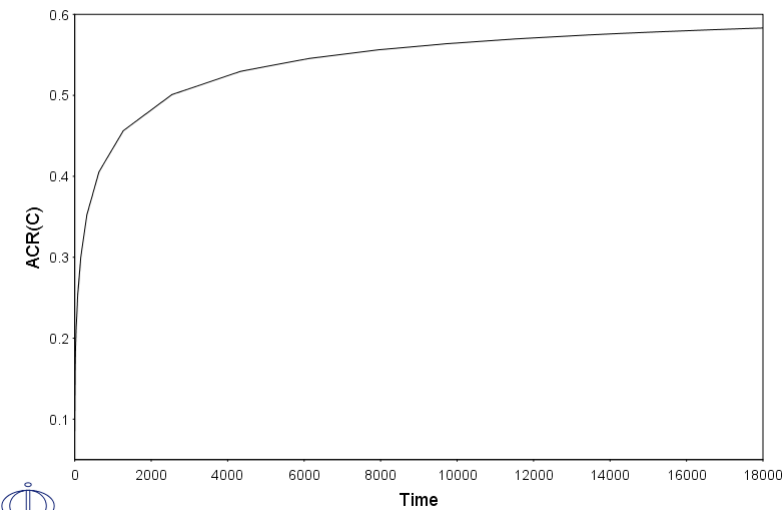
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa5\plot.DCM"DIC>
DIC>
DIC> @@ exa5_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE a5
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 1.80000E+04
*** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
DIC> read exa5
OK
DIC>
DIC> @@
DIC> @@ ENTER THE POST PROCESSOR
DIC> @@
DIC> post
```

POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson

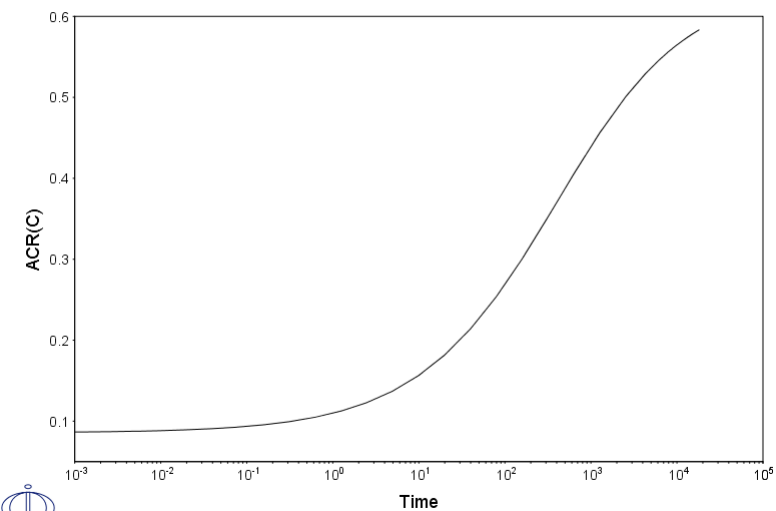
```
POST-1:
POST-1: @@
POST-1: @@ PLOT SOME DIFFERENT CONCENTRATION PROFILES
POST-1: @@
POST-1: s-d-a x dist glo
INFO: Distance is set as independent variable
POST-1: s-d-a y w-p c
POST-1: s-p-c time 100 1000 5000 18000
POST-1:
POST-1: plot
2018.02.18.18.41.57
Time=100,1000,5000,18000
CELL#1
```



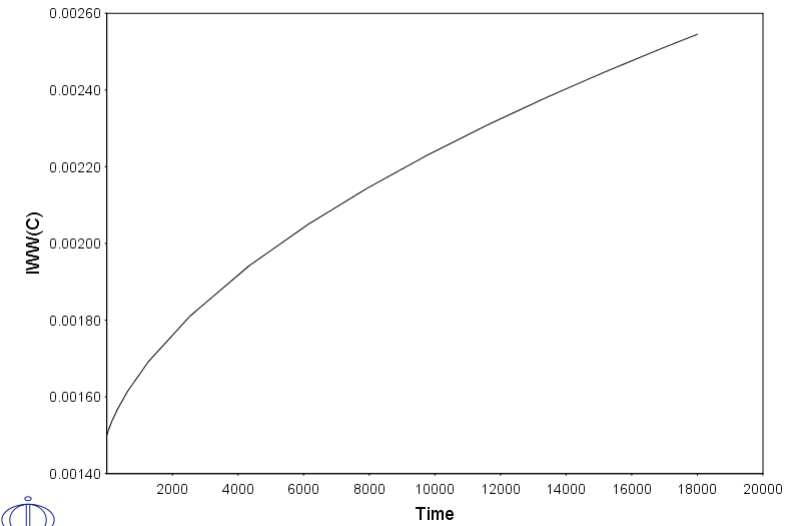
```
POST-1:
POST-1:
POST-1:
POST-1: @?<Hit_return_to_continue>
POST-1:
POST-1: @@
POST-1: @@ PLOT THE VARIATION OF THE C ACTIVITY AT THE SURFACE
POST-1: @@
POST-1: s-d-a y acr(c)
POST-1:
POST-1: s-d-a x time
INFO: Time is set as independent variable
POST-1:
POST-1: s-p-c
CONDITION /TIME/: interface
INTERFACE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



```
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: @@
POST-1: @@ USE A LOGARITHMIC SCALE ON THE X-AXIS
POST-1: @@
POST-1: set-axis-type
AXIS (X, Y OR Z) : x
AXIS TYPE /LINEAR/: logarithmic
POST-1:
POST-1: s-s-s x n 0.001 2e4
POST-1:
POST-1: plot
2018.02.18.18.41.58
"FIRST" INTERFACE OF SYSTEM
CELL #1
```



```
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: @@
POST-1: @@ PLOT THE AVERAGE WEIGHT FRACTION OF C IN THE SPECIMEN
POST-1: @@
POST-1: s-d-a y iww(c)
POST-1:
POST-1: set-ax-ty
AXIS (X, Y OR Z) : x
AXIS TYPE /LINEAR/: linear
POST-1:
POST-1: plot
```



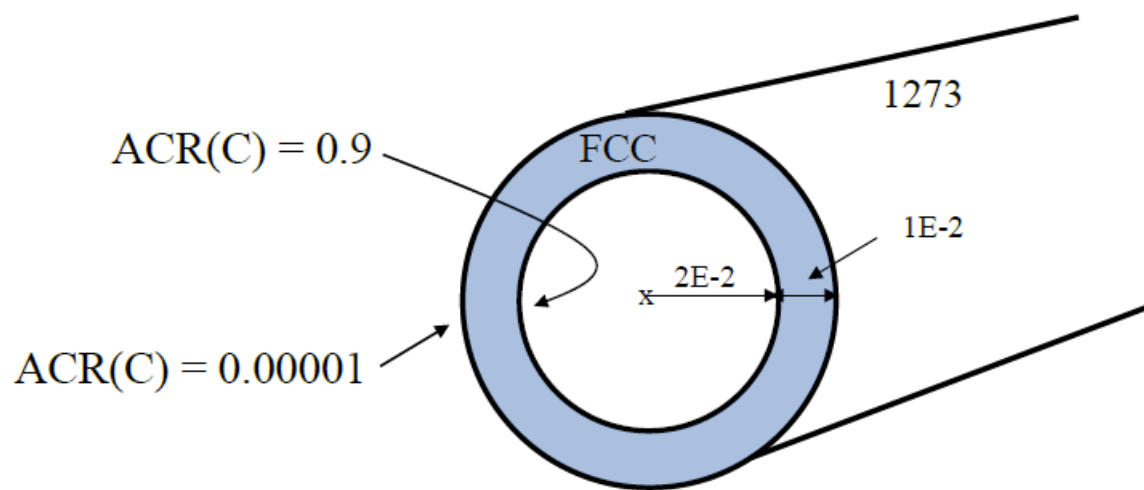
POST-1:
POST-1:
POST-1:
POST-1: @?<Hit_return_to_continue>
POST-1:
POST-1:
POST-1: set-inter
--OK--
POST-1:



Example exa6

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

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



exa6-setup

About Stockholm, Sweden

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

SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa6\setup.DCM"SYS: @@

SYS: @@ One-phase problem.

SYS: @@ Diffusion through a tube wall.

SYS: @@ A simple example about diffusion through a tube wall.

SYS: @@ The tube material is an Fe-0.6%Mn-0.7%Si-0.05%C alloy. On

SYS: @@ the inside wall a carbon activity of 0.9 is maintained whereas on

SYS: @@ the outside the C-activity is very low. This example demonstrates

SYS: @@ the use of the command SET-FIRST-INTERFACE as well as the MIXED

SYS: @@ boundary conditions.

SYS: -----

NO SUCH COMMAND, USE HELP

SYS:

SYS: @@ setup.DCM

SYS:

SYS:

SYS: @@

SYS: @@ GO TO THE DATABASE MODULE

SYS: @@

SYS: go da

THERMODYNAMIC DATABASE module

Current database: Steels/Fe-Alloys v9.0

VA /- DEFINED
L12_FCC B2_BCC DICTRA_FCC_A1
REJECTED

TDB_TCFE9:

TDB_TCFE9: @@

TDB_TCFE9: @@ USE THE TCFE DATABASE FOR THERMODYNAMIC DATA

TDB_TCFE9: @@

TDB_TCFE9: sw tcfe7

Current database: Steels/Fe-Alloys v7.0

VA DEFINED
L12_FCC B2_BCC B2_VACANCY
HIGH SIGMA DICTRA_FCC_A1 REJECTED

TDB_TCFE7: def-sys fe si mn c

FE SI MN

C DEFINED

TDB_TCFE7: rej ph * all

GAS:G LIQUID:L BCC_A2
FCC_A1 HCP_A3 DIAMOND_FCC_A4
GRAPHITE CEMENTITE M23C6
M7C3 M5C2 KSI_CARBIDE
A1_KAPPA KAPPA FE4N_LP1
FECN_CHI LAVES_PHASE_C14 M3SI
G_PHASE CR3SI FE2SI
MSI M5SI3 AL4C3
FE8SI2C SIC REJECTED

TDB_TCFE7: res ph fcc,grap
FCC_A1 GRAPHITE RESTORED

TDB_TCFE7: get

REINITIATING GES

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

FUNCTIONS

List of references for assessed data

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

-OK-

TDB_TCFE7:

TDB_TCFE7: @@

TDB_TCFE7: @@ SWITCH TO A MOBILITY DATABASE TO RETRIVE KINETIC DATA

TDB_TCFE7: @@

TDB_TCFE7: app

Use one of these databases

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

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

DATABASE NAME /TCFE7/: mobfe2

Current database: Steels/Fe-Alloys Mobility v2.0

TCS Steel Mobility Database Version 2.0 from 2011-12-09.

VA DEFINED

APP: def-sys fe si mn c

FE SI MN

C DEFINED

APP: rej ph * all

BCC_A2 CEMENTITE FCC_A1

FE4N_LP1 HCP_A3 LIQUID:L

REJECTED

APP: res ph fcc

FCC_A1 RESTORED

APP: get

ELEMENTS

SPECIES

PHASES

PARAMETERS ...
FUNCTIONS

List of references for assessed data

'This parameter has not been assessed'
'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'
'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
-Ni'
'Bae et al.: Z. Metallkunde 91(2000)672-674; fcc Fe-Mn
Mn-Ni'
'D. Bergner et al., Defect and Diffusion Forum 66-69(1989)409. Impurity
diffusion of Si in fcc Fe.'

-OK-

APP: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE PROBLEM IS SET UP
APP: @@
APP: go d-m
NO TIME STEP DEFINED
*** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
DIC>
DIC> @@
DIC> @@ ENTER GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 1273; * N

DIC>
DIC> @@
DIC> @@ SET THE REFERENCE STATE FOR CARBON
DIC> @@
DIC> set-ref C grap * 101325
DIC>
DIC> @@
DIC> @@ ENTER A REGION
DIC> @@
DIC> enter-region aus
DIC>
DIC> @@
DIC> @@ ENTER A DOUBLE GEOMETRIC GRID INTO THE REGION
DIC> @@
DIC> enter-grid
REGION NAME : /AUS/: aus
WIDTH OF REGION /1/: 1e-2
TYPE /LINEAR/: AUTO
DIC>
DIC> @@
DIC> @@ SET THE GEOMETRY (1 = CYLINDER)
DIC> @@
DIC> enter-geo
GEOMETRICAL EXPONENT /0/: 1
DIC>
DIC> @@
DIC> @@ SET THE FIRST INTERFACE => TUBE
DIC> @@
DIC> set-first-interface
COORDINATE FOR FIRST INTERFACE /0/: 2e-2
DIC>
DIC> @@
DIC> @@ ENTER AN active PHASE IN THE REGION
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /AUS/: aus
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc_al#1
DIC>
DIC> @@
DIC> @@ ENTER INITIAL COMPOSITIONS INTO THE PHASE
DIC> @@
DIC> enter-composition
REGION NAME : /AUS/: aus
PHASE NAME: /FCC A1/: fcc#1
DEPENDENT COMPONENT ? /SI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: si lin 0.7 0.7
PROFILE FOR /MN/: mn lin 0.6 0.6
PROFILE FOR /SI/: c lin 5e-2 5e-2
DIC>
DIC> @@
DIC> @@ SET THE BOUNDARY CONDITIONS ON BOTH THE LOWER AND UPPER PART OF THE REGION
DIC> @@
DIC> @@ USE MIXED CONDITIONS: AN ACTIVITY CONDITION FOR C AND CLOSED
DIC> @@ SYSTEMS FOR MN AND SI.
DIC> @@
DIC> set-cond

GLOBAL OR BOUNDARY CONDITION /GLOBAL/: boundary
BOUNDARY /LOWER/: lower
CONDITION TYPE /CLOSED_SYSTEM/: mixed
Dependent substitutional element:FE
Dependent interstitial element:VA
TYPE OF CONDITION FOR COMPONENT C /ZERO_FLUX/: activity
LOW TIME LIMIT /0/: 0
ACR(C)(TIME)= 0.9;
HIGH TIME LIMIT /*/: *
ANY MORE RANGES /N/: N
TYPE OF CONDITION FOR COMPONENT MN /ZERO_FLUX/: zero_flux
TYPE OF CONDITION FOR COMPONENT SI /ZERO_FLUX/: zero_flux
DIC>
DIC> set-cond

GLOBAL OR BOUNDARY CONDITION /GLOBAL/: boundary
BOUNDARY /UPPER/: upper
CONDITION TYPE /CLOSED_SYSTEM/: mixed
Dependent substitutional element:FE
Dependent interstitial element:VA
TYPE OF CONDITION FOR COMPONENT C /ZERO_FLUX/: activity
LOW TIME LIMIT /0/: 0
ACR(C)(TIME)= 1e-5;
HIGH TIME LIMIT /*/: *


```
ANY MORE RANGES /N/: N
TYPE OF CONDITION FOR COMPONENT MN /ZERO_FLUX/: zero_flux
TYPE OF CONDITION FOR COMPONENT SI /ZERO_FLUX/: zero_flux
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 1e9
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /100000000/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC> @@
DIC> @@ SAVE TO FILE
DIC> @@
DIC> save exa6 y
DIC>
DIC> set-inter
--OK--
DIC>
```

exa6-run

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa6\run.DCM"DIC>
DIC>
DIC> @@ run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING exa6
DIC> @@
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 0.00000E+00
*** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
DIC> read exa6
OK
DIC>
DIC> @@
DIC> @@ Start the simulation
DIC> @@
DIC> simulate
Region: AUS
double geometric
dense at outer boundaries, coarse at 0.50000E-02
lower part 1.2500 22
upper part 0.80000 22
U-FRACTION IN SYSTEM: C = .00115488575879621 FE = .490055682684517
MN = .00302988813183617 SI = .00691442924890045
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
U-FRACTION IN SYSTEM: C = .00115488575879621 FE = .490055682684517
MN = .00302988813183617 SI = .00691442924890045
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .001168232207708 FE = .490055682684517
MN = .00302988813183617 SI = .00691442924890045
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds
TIME = 0.10010000E-03 DT = 0.10000000E-03 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00116829562757795 FE = .490055682684517
MN = .00302988813183617 SI = .00691442924889595
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds
TIME = 3.0557506 DT = 3.0556505 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00118960627023709 FE = .490055682684521
MN = .00302988813183657 SI = .00691442924889595
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds
TIME = 9.1670515 DT = 6.1113009 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00121114065253319 FE = .490055682684524
MN = .00302988813183688 SI = .00691442924889252
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds
TIME = 21.389653 DT = 12.222602 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00123894224179207 FE = .490055682684528
MN = .00302988813183725 SI = .00691442924888855
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 1 seconds
TIME = 45.834857 DT = 24.445204 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00127675531962732 FE = .490055682684532
MN = .00302988813183768 SI = .00691442924888393
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds
TIME = 94.725265 DT = 48.890408 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00132929244094337 FE = .490055682684536
MN = .00302988813183816 SI = .0069144292488789
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds
TIME = 192.50608 DT = 97.780815 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00140301692405163 FE = .490055682684541
MN = .00302988813183861 SI = .00691442924887446
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds
TIME = 388.06771 DT = 195.56163 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00150699028673373 FE = .490055682684541
MN = .0030298881318388 SI = .00691442924887331
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds
TIME = 779.19097 DT = 391.12326 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00165403563506009 FE = .490055682684533
MN = .00302988813183819 SI = .00691442924888217
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 1 seconds
TIME = 1561.4375 DT = 782.24652 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00186239344623103 FE = .49005568268452
MN = .00302988813183713 SI = .00691442924889648
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds
TIME = 3125.9305 DT = 1564.4930 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00215807121249969 FE = .490055682684546
MN = .00302988813183974 SI = .00691442924886796
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds
TIME = 6254.9166 DT = 3128.9861 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00257823536978672 FE = .490055682684616
MN = .00302988813184698 SI = .00691442924879113
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds
TIME = 12512.889 DT = 6257.9722 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00317699718807945 FE = .490055682684705
MN = .0030298881318573 SI = .00691442924869157
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds
TIME = 25028.833 DT = 12515.944 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00403336961093126 FE = .490055682684793
MN = .00302988813186931 SI = .00691442924859118
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 1 seconds
TIME = 50060.722 DT = 25031.889 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00526363637174368 FE = .490055682684873
MN = .00302988813188164 SI = .00691442924849893
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds
```

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

output ignored...

... output resumed

```
CPU time used in timestep 1 seconds
TIME = 1602037.8 DT = 801020.44 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0165218937291276 FE = .490055682687136
MN = .00302988813210615 SI = .00691442924601151
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds
TIME = 3070759.8 DT = 1468722.0 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0165306302137249 FE = .490055682689487
MN = .00302988813231524 SI = .00691442924345072
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds
TIME = 5520081.8 DT = 2449321.9 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0165307407276147 FE = .49005568269412
MN = .00302988813270145 SI = .0069144292384322
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 1 seconds
TIME = 9712140.3 DT = 4192058.5 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0165306049407457 FE = .49005568270373
MN = .00302988813346508 SI = .00691442922805808
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds
TIME = 17804358. DT = 8092217.5 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0165302884173806 FE = .490055682726962
MN = .00302988813524102 SI = .00691442920305048
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 1 seconds
TIME = 33988793. DT = 16184435. SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0165299095291916 FE = .490055682786251
MN = .00302988813967787 SI = .00691442913932503
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds
TIME = 66357663. DT = 32368870. SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0165296370794655 FE = .490055682925557
MN = .00302988815056947 SI = .00691442898912743
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds
TIME = 0.13109540E+09 DT = 64737740. SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0165297311657981 FE = .490055683202508
MN = .00302988817529088 SI = .0069144286874545
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 1 seconds
TIME = 0.23051887E+09 DT = 99423470. SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0165316513851906 FE = .490055683573445
MN = .0030298882136918 SI = .00691442827811698
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds
TIME = 0.33003492E+09 DT = 99516053. SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0165355763010635 FE = .49005568389079
MN = .00302988824987424 SI = .0069144279245888
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 1 seconds
TIME = 0.42961658E+09 DT = 99581650. SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0165388724264922 FE = .490055684170609
MN = .00302988828351862 SI = .00691442761112566
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds
TIME = 0.52925282E+09 DT = 99636240. SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0165418605270749 FE = .490055684422996
MN = .00302988831490655 SI = .00691442732735122
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds
TIME = 0.62893535E+09 DT = 99682537. SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0165446599910542 FE = .490055684654308
MN = .00302988834435435 SI = .00691442706659145
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 1 seconds
TIME = 0.72865867E+09 DT = 99723322. SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0165473274287305 FE = .490055684868825
MN = .00302988837213727 SI = .00691442682429134
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds
TIME = 0.82841842E+09 DT = 99759750. SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0165498943962927 FE = .490055685069575
MN = .00302988839848144 SI = .00691442659719764
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 1 seconds
TIME = 0.92821105E+09 DT = 99792624. SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0165523804304784 FE = .490055685258784
MN = .00302988842357088 SI = .00691442638289816
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 0 seconds
TIME = 0.98981461E+09 DT = 61603559. SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0165550594430682 FE = .490055685370543
MN = .00302988843849379 SI = .0069144262562169
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
CPU time used in timestep 1 seconds
TIME = 0.10000000E+10 DT = 10185394. SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0165567958948894 FE = .490055685388685
MN = .00302988844092304 SI = .00691442623564514
TOTAL SIZE OF SYSTEM: .00314159265359 [m^2]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
```

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

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

```
TIMESTEP AT      0.100000000E+10 SELECTED
```

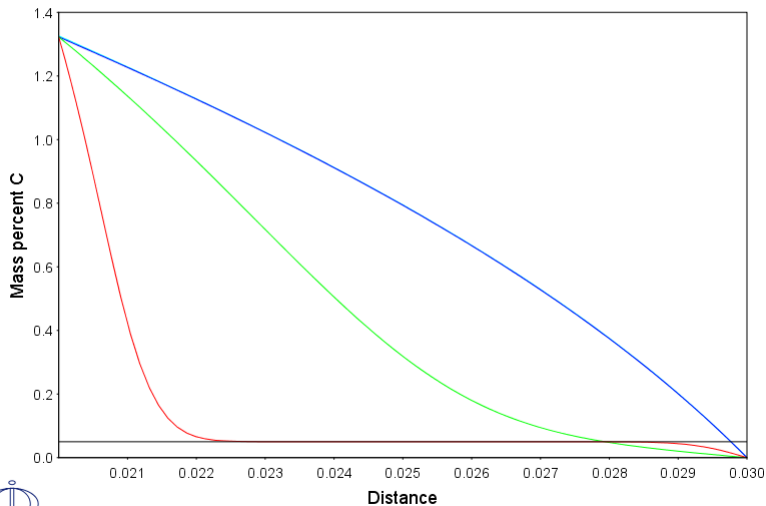
```
DIC>
DIC> @@
DIC> @@ THE SIMULATION IS FINISHED
DIC> @@
DIC>
DIC> set-inter
--OK--
DIC>
```

exa6-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa6\plot.DCM"DIC>
DIC>
DIC> @@ exa6_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE exa6
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 1.00000E+09
*** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
DIC> read exa6
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
```

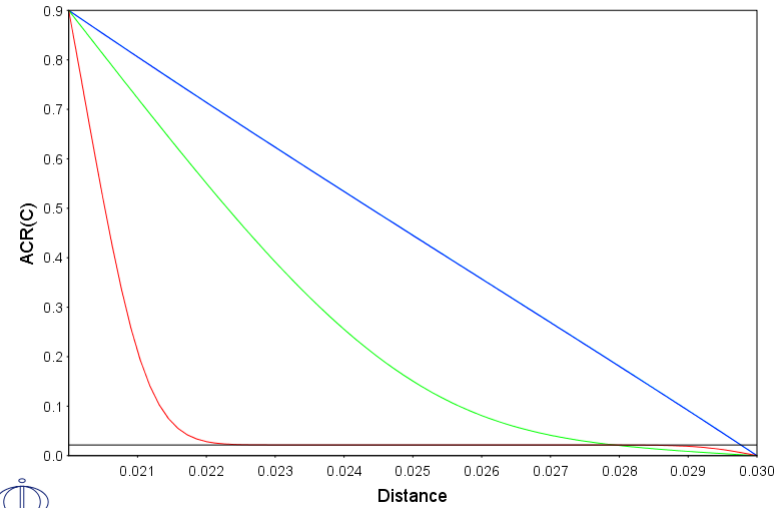
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson

```
POST-1:
POST-1:
POST-1: @@
POST-1: @@ PLOT THE CONCENTRATION OF C AT DIFFERENT TIMES
POST-1: @@
POST-1: s-d-a x distance global
INFO: Distance is set as independent variable
POST-1: s-d-a y w-p c
POST-1: s-p-c time 0,1e4,2e5,1e7,1e9
POST-1:
POST-1: plot
2018.02.18.18.45.13
Time=0,10000,200000,1E+07,1E+09
CELL #1
```

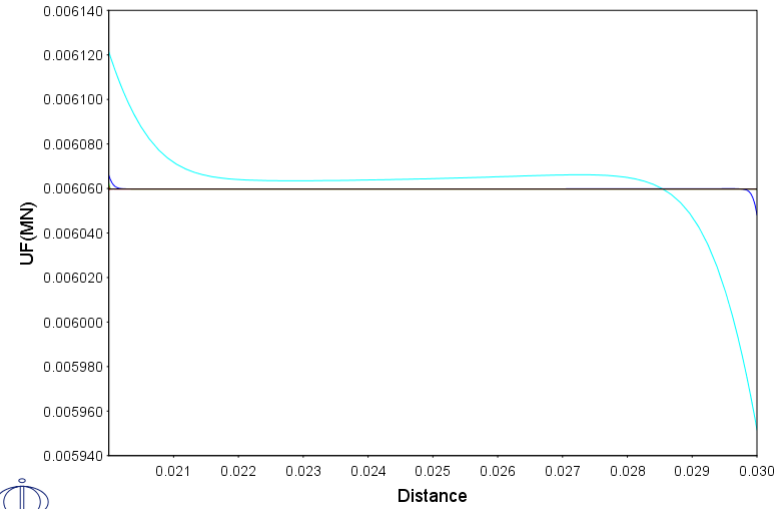


```
POST-1:
POST-1:
POST-1: Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ PLOT THE ACTIVITY OF C
POST-1: @@
POST-1:
POST-1: s-d-a y acr(c)
POST-1:
POST-1: plot
```

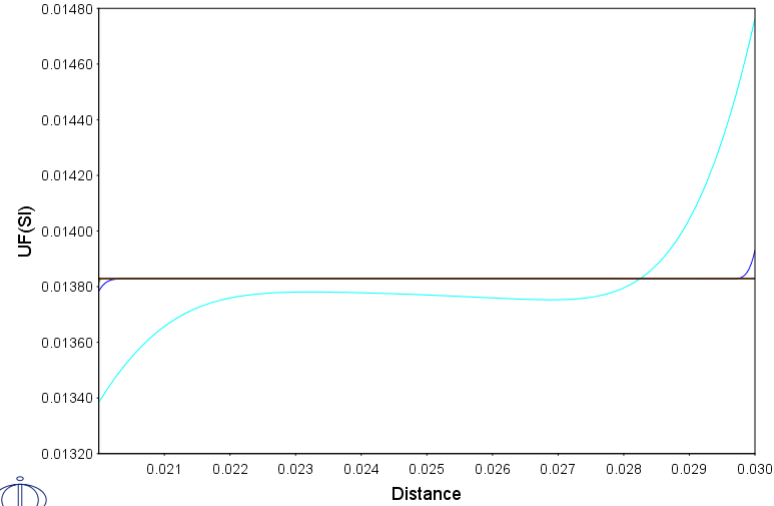
2018.02.18.18.45.15
Time = 0,10000,200000,1E+07,1E+09
CELL #1



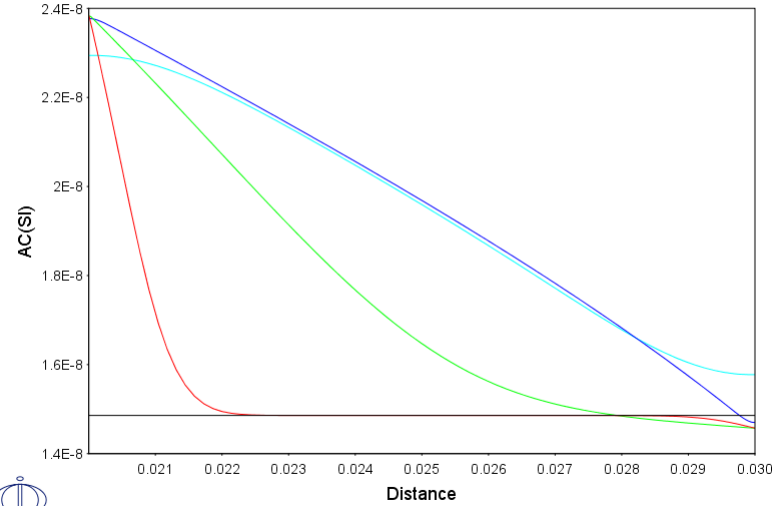
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ LET US LOOK AT THE MN AND SI PROFILES
POST-1: @@
POST-1: @@ WE PLOT THE U-FRACTION OF MN AND SI WHICH WILL BE INDEPENDENT
POST-1: @@ OF THE C-CONCENTRATION.
POST-1: @@
POST-1: s-d-a y u-f mn
POST-1:
POST-1: plot
2018.02.18.18.45.16
Time = 0,10000,200000,1E+07,1E+09
CELL #1



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



```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ FINALLY, LOOK AT THE ACTIVITY PROFILES OF SI
POST-1: @@
POST-1: s-d-a y ac(si)
POST-1:
POST-1: plot
2018.02.18.18.45.18
Time = 0.10000,200000.1E+07,1E+09
CELL #1
```



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

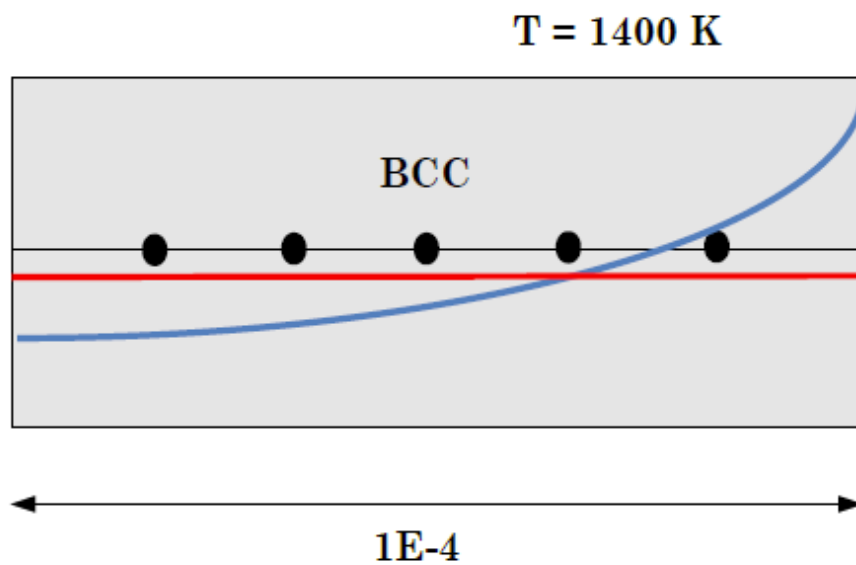


Example exa7

Homogenization heat-treatment

(Initial profile imported from Scheil simulation)

The initial segregation profile is created from a Scheil calculation (see macro `create_initial_profile.TCM`). The command `INPUT_SCHEIL_PROFILE` in the DICTRA monitor performs most of the setup. Only time and temperature must be entered after the `INPUT_SCHEIL_PROFILE` command is executed.



exa7-setup

About Stockholm, Sweden

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

SYS: **SYS:MACRO** "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa7\setup.DCM" @@ One phase example.

SYS: @@ Homogenization heat treatment

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

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

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

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

SYS: @@ INPUT_SCHEIL_PROFILE command is executed.

SYS: -----

NO SUCH COMMAND, USE HELP

SYS:

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

SYS: go da

THERMODYNAMIC DATABASE module

Current database: Steels/Fe-Alloys v9.0

VA /- DEFINED
L12_FCC B2_BCC DICTRA_FCC_A1
REJECTED

TDB_TCFE9: sw FEDEMO

Current database: Iron Demo Database v2.0

VA /- DEFINED

TDB_FEDEMO: def-sys fe cr ni mn

FE CR NI

MN DEFINED

TDB_FEDEMO: rej ph *

LIQUID:L BCC_A2 CHI_A12

DIAMOND_FCC_A4 FCC_A1 HCP_A3

LAVES_PHASE_C14 SIGMA REJECTED

TDB_FEDEMO: rest ph bcc

BCC_A2 RESTORED

TDB_FEDEMO: get

REINITIATING GES

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

FUNCTIONS

List of references for assessed data

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

-OK-

TDB_FEDEMO:

TDB_FEDEMO: app MFEDEMO

Current database: Fe-Alloys Mobility demo database v2.0

VA DEFINED

APP: def-sys fe cr ni mn

FE CR NI

MN DEFINED

APP: rej ph *

BCC_A2 FCC_A1 REJECTED

APP: rest ph bcc

BCC_A2 RESTORED

APP: get

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

FUNCTIONS

List of references for assessed data

'This parameter has not been assessed'
'B. Jonsson: ISIJ International, 35(1995)1415-1421; Cr, Fe and Ni diffusion bcc Cr-Fe-Ni'
'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion in bcc Fe'
'Assessed from data presented in Landholt-Bornstein, Vol. 26, ed. H. Mehrer, springer (1990); Impurity diff of Mn in bcc Fe.'

-OK-

APP:

APP: go dict-mon

NO TIME STEP DEFINED

DIC>

DIC>

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

DIC> input_scheil_profile

INFO: SCHEIL_REGION CREATED

FILE NAME /XF.TXT/: segregation_profile.TXT

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

INFO: LINEAR GRID IN SCHEIL_REGION ENTERED WITH 100 GRID POINTS

ENTER MAIN SOLID SOLUTION PHASE

PHASE NAME: bcc#1

INFO: COMPOSITION PROFILE ENTERED IN REGION

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

INFO: TO COMPLETE SETUP, ENTER TEMPERATURE AND

```
SIMULATION TIME
DIC>
DIC>
DIC> @@ ENTER THE HEAT TREATMENT TEMPERATURE
DIC> s-cond

GLOBAL OR BOUNDARY CONDITION /GLOBAL/: glob
VARIABLE : t
LOW TIME LIMIT /0/: 0 1473; * n
DIC>
DIC>
DIC> @@ ENTER A SIMULATION TIME
DIC> se-si-ti
END TIME FOR INTEGRATION /.1/: 3600
AUTOMATIC TIMESTEP CONTROL /YES/: y
MAX TIMESTEP DURING INTEGRATION /360/: 360
INITIAL TIMESTEP : /1E-07/: 1e-7
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/: 1e-9
DIC>
DIC>
DIC> save exa7 y
DIC>
DIC> set-inter
--OK--
DIC>
```

exa7-run

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa7\run.DCM"DIC> go dict-mon
TIME STEP AT TIME 0.00000E+00
DIC>
DIC> read exa7
OK
DIC>
DIC> sim
U-FRACTION IN SYSTEM: CR = .180420497424242 FE = .796498787878788
MN = .00999016878282829 NI = .0130905459141414
TOTAL SIZE OF SYSTEM: 1E-04 [m]
U-FRACTION IN SYSTEM: CR = .180420497424242 FE = .796498787878788
MN = .00999016878282829 NI = .0130905459141414
TOTAL SIZE OF SYSTEM: 1E-04 [m]
TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .180420497424242 FE = .796498787878787
MN = .00999016878282828 NI = .0130905459141415
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.10010000E-03 DT = 0.10000000E-03 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .180420497424243 FE = .796498787878788
MN = .00999016878282829 NI = .0130905459141415
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.41908397 DT = 0.41898387 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .180420497424242 FE = .796498787878788
MN = .0099901687828279 NI = .0130905459141419
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 1.2570517 DT = 0.83796774 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .180420497424242 FE = .796498787878788
MN = .0099901687828279 NI = .0130905459141418
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 2.9329872 DT = 1.6759355 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .180420497424243 FE = .796498787878789
MN = .00999016878282889 NI = .0130905459141397
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 1 seconds
TIME = 6.2848581 DT = 3.3518710 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .180420497424257 FE = .796498787878809
MN = .00999016878284567 NI = .0130905459140889
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 12.988600 DT = 6.7037419 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .180420497424302 FE = .796498787878888
MN = .0099901687828762 NI = .0130905459139341
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 26.396084 DT = 13.407484 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .180420497424318 FE = .796498787878861
MN = .0099901687829013 NI = .0130905459139194
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 53.211052 DT = 26.814968 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .180420497424435 FE = .796498787878771
MN = .00999016878299364 NI = .0130905459138002
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 106.84099 DT = 53.629935 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .180420497424575 FE = .796498787878385
MN = .00999016878336974 NI = .0130905459136702
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 1 seconds
TIME = 214.10086 DT = 107.25987 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .180420497424432 FE = .796498787878199
MN = .00999016878339541 NI = .0130905459139735
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 428.62060 DT = 214.51974 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .18042049742409 FE = .7964987877756
MN = .00999016878350895 NI = .0130905459146442
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 788.62060 DT = 360.00000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .180420497424077 FE = .796498787877899
MN = .00999016878346233 NI = .0130905459145616
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 1148.6206 DT = 360.00000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .180420497423613 FE = .796498787877388
MN = .00999016878332526 NI = .0130905459156739
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 1 seconds
TIME = 1508.6206 DT = 360.00000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .180420497423265 FE = .796498787877026
MN = .0099901687831702 NI = .0130905459165386
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 1868.6206 DT = 360.00000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .180420497422966 FE = .796498787875233
MN = .00999016878344972 NI = .0130905459183517
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 2228.6206 DT = 360.00000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .180420497422686 FE = .79649878787269
MN = .00999016878399045 NI = .0130905459206335
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 2588.6206 DT = 360.00000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .180420497422472 FE = .796498787870928
MN = .00999016878437055 NI = .0130905459222304
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 2948.6206 DT = 360.00000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .180420497422317 FE = .796498787869701
MN = .00999016878464137 NI = .0130905459233406
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 3308.6206 DT = 360.00000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .180420497422203 FE = .796498787868854
MN = .00999016878483073 NI = .0130905459241122
TOTAL SIZE OF SYSTEM: 1E-04 [m]
```

```
CPU time used in timestep          1 seconds
TIME = 3600.0000    DT = 291.37940    SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .180420497422138  FE = .796498787868426
MN = .00999016878491876  NI = .0130905459245169
TOTAL SIZE OF SYSTEM: 1E-04 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME      0.0000000
DELETING TIME-RECORD FOR TIME      0.10000000E-06
DELETING TIME-RECORD FOR TIME      0.10010000E-03
DELETING TIME-RECORD FOR TIME      0.41908397
DELETING TIME-RECORD FOR TIME      1.2570517
DELETING TIME-RECORD FOR TIME      2.9329872
DELETING TIME-RECORD FOR TIME      6.2848581
DELETING TIME-RECORD FOR TIME      12.988600
DELETING TIME-RECORD FOR TIME      26.396084
DELETING TIME-RECORD FOR TIME      53.211052
DELETING TIME-RECORD FOR TIME      106.84099
DELETING TIME-RECORD FOR TIME      214.10086
DELETING TIME-RECORD FOR TIME      428.62060
DELETING TIME-RECORD FOR TIME      788.62060
DELETING TIME-RECORD FOR TIME      1148.6206
DELETING TIME-RECORD FOR TIME      1508.6206
DELETING TIME-RECORD FOR TIME      1868.6206
DELETING TIME-RECORD FOR TIME      2228.6206
DELETING TIME-RECORD FOR TIME      2588.6206
DELETING TIME-RECORD FOR TIME      2948.6206

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

TIMESTEP AT      3600.00000    SELECTED
```

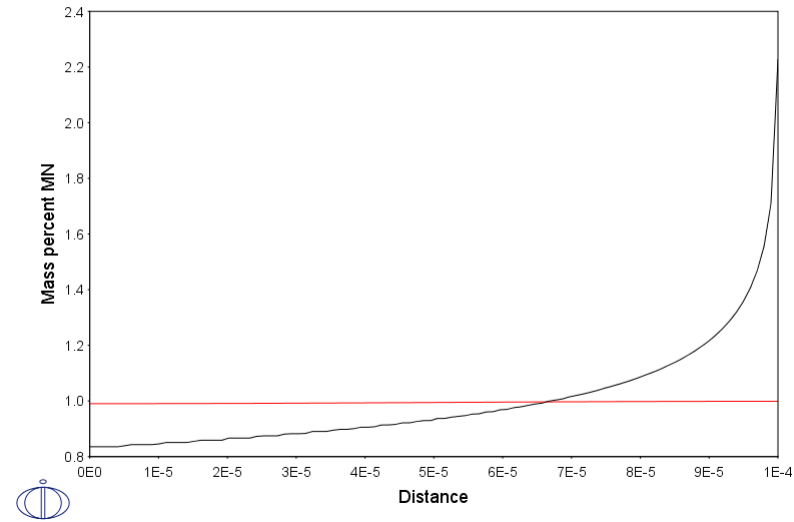
```
DIC>
DIC> set-inter
--OK--
DIC>
```

exa7-plot

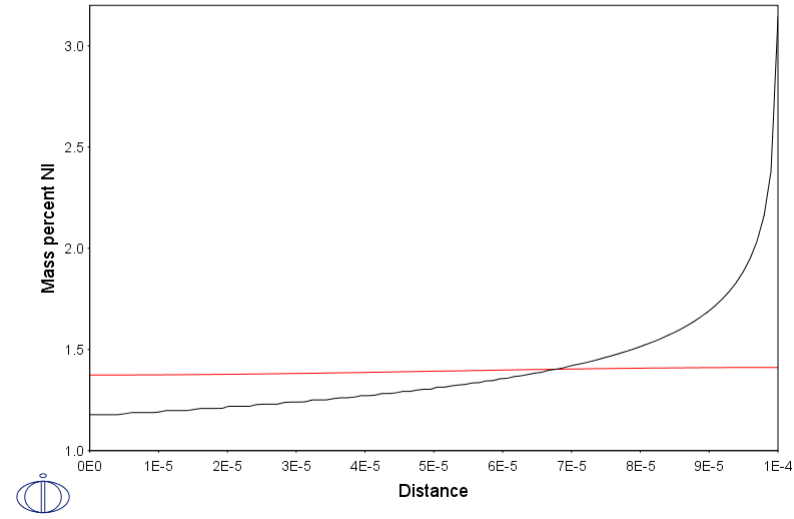
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exa7\plot.DCM"DIC> go dict-mon
TIME STEP AT TIME 3.60000E+03
DIC>
DIC> read exa7
OK
DIC>
DIC> post

POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson

POST-1:
POST-1: s-p-c time 0,3600
POST-1: s-d-a x d g
INFO: Distance is set as independent variable
POST-1: s-d-a y w-p mn
POST-1: plot
2018.02.18.18.48.22
Time=0,3600
CELL #1
```



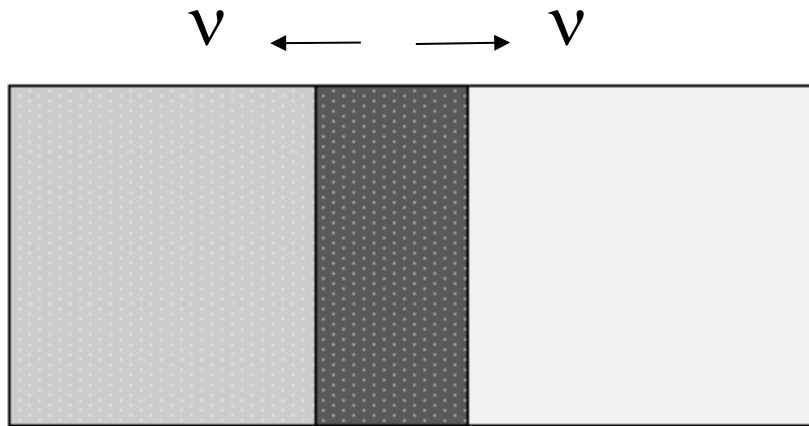
```
POST-1:
POST-1: @@ Hit enter for the next plot
POST-1:e?
POST-1:
POST-1: s-d-a y w-p ni
POST-1: plot
2018.02.18.18.48.22
Time=0,3600
CELL #1
```



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



Moving Boundary Problems



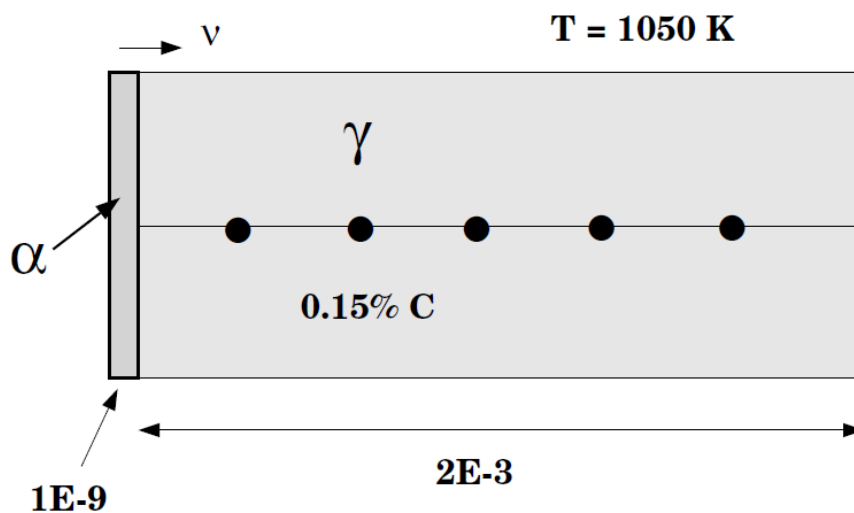
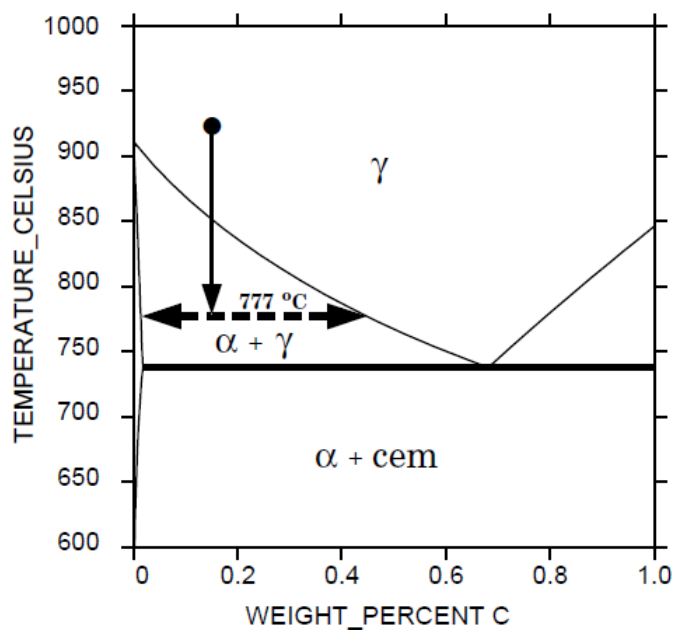


Example exb1a

γ to α transformation in a binary Fe-C alloy

This example calculates a ferrite (BCC)/austenite (FCC) transformation in a binary Fe-C alloy. The initial state is an austenite of 2 mm thickness. The composition of the austenite is Fe-0.15wt%C. After austenitization the specimen has been quenched down to 1050K. The system is assumed closed, no boundary conditions are set (a closed system is the default). Ferrite is expected to grow into the austenite. For this reason you start with a thin region with ferrite adjacent to the austenite.

Fe - C Phase diagram



exbla-setup

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

```
SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exbla\setup.DCM" @@
SYS: @@ Moving boundary problem.
SYS: @@ Austenite to ferrite transformation in a binary Fe-C alloy
SYS: @@ This example calculates a ferrite(BCC)/austenite(FCC)transformation
SYS: @@ in a binary Fe-C alloy. The initial state is an austenite of 2mm
SYS: @@ thickness. The composition of the austenite is Fe-0.15wt%C.
SYS: @@
SYS: @@ After austenitization the specimen is quenched down to 1050K.
SYS: @@ The system is assumed closed, so no boundary conditions are set
SYS: @@ (a closed system is the default). Ferrite is expected to grow
SYS: @@ into the austenite, which is why we start with a thin
SYS: @@ region with ferrite adjacent to the austenite.
SYS: -----
NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exbla_setup.DCM
SYS:
SYS:
SYS: @@
SYS: @@ START BY GOING TO THE DATABASE MODULE
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Current database: Steels/Fe-Alloys v9.0

VA                /-  DEFINED
L12_FCC            B2_BCC                DICTRA_FCC_A1
REJECTED

TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE THE DATA
TDB_TCFE9: @@
TDB_TCFE9: sw FEDEMO
Current database: Iron Demo Database v2.0

VA                /-  DEFINED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ DEFINE THE SYSTEM TO WORK WITH
TDB_FEDEMO: @@
TDB_FEDEMO: def-sys fe c
FE                C  DEFINED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ EXCLUDE THE THERMODYNAMIC DATA FOR THE PHASES THAT ARE NOT NEEDED
TDB_FEDEMO: @@
TDB_FEDEMO: rej ph * all
GAS:G             LIQUID:L                BCC_A2
CEMENTITE          DIAMOND_FCC_A4          FCC_A1
GRAPHITE           HCP_A3                 KSI_CARBIDE
LAVES_PHASE_C14    M23C6                  M5C2
M7C3 REJECTED
TDB_FEDEMO: res ph fcc bcc
FCC_A1            BCC_A2  RESTORED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ RETRIEVE DATA FROM THE DATABASE FILE
TDB_FEDEMO: @@
TDB_FEDEMO: get
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

List of references for assessed data

'P. Franke, Estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-Fe'
'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
volumes'
'X.-G. Lu, M. Selleby, B. Sundman, CALPHAD, 29 (2005) 49-55; Fe P-T diagram'
'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
-OK-
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ MOBILITY/DIFFUSIVITY DATA ARE STORED IN A SEPARATE DATABASE FILE.
TDB_FEDEMO: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE DATA
TDB_FEDEMO: @@
TDB_FEDEMO: append
Use one of these databases

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


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

DATABASE NAME /FEDEMO/: MFEDEMO

Current database: Fe-Alloys Mobility demo database v2.0

```

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

List of references for assessed data

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

```

'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
-Ni'
'B. Jonsson: Z. Metallkunde 85(1994)498-501; C and N diffusion in bcc Cr
-Fe-Ni'
'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
in bcc Fe'

-OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP
APP: @@
APP: go d-m
NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER GLOBAL CONDITION T
DIC> @@
DIC> set-condition global T 0 1050; * N

DIC>
DIC> @@
DIC> @@ START BY ENTERING THE REGIONS ferrite AND austenite WHERE WE
DIC> @@ PUT THE BCC AND FCC PHASE, RESPECTIVELY. THE FERRITE REGION IS
DIC> @@ ASSUMED INITIALLY TO BE VERY THIN, 1E-9 METERS.
DIC> @@
DIC> enter-region
REGION NAME : ferrite
DIC>
DIC> enter-region
REGION NAME : austenite
ATTACH TO REGION NAMED /FERRITE/:
ATTACHED TO THE RIGHT OF FERRITE /YES/:
DIC>
DIC> @@
DIC> @@ ENTER GRIDS INTO THE REGIONS
DIC> @@
DIC> enter-grid
REGION NAME : /FERRITE/: ferrite
WIDTH OF REGION /1/: 1e-9
TYPE /LINEAR/: AUTO
DIC>
DIC> enter-grid austenite
WIDTH OF REGION /1/: 20e-4
TYPE /LINEAR/: AUTO
DIC>
DIC> @@
DIC> @@ ENTER active PHASES INTO THE REGIONS
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /FERRITE/: ferrite
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: bcc
DIC>
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /AUSTENITE/: austenite
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ ENTER AN INITIAL COMPOSITION INTO BCC
DIC> @@
DIC> enter-composition
REGION NAME : /FERRITE/: ferrite
PHASE NAME: /BCC_A2/: bcc
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: C
TYPE /LINEAR/: linear
VALUE OF FIRST POINT : 0.01
VALUE OF LAST POINT : /1E-2/: 0.01
DIC>
DIC> @@
DIC> @@ ENTER AN INITIAL COMPOSITION INTO FCC
DIC> @@
DIC> enter-composition
REGION NAME : /AUSTENITE/: austenite
PHASE NAME: /FCC_A1/: fcc#1
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: C
TYPE /LINEAR/: linear
VALUE OF FIRST POINT : 0.15
VALUE OF LAST POINT : /0.15/: 0.15
DIC>
DIC> @@
DIC> @@ THE BOUNDARY CONDITION IS A CLOSED SYSTEM AS WE DO NOT SPECIFY
DIC> @@ ANYTHING ELSE
DIC> @@
DIC>
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 1e9
AUTOMATIC TIMESTEP CONTROL /YES/: YES
MAX TIMESTEP DURING INTEGRATION /100000000/: 1e8
INITIAL TIMESTEP : /1E-07/: 1E-5
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/: 1E-5
DIC>
DIC>
DIC> @@
DIC> @@ IMPLICIT (1) TIME INTEGRATION IS USED INSTEAD OF THE MORE ACCURATE
DIC> @@ (BUT LESS STABLE) TRAPETZOIDAL METHOD WHICH IS THE DEFAULT.
DIC> @@
DIC> s-s-c
NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDF: /2/:

```

```
CHECK INTERFACE POSITION /NO/:
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPLICIT WHEN INTEGRATING PDEs (0 -> 0.5 -> 1): /.5/: 1.0
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /NO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/:
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exbla Y
DIC>
DIC> set-inter
--OK--
DIC>
```

exbla-run

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exbla\run.DCM"DIC>
DIC>
DIC> @@ exbla_run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING EXAMPLE bla
DIC> @@
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 0.00000E+00
DIC> read exbla
OK
DIC>
DIC> @@
DIC> @@ START THE SIMULATION
DIC> @@
DIC> simulate
Region: FERRITE
single geometric dense at 0.10000E-08
1.0000 24
Region: AUSTENITE
single geometric dense at 0.0000
1.1762 99
Trying old scheme 3
U-FRACTION IN SYSTEM: C = .00698495590385911 FE = 1
TOTAL SIZE OF SYSTEM: .002000001 [m]
U-FRACTION IN SYSTEM: C = .00698495590385911 FE = 1
TOTAL SIZE OF SYSTEM: .002000001 [m]
3.981486698393685E-005 3.982285206222398E-005 1.590375607321276E-012 8.419473575737259E-020 TIME = 0.10000000E-
04 DT = 0.10000000E-04 SUM OF SQUARES = 0.84194736E-19
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.29175547E-02 AND 0.29175547E-02
POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.30175547E-07
U-FRACTION IN SYSTEM: C = .00698495590212148 FE = 1
TOTAL SIZE OF SYSTEM: .002000001 [m]
13 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: AUSTENITE

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

output ignored...

... output resumed

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

CPU time used in timestep 1 seconds
7.87643036807491E-006 7.877230502301119E-006 8.670326884772467E-
020 TIME = 0.67592186E+09 DT = 0.10000000E+09 SUM OF SQUARES = 0.86703269E-19
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.67714996E-17 AND 0.67714996E-17
POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.13795049E-02
U-FRACTION IN SYSTEM: C = .00698537447225076 FE = 1
TOTAL SIZE OF SYSTEM: .002000001 [m]
1 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: FERRITE

CPU time used in timestep 0 seconds
1.197224211328478E-004 1.197253828931874E-004 2.219521099311381E-
025 TIME = 0.77592186E+09 DT = 0.10000000E+09 SUM OF SQUARES = 0.22195211E-24
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.47013865E-16 AND -0.47013865E-16
```

```

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

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

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

CPU time used in timestep 0 seconds
3.580785187466553E-006 3.581416153708028E-006 4.119529880739355E-
020 TIME = 0.10000000E+10 DT = 24078140. SUM OF SQUARES = 0.41195299E-19
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.11040702E-15 AND -0.11040702E-15
POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.13794921E-02
U-FRACTION IN SYSTEM: C = .00698550549904436 FE = 1
TOTAL SIZE OF SYSTEM: .002000001 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 0.00000000
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 0.10000000E+10 SELECTED

```

```

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

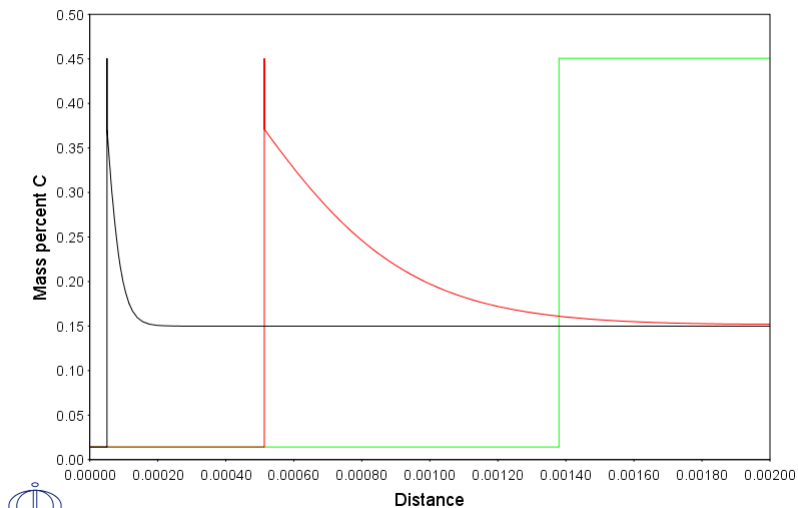
```

exbia-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exbia\plot.DCM"DIC>
DIC>
DIC> @@ exbia_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE bla
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 1.00000E+09
DIC> read exbia
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
```

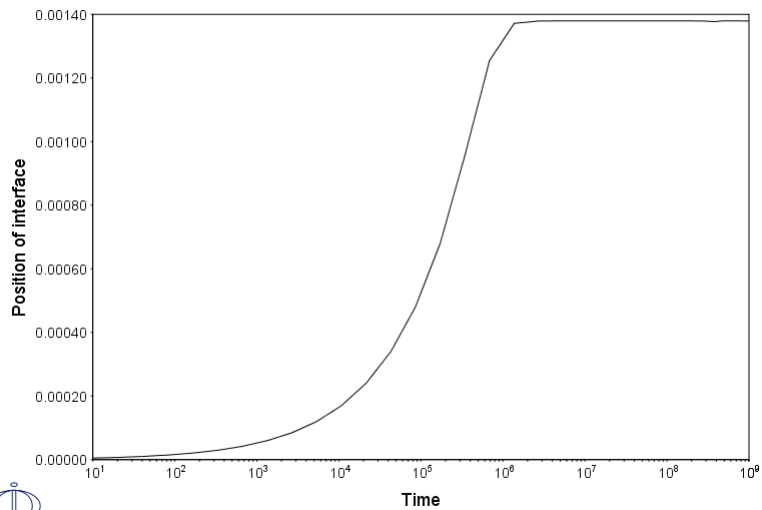
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson

```
POST-1:
POST-1:
POST-1: @@
POST-1: @@ PLOT THE CARBON CONCENTRATIONS AT DIFFERENT TIMES
POST-1: @@
POST-1: s-d-a x distance global
INFO: Distance is set as independent variable
POST-1: s-d-a y w-p c
POST-1: s-p-c time 1e3,1e5,1e9
POST-1:
POST-1: plot
2018.02.18.18.51.24
Time=1000,100000,1E+09
CELL #1
```

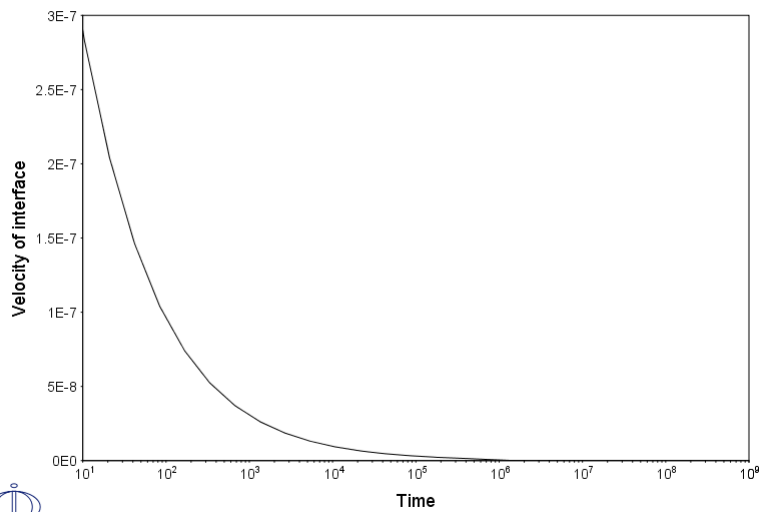


```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ PLOT THE POSITION OF THE BCC/FCC INTERPHASE
POST-1: @@
POST-1: s-d-a x time
INFO: Time is set as independent variable
POST-1: s-d-a y
VARIABLE : pos
INTERFACE : aus
UPPER OR LOWER INTERFACE OF REGION AUSTENITE#1 /LOWER/: lower
POST-1:
POST-1: set_axis_type
AXIS (X, Y OR Z) : x
AXIS TYPE /LINEAR/: log
POST-1:
POST-1: s-s-s
AXIS (X, Y OR Z) : x
AUTOMATIC SCALING (Y OR N) /N/: n
MIN VALUE : 10
MAX VALUE : 1e9
POST-1:
POST-1: plot
```

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



```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ PLOT THE VELOCITY OF THE BCC/FCC INTERPHASE
POST-1: @@
POST-1: s-d-a
AXIS (X, Y OR Z) : y
VARIABLE : velocity
INTERFACE : aus
UPPER OR LOWER INTERFACE OF REGION AUSTENITE#1 /LOWER/: lower
POST-1:
POST-1: plot
2018.02.18.18.51.25
LOWER INTERFACE OF REGION "AUSTENITE#1"
CELL #1
```



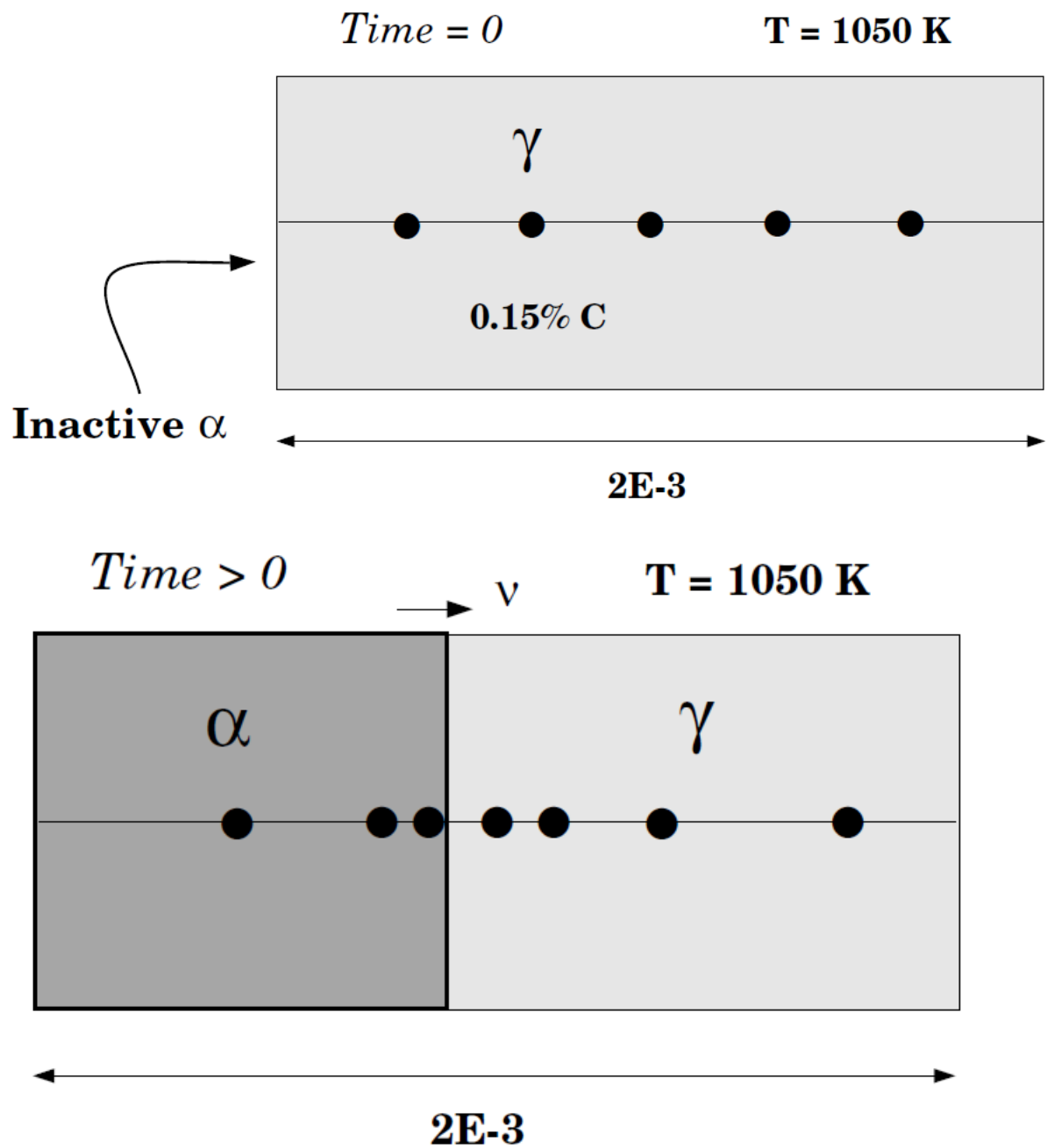
```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: set-inter
--OK--
POST-1:
```



Example exb1b

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

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



exblb-setup

About Stockholm, Sweden

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

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

SYS: @@ Moving boundary problem.

SYS: @@ Austenite to ferrite transformation in a binary Fe-C alloy

SYS: @@ This is the same example as in exbla but now the problem is with

SYS: @@ ferrite as an inactive phase adjacent to the initial austenite.

SYS: -----

NO SUCH COMMAND, USE HELP

SYS:

SYS: @@ exblb_setup.DCM

SYS:

SYS: @@

SYS: @@ START BY GOING TO THE DATABASE MODULE

SYS: @@

SYS: go da

THERMODYNAMIC DATABASE module

Current database: Steels/Fe-Alloys v9.0

VA /- DEFINED

L12_FCC B2_BCC DICTRA_FCC_A1

REJECTED

TDB_TCFE9:

TDB_TCFE9: @@

TDB_TCFE9: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA

TDB_TCFE9: @@

TDB_TCFE9: sw FEDEMO

Current database: Iron Demo Database v2.0

VA /- DEFINED

TDB_FEDEMO:

TDB_FEDEMO: @@

TDB_FEDEMO: @@ DEFINE THE SYSTEM TO WORK WITH

TDB_FEDEMO: @@

TDB_FEDEMO: def-sys fe c

FE C DEFINED

TDB_FEDEMO:

TDB_FEDEMO: @@

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

TDB_FEDEMO: @@

TDB_FEDEMO: rej ph * all

GAS:G	LIQUID:L	BCC_A2
CEMENTITE	DIAMOND_FCC_A4	FCC_A1
GRAPHITE	HCP_A3	KSI_CARBIIDE
LAVES_PHASE_C14	M23C6	M5C2
M7C3_REJECTED		

TDB_FEDEMO: res ph fcc bcc

FCC_A1 BCC_A2 RESTORED

TDB_FEDEMO:

TDB_FEDEMO: @@

TDB_FEDEMO: @@ RETRIEVE DATA FROM THE DATABASE FILE

TDB_FEDEMO: @@

TDB_FEDEMO: get

REINITIATING GES

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

FUNCTIONS

List of references for assessed data

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

TDB_FEDEMO:

TDB_FEDEMO: @@

TDB_FEDEMO: @@ MOBILITY/DIFFUSIVITY DATA ARE STORED IN A SEPARATE DATABASE FILE.

TDB_FEDEMO: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE THE DATA.

TDB_FEDEMO: @@

TDB_FEDEMO: app

Use one of these databases

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

TCMG3 = Mg-Alloys v3.0
TCMG2 = Mg-Alloys v2.0
TCMG1 = Mg-Alloys v1.1
TCTI1 = Ti-Alloys v1.0
TCCU2 = Cu-Alloys v2.0
TCCU1 = Cu-Alloys v1.0
TCCC1 = Cemented carbide v1.0
TCHEA2 = High Entropy Alloy v2.1
TCHEA1 = High Entropy Alloy v1.0
SSOL6 = SGTE Alloy Solutions Database v6.0
SSOL5 = SGTE Alloy Solutions Database v5.0
SSOL4 = SGTE Alloy Solutions Database v4.9g
SSOL2 = SGTE Alloy Solutions Database v2.1
SSUB6 = SGTE Substances Database v6.0
SSUB5 = SGTE Substances Database v5.2
SSUB4 = SGTE Substances Database v4.1
SSUB3 = SGTE Substances Database v3.3
SSUB2 = SGTE Substances Database v2.2
SNOB3 = SGTE Noble Metal Alloys Database v3.1
STBC2 = SGTE Thermal Barrier Coating TDB v2.2
STBC1 = SGTE Thermal Barrier Coating TDB v1.1
SALT1 = SGTE Molten Salts Database v1.2
SEMC2 = TC Semi-Conductors v2.1
SLAG4 = Fe-containing Slag v4.1
SLAG3 = Fe-containing Slag v3.2
SLAG2 = Fe-containing Slag v2.2
SLAG1 = Fe-containing Slag v1.2
TCOX7 = Metal Oxide Solutions v7.0
TCOX6 = Metal Oxide Solutions v6.0
TCOX5 = Metal Oxide Solutions v5.1
TCOX4 = Metal Oxide Solutions v4.1
ION3 = Ionic Solutions v3.0
ION2 = Ionic Solutions v2.6
ION1 = Ionic Solutions v1.5
NOX2 = NPL Oxide Solutions Database v2.1
TCNOBL1 = Noble Metals Alloys v1.0
TCSLD3 = Solder Alloys v3.2
TCSLD2 = Solder Alloys v2.0
TCSI1 = Ultrapure Silicon v1.2
TCMP2 = Materials Processing v2.5
TCES1 = Combustion/Sintering v1.1
TCSC1 = Super Conductor v1.0
TCFC1 = SOFC Database v1.0
NUMT2 = Nuclear Materials v2.1
NUOX4 = Nuclear Oxides v4.2
NUCL15 = IRSN NUCLEA-15_4
NUCL10 = ThermoData NUCLEA Alloys-oxides TDB v10.2
MEPH15 = IRSN Mephista-15_1
MEPH11 = ThermoData MEPHISTA Nuclear Fuels TDB v11.2
TCAQ3 = Aqueous Solution v3.0
TCAQ2 = Aqueous Solution v2.6
AQS2 = TGG Aqueous Solution Database v2.6
GCE2 = TGG Geochemical/Environmental TDB v2.3
FEDEMO = Iron Demo Database v2.0
ALDEMO = Aluminum Demo Database v2.0
NIDEMO = Nickel Demo Database v1.0
CUDEMO = Copper Demo Database v1.0
SLDEMO = Solder Demo Database v1.0
OXDEMO = Oxide Demo Database v1.0
SUBDEMO = Substance Demo Database v1.0
PTERN = Public Ternary Alloys TDB v1.3
PAQ2 = Public Aqueous Soln (SIT) TDB v2.4
PG35 = G35 Binary Semi-Conductors TDB v1.2
PURE5 = SGTE Unary (Pure Elements) TDB v5.1
MOB2 = Alloys Mobility v2.7
MOB1 = Alloys Mobility v1.3
MOBFE1 = Steels/Fe-Alloys Mobility v1.0
MOBFE2 = Steels/Fe-Alloys Mobility v2.0
MOBFE3 = Steels/Fe-Alloys Mobility v3.0
MOBFE4 = Steels/Fe-Alloys Mobility v4.0
MOBNI4 = Ni-Alloys Mobility v4.0
MOBNI3 = Ni-Alloys Mobility v3.1
MOBNI2 = Ni-Alloys Mobility v2.4
MOBNI1 = Ni-Alloys Mobility v1.0
MOBAL3 = Al-Alloys Mobility v3.0
MOBAL2 = Al-Alloys Mobility v2.0
MOBAL1 = Al-Alloys Mobility v1.0
MOBCU1 = Cu-Alloys Mobility v1.0
MOBCU2 = Cu-Alloys Mobility v2.0
MOBMC1 = Mg-Alloys Mobility v1.0
MOBSI1 = Si-Alloys Mobility v1.0
MOBSLD1 = Solder-Alloys Mobility v1.0
MOBTI2 = Ti-Alloys Mobility v2.0 SNAPSHOT
MOBTI1 = Ti-Alloys Mobility v1.0
MALDEMO = Al-Alloys Mobility demo database v1.0
MFEDEMO = Fe-Alloys Mobility demo database v2.0
MNIDEMO = Ni-Alloys Mobility demo database v1.0
MCUDEMO = Cu-Alloys Mobility demo database v1.0
USER = User defined Database

DATABASE NAME /FEDEMO/: MFEDEMO

Current database: Fe-Alloys Mobility demo database v2.0

```

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

```

List of references for assessed data

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

```

      in bcc Fe'
-OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP
APP: @@
APP: go d-m
      NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 1050; * N

DIC>
DIC> @@
DIC> @@ START BY ENTERING THE REGION austenite WHERE WE PUT THE fcc PHASE
DIC> @@
DIC> enter-region
REGION NAME : austenite
DIC>
DIC> @@
DIC> @@ ENTER THE GRID INTO THE REGION
DIC> @@
DIC> enter-grid
REGION NAME : /AUSTENITE/: austenite
WIDTH OF REGION /1/: 20e-4
TYPE /LINEAR/: AUTO
DIC>
DIC> @@
DIC> @@ ENTER THE active PHASES INTO THE REGIONS
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /AUSTENITE/: austenite
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC> @@
DIC> @@ ENTER THE inactive PHASES INTO THE REGIONS
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inactive
ATTACH TO REGION NAMED /AUSTENITE/: austenite
ATTACHED TO THE RIGHT OF AUSTENITE /YES/: no
PHASE NAME: /NONE/: bcc
      REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-5
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITION FOR FCC
DIC> @@
DIC> enter-composition
REGION NAME : /AUSTENITE/: austenite
PHASE NAME: /FCC_A1/: fcc#1
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: C
TYPE /LINEAR/: lin
VALUE OF FIRST POINT : 0.15
VALUE OF LAST POINT : /0.15/: 0.15
DIC>
DIC> @@
DIC> @@ THE BOUNDARY CONDITION IS A CLOSED SYSTEM AS WE DO NOT SPECIFY
DIC> @@ ANYTHING ELSE
DIC> @@
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 1e9
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /100000000/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ IMPLICIT (1) TIME INTEGRATION IS USED INSTEAD OF THE MORE ACCURATE
DIC> @@ (BUT LESS STABLE) TRAPETZOIDAL METHOD WHICH IS THE DEFAULT.
DIC> @@
DIC> s-s-c
NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIFF: /2/:
CHECK INTERFACE POSITION /NO/:
VARY POTENTIALS OR ACTIVITIES OR LNAc : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPLICIT WHEN INTEGRATING PDEs (0 -> 0.5 -> 1): /.5/: 1.0
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /NO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIFF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/:
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exblb Y

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

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

```

exbib-run

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exbib\run.DCM"DIC>
DIC>
DIC> @@ exbib_run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING EXAMPLE blb
DIC> @@
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 0.00000E+00
DIC> read exbib
OK
DIC>
DIC> @@
DIC> @@ START THE SIMULATION
DIC> @@
DIC> sim
Region: AUSTENITE
single geometric dense at 0.0000
1.2284 102
U-FRACTION IN SYSTEM: C = .00698495916383108 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
U-FRACTION IN SYSTEM: C = .00698495916383108 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
INFO: PHASE BCC_A2 IS SCHEDULED TO APPEAR
REGION STATUS CHANGE, ITERATING: TIME= 0.50000000E-07
REGION STATUS CHANGE, ITERATING: TIME= 0.25000000E-07
TIME = 0.25000000E-07 DT = 0.25000000E-07
U-FRACTION IN SYSTEM: C = .00698495916383108 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE

KEEPING TIME-RECORD FOR TIME 0.0000000
AND FOR TIME 0.25000000E-07
WORKSPACE RECLAIMED
WIDTH OF NEW REGION R_BCC_A2 /1E-06/:
Trying old scheme 3
START VALUE(S) FOR INTERFACE #2 R_BCC_A2/AUSTENITE, CELL #1
-----
VELOCITY /1/:
25 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: AUSTENITE

Trying old scheme 3
U-FRACTION IN SYSTEM: C = .00698156310125389 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
U-FRACTION IN SYSTEM: C = .00698156310125389 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
1 GRIDPOINT(S) ADDED TO CELL #1 REGION: R_BCC_A2
2.641796457611307E-003 2.641820164602526E-003 0.237813344814168 2.896595832939294E-003 2.863309992288289E-
003 2.465854448694629E-003 3.038053031129606E-003 2.558808985662677E-003 2.415833959662654E-
003 2.363564691276574E-003 3.038053031129606E-003 2.415833959662654E-003 2.496303854395677E-
003 2.376837933638304E-003 2.369135026131276E-003 2.366895703929962E-003 2.36189602229608E-
003 2.360225248520155E-003 2.369135026131276E-003 2.36189602229608E-003 2.359389073324242E-
003 2.358662147350008E-003 2.369135026131276E-003 2.359389073324242E-003 2.361278827669174E-
003 2.358761597295600E-003 2.358656989247688E-003 2.358709294258692E-003 2.358624351344181E-
003 2.358591712679603E-003 2.358824313562941E-003 2.358624351344181E-003 2.358620260492668E-
003 2.358624351344181E-003 2.358620260492668E-003 2.358624351344181E-003

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

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

output ignored...

... output resumed

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

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

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

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

```

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

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

CPU time used in timestep 0 seconds
2.098982308023776E-007 2.099906631861657E-007 4.239461125711217E-
020 TIME = 0.10000000E+10 DT = 94976699. SUM OF SQUARES = 0.42394611E-19
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.26992581E-16 AND 0.26992581E-16
POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS 0.13796720E-02
U-FRACTION IN SYSTEM: C = .00698366332775786 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 0.0000000
DELETING TIME-RECORD FOR TIME 0.25000000E-07
DELETING TIME-RECORD FOR TIME 0.12500000E-06
DELETING TIME-RECORD FOR TIME 0.60948835E-05
DELETING TIME-RECORD FOR TIME 0.18034650E-04
DELETING TIME-RECORD FOR TIME 0.41914184E-04
DELETING TIME-RECORD FOR TIME 0.89673252E-04
DELETING TIME-RECORD FOR TIME 0.18519139E-03
DELETING TIME-RECORD FOR TIME 0.37622766E-03
DELETING TIME-RECORD FOR TIME 0.75830020E-03
DELETING TIME-RECORD FOR TIME 0.15224453E-02
DELETING TIME-RECORD FOR TIME 0.30507355E-02
DELETING TIME-RECORD FOR TIME 0.61073158E-02
DELETING TIME-RECORD FOR TIME 0.12220476E-01
DELETING TIME-RECORD FOR TIME 0.24446798E-01
DELETING TIME-RECORD FOR TIME 0.48899441E-01
DELETING TIME-RECORD FOR TIME 0.97804726E-01
DELETING TIME-RECORD FOR TIME 0.19561530
DELETING TIME-RECORD FOR TIME 0.39123644
DELETING TIME-RECORD FOR TIME 0.78247872
DELETING TIME-RECORD FOR TIME 1.5649633
DELETING TIME-RECORD FOR TIME 3.1299324
DELETING TIME-RECORD FOR TIME 6.2598707
DELETING TIME-RECORD FOR TIME 12.519747
DELETING TIME-RECORD FOR TIME 25.039500
DELETING TIME-RECORD FOR TIME 50.079006
DELETING TIME-RECORD FOR TIME 100.15802
DELETING TIME-RECORD FOR TIME 200.31604
DELETING TIME-RECORD FOR TIME 400.63209
DELETING TIME-RECORD FOR TIME 801.26419
DELETING TIME-RECORD FOR TIME 1602.5284
DELETING TIME-RECORD FOR TIME 3205.0568
DELETING TIME-RECORD FOR TIME 6410.1136
DELETING TIME-RECORD FOR TIME 12820.227
DELETING TIME-RECORD FOR TIME 25640.454
DELETING TIME-RECORD FOR TIME 51280.909
DELETING TIME-RECORD FOR TIME 102561.82
DELETING TIME-RECORD FOR TIME 205123.63
DELETING TIME-RECORD FOR TIME 410247.27
DELETING TIME-RECORD FOR TIME 820494.54
DELETING TIME-RECORD FOR TIME 1640989.1
DELETING TIME-RECORD FOR TIME 3281978.2
DELETING TIME-RECORD FOR TIME 6563956.3
DELETING TIME-RECORD FOR TIME 13127913.
DELETING TIME-RECORD FOR TIME 26255825.
DELETING TIME-RECORD FOR TIME 52511650.
DELETING TIME-RECORD FOR TIME 0.10502330E+09
DELETING TIME-RECORD FOR TIME 0.20502330E+09
DELETING TIME-RECORD FOR TIME 0.30502330E+09
DELETING TIME-RECORD FOR TIME 0.40502330E+09
DELETING TIME-RECORD FOR TIME 0.50502330E+09
DELETING TIME-RECORD FOR TIME 0.60502330E+09
DELETING TIME-RECORD FOR TIME 0.70502330E+09
DELETING TIME-RECORD FOR TIME 0.80502330E+09

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

TIMESTEP AT 0.10000000E+10 SELECTED

```

```

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

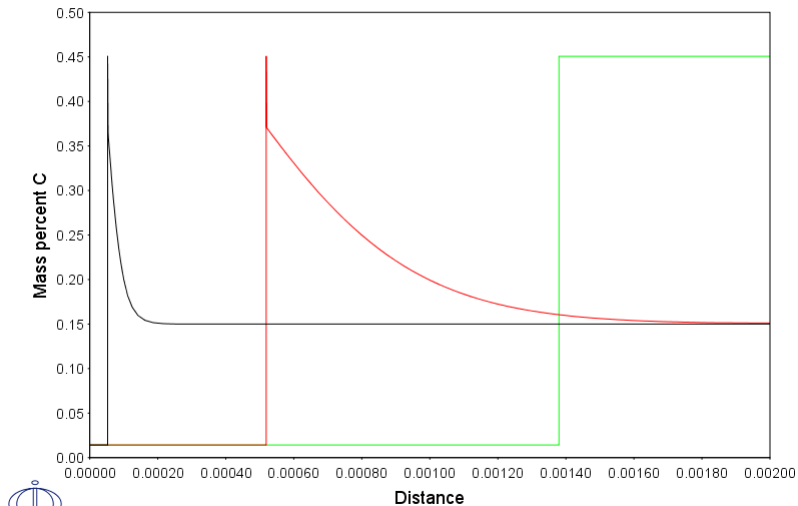
```

exbib-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exbib\plot.DCM"DIC>
DIC>
DIC> @@ exbib_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE bib
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 1.00000E+09
DIC> read exbib
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
```

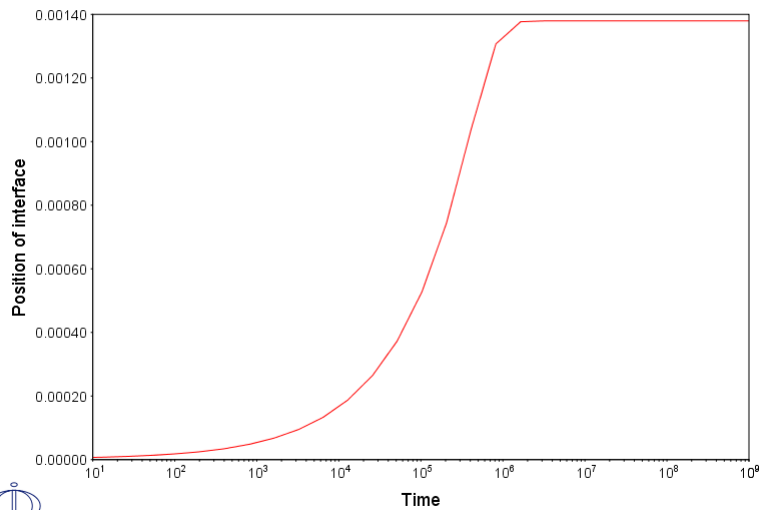
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson

```
POST-1:
POST-1:
POST-1: @@
POST-1: @@ PLOT THE CARBON CONCENTRATIONS AT DIFFERENT TIMES
POST-1: @@
POST-1: s-d-a y w-p c
POST-1: s-d-a x dist glob
INFO: Distance is set as independent variable
POST-1: s-p-c time 1e3,1e5,1e9
POST-1:
POST-1: plot
2018.02.18.18.54.27
Time=1000,100000,1E+09
CELL #1
```

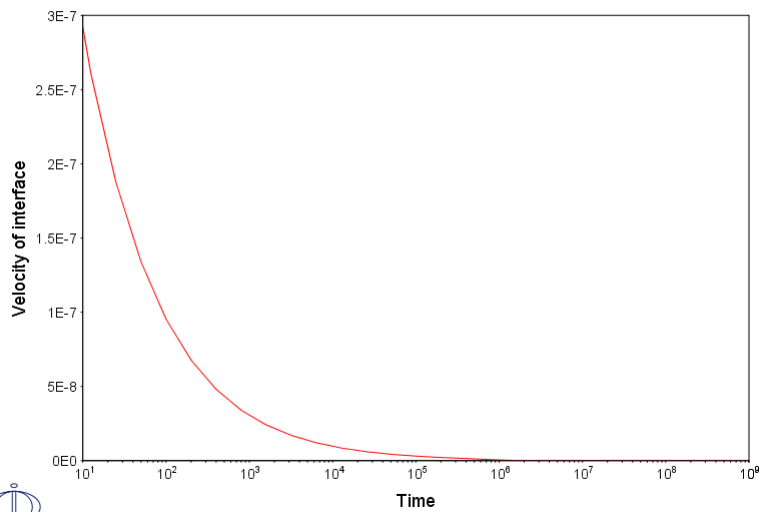


```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ PLOT THE POSITION OF THE BCC/FCC INTERPHASE
POST-1: @@
POST-1: s-d-a x time
INFO: Time is set as independent variable
POST-1: s-d-a y
VARIABLE : pos
INTERFACE : aus
UPPER OR LOWER INTERFACE OF REGION AUSTENITE#1 /LOWER/: lower
POST-1:
POST-1: set_axis_type
AXIS (X, Y OR Z) : x
AXIS TYPE /LINEAR/: log
POST-1:
POST-1: s-s-s
AXIS (X, Y OR Z) : x
AUTOMATIC SCALING (Y OR N) /N/: n
MIN VALUE : 10
MAX VALUE : 1e9
POST-1:
POST-1: plot
```

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



```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ PLOT THE VELOCITY OF THE BCC/FCC INTERPHASE
POST-1: @@
POST-1: s-d-a
AXIS (X, Y OR Z) : y
VARIABLE : velocity
INTERFACE : aus
UPPER OR LOWER INTERFACE OF REGION AUSTENITE#1 /LOWER/: lower
POST-1:
POST-1: plot
2018.02.18.18.54.28
LOWER INTERFACE OF REGION "AUSTENITE#1"
CELL #1
```



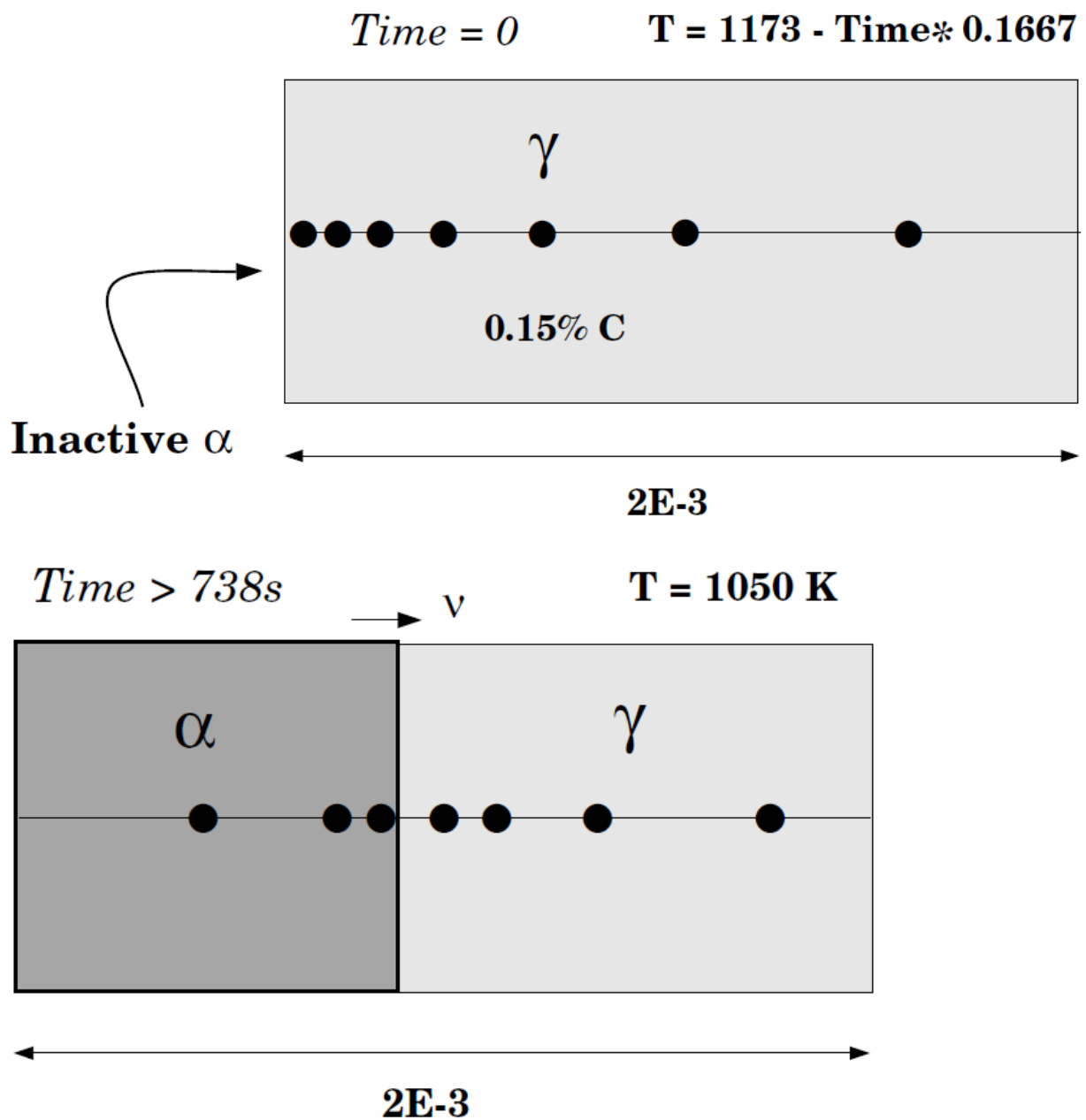
```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: set-inter
--OK--
POST-1:
```



Example exb1c

γ to α transformation in a binary Fe-C alloy: Gradual cool down to 1050 K

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



exblc-setup

About Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

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

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

SYS: @@ Moving boundary problem.

SYS: @@ Austenite to ferrite transformation in a binary Fe-C alloy

SYS: @@ This is the same example as in exbla and exblb but now the

SYS: @@ simulation starts at a higher temperature and assumes a gradual cooling

SYS: @@ down to 1050 K.

SYS: @@

SYS: @@ When 1050 K is reached, the temperature is kept constant and thus has an

SYS: @@ isothermal transformation. As in exblb ferrite is an inactive

SYS: @@ phase adjacent to the initial austenite.

SYS: -----

NO SUCH COMMAND, USE HELP

SYS:

SYS: @@ exblc_setup.DCM

SYS:

SYS: @@

SYS: @@ START BY GOING TO THE DATABASE MODULE

SYS: @@

SYS: go da

THERMODYNAMIC DATABASE module

Current database: Steels/Fe-Alloys v9.0

VA /- DEFINED

L12_FCC B2_BCC DICTRA_FCC_A1

REJECTED

TDB_TCFE9:

TDB_TCFE9: @@

TDB_TCFE9: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA

TDB_TCFE9: @@

TDB_TCFE9: sw FEDEMO

Current database: Iron Demo Database v2.0

VA /- DEFINED

TDB_FEDEMO:

TDB_FEDEMO: @@

TDB_FEDEMO: @@ DEFINE THE SYSTEM TO WORK WITH

TDB_FEDEMO: @@

TDB_FEDEMO: def-sys fe c

FE C DEFINED

TDB_FEDEMO:

TDB_FEDEMO: @@

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

TDB_FEDEMO: @@

TDB_FEDEMO: rej ph * all

GAS:G LIQUID:L BCC_A2

CEMENTITE DIAMOND_FCC_A4 FCC_A1

GRAPHITE HCP_A3 KSI_CARBIIDE

LAVES_PHASE_C14 M23C6 M5C2

M7C3 _REJECTED

TDB_FEDEMO: res ph fcc bcc

FCC_A1 BCC_A2 RESTORED

TDB_FEDEMO:

TDB_FEDEMO: @@

TDB_FEDEMO: @@ RETRIEVE DATA FROM THE DATABASE FILE

TDB_FEDEMO: @@

TDB_FEDEMO: get

REINITIATING GES

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

FUNCTIONS

List of references for assessed data

'P. Franke, Estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'

'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-Fe'

'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'

'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'

'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar

volumes'

'X.-G. Lu, M. Selleby, B. Sundman, CALPHAD, 29 (2005) 49-55; Fe P-T diagram'

'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'

-OK-

TDB_FEDEMO:

TDB_FEDEMO: @@

TDB_FEDEMO: @@ MOBILITY/DIFFUSIVITY DATA ARE STORED IN A SEPARATE DATABASE FILE.

TDB_FEDEMO: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE DATA

TDB_FEDEMO: @@

TDB_FEDEMO: app

Use one of these databases

TCFE9 = Steels/Fe-Alloys v9.0

TCFE10 = Steels/Fe-Alloys v10.0 SNAPSHOT

TCFE8 = Steels/Fe-Alloys v8.1

FROST1 = FROST database v1.0

TCFE7 = Steels/Fe-Alloys v7.0

TCFE6 = Steels/Fe-Alloys v6.2

TCFE5 = Steels/Fe-Alloys v5.0

TCFE4 = Steels/Fe-Alloys v4.1

TCFE3 = Steels/Fe-Alloys v3.1

TCFE2 = Steels/Fe-Alloys v2.1

TCFE1 = Steels/Fe-Alloys v1.0

TCNI9 = Ni-Alloys v9.0 SNAPSHOT

NI25 = NI25 database

TCNI8 = Ni-Alloys v8.1

TCNI7 = Ni-Alloys v7.1

TCNI6 = Ni-Alloys v6.0

TCNI5 = Ni-Alloys v5.1

TCNI4 = Ni-Alloys v4.0

TCNI1 = Ni-Alloys v1.3

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

DATABASE NAME /FEDEMO/: MFEDEMO

Current database: Fe-Alloys Mobility demo database v2.0

```

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

List of references for assessed data

'This parameter has not been assessed'

```

'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'
'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
-Ni'
'B. Jonsson: Z. Metallkunde 85(1994)498-501; C and N diffusion in bcc Cr
-Fe-Ni'
'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
in bcc Fe'
-OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP
APP: @@
APP: go d-m
NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER GLOBAL CONDITION T
DIC> @@
DIC> @@ ASSUME THAT THE COOLING RATE IS 10K/MINUTE DOWN TO 1050K
DIC> @@
DIC> set-cond

GLOBAL OR BOUNDARY CONDITION /GLOBAL/: glob
VARIABLE : T
LOW TIME LIMIT /0/: 0
T(TIME,X)= 1173-time*0.1667;
HIGH TIME LIMIT /*/: 738
ANY MORE RANGES /N/: y
T(TIME,X)= 1050;
HIGH TIME LIMIT /*/: *
ANY MORE RANGES /N/: N
DIC>
DIC> @@
DIC> @@ START BY ENTERING THE REGION austenite WHERE WE PUT THE fcc PHASE
DIC> @@
DIC> enter-region
REGION NAME : austenite
DIC>
DIC> @@
DIC> @@ ENTER THE GRID INTO THE REGION
DIC> @@
DIC> enter-grid
REGION NAME : /AUSTENITE/: austenite
WIDTH OF REGION /1/: 20e-4
TYPE /LINEAR/: AUTO
DIC>
DIC> @@
DIC> @@ ENTER THE active PHASES INTO THE REGIONS
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /AUSTENITE/: austenite
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC> @@
DIC> @@ ENTER THE inactive PHASES INTO THE REGIONS
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inact
ATTACH TO REGION NAMED /AUSTENITE/: austenite
ATTACHED TO THE RIGHT OF AUSTENITE /YES/: no
PHASE NAME: /NONE/: bcc
REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-5
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITION FOR FCC
DIC> @@
DIC> enter-composition
REGION NAME : /AUSTENITE/: austenite
PHASE NAME: /FCC_A1/: fcc#1
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: C
TYPE /LINEAR/: lin
VALUE OF FIRST POINT : 0.15
VALUE OF LAST POINT : /0.15/: 0.15
DIC>
DIC> @@
DIC> @@ THE BOUNDARY CONDITION IS A CLOSED SYSTEM AS WE DO NOT SPECIFY
DIC> @@ ANYTHING ELSE.
DIC> @@
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 738
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /73.8/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC> @@
DIC> @@ IMPLICIT (1) TIME INTEGRATION IS USED INSTEAD OF THE MORE ACCURATE
DIC> @@ (BUT LESS STABLE) TRAPETZOIDAL METHOD WHICH IS THE DEFAULT.
DIC> @@
DIC> s-s-c
NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIFF : /2/:
CHECK INTERFACE POSITION /NO/:
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPLICIT WHEN INTEGRATING PDES (0 -> 0.5 -> 1): /.5/: 1.0
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /NO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIFF /YES/:

```

```
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/:  
DIC> @@  
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT  
DIC> @@  
DIC> save exblc Y  
DIC>  
DIC> set-inter  
--OK--  
DIC>
```

exb1c-run

```
DIC>AboutDIC>DIC>MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb1c\run.DCM"DIC>
DIC>
DIC> @@ exb1c_run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING EXAMPLE exb1c
DIC> @@
DIC> go d-m
    TIME STEP AT TIME 0.00000E+00
DIC> read exb1c
OK
DIC>
DIC> @@
DIC> @@ START THE SIMULATION
DIC> @@
DIC> sim
    Region: AUSTENITE
    single geometric dense at 0.0000
    1.2084 101
    U-FRACTION IN SYSTEM: C = .0069849591638311 FE = 1
    TOTAL SIZE OF SYSTEM: .002 [m]
    U-FRACTION IN SYSTEM: C = .0069849591638311 FE = 1
    TOTAL SIZE OF SYSTEM: .002 [m]
    TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.0000000
    U-FRACTION IN SYSTEM: C = .0069849591638311 FE = 1
    TOTAL SIZE OF SYSTEM: .002 [m]
    CPU time used in timestep 0 seconds
    TIME = 0.24660033E-05 DT = 0.23660033E-05 SUM OF SQUARES = 0.0000000
    U-FRACTION IN SYSTEM: C = .00698495916383109 FE = 1
    TOTAL SIZE OF SYSTEM: .002 [m]
    CPU time used in timestep 0 seconds
    TIME = 0.71980098E-05 DT = 0.47320065E-05 SUM OF SQUARES = 0.0000000
    U-FRACTION IN SYSTEM: C = .00698495916383109 FE = 1
    TOTAL SIZE OF SYSTEM: .002 [m]
    CPU time used in timestep 0 seconds
    TIME = 0.16662023E-04 DT = 0.94640131E-05 SUM OF SQUARES = 0.0000000
    U-FRACTION IN SYSTEM: C = .00698495916383109 FE = 1
    TOTAL SIZE OF SYSTEM: .002 [m]
    CPU time used in timestep 0 seconds
    TIME = 0.35590049E-04 DT = 0.18928026E-04 SUM OF SQUARES = 0.0000000
    U-FRACTION IN SYSTEM: C = .00698495916383109 FE = 1
    TOTAL SIZE OF SYSTEM: .002 [m]
    CPU time used in timestep 0 seconds
    TIME = 0.73446101E-04 DT = 0.37856052E-04 SUM OF SQUARES = 0.0000000
    U-FRACTION IN SYSTEM: C = .00698495916383109 FE = 1
    TOTAL SIZE OF SYSTEM: .002 [m]
    CPU time used in timestep 0 seconds
    TIME = 0.14915821E-03 DT = 0.75712105E-04 SUM OF SQUARES = 0.0000000
    U-FRACTION IN SYSTEM: C = .00698495916383109 FE = 1
    TOTAL SIZE OF SYSTEM: .002 [m]
    CPU time used in timestep 0 seconds
    TIME = 0.30058241E-03 DT = 0.15142421E-03 SUM OF SQUARES = 0.0000000
    U-FRACTION IN SYSTEM: C = .00698495916383109 FE = 1
    TOTAL SIZE OF SYSTEM: .002 [m]
    CPU time used in timestep 0 seconds
    TIME = 0.60343083E-03 DT = 0.30284842E-03 SUM OF SQUARES = 0.0000000
    U-FRACTION IN SYSTEM: C = .00698495916383109 FE = 1
    TOTAL SIZE OF SYSTEM: .002 [m]
    CPU time used in timestep 0 seconds
    TIME = 0.12091277E-02 DT = 0.60569684E-03 SUM OF SQUARES = 0.0000000
    U-FRACTION IN SYSTEM: C = .00698495916383109 FE = 1
    TOTAL SIZE OF SYSTEM: .002 [m]
    CPU time used in timestep 0 seconds
    TIME = 0.24205213E-02 DT = 0.12113937E-02 SUM OF SQUARES = 0.0000000
    U-FRACTION IN SYSTEM: C = .00698495916383109 FE = 1
    TOTAL SIZE OF SYSTEM: .002 [m]
    CPU time used in timestep 0 seconds
    TIME = 0.48433087E-02 DT = 0.24227873E-02 SUM OF SQUARES = 0.0000000
    U-FRACTION IN SYSTEM: C = .00698495916383109 FE = 1
    TOTAL SIZE OF SYSTEM: .002 [m]
    CPU time used in timestep 0 seconds
    TIME = 0.96888834E-02 DT = 0.48455747E-02 SUM OF SQUARES = 0.0000000
    U-FRACTION IN SYSTEM: C = .00698495916383109 FE = 1
    TOTAL SIZE OF SYSTEM: .002 [m]
    CPU time used in timestep 0 seconds
    TIME = 0.19380033E-01 DT = 0.96911494E-02 SUM OF SQUARES = 0.0000000
    U-FRACTION IN SYSTEM: C = .00698495916383109 FE = 1
    TOTAL SIZE OF SYSTEM: .002 [m]
    CPU time used in timestep 0 seconds
    TIME = 0.38762332E-01 DT = 0.19382299E-01 SUM OF SQUARES = 0.0000000
    U-FRACTION IN SYSTEM: C = .00698495916383109 FE = 1
    TOTAL SIZE OF SYSTEM: .002 [m]
    CPU time used in timestep 0 seconds
    TIME = 0.77526929E-01 DT = 0.38764598E-01 SUM OF SQUARES = 0.0000000
    U-FRACTION IN SYSTEM: C = .00698495916383109 FE = 1
    TOTAL SIZE OF SYSTEM: .002 [m]
    CPU time used in timestep 0 seconds
    TIME = 0.15505612 DT = 0.77529195E-01 SUM OF SQUARES = 0.0000000
    U-FRACTION IN SYSTEM: C = .00698495916383109 FE = 1
    TOTAL SIZE OF SYSTEM: .002 [m]
    CPU time used in timestep 0 seconds
    TIME = 0.31011451 DT = 0.15505839 SUM OF SQUARES = 0.0000000
    U-FRACTION IN SYSTEM: C = .00698495916383109 FE = 1
    TOTAL SIZE OF SYSTEM: .002 [m]
    CPU time used in timestep 0 seconds
    TIME = 0.62023129 DT = 0.31011678 SUM OF SQUARES = 0.0000000
    U-FRACTION IN SYSTEM: C = .00698495916383109 FE = 1
    TOTAL SIZE OF SYSTEM: .002 [m]
    CPU time used in timestep 0 seconds
    TIME = 1.2404649 DT = 0.62023356 SUM OF SQUARES = 0.0000000
    U-FRACTION IN SYSTEM: C = .0069849591638311 FE = 1
    TOTAL SIZE OF SYSTEM: .002 [m]
    CPU time used in timestep 0 seconds
    TIME = 2.4809320 DT = 1.2404671 SUM OF SQUARES = 0.0000000
    U-FRACTION IN SYSTEM: C = .0069849591638311 FE = 1
    TOTAL SIZE OF SYSTEM: .002 [m]
    CPU time used in timestep 0 seconds
    TIME = 4.9618662 DT = 2.4809342 SUM OF SQUARES = 0.0000000
    U-FRACTION IN SYSTEM: C = .00698495916383109 FE = 1
    TOTAL SIZE OF SYSTEM: .002 [m]
    CPU time used in timestep 0 seconds
    TIME = 9.9237347 DT = 4.9618685 SUM OF SQUARES = 0.0000000
```

U-FRACTION IN SYSTEM: C = .00698495916383108 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 0 seconds
TIME = 19.847472 DT = 9.9237370 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0069849591638311 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 0 seconds
TIME = 39.694946 DT = 19.847474 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0069849591638311 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 0 seconds
TIME = 76.594946 DT = 36.900000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698495916383102 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 0 seconds
TIME = 113.49495 DT = 36.900000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00698495916383101 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]

output ignored...

... output resumed

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

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

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

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

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

CPU time used in timestep 0 seconds
1.440034499273632E-005 1.440179063999719E-005 7.407006665689525E-
029 TIME = 0.93290424E+09 DT = 0.10000000E+09 SUM OF SQUARES = 0.74070067E-28
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.92672920E-15 AND -0.92672920E-15
POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS 0.13797192E-02
U-FRACTION IN SYSTEM: C = .00698318213512128 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 0 seconds
3.754518665345077E-006 3.755236501551250E-006 2.175886568427993E-
023 TIME = 0.10000000E+10 DT = 67095763. SUM OF SQUARES = 0.21758866E-22
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.41881901E-16 AND 0.41881901E-16
POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS 0.13797220E-02
U-FRACTION IN SYSTEM: C = .00698315347948737 FE = 1
TOTAL SIZE OF SYSTEM: .002 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 738.00000
DELETING TIME-RECORD FOR TIME 769.68667
DELETING TIME-RECORD FOR TIME 833.06001
DELETING TIME-RECORD FOR TIME 959.80670
DELETING TIME-RECORD FOR TIME 1213.3001
DELETING TIME-RECORD FOR TIME 1720.2868
DELETING TIME-RECORD FOR TIME 2734.2603
DELETING TIME-RECORD FOR TIME 4762.2072
DELETING TIME-RECORD FOR TIME 8818.1011
DELETING TIME-RECORD FOR TIME 16929.889
DELETING TIME-RECORD FOR TIME 33153.464
DELETING TIME-RECORD FOR TIME 65600.616
DELETING TIME-RECORD FOR TIME 130494.92
DELETING TIME-RECORD FOR TIME 260283.52
DELETING TIME-RECORD FOR TIME 519860.73
DELETING TIME-RECORD FOR TIME 1039015.1
DELETING TIME-RECORD FOR TIME 2077324.0
DELETING TIME-RECORD FOR TIME 4153941.7
DELETING TIME-RECORD FOR TIME 8307177.0
DELETING TIME-RECORD FOR TIME 16613648.
DELETING TIME-RECORD FOR TIME 33226589.
DELETING TIME-RECORD FOR TIME 66452472.
DELETING TIME-RECORD FOR TIME 0.13290424E+09
DELETING TIME-RECORD FOR TIME 0.23290424E+09
DELETING TIME-RECORD FOR TIME 0.33290424E+09
DELETING TIME-RECORD FOR TIME 0.43290424E+09
DELETING TIME-RECORD FOR TIME 0.53290424E+09
DELETING TIME-RECORD FOR TIME 0.63290424E+09
DELETING TIME-RECORD FOR TIME 0.73290424E+09

DELETING TIME-RECORD FOR TIME 0.83290424E+09

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

TIMESTEP AT 0.10000000E+10 SELECTED

DIC>

DIC>

DIC>

DIC>

DIC>

DIC>

DIC>

DIC> @@

DIC> @@ THE SIMULATION IS FINISHED

DIC> @@

DIC>

DIC> set-inter

--OK--

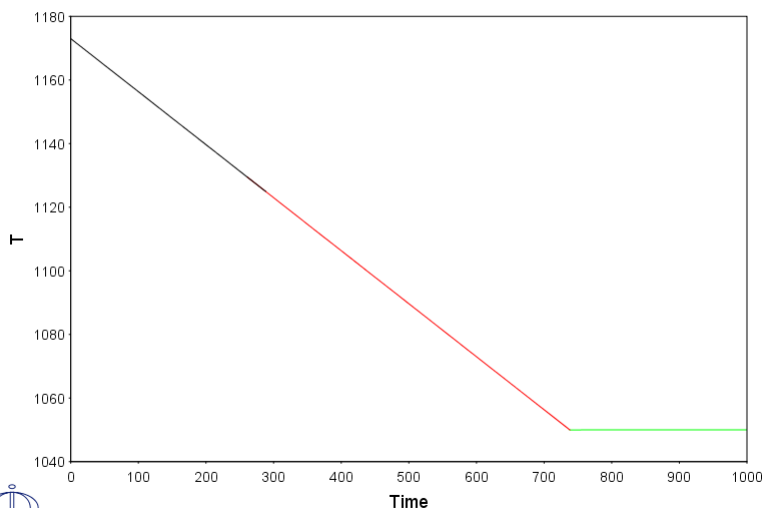
DIC>

exb1c-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb1c\plot.DCM"DIC>
DIC>
DIC> @@ exb1c_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE b1c
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 1.00000E+09
DIC> read exb1c
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post

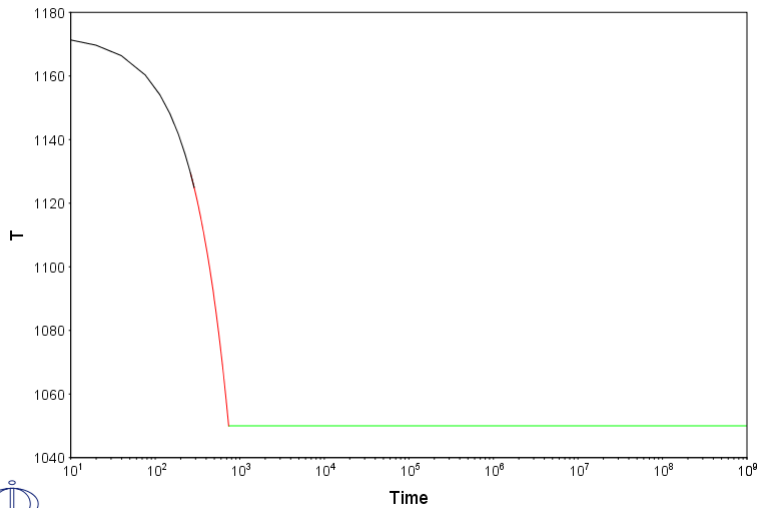
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
```

```
POST-1:
POST-1:
POST-1: @@
POST-1: @@ PLOT TEMPERATURE VS. TIME
POST-1: @@
POST-1: s-d-a y t
POST-1: s-d-a x time
INFO: Time is set as independent variable
POST-1: s-p-c
CONDITION /TIME/: interface
INTERFACE : austenite
UPPER OR LOWER INTERFACE OF REGION AUSTENITE#1 /LOWER/: lower
POST-1: s-s-s x n 0 1000
POST-1:
POST-1: plot
2018.02.18.18.57.32
LOWER INTERFACE OF REGION "AUSTENITE#1"
CELL #1
```

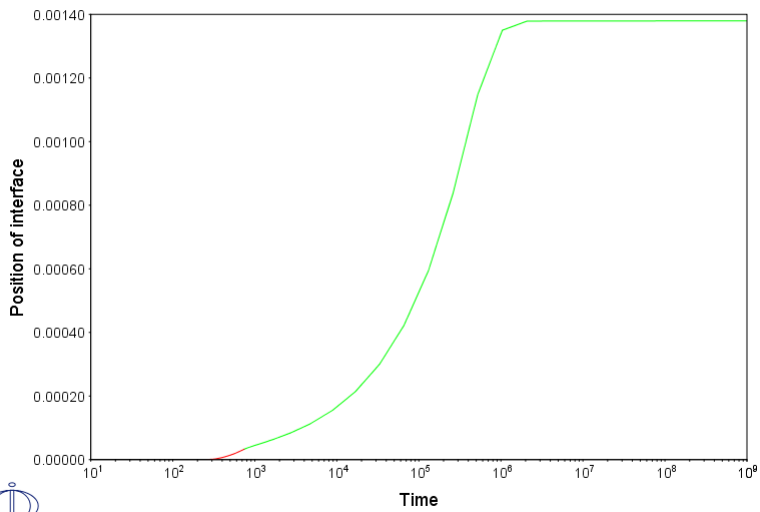


```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1: @@?<Hit_return_to_continue>
POST-1:
POST-1: @@
POST-1: @@ PLOT VS. LOG TIME
POST-1: @@
POST-1: set-axis-type x log
POST-1: s-s-s x n 10 1e9
POST-1:
POST-1: plot
```

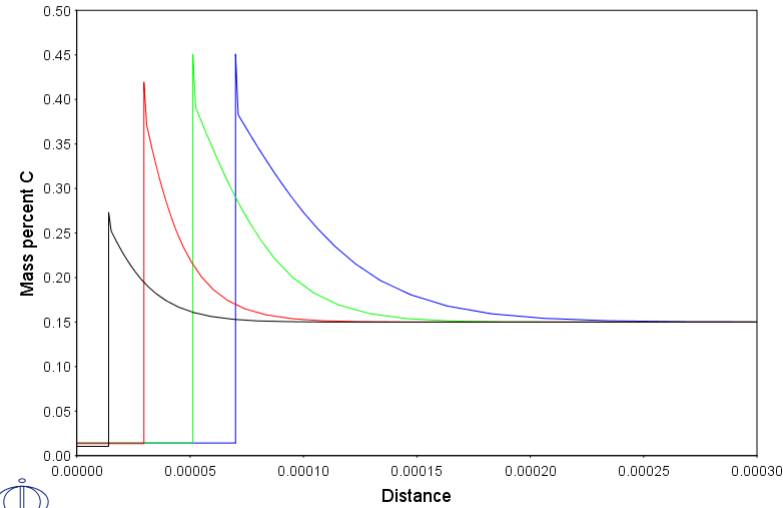

2018.02.18.18.57.32
 LOWER INTERFACE OF REGION "AUSTENITE#1"
 CELL #1



```
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: @@
POST-1: @@ PLOT THE POSITION OF THE BCC/FCC INTERPHASE
POST-1: @@
POST-1: s-d-a
POST-1: AXIS (X, Y OR Z) : y
POST-1: VARIABLE : position
POST-1: INTERFACE : austenite
POST-1: UPPER OR LOWER INTERFACE OF REGION AUSTENITE#1 /LOWER/: lower
POST-1:
POST-1: plot
2018.02.18.18.57.33
LOWER INTERFACE OF REGION "AUSTENITE#1"
CELL #1
```



```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: @@
POST-1: @@ PLOT THE CARBON CONCENTRATION VS. DISTANCE
POST-1: @@
POST-1: s-d-a y w-p c
POST-1: s-d-a x dis glob
POST-1: INFO: Distance is set as independent variable
POST-1: s-p-c time 500,700,1200,2000
POST-1: set-axis-type x lin
POST-1: s-s-s x n 0 3e-4
POST-1:
POST-1: plot
```



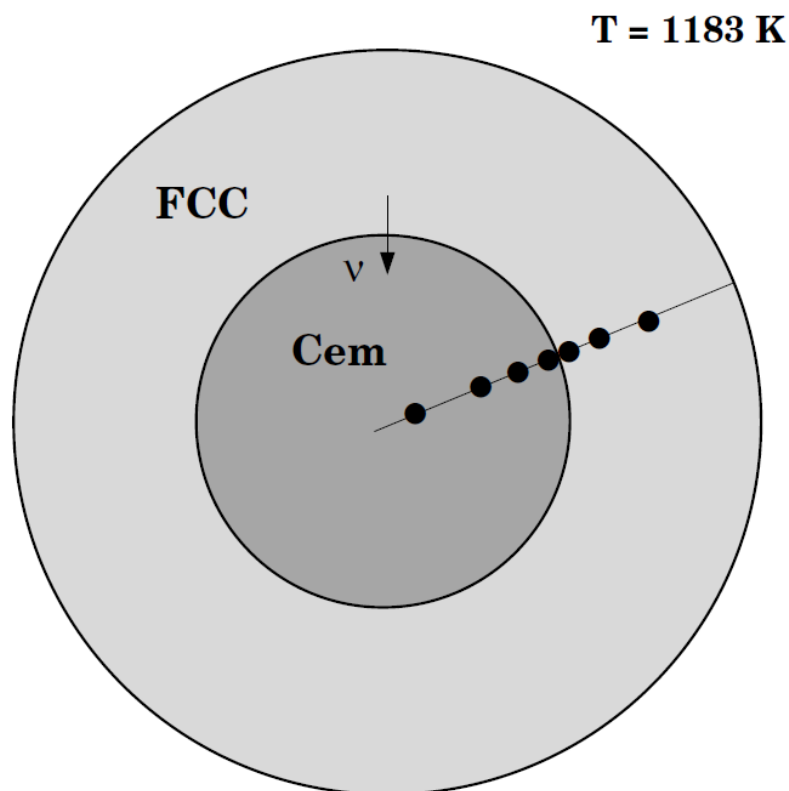
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:??<Hit_return_to_continue>
POST-1: set-inter
--OK--
POST-1:



Example exb2

Cementite dissolution in an Fe-Cr-C alloy

This example calculates the dissolution of a spherical cementite particle in an austenite matrix. This case is from Z.-K. Liu, L. Höglund, B. Jönsson and J. Ågren (Metall. Trans.A, v.22A, 1991, pp. 1745-1752). In order to achieve the correct average composition in the calculation it is necessary to take into account the fact that the calculation is set up using the volume fraction of the phases. To calculate the initial state at the heat treatment temperature we need first to determine the state at the normalizing temperature. To calculate the volume fraction of the phases we need to enter a number of functions that calculate these quantities.



exb2-setup

About Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

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

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

VA      /- DEFINED
LI12_FCC      B2_BCC      DICTRA_FCC_A1
REJECTED
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE THE DATA
TDB_TCFE9: @@
TDB_TCFE9: sw FEDEMO
Current database: Iron Demo Database v2.0

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

List of references for assessed data

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

```

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

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

List of references for assessed data

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

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

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

```

```

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

```

exb2-run

DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb2\run.DCM"DIC>

DIC>

DIC> @@ exb2_run.DCM

DIC>

DIC> @@

DIC> @@ READ THE SET UP FROM FILE AND START THE SIMULATION

DIC> @@

DIC>

DIC> go d-m

TIME STEP AT TIME 0.00000E+00

*** ENTERING BCC_A2 AS A DIFFUSION NONE PHASE

DIC> read exb2

OK

DIC> sim

Region: CARB

single geometric dense at 0.52550E-06

0.85084 96

Region: AUS

single geometric dense at 0.0000

1.0072 63

Trying old scheme 4

GENERATING STARTING VALUES FOR CELL # 1 INTERFACE # 2

DETERMINING INITIAL EQUILIBRIUM VALUES

CALCULATING STARTING VALUES: 9 EQUILIBRIUM CALCULATIONS

DONE 6 OUT OF 9

04

U-FRACTION IN SYSTEM: C = .0406910188418179 CR = .0214382349908299

FE = .978561765139677

TOTAL SIZE OF SYSTEM: 5.0562665819E-18 [m^3]

U-FRACTION IN SYSTEM: C = .0406910188418179 CR = .0214382349908299

FE = .978561765139677

TOTAL SIZE OF SYSTEM: 5.0562665819E-18 [m^3]

0.175650481269751 0.175691744058966 0.175650536404886 2.957532104484168E-003 7.754436530875758E-

005 5.789654735166348E-006 8.570960213922231E-007 3.747799259728377E-007 3.453263876444000E-

007 1.349945939910680E-007 1.350781757709255E-007 1.346762090320248E-007 1.361220011258119E-

007 1.343486474217425E-007 1.340758203772263E-007 1.335307568888863E-007 1.344901942324164E-

007 1.324431404508194E-007 1.302779893773460E-007 1.259883039615329E-007 1.269270720671105E-

007 1.175748901910759E-007 1.014429630745407E-007 7.217938870756822E-008 7.299666432258670E-

008 2.728114977158535E-008 7.241529806521035E-011 4.088996652349226E-014 7.514509141967509E-

019 TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.75145091E-18

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.39436719E-02 AND -0.39436719E-02

POSITION OF INTERFACE CARB / AUS IS 0.52510563E-06

U-FRACTION IN SYSTEM: C = .0407290154735827 CR = .0214383281160798

FE = .978561672014427

TOTAL SIZE OF SYSTEM: 5.0562665819E-18 [m^3]

15 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: CARB

CPU time used in timestep 1 seconds

2.248317823774132E-005 2.248767785871598E-005 2.248316234366775E-005 1.887681598926652E-009 1.633889034216790E-

009 1.019554044105679E-009 6.882193013883610E-010 6.885272455086273E-010 2.216753491915168E-

010 6.151361467432378E-014 2.128398762358501E-017 TIME = 0.30000000E-06 DT = 0.20000000E-

06 SUM OF SQUARES = 0.21283988E-16

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.22443467E-04 AND -0.22443467E-04

POSITION OF INTERFACE CARB / AUS IS 0.52510114E-06

U-FRACTION IN SYSTEM: C = .0407297653418501 CR = .0214383291133005

FE = .978561671017207

TOTAL SIZE OF SYSTEM: 5.0562665819E-18 [m^3]

CPU time used in timestep 0 seconds

6.026883998584040E-004 6.026580888942288E-004 6.026721103974375E-004 8.498819122335174E-005 3.515893844060556E-

005 2.728074750064295E-007 4.049324254833804E-010 6.350550454746669E-015 2.881437473850283E-

018 TIME = 0.70000000E-06 DT = 0.40000000E-06 SUM OF SQUARES = 0.28814375E-17

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.46375369E-05 AND -0.46375369E-05

POSITION OF INTERFACE CARB / AUS IS 0.52509929E-06

U-FRACTION IN SYSTEM: C = .0407315536282503 CR = .0214383294271359

FE = .978561670703371

TOTAL SIZE OF SYSTEM: 5.0562665819E-18 [m^3]

CPU time used in timestep 1 seconds

2.365053298194977E-004 2.365033654325256E-004 2.364987107717018E-004 7.190732024202641E-005 1.444209573214119E-

007 4.667964222950008E-011 2.104118921106627E-014 2.043518107460929E-017 TIME = 0.15000000E-05 DT = 0.80000000E-

06 SUM OF SQUARES = 0.20435181E-16

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.40628860E-05 AND -0.40628860E-05

POSITION OF INTERFACE CARB / AUS IS 0.52509604E-06

U-FRACTION IN SYSTEM: C = .0407314706589161 CR = .0214383297891356

FE = .978561670341372

TOTAL SIZE OF SYSTEM: 5.0562665819E-18 [m^3]

CPU time used in timestep 0 seconds

3.788612455941237E-005 3.788586871828255E-005 3.788453387382108E-005

output ignored...

... output resumed

2.983577615403479E-009 6.454633484857469E-014 4.765435236071551E-

019 TIME = 8179.7139 DT = 1000.0000 SUM OF SQUARES = 0.47654352E-18

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.10807344E-10 AND -0.10807344E-10

POSITION OF INTERFACE CARB / AUS IS 0.24757819E-06

U-FRACTION IN SYSTEM: C = .0407635155644673 CR = .0214383980828099

FE = .978561602047697

TOTAL SIZE OF SYSTEM: 5.0562665819E-18 [m^3]

CPU time used in timestep 1 seconds

9.541491481690836E-009 9.602297615637573E-009 9.559945434056129E-009 3.099188909764701E-009 1.052631177236939E-

009 7.570945912359031E-015 2.435855150451165E-

018 TIME = 9179.7139 DT = 1000.0000 SUM OF SQUARES = 0.24358552E-17

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.10178497E-10 AND -0.10178497E-10

POSITION OF INTERFACE CARB / AUS IS 0.23739969E-06

U-FRACTION IN SYSTEM: C = .0407635351055688 CR = .0214383969215681

FE = .978561603208939

TOTAL SIZE OF SYSTEM: 5.0562665819E-18 [m^3]

CPU time used in timestep 1 seconds

1.943033399345351E-007 1.941096197641130E-007 1.939935593089594E-007 2.953461423144300E-008 3.247208203742438E-

009 3.923651150138315E-017 TIME = 10000.000 DT = 820.28605 SUM OF SQUARES = 0.39236512E-16

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.96946211E-11 AND -0.96946211E-11

POSITION OF INTERFACE CARB / AUS IS 0.22944733E-06

U-FRACTION IN SYSTEM: C = .0407635386763659 CR = .0214383960997853

FE = .978561604030722

TOTAL SIZE OF SYSTEM: 5.0562665819E-18 [m^3]

MUST SAVE WORKSPACE ON FILE

WORKSPACE SAVED ON FILE

RECLAIMING WORKSPACE

DELETING TIME-RECORD FOR TIME 0.0000000

```
DELETING TIME-RECORD FOR TIME 0.10000000E-06
DELETING TIME-RECORD FOR TIME 0.30000000E-06
DELETING TIME-RECORD FOR TIME 0.70000000E-06
DELETING TIME-RECORD FOR TIME 0.15000000E-05
DELETING TIME-RECORD FOR TIME 0.31000000E-05
DELETING TIME-RECORD FOR TIME 0.63000000E-05
DELETING TIME-RECORD FOR TIME 0.12700000E-04
DELETING TIME-RECORD FOR TIME 0.25500000E-04
DELETING TIME-RECORD FOR TIME 0.51100000E-04
DELETING TIME-RECORD FOR TIME 0.99418868E-04
DELETING TIME-RECORD FOR TIME 0.17900397E-03
DELETING TIME-RECORD FOR TIME 0.30071451E-03
DELETING TIME-RECORD FOR TIME 0.47831845E-03
DELETING TIME-RECORD FOR TIME 0.72934499E-03
DELETING TIME-RECORD FOR TIME 0.10758345E-02
DELETING TIME-RECORD FOR TIME 0.15428996E-02
DELETING TIME-RECORD FOR TIME 0.21467218E-02
DELETING TIME-RECORD FOR TIME 0.29017296E-02
DELETING TIME-RECORD FOR TIME 0.38194698E-02
DELETING TIME-RECORD FOR TIME 0.49085555E-02
DELETING TIME-RECORD FOR TIME 0.61737650E-02
DELETING TIME-RECORD FOR TIME 0.76141364E-02
DELETING TIME-RECORD FOR TIME 0.92226414E-02
DELETING TIME-RECORD FOR TIME 0.10986320E-01
DELETING TIME-RECORD FOR TIME 0.12887767E-01
DELETING TIME-RECORD FOR TIME 0.14913901E-01
DELETING TIME-RECORD FOR TIME 0.17051564E-01
DELETING TIME-RECORD FOR TIME 0.19291247E-01
DELETING TIME-RECORD FOR TIME 0.21633944E-01
DELETING TIME-RECORD FOR TIME 0.24076983E-01
DELETING TIME-RECORD FOR TIME 0.26620133E-01
DELETING TIME-RECORD FOR TIME 0.29265465E-01
DELETING TIME-RECORD FOR TIME 0.32011145E-01
DELETING TIME-RECORD FOR TIME 0.34863203E-01
DELETING TIME-RECORD FOR TIME 0.37830557E-01
DELETING TIME-RECORD FOR TIME 0.40922463E-01
DELETING TIME-RECORD FOR TIME 0.44137344E-01
DELETING TIME-RECORD FOR TIME 0.47481808E-01
DELETING TIME-RECORD FOR TIME 0.50962589E-01
DELETING TIME-RECORD FOR TIME 0.54594558E-01
DELETING TIME-RECORD FOR TIME 0.58385150E-01
DELETING TIME-RECORD FOR TIME 0.62359088E-01
DELETING TIME-RECORD FOR TIME 0.66523452E-01
DELETING TIME-RECORD FOR TIME 0.68804369E-01
DELETING TIME-RECORD FOR TIME 0.71498821E-01
DELETING TIME-RECORD FOR TIME 0.74614406E-01
DELETING TIME-RECORD FOR TIME 0.78161085E-01
DELETING TIME-RECORD FOR TIME 0.82117495E-01
DELETING TIME-RECORD FOR TIME 0.86493409E-01
DELETING TIME-RECORD FOR TIME 0.91279391E-01
DELETING TIME-RECORD FOR TIME 0.96476033E-01
DELETING TIME-RECORD FOR TIME 0.10206367
DELETING TIME-RECORD FOR TIME 0.10805208
DELETING TIME-RECORD FOR TIME 0.11445447
DELETING TIME-RECORD FOR TIME 0.12133499
DELETING TIME-RECORD FOR TIME 0.12873941
DELETING TIME-RECORD FOR TIME 0.13675470
DELETING TIME-RECORD FOR TIME 0.14544308
DELETING TIME-RECORD FOR TIME 0.15495431
DELETING TIME-RECORD FOR TIME 0.16561997
DELETING TIME-RECORD FOR TIME 0.17787509
DELETING TIME-RECORD FOR TIME 0.19240719
DELETING TIME-RECORD FOR TIME 0.21036557
DELETING TIME-RECORD FOR TIME 0.23443130
DELETING TIME-RECORD FOR TIME 0.27070025
DELETING TIME-RECORD FOR TIME 0.33547552
DELETING TIME-RECORD FOR TIME 0.41276116
DELETING TIME-RECORD FOR TIME 0.50861425
DELETING TIME-RECORD FOR TIME 0.63495278
DELETING TIME-RECORD FOR TIME 0.81541856
DELETING TIME-RECORD FOR TIME 0.91426374
DELETING TIME-RECORD FOR TIME 1.0967390
DELETING TIME-RECORD FOR TIME 1.4417612
DELETING TIME-RECORD FOR TIME 1.6307377
DELETING TIME-RECORD FOR TIME 1.9963541
DELETING TIME-RECORD FOR TIME 2.7114648
DELETING TIME-RECORD FOR TIME 4.0769542
DELETING TIME-RECORD FOR TIME 6.6739896
DELETING TIME-RECORD FOR TIME 11.677852
DELETING TIME-RECORD FOR TIME 21.553167
DELETING TIME-RECORD FOR TIME 41.303796
DELETING TIME-RECORD FOR TIME 80.805054
DELETING TIME-RECORD FOR TIME 159.80757
DELETING TIME-RECORD FOR TIME 317.81260
DELETING TIME-RECORD FOR TIME 633.82267
DELETING TIME-RECORD FOR TIME 1265.8428
DELETING TIME-RECORD FOR TIME 2196.1016
DELETING TIME-RECORD FOR TIME 3179.7139
DELETING TIME-RECORD FOR TIME 4179.7139
DELETING TIME-RECORD FOR TIME 5179.7139
DELETING TIME-RECORD FOR TIME 6179.7139
DELETING TIME-RECORD FOR TIME 7179.7139
DELETING TIME-RECORD FOR TIME 8179.7139

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

```
TIMESTEP AT 10000.0000 SELECTED
```

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


exb2-plot

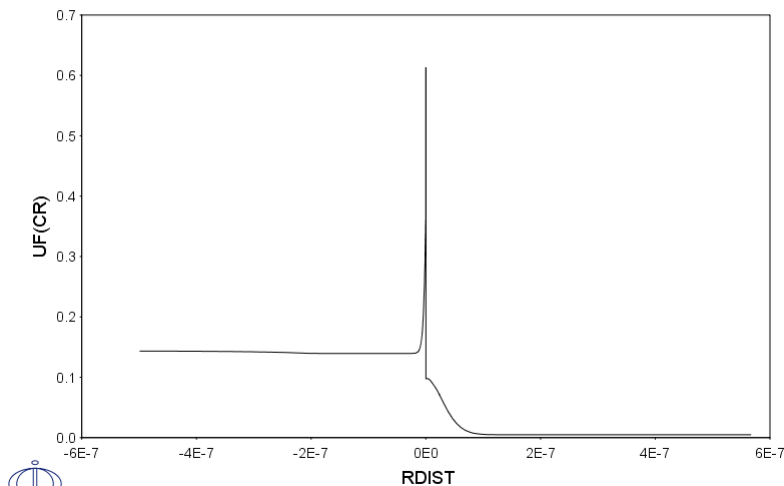
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb2\plot.DCM"DIC>
DIC>
DIC> @@ exb2_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE b2
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go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

POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
```

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

Figure b2.1

2018.02.18.19.03.41
Time=10
CELL#1



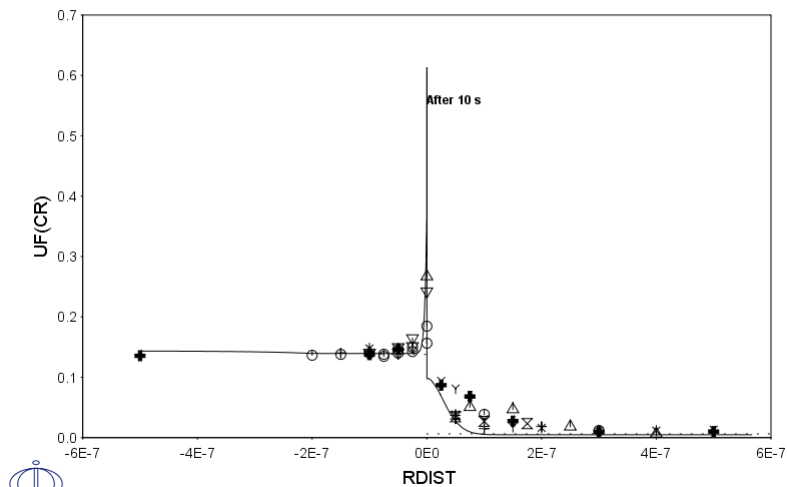
```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: @@
POST-1: @@ INCLUDE EXPERIMENTAL DATA POINTS ON THE PLOT FOR COMPARISON
POST-1: @@
POST-1: @@ FIRST LIST DATASETS
POST-1: @@
POST-1: app y exb2.exp
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: -1
DATASET 1 CONCENTRATION PROFILE T=10S
DATASET 2 CONCENTRATION PROFILE T=100S
DATASET 3 CONCENTRATION PROFILE T=1000S
DATASET 4 CONCENTRATION PROFILE T=10000S
DATASET 5 VOLUME FRACTION CEMENTITE VS. TIME
```

DATASET 6 MEAN PARTICLE DIAMETER VS. TIME

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

Figure b2.2

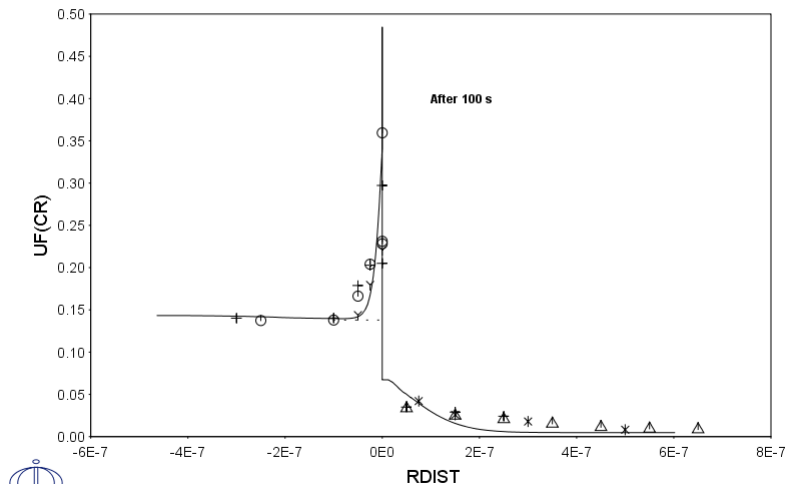
2018.02.18.19.03.42
Time=10
CELL#1



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

Figure b2.3

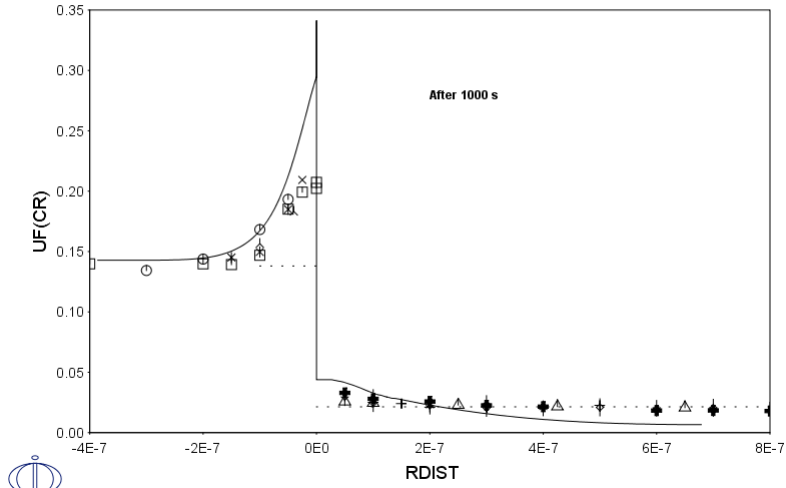
2018.02.18.19.03.43
Time=100
CELL#1



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

Figure b2.4

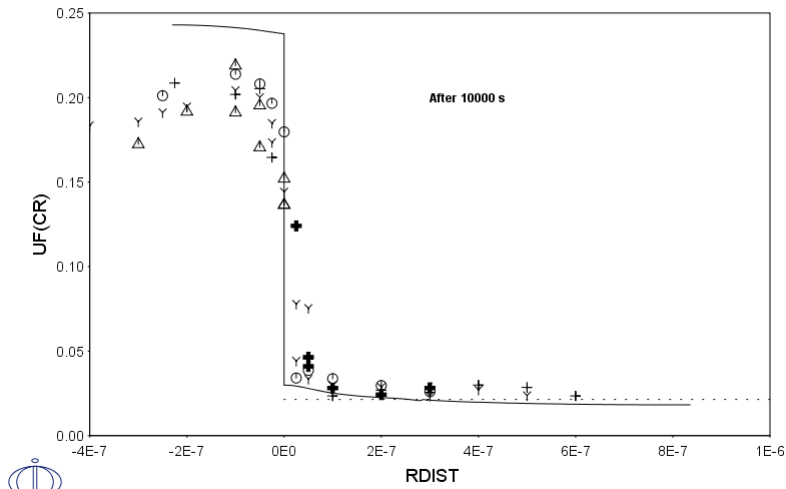
2018.02.18.19.03.44
Time = 1000
CELL #1



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

Figure b2.5

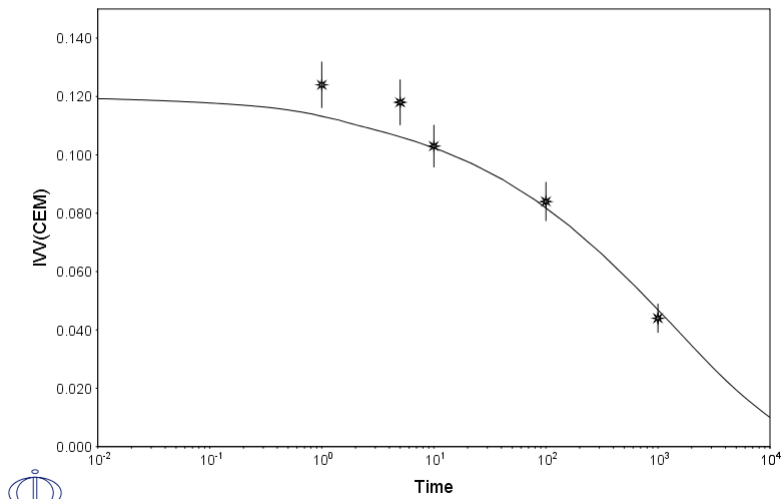
2018.02.18.19.03.45
Time = 10000
CELL #1



```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: @@
POST-1: @@ ALSO PLOT HOW THE VOLUME FRACTION OF CEMENTITE VARIES
POST-1: @@ WITH TIME
POST-1: @@
POST-1: s-d-a y ivv(cem)
POST-1: s-s-s y n 0 .15
POST-1:
POST-1: s-d-a x time
INFO: Time is set as independent variable
POST-1: set-axis-type x log
POST-1: s-s-s x n .01 10000
POST-1:
POST-1: s-p-c integral
POST-1:
POST-1: app y exb2.exp
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 5
POST-1:
POST-1: set-title Figure b2.6
POST-1: plo
```

Figure b2.6

2018.02.18.19.03.46
CELL #1

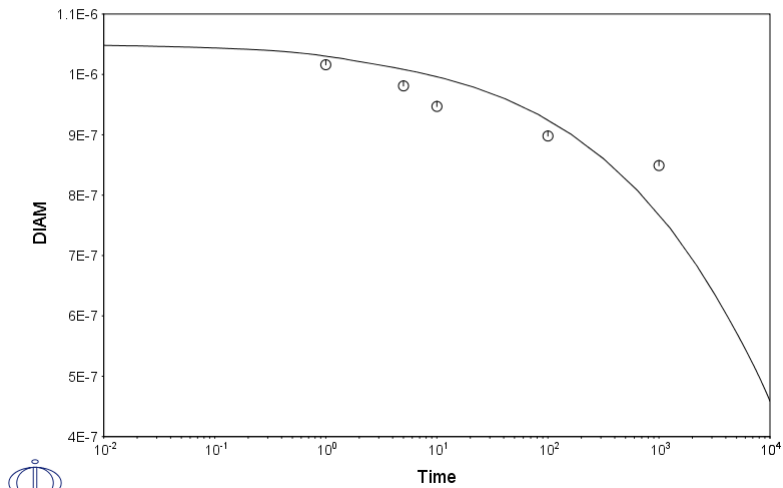


```

POST-1:
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: @@
POST-1: @@ ALSO PLOT HOW THE DIAMETER OF CEMENTITE VARIES WITH TIME
POST-1: @@
POST-1: enter func diam=2*poi(carb,u);
POST-1: s-d-a y diam
POST-1:
POST-1: s-p-c interface carb upper
POST-1:
POST-1: app y exb2.exp
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 6
POST-1:
POST-1: set-title Figure b2.7
POST-1: plo
  
```

Figure b2.7

2018.02.18.19.03.47
UPPER INTERFACE OF REGION "CARB#1"
CELL #1



```

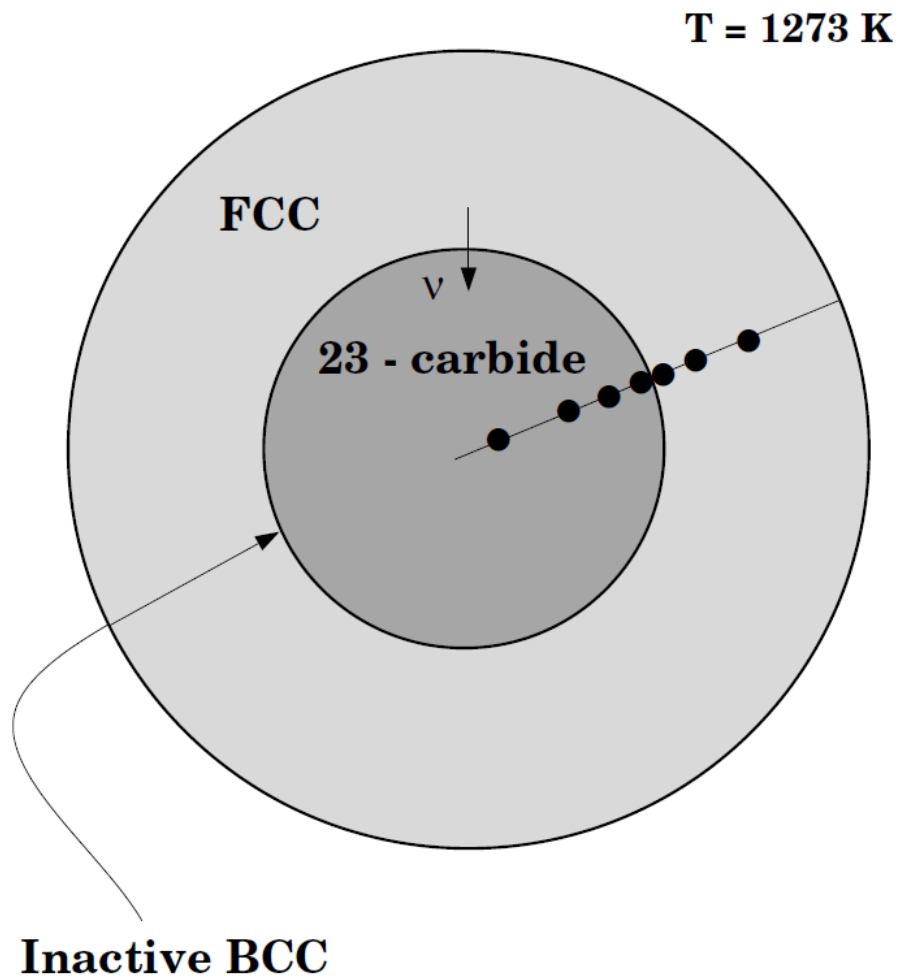
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: set-inter
OK--
POST-1:
  
```



Example exb3

Dissolution of 23-carbide in an austenitic matrix

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



exb3-setup

AboutSYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb3\setup.DCM"

SYS: @@ Moving boundary example.

SYS: @@ Dissolution of 23-carbide in an austenitic matrix

SYS: @@ This example calculates the dissolution of an M23C6 particle in an

SYS: @@ austenite matrix. A film of ferrite is allowed to nucleate around the

SYS: @@ carbide during the precipitation.

SYS: -----

NO SUCH COMMAND, USE HELP

SYS:

SYS: @@

SYS: @@ RETRIEVE DATA FROM THE DATABASES

SYS: @@

SYS: go da

THERMODYNAMIC DATABASE module

Current database: Steels/Fe-Alloys v9.0

VA /- DEFINED
L12_FCC B2_BCC DICTRA_FCC_A1

REJECTED

TDB_TCFE9:

TDB_TCFE9: @@

TDB_TCFE9: @@ USE A DATABASE FOR THERMODYNAMIC DATA

TDB_TCFE9: @@

TDB_TCFE9: sw fedemo

Current database: Iron Demo Database v2.0

VA /- DEFINED

TDB_FEDEMO: def-sys fe c cr

FE C CR

DEFINED

TDB_FEDEMO: rej ph *

GAS:G LIQUID:L BCC_A2
CEMENTITE CHI_A12 DIAMOND_FCC_A4
FCC_A1 GRAPHITE HCP_A3
KSI_CARBIDE LAVES_PHASE_C14 M23C6
M3C2 M5C2 M7C3

SIGMA REJECTED

TDB_FEDEMO: res ph fcc bcc m23

FCC_A1 BCC_A2 M23C6

RESTORED

TDB_FEDEMO: get

REINITIATING GES

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

FUNCTIONS

List of references for assessed data

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

-OK-

TDB_FEDEMO:

TDB_FEDEMO: @@

TDB_FEDEMO: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE THE MOBILITY DATA

TDB_FEDEMO: @@

TDB_FEDEMO: app mfedemo

Current database: Fe-Alloys Mobility demo database v2.0

VA DEFINED

APP: def-sys c cr fe

C CR FE

DEFINED

APP: rej ph *

BCC_A2 FCC_A1 REJECTED

APP: res ph fcc bcc

FCC_A1 BCC_A2 RESTORED

APP: get

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

FUNCTIONS

List of references for assessed data

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

-OK-

APP:

APP: @@

```

APP: @@ ENTER THE DICTRA MONITOR
APP: @@
APP: go d-m
NO TIME STEP DEFINED
*** ENTERING M23C6 AS A DIFFUSION NONE PHASE
DIC>
DIC>
DIC> @@ THE MOBILITY DATABASE LACKS KINETIC DATA FOR THE M23-CARBIDE
DIC> @@ SO AN ESTIMATE FOR THE MOBILITIES IN THIS PHASE ARE ENTERED.
DIC> ent-mob-est M23 c
M[M23,C] (T)= 0;
DIC>
DIC> ent-mob-est M23 cr
M[M23,CR] (T)= 3e-11*exp(-278000/8.3145/T);
DIC>
DIC> ent-mob-est M23 fe
M[M23,FE] (T)= 1e-11*exp(-275000/8.3145/T);
DIC>
DIC> @@
DIC> @@ ENTER GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 1273; * N

DIC>
DIC> @@
DIC> @@ ENTER THE REGIONS carbide AND matrix
DIC> @@
DIC> enter-region carbide
DIC> enter-region matrix
ATTACH TO REGION NAMED /CARBIDE/:
ATTACHED TO THE RIGHT OF CARBIDE /YES/:
DIC> @@
DIC> @@ ASSUME SOME REASONABLE SIZE OF THE CARBIDE PARTICLE
DIC> @@
DIC> enter-grid carbide 5.00000000E-7 AUTO
DIC> @@
DIC> @@ THE SIZE OF THE FCC REGION WE CAN CALCULATE FROM A MASS BALANCE
DIC> @@ AFTER ESTIMATING THE INITIAL COMPOSITIONS IN THE TWO PHASES.
DIC> @@
DIC> enter-grid matrix 5.55859755E-7 AUTO
DIC> @@
DIC> @@ ENTER PHASES INTO THE REGION MATRIX. BOUNDARY CONDITIONS ARE GIVEN
DIC> @@ IF THE INACTIVE PHASE bcc IS NUCLEATED
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /CARBIDE/: matrix
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inact
ATTACH TO REGION NAMED /MATRIX/: matrix
ATTACHED TO THE RIGHT OF MATRIX /YES/: no
PHASE NAME: /NONE/: bcc#1
DEPENDENT COMPONENT ? /FE/: fe
REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/:
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> @@
DIC> @@ ENTER THE PHASE INTO THE REGION carbide
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /CARBIDE/: carbide
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: m23c6
DIC>
DIC> @@
DIC> @@ ENTER COMPOSITIONS INTO THE PHASES
DIC> @@
DIC> enter-composition
REGION NAME : /CARBIDE/: carbide
PHASE NAME: /M23C6/: m23c6
DEPENDENT COMPONENT ? /FE/: fe
COMPOSITION TYPE /MOLE_FRACTION/: mole-fraction
PROFILE FOR /CR/: cr lin 0.55079807 0.55079807
DIC>
DIC>
DIC> enter-composition
REGION NAME : /MATRIX/: matrix
PHASE NAME: /FCC_A1#1/: fcc#1
DEPENDENT COMPONENT ? /FE/: fe
COMPOSITION TYPE /MOLE_FRACTION/: mole-fraction
PROFILE FOR /C/: cr lin 8.5203899E-2 8.5203899E-2
PROFILE FOR /CR/: c lin 1.8072433E-4 1.8072433E-4
DIC>
DIC> @@
DIC> @@ SET TO A SPHERICAL GEOMETRY
DIC> @@
DIC> enter-geo
GEOMETRICAL EXPONENT /0/: 2
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME AND OTHER SIMULATION PARAMETERS
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 8000
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /800/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exb3 Y
DIC>
DIC>
DIC>
DIC> set-inter

```


exb3-run

DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb3\run.DCM"DIC>

DIC>
DIC> @@ exb3_run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING EXAMPLE b3
DIC> @@
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA MONITOR AND READ THE SET UP FROM FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 0.00000E+00

DIC> read exb3

OK

DIC>

DIC> @@

DIC> @@ WHEN THE FERRITE NUCLEATES WE USE DEFAULT VALUES

DIC> @@ AS STARTING VALUES FOR THE WIDTH OF THE NEW REGION

DIC> @@ AND THE VELOCITY OF THE INTERFACES

DIC> @@

DIC>

DIC> @@

DIC> @@ START THE SIMULATION

DIC> @@

DIC> sim yes

Region: CARBIDE

single geometric dense at 0.50000E-06

0.83296 92

Region: MATRIX

single geometric dense at 0.0000

1.0051 62

Trying old scheme 4

GENERATING STARTING VALUES FOR CELL # 1 INTERFACE # 2

DETERMINING INITIAL EQUILIBRIUM VALUES

CALCULATING STARTING VALUES: 9 EQUILIBRIUM CALCULATIONS

DONE 6 OUT OF 9

U-FRACTION IN SYSTEM: C = .0278637912207471 CR = .149918318671311

FE = .850081681459196

TOTAL SIZE OF SYSTEM: 4.93068569406E-18 [m^3]

U-FRACTION IN SYSTEM: C = .0278637912207471 CR = .149918318671311

FE = .850081681459196

TOTAL SIZE OF SYSTEM: 4.93068569406E-18 [m^3]

0.565663007975143 0.565797019192577 0.565663812089356 1.015925208865390E-002 3.012654895008019E-

004 4.777345249237744E-005 2.965739032002669E-006 7.215362048263626E-007 8.262638023301182E-

007 4.246506051605422E-008 4.119324775682431E-008 3.974271203721860E-008 4.355497133554406E-

008 3.870625295026483E-008 3.673410108968729E-008 3.294771044059294E-008 3.668595704949160E-

008 2.600355360941065E-008 1.460917533598369E-008 1.658190571554172E-009 4.335933723645985E-

012 1.279149078571039E-015 2.899183529819540E-017 TIME = 0.100000000E-06 DT = 0.100000000E-

06 SUM OF SQUARES = 0.28991835E-16

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.17310735E-02 AND -0.17310735E-02

POSITION OF INTERFACE CARBIDE / MATRIX IS 0.49982689E-06

U-FRACTION IN SYSTEM: C = .0278769048021911 CR = .149918499752463

FE = .850081500378044

TOTAL SIZE OF SYSTEM: 4.93068569406E-18 [m^3]

16 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: CARBIDE

CPU time used in timestep 1 seconds

1.096405342623862E-004 1.0966264445879963E-004 1.096405350851704E-004 5.301312531052159E-008 2.238795214918746E-

008 6.726062310361936E-011 8.232621485718108E-014 3.182662037225323E-019 TIME = 0.300000000E-06 DT = 0.200000000E-

06 SUM OF SQUARES = 0.3182620E-18

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.29934902E-05 AND -0.29934902E-05

POSITION OF INTERFACE CARBIDE / MATRIX IS 0.49982629E-06

U-FRACTION IN SYSTEM: C = .0278774003819474 CR = .149918500361418

FE = .850081499769089

TOTAL SIZE OF SYSTEM: 4.93068569406E-18 [m^3]

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

CPU time used in timestep 1 seconds

1.217834959639798E-004 1.217822143860332E-004 1.217736602728715E-004 6.952194334566076E-007 2.897690349262264E-

009 5.944810708355392E-012 3.496240359029881E-016 2.032256660449822E-022 TIME = 0.700000000E-06 DT = 0.400000000E-

06 SUM OF SQUARES = 0.20322567E-21

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.28086480E-05 AND -0.28086480E-05

POSITION OF INTERFACE CARBIDE / MATRIX IS 0.49982517E-06

U-FRACTION IN SYSTEM: C = .0278774419496498 CR = .149918501468152

FE = .850081498662355

TOTAL SIZE OF SYSTEM: 4.93068569406E-18 [m^3]

CPU time used in timestep 0 seconds

6.892011300109831E-006 6.891932131748709E-006 6.890942061713327E-006

output ignored...

... output resumed

3.596091136776303E-008 8.216033691580668E-012 6.248152751737216E-

017 TIME = 5410.4257 DT = 800.00000 SUM OF SQUARES = 0.62481528E-16

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.74030235E-12 AND -0.74030235E-12

POSITION OF INTERFACE CARBIDE / MATRIX IS 0.39236306E-06

U-FRACTION IN SYSTEM: C = .0277635741857872 CR = .149675658318268

FE = .850324341812239

TOTAL SIZE OF SYSTEM: 4.93068569406E-18 [m^3]

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

CPU time used in timestep 1 seconds

7.397554469224484E-008 7.399690832891322E-008 7.390401694592549E-008 4.729538433889559E-008 3.738284861005563E-

008 1.904030934350095E-008 7.062238354706955E-010 1.249316828613806E-015 9.774450116579076E-

022 TIME = 6210.4257 DT = 800.00000 SUM OF SQUARES = 0.97744501E-21

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.30089948E-12 AND -0.30089948E-12

POSITION OF INTERFACE CARBIDE / MATRIX IS 0.39212234E-06

U-FRACTION IN SYSTEM: C = .0277635755152104 CR = .149675658812231

FE = .850324341318276

TOTAL SIZE OF SYSTEM: 4.93068569406E-18 [m^3]

CPU time used in timestep 1 seconds

2.558036433460315E-008 2.558546174339629E-008 2.553729557831349E-008 1.697014320315236E-008 1.554273078104043E-

008 1.249746186331826E-008 7.595600812641111E-009 7.591676980921429E-009 1.359289190143328E-

009 1.010790598659928E-015 6.469467549519251E-

020 TIME = 7010.4257 DT = 800.00000 SUM OF SQUARES = 0.64694675E-19

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.48195675E-13 AND -0.48195675E-13

POSITION OF INTERFACE CARBIDE / MATRIX IS 0.39208379E-06

U-FRACTION IN SYSTEM: C = .0277635745417878 CR = .149675659024147
FE = .85032434110636
TOTAL SIZE OF SYSTEM: 4.93068569406E-18 [m^3]
1 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: MATRIX

CPU time used in timestep 1 seconds
8.755707216979695E-009 8.756183722699488E-009 8.729902660904552E-009 5.724347401567462E-009 5.650604863023250E-
009 5.461702834959989E-009 5.134317922419642E-009 5.136158545777380E-009 4.471776075599300E-
009 3.316831595143683E-009 1.518492536949695E-009 1.518354498850523E-009 4.843822582897689E-
012 1.867506911066414E-018 TIME = 7810.4257 DT = 800.00000 SUM OF SQUARES = 0.18675069E-17
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.97015850E-13 AND 0.97015850E-13
POSITION OF INTERFACE CARBIDE / MATRIX IS 0.39216140E-06
U-FRACTION IN SYSTEM: C = .0277635652652809 CR = .1496756590339302
FE = .850324341091205
TOTAL SIZE OF SYSTEM: 4.93068569406E-18 [m^3]
30 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: CARBIDE

CPU time used in timestep 1 seconds
7.291179747246321E-008 7.290978922893142E-008 7.324387881826405E-008 2.924239425496701E-008 2.882473950708875E-
008 2.785550866674718E-008 2.609831532441511E-008 2.608909518860428E-008 2.264366027348484E-
008 1.655035603339147E-008 7.188348968447023E-009 3.836741804380008E-016 1.042063658795509E-
018 TIME = 8000.0000 DT = 189.57432 SUM OF SQUARES = 0.10420637E-17
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.40784293E-12 AND 0.40784293E-12
POSITION OF INTERFACE CARBIDE / MATRIX IS 0.39223872E-06
U-FRACTION IN SYSTEM: C = .0277635584898389 CR = .149675659044322
FE = .850324341086185
TOTAL SIZE OF SYSTEM: 4.93068569406E-18 [m^3]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 45.271088
DELETING TIME-RECORD FOR TIME 68.248413
DELETING TIME-RECORD FOR TIME 68.248423
DELETING TIME-RECORD FOR TIME 68.248443
DELETING TIME-RECORD FOR TIME 68.248483
DELETING TIME-RECORD FOR TIME 68.248563
DELETING TIME-RECORD FOR TIME 68.248723
DELETING TIME-RECORD FOR TIME 68.249043
DELETING TIME-RECORD FOR TIME 68.249683
DELETING TIME-RECORD FOR TIME 68.250963
DELETING TIME-RECORD FOR TIME 68.253523
DELETING TIME-RECORD FOR TIME 68.258643
DELETING TIME-RECORD FOR TIME 68.268883
DELETING TIME-RECORD FOR TIME 68.289363
DELETING TIME-RECORD FOR TIME 68.330323
DELETING TIME-RECORD FOR TIME 68.412243
DELETING TIME-RECORD FOR TIME 68.576083
DELETING TIME-RECORD FOR TIME 68.903763
DELETING TIME-RECORD FOR TIME 69.559123
DELETING TIME-RECORD FOR TIME 70.869843
DELETING TIME-RECORD FOR TIME 73.491283
DELETING TIME-RECORD FOR TIME 78.734163
DELETING TIME-RECORD FOR TIME 89.219923
DELETING TIME-RECORD FOR TIME 110.19144
DELETING TIME-RECORD FOR TIME 152.13448
DELETING TIME-RECORD FOR TIME 236.02056
DELETING TIME-RECORD FOR TIME 403.79272
DELETING TIME-RECORD FOR TIME 739.33704
DELETING TIME-RECORD FOR TIME 1410.4257
DELETING TIME-RECORD FOR TIME 2210.4257
DELETING TIME-RECORD FOR TIME 3010.4257
DELETING TIME-RECORD FOR TIME 3810.4257
DELETING TIME-RECORD FOR TIME 4610.4257
DELETING TIME-RECORD FOR TIME 5410.4257
DELETING TIME-RECORD FOR TIME 6210.4257
DELETING TIME-RECORD FOR TIME 7010.4257

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

TIMESTEP AT 8000.00000 SELECTED

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

exb3-plot

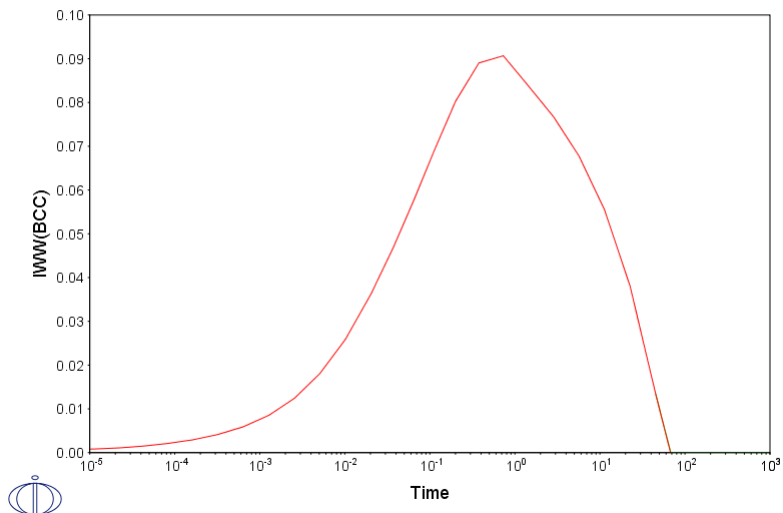
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb3\plot.DCM"DIC>
DIC>
DIC> @@ exb3_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE b3
DIC> @@
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA MODULE AND SPECIFY THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 8.00000E+03
DIC> read exb3
OK
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA POST PROCESSOR
DIC> @@
DIC> post
```

POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson

```
POST-1:
POST-1: @@
POST-1: @@ LET US SEE HOW THE AMOUNT OF FERRITE VARIED DURING THE
POST-1: @@ SIMULATION
POST-1: @@
POST-1: s-d-a y iww(bcc)
POST-1: s-d-a x time
INFO: Time is set as independent variable
POST-1: s-ax-typ x log
POST-1: s-s-s x n 1E-5 1E3
POST-1: s-s-s y n 0 0.1
POST-1:
POST-1: set-tit Figure b3.1
POST-1:
POST-1: plot
```

Figure b3.1

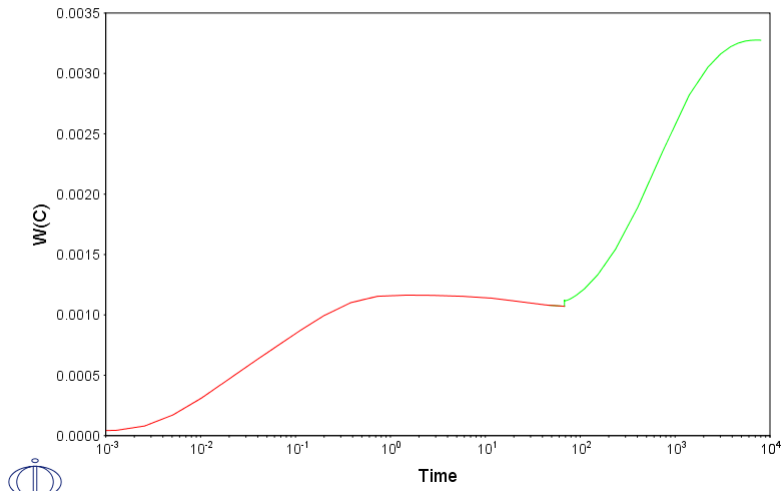
2018.02.18.19.13.11
CELL #1



```
POST-1:
POST-1:
POST-1: @?<_hit_return_to_continue_>
POST-1:
POST-1: @@
POST-1: @@ NOW LOOK AT THE ALLOYING ELEMENTS AT THE UPPER BOUND OF THE SYSTEM
POST-1: @@
POST-1: s-d-a y w(c)
POST-1: s-s-s x n 1E-3 1E4
POST-1: s-p-c interface last
POST-1:
POST-1: set-tit Figure b3.2
POST-1:
POST-1: plot
```

Figure b3.2

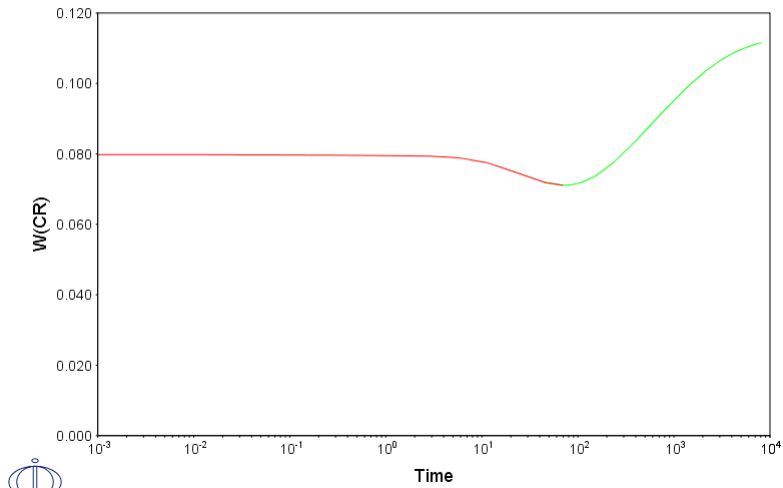
2018.02.18.19.13.12
UPPER INTERFACE OF REGION "LAST"
CELL #1



```
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: s-d-a y w(cr)
POST-1: s-s-s y n 0 0.12
POST-1:
POST-1: set-tit Figure b3.3
POST-1:
POST-1: plot
```

Figure b3.3

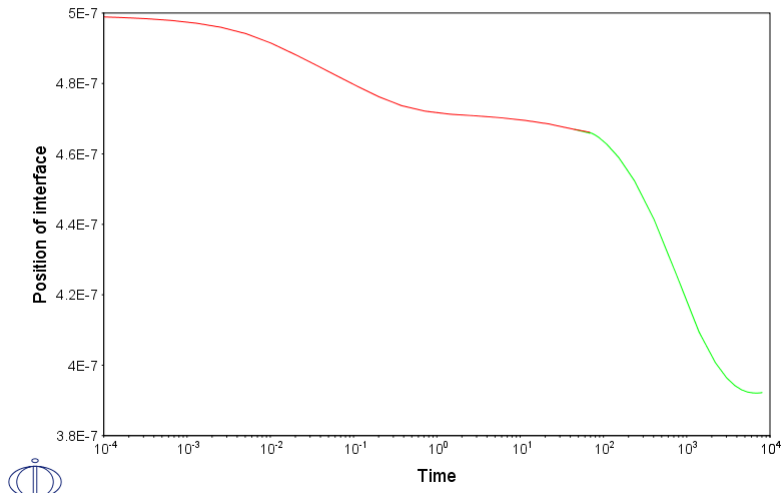
2018.02.18.19.13.13
UPPER INTERFACE OF REGION "LAST"
CELL #1



```
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: @@
POST-1: @@ AND FINALLY LOOK AT THE CHANGE OF RADIUS OF THE M23-CARBIDE
POST-1: @@
POST-1: s-d-a y position carbide upper
POST-1: s-s-s x n 1E-4 1E4
POST-1:
POST-1: set-tit Figure b3.4
POST-1:
POST-1: plot
```

Figure b3.4

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



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



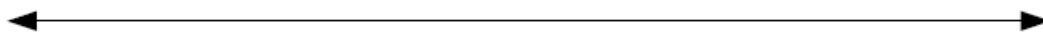
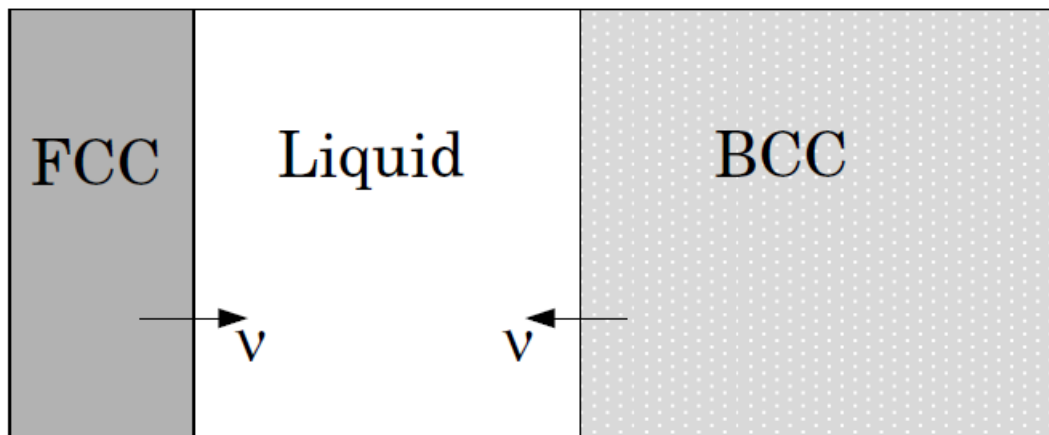
Example exb4a

Solidification path of a Fe-18%Cr-8%Ni alloy: Eutectic reaction

This example demonstrates the solidification path of an Fe-18%Cr-8%Ni alloy. A eutectic reaction is assumed, LIQUID $\rightarrow$ BCC + FCC. Hence the BCC and FCC regions should be on separate sides of the liquid region. Comparison is made with both a Scheil-Gulliver simulation and equilibrium solidification conditions, both made with Thermo-Calc.

Time > 0

T = 1900 - 1 * Time K



1E-4

exb4a-setup

About Stockholm, Sweden

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

```
SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb4a\setup.DCM" @@
SYS: @@ Moving boundary problem.
SYS: @@ Solidification path of an Fe-18%Cr-8%Ni alloy: Eutectic reaction
SYS: @@ This example demonstrates the solidification path of an Fe-18%Cr-8%Ni
SYS: @@ alloy. A eutectic reaction is assumed, LIQUID -> BCC + FCC. Hence the
SYS: @@ BCC and FCC regions should be on separate sides of the liquid region.
SYS: @@ Comparison is made with both a Scheil-Gulliver simulation and equilibrium
SYS: @@ solidification conditions, both done in Thermo-Calc.
SYS: -----
NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exb4a_setup.DCM
SYS:
SYS:
SYS: @@
SYS: @@ START BY GOING TO THE DATABASE MODULE
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Current database: Steels/Fe-Alloys v9.0

VA                /- DEFINED
L12_FCC            B2_BCC                DICTRA_FCC_A1
REJECTED

TDB_TCFE9:
TDB_TCFE9: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA
TDB_TCFE9: sw fedemo
Current database: Iron Demo Database v2.0

VA                /- DEFINED
TDB_FEDEMO:
TDB_FEDEMO: @@ DEFINE THE SYSTEM TO WORK WITH
TDB_FEDEMO: def-sys fe ni cr
FE                NI                CR
DEFINED
TDB_FEDEMO:
TDB_FEDEMO: @@ EXCLUDE THE THERMODYNAMIC DATA FOR THE PHASES THAT ARE NOT NEEDED
TDB_FEDEMO: rej ph /all
LIQUID:L          BCC_A2                CHI_A12
FCC_A1            HCP_A3                LAVES_PHASE_C14
SIGMA REJECTED
TDB_FEDEMO: res ph fcc liq bcc
FCC_A1            LIQUID:L                BCC_A2
RESTORED
TDB_FEDEMO:
TDB_FEDEMO: @@ RETRIEVE DATA FROM THE DATABASE FILE
TDB_FEDEMO: get
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

List of references for assessed data

'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
'X.-G. Lu, M. Selleby, B. Sundman, CALPHAD, 29 (2005) 49-55; Fe P-T diagram'
'J. Brillo and I. Egry, Int. J. Thermophysics, 24, 1155-1170'
'B.-J. Lee, CALPHAD, 17 (1993) 251-268; revision of Fe-Cr and Fe -Ni liquid'
'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
'B.-J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
volumes'
'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270
(1986); CR-FE'
'A. Dinsdale and T. Chart, MTDS NPL, Unpublished work (1986); CR -NI'
'A. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); FE-NI'
-OK-
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ MOBILITY/DIFFUSIVITY DATA ARE STORED IN A SEPARATE DATABASE FILE.
TDB_FEDEMO: @@ SWITCH TO A MOBILITY DATABASE AND APPEND THE DATA
TDB_FEDEMO: @@
TDB_FEDEMO: app
Use one of these databases

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

```

TCMG3 = Mg-Alloys v3.0
TCMG2 = Mg-Alloys v2.0
TCMG1 = Mg-Alloys v1.1
TCTI1 = Ti-Alloys v1.0
TCCU2 = Cu-Alloys v2.0
TCCU1 = Cu-Alloys v1.0
TCCC1 = Cemented carbide v1.0
TCHEA2 = High Entropy Alloy v2.1
TCHEA1 = High Entropy Alloy v1.0
SSOL6 = SGTE Alloy Solutions Database v6.0
SSOL5 = SGTE Alloy Solutions Database v5.0
SSOL4 = SGTE Alloy Solutions Database v4.9g
SSOL2 = SGTE Alloy Solutions Database v2.1
SSUB6 = SGTE Substances Database v6.0
SSUB5 = SGTE Substances Database v5.2
SSUB4 = SGTE Substances Database v4.1
SSUB3 = SGTE Substances Database v3.3
SSUB2 = SGTE Substances Database v2.2
SNOB3 = SGTE Noble Metal Alloys Database v3.1
STBC2 = SGTE Thermal Barrier Coating TDB v2.2
STBC1 = SGTE Thermal Barrier Coating TDB v1.1
SALT1 = SGTE Molten Salts Database v1.2
SEMC2 = TC Semi-Conductors v2.1
SLAG4 = Fe-containing Slag v4.1
SLAG3 = Fe-containing Slag v3.2
SLAG2 = Fe-containing Slag v2.2
SLAG1 = Fe-containing Slag v1.2
TCOX7 = Metal Oxide Solutions v7.0
TCOX6 = Metal Oxide Solutions v6.0
TCOX5 = Metal Oxide Solutions v5.1
TCOX4 = Metal Oxide Solutions v4.1
ION3 = Ionic Solutions v3.0
ION2 = Ionic Solutions v2.6
ION1 = Ionic Solutions v1.5
NOX2 = NPL Oxide Solutions Database v2.1
TCNOBL1 = Noble Metals Alloys v1.0
TCSLD3 = Solder Alloys v3.2
TCSLD2 = Solder Alloys v2.0
TCSI1 = Ultrapure Silicon v1.2
TCMP2 = Materials Processing v2.5
TCES1 = Combustion/Sintering v1.1
TCSC1 = Super Conductor v1.0
TCFC1 = SOFC Database v1.0
NUMT2 = Nuclear Materials v2.1
NUOX4 = Nuclear Oxides v4.2
NUCL15 = IRSN NUCLEA-15_4
NUCL10 = ThermoData NUCLEA Alloys-oxides TDB v10.2
MEPH15 = IRSN Mephista-15_1
MEPH11 = ThermoData MEPHISTA Nuclear Fuels TDB v11.2
TCAQ3 = Aqueous Solution v3.0
TCAQ2 = Aqueous Solution v2.6
AQS2 = TGG Aqueous Solution Database v2.6
GCE2 = TGG Geochemical/Environmental TDB v2.3
FEDEMO = Iron Demo Database v2.0
ALDEMO = Aluminum Demo Database v2.0
NIDEMO = Nickel Demo Database v1.0
CUDEMO = Copper Demo Database v1.0
SLDEMO = Solder Demo Database v1.0
OXDEMO = Oxide Demo Database v1.0
SUBDEMO = Substance Demo Database v1.0
PTERN = Public Ternary Alloys TDB v1.3
PAQ2 = Public Aqueous Soln (SIT) TDB v2.4
PG35 = G35 Binary Semi-Conductors TDB v1.2
PURE5 = SGTE Unary (Pure Elements) TDB v5.1
MOB2 = Alloys Mobility v2.7
MOB1 = Alloys Mobility v1.3
MOBFE1 = Steels/Fe-Alloys Mobility v1.0
MOBFE2 = Steels/Fe-Alloys Mobility v2.0
MOBFE3 = Steels/Fe-Alloys Mobility v3.0
MOBFE4 = Steels/Fe-Alloys Mobility v4.0
MOBNI4 = Ni-Alloys Mobility v4.0
MOBNI3 = Ni-Alloys Mobility v3.1
MOBNI2 = Ni-Alloys Mobility v2.4
MOBNI1 = Ni-Alloys Mobility v1.0
MOBAL3 = Al-Alloys Mobility v3.0
MOBAL2 = Al-Alloys Mobility v2.0
MOBAL1 = Al-Alloys Mobility v1.0
MOBCU1 = Cu-Alloys Mobility v1.0
MOBCU2 = Cu-Alloys Mobility v2.0
MOBMC1 = Mg-Alloys Mobility v1.0
MOBSI1 = Si-Alloys Mobility v1.0
MOBSLD1 = Solder-Alloys Mobility v1.0
MOBTI2 = Ti-Alloys Mobility v2.0 SNAPSHOT
MOBTI1 = Ti-Alloys Mobility v1.0
MALDEMO = Al-Alloys Mobility demo database v1.0
MFEDEMO = Fe-Alloys Mobility demo database v2.0
MNIDEMO = Ni-Alloys Mobility demo database v1.0
MCUDEMO = Cu-Alloys Mobility demo database v1.0
USER = User defined Database

```

```

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

```

```

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

```

List of references for assessed data

```

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

```



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

DIC>
DIC> @@
DIC> @@ ENTER A REGION CALLED smalta
DIC> @@
DIC> enter-region smalta
DIC>
DIC> @@
DIC> @@ ENTER A DOUBLE GEOMETRIC GRID INTO THE REGION
DIC> @@
DIC> enter-grid
REGION NAME : /SMALTA/: smalta
WIDTH OF REGION /1/: 1e-4
TYPE /LINEAR/: AUTO
DIC>
DIC>
DIC> @@
DIC> @@ ENTER active PHASES INTO THE REGION
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /SMALTA/: smalta
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: liq
SETTING CHECK INTERFACE POSITION ON
DIC>
DIC> @@
DIC> @@ ENTER inactive PHASES INTO THE REGION; ONE PHASE ON EACH SIDE OF THE LIQUID
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inact
ATTACH TO REGION NAMED /SMALTA/: smalta
ATTACHED TO THE RIGHT OF SMALTA /YES/: no
PHASE NAME: /NONE/: fcc#1
DEPENDENT COMPONENT ? /NI/: fe
    REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-5
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inact
ATTACH TO REGION NAMED /SMALTA/: smalta
ATTACHED TO THE RIGHT OF SMALTA /YES/: yes
PHASE NAME: /NONE/: bcc#1
DEPENDENT COMPONENT ? /NI/: fe
    REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-5
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> @@
DIC> @@ ENTER A START COMPOSITION FOR THE LIQUID
DIC> @@
DIC> enter-composition
REGION NAME : /SMALTA/: smalta
PHASE NAME: /LIQUID/: liq
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /CR/: cr lin 18 18
PROFILE FOR /NI/: ni lin 8 8
DIC>
DIC> @@
DIC> @@ THE BOUNDARY CONDITION IS A CLOSED SYSTEM (THE DEFAULT) AS WE DO NOT SPECIFY
DIC> @@ ANYTHING ELSE.
DIC> @@
DIC>
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 200
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /20/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC> @@
DIC> @@ CHECK THE INTERFACE POSITION. THIS IS TO MAKE SURE THAT THE
DIC> @@ LIQUID REGION DOES NOT SHRINK TOO MUCH DURING A TIMESTEP.
DIC> @@ IN ADDITION THE TIMESTEP IS CONTROLLED BY THE PHASE INTERFACE
DIC> @@ DISPLACEMENT DURING THE SIMULATION.
DIC> @@
DIC> s-s-c
NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDF: /2/:
CHECK INTERFACE POSITION /YES/: yes
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:

```

```
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (0 -> 0.5 -> 1): /.5/:
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /NO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/:
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exb4a Y
DIC>
DIC> set-inter
--OK--
DIC>
```

exb4a-run

DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb4a\run.DCM"DIC>

DIC>

DIC> @@ exb4a_run.DCM

DIC>

DIC> @@

DIC> @@ FILE FOR RUNNING EXAMPLE b4a

DIC> @@

DIC>

DIC> @@

DIC> @@ ENTER THE DICTRA MONITOR AND READ THE SET UP FROM FILE

DIC> @@

DIC> go d-m

TIME STEP AT TIME 0.00000E+00

DIC> read exb4a

OK

DIC>

DIC> @@

DIC> @@ START THE SIMULATION

DIC> @@

DIC> sim yes

Region: SMALTA

double geometric

dense at outer boundaries, coarse at 0.50000E-04

lower part 1.2500 22

upper part 0.80000 22

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882254

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

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882254

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

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

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882254

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

CPU time used in timestep 0 seconds

TIME = 0.65057363E-05 DT = 0.64057363E-05 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882254

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

CPU time used in timestep 0 seconds

TIME = 0.19317209E-04 DT = 0.12811473E-04 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882254

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

CPU time used in timestep 0 seconds

TIME = 0.44940154E-04 DT = 0.25622945E-04 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882254

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

CPU time used in timestep 0 seconds

TIME = 0.96186044E-04 DT = 0.51245890E-04 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882254

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

CPU time used in timestep 1 seconds

TIME = 0.19867782E-03 DT = 0.10249178E-03 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882254

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

CPU time used in timestep 0 seconds

TIME = 0.40366139E-03 DT = 0.20498356E-03 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882254

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

CPU time used in timestep 0 seconds

TIME = 0.81362851E-03 DT = 0.40996712E-03 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882254

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

CPU time used in timestep 0 seconds

TIME = 0.16335628E-02 DT = 0.81993424E-03 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882254

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

CPU time used in timestep 0 seconds

TIME = 0.32734312E-02 DT = 0.16398685E-02 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882254

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

CPU time used in timestep 0 seconds

TIME = 0.65531682E-02 DT = 0.32797370E-02 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882254

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

CPU time used in timestep 0 seconds

TIME = 0.13112642E-01 DT = 0.65594740E-02 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882254

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

CPU time used in timestep 0 seconds

TIME = 0.26231590E-01 DT = 0.13118948E-01 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882255

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

CPU time used in timestep 0 seconds

TIME = 0.52469486E-01 DT = 0.26237896E-01 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882254

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

CPU time used in timestep 0 seconds

TIME = 0.10494528 DT = 0.52475792E-01 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882255

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

CPU time used in timestep 0 seconds

TIME = 0.20989686 DT = 0.10495158 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992482 FE = .733068011219292
NI = .0754116207882253

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

CPU time used in timestep 0 seconds

TIME = 0.41980003 DT = 0.20990317 SUM OF SQUARES = 0.0000000

```
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292
NI = .0754116207882252
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.83960636 DT = 0.41980633 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992484 FE = .733068011219292
NI = .0754116207882248
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 1.6792190 DT = 0.83961267 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291
NI = .0754116207882252
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 3.3584444 DT = 1.6792253 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .191520367992488 FE = .73306801121929
```

output ignored...

... output resumed

```
5.514005299448755E-006 5.509376563838510E-006 7.547294441383454E-010 5.022583224199097E-014 5.481369063070259E-
019 TIME = 178.06453 DT = 1.3107200 SUM OF SQUARES = 0.54813691E-18
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.60791645E-07 AND -0.60791645E-07
POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS 0.64305088E-05
U-FRACTION IN SYSTEM: CR = .191499811939236 FE = .733100727058195
NI = .0753994610025692
TOTAL SIZE OF SYSTEM: 1E-04 [m]
2 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: R_BCC_A2
CPU time used in timestep 2 seconds
1.053156852724598E-005 1.053152073815954E-005 1.052555445432811E-005 4.057250259300867E-007 3.528412544722028E-
011 3.011930265008765E-016 4.421460299214064E-
021 TIME = 180.68597 DT = 2.6214400 SUM OF SQUARES = 0.44214603E-20
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.44074694E-07 AND -0.44074694E-07
POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS 0.63149697E-05
U-FRACTION IN SYSTEM: CR = .191499811958015 FE = .73310072702147
NI = .075399461020515
TOTAL SIZE OF SYSTEM: 1E-04 [m]
3 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: R_BCC_A2
CPU time used in timestep 3 seconds
7.659975284018353E-006 7.660132765574592E-006 7.656721414781887E-006 1.049739953313493E-006 2.121510544843710E-
007 2.260034806150486E-012 4.796864873246992E-
017 TIME = 185.92885 DT = 5.2428800 SUM OF SQUARES = 0.47968649E-16
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.16957857E-07 AND -0.16957857E-07
POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS 0.62260617E-05
U-FRACTION IN SYSTEM: CR = .191499811977765 FE = .733100726963597
NI = .0753994610586384
TOTAL SIZE OF SYSTEM: 1E-04 [m]
3 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: R_BCC_A2
CPU time used in timestep 2 seconds
5.642974296566065E-006 5.643125095318699E-006 5.641517484928644E-006 2.458262515757805E-006 1.706103643042057E-
006 5.102549567539333E-007 4.488461283369183E-011 3.063522581558072E-015 6.513585356447460E-
019 TIME = 196.41461 DT = 10.485760 SUM OF SQUARES = 0.65135854E-18
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.23346098E-07 AND 0.23346098E-07
POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS 0.64708632E-05
U-FRACTION IN SYSTEM: CR = .191499811977631 FE = .733100726947108
NI = .0753994610762612
TOTAL SIZE OF SYSTEM: 1E-04 [m]
5 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: R_FCC_A1
CPU time used in timestep 2 seconds
1.293494529309763E-005 1.293515101167310E-005 1.293008550633410E-005 2.658335068138821E-008 8.679707504660311E-
012 1.146811880809633E-016 TIME = 200.00000 DT = 3.5853947 SUM OF SQUARES = 0.11468119E-15
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.18287074E-07 AND 0.18287074E-07
POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS 0.65364296E-05
U-FRACTION IN SYSTEM: CR = .191499811977615 FE = .733100726940699
NI = .0753994610816858
TOTAL SIZE OF SYSTEM: 1E-04 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 175.02035
DELETING TIME-RECORD FOR TIME 175.44310
DELETING TIME-RECORD FOR TIME 175.44311
DELETING TIME-RECORD FOR TIME 175.44313
DELETING TIME-RECORD FOR TIME 175.44317
DELETING TIME-RECORD FOR TIME 175.44325
DELETING TIME-RECORD FOR TIME 175.44341
DELETING TIME-RECORD FOR TIME 175.44373
DELETING TIME-RECORD FOR TIME 175.44437
DELETING TIME-RECORD FOR TIME 175.44565
DELETING TIME-RECORD FOR TIME 175.44821
DELETING TIME-RECORD FOR TIME 175.45333
DELETING TIME-RECORD FOR TIME 175.46357
DELETING TIME-RECORD FOR TIME 175.48405
DELETING TIME-RECORD FOR TIME 175.52501
DELETING TIME-RECORD FOR TIME 175.60693
DELETING TIME-RECORD FOR TIME 175.77077
DELETING TIME-RECORD FOR TIME 176.09845
DELETING TIME-RECORD FOR TIME 176.75381
DELETING TIME-RECORD FOR TIME 178.06453
DELETING TIME-RECORD FOR TIME 180.68597
DELETING TIME-RECORD FOR TIME 185.92885
KEEPING TIME-RECORD FOR TIME 196.41461
AND FOR TIME 200.00000
WORKSPACE RECLAIMED
TIMESTEP AT 200.000000 SELECTED
```

DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
DIC>

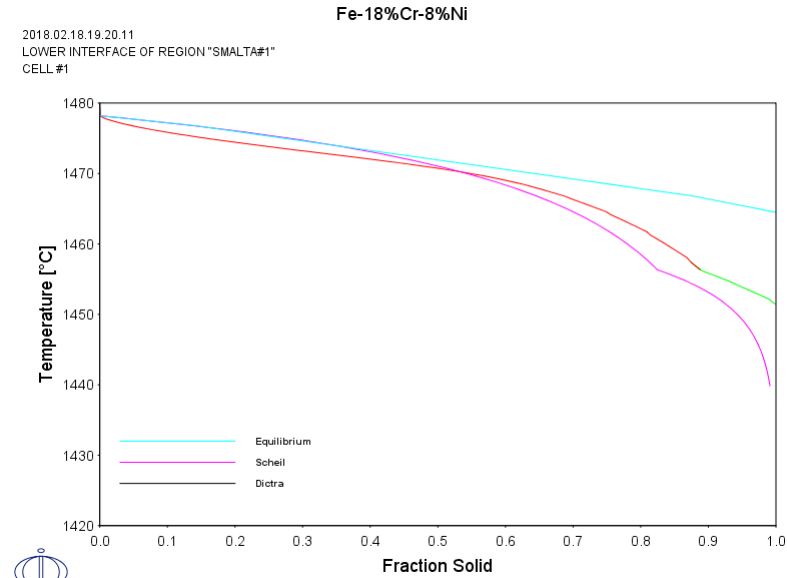
```
DIC>  
DIC>  
DIC> @@  
DIC> @@ THE SIMULATION IS FINISHED  
DIC> @@  
DIC>  
DIC> set-inter  
--OK--  
DIC>
```

exb4a-plot

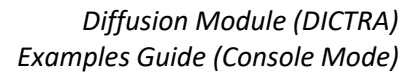
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb4a\plot.DCM"DIC>
DIC>
DIC> @@ exb4a_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE b4a
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 2.00000E+02
DIC> read exb4a
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post

POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
```

```
POST-1:
POST-1: set-title Fe-18%Cr-8%Ni
POST-1:
POST-1: @@
POST-1: @@ PLOT THE FRACTION OF SOLID AND COMPARE WITH A SCHEIL-GULLIVER SIMULATION
POST-1: @@ AND EQUILIBRIUM SOLIDIFICATION (DATA ON FILE exb4.exp)
POST-1: @@
POST-1: enter function fs=1-ivv(liquid);
POST-1: s-d-a x fs
POST-1: s-s-s x n 0 1
POST-1: set-axis-text
AXIS (X, Y OR Z) : x
AUTOMATIC AXIS TEXT (Y OR N) /N/: n
AXIS TEXT : Fraction Solid
POST-1:
POST-1: s-d-a y t-c
POST-1: s-s-s y n 1420 1480
POST-1:
POST-1: s-p-c interface smalta lower
POST-1:
POST-1: app y exb4a.exp 0; 1
POST-1: plo
```



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



Solidification path of an Fe-18%Cr-8%Ni alloy: Peritectic reaction

Time > 0

T = 1900 - 1 * Time K

Liquid

FCC

BCC

v

v

1E-4

exb4b-setup

About Stockholm, Sweden

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

```
SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb4b\setup.DCM" @@
SYS: @@ Moving boundary problem.
SYS: @@ Solidification path of an Fe-18%Cr-8%Ni alloy: Peritectic reaction
SYS: @@ This example is the same as exb4a but now a peritectic reaction is assumed:
SYS: @@ LIQUID + BCC -> FCC. Hence the FCC region should appear in between the LIQUID
SYS: @@ and the BCC. Comparison is made with both a Scheil-Gulliver simulation and
SYS: @@ equilibrium solidification conditions, both done in Thermo-Calc.
SYS: -----
NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exb4b_setup.DCM
SYS:
SYS:
SYS: @@
SYS: @@ START BY GOING TO THE DATABASE MODULE
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Current database: Steels/Fe-Alloys v9.0

VA                      /-  DEFINED
L12 FCC                  B2_BCC                      DICTRA_FCC_A1
REJECTED
TDB_TCFE9:
TDB_TCFE9: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA
TDB_TCFE9: sw fedemo
Current database: Iron Demo Database v2.0

VA                      /-  DEFINED
TDB_FEDEMO:
TDB_FEDEMO: @@ DEFINE THE SYSTEM TO WORK WITH
TDB_FEDEMO: def-sys fe ni cr
FE                      NI                      CR
DEFINED
TDB_FEDEMO:
TDB_FEDEMO: @@ EXCLUDE THE THERMODYNAMIC DATA FOR THE PHASES THAT ARE NOT NEEDED
TDB_FEDEMO: rej ph /all
LIQUID:L                BCC_A2                      CHI_A12
FCC_A1                  HCP_A3                      LAVES_PHASE_C14
SIGMA REJECTED
TDB_FEDEMO: res ph fcc liq bcc
FCC_A1                  LIQUID:L                      BCC_A2
RESTORED
TDB_FEDEMO:
TDB_FEDEMO: @@ RETRIEVE DATA FROM THE DATABASE FILE
TDB_FEDEMO: get
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

List of references for assessed data

'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
'X.-G. Lu, M. Selleby, B. Sundman, CALPHAD, 29 (2005) 49-55; Fe P-T diagram'
'J. Brillo and I. Egry, Int. J. Thermophysics, 24, 1155-1170'
'B.-J. Lee, CALPHAD, 17 (1993) 251-268; revision of Fe-Cr and Fe -Ni liquid'
'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
'B.-J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
volumes'
'J.-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270
(1986); CR-FE'
'A. Dinsdale and T. Chart, MTDS NPL, Unpublished work (1986); CR -NI'
'A. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); FE-NI'
-OK-
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ MOBILITY/DIFFUSIVITY DATA ARE STORED IN A SEPARATE DATABASE FILE.
TDB_FEDEMO: @@ SWITCH TO A MOBILITY DATABASE AND APPEND THE DATA.
TDB_FEDEMO: @@
TDB_FEDEMO: app
Use one of these databases

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


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

DATABASE NAME /FEDEMO/: mobfe2

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

VA DEFINED

APP: def-sys fe ni cr

FE NI CR
DEFINED

APP: rej ph /all

BCC_A2 FCC_A1 HCP_A3

LIQUID:L REJECTED

APP: res ph fcc liq bcc

FCC_A1 LIQUID:L BCC_A2

RESTORED

APP: get

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

FUNCTIONS

List of references for assessed data

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

```

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

DIC>
DIC> @@
DIC> @@ ENTER A REGION CALLED smalta
DIC> @@
DIC> enter-region smalta
DIC>
DIC> @@
DIC> @@ ENTER A GEOMETRIC GRID INTO THE REGION
DIC> @@
DIC> enter-grid
REGION NAME : /SMALTA/: smalta
WIDTH OF REGION /1/: 1e-4
TYPE /LINEAR/: AUTO
DIC>
DIC> @@
DIC> @@ ENTER active PHASES INTO THE REGION
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /SMALTA/: smalta
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: liq
      SETTING CHECK INTERFACE POSITION ON
DIC>
DIC> @@
DIC> @@ ENTER inactive PHASES INTO THE REGION, WITH BOTH PHASES ON THE SAME
DIC> @@ SIDE OF THE LIQUID REGION IN ORDER TO GET A PERITECTIC REACTION.
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inact
ATTACH TO REGION NAMED /SMALTA/: smalta
ATTACHED TO THE RIGHT OF SMALTA /YES/: yes
PHASE NAME: /NONE/: fcc#1
DEPENDENT COMPONENT ? /NI/: fe
      REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-5
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inact
ATTACH TO REGION NAMED /SMALTA/: smalta
ATTACHED TO THE RIGHT OF SMALTA /YES/: yes
PHASE NAME: /NONE/: bcc#1
DEPENDENT COMPONENT ? /NI/: fe
      REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-5
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> @@
DIC> @@ ENTER THE START COMPOSITION FOR THE LIQUID
DIC> @@
DIC> enter-composition
REGION NAME : /SMALTA/: smalta
PHASE NAME: /LIQUID/: liq
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /CR/: cr lin 18 18
PROFILE FOR /NI/: ni lin 8 8
DIC>
DIC> @@
DIC> @@ THE BOUNDARY CONDITION IS A CLOSED SYSTEM (DEFAULT) AS WE DO NOT SPECIFY
DIC> @@ ANYTHING ELSE.
DIC> @@
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 200
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /20/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ CHECK THE INTERFACE POSITION. THIS IS TO MAKE SURE THAT THE LIQUID REGION
DIC> @@ DOES NOT SHRINK TOO MUCH DURING A TIMESTEP. IN ADDITION, THE TIMESTEP IS
DIC> @@ CONTROLLED BY THE PHASE INTERFACE DISPLACEMENT DURING THE SIMULATION.
DIC> @@
DIC> s-s-c
NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDEF: /2/:
CHECK INTERFACE POSITION /YES/: yes
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:

```

```
DEGREE OF IMPLICIT WHEN INTEGRATING PDEs (0 -> 0.5 -> 1): /.5/:
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /NO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIFF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/: @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exb4b Y
DIC>
DIC> set-inter
--OK--
DIC>
```

exb4b-run

DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb4b\run.DCM"DIC>

DIC> @@ exb4b_run.DCM

DIC>

DIC> @@

DIC> @@ FILE FOR RUNNING EXAMPLE b4b

DIC> @@

DIC> @@

DIC> @@

DIC> @@ ENTER THE DICTRA MONITOR AND READ THE SET UP FROM FILE

DIC> @@

DIC> go d-m

TIME STEP AT TIME 0.00000E+00

DIC> read exb4b

OK

DIC>

DIC> @@

DIC> @@ START THE SIMULATION

DIC> @@

DIC> sim yes

Region: SMALTA

single geometric dense at 0.10000E-03

0.92197 87

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291

NI = .0754116207882254

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

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291

NI = .0754116207882254

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

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

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291

NI = .0754116207882254

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

CPU time used in timestep 0 seconds

TIME = 0.26002472E-05 DT = 0.25002472E-05 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291

NI = .0754116207882254

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

CPU time used in timestep 0 seconds

TIME = 0.76007416E-05 DT = 0.50004944E-05 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291

NI = .0754116207882254

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

CPU time used in timestep 0 seconds

TIME = 0.17601730E-04 DT = 0.10000989E-04 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291

NI = .0754116207882254

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

CPU time used in timestep 0 seconds

TIME = 0.37603708E-04 DT = 0.20001978E-04 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291

NI = .0754116207882254

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

CPU time used in timestep 0 seconds

TIME = 0.77607664E-04 DT = 0.40003955E-04 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291

NI = .0754116207882254

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

CPU time used in timestep 0 seconds

TIME = 0.15761557E-03 DT = 0.80007911E-04 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291

NI = .0754116207882254

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

CPU time used in timestep 0 seconds

TIME = 0.31763140E-03 DT = 0.16001582E-03 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291

NI = .0754116207882254

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

CPU time used in timestep 0 seconds

TIME = 0.63766304E-03 DT = 0.32003164E-03 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291

NI = .0754116207882254

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

CPU time used in timestep 1 seconds

TIME = 0.12777263E-02 DT = 0.64006329E-03 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291

NI = .0754116207882254

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

CPU time used in timestep 0 seconds

TIME = 0.25578529E-02 DT = 0.12801266E-02 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291

NI = .0754116207882254

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

CPU time used in timestep 0 seconds

TIME = 0.51181060E-02 DT = 0.25602531E-02 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291

NI = .0754116207882254

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

CPU time used in timestep 0 seconds

TIME = 0.10238612E-01 DT = 0.51205063E-02 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291

NI = .0754116207882254

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

CPU time used in timestep 0 seconds

TIME = 0.20479625E-01 DT = 0.10241013E-01 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882254

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

CPU time used in timestep 0 seconds

TIME = 0.40961650E-01 DT = 0.20482025E-01 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992482 FE = .733068011219292

NI = .0754116207882253

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

CPU time used in timestep 0 seconds

TIME = 0.81925700E-01 DT = 0.40964050E-01 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992482 FE = .733068011219293

NI = .0754116207882251

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

CPU time used in timestep 0 seconds

TIME = 0.16385380 DT = 0.81928101E-01 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992481 FE = .733068011219295

NI = .0754116207882247

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

[illegible]

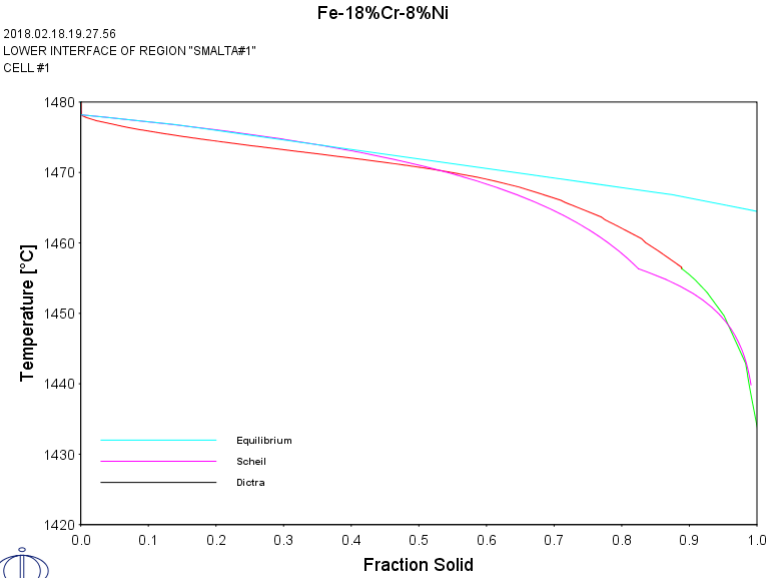
```
DIC>  
DIC> set-inter  
--OK--  
DIC>
```

exb4b-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb4b\plot.DCM"DIC>
DIC>
DIC> @@ exb4b_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE b4b
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 2.00000E+02
DIC> read exb4b
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post

POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
```

```
POST-1:
POST-1: set-title Fe-18%Cr-8%Ni
POST-1:
POST-1: @@
POST-1: @@ PLOT THE FRACTION OF SOLID AND COMPARE WITH A SCHEIL-GULLIVER
POST-1: @@ SIMULATION AND EQUILIBRIUM SOLIDIFICATION (DATA ON FILE exb4.exp)
POST-1: @@
POST-1: enter func fs=l-ivv(liquid);
POST-1: s-d-a x fs
POST-1: s-s-s x n 0 1
POST-1: s-ax-te x n Fraction Solid
POST-1:
POST-1: s-d-a y t-c
POST-1: s-s-s y n 1420 1480
POST-1:
POST-1: s-p-c interf smalta lower
POST-1:
POST-1: app y exb4b.exp 0; 1
POST-1: plo
```





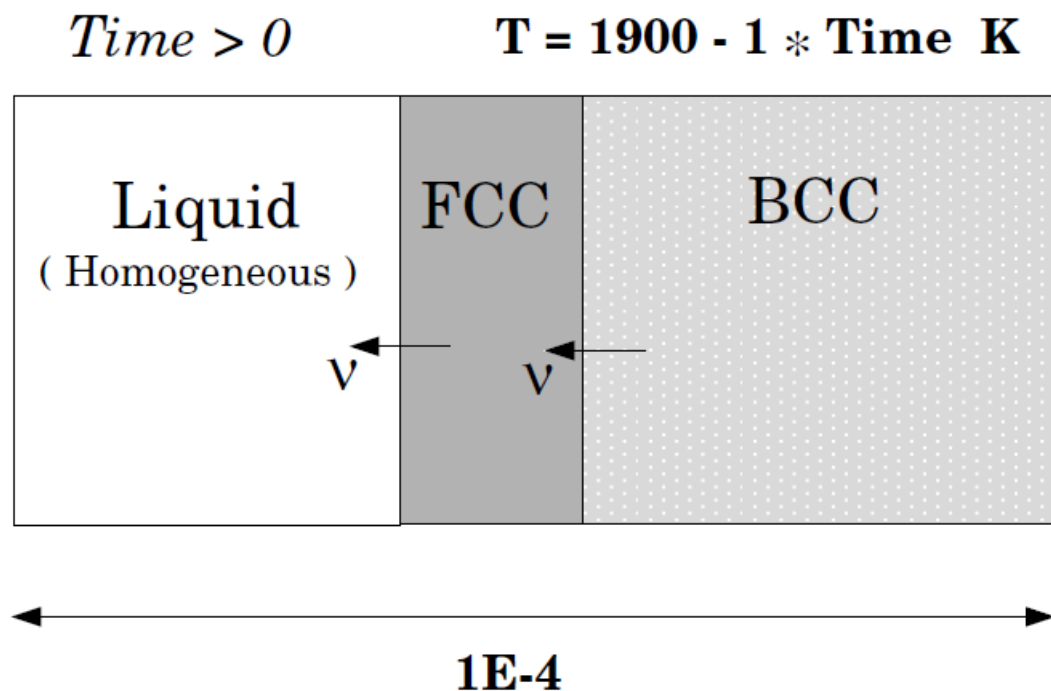
```
POST-1:
POST-1:
POST-1:
POST-1: set-inter
--OK--
POST-1:
```



Example exb4c

Solidification path of an Fe-18%Cr-8%Ni alloy: Peritectic reaction, homogeneous liquid

This example is the same as exb4b but now the diffusivity data is amended for the LIQUID and a very high value for the diffusivity is used in order to simulate a case where we assume that the composition in the LIQUID is always homogeneous. This case should be considered less realistic than exb4b. Comparison is made with both a Scheil-Gulliver simulation and equilibrium solidification conditions, both made with Thermo-Calc.



exb4c-setup

About

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

```
SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb4c\setup.DCM" @@
```

```
SYS: @@ Moving boundary problem.
```

```
SYS: @@ Solidification path of an Fe-18%Cr-8%Ni alloy
```

```
SYS: @@ This example is the same as exb4b but now the diffusivity data is amended
```

```
SYS: @@ for the LIQUID and a high value for the diffusivity is used to simulate a
```

```
SYS: @@ case where it is assumed that the composition in the LIQUID is always
```

```
SYS: @@ homogeneous. This example is less realistic than exb4b.
```

```
SYS: @@ Comparison is made with both a Scheil-Gulliver simulation and equilibrium
```

```
SYS: @@ solidification conditions, both done in Thermo-Calc.
```

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

```
NO SUCH COMMAND, USE HELP
```

```
SYS:
```

```
SYS: @@ exb4c_setup.DCM
```

```
SYS:
```

```
SYS: @@
```

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

```
SYS: @@
```

```
SYS: go da
```

```
THERMODYNAMIC DATABASE module
```

```
Current database: Steels/Fe-Alloys v9.0
```

```
VA /- DEFINED
```

```
L12_FCC B2_BCC DICTRA_FCC_A1
```

```
REJECTED
```

```
TDB_TCFE9:
```

```
TDB_TCFE9: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA
```

```
TDB_TCFE9: sw fedemo
```

```
Current database: Iron Demo Database v2.0
```

```
VA /- DEFINED
```

```
TDB_FEDEMO:
```

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

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

```
FE NI CR
```

```
DEFINED
```

```
TDB_FEDEMO:
```

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

```
TDB_FEDEMO: rej ph /all
```

```
LIQUID:L BCC_A2 CHI_A12
```

```
FCC_A1 HCP_A3 LAVES_PHASE_C14
```

```
SIGMA REJECTED
```

```
TDB_FEDEMO: res ph fcc liq bcc
```

```
FCC_A1 LIQUID:L BCC_A2
```

```
RESTORED
```

```
TDB_FEDEMO:
```

```
TDB_FEDEMO: @@ RETRIEVE DATA FROM THE DATABASE FILE
```

```
TDB_FEDEMO: get
```

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

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

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

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

```
PARAMETERS ...
```

```
FUNCTIONS ....
```

```
List of references for assessed data
```

```
'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
```

```
'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
```

```
'X.-G. Lu, M. Selleby, B. Sundman, CALPHAD, 29 (2005) 49-55; Fe P-T diagram'
```

```
'J. Brillo and I. Egry, Int. J. Thermophysics, 24, 1155-1170'
```

```
'B.-J. Lee, CALPHAD, 17 (1993) 251-268; revision of Fe-Cr and Fe -Ni liquid'
```

```
'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
```

```
'B.-J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
```

```
'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
```

```
volumes'
```

```
'J.-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270
```

```
(1986); CR-FE'
```

```
'A. Dinsdale and T. Chart, MTDS NPL, Unpublished work (1986); CR -NI'
```

```
'A. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); FE-NI'
```

```
-OK-
```

```
TDB_FEDEMO:
```

```
TDB_FEDEMO: @@
```

```
TDB_FEDEMO: @@ MOBILITY/DIFFUSIVITY DATA ARE STORED IN A SEPARATE DATABASE FILE.
```

```
TDB_FEDEMO: @@ SWITCH TO A MOBILITY DATABASE AND APPEND THE DATA.
```

```
TDB_FEDEMO: @@
```

```
TDB_FEDEMO: app
```

```
Use one of these databases
```

```
TCFE9 = Steels/Fe-Alloys v9.0
```

```
TCFE10 = Steels/Fe-Alloys v10.0 SNAPSHOT
```

```
TCFE8 = Steels/Fe-Alloys v8.1
```

```
FROST1 = FROST database v1.0
```

```
TCFE7 = Steels/Fe-Alloys v7.0
```

```
TCFE6 = Steels/Fe-Alloys v6.2
```

```
TCFE5 = Steels/Fe-Alloys v5.0
```

```
TCFE4 = Steels/Fe-Alloys v4.1
```

```
TCFE3 = Steels/Fe-Alloys v3.1
```

```
TCFE2 = Steels/Fe-Alloys v2.1
```

```
TCFE1 = Steels/Fe-Alloys v1.0
```

```
TCNI9 = Ni-Alloys v9.0 SNAPSHOT
```

```
NI25 = NI25 database
```

```
TCNI8 = Ni-Alloys v8.1
```

```
TCNI7 = Ni-Alloys v7.1
```

```
TCNI6 = Ni-Alloys v6.0
```

```
TCNI5 = Ni-Alloys v5.1
```

```
TCNI4 = Ni-Alloys v4.0
```

```
TCNI1 = Ni-Alloys v1.3
```

```
TCAL5 = Al-Alloys v5.0
```

```
TCAL4 = Al-Alloys v4.0
```

```
TCAL3 = Al-Alloys v3.0
```

```
TCAL2 = Al-Alloys v2.1
```

```
TCAL1 = Al-Alloys v1.2
```

```
TCMG4 = Mg-Alloys v4.0
```

```
TCMG3 = Mg-Alloys v3.0
```

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

DATABASE NAME /FEDEMO/: mobfe2

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

VA DEFINED

APP: def-sys fe ni cr

FE NI CR
DEFINED

APP: rej ph /all

BCC_A2 FCC_A1 HCP_A3

LIQUID:L REJECTED

APP: res ph fcc liq bcc

FCC_A1 LIQUID:L BCC_A2

RESTORED

APP: get

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

FUNCTIONS

List of references for assessed data

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

```

      Cr-Fe-Ni'
'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
-Ni'
'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Ni self-diffusion'
'B. Jonsson: ISIJ International, 35(1995)1415-1421; Cr, Fe and Ni
diffusion bcc Cr-Fe-Ni'
'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
in bcc Fe'
-OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP
APP: @@
APP: go d-m
      NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ LIST THE MOBILITIES IN THE LIQUID
DIC> @@
DIC> list-mobility-data
      Sorry, LIST-DATA disabled for this database
DIC>
DIC>
DIC> liquid
      NO SUCH COMMAND, USE HELP
DIC>
DIC>
DIC> @@
DIC> @@ AMEND THE DIFFUSIVITY DATA IN THE LIQUID
DIC> @@
DIC> @@ CHANGE TO A DIFFUSIVITY THAT IS 1000 TIMES HIGHER THAN THE
DIC> @@ VALUE IN THE MOBILITY DATABASE. THIS SHOULD BE ENOUGH IN ORDER TO
DIC> @@ ASSUME THAT THE COMPOSITION IN THE LIQUID IS AT ALL TIMES HOMOGENEOUS.
DIC> @@
DIC> amend_mobility_data
PARAMETER:
*** ERROR, PLEASE RE-ENTER EACH PART SEPARATELY
IDENTIFIER: dq
PHASE NAME: liquid&cr
CONSTITUENT: cr
INTERACTING CONSTITUENT:
      DQ(LIQUID&CR#1,CR;0) = Sorry, database encrypted
DO YOU WANT TO CHANGE THE NUMBER OF RANGES /NO/: yes
      I AM SORRY BUT YOU MUST THEN REENTER ALL RANGES
      DQ(LIQUID&CR#1,CR;0) =
LOW TEMPERATURE LIMIT /298.15/: 298.15
FUNCTION: +R*T*LN(1E-06);
HIGH TEMPERATURE LIMIT /6000/: 6000
ANY MORE RANGES /N/: no
DIC>
DIC> amend_mobility_data
PARAMETER: dq(liquid&cr,fe;0)
      DQ(LIQUID&CR#1,FE;0) = Sorry, database encrypted
DO YOU WANT TO CHANGE THE NUMBER OF RANGES /NO/: y
      I AM SORRY BUT YOU MUST THEN REENTER ALL RANGES
      DQ(LIQUID&CR#1,FE;0) =
LOW TEMPERATURE LIMIT /298.15/: 298.15 +R*T*LN(1E-06); 6000 n
DIC>
DIC> am-mob dq(liquid&cr,ni;0)
      DQ(LIQUID&CR#1,NI;0) = Sorry, database encrypted
DO YOU WANT TO CHANGE THE NUMBER OF RANGES /NO/: y
      I AM SORRY BUT YOU MUST THEN REENTER ALL RANGES
      DQ(LIQUID&CR#1,NI;0) =
LOW TEMPERATURE LIMIT /298.15/: 298.15 +R*T*LN(1E-06); 6000 n
DIC>
DIC> am-mob dq(liquid&ni,cr;0)
      DQ(LIQUID&NI#1,CR;0) = Sorry, database encrypted
DO YOU WANT TO CHANGE THE NUMBER OF RANGES /NO/: y
      I AM SORRY BUT YOU MUST THEN REENTER ALL RANGES
      DQ(LIQUID&NI#1,CR;0) =
LOW TEMPERATURE LIMIT /298.15/: 298.15 +R*T*LN(1E-06); 6000 n
DIC>
DIC> am-mob dq(liquid&ni,fe;0)
      DQ(LIQUID&NI#1,FE;0) = Sorry, database encrypted
DO YOU WANT TO CHANGE THE NUMBER OF RANGES /NO/: y
      I AM SORRY BUT YOU MUST THEN REENTER ALL RANGES
      DQ(LIQUID&NI#1,FE;0) =
LOW TEMPERATURE LIMIT /298.15/: 298.15 +R*T*LN(1E-06); 6000 n
DIC>
DIC> am-mob dq(liquid&ni,ni;0)
      DQ(LIQUID&NI#1,NI;0) = Sorry, database encrypted
DO YOU WANT TO CHANGE THE NUMBER OF RANGES /NO/: y
      I AM SORRY BUT YOU MUST THEN REENTER ALL RANGES
      DQ(LIQUID&NI#1,NI;0) =
LOW TEMPERATURE LIMIT /298.15/: 298.15 +R*T*LN(1E-06); 6000 n
DIC>
DIC> am-mob dq(liquid&fe,cr;0)
      DQ(LIQUID&FE#1,CR;0) = Sorry, database encrypted
DO YOU WANT TO CHANGE THE NUMBER OF RANGES /NO/: y
      I AM SORRY BUT YOU MUST THEN REENTER ALL RANGES
      DQ(LIQUID&FE#1,CR;0) =
LOW TEMPERATURE LIMIT /298.15/: 298.15 +R*T*LN(1E-06); 6000 n
DIC>
DIC> am-mob dq(liquid&fe,fe;0)
      DQ(LIQUID&FE#1,FE;0) = Sorry, database encrypted
DO YOU WANT TO CHANGE THE NUMBER OF RANGES /NO/: y
      I AM SORRY BUT YOU MUST THEN REENTER ALL RANGES
      DQ(LIQUID&FE#1,FE;0) =
LOW TEMPERATURE LIMIT /298.15/: 298.15 +R*T*LN(1E-06); 6000 n
DIC>
DIC> am-mob dq(liquid&fe,ni;0)
      DQ(LIQUID&FE#1,NI;0) = Sorry, database encrypted
DO YOU WANT TO CHANGE THE NUMBER OF RANGES /NO/: y
      I AM SORRY BUT YOU MUST THEN REENTER ALL RANGES
      DQ(LIQUID&FE#1,NI;0) =
LOW TEMPERATURE LIMIT /298.15/: 298.15 +R*T*LN(1E-06); 6000 n
DIC>
DIC> li-mob
      AMBIGUOUS COMMAND, USE HELP
DIC>
DIC>
DIC> liquid

```

```

NO SUCH COMMAND, USE HELP
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> @@ LOWER THE TEMPERATURE TO A RATE OF 1 K/s
DIC> set-cond glob T 0 1900-1*TIME; * N

DIC>
DIC> @@
DIC> @@ ENTER A REGION CALLED smalta
DIC> @@
DIC> enter-region smalta
DIC>
DIC> @@
DIC> @@ ENTER A GEOMETRIC GRID INTO THE REGION
DIC> @@
DIC> enter-grid
REGION NAME : /SMALTA/: smalta
WIDTH OF REGION /1/: 1e-4
TYPE /LINEAR/: AUTO
DIC>
DIC> @@
DIC> @@ ENTER active PHASES INTO THE REGION
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /SMALTA/: smalta
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: liq
SETTING CHECK INTERFACE POSITION ON
DIC>
DIC> @@
DIC> @@ ENTER inactive PHASES INTO THE REGION, BOTH PHASES ON THE SAME SIDE
DIC> @@ OF THE LIQUID REGION IN ORDER TO GET A PERITECTIC REACTION.
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inact
ATTACH TO REGION NAMED /SMALTA/: smalta
ATTACHED TO THE RIGHT OF SMALTA /YES/: yes
PHASE NAME: /NONE/: fcc#1
DEPENDENT COMPONENT ? /NI/: fe
REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-5
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inact
ATTACH TO REGION NAMED /SMALTA/: smalta
ATTACHED TO THE RIGHT OF SMALTA /YES/: yes
PHASE NAME: /NONE/: bcc#1
DEPENDENT COMPONENT ? /NI/: fe
REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-5
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> @@
DIC> @@ ENTER THE START COMPOSITION FOR THE LIQUID
DIC> @@
DIC> enter-composition
REGION NAME : /SMALTA/: smalta
PHASE NAME: /LIQUID/: liq
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /CR/: cr lin 18 18
PROFILE FOR /NI/: ni lin 8 8
DIC>
DIC> @@
DIC> @@ THE BOUNDARY CONDITION IS A CLOSED SYSTEM (DEFAULT) AS WE DO NOT SPECIFY
DIC> @@ ANYTHING ELSE
DIC> @@
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 200
AUTOMATIC TIMESTEP CONTROL /YES/: yes
MAX TIMESTEP DURING INTEGRATION /20/: 1
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ CHECK THE INTERFACE POSITION. THIS IS TO MAKE SURE THAT THE LIQUID
DIC> @@ REGION DOES NOT SHRINK TOO MUCH DURING A TIMESTEP. IN ADDITION THE TIMESTEP
DIC> @@ IS CONTROLLED BY THE PHASE INTERFACE DISPLACEMENT DURING THE SIMULATION.
DIC> @@
DIC> s-s-c
NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDF: /2/:
CHECK INTERFACE POSITION /YES/: yes
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPLICITY WHEN INTEGRATING PDES (0 -> 0.5 -> 1): /.5/:
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /NO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/: @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exb4c Y
DIC>
DIC> set-inter
--OK--
DIC>

```


exb4c-run

DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb4c\run.DCM"DIC>

DIC> @@ exb4c_run.DCM

DIC>

DIC> @@

DIC> @@ FILE FOR RUNNING EXAMPLE b4b

DIC> @@

DIC>

DIC> @@

DIC> @@ ENTER THE DICTRA MONITOR AND READ THE SET UP FROM FILE

DIC> @@

DIC> go d-m

TIME STEP AT TIME 0.00000E+00

DIC> read exb4c

OK

DIC>

DIC> @@

DIC> @@ START THE SIMULATION

DIC> @@

DIC> sim yes

Region: SMALTA

single geometric dense at 0.10000E-03

0.99375 62

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882255

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

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882255

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

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

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882254

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

CPU time used in timestep 0 seconds

TIME = 0.10874528E-05 DT = 0.98745278E-06 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882254

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

CPU time used in timestep 0 seconds

TIME = 0.30623583E-05 DT = 0.19749056E-05 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882254

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

CPU time used in timestep 0 seconds

TIME = 0.70121695E-05 DT = 0.39498111E-05 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882254

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

CPU time used in timestep 0 seconds

TIME = 0.14911792E-04 DT = 0.78996222E-05 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882254

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

CPU time used in timestep 0 seconds

TIME = 0.30711036E-04 DT = 0.15799244E-04 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882254

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

CPU time used in timestep 0 seconds

TIME = 0.62309525E-04 DT = 0.31598489E-04 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882254

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

CPU time used in timestep 0 seconds

TIME = 0.12550650E-03 DT = 0.63196978E-04 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882254

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

CPU time used in timestep 0 seconds

TIME = 0.25190046E-03 DT = 0.12639396E-03 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882254

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

CPU time used in timestep 0 seconds

TIME = 0.50468837E-03 DT = 0.25278791E-03 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291

NI = .0754116207882256

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

CPU time used in timestep 0 seconds

TIME = 0.10102642E-02 DT = 0.50557582E-03 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219292

NI = .0754116207882255

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

CPU time used in timestep 0 seconds

TIME = 0.20214158E-02 DT = 0.10111516E-02 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291

NI = .0754116207882259

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

CPU time used in timestep 0 seconds

TIME = 0.40437191E-02 DT = 0.20223033E-02 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291

NI = .0754116207882259

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

CPU time used in timestep 0 seconds

TIME = 0.80883257E-02 DT = 0.40446066E-02 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992477 FE = .733068011219298

NI = .0754116207882252

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

CPU time used in timestep 1 seconds

TIME = 0.16177539E-01 DT = 0.80892132E-02 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992482 FE = .733068011219295

NI = .0754116207882228

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

CPU time used in timestep 0 seconds

TIME = 0.32355965E-01 DT = 0.16178426E-01 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992504 FE = .733068011219263

NI = .0754116207882329

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

CPU time used in timestep 0 seconds

TIME = 0.64712818E-01 DT = 0.32356853E-01 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: CR = .191520367992551 FE = .733068011219194

NI = .0754116207882548

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

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

output ignored...

... output resumed

```
2.086373647587891E-015      4.787229045784939E-014      1.971385888754113E-
016      TIME = 199.16151      DT = 1.0000000      SUM OF SQUARES = 0.19713859E-15
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.10033934E-06 AND -0.10033934E-06
POSITION OF INTERFACE SMALTA / R_FCC_A1 IS 0.46441749E-06
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.11516775E-07 AND 0.11516775E-07
POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS 0.10970287E-04
U-FRACTION IN SYSTEM:  CR = .191211086169418 FE = .733433260812751
NI = .0753556530178301
TOTAL SIZE OF SYSTEM: 1E-04 [m]
32 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: R_FCC_A1

CPU time used in timestep          4 seconds
3.780876991451475E-007      3.786514022577464E-007      3.780834027702343E-007      3.780917218658302E-007      3.779744598558534E-
007      2.326746685393648E-008      9.107557821247557E-010      7.162247005586656E-013      1.756975994127614E-
014      1.047100422739898E-015      5.726994848012839E-013      1.904683817878645E-
016      TIME = 200.00000      DT = 0.83849346      SUM OF SQUARES = 0.19046838E-15
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.85423816E-07 AND -0.85423816E-07
POSITION OF INTERFACE SMALTA / R_FCC_A1 IS 0.39279018E-06
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.13581454E-07 AND 0.13581454E-07
POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS 0.10981675E-04
U-FRACTION IN SYSTEM:  CR = .191211078394994 FE = .733433268342357
NI = .075355653262649
TOTAL SIZE OF SYSTEM: 1E-04 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 170.39980
DELETING TIME-RECORD FOR TIME 170.48379
DELETING TIME-RECORD FOR TIME 170.48379
DELETING TIME-RECORD FOR TIME 170.48379
DELETING TIME-RECORD FOR TIME 170.48379
DELETING TIME-RECORD FOR TIME 170.48379
DELETING TIME-RECORD FOR TIME 170.48379
DELETING TIME-RECORD FOR TIME 170.48379
DELETING TIME-RECORD FOR TIME 170.48380
DELETING TIME-RECORD FOR TIME 170.48381
DELETING TIME-RECORD FOR TIME 170.48384
DELETING TIME-RECORD FOR TIME 170.48389
DELETING TIME-RECORD FOR TIME 170.48399
DELETING TIME-RECORD FOR TIME 170.48419
DELETING TIME-RECORD FOR TIME 170.48460
DELETING TIME-RECORD FOR TIME 170.48542
DELETING TIME-RECORD FOR TIME 170.48706
DELETING TIME-RECORD FOR TIME 170.49034
DELETING TIME-RECORD FOR TIME 170.49689
DELETING TIME-RECORD FOR TIME 170.51000
DELETING TIME-RECORD FOR TIME 170.53621
DELETING TIME-RECORD FOR TIME 170.58864
DELETING TIME-RECORD FOR TIME 170.69350
DELETING TIME-RECORD FOR TIME 170.90322
DELETING TIME-RECORD FOR TIME 171.32265
DELETING TIME-RECORD FOR TIME 172.16151
DELETING TIME-RECORD FOR TIME 173.16151
DELETING TIME-RECORD FOR TIME 174.16151
DELETING TIME-RECORD FOR TIME 175.16151
DELETING TIME-RECORD FOR TIME 176.16151
DELETING TIME-RECORD FOR TIME 177.16151
DELETING TIME-RECORD FOR TIME 178.16151
DELETING TIME-RECORD FOR TIME 179.16151
DELETING TIME-RECORD FOR TIME 180.16151
DELETING TIME-RECORD FOR TIME 181.16151
DELETING TIME-RECORD FOR TIME 182.16151
DELETING TIME-RECORD FOR TIME 183.16151
DELETING TIME-RECORD FOR TIME 184.16151
DELETING TIME-RECORD FOR TIME 185.16151
DELETING TIME-RECORD FOR TIME 186.16151
DELETING TIME-RECORD FOR TIME 187.16151
DELETING TIME-RECORD FOR TIME 188.16151
DELETING TIME-RECORD FOR TIME 189.16151
DELETING TIME-RECORD FOR TIME 190.16151
DELETING TIME-RECORD FOR TIME 191.16151
DELETING TIME-RECORD FOR TIME 192.16151
DELETING TIME-RECORD FOR TIME 193.16151
DELETING TIME-RECORD FOR TIME 194.16151
DELETING TIME-RECORD FOR TIME 195.16151
DELETING TIME-RECORD FOR TIME 196.16151
DELETING TIME-RECORD FOR TIME 197.16151
DELETING TIME-RECORD FOR TIME 198.16151

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

TIMESTEP AT 200.000000 SELECTED
```

DIC>
DIC>
DIC>
DIC>
DIC>
DIC>

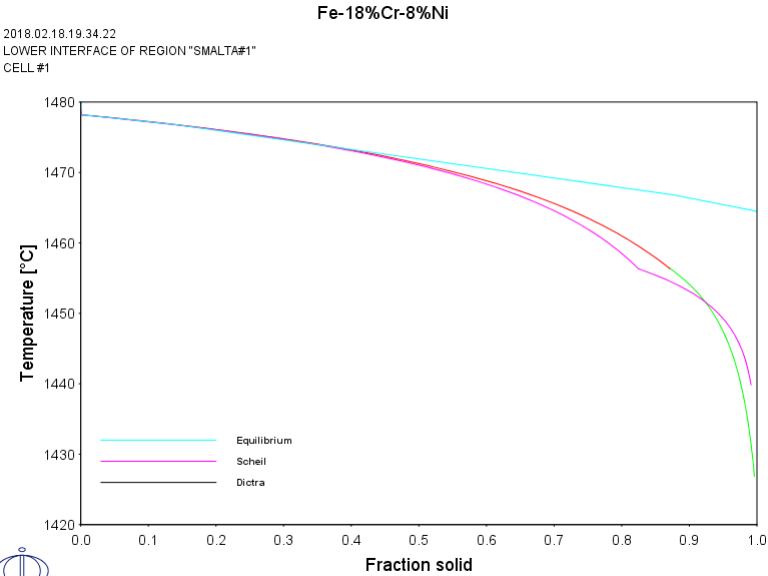
```
DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ THE SIMULATION IS FINISHED
DIC> @@
DIC>
DIC> set-inter
--OK--
DIC>
```


exb4c-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb4c\plot.DCM"DIC>
DIC>
DIC> @@ exb4c_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE b4c
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
    TIME STEP AT TIME  2.00000E+02
DIC> read exb4c
    OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post

    POST PROCESSOR VERSION  1.7
    Implemented by Bjorn Jonsson
```

```
POST-1:
POST-1: set-title Fe-18%Cr-8%Ni
POST-1:
POST-1: @@
POST-1: @@ PLOT THE FRACTION OF SOLID AND COMPARE WITH A SCHEIL-GULLIVER
POST-1: @@ SIMULATION AND EQUILIBRIUM SOLIDIFICATION (DATA ON FILE exb4.exp).
POST-1: @@ IN THIS CASE WE CAN SEE THAT ALL THREE LINES INITIALLY FALL
POST-1: @@ ON THE SAME LINE.
POST-1: @@
POST-1: enter func fs=1-ivv(liquid);
POST-1: s-d-a x fs
POST-1: s-s-s x n 0 1
POST-1: s-ax-te x n Fraction solid
POST-1:
POST-1: s-d-a y t-c
POST-1: s-s-s y n 1420 1480
POST-1:
POST-1: s-p-c interf smalta lower
POST-1:
POST-1: app y exb4c.exp 0; 1
POST-1: plo
```



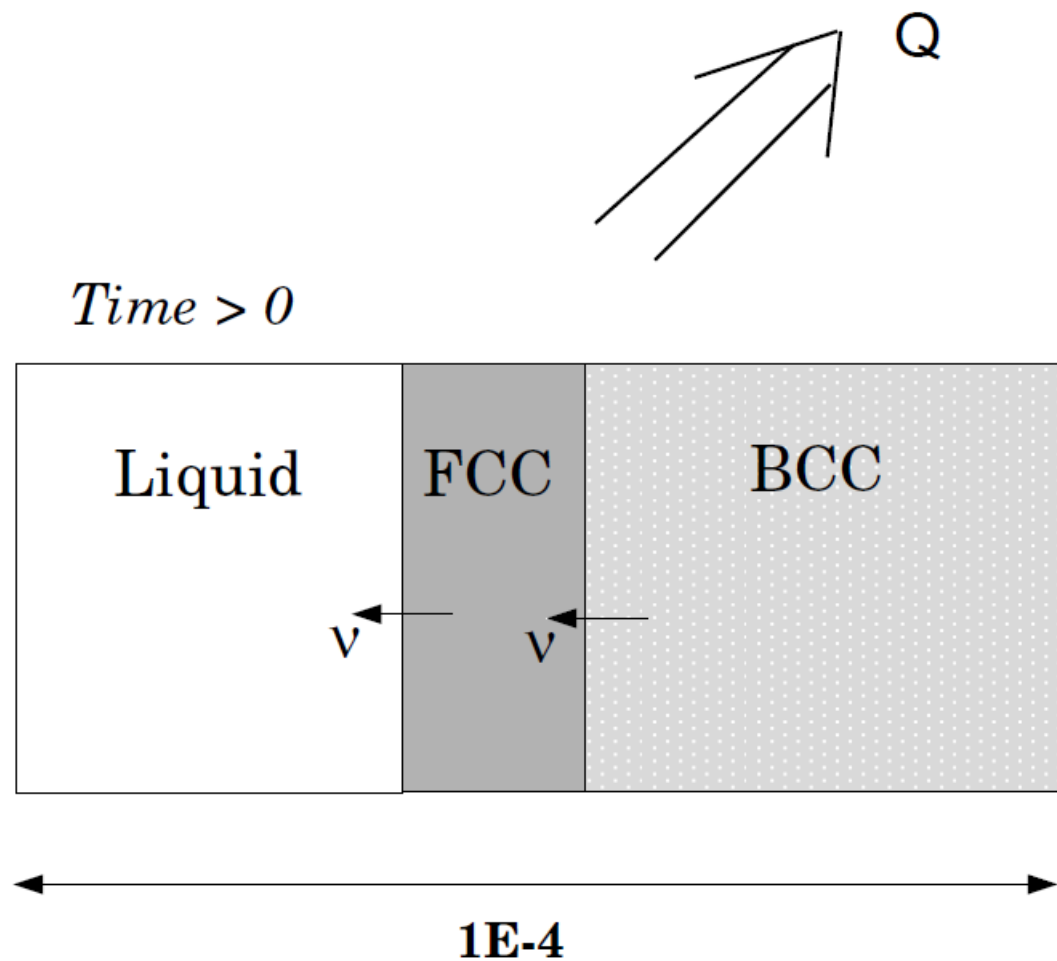
```
POST-1:
POST-1:
POST-1:
POST-1: set-inter
--OK--
POST-1:
```



Example exb4d

Solidification path of an Fe-18%Cr-8%Ni alloy: Peritectic reaction, heat-flux controls the temperature

This example is the same as exb4b but instead of controlling the temperature the amount heat extracted is given. Comparison is made with both a Scheil-Gulliver simulation and equilibrium solidification conditions, both made with Thermo-Calc.



exb4d-setup

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

```
SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb4d\setup.DCM"SYS: @@
SYS: @@ Moving boundary problem.
SYS: @@ Solidification path of an Fe-18%Cr-8%Ni alloy
SYS: @@ This example is the same as exb4b but instead of controlling the temperature
SYS: @@ the amount of heat extracted is given. Comparison is made with both a
SYS: @@ Scheil-Gulliver simulation and equilibrium solidification conditions,
SYS: @@ both done in Thermo-Calc.
SYS: -----
NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exb4d_setup.DCM
SYS:
SYS: @@
SYS: @@ START BY GOING TO THE DATABASE MODULE
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Current database: Steels/Fe-Alloys v9.0

VA          /-  DEFINED
LI2_FCC      B2_BCC          DICTRA_FCC_A1
REJECTED

TDB_TCFE9:
TDB_TCFE9: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA
TDB_TCFE9: sw fedemo
Current database: Iron Demo Database v2.0

VA          /-  DEFINED
TDB_FEDEMO:
TDB_FEDEMO: @@ DEFINE THE SYSTEM TO WORK WITH
TDB_FEDEMO: def-sys fe ni cr
FE          NI          CR
DEFINED
TDB_FEDEMO:
TDB_FEDEMO: @@ EXCLUDE THE THERMODYNAMIC DATA FOR THE PHASES THAT ARE NOT NEEDED
TDB_FEDEMO: rej ph /all
LIQUID:L          BCC_A2          CHI_A12
FCC_A1          HCP_A3          LAVES_PHASE_C14
SIGMA REJECTED
TDB_FEDEMO: res ph fcc liq bcc
FCC_A1          LIQUID:L          BCC_A2
RESTORED
TDB_FEDEMO:
TDB_FEDEMO: @@ RETRIEVE DATA FROM THE DATABASE FILE
TDB_FEDEMO: get
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

List of references for assessed data

'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
'X.-G. Lu, M. Selleby, B. Sundman, CALPHAD, 29 (2005) 49-55; Fe P-T diagram'
'J. Brillo and I. Egry, Int. J. Thermophysics, 24, 1155-1170'
'B.-J. Lee, CALPHAD, 17 (1993) 251-268; revision of Fe-Cr and Fe -Ni liquid'
'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
'B.-J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
volumes'
'J.-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270
(1986); CR-FE'
'A. Dinsdale and T. Chart, MTDS NPL, Unpublished work (1986); CR -NI'
'A. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); FE-NI'
-OK-
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ MOBILITY/DIFFUSIVITY DATA ARE STORED IN A SEPARATE DATABASE FILE.
TDB_FEDEMO: @@ SWITCH TO THE MOBILITY DATABASE AND APPEND THE DATA
TDB_FEDEMO: @@
TDB_FEDEMO: app
Use one of these databases

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

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

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

```

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

```

List of references for assessed data

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

```

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

DIC>
DIC> @@
DIC> @@ ENTER AN INITIAL TEMPERATURE
DIC> @@
DIC> set-initial-temp 1900
DIC>
DIC> @@
DIC> @@ ENTER A REGION CALLED smalta
DIC> @@
DIC> enter-region smalta
DIC>
DIC> @@
DIC> @@ ENTER A GEOMETRIC GRID INTO THE REGION
DIC> @@
DIC> enter-grid
REGION NAME : /SMALTA/: smalta
WIDTH OF REGION /1/: 1e-4
TYPE /LINEAR/: AUTO
DIC>
DIC>
DIC> @@
DIC> @@ ENTER active PHASES INTO THE REGION
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /SMALTA/: smalta
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: liq
SETTING CHECK INTERFACE POSITION ON
DIC>
DIC> @@
DIC> @@ ENTER inactive PHASES INTO THE REGION, BOTH PHASES ON THE
DIC> @@ SAME SIDE OF THE LIQUID REGION TO GET A PERITECTIC REACTION.
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inact
ATTACH TO REGION NAMED /SMALTA/: smalta
ATTACHED TO THE RIGHT OF SMALTA /YES/: yes
PHASE NAME: /NONE/: fcc#1
DEPENDENT COMPONENT ? /NI/: fe
REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-3
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inact
ATTACH TO REGION NAMED /SMALTA/: smalta
ATTACHED TO THE RIGHT OF SMALTA /YES/: yes
PHASE NAME: /NONE/: bcc#1
DEPENDENT COMPONENT ? /NI/: fe
REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-3
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> @@
DIC> @@ ENTER A START COMPOSITION FOR THE LIQUID
DIC> @@
DIC> enter-composition
REGION NAME : /SMALTA/: smalta
PHASE NAME: /LIQUID/: liq
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /CR/: cr lin 18 18
PROFILE FOR /NI/: ni lin 8 8
DIC>
DIC> @@
DIC> @@ THE BOUNDARY CONDITION IS A CLOSED SYSTEM (DEFAULT) AS WE DO NOT SPECIFY
DIC> @@ ANYTHING ELSE
DIC> @@
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 200
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /20/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ CHECK THE INTERFACE POSITION. THIS IS TO MAKE SURE THAT THE LIQUID REGION
DIC> @@ DOES NOT SHRINK TOO MUCH DURING A TIMESTEP. IN ADDITION THE TIMESTEP IS
DIC> @@ CONTROLLED BY THE PHASE INTERFACE DISPLACEMENT DURING THE SIMULATION.
DIC> @@
DIC> s-s-c
NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDF: /2/:
CHECK INTERFACE POSITION /YES/: yes
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/: no
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:

```

```
DEGREE OF IMPLICIT WHEN INTEGRATING PDEs (0 -> 0.5 -> 1): /.5/:
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /NO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIFF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/: @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exb4d Y
DIC>
DIC> set-inter
--OK--
DIC>
```

exb4d-run

DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb4d\run.DCM"DIC>

DIC> @@ exb4d_run.DCM

DIC>

DIC> @@

DIC> @@ FILE FOR RUNNING EXAMPLE b4b

DIC> @@

DIC> @@

DIC> @@

DIC> @@ ENTER THE DICTRA MONITOR AND READ THE SET UP FROM FILE

DIC> @@

DIC> go d-m

TIME STEP AT TIME 0.00000E+00

DIC> read exb4d

OK

DIC>

DIC> @@

DIC> @@ START THE SIMULATION

DIC> @@

DIC> sim

Region: SMALTA

single geometric dense at 0.10000E-03

0.92197 87

TEMPERATURE: 1900. ENTHALPY: 0.7394E+05

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291

NI = .0754116207882254

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

TEMPERATURE: 1900. ENTHALPY: 0.7394E+05

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291

NI = .0754116207882254

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

3.863918610053681E-007 3.864691456620901E-007 3.837979016399162E-016 3.830845290529296E-025 TIME = 0.10000000E-

06 DT = 0.10000000E-06 SUM OF SQUARES = 0.38308453E-24

TEMPERATURE: 1900. ENTHALPY: 0.7394E+05

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291

NI = .0754116207882254

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

CPU time used in timestep 0 seconds

9.508207427607264E-018 TIME = 0.26002472E-05 DT = 0.25002472E-05 SUM OF SQUARES = 0.95082074E-17

TEMPERATURE: 1900. ENTHALPY: 0.7394E+05

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291

NI = .0754116207882254

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

CPU time used in timestep 0 seconds

3.803282971042906E-017 TIME = 0.76007416E-05 DT = 0.50004944E-05 SUM OF SQUARES = 0.38032830E-16

TEMPERATURE: 1900. ENTHALPY: 0.7394E+05

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291

NI = .0754116207882254

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

CPU time used in timestep 0 seconds

1.521313188417162E-016 1.521313188417162E-016

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

*** ERROR 1890 IN DCNS01

*** ERROR RETURN FROM NS01A

1.521313188417162E-016 1.521313188417162E-016 1.521313188417162E-016 9.303850408268813E-020 1.431856390077847E-

016 3.399472344393975E-017 3.399472344393975E-017 1.089191126797645E-019 1.089191126797645E-

019 1.089191126797645E-019 1.089191126797645E-019 2.673347549794903E-017 1.089185930657826E-

019 1.089185930657826E-019 1.089185930657826E-019 1.089185930657826E-019 1.092210507539688E-

018 1.089191126797645E-019 TIME = 0.17601730E-04 DT = 0.10000989E-04 SUM OF SQUARES = 0.10891911E-18

TEMPERATURE: 1900. ENTHALPY: 0.7394E+05

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291

NI = .0754116207882254

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

CPU time used in timestep 0 seconds

1.666578502523493E-016 1.666578502523493E-016

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

*** ERROR 1890 IN DCNS01

*** ERROR RETURN FROM NS01A

1.666578502523493E-016 1.666578502523493E-016 1.666578502523493E-016 1.352477274150108E-012 1.666578502523493E-

016 1.038241667728256E-035 1.038241667728256E-035 1.038241667728256E-035 1.038241667728256E-

035 1.038241667728256E-035 1.038241667728256E-035 1.038241667728256E-035 1.038241667728256E-

035 1.038241667728256E-035 1.038241667728256E-035 1.038241667728256E-035 TIME = 0.37603708E-04 DT = 0.20001978E-

04 SUM OF SQUARES = 0.10382417E-34

TEMPERATURE: 1900. ENTHALPY: 0.7394E+05

U-FRACTION IN SYSTEM: CR = .191520367992483 FE = .733068011219291

NI = .0754116207882254

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

output ignored...

... output resumed

POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS 0.55694300E-05

TEMPERATURE: 1705. ENTHALPY: 0.5598E+05

U-FRACTION IN SYSTEM: CR = .191419766484522 FE = .73319305074855

NI = .075387182766928

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

2 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: R_FCC_A1

CPU time used in timestep 1 seconds

2.851700635661659E-007 2.851708831145793E-007 2.851624308208675E-007 2.851128595190466E-007 3.297264654510150E-

008 3.644973198683710E-013 1.151450973113358E-

017 TIME = 196.69085 DT = 0.66250000 SUM OF SQUARES = 0.11514510E-16

CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.77639011E-07 AND 0.77639011E-07

POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS 0.56208658E-05

TEMPERATURE: 1704. ENTHALPY: 0.5592E+05

U-FRACTION IN SYSTEM: CR = .191419766484524 FE = .733193050748551

NI = .0753871827669249

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

3 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: R_FCC_A1

CPU time used in timestep 1 seconds

1.454026536091647E-006 1.454359117619401E-006 1.454001659786809E-006 1.453664261497834E-006 8.606587472876681E-

007 4.249638417202260E-007 3.262596954381343E-008 1.388431396930162E-012 1.963259591187198E-

```
017      TIME =    198.01585          DT   1.3250000          SUM OF SQUARES =    0.19632596E-16  
CELL # 1 VELOCITY AT INTERFACE # 2 IS    0.91803141E-07 AND    0.91803141E-07  
POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS    0.57425050E-05  
TEMPERATURE:    1701.           ENTHALPY:    0.5580E+05  
U-FRACTION IN SYSTEM: CR = .191419766484521 FE = .733193050748554  
NI = .0753871827669252  
TOTAL SIZE OF SYSTEM: 1E-04 [m]  
10 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: R_FCC_A1  
  
CPU time used in timestep                2 seconds  
1.244319273883474E-006        1.244443998637513E-006        1.244744746398433E-006        1.243773368185792E-006        8.842480260593866E-  
007        5.113987890663018E-007        1.095007729722212E-007        1.184043441071940E-011        4.534939770399833E-  
016        7.718568589832551E-020        TIME =    200.00000        DT =    1.9841508        SUM OF SQUARES =    0.77185686E-19  
CELL # 1 VELOCITY AT INTERFACE # 2 IS    0.10665583E-06 AND    0.10665583E-06  
POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS    0.59541262E-05  
TEMPERATURE:    1696.           ENTHALPY:    0.5562E+05  
U-FRACTION IN SYSTEM: CR = .191419766484487 FE = .733193050748579  
NI = .0753871827669334  
TOTAL SIZE OF SYSTEM: 1E-04 [m]  
MUST SAVE WORKSPACE ON FILE  
WORKSPACE SAVED ON FILE  
RECLAIMING WORKSPACE  
DELETING TIME-RECORD FOR TIME    194.62054  
DELETING TIME-RECORD FOR TIME    195.44866  
DELETING TIME-RECORD FOR TIME    195.53147  
DELETING TIME-RECORD FOR TIME    195.69710  
DELETING TIME-RECORD FOR TIME    196.02835  
DELETING TIME-RECORD FOR TIME    196.69085  
  
KEEPING TIME-RECORD FOR TIME    198.01585  
AND FOR TIME    200.00000  
WORKSPACE RECLAIMED  
  
TIMESTEP AT    200.000000    SELECTED  
  
DIC>  
DIC>  
DIC>  
DIC>  
DIC>  
DIC>  
DIC>  
DIC>  
DIC>  
DIC>  
DIC>  
DIC>  
DIC>  
DIC>  
DIC>  
DIC>  
DIC>  
DIC>  
DIC>  
DIC>  
DIC>  
DIC>  
DIC> @@  
DIC> @@ THE SIMULATION IS FINISHED  
DIC> @@  
DIC>  
DIC> set-inter  
--OK---
```


exb4d-plot

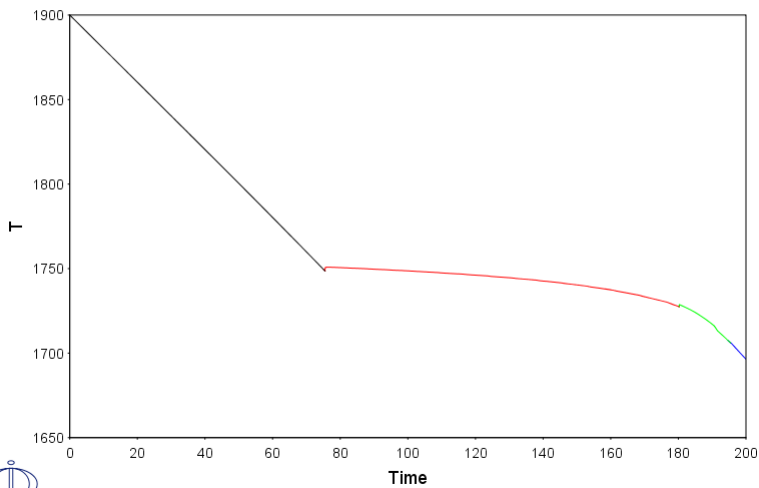
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb4d\plot.DCM"DIC>
DIC>
DIC> @@ exb4d_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE b4b
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 2.00000E+02
DIC> read exb4d
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
```

POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson

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

Fe-18%Cr-8%Ni

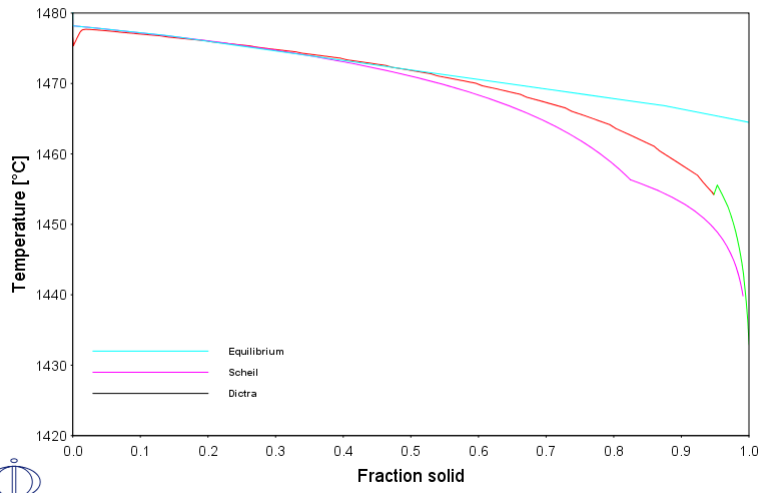
2018.02.18.19.40.37
"FIRST" INTERFACE OF SYSTEM
CELL #1



```
POST-1:
POST-1:Hit RETURN to continue
POST-1: enter func fs=1-ivv(liquid);
POST-1: s-d-a x fs
POST-1: s-s-s x n 0 1
POST-1: s-ax-te x n Fraction solid
POST-1:
POST-1: s-d-a y t-c
POST-1: s-s-s y n 1420 1480
POST-1:
POST-1: s-p-c interf smalta lower
POST-1:
POST-1: app y exb4d.exp 0; 1
POST-1: plo
```

Fe-18%Cr-8%Ni

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



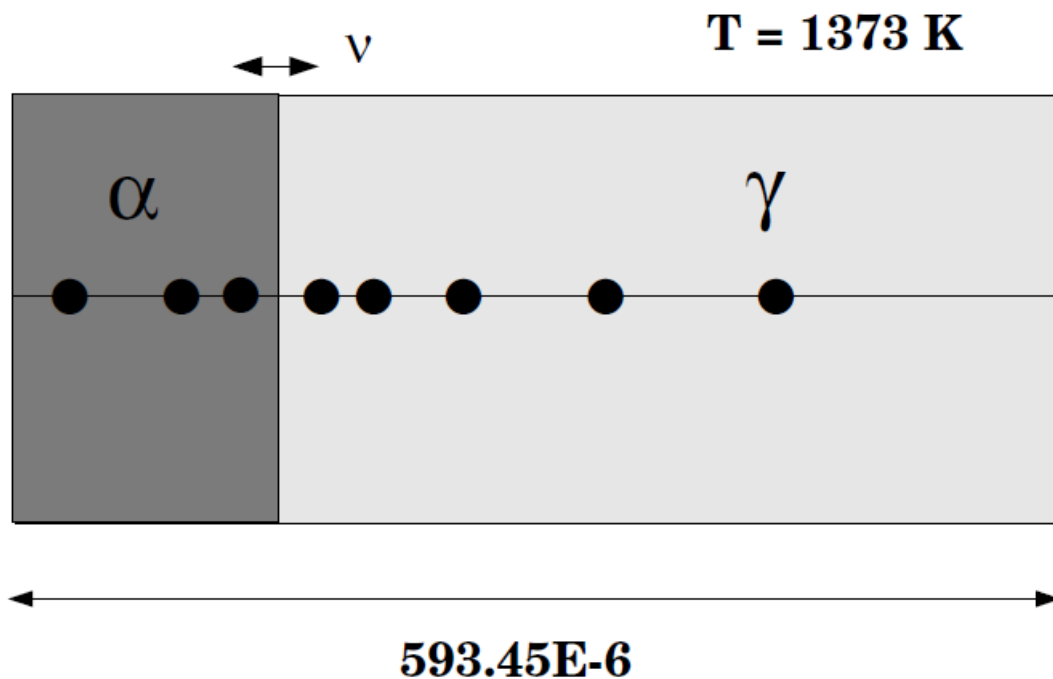
POST-1:
POST-1:
POST-1:
POST-1: set-inter
--OK--
POST-1:



Example exb5

$\gamma/\alpha/\gamma$ diffusion couple of Fe-Ni-Cr alloys

This example demonstrates the evaluation of a ternary Fe-Cr-Ni diffusion couple. A thin slice of 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. Kikuchi: Acta Metall.Mater. 41 (1993), pp.2045-2059.



exb5-setup

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

```
SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb5\setup.DCM" @@
SYS: @@ Moving boundary problem.
SYS: @@ Ternary diffusion couple of Fe-Ni-Cr alloys
SYS: @@ This example demonstrates the evaluation of a ternary Fe-Cr-Ni diffusion
SYS: @@ couple. A thin slice of alpha phase (38%Cr, 0%Ni) is clamped between
SYS: @@ two thicker slices of gamma phase (27%Cr, 20%Ni). The assembly is
SYS: @@ subsequently heat treated at 1373 K. This example corresponds to diffusion
SYS: @@ couple A in M. Kajihara, C.-B. Lim and M. Kikuchi: ISIJ International
SYS: @@ 33 (1993), pp. 498-507. See also M. Kajihara and M. Kikuchi: Acta Metall.Mater.
SYS: @@ 41 (1993), pp.2045-2059.
SYS: -----
NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exb5_setup.DCM
SYS:
SYS: @@
SYS: @@ GO TO A DATABASE AND READ THE THERMODYNAMIC AND KINETIC DATA
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Current database: Steels/Fe-Alloys v9.0

VA /- DEFINED
LI2_FCC B2_BCC DICTRA_FCC_A1
REJECTED
TDB_TCFE9: sw fedemo
Current database: Iron Demo Database v2.0

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

List of references for assessed data

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

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

```

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

```

DATABASE NAME /FEDEMO/: mfedemo

Current database: Fe-Alloys Mobility demo database v2.0

```

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

```

List of references for assessed data

```

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

```

-OK-

```

APP:
APP: @@
APP: @@ GO TO THE DICTRA MODULE TO SET UP THE SIMULATION
APP: @@
APP: go d-m
NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ SET THE GLOBAL CONDITIONS
DIC> @@

```

```

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

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

```

exb5-run

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb5\run.DCM"DIC>
DIC>
DIC> @@ exb5_run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING EXAMPLE b5
DIC> @@
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA MONITOR AND READ THE SET UP FROM FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 0.00000E+00
DIC> read exb5
OK
DIC>
DIC> @@
DIC> @@ START THE SIMULATION
DIC> @@
DIC> simulate
Region: ALPHA
single geometric dense at 0.93450E-04
0.80000 36
Region: GAMMA
single geometric dense at 0.0000
1.2500 103
Trying old scheme 4
GENERATING STARTING VALUES FOR CELL # 1 INTERFACE # 2
DETERMINING INITIAL EQUILIBRIUM VALUES
CALCULATING STARTING VALUES: 9 EQUILIBRIUM CALCULATIONS
*** ERROR 1611 IN QTHISS
*** TOO MANY ITERATIONS
Give the command INFO TROUBLE for help
DONE 6 OUT OF 9
*** ERROR 1611 IN QTHISS
*** TOO MANY ITERATIONS
Give the command INFO TROUBLE for help
DONE 9 OUT OF 9 try 1 failed
try 2 failed
try 3 failed
DETERMINED ACTIVITIES ACR(NI) 2.00457405352E-04

UNABLE TO OBTAIN GOOD STARTING VALUE USING THE OLD SCHEME
USE NEW SCHEME /YES/:

Trying new scheme
GENERATING STARTING VALUES FOR CELL # 1 INTERFACE # 2
DETERMINING INITIAL EQUILIBRIUM VALUES
CALCULATING STARTING VALUES: 18 EQUILIBRIUM CALCULATIONS DONE 1 OUT OF 18
04

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

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

output ignored...

... output resumed

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

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

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

```

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

CPU time used in timestep 1 seconds
4.278373565459864E-009 4.280902901842744E-009 4.297285706959512E-009 1.879840611235033E-009 8.591834998963679E-
010 4.289222548337157E-016 1.381416581816048E-
024 TIME = 3600000.0 DT = 317931.12 SUM OF SQUARES = 0.13814166E-23
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.49338740E-11 AND -0.49338740E-11
POSITION OF INTERFACE ALPHA / GAMMA IS 0.87487243E-04
U-FRACTION IN SYSTEM: CR = .30528044638003 FE = .471672022864279
NI = .223047530755692
TOTAL SIZE OF SYSTEM: 5.9345E-04 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 0.0000000
DELETING TIME-RECORD FOR TIME 0.10000000E-06
DELETING TIME-RECORD FOR TIME 0.93355784E-05
DELETING TIME-RECORD FOR TIME 0.27806735E-04
DELETING TIME-RECORD FOR TIME 0.64749049E-04
DELETING TIME-RECORD FOR TIME 0.13863368E-03
DELETING TIME-RECORD FOR TIME 0.28640293E-03
DELETING TIME-RECORD FOR TIME 0.58194144E-03
DELETING TIME-RECORD FOR TIME 0.11730185E-02
DELETING TIME-RECORD FOR TIME 0.23551725E-02
DELETING TIME-RECORD FOR TIME 0.47194806E-02
DELETING TIME-RECORD FOR TIME 0.94480967E-02
DELETING TIME-RECORD FOR TIME 0.18905329E-01
DELETING TIME-RECORD FOR TIME 0.37819794E-01
DELETING TIME-RECORD FOR TIME 0.75648723E-01
DELETING TIME-RECORD FOR TIME 0.15130658
DELETING TIME-RECORD FOR TIME 0.19274610
DELETING TIME-RECORD FOR TIME 0.21544345
DELETING TIME-RECORD FOR TIME 0.26083817
DELETING TIME-RECORD FOR TIME 0.35162760
DELETING TIME-RECORD FOR TIME 0.40135502
DELETING TIME-RECORD FOR TIME 0.50080986
DELETING TIME-RECORD FOR TIME 0.69971953
DELETING TIME-RECORD FOR TIME 0.91386552
DELETING TIME-RECORD FOR TIME 1.3421575
DELETING TIME-RECORD FOR TIME 2.0765292
DELETING TIME-RECORD FOR TIME 3.2890531
DELETING TIME-RECORD FOR TIME 5.5909634
DELETING TIME-RECORD FOR TIME 10.194784
DELETING TIME-RECORD FOR TIME 13.853759
DELETING TIME-RECORD FOR TIME 21.171708
DELETING TIME-RECORD FOR TIME 35.807606
DELETING TIME-RECORD FOR TIME 65.079402
DELETING TIME-RECORD FOR TIME 89.577448
DELETING TIME-RECORD FOR TIME 138.57354
DELETING TIME-RECORD FOR TIME 236.56573
DELETING TIME-RECORD FOR TIME 319.77973
DELETING TIME-RECORD FOR TIME 486.20775
DELETING TIME-RECORD FOR TIME 761.28537
DELETING TIME-RECORD FOR TIME 1232.2152
DELETING TIME-RECORD FOR TIME 2093.9211
DELETING TIME-RECORD FOR TIME 3662.4504
DELETING TIME-RECORD FOR TIME 6799.5089
DELETING TIME-RECORD FOR TIME 13073.626
DELETING TIME-RECORD FOR TIME 25621.860
DELETING TIME-RECORD FOR TIME 50718.328
DELETING TIME-RECORD FOR TIME 100911.26
DELETING TIME-RECORD FOR TIME 201297.14
DELETING TIME-RECORD FOR TIME 402068.88
DELETING TIME-RECORD FOR TIME 762068.88
DELETING TIME-RECORD FOR TIME 1122068.9
DELETING TIME-RECORD FOR TIME 1482068.9
DELETING TIME-RECORD FOR TIME 1842068.9
DELETING TIME-RECORD FOR TIME 2202068.9
DELETING TIME-RECORD FOR TIME 2562068.9
DELETING TIME-RECORD FOR TIME 2922068.9

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

TIMESTEP AT 3600000.00 SELECTED

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

```


exb5-plot

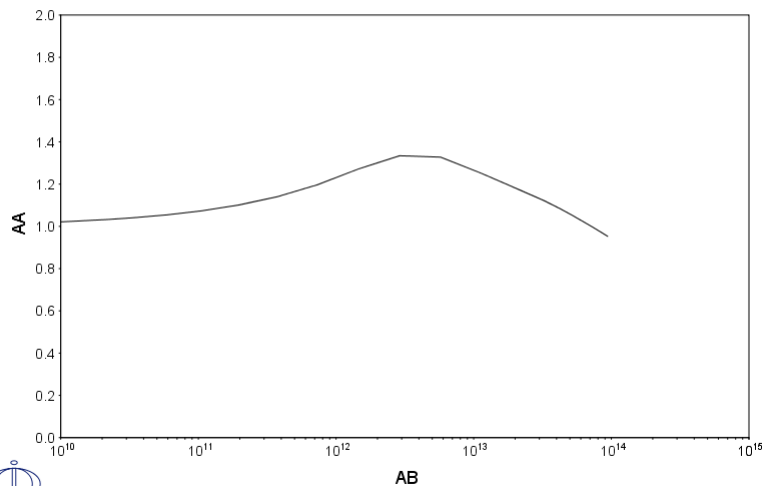
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb5\plot.DCM"DIC>
DIC>
DIC> @@ exb5_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE b5
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 3.60000E+06
DIC> read exb5
OK
DIC>
DIC> @@
DIC> @@ ENTER THE POST PROCESSOR, PLOT SOME QUANTITIES AND COMPARE WITH EXPERIMENTS
DIC> @@
DIC> post
```

```
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
```

```
POST-1:
POST-1: set-title Diffusion Couple A
POST-1:
POST-1: @@
POST-1: @@ WE ARE INTERESTED IN THE POSITION OF THE UPPER INTERFACE OF REGION ALPHA
POST-1: @@
POST-1: s-p-c interf alpha upper
POST-1:
POST-1: @@
POST-1: @@ 10 IS THE INITIAL THICKNESS USED FOR NORMALIZATION
POST-1: @@
POST-1: enter func l0=186.9e-6;
POST-1: enter func aa=2*poi(alpha,u)/l0;
POST-1: enter func ab=time/l0**2;
POST-1: s-i-v time
POST-1:
POST-1: s-d-a x ab
POST-1: s-s-s x n 1e10 1e15
POST-1: s-ax-ty x log
POST-1:
POST-1: s-d-a y aa
POST-1: s-s-s y n 0 2
POST-1:
POST-1: app y exb5.exp
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 7
POST-1:
POST-1: plo
```

Diffusion Couple A

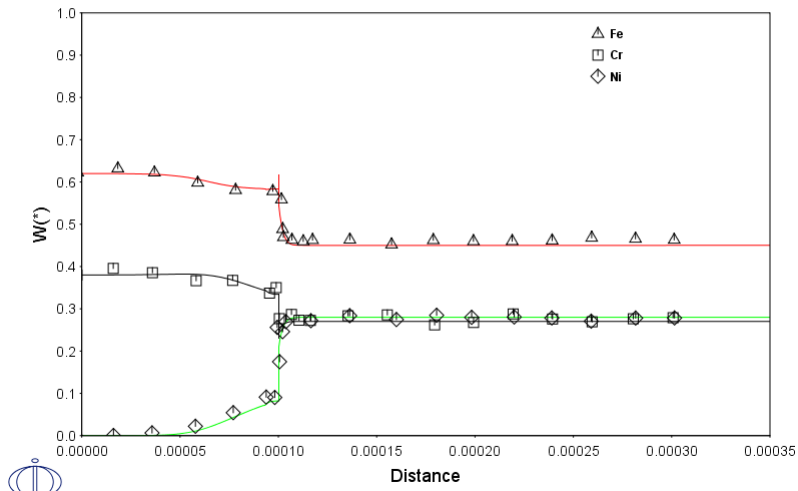
2018.02.18.19.44.46
UPPER INTERFACE OF REGION "ALPHA#1"
CELL#1



```
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ PLOT THE CONCENTRATION PROFILES FOR DIFFERENT ANNEALING TIMES
POST-1: @@
POST-1: s-d-a x dist glo
INFO: Distance is set as independent variable
POST-1: s-ax-ty x lin
POST-1: s-s-s x n 0 350e-6
POST-1:
POST-1: s-d-a y w(*)
POST-1: s-s-s y n 0 1
POST-1:
POST-1: s-p-c time 3600
POST-1:
POST-1: app y exb5.exp 0; 1
POST-1: plo
```

2018.02.18 19:44.46
Time = 3600
CELL #1

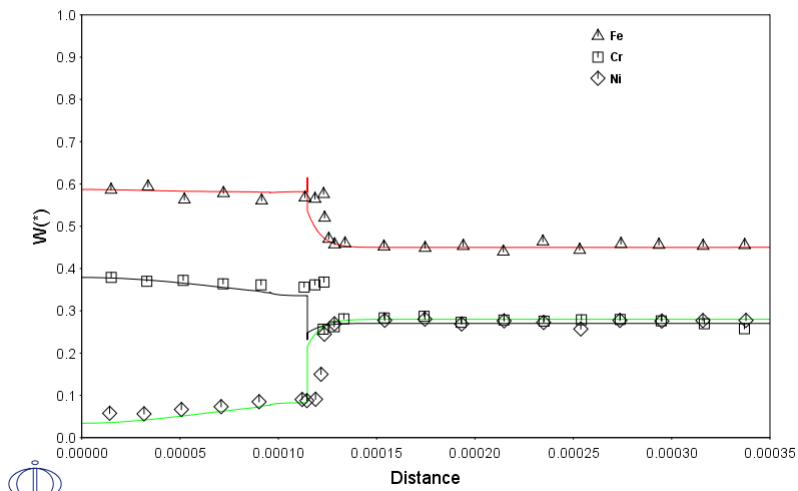
Diffusion Couple A



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

Diffusion Couple A

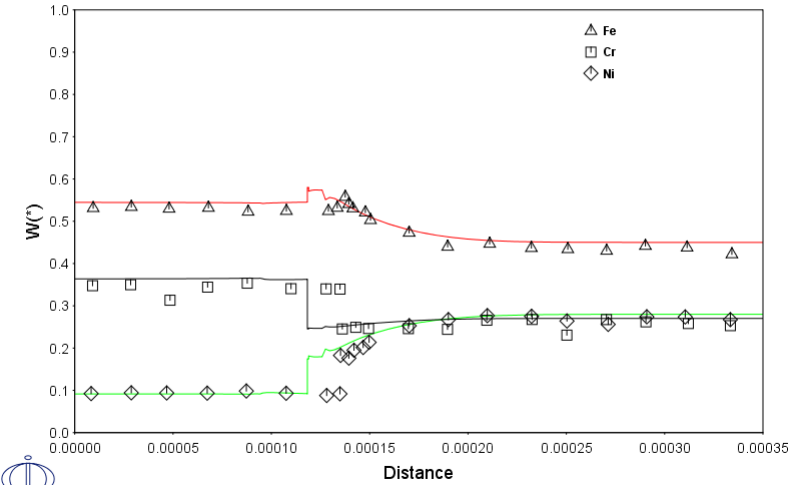
2018.02.18 19:44.47
Time = 36000
CELL #1



POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: s-p-c time 360000
POST-1: app y exb5.exp 0; 3
POST-1: plo

2018.02.18 19:44.48
Time = 360000
CELL #1

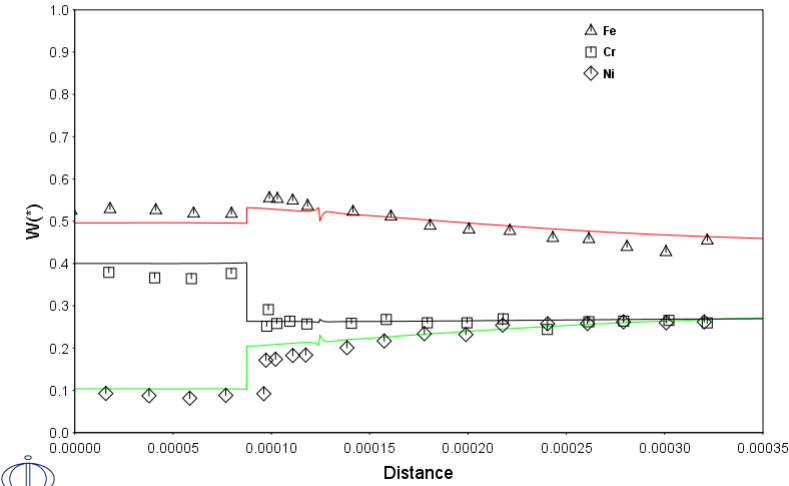
Diffusion Couple A



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

Diffusion Couple A

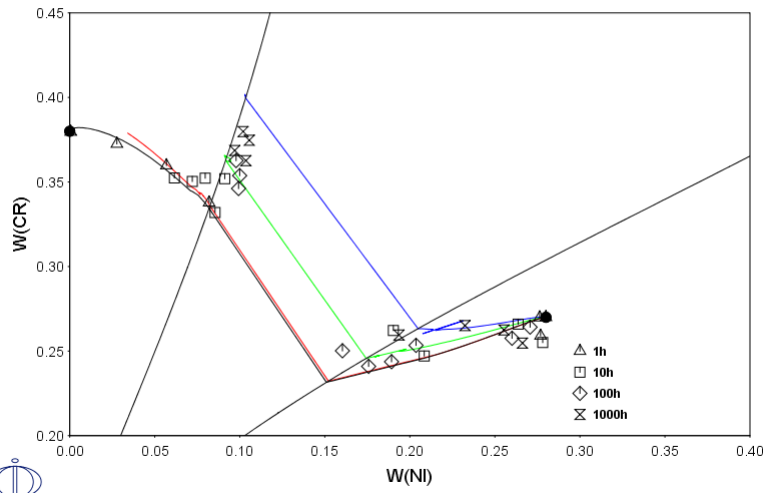
2018.02.18 19:44.49
Time = 3600000
CELL #1



POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ FINALLY PLOT DIFFERENT DIFFUSION PATHS.
POST-1: @@
POST-1: s-d-a x w(ni)
POST-1: s-s-s x n .00 .40
POST-1:
POST-1: s-d-a y w(cr)
POST-1: s-s-s y n .20 .45
POST-1:
POST-1: s-i-v dist glob
POST-1:
POST-1: s-p-c time 3600,36000,360000,3600000
POST-1:
POST-1: app y exb5.exp 0; 5 6
POST-1: plo

Diffusion Couple A

2018.02.18 19:44.49
Time = 3600,36000,360000,3600000
CELL #1



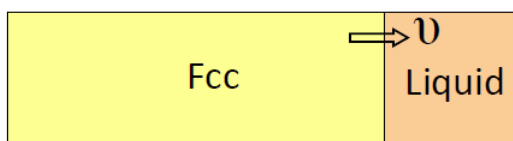
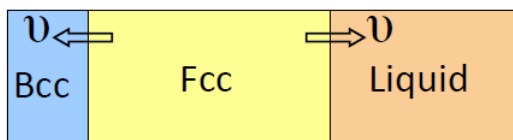
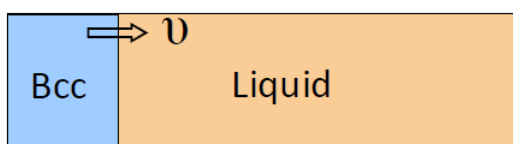
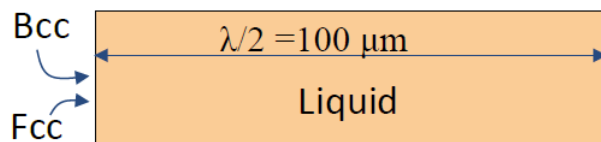
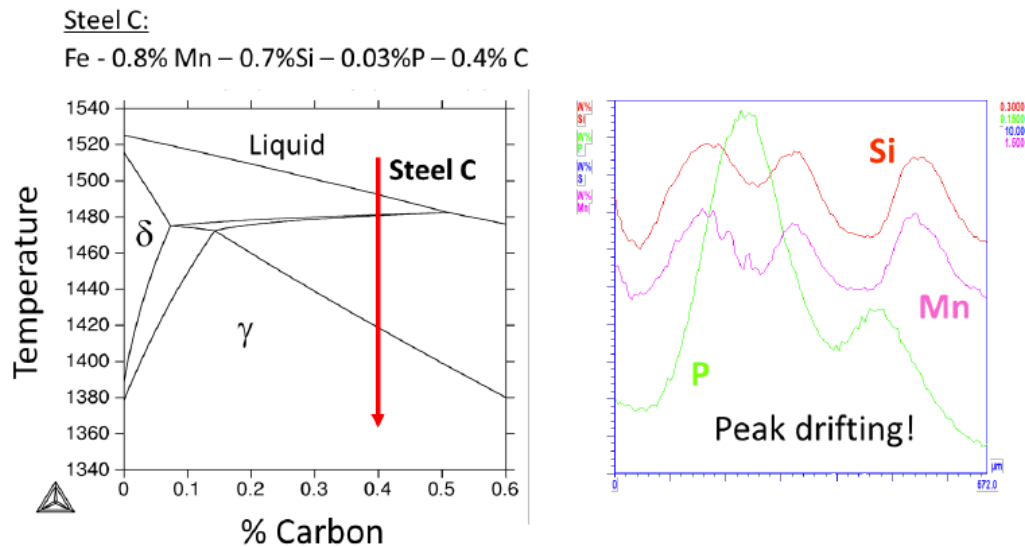
POST-1:
POST-1:
POST-1:
POST-1: set-inter
--OK--
POST-1:



Example exb6

Micro-segregation of phosphorus

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



exb6-setup

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

SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb6\setup.DCM" @@

SYS: @@ Moving boundary problem.

SYS: @@ Microsegregation of phosphorus

SYS: @@ This example illustrates the effect of microsegregation

SYS: @@ of phosphorus during peritectic solidification in steel.

SYS: -----

NO SUCH COMMAND, USE HELP

SYS:

SYS: @@

SYS: @@ START BY GOING TO THE DATABASE MODULE

SYS: @@

SYS: go da

THERMODYNAMIC DATABASE module

Current database: Steels/Fe-Alloys v9.0

VA /- DEFINED
L12_FCC B2_BCC DICTRA_FCC_A1
REJECTED

TDB_TCFE9:

TDB_TCFE9: @@ USE A TCFE DATABASE FOR THERMODYNAMIC DATA

TDB_TCFE9: sw tcfe7

Current database: Steels/Fe-Alloys v7.0

VA DEFINED
L12_FCC B2_BCC B2_VACANCY
HIGH SIGMA DICTRA_FCC_A1 REJECTED

TDB_TCFE7:

TDB_TCFE7: @@ DEFINE THE SYSTEM TO WORK WITH

TDB_TCFE7: def-sys fe c si mn p

FE C SI
MN P DEFINED

TDB_TCFE7:

TDB_TCFE7: @@ EXCLUDE THE THERMODYNAMIC DATA FOR THE PHASES THAT ARE NOT NEEDED

TDB_TCFE7: rej ph /all

GAS:G LIQUID:L BCC_A2
FCC_A1 HCP_A3 DIAMOND_FCC_A4
RED_P WHITE_P GRAPHITE
CEMENTITE M23C6 M7C3
M5C2 KSI_CARBIIDE A1_KAPPA
KAPPA FE4N_LP1 FECN_CHI
LAVES_PHASE_C14 M3SI G_PHASE
CR3SI FE2SI MSI
M5SI3 AL4C3 FE8SI2C
SIC FEP CU3P
M2P M3P REJECTED

TDB_TCFE7: res ph fcc liq bcc

FCC_A1 LIQUID:L BCC_A2
RESTORED

TDB_TCFE7:

TDB_TCFE7: @@ RETRIEVE DATA FROM THE DATABASE FILE

TDB_TCFE7: get

REINITIATING GES

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

FUNCTIONS

List of references for assessed data

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

-OK-

TDB_TCFE7:

TDB_TCFE7: @@

TDB_TCFE7: @@ MOBILITY/DIFFUSIVITY DATA ARE STORED IN A SEPARATE DATABASE FILE.

TDB_TCFE7: @@ SWITCH TO A MOBILITY DATABASE AND APPEND THE DATA.

TDB_TCFE7: @@

TDB_TCFE7: app

Use one of these databases

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

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

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

VA DEFINED
APP: def-sys fe c si mn p
FE C SI
MN P DEFINED
APP: rej ph /all
BCC_A2 CEMENTITE FCC_A1
FE4N_LP1 HCP_A3 LIQUID:L

```

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

List of references for assessed data

'This parameter has not been assessed'
'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'
'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
-Ni'
'Bae et al.: Z. Metallkunde 91(2000)672-674; fcc Fe-Mn
Mn-Ni'
'V. V. Mural and P. L. Gruzin, Phys. Met. Metallogr. (English Transl.) 17
(5) (1964)154.; Impurity diff of P in fcc Fe.'
'D. Bergner et al., Defect and Diffusion Forum 66-69(1989)409. Impurity
diffusion of Si in fcc Fe.'
'B. Jonsson: Z. Metallkunde 85(1994)498-501; C and N diffusion in bcc Cr
-Fe-Ni'
'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
in bcc Fe'
'B. Jonsson: Unpublished research bcc Fe-Si 1994'
'Assessed from data presented in Landholt-Bornstein, Vol. 26, ed. H.
Mehrer, springer (1990); Impurity diff of Mn in bcc Fe.'
'Assessed from data presented in Landholt-Bornstein, Vol. 26, ed. H.
Mehrer, springer (1990); Impurity diff of P in bcc Fe.'

-OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP
APP: @@
APP: go d-m
NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> @@ LOWER THE TEMPERATURE TO A RATE OF 0.2 K/s
DIC> @@
DIC> set-cond glob T 0 1780-0.2*TIME; * N

DIC>
DIC> @@
DIC> @@ ENTER A REGION CALLED smalta
DIC> @@
DIC> enter-region smalta
DIC>
DIC> @@
DIC> @@ ENTER A DOUBLE GEOMETRIC GRID INTO THE REGION
DIC> @@
DIC> enter-grid
REGION NAME : /SMALTA/: smalta
WIDTH OF REGION /1/: 1e-4
TYPE /LINEAR/: AUTO
DIC>
DIC> @@
DIC> @@ ENTER active PHASES INTO THE REGION
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /SMALTA/: smalta
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: liq
SETTING CHECK INTERFACE POSITION ON
DIC>
DIC> @@
DIC> @@ ENTER inactive PHASES INTO THE REGION, BOTH PHASES ON THE SAME SIDE
DIC> @@ OF THE LIQUID REGION TO GET A PERITECTIC REACTION.
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inact
ATTACH TO REGION NAMED /SMALTA/: smalta
ATTACHED TO THE RIGHT OF SMALTA /YES/: no
PHASE NAME: /NONE/: fcc#1
DEPENDENT COMPONENT ? /SI/: fe
REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-5
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inact
ATTACH TO REGION NAMED /SMALTA/: smalta
ATTACHED TO THE RIGHT OF SMALTA /YES/: no
PHASE NAME: /NONE/: bcc#1
DEPENDENT COMPONENT ? /SI/: fe
REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-5
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> @@
DIC> @@ ENTER A START COMPOSITION FOR THE LIQUID
DIC> @@
DIC> enter-composition
REGION NAME : /SMALTA/: smalta
PHASE NAME: /LIQUID/: liq
DEPENDENT COMPONENT ? /SI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: c lin 0.4 0.4
PROFILE FOR /MN/: si lin 0.7 0.7
PROFILE FOR /P/: mn lin 0.8 0.8
PROFILE FOR /SI/: p lin 0.03 0.03
DIC>
DIC> @@
DIC> @@ THE BOUNDARY CONDITION IS A CLOSED SYSTEM (DEFAULT) AS WE DO NOT SPECIFY
DIC> @@ ANYTHING ELSE
DIC> @@
DIC>
DIC> @@

```



```
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 3000
AUTOMATIC TIMESTEP CONTROL /YES/: yes
MAX TIMESTEP DURING INTEGRATION /300/: 15
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC>
DIC>
DIC> @@ CHECK THE INTERFACE POSITION. THIS IS TO MAKE SURE THAT THE LIQUID REGION
DIC> @@ DOES NOT SHRINK TOO MUCH DURING A TIMESTEP. IN ADDITION THE TIMESTEP IS
DIC> @@ CONTROLLED BY THE PHASE INTERFACE DISPLACEMENT DURING THE SIMULATION.
DIC> @@
DIC> s-s-c
NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDF: /2/:
CHECK INTERFACE POSITION /YES/: yes
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (0 -> 0.5 -> 1): /.5/:
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /NO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/:
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exb6 Y
DIC>
DIC> set-inter
--OK--
DIC>
```

exb6-run

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb6\run.DCM"DIC>
DIC>
DIC> @@ exb6_run.DCM
DIC>
DIC> @@
DIC> @@ READ THE SET UP FROM FILE AND START THE SIMULATION
DIC> @@
DIC>
DIC> go d-m
TIME STEP AT TIME 0.00000E+00
DIC> read exb6
OK
DIC> sim
Region: SMALTA
single geometric dense at 0.0000
1.0846 88
U-FRACTION IN SYSTEM: C = .0185375871047351 FE = .97748186120908
MN = .00810568126669965 P = 5.39133528237326E-04
SI = .0138733239959838
TOTAL SIZE OF SYSTEM: 1E-04 [m]
U-FRACTION IN SYSTEM: C = .0185375871047351 FE = .97748186120908
MN = .00810568126669965 P = 5.39133528237326E-04
SI = .0138733239959838
TOTAL SIZE OF SYSTEM: 1E-04 [m]
TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0185375871047351 FE = .977481861209079
MN = .00810568126669965 P = 5.39133528237326E-04
SI = .0138733239959838
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.26002472E-05 DT = 0.25002472E-05 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0185375871047351 FE = .977481861209079
MN = .00810568126669965 P = 5.39133528237326E-04
SI = .0138733239959838
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.76007416E-05 DT = 0.50004944E-05 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0185375871047351 FE = .97748186120908
MN = .00810568126669965 P = 5.39133528237326E-04
SI = .0138733239959838
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.17601730E-04 DT = 0.10000989E-04 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0185375871047351 FE = .97748186120908
MN = .00810568126669965 P = 5.39133528237326E-04
SI = .0138733239959838
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.37603708E-04 DT = 0.20001978E-04 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0185375871047351 FE = .977481861209079
MN = .00810568126669965 P = 5.39133528237326E-04
SI = .0138733239959838
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 1 seconds
TIME = 0.77607664E-04 DT = 0.40003955E-04 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0185375871047351 FE = .977481861209079
MN = .00810568126669965 P = 5.39133528237326E-04
SI = .0138733239959838
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.15761557E-03 DT = 0.80007911E-04 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0185375871047351 FE = .977481861209079
MN = .00810568126669965 P = 5.39133528237326E-04
SI = .0138733239959838
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.31763140E-03 DT = 0.16001582E-03 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0185375871047351 FE = .97748186120908
MN = .00810568126669965 P = 5.39133528237326E-04
SI = .0138733239959838
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.63766304E-03 DT = 0.32003164E-03 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0185375871047351 FE = .97748186120908
MN = .00810568126669965 P = 5.39133528237326E-04
SI = .0138733239959838
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.12777263E-02 DT = 0.64006329E-03 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0185375871047351 FE = .97748186120908
MN = .00810568126669965 P = 5.39133528237326E-04
SI = .0138733239959838
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.25578529E-02 DT = 0.12801266E-02 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0185375871047351 FE = .97748186120908
MN = .00810568126669966 P = 5.39133528237326E-04
SI = .0138733239959838
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.51181060E-02 DT = 0.25602531E-02 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0185375871047351 FE = .97748186120908
MN = .00810568126669966 P = 5.39133528237326E-04
SI = .0138733239959838
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 1 seconds
TIME = 0.10238612E-01 DT = 0.51205063E-02 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .018537587104735 FE = .97748186120908
MN = .00810568126669965 P = 5.39133528237326E-04
SI = .0138733239959838
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.20479625E-01 DT = 0.10241013E-01 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .018537587104735 FE = .97748186120908
MN = .00810568126669965 P = 5.39133528237325E-04
SI = .0138733239959838
TOTAL SIZE OF SYSTEM: 1E-04 [m]
CPU time used in timestep 0 seconds
TIME = 0.40961650E-01 DT = 0.20482025E-01 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .018537587104735 FE = .97748186120908
MN = .00810568126669964 P = 5.39133528237325E-04
SI = .0138733239959838
```

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

output ignored...

... output resumed

```
DELETING TIME-RECORD FOR TIME 896.69665
DELETING TIME-RECORD FOR TIME 911.69665
DELETING TIME-RECORD FOR TIME 926.69665
DELETING TIME-RECORD FOR TIME 941.69665
DELETING TIME-RECORD FOR TIME 956.69665
DELETING TIME-RECORD FOR TIME 971.69665
DELETING TIME-RECORD FOR TIME 986.69665
DELETING TIME-RECORD FOR TIME 1001.6966
DELETING TIME-RECORD FOR TIME 1016.6966
DELETING TIME-RECORD FOR TIME 1031.6966
DELETING TIME-RECORD FOR TIME 1046.6966
DELETING TIME-RECORD FOR TIME 1061.6966
DELETING TIME-RECORD FOR TIME 1076.6966
DELETING TIME-RECORD FOR TIME 1091.6966
DELETING TIME-RECORD FOR TIME 1106.6966
DELETING TIME-RECORD FOR TIME 1121.6966
DELETING TIME-RECORD FOR TIME 1136.6966
DELETING TIME-RECORD FOR TIME 1151.6966
DELETING TIME-RECORD FOR TIME 1166.6966
DELETING TIME-RECORD FOR TIME 1181.6966
DELETING TIME-RECORD FOR TIME 1196.6966
DELETING TIME-RECORD FOR TIME 1211.6966
DELETING TIME-RECORD FOR TIME 1226.6966
DELETING TIME-RECORD FOR TIME 1241.6966
DELETING TIME-RECORD FOR TIME 1256.6966
DELETING TIME-RECORD FOR TIME 1271.6966
DELETING TIME-RECORD FOR TIME 1286.6966
DELETING TIME-RECORD FOR TIME 1301.6966
DELETING TIME-RECORD FOR TIME 1316.6966
DELETING TIME-RECORD FOR TIME 1331.6966
DELETING TIME-RECORD FOR TIME 1346.6966
DELETING TIME-RECORD FOR TIME 1361.6966
DELETING TIME-RECORD FOR TIME 1376.6966
DELETING TIME-RECORD FOR TIME 1391.6966
DELETING TIME-RECORD FOR TIME 1406.6966
DELETING TIME-RECORD FOR TIME 1421.6966
DELETING TIME-RECORD FOR TIME 1436.6966
DELETING TIME-RECORD FOR TIME 1451.6966
DELETING TIME-RECORD FOR TIME 1466.6966
DELETING TIME-RECORD FOR TIME 1481.6966
DELETING TIME-RECORD FOR TIME 1496.6966
DELETING TIME-RECORD FOR TIME 1511.6966
DELETING TIME-RECORD FOR TIME 1526.6966
DELETING TIME-RECORD FOR TIME 1541.6966
DELETING TIME-RECORD FOR TIME 1556.6966
DELETING TIME-RECORD FOR TIME 1571.6966
DELETING TIME-RECORD FOR TIME 1586.6966
DELETING TIME-RECORD FOR TIME 1601.6966
DELETING TIME-RECORD FOR TIME 1616.6966
DELETING TIME-RECORD FOR TIME 1631.6966
DELETING TIME-RECORD FOR TIME 1646.6966
DELETING TIME-RECORD FOR TIME 1661.6966
DELETING TIME-RECORD FOR TIME 1676.6966
DELETING TIME-RECORD FOR TIME 1691.6966
DELETING TIME-RECORD FOR TIME 1706.6966
DELETING TIME-RECORD FOR TIME 1721.6966
DELETING TIME-RECORD FOR TIME 1736.6966
DELETING TIME-RECORD FOR TIME 1751.6966
DELETING TIME-RECORD FOR TIME 1766.6966
DELETING TIME-RECORD FOR TIME 1781.6966
DELETING TIME-RECORD FOR TIME 1796.6966
DELETING TIME-RECORD FOR TIME 1811.6966
DELETING TIME-RECORD FOR TIME 1826.6966
DELETING TIME-RECORD FOR TIME 1841.6966
DELETING TIME-RECORD FOR TIME 1856.6966
DELETING TIME-RECORD FOR TIME 1871.6966
DELETING TIME-RECORD FOR TIME 1886.6966
DELETING TIME-RECORD FOR TIME 1901.6966
DELETING TIME-RECORD FOR TIME 1916.6966
DELETING TIME-RECORD FOR TIME 1931.6966
DELETING TIME-RECORD FOR TIME 1946.6966
DELETING TIME-RECORD FOR TIME 1961.6966
DELETING TIME-RECORD FOR TIME 1976.6966
DELETING TIME-RECORD FOR TIME 1991.6966
DELETING TIME-RECORD FOR TIME 2006.6966
DELETING TIME-RECORD FOR TIME 2021.6966
DELETING TIME-RECORD FOR TIME 2036.6966
DELETING TIME-RECORD FOR TIME 2051.6966
DELETING TIME-RECORD FOR TIME 2066.6966
DELETING TIME-RECORD FOR TIME 2081.6966
DELETING TIME-RECORD FOR TIME 2096.6966
DELETING TIME-RECORD FOR TIME 2111.6966
DELETING TIME-RECORD FOR TIME 2126.6966
DELETING TIME-RECORD FOR TIME 2141.6966
DELETING TIME-RECORD FOR TIME 2156.6966
```

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

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

```
TIMESTEP AT 3000.00000 SELECTED
```

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

exb6-plot

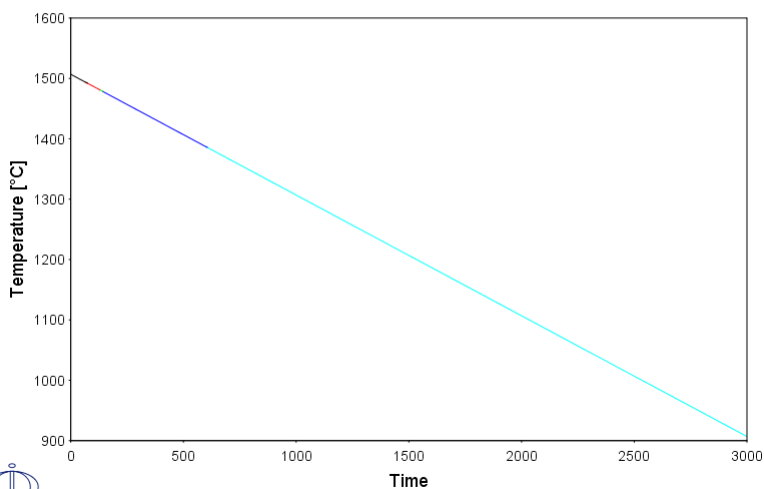
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb6\plot.DCM"DIC>
DIC>
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
      TIME STEP AT TIME 3.00000E+03
DIC> read exb6
      OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
```

```
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
```

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

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

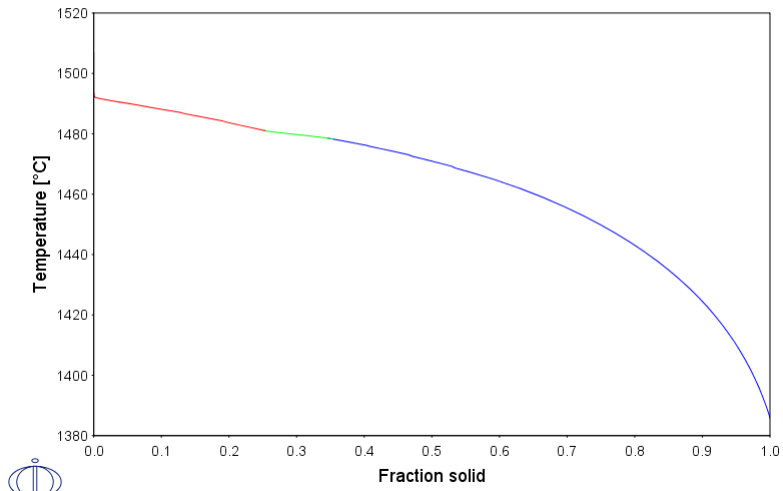
2018.02.18.20.25.24
"FIRST" INTERFACE OF SYSTEM
CELL #1



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

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

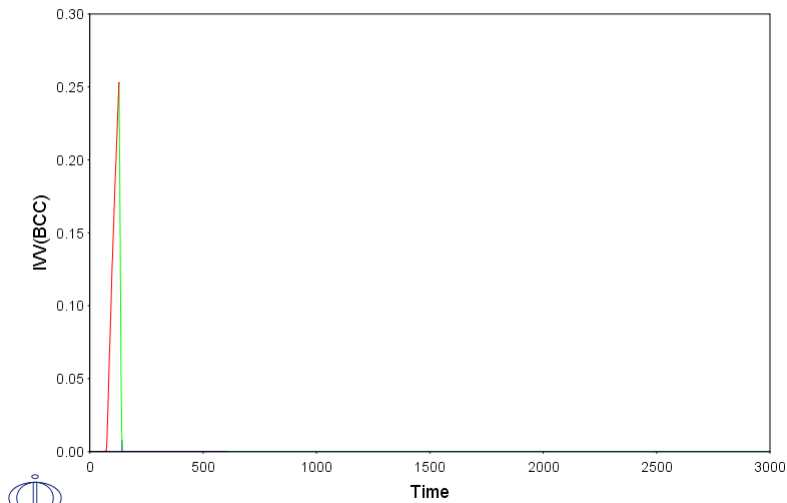
2018.02.18.20.25.27
LOWER INTERFACE OF REGION "SMALTA#1"
CELL #1



POST-1:
POST-1:Hit RETURN to continue
POST-1: s-d-a y ivv(bcc)
POST-1: s-d-a x time
INFO: Time is set as independent variable
POST-1:
POST-1: plot

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

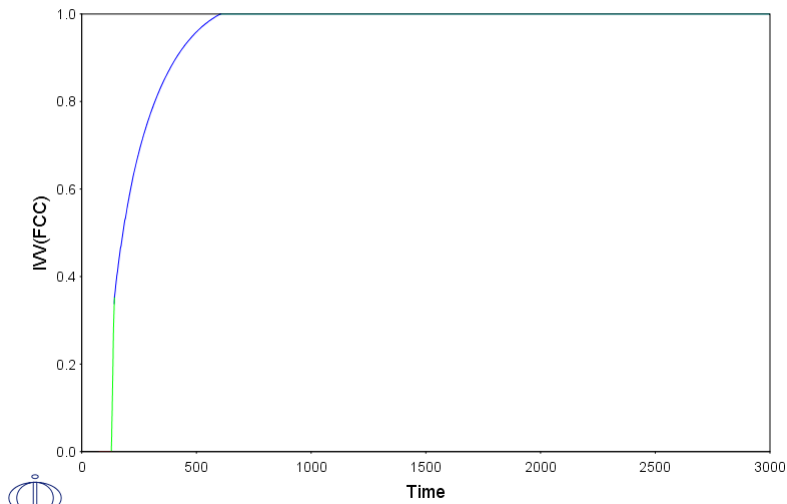
2018.02.18.20.25.30
CELL #1



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

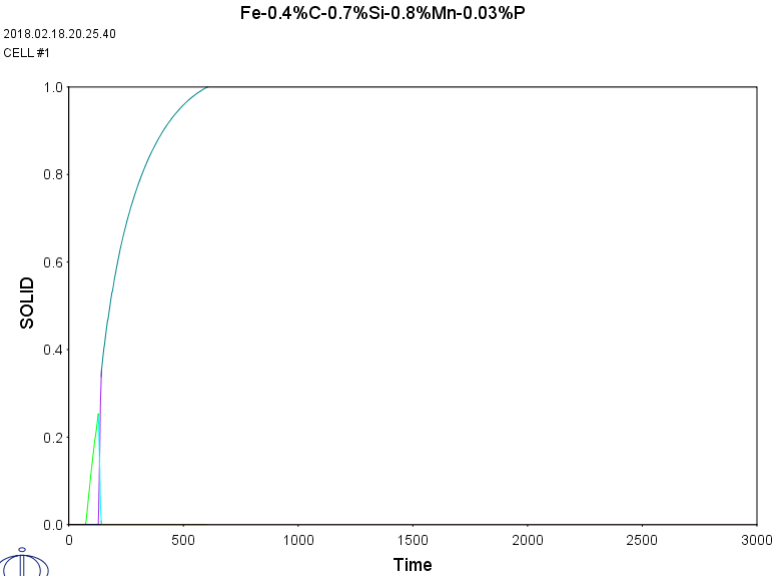
Fe-0.4%C-0.7%Si-0.8%Mn-0.03%P

2018.02.18.20.25.34
CELL #1

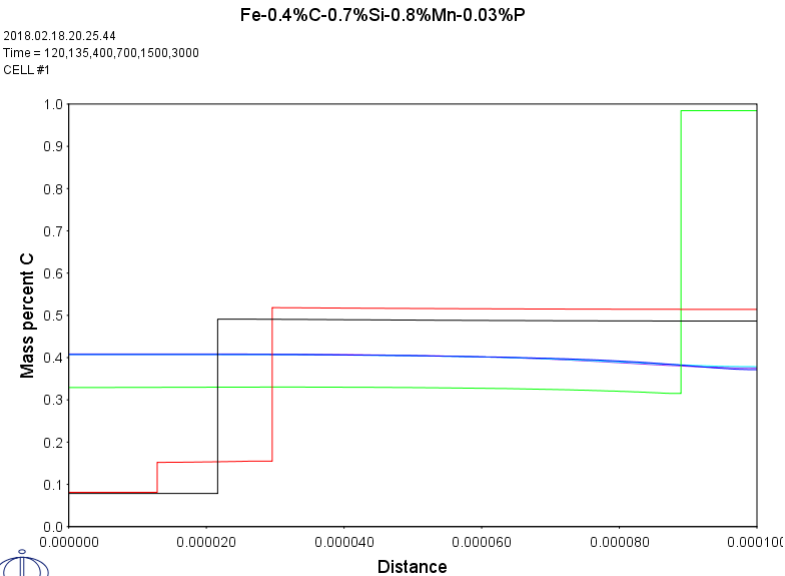


POST-1:
POST-1:Hit RETURN to continue
POST-1: ent table solid

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



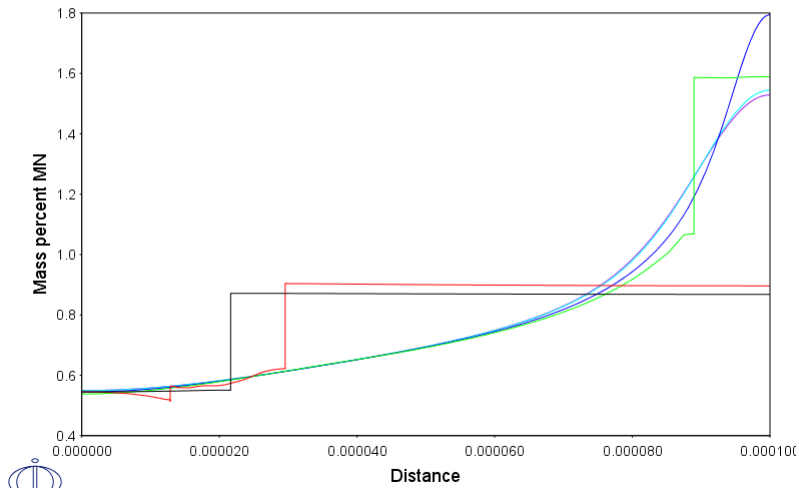
```
POST-1:
POST-1:Hit RETURN to continue
POST-1: s-d-a y w-p c
POST-1: s-d-a x dis gl
INFO: Distance is set as independent variable
POST-1: s-p-c time 120,135,400,700,1500,3000
POST-1:
POST-1: plot
```



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

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

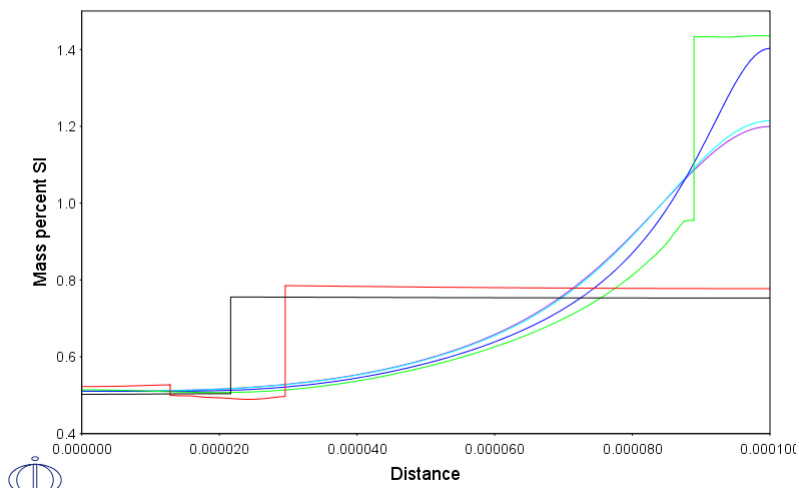
2018.02.18.20.25.46
Time = 120,135,400,700,1500,3000
CELL #1



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

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

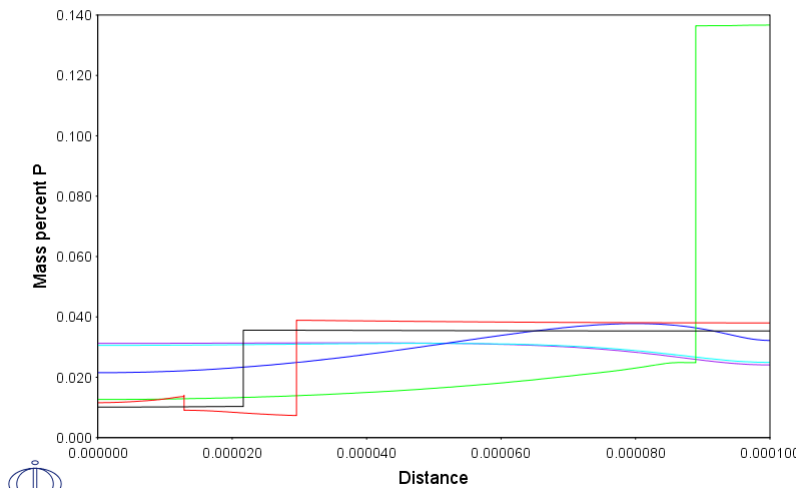
2018.02.18.20.25.48
Time = 120,135,400,700,1500,3000
CELL #1



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

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

2018.02.18.20.25.50
Time = 120,135,400,700,1500,3000
CELL #1

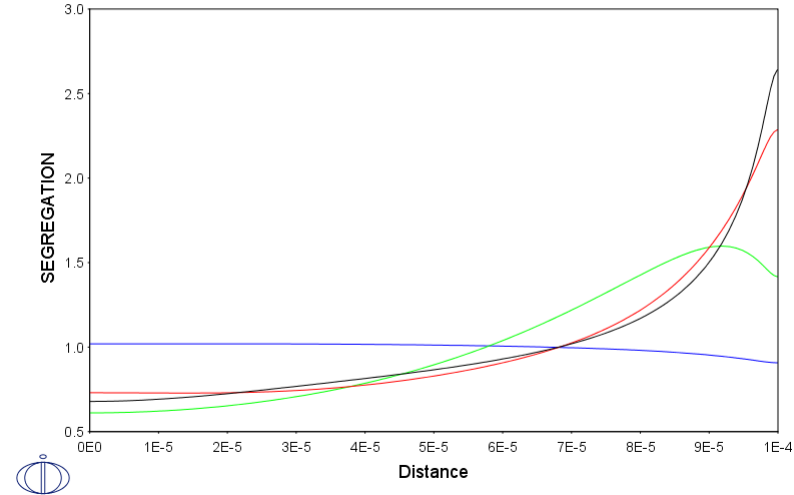


POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: ent function mnn
FUNCTION: w(mn)/0.008
&
POST-1: ent function sin


```
FUNCTION: w(si)/0.007
&
POST-1: ent function pn
FUNCTION: w(p)/0.0003
&
POST-1: ent function cn
FUNCTION: w(c)/0.004
&
POST-1: ent tabel segregation
Variable(s) mnn sin pn cn
POST-1:
POST-1:
POST-1: s-d-a y segregation
COLUMN NUMBER /*/:
POST-1:
POST-1:
POST-1: s-p-c time 610
POST-1: plot
```

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

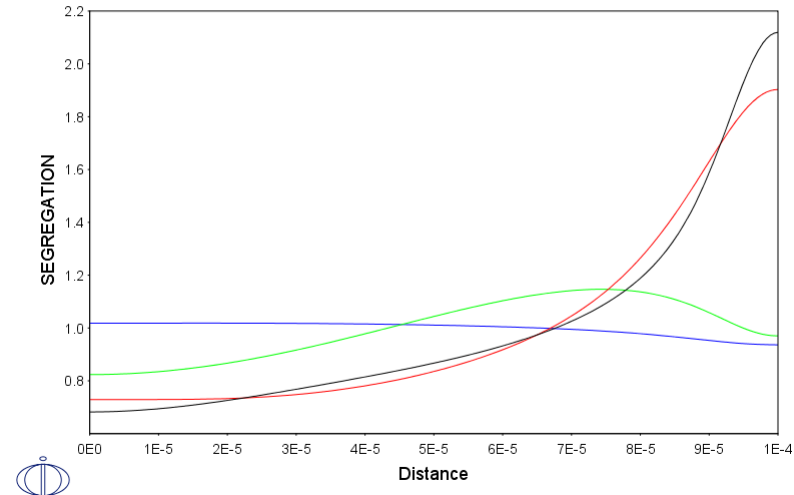
2018.02.18.20.25.52
Time=610
CELL#1



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

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

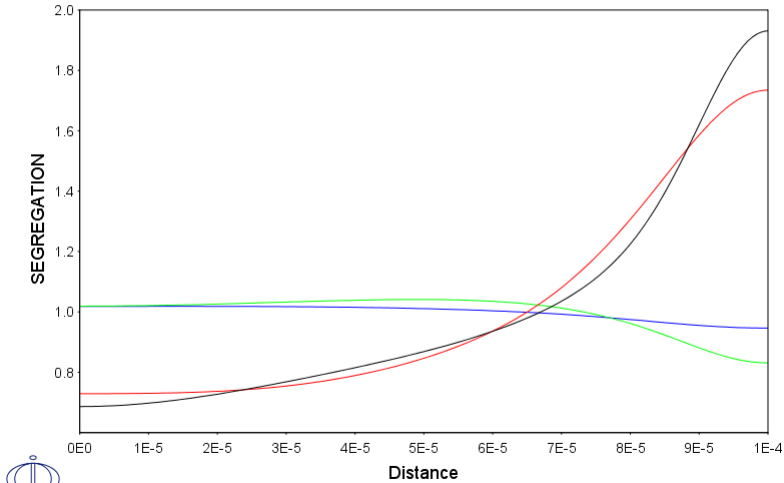
2018.02.18.20.25.54
Time=800
CELL#1



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

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

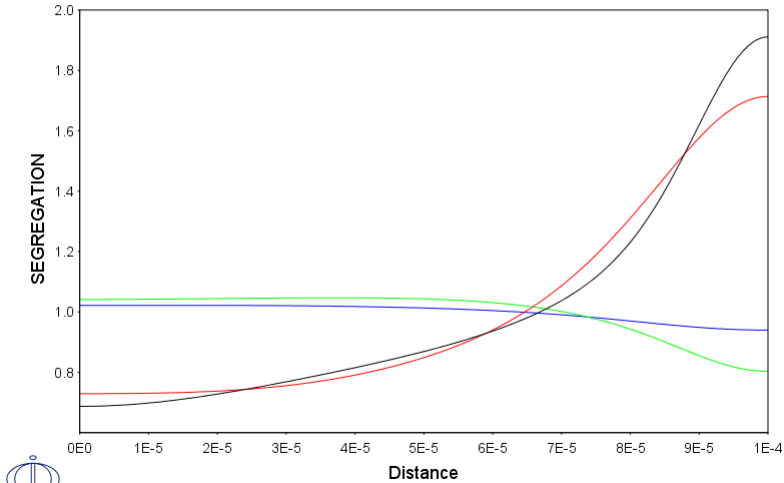
2018.02.18.20.25.55
Time = 1500
CELL #1



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

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

2018.02.18.20.25.57
Time = 3000
CELL #1



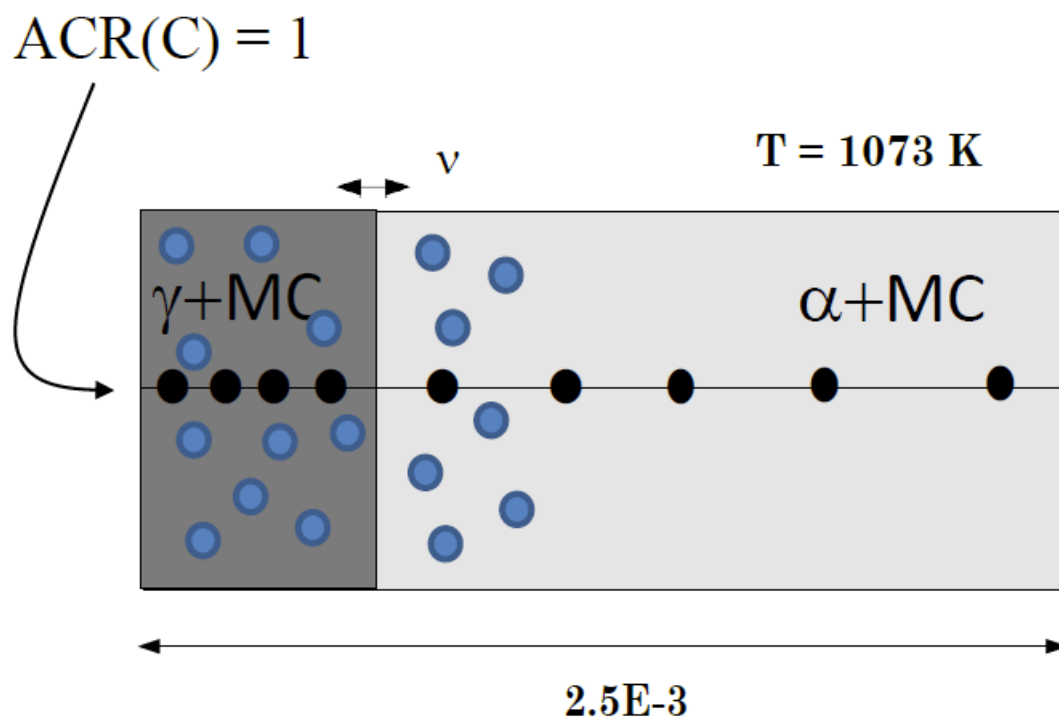
POST-1:
POST-1:Hit RETURN to continue
POST-1: set-inter
--OK--
POST-1:



Example exb7

Moving boundary problem with multiple phases on each side of the boundary

This example shows how to enter dispersed phases on either side of a phase interface. The particular case shows how the kinetics of a ferrite to austenite transformation is affected by simultaneous precipitation of niobium carbide. The transformation is caused by carburization.



exb7-setup

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

```
SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb7\setup.DCM" @@
SYS: @@ Moving boundary problem.
SYS: @@ Moving boundary problem with multiple phases on each side
SYS: @@ This example shows how to enter dispersed phases on either side
SYS: @@ of a phase interface. The particular case shows how
SYS: @@ the kinetics of a ferrite to austenite transformation is
SYS: @@ affected by simultaneous precipitation of niobium carbide.
SYS: @@ The transformation is caused by carburization.
SYS: -----
NO SUCH COMMAND, USE HELP
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASE
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Current database: Steels/Fe-Alloys v9.0

VA      /-  DEFINED
L12_FCC      B2_BCC      DICTRA_FCC_A1
REJECTED

TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ USE A TCFE DATABASE FOR THERMODYNAMIC DATA
TDB_TCFE9: @@
TDB_TCFE9: sw tcfe7
Current database: Steels/Fe-Alloys v7.0

VA      DEFINED
L12_FCC      B2_BCC      B2_VACANCY
HIGH_SIGMA   DICTRA_FCC_A1  REJECTED

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

List of references for assessed data

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

VA      DEFINED
APP: def-sys fe c nb      C      NB
FE      DEFINED
APP: rej ph *
GAS:G      GRAPHITE      GRAPHITE_L
DIAMOND     CO_749NB1_S   CO_877NB1_S
CO_98NB1_S  C1FE3_S        C1NB1_S
C1NB2_S     C60_S         FE_S
FE_S2       FE_S3        FE_L
FE2NB1_S    NB_S         NB_L
REJECTED
APP: rest ph c1nb1_s
```

```

CINB1_S RESTORED
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

List of references for assessed data

CINB1 I. BARIN 3rd. Edition
CINB1 NbC
Data taken from BARIN 3rd. Ed. (1995)

-OK-
APP:
APP: @@
APP: @@ MOBILITY/DIFFUSIVITY DATA ARE STORED IN A SEPARATE DATABASE FILE.
APP: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE THE DATA
APP: @@
APP: app mobfe2
Current database: Steels/Fe-Alloys Mobility v2.0
TCS Steel Mobility Database Version 2.0 from 2011-12-09.

VA DEFINED
APP: def-sys fe c nb
FE C NB
DEFINED
APP: rej ph * all
BCC_A2 CEMENTITE FCC_A1
FE4N LP1 HCP_A3 LIQUID:L
REJECTED
APP: res ph fcc bcc
FCC_A1 BCC_A2 RESTORED
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

List of references for assessed data

'This parameter has not been assessed'
'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'
'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
-Ni'
'J. Geise and Ch. Herzig, Z. Metallkd. 76(1985)622.; Impurity diffusion of
Nb in fcc Fe.'
'Assessed from data presented by B. B. Yu and R. F. Davis J. Phys. Chem.
Solids 40(1979)997.; C Self-Diff in NbC.'
'B. Jonsson: Z. Metallkunde 85(1994)498-501; C and N diffusion in bcc Cr
-Fe-Ni'
'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
in bcc Fe'
'R. F. Peart, Acta Metall. 10(1962)519.; Impurity diffusion of Fe in bcc
Nb.'
'Assessed from data presented in Landholt-Bornstein, Vol. 26, ed. H.
Mehrer, springer (1990); Impurity diff of Nb in bcc Fe.'
'R. E. Einziger et al., Phys. Rev. B 17(1978)440.; self-diffusion of Nb in
bcc Nb.'

-OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP
APP: @@
APP: go d-m
NO TIME STEP DEFINED
*** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
*** ENTERING CINB1_S AS A DIFFUSION NONE PHASE
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 1073.15; * N

DIC>
DIC> @@
DIC> @@ ENTER REGIONS ferr AND aus
DIC> @@
DIC> enter-region
REGION NAME : ferr
DIC>
DIC> ent-reg
REGION NAME : aus
ATTACH TO REGION NAMED /FERR/: ferr
ATTACHED TO THE RIGHT OF FERR /YES/: n
DIC>
DIC> @@
DIC> @@ ENTER GRIDS INTO REGIONS
DIC> @@
DIC> enter-grid
REGION NAME : /AUS/: ferr
WIDTH OF REGION /1/: 2.499999e-3
TYPE /LINEAR/: AUTO
DIC>
DIC>
DIC> enter-grid
REGION NAME : /AUS/: aus
WIDTH OF REGION /1/: 1e-9
TYPE /LINEAR/: AUTO
DIC>
DIC>
DIC> @@
DIC> @@ ENTER active PHASES INTO REGIONS
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /AUS/: ferr
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: bcc
DIC>
DIC>

```

```

DIC> en-ph
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /AUS/: ferr
PHASE TYPE /MATRIX/: sph
PHASE NAME: /NONE/: c1nb1_s
DIC>
DIC>
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /AUS/: aus
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC>
DIC> en-ph
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /AUS/: aus
PHASE TYPE /MATRIX/: sph
PHASE NAME: /NONE/: c1nb1_s
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITIONS OF THE PHASES
DIC> @@
DIC> enter-composition
REGION NAME : /AUS/: ferr
PHASE NAME: /BCC_A2/: bcc
DEPENDENT COMPONENT ? /NB/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: C
TYPE /LINEAR/: lin
VALUE OF FIRST POINT : 1e-3
VALUE OF LAST POINT : /1E-3/: 1e-3
PROFILE FOR /NB/: nb
TYPE /LINEAR/: lin
VALUE OF FIRST POINT : 0.28
VALUE OF LAST POINT : /0.28/: 0.28
DIC>
DIC> en-co
REGION NAME : /AUS/: ferr
PHASE NAME: /BCC_A2/: c1nb1_s
USE EQUILIBRIUM VALUE /Y/: y
DIC>
DIC> enter-composition
REGION NAME : /AUS/: aus
PHASE NAME: /FCC_A1#1/: fcc#1
DEPENDENT COMPONENT ? /NB/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: C
TYPE /LINEAR/: lin
VALUE OF FIRST POINT : 0.89
VALUE OF LAST POINT : /0.89/: 0.89
PROFILE FOR /NB/: nb
TYPE /LINEAR/: lin
VALUE OF FIRST POINT : 0.28
VALUE OF LAST POINT : /0.28/: 0.28
DIC>
DIC> en-co
REGION NAME : /AUS/: aus
PHASE NAME: /FCC_A1#1/: c1nb1_s
USE EQUILIBRIUM VALUE /Y/: y
DIC>
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 32400
AUTOMATIC TIMESTEP CONTROL /YES/: y
MAX TIMESTEP DURING INTEGRATION /3240/: 3240
INITIAL TIMESTEP : /1E-07/: 1e-8
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/: 1e-15
DIC>
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ SET THE REFERENCE PHASE OF CARBON AS GRAPHITE
DIC> @@
DIC> s-ref
Component: c
Reference state: grap
Temperature /*/: *
Pressure /100000/: 1e5
DIC>
DIC> @@
DIC> @@ SET THE BOUNDARY CONDITION.
DIC> @@ THE CARBON ACTIVITY IS THE ONE ON THE BOUNDARY
DIC> @@
DIC> s-cond

GLOBAL OR BOUNDARY CONDITION /GLOBAL/: bound
BOUNDARY /LOWER/: low
CONDITION TYPE /CLOSED_SYSTEM/: mix
Dependent substitutional element:FE
Dependent interstitial element:VA
TYPE OF CONDITION FOR COMPONENT C /ZERO_FLUX/: act
LOW TIME LIMIT /0/: 0
ACR(C)(TIME)= 1.0;
HIGH TIME LIMIT /*/: *
ANY MORE RANGES /N/: N
TYPE OF CONDITION FOR COMPONENT NB /ZERO_FLUX/: zero
DIC>
DIC> @@
DIC> @@ ENABLE THE HOMOGENIZATION MODEL
DIC> @@
DIC> ho y y
INFO: HOMOGENIZATION MODEL ENABLED
DIC>
DIC>
DIC>

```

```
DIC>  
DIC> @@  
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT  
DIC> @@  
DIC> save exb7 Y  
DIC>  
DIC>  
DIC> set-inter  
--OK--  
DIC>
```

exb7-run

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb7\run.DCM"DIC> @@
DIC> @@ READ THE SET UP FROM FILE AND START THE SIMULATION
DIC> @@
DIC>
DIC> go d-m
TIME STEP AT TIME 0.00000E+00
*** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
*** ENTERING C1NB1_S AS A DIFFUSION NONE PHASE
DIC> read exb7
OK
DIC> sim yes
Region: AUS
double geometric
dense at outer boundaries, coarse at 0.50000E-09
lower part 1.0800 16
upper part 0.92593 16
Region: FERR
single geometric dense at 0.0000
1.0800 114
STARTING SIMULATION USING HOMOGENIZATION MODEL
-----
WARNING: ELEMENT C
IS BOTH INTERSTITIAL AND SUBSTITUTIONAL
AND RESULTS MUST BE INTERPRETED WITH CARE
INFO: PHASE WITH LIMITED SOLUBILITY OF ELEMENT(S) EXIST
A FALLBACK PHASE ZZDICTRA_GHOST WILL BE DEFINED
ALONG WITH THE FOLLOWING PARAMETERS:
G(ZZDICTRA_GHOST,C;0)-H298 (GRAPHITE,C;0)
G(ZZDICTRA_GHOST,FE;0)-H298 (BCC_A2,FE;0)
G(ZZDICTRA_GHOST,NB;0)-H298 (BCC_A2,NB;0)
L(ZZDICTRA_GHOST,C,FE;0)
L(ZZDICTRA_GHOST,C,NB;0)
L(ZZDICTRA_GHOST,FE,NB;0)
Saving results
-----
WARNING:C1NB1_S HAS NO VOLUME FRACTION, CREATING ONE
WARNING:C1NB1_S HAS NO VOLUME FRACTION, CREATING ONE
Starting time-step t0= 0.0000000 dt= 0.10000000E-07
Stage 1
Evaluating Jacobian
Iteration # 1 sum residual **2: 0.44222132E+15
Iteration # 2 sum residual **2: 0.43975158E+15
Evaluating Jacobian
Iteration # 3 sum residual **2: 0.51145294E+15
Reducing dt to 5.000000000000000E-009
Stage 1
Evaluating Jacobian
Iteration # 1 sum residual **2: 0.10858850E+15
Iteration # 2 sum residual **2: 0.10768159E+15
Evaluating Jacobian
Iteration # 3 sum residual **2: 0.47896705E+14
Error 408
Reducing dt to 2.500000000000000E-009
Stage 1
Evaluating Jacobian
Iteration # 1 sum residual **2: 0.26436925E+14
Iteration # 2 sum residual **2: 0.26156665E+14
Iteration # 3 sum residual **2: 0.19671471E+14
Iteration # 4 sum residual **2: 0.15909309E+14
Iteration # 5 sum residual **2: 0.13449818E+14
Iteration # 6 sum residual **2: 0.11738463E+14
Iteration # 7 sum residual **2: 0.10482765E+14
Iteration # 8 sum residual **2: 0.95259408E+13
Iteration # 9 sum residual **2: 0.87784754E+13
Iteration # 10 sum residual **2: 0.81854606E+13
Iteration # 11 sum residual **2: 0.77115365E+13
Iteration # 12 sum residual **2: 0.73332751E+13
Iteration # 13 sum residual **2: 0.70494151E+13
Iteration # 14 sum residual **2: 0.67771939E+13
Iteration # 15 sum residual **2: 0.66328406E+13
Iteration # 16 sum residual **2: 0.65465027E+13
Error 408
Reducing dt to 1.250000000000000E-009
Stage 1
Evaluating Jacobian
Iteration # 1 sum residual **2: 0.63517503E+13
Iteration # 2 sum residual **2: 0.48482644E+13
Iteration # 3 sum residual **2: 0.37734642E+13
Iteration # 4 sum residual **2: 0.30347657E+13
Iteration # 5 sum residual **2: 0.25629830E+13
Iteration # 6 sum residual **2: 0.22401447E+13
Iteration # 7 sum residual **2: 0.20098774E+13
Iteration # 8 sum residual **2: 0.18423841E+13
Iteration # 9 sum residual **2: 0.17206673E+13
Iteration # 10 sum residual **2: 0.16346439E+13
Iteration # 11 sum residual **2: 0.15783334E+13
Error 408
Reducing dt to 6.250000000000000E-010
Stage 1
Evaluating Jacobian
Iteration # 1 sum residual **2: 0.15173761E+13
Iteration # 2 sum residual **2: 0.92807494E+12
Iteration # 3 sum residual **2: 0.68227945E+12
Iteration # 4 sum residual **2: 0.55087278E+12
Iteration # 5 sum residual **2: 0.47067619E+12
Iteration # 6 sum residual **2: 0.41909384E+12
Iteration # 7 sum residual **2: 0.38590443E+12
Iteration # 8 sum residual **2: 0.36635838E+12
Error 408
Reducing dt to 3.125000000000000E-010
Stage 1
Evaluating Jacobian
Iteration # 1 sum residual **2: 0.27840998E+12
Iteration # 2 sum residual **2: 0.17201055E+12
Iteration # 3 sum residual **2: 0.12687021E+12
Iteration # 4 sum residual **2: 0.10303215E+12
Iteration # 5 sum residual **2: 0.89261308E+11
Error 408
Reducing dt to 1.562500000000000E-010
Stage 1
Evaluating Jacobian
Iteration # 1 sum residual **2: 0.50738890E+11
```



```

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

```

output ignored...

... output resumed

```

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

```

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

KEEPING TIME-RECORD FOR TIME 32386.152
AND FOR TIME 32400.000
WORKSPACE RECLAIMED

INTERPOLATION SCHEME USED THIS FRACTION OF
THE ALLOCATED MEMORY: 0.979204858989315
EFFICIENCY FACTOR: 31.4799576717506
MEMORY FRACTION USAGE PER BRANCH:
1.000000000000000
0.906424464627948
1.000000000000000

DEALLOCATING

TIMESTEP AT 32400.0000 SELECTED

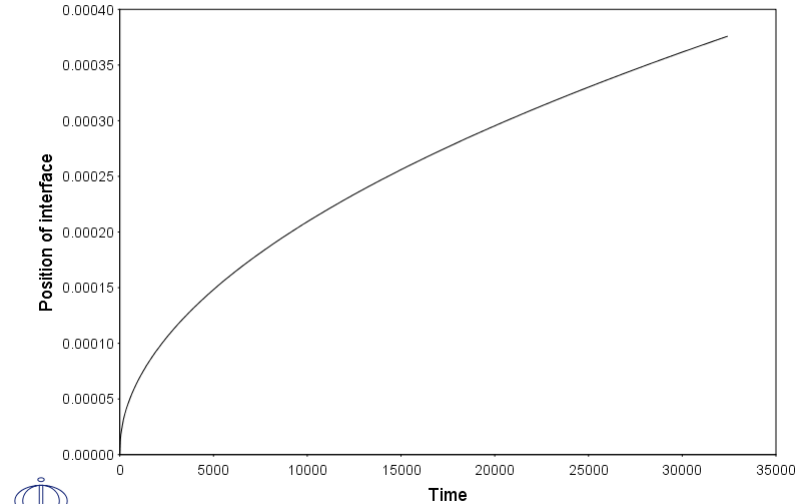
DIC>
DIC> set-inter
--OK--
DIC>

exb7-plot

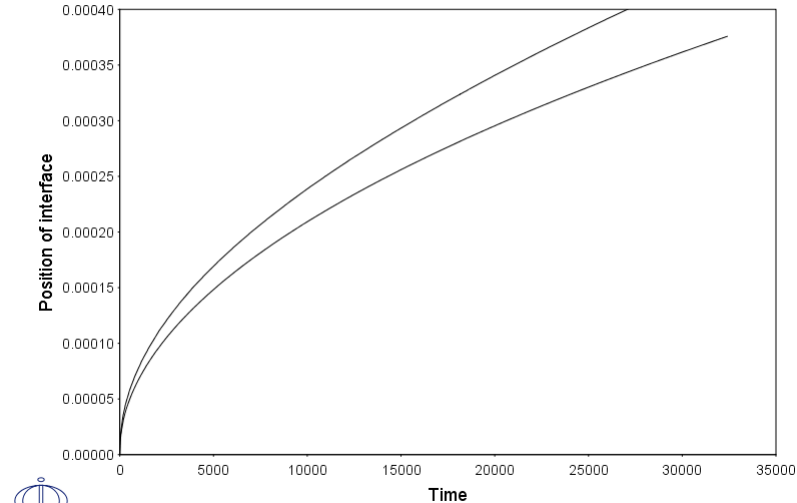
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exb7\plot.DCM"DIC>
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 3.24000E+04
*** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
*** ENTERING CINb1_S AS A DIFFUSION NONE PHASE
DIC> read exb7
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post

POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
```

```
POST-1:
POST-1: @@
POST-1: @@ PLOT THE INTERFACE POSITION AS A FUNCTION OF TIME
POST-1: @@
POST-1: s-d-a x time
INFO: Time is set as independent variable
POST-1: s-d-a y po-o-in aus upp
POST-1:
POST-1: plot
2018.02.18.20.44.43
UPPER INTERFACE OF REGION "AUS#1"
CELL #1
```



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

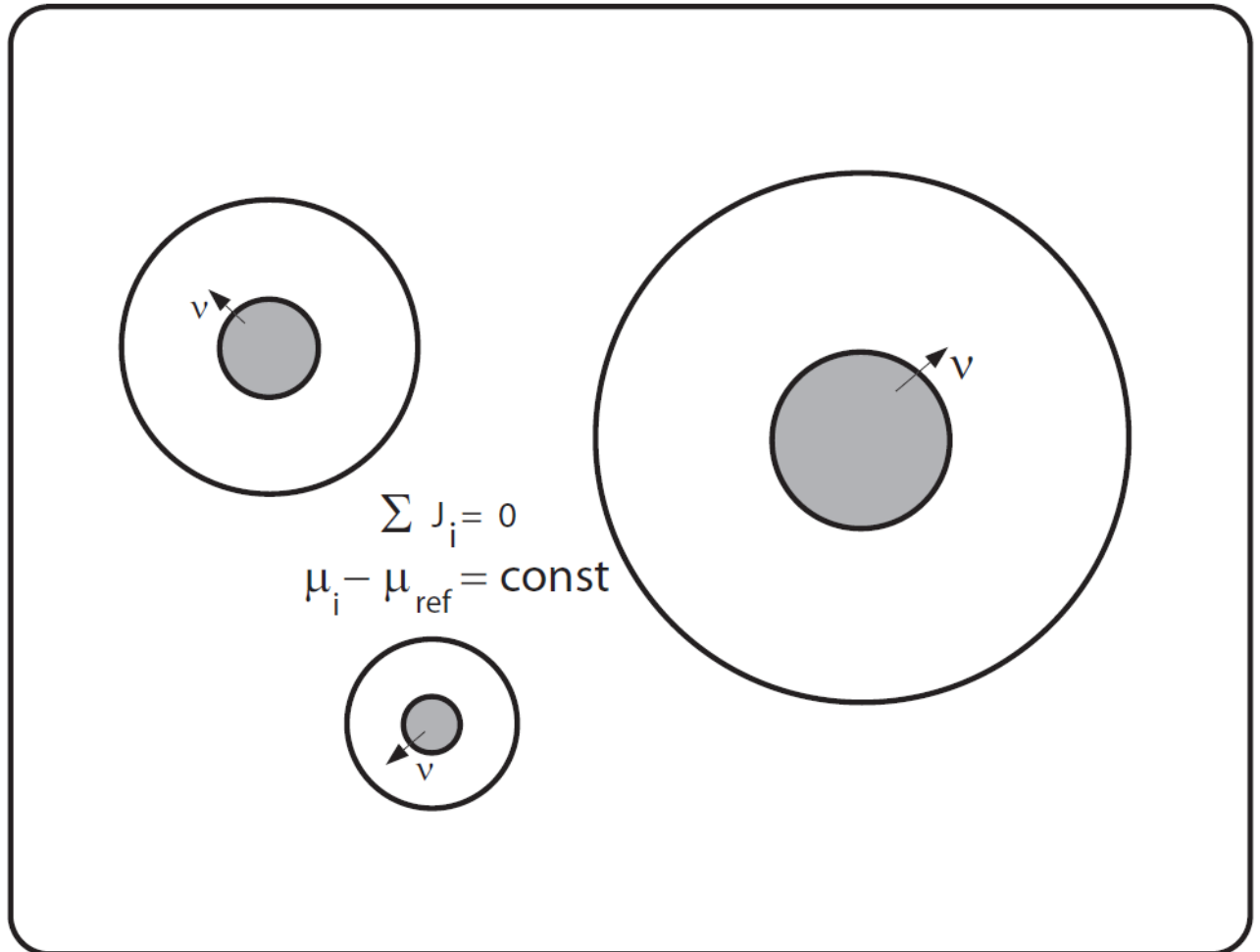


```
POST-1:
POST-1: set-inter
```

--OK--
POST-1:



Cell Calculations



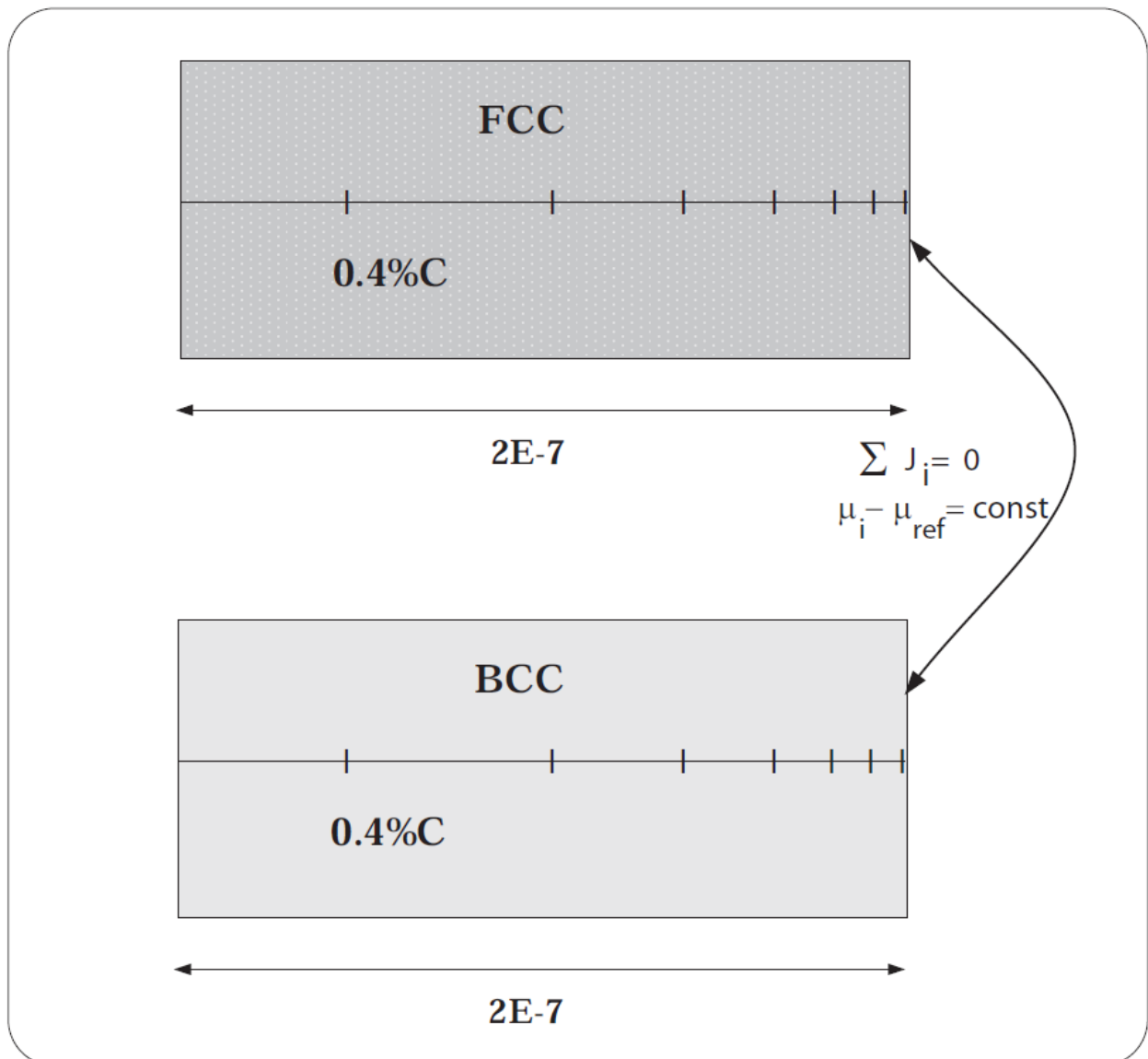


Example exc1

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

This example simulates what happens to a ferrite plate that has inherited the carbon content of its parent austenite. The ferrite plate formed is embedded in an austenite matrix. This setup corresponds to a proposed mechanism for formation of Widmannstätten ferrite or for the ferrite phase of the bainite structure. It is assumed that the phase boundary between ferrite and austenite is immobile, this is achieved in the simulation by putting the ferrite and the austenite in two different cells. See also M. Hillert, L. Höglund and J. Ågren: Acta Metall. Mater. 41 (1993), pp.1951-1957.

$$T = 673K$$



excl-setup

About Stockholm, Sweden

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

```
SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\excl\setup.DCM" ?@@
NO SUCH COMMAND, USE HELP
SYS: @@ Cell calculation.
SYS: @@ Carbon cannon in ferrite/austenite: Fe-C system, 2-cell calculation
SYS: @@ This example simulates what happens to a ferrite plate that has
SYS: @@ inherited the carbon content of its parent austenite. The ferrite
SYS: @@ plate formed is embedded in an austenite matrix. This setup
SYS: @@ corresponds to a proposed mechanism for formation of Widmannstätten
SYS: @@ ferrite or for the ferrite phase of the bainite structure. It is
SYS: @@ assumed that the phase boundary between ferrite and austenite is
SYS: @@ immobile, this is achieved in the simulation by putting the ferrite
SYS: @@ and the austenite in two different cells. See also M. Hillert,
SYS: @@ L. Höglund and J. Ågren: Acta Metall. Mater. 41 (1993), pp.1951-1957.
SYS: -----
NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ excl_setup.DCM
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASE
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Current database: Steels/Fe-Alloys v9.0

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

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

List of references for assessed data

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

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

List of references for assessed data

'This parameter has not been assessed'
'J. Ågren: 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 MULDF: /2/:
CHECK INTERFACE POSITION /NO/:
VARY POTENTIALS OR ACTIVITIES OR LNAC : /POTENTIAL/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPLICIT WHEN INTEGRATING PDES (0 -> 0.5 -> 1): /.5/: 1.0
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /NO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDF /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 excl Y
DIC-2>
DIC-2> set-inter
--OK--
DIC-2>

```


excl-run

```
DIC-2>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\excl\run.DCM"DIC-2>
DIC-2>
DIC-2> @@ excl_run.DCM
DIC-2>
DIC-2> @@
DIC-2> @@ READ THE WORKSPACE AND START THE SIMULATION
DIC-2> @@
DIC-2> go d-m
TIME STEP AT TIME 0.00000E+00
DIC-2> read excl
OK
DIC> sim
Region: AUS
single geometric dense at 0.20000E-06
0.89105 93
Region: FER
single geometric dense at 0.20000E-06
0.96940 72
U-FRACTION IN SYSTEM: C = .018673311178274 FE = 1
TOTAL SIZE OF SYSTEM: 4E-07 [m]
U-FRACTION IN SYSTEM: C = .018673311178274 FE = 1
TOTAL SIZE OF SYSTEM: 4E-07 [m]
2.570491440876833E-002 2.570457646507204E-002 1.632468496708230E-002 1.481595250675601E-003 4.374341462051788E-
005 2.088305124067901E-007 2.465148837668976E-011 1.324756764297081E-017 TIME = 0.10000000E-06 DT = 0.10000000E-
06 SUM OF SQUARES = 0.13247568E-16
U-FRACTION IN SYSTEM: C = .018673311178092 FE = 1
TOTAL SIZE OF SYSTEM: 4E-07 [m]
CPU time used in timestep 0 seconds
1.721271285522132E-002 1.721309826251375E-002 1.320114685474547E-003 1.780264104372174E-004 4.883616119764177E-
006 2.701426733646338E-008 4.894446543282404E-012 5.060987976361818E-018 TIME = 0.30000000E-06 DT = 0.20000000E-
06 SUM OF SQUARES = 0.50609880E-17
U-FRACTION IN SYSTEM: C = .018673311178317 FE = 1
TOTAL SIZE OF SYSTEM: 4E-07 [m]
CPU time used in timestep 1 seconds
1.723030673037079E-002 1.722973038975870E-002 6.546665653188744E-004 1.540163381854436E-005 9.847914086370379E-
009 1.575452822349616E-013 1.593769930090315E-021 TIME = 0.70000000E-06 DT = 0.40000000E-
06 SUM OF SQUARES = 0.15937699E-20
U-FRACTION IN SYSTEM: C = .0186733111783162 FE = 1
TOTAL SIZE OF SYSTEM: 4E-07 [m]
CPU time used in timestep 0 seconds
2.046536420972098E-003 2.046359859030639E-003 1.093843934644341E-005 4.894916965478312E-008 1.003356508283692E-
012 9.302414829459864E-020 TIME = 0.15000000E-05 DT = 0.80000000E-06 SUM OF SQUARES = 0.93024148E-19
U-FRACTION IN SYSTEM: C = .0186733111783284 FE = 1
TOTAL SIZE OF SYSTEM: 4E-07 [m]
CPU time used in timestep 1 seconds
1.307886964750396E-003 1.307786277164665E-003 8.937183842406468E-006 4.994501913148052E-008 1.605937233342920E-
012 2.925328975717250E-019 TIME = 0.31000000E-05 DT = 0.16000000E-05 SUM OF SQUARES = 0.29253290E-18
U-FRACTION IN SYSTEM: C = .0186733111783716 FE = 1
TOTAL SIZE OF SYSTEM: 4E-07 [m]
CPU time used in timestep 0 seconds
5.482172962189864E-004 5.481699846891220E-004 2.979475699821687E-006 1.354117993457866E-008 2.862902386732131E-
013 2.781528300460643E-020 TIME = 0.63000000E-05 DT = 0.32000000E-05 SUM OF SQUARES = 0.27815283E-19
U-FRACTION IN SYSTEM: C = .0186733111783983 FE = 1
TOTAL SIZE OF SYSTEM: 4E-07 [m]
CPU time used in timestep 1 seconds
2.615717394236350E-002 2.615484476818204E-002 1.336512838121405E-004 5.745045707598120E-007 1.084421168367715E-
011 8.892868844306621E-019 TIME = 0.12700000E-04 DT = 0.64000000E-05 SUM OF SQUARES = 0.88928688E-18
U-FRACTION IN SYSTEM: C = .0186733111784285 FE = 1
TOTAL SIZE OF SYSTEM: 4E-07 [m]
CPU time used in timestep 0 seconds
1.276911017788254E-002 1.276795521545566E-002 6.327039393406848E-005 2.645588403126521E-007 4.737846880516210E-
012 3.569977336034442E-019 TIME = 0.25500000E-04 DT = 0.12800000E-04 SUM OF SQUARES = 0.35699773E-18
U-FRACTION IN SYSTEM: C = .0186733111784667 FE = 1
TOTAL SIZE OF SYSTEM: 4E-07 [m]
CPU time used in timestep 1 seconds
6.319101225966472E-003 6.318525707093593E-003 3.090594428117439E-005 1.275882533925475E-007 2.220821508127569E-
012 1.611800391932045E-019 TIME = 0.51100000E-04 DT = 0.25600000E-04 SUM OF SQUARES = 0.16118004E-18
U-FRACTION IN SYSTEM: C = .0186733111785181 FE = 1
TOTAL SIZE OF SYSTEM: 4E-07 [m]
CPU time used in timestep 0 seconds
output ignored...

... output resumed

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

```

TOTAL SIZE OF SYSTEM: 4E-07 [m]
CPU time used in timestep 0 seconds
2.924257073550977E-005 2.922561803227903E-005 1.420221635556956E-009 5.383694526367622E-014 1.053517999033209E-
022 TIME = 0.49683922 DT = 0.50000000E-01 SUM OF SQUARES = 0.10535180E-21
U-FRACTION IN SYSTEM: C = .0186734961806317 FE = 1
TOTAL SIZE OF SYSTEM: 4E-07 [m]
CPU time used in timestep 1 seconds
1.311639930578495E-002 1.311509713869623E-002 1.933611102012263E-005 2.528801921586462E-008 6.842159294738176E-
014 9.431797172291871E-023 TIME = 0.50000000 DT = 0.31607821E-02 SUM OF SQUARES = 0.94317972E-22
U-FRACTION IN SYSTEM: C = .0186734961806332 FE = 1
TOTAL SIZE OF SYSTEM: 4E-07 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 0.00000000
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>

```

excl-plot

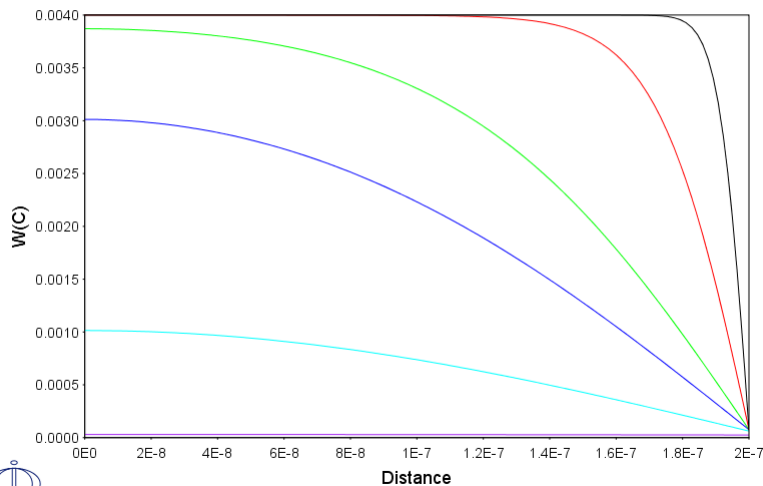
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\excl\plot.DCM"DIC>
DIC>
DIC> @@ excl_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE c1
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 5.00000E-01
DIC> read excl
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post

POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
```

```
POST-1:
POST-1: @@
POST-1: @@ FIRST PLOT CARBON CONCENTRATION PROFILES IN FERRITE (CELL-2)
POST-1: @@ THEN SET THE DISTANCE AS X-AXIS (NOT THAT DISTANCE IS SET INDEPENDENT
POST-1: @@ VARIABLE AUTOMATICALLY) AND W-FRACTION CARBON AS Y-AXIS
POST-1: @@ REMEMBER THAT THE PLOT CONDITION ALSO MUST BE SET.
POST-1: @@
POST-1: select-cell
Number /NEXT/: 2
CELL 2 SELECTED
POST-2:
POST-2: @@
POST-2: @@ NOTICE THAT THE PROMPT INCLUDES THE CURRENT CELL NUMBER
POST-2: @@
POST-2: s-d-a x dist glo
INFO: Distance is set as independent variable
POST-2: s-d-a y w(c)
POST-2: s-p-c time .0001 .001 .01 .03 .1 .5
POST-2:
POST-2: @@
POST-2: @@ SET THE TITLE ON THE PLOTS
POST-2: @@
POST-2: set-title Figure c1.1
POST-2: plo
```

Figure c1.1

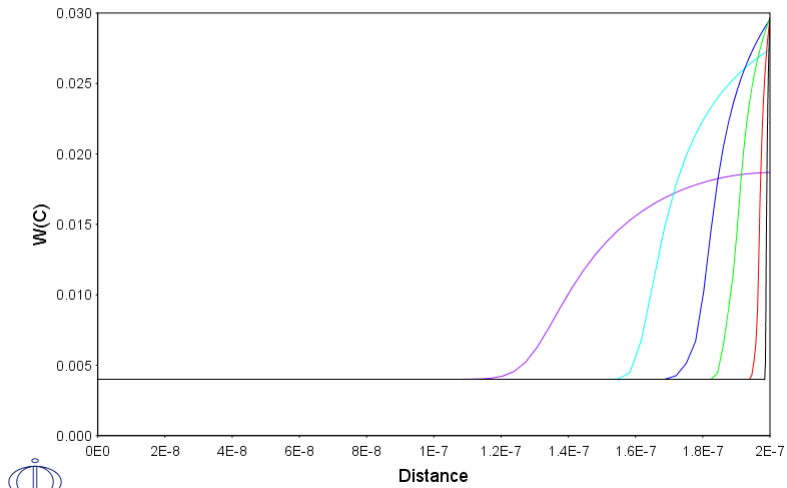
2018.02.18.20.48.16
Time=1E-04,.001,.01,.03,.1,.5
CELL#2



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

Figure c1.2

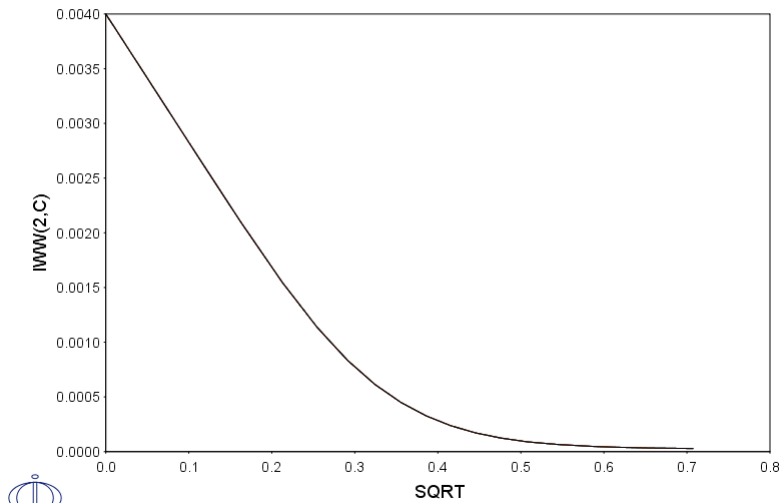
2018.02.18.20.48.16
Time = 1E-04, 0.01, 0.1, 0.3, 1, 5
CELL #1



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

Figure c1.3

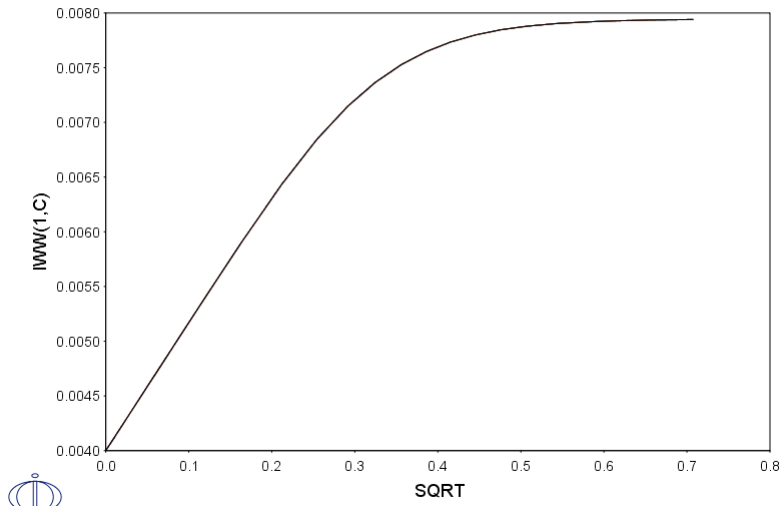
2018.02.18.20.48.17
CELL #2



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

Figure c1.4

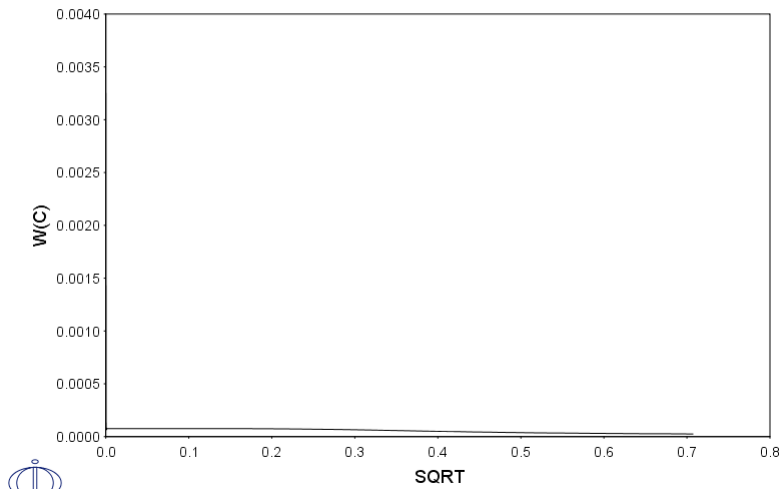
2018.02.18.20.48.18
CELL #1



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

Figure c1.5

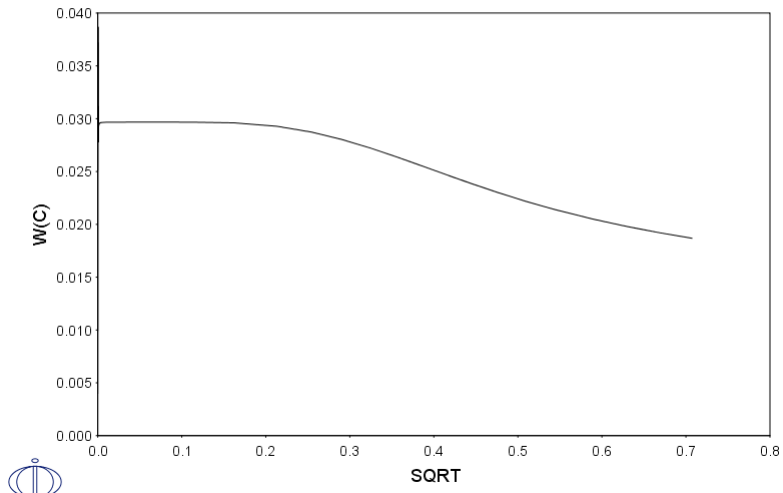
2018.02.18.20.48.19
UPPER INTERFACE OF REGION "LAST"
CELL #2



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

Figure c1.6

2018.02.18.20.48.19
UPPER INTERFACE OF REGION "LAST"
CELL #1



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

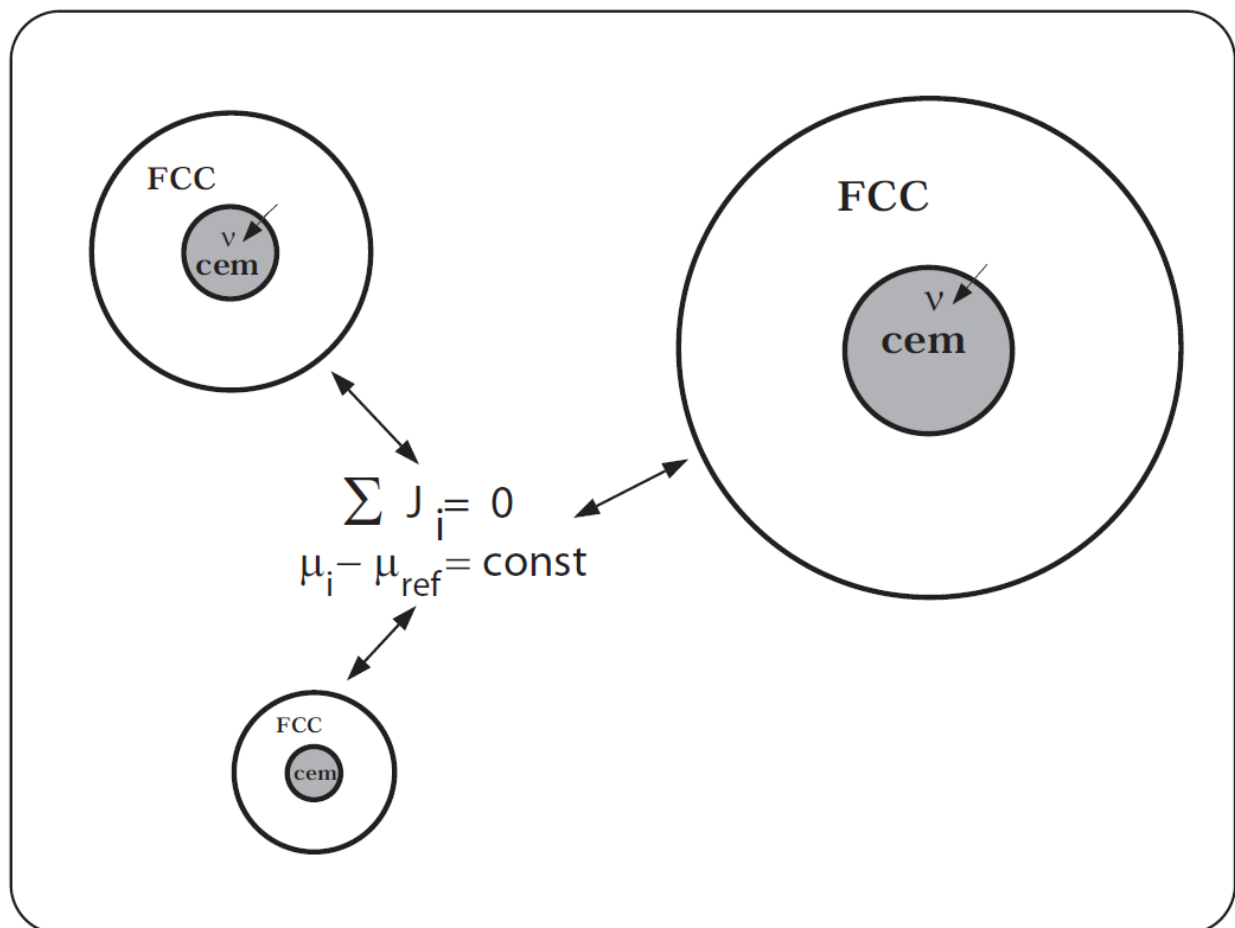


Example exc2

Cementite dissolution in an Fe-Cr-C alloy: Three particle sizes and three different cells

This example calculates the dissolution of cementite particles in an austenite matrix. This is the same as exc1 except that there are three particle sizes. Altogether six particles are considered using three different cells. This is to be able to represent some size distribution among the cementite particles. See also Z.-K. Liu, L. Höglund, B. Jönsson and J. Ågren: Metall.Trans.A, v. 22A (1991), pp. 1745-1752.

$$T = 1183\text{K}$$



exc2-setup

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

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

NO SUCH COMMAND, USE HELP

SYS: @@ Cell calculation.

SYS: @@ Cementite dissolution in an Fe-Cr-C alloy: Three particle sizes and

SYS: @@ three different cells

SYS: @@ This example calculates the dissolution of cementite particles

SYS: @@ in an austenite matrix. This example is the same as exc1 but

SYS: @@ instead there are three particle sizes. A total of six

SYS: @@ particles are considered using three different cells. This is to

SYS: @@ represent some size distribution among the cementite particles.

SYS: @@ See also Z.-K. Liu, L. Höglund, B. Jönsson and J. Ågren:

SYS: @@ Metall.Trans.A, v. 22A (1991), pp. 1745-1752.

SYS: -----

NO SUCH COMMAND, USE HELP

SYS:

SYS: @@ exc2_setup.DCM

SYS:

SYS: @@

SYS: @@ RETRIEVE DATA FROM THE DATABASE

SYS: @@

SYS: go da

THERMODYNAMIC DATABASE module

Current database: Steels/Fe-Alloys v9.0

VA /- DEFINED

L12_FCC B2_BCC DICTRA_FCC_A1

REJECTED

TDB_TCFE9:

TDB_TCFE9: @@

TDB_TCFE9: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA

TDB_TCFE9: @@

TDB_TCFE9: switch fedemo

Current database: Iron Demo Database v2.0

VA /- DEFINED

TDB_FEDEMO: def-sys fe cr c

FE CR C

DEFINED

TDB_FEDEMO: rej ph * all

GAS:G LIQUID:L

CEMENTITE CHI_A12 DIAMOND_FCC_A4

FCC_A1 GRAPHITE HCP_A3

KSI_CARBIIDE LAVES_PHASE_C14 M23C6

M3C2 M5C2 M7C3

SIGMA REJECTED

TDB_FEDEMO: res ph fcc cementite

FCC_A1 CEMENTITE RESTORED

TDB_FEDEMO: get

REINITIATING GES

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

FUNCTIONS

List of references for assessed data

'B.-J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'

'P. Villars and L.D. Calvert (1985). Pearson's handbook of
crystallographic data for intermetallic phases. Metals park, Ohio.
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'B. Hallstedt, D. Djurovic, J. von Appen, R. Dronskowski, A. Dick, F.
Koermann, T. Hickel, J. Neugebauer, CALPHAD, 34, 129 -33(2010); Fe-C'

'A.V. Khvan, B. Hallstedt, C. Broeckmann, CALPHAD, 46, 24 -33(2014); Cr-Fe
-C'

'J. Bratberg, Z. Metallkd., 96 (2005) 335-344; Fe-Cr-Mo-C'

'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'

'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'

'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'

'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
volumes'

'X.-G. Lu, M. Selleby, B. Sundman, CALPHAD, 29 (2005) 49-55; Fe P-T diagram'

'R. Naraghi, Thermo-Calc Software AB, Sweden, 2016; FCC Fe-Cr-C and C-Cr-Ni'

'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'

'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270
(1986); CR-FE'

-OK-

TDB_FEDEMO:

TDB_FEDEMO: @@

TDB_FEDEMO: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE MOBILITY DATA

TDB_FEDEMO: @@

TDB_FEDEMO: app mobfe2

Current database: Steels/Fe-Alloys Mobility v2.0

TCS Steel Mobility Database Version 2.0 from 2011-12-09.

VA DEFINED

APP: def-sys fe cr c

FE CR C

DEFINED

APP: rej ph * all

BCC_A2 CEMENTITE FCC_A1

FE4N_LP1 HCP_A3 LIQUID:L

REJECTED

APP: res ph fcc cementite

FCC_A1 CEMENTITE RESTORED

APP: get

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

FUNCTIONS

List of references for assessed data

'This parameter has not been assessed'


```

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

DIC>
DIC> @@-----
DIC> @@ CELL NUMBER ONE
DIC> @@-----
DIC>
DIC> @@
DIC> @@ ENTER REGIONS carb AND aus
DIC> @@
DIC> enter-region carb
DIC> enter-region aus
ATTACH TO REGION NAMED /CARB/:
ATTACHED TO THE RIGHT OF CARB /YES/:
DIC> @@
DIC> @@ ENTER GEOMETRICAL GRIDS INTO THE REGIONS
DIC> @@
DIC>
DIC> @@
DIC> @@ THE SIZE OF THE CEMENTITE PARTICLES ARE KNOWN AS WE ASSUME
DIC> @@ IT HAS BEEN MEASURED.
DIC> @@
DIC> enter-grid
REGION NAME : /CARB/: carb
WIDTH OF REGION /1/: 0.700000e-6
TYPE /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 GEOMETRICAL 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 GEOMETRICAL 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 /C/: 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-1
's-n-1' 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> @@ SET THE SIMULATION TIME
DIC-3> @@
DIC-3> set-simulation-time
END TIME FOR INTEGRATION /.1/: 10000
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /1000/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC-3>
DIC-3> @@
DIC-3> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC-3> @@
DIC-3> save exc2 Y
DIC-3>
DIC-3>
DIC-3> set-inter
--OK--
DIC-3>

```

exc2-run

```
DIC-3>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exc2\run.DCM"DIC-3>
DIC-3>
DIC-3> @@ exc2_run.DCM
DIC-3>
DIC-3> @@
DIC-3> @@ READ THE SET UP FROM FILE AND START THE SIMULATION
DIC-3> @@
DIC-3>
DIC-3> go d-m
TIME STEP AT TIME 0.00000E+00
DIC-3> read exc2
OK
DIC> sim yes
Region: CARB
single geometric dense at 0.70000E-06
0.84611 96
Region: AUS
double geometric
dense at outer boundaries, coarse at 0.35916E-06
lower part 1.0486 22
upper part 0.95367 22
Region: CARB
single geometric dense at 0.30000E-06
0.86023 95
Region: AUS
double geometric
dense at outer boundaries, coarse at 0.15393E-06
lower part 1.0067 22
upper part 0.99334 22
Region: CARB
single geometric dense at 0.52550E-06
0.85084 96
Region: AUS
double geometric
dense at outer boundaries, coarse at 0.26963E-06
lower part 1.0222 22
upper part 0.97828 22
Trying old scheme 4
GENERATING STARTING VALUES FOR CELL # 1 INTERFACE # 2
DETERMINING INITIAL EQUILIBRIUM VALUES
CALCULATING STARTING VALUES: 9 EQUILIBRIUM CALCULATIONS DONE 6 OUT OF 9
89434.0516915

Trying old scheme 4
GENERATING STARTING VALUES FOR CELL # 2 INTERFACE # 2
DETERMINING INITIAL EQUILIBRIUM VALUES
CALCULATING STARTING VALUES: 9 EQUILIBRIUM CALCULATIONS DONE 6 OUT OF 9
89434.0516915

Trying old scheme 4
GENERATING STARTING VALUES FOR CELL # 3 INTERFACE # 2
DETERMINING INITIAL EQUILIBRIUM VALUES
CALCULATING STARTING VALUES: 9 EQUILIBRIUM CALCULATIONS DONE 6 OUT OF 9
89434.0516915

U-FRACTION IN SYSTEM: C = .0406910187346776 CR = .0214382352304608
FE = .978561764900046
TOTAL SIZE OF SYSTEM: 2.90023192349E-17 [m^3]
U-FRACTION IN SYSTEM: C = .0406910187346776 CR = .0214382352304608
FE = .978561764900046
TOTAL SIZE OF SYSTEM: 2.90023192349E-17 [m^3]
0.549881621022645 0.549917064641365 0.549938978099241 0.549921828506971 0.549881463442405 0.549881396770026
002 3.584789099973641E-004 4.707896215169447E-005 1.368538548719131E-006 9.616968067506565E-
006 1.052143984005091E-006 9.010518126001122E-007 8.267746915912355E-007 8.321573838165257E-
007 8.024773009998710E-007 8.036126148068533E-007 7.984608479813919E-007 8.050009081216152E-
007 8.000667876669771E-007 7.984620140526977E-007 7.984782243626459E-007 8.003049929700262E-
007 8.048504050500911E-007 8.013658009077427E-007 7.869048260291603E-007 7.845298608518584E-
007 7.828052493081366E-007 7.795100507715870E-007 7.765420050192562E-007 7.772966895125170E-
007 7.719168100439892E-007 7.729228850442111E-007 7.669031199779128E-007 7.600329286473438E-
007 7.604611933884462E-007 7.600341337121120E-007 7.600503467478045E-007 7.525562577038541E-
007 7.561970193980981E-007 7.540768031118053E-007 7.401555177117967E-007 7.236762721884894E-
007 7.065875831403977E-007 6.785553058049482E-007 6.488672003692035E-007 6.495030277159912E-
007 5.991860198842355E-007 6.000961686264694E-007 5.458302380562768E-007 4.547576422565395E-
007 4.549588595027279E-007 4.54758859509569E-007 4.547750687468223E-007 3.591727483757561E-
007 3.588608067310060E-007 3.590808326814583E-007 5.291229251797131E-007

output ignored...

... output resumed

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

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

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

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

exc2-plot

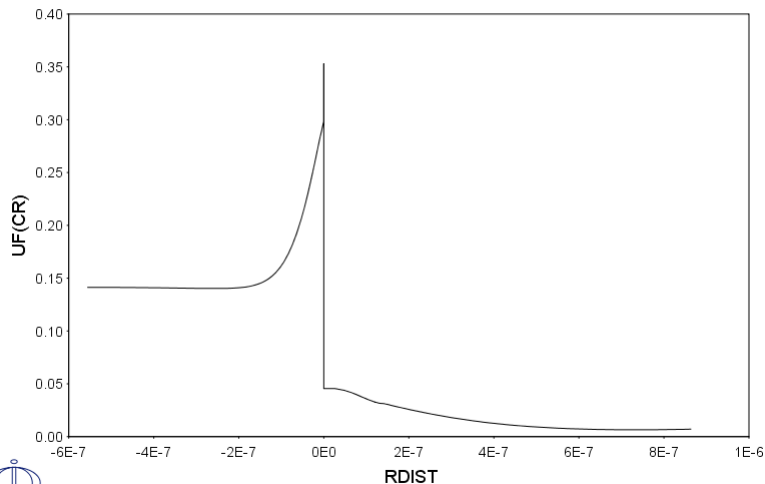
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exc2\plot.DCM"DIC>
DIC>
DIC> @@ exc2_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE c2
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go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

```
POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
```

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

Figure C2.1

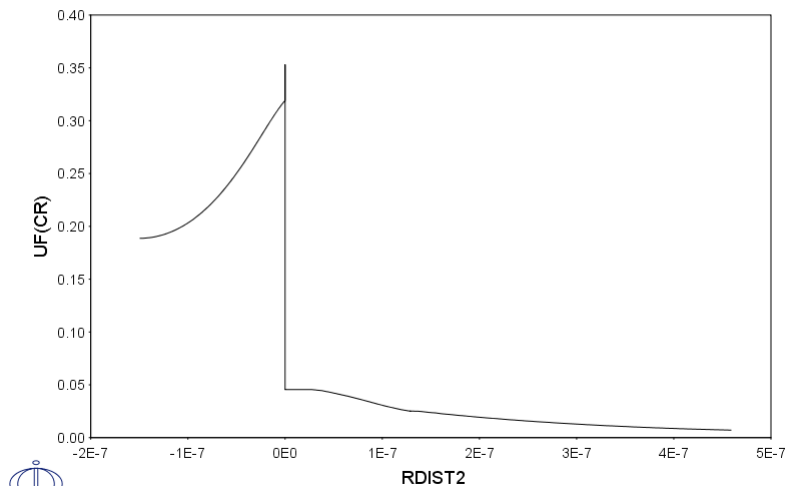
2018.02.18 21.42.26
Time=1000
CELL#1



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

Figure C2.2

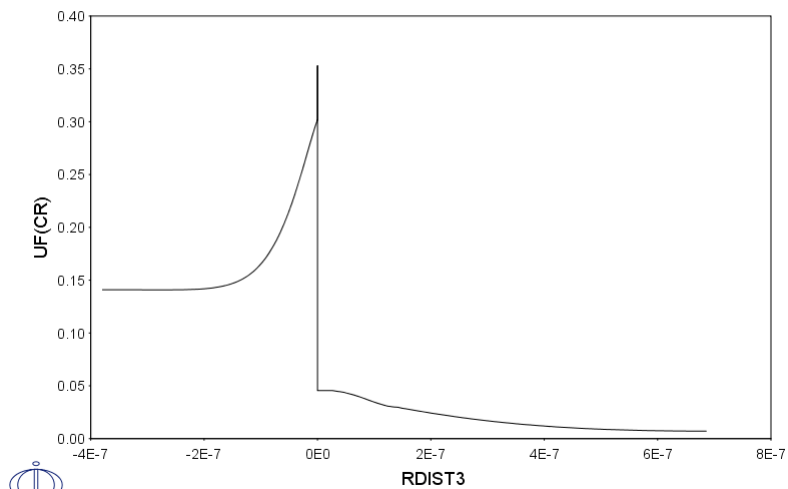
2018.02.18.21.42.30
Time = 1000
CELL #2



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

Figure C2.3

2018.02.18.21.42.33
Time = 1000
CELL #3



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

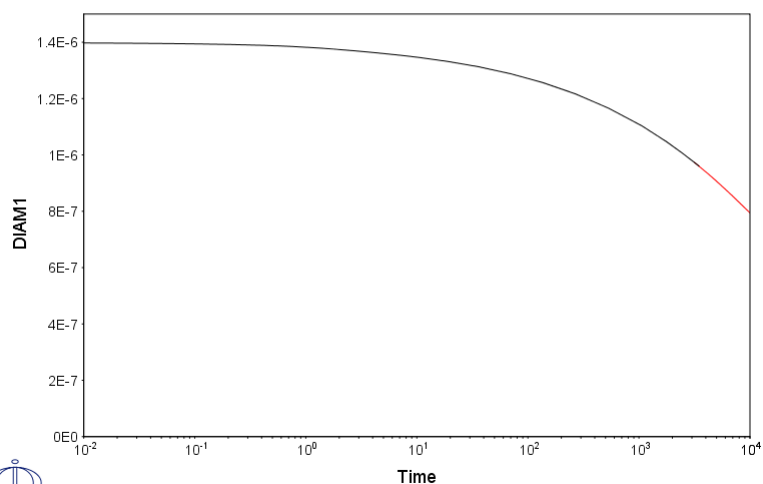
```

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

```

Figure C2.4

2018.02.18.21.42.37
UPPER INTERFACE OF REGION "CARB#1"
CELL #1



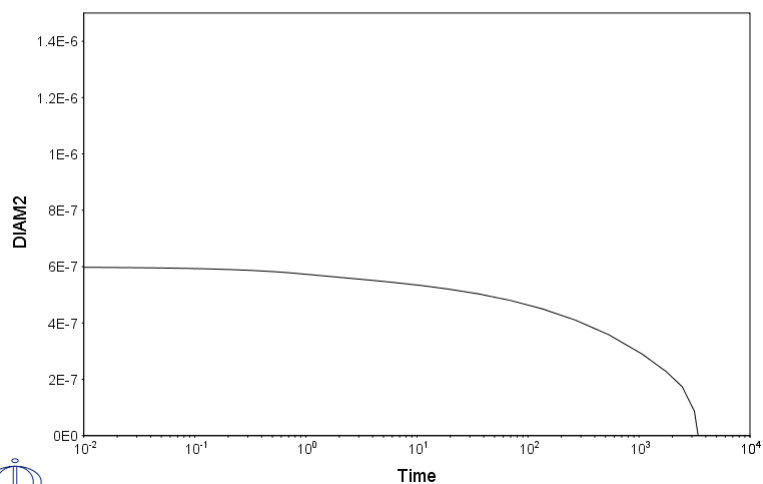
```

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

```

Figure C2.5

2018.02.18.21.42.41
UPPER INTERFACE OF REGION "CARB#2"
CELL #2



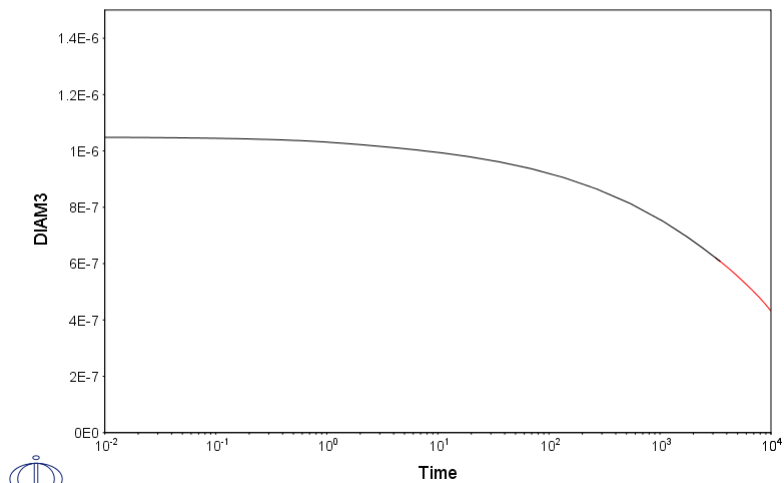
```

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

```

Figure C2.6

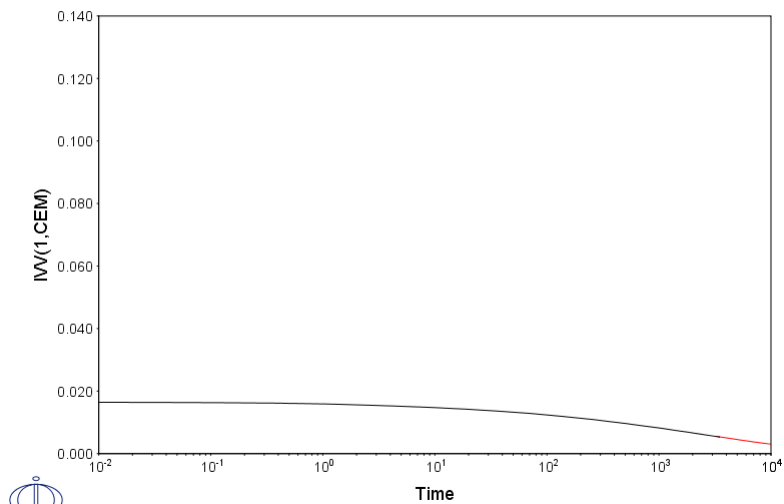
2018.02.18.21.42.45
UPPER INTERFACE OF REGION "CARB#3"
CELL #3



```
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: plo
```

Figure C2.7

2018.02.18.21.42.51
CELL #3

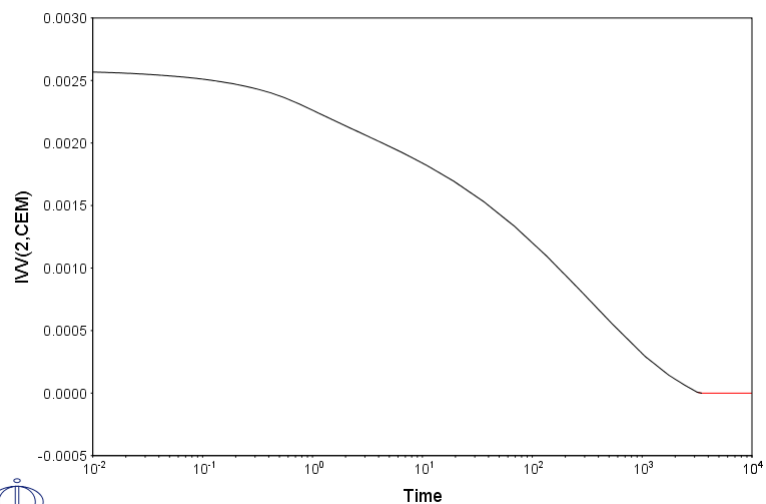


```
POST-3:
POST-3:
POST-3:
POST-3:
POST-3:@?<_hit_return_to_continue_>
POST-3:
POST-3: @@
POST-3: @@ CELL 2
POST-3: @@
POST-3: s-d-a y ivv(2,cem)
POST-3:
POST-3: set-title Figure C2.8
POST-3: plo
```


Figure C2.8

2018.02.18.21.43.00

CELL #3



```

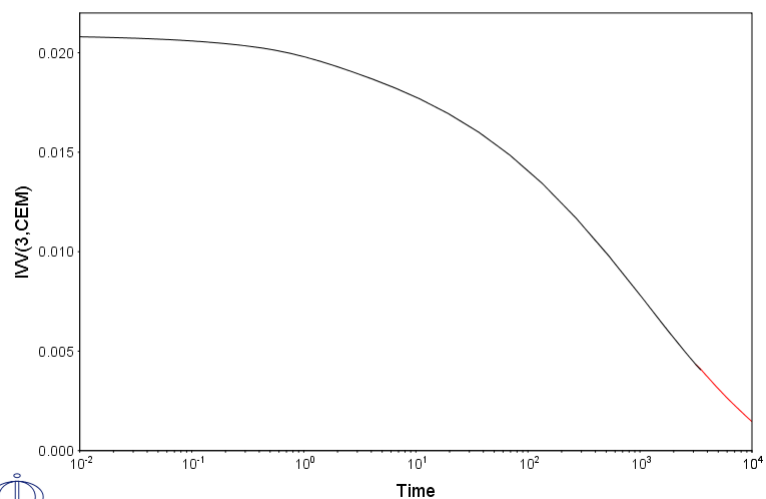
POST-3:
POST-3:
POST-3:
POST-3:
POST-3:@?<_hit_return_to_continue_>
POST-3:
POST-3: @@
POST-3: @@ CELL 3
POST-3: @@
POST-3: s-d-a y ivv(3,cem)
POST-3:
POST-3: set-title Figure C2.9
POST-3: plo

```

Figure C2.9

2018.02.18.21.43.10

CELL #3



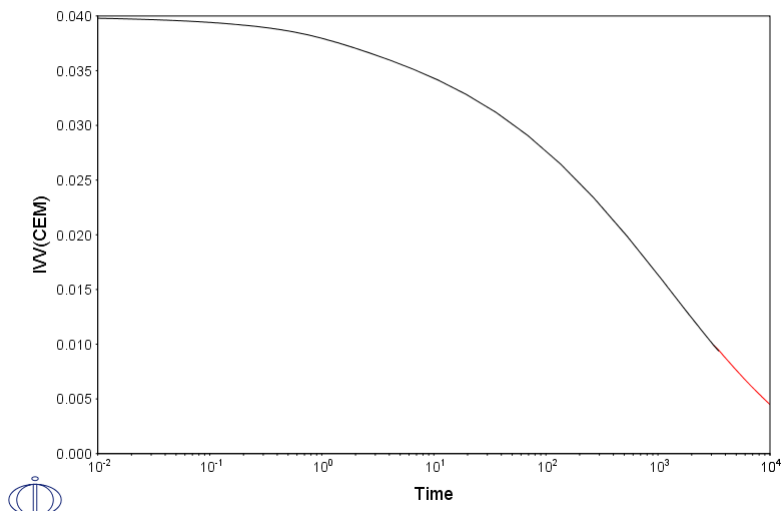
```

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

```

Figure C2.10

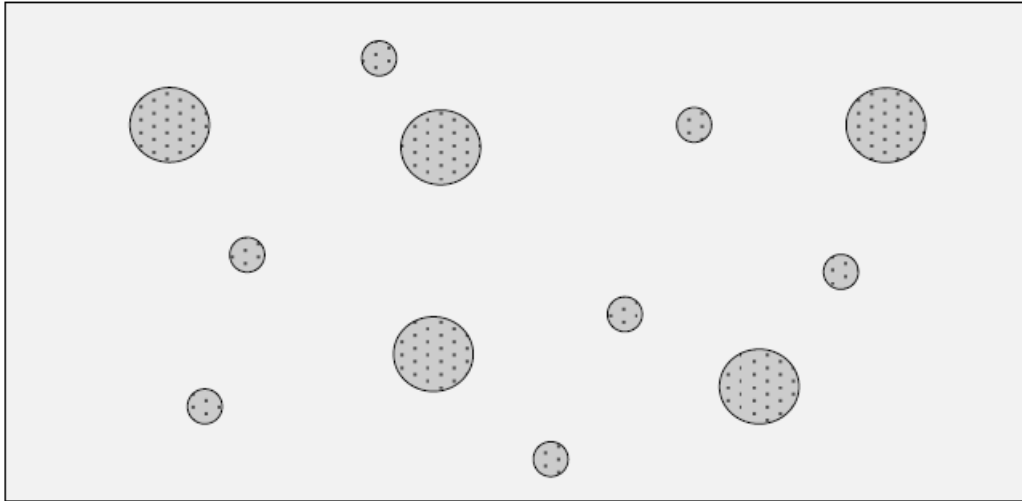
2018.02.18.21.43.19
CELL #3



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



Diffusion in Dispersed Systems

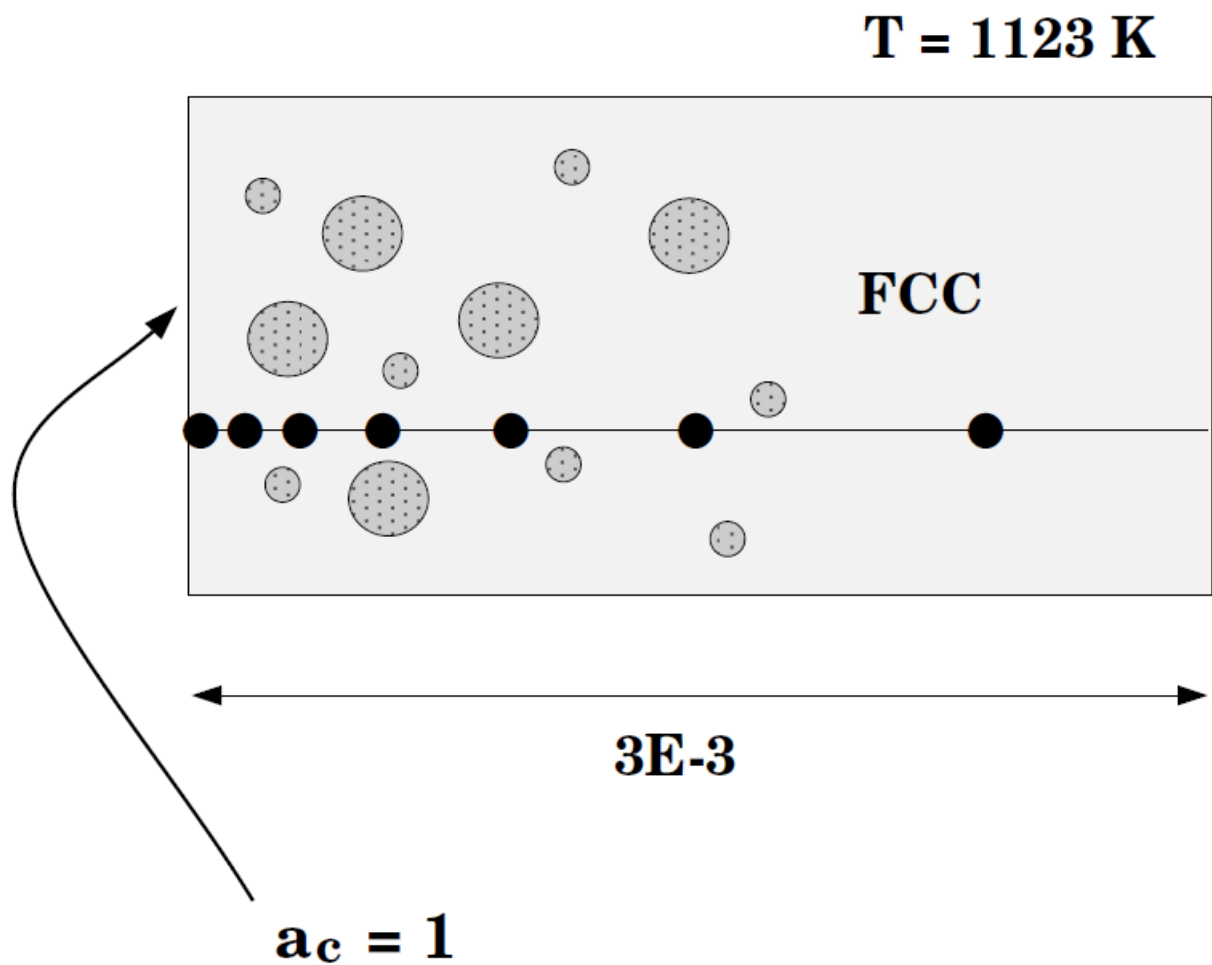




Example exd1a

Carburization of a Ni-25% Cr alloy: Dispersed system model

This example is about carburization of a Ni-25Cr alloy. In this case the M₃C₂ and M₇C₃ carbides are entered as spheroid phases in a FCC matrix. In this example the DISPERSED SYSTEM MODEL is used. This case is from A. Engström, L. Höglund and J. Ågren: Metall.Trans.A v. 25A (1994), pp. 1127-1134.



exdla-setup

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

```
SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exdla\setup.DCM" ?@@
NO SUCH COMMAND, USE HELP
SYS: @@ Diffusion in dispersed systems.
SYS: @@ Carburization of Ni-25%Cr alloy: Dispersed system model
SYS: @@ This example is about carburization of a Ni-25Cr alloy.
SYS: @@ In this case the M3C2 and M7C3 carbides are entered as
SYS: @@ spheroid phases in a FCC matrix. This simulation can be run
SYS: @@ with either the DISPERSED SYSTEM MODEL or the HOMOGENIZATION MODEL.
SYS: @@ In this example the DISPERSED SYSTEM MODEL is used, which requires
SYS: @@ that the default HOMOGENIZATION MODEL is disabled.
SYS: @@ With the DISPERSED SYSTEM MODEL the command
SYS: @@ ENTER_LABYRINTH_FUNCTION is used to take into account the
SYS: @@ impeding effect of dispersed phases on long-range diffusion.
SYS: @@ For the HOMOGENIZATION MODEL the command
SYS: @@ ENTER_HOMOGENIZATION_FUNCTION should be used.
SYS: @@ This case is from A. Engström, L. Höglund and J. Ågren:
SYS: @@ Metall.Trans.A v. 25A (1994), pp. 1127-1134.
SYS: -----
NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exd1_setup.DCM
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASE
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Current database: Steels/Fe-Alloys v9.0

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

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

List of references for assessed data

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

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

List of references for assessed data

```
'This parameter has not been assessed'
'B. Jonsson: Z. Metallkunde 85(1994)502-509;
  C diffusion in fcc Cr-Fe-Ni'
'B. Jonsson: Scand. J. Metall. 24(1995)21-27;
  Cr and Fe diffusion fcc Cr-Fe'
'B. Jonsson: Scand. J. Metall. 24(1995)21-27;
  Cr and Ni diffusion fcc Cr-Ni'
'B. Jonsson: Scand. J. Metall. 24(1995)21-27;
  Ni self-diffusion'
-OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR
APP: @@
APP: go d-m
NO TIME STEP DEFINED
*** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
*** ENTERING M3C2 AS A DIFFUSION NONE PHASE
*** ENTERING M7C3 AS A DIFFUSION NONE PHASE
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 1123; * N

DIC>
DIC> @@
DIC> @@ SET THE REFERENCE STATE FOR CARBON
DIC> @@
DIC> set-reference-state
Component: C
Reference state: grap
Temperature /*/: *
Pressure /100000/: 101325
DIC>
DIC> @@
DIC> @@ ENTER THE REGION aus
DIC> @@
DIC> enter-region aus
DIC>
DIC> @@
DIC> @@ ENTER A GEOMETRICAL GRID INTO THE REGION
DIC> @@
DIC> enter-grid aus 3e-3 geo 100 1.02
DIC>
DIC> @@
DIC> @@ ENTER A MATRIX PHASE IN THE REGION
DIC> @@
DIC> enter-phase act aus matrix fcc_a1#1
DIC>
DIC> @@
DIC> @@ ENTER THE START COMPOSITION FOR THE MATRIX PHASE
DIC> @@
DIC> enter-composition
REGION NAME : /AUS/: aus
PHASE NAME: /FCC_A1#1/: fcc#1
DEPENDENT COMPONENT ? /NI/: ni
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: cr
TYPE /LINEAR/: lin 25 25
PROFILE FOR /CR/: c
TYPE /LINEAR/: lin 1e-4 1e-4
DIC>
DIC> @@
DIC> @@ ENTER SPHEROIDAL PHASES IN THE REGION
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /AUS/: aus
PHASE TYPE /MATRIX/: sph
PHASE NAME: /NONE/: m7c3
DIC>
DIC> @@
DIC> @@ ENTER A STOICHOOMETRIC SPHEROIDAL PHASE IN THE REGION
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /AUS/: aus
PHASE TYPE /MATRIX/: sph
PHASE NAME: /NONE/: m3c2
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 TO SAVE SOME SPACE ON THE DISK THE RESULT IS STORED
DIC> @@ SELECTIVELY. OTHERWISE THE STORE-RESULT-FILE FROM THIS EXAMPLE
DIC> @@ WOULD BE VERY LARGE.
DIC> @@
DIC> set-simulation-condition
NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDF: /2/:
CHECK INTERFACE POSITION /NO/:
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/: 99
DEGREE OF IMPLICIT WHEN INTEGRATING PDEs (0 -> 0.5 -> 1): /.5/:
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /NO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDF /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 exdl y
DIC>
DIC> set-inter
--OK--
DIC>

```

exdia-run

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exdia\run.DCM"DIC>
DIC>
DIC> @@ exdl_run.DCM
DIC>
DIC> @@
DIC> @@ READ THE SETUP FILE AND START THE SIMULATION
DIC> @@
DIC> go d-m
TIME STEP AT TIME 0.000000E+00
*** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
*** ENTERING M3C2 AS A DIFFUSION NONE PHASE
*** ENTERING M7C3 AS A DIFFUSION NONE PHASE
DIC> read exdl
OK
DIC> sim
U-FRACTION IN SYSTEM: C = 4.73399698964897E-06 CR = .273386070506604
NI = .726613929493396
TOTAL SIZE OF SYSTEM: .003 [m]
WARNING:M7C3 HAS NO VOLUME FRACTION, CREATING ONE

WARNING:M3C2 HAS NO VOLUME FRACTION, CREATING ONE

U-FRACTION IN SYSTEM: C = 4.73399698964898E-06 CR = .273386070506604
NI = .726613929493396
TOTAL SIZE OF SYSTEM: .003 [m]
TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = 7.37829265031503E-05 CR = .273386070506603
NI = .726613929493397
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 0.10010000E-03 DT = 0.10000000E-03 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = 1.07765273658403E-04 CR = .273386070506579
NI = .726613929493421
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 0.40010010 DT = 0.40000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = 1.29844980713891E-04 CR = .273386070500949
NI = .726613929499051
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 61.221707 DT = 60.821607 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = 1.67985911285438E-04 CR = .273386069358852
NI = .726613930641148
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 135.34814 DT = 74.126429 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = 2.08836403949596E-04 CR = .273386068335922
NI = .726613931664078
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 242.67634 DT = 107.32821 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = 2.57253556459827E-04 CR = .273386067317191
NI = .726613932682809
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 1 seconds
TIME = 408.61790 DT = 165.94156 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = 3.16829365327122E-04 CR = .273386066351575
NI = .726613933648425
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 677.99375 DT = 269.37585 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = 3.91398501422706E-04 CR = .273386065452222
NI = .726613934547778
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 1140.3108 DT = 462.31701 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = 4.86579533187512E-04 CR = .273386064383137
NI = .726613935616863
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 2003.0736 DT = 862.76284 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = 6.16999894543263E-04 CR = .273386063110096
NI = .726613936889904
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 3701.3810 DT = 1698.3074 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = 8.03308317133761E-04 CR = .273386061634911
NI = .726613938365089
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 5501.3810 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = 9.81626963664688E-04 CR = .273386060762439
NI = .726613939237561
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 7301.3810 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0011473629203206 CR = .273386060181809
NI = .726613939818191
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 1 seconds
TIME = 9101.3810 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00130395620915009 CR = .273386059222275
NI = .726613940777725
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 10901.381 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00145171605713694 CR = .27338605759019
NI = .72661394240981
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 12701.381 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00159094848225919 CR = .273386055196014
```



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

output ignored...

... output resumed

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

```

TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 3594359.7 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0316569773322023 CR = .273385942325503
NI = .726614057674497
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 1 seconds
TIME = 3596159.7 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0316648959325256 CR = .273385942293274
NI = .726614057706726
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 3597959.7 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0316728128781564 CR = .273385942260811
NI = .726614057739189
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 3599759.7 DT = 1800.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0316807281854782 CR = .273385942228113
NI = .726614057771886
TOTAL SIZE OF SYSTEM: .003 [m]
CPU time used in timestep 0 seconds
TIME = 3600000.0 DT = 240.30748 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0316817891333221 CR = .273385942223672
NI = .726614057776328
TOTAL SIZE OF SYSTEM: .003 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 0.0000000
DELETING TIME-RECORD FOR TIME 0.10000000E-06
DELETING TIME-RECORD FOR TIME 0.10010000E-03
DELETING TIME-RECORD FOR TIME 163559.69
DELETING TIME-RECORD FOR TIME 341759.69
DELETING TIME-RECORD FOR TIME 519959.69
DELETING TIME-RECORD FOR TIME 698159.69
DELETING TIME-RECORD FOR TIME 876359.69
DELETING TIME-RECORD FOR TIME 1054559.7
DELETING TIME-RECORD FOR TIME 1232759.7
DELETING TIME-RECORD FOR TIME 1410959.7
DELETING TIME-RECORD FOR TIME 1589159.7
DELETING TIME-RECORD FOR TIME 1767359.7
DELETING TIME-RECORD FOR TIME 1945559.7
DELETING TIME-RECORD FOR TIME 2123759.7
DELETING TIME-RECORD FOR TIME 2301959.7
DELETING TIME-RECORD FOR TIME 2480159.7
DELETING TIME-RECORD FOR TIME 2658359.7
DELETING TIME-RECORD FOR TIME 2836559.7
DELETING TIME-RECORD FOR TIME 3014759.7
DELETING TIME-RECORD FOR TIME 3192959.7
DELETING TIME-RECORD FOR TIME 3371159.7
DELETING TIME-RECORD FOR TIME 3549359.7
DELETING TIME-RECORD FOR TIME 3596159.7
DELETING TIME-RECORD FOR TIME 3597959.7

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

TIMESTEP AT 3600000.00 SELECTED

```

```

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

```

exdia-plot

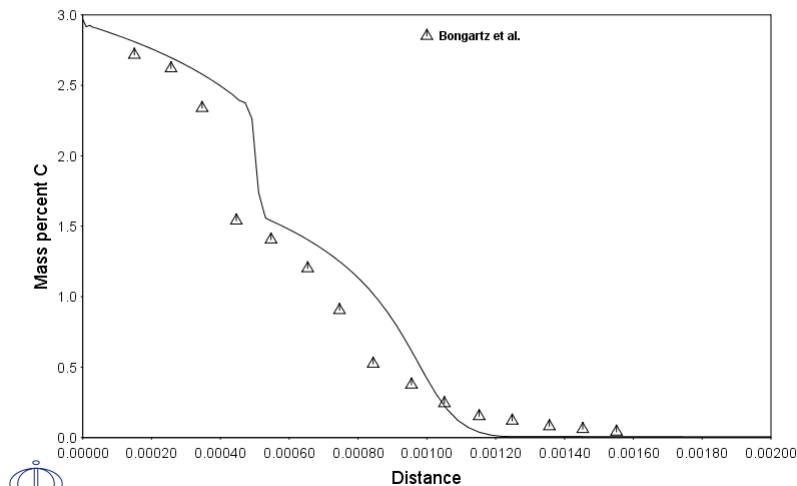
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exdia\plot.DCM"DIC>
DIC>
DIC> @@ exd1_plot.DCM
DIC>
DIC> @@
DIC> @@ FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE exd1
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 3.60000E+06
*** ENTERING GRAPHITE 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
```

d1.1

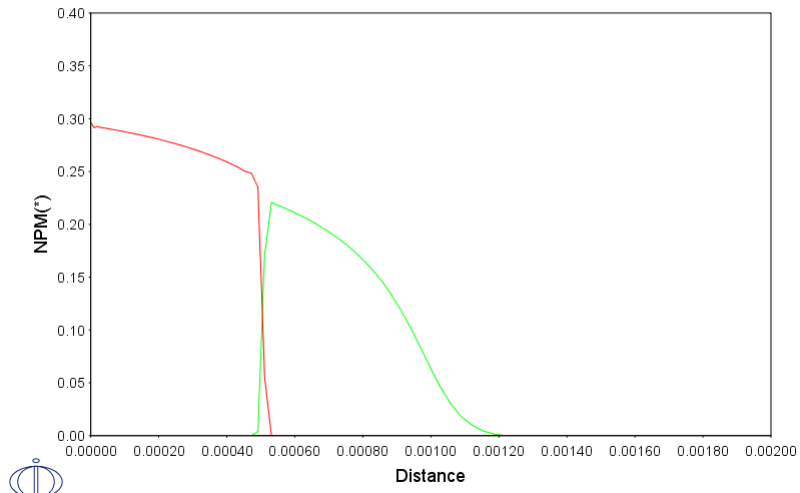
2018.02.18.21.53.30
Time=3600000
CELL#1



```
POST-1:
POST-1:
POST-1:
POST-1: @?<_hit_return_to_continue_>
POST-1:
POST-1: @@
POST-1: @@ NOW PLOT THE AMOUNT OF CARBIDES FORMED
POST-1: @@
POST-1: s-d-a y npm(*)
POST-1: s-s-s y n 0 0.4
POST-1: app n
POST-1:
POST-1: set-tit d1.2
POST-1: plot
```

d1.2

2018.02.18.21.53.31
Time = 3600000
CELL #1



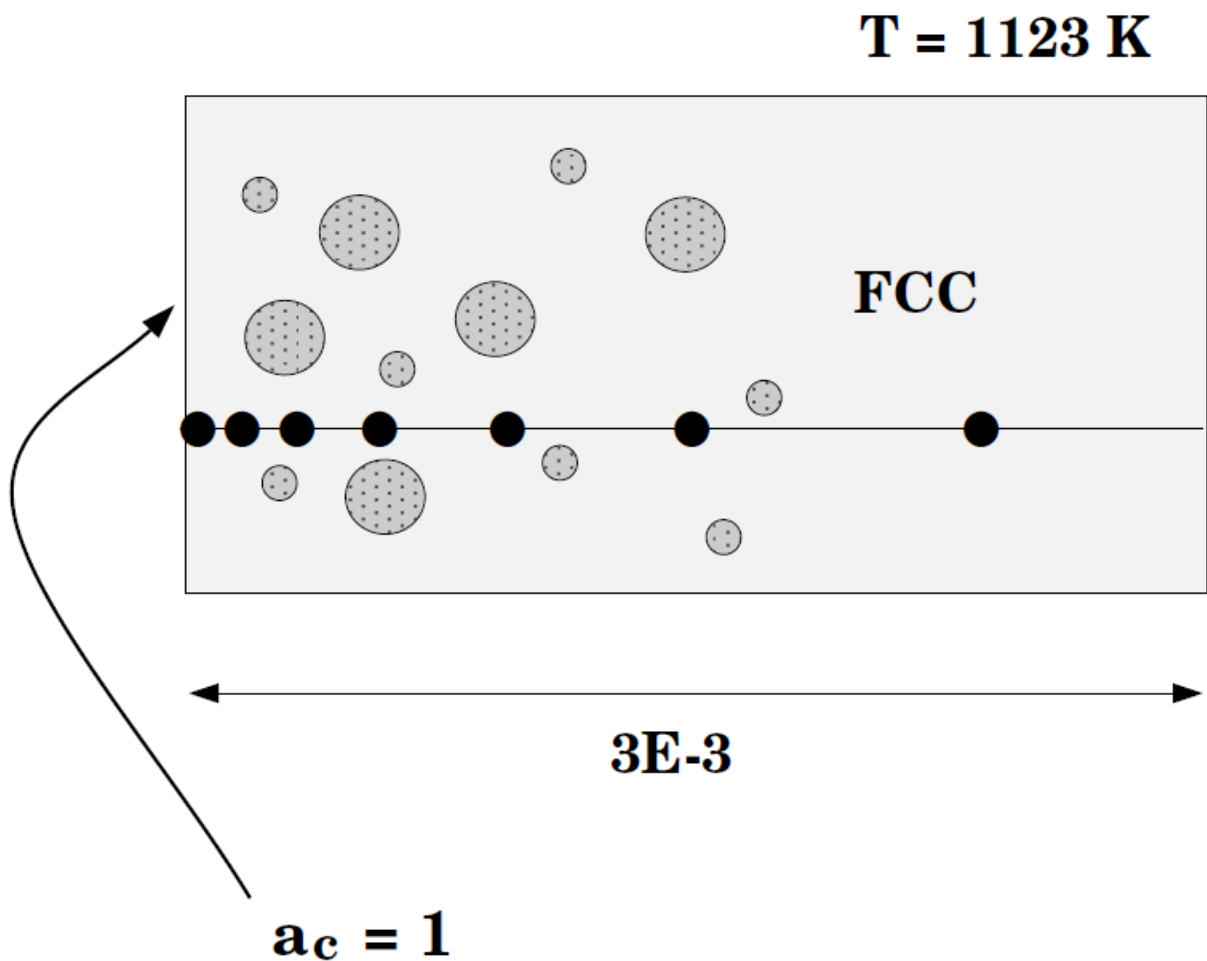
POST-1:
POST-1:
POST-1:
POST-1: @?<_hit_return_to_continue_>
POST-1:
POST-1: set-inter
--OK--
POST-1:



Example exd1b

Carburization of a Ni-25% Cr alloy: Homogenization model

This example is about carburization of a Ni-25Cr alloy. In this case the M3C2 and M7C3 carbides are entered as spheroid phases in a FCC matrix. It is similar to exd1a except the default HOMOGENIZATION MODEL is used and then ENTER_HOMOGENIZATION_FUNCTION should be used instead of ENTER_LABYRINTH_FUNCTION. This case is from A. Engström, L. Höglund and J. Ågren: Metall.Trans. A, v.25A (1994), pp. 1127-1134.



exdlb-setup

About Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

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

```
SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exdlb\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: @@ exdlb_setup.DCM
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASE
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Current database: Steels/Fe-Alloys v9.0
```

```
VA /- DEFINED
L12_FCC B2_BCC DICTRA_FCC_A1
REJECTED
```

```
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ USE THE SSOL DATABASE FOR THERMODYNAMIC DATA
TDB_TCFE9: @@
TDB_TCFE9: sw ssol2
Current database: SGTE Alloy Solutions Database v2.1
```

```
VA DEFINED
B2_BCC L12_FCC AL5FE4:
REJECTED
GAS:G AQUEOUS:A WATER:A
REJECTED
```

```
TDB_SSOL2: def-sys ni cr c
NI CR C
DEFINED
TDB_SSOL2: rej ph * all
LIQUID:L FCC_A1 BCC_A2
HCP_A3 DIAMOND_A4 CHI_A12
CBCC_A12 CUB_A13 SIGMA
GRAPHITE CEMENTITE KSI_CARBIDE
M23C6 M7C3 M3C2
FE4N AL3NI2 ALNI_B2
CR3SI CRSI2 REJECTED
```

```
TDB_SSOL2: res ph fcc,m7c3,m3c2,grap
FCC_A1 M7C3 M3C2
GRAPHITE RESTORED
```

```
TDB_SSOL2: get
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....
```

List of references for assessed data

```
'Byeong-Joo Lee, unpublished revision (1991); C-Cr-Fe-Ni'
'Alan Dinsdale, SGTE Data for Pure Elements, NPL Report DMA(A)195
September 1989'
'Alan Dinsdale, SGTE Data for Pure Elements,
Calphad Vol 15(1991) p 317-425,
also in NPL Report DMA(A)195 Rev. August 1990'
'A. Gabriel, C. Chatillon, I. Ansara, to be published in
High Temp. Sci. (parameters listed in
Calphad Vol 11 (1987) pp 203-218); C-Ni'
'A. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); CR-Ni'
'NPL, unpublished work (1989); C-Cr-Ni'
-OK-
```

```
TDB_SSOL2:
TDB_SSOL2: @@
TDB_SSOL2: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE MOBILITY DATA
TDB_SSOL2: @@
TDB_SSOL2: app mob2
Current database: Alloys Mobility v2.7
```

```
VA DEFINED
GAS:G REJECTED
APP: def-sys ni c cr
NI C CR
DEFINED
APP: rej ph * all
BCC_A2 CEMENTITE DIAMOND_A4
FCC_A1 M4N GRAPHITE
HCP_A3 KSI_CARBIDE LIQUID:L
M23C6 M3C2 M7C3
SIGMA REJECTED
```

```
APP: res ph fcc,m7c3,m3c2,grap
FCC_A1 M7C3 M3C2
GRAPHITE RESTORED
```

```
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
```

PARAMETERS ...
FUNCTIONS

List of references for assessed data

'This parameter has not been assessed'
'B. Jonsson: Z. Metallkunde 85(1994)502-509;
C diffusion in fcc Cr-Fe-Ni'
'B. Jonsson: Scand. J. Metall. 24(1995)21-27;
Cr and Fe diffusion fcc Cr-Fe'
'B. Jonsson: Scand. J. Metall. 24(1995)21-27;
Cr and Ni diffusion fcc Cr-Ni'
'B. Jonsson: Scand. J. Metall. 24(1995)21-27;
Ni self-diffusion'

-OK-

APP:

APP: @@

APP: @@ ENTER THE DICTRA MONITOR

APP: @@

APP: go d-m

NO TIME STEP DEFINED

*** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE

*** ENTERING M3C2 AS A DIFFUSION NONE PHASE

*** ENTERING M7C3 AS A DIFFUSION NONE PHASE

DIC>

DIC> @@

DIC> @@ ENTER THE GLOBAL CONDITION T

DIC> @@

DIC> set-cond glob T 0 1123; * N

DIC>

DIC> @@

DIC> @@ SET THE REFERENCE STATE FOR CARBON

DIC> @@

DIC> set-reference-state

Component: C

Reference state: grap

Temperature /*/: *

Pressure /100000/: 101325

DIC>

DIC> @@

DIC> @@ ENTER THE REGION aus

DIC> @@

DIC> enter-region aus

DIC>

DIC> @@

DIC> @@ ENTER A GEOMETRICAL GRID INTO THE REGION

DIC> @@

DIC> enter-grid aus 3e-3 geo 100 1.02

DIC>

DIC> @@

DIC> @@ ENTER A MATRIX PHASE IN THE REGION

DIC> @@

DIC> enter-phase act aus matrix fcc_a1#1

DIC>

DIC> @@

DIC> @@ ENTER THE START COMPOSITION FOR THE MATRIX PHASE

DIC> @@

DIC> enter-composition

REGION NAME : /AUS/: aus

PHASE NAME: /FCC_A1#1/: fcc#1

DEPENDENT COMPONENT ? /NI/: ni

COMPOSITION TYPE /MOLE_FRACTION/: w-p

PROFILE FOR /C/: cr

TYPE /LINEAR/: lin 25 25

PROFILE FOR /CR/: c

TYPE /LINEAR/: lin 1e-4 1e-4

DIC>

DIC> @@

DIC> @@ ENTER SPHEROIDAL PHASES IN THE REGION

DIC> @@

DIC> enter-phase

ACTIVE OR INACTIVE PHASE /ACTIVE/: act

REGION NAME : /AUS/: aus

PHASE TYPE /MATRIX/: sph

PHASE NAME: /NONE/: m7c3

DIC>

DIC> @@

DIC> @@ ENTER A STOICHOMETRIC SPHEROIDAL PHASE IN THE REGION

DIC> @@

DIC> enter-phase

ACTIVE OR INACTIVE PHASE /ACTIVE/: act

REGION NAME : /AUS/: aus

PHASE TYPE /MATRIX/: sph

PHASE NAME: /NONE/: m3c2

DIC>

DIC>

DIC> @@

DIC> @@ ENTER A START COMPOSITION FOR THE SPHEROIDAL PHASES

DIC> @@

DIC> enter-composition

REGION NAME : /AUS/: aus

PHASE NAME: /FCC_A1#1/: m7c3

USE EQUILIBRIUM VALUE /Y/: Y

DIC> enter-composition

REGION NAME : /AUS/: aus

PHASE NAME: /FCC_A1#1/: m3c2

USE EQUILIBRIUM VALUE /Y/: Y

DIC>

DIC> @@

DIC> @@ SET THE BOUNDARY CONDITION

DIC> @@

DIC> set-cond

GLOBAL OR BOUNDARY CONDITION /GLOBAL/: boundary

BOUNDARY /LOWER/: lower

CONDITION TYPE /CLOSED_SYSTEM/: mixed

Dependent substitutional element:NI

Dependent interstitial element:VA

TYPE OF CONDITION FOR COMPONENT C /ZERO_FLUX/: activity

LOW TIME LIMIT /0/: 0

```

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

```


exd1b-run

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exd1b\run.DCM"DIC>
DIC>
DIC> @@ exd1_run.DCM
DIC>
DIC> @@
DIC> @@ READ THE SETUP FILE AND START THE SIMULATION
DIC> @@
DIC> go d-m
TIME STEP AT TIME 0.000000E+00
*** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
*** ENTERING M3C2 AS A DIFFUSION NONE PHASE
*** ENTERING M7C3 AS A DIFFUSION NONE PHASE
DIC> read exd1
OK
DIC> sim
STARTING SIMULATION USING HOMOGENIZATION MODEL
-----
INFO: PHASE WITH LIMITED SOLUBILITY OF ELEMENT(S) EXIST
A FALLBACK PHASE ZZDICTRA_GHOST WILL BE DEFINED
ALONG WITH THE FOLLOWING PARAMETERS:
G(ZZDICTRA_GHOST,C;0)-H298 (GRAPHITE,C;0)
G(ZZDICTRA_GHOST,CR;0)-H298 (BCC_A2,CR;0)
G(ZZDICTRA_GHOST,NI;0)-H298 (FCC_A1,NI;0)
L(ZZDICTRA_GHOST,C,CR;0)
L(ZZDICTRA_GHOST,C,NI;0)
L(ZZDICTRA_GHOST,CR,NI;0)
Saving results
-----
WARNING:M7C3 HAS NO VOLUME FRACTION, CREATING ONE
WARNING:M3C2 HAS NO VOLUME FRACTION, CREATING ONE
Starting time-step t0= 0.0000000 dt= 0.100000000E-06
Stage 1
Stage 2
Stage 3
Moles of elements / mole fractions in system:
C 0.14201992E-07 / 0.47339748E-05
CR 0.82015821E-03 / 0.27338478
NI 0.21798418E-02 / 0.72661049

Time-step converged t0= 0.0000000 dt= 0.100000000E-06
-----
Saving results
-----
Starting time-step t0= 0.100000000E-06 dt= 0.200000000E-06
Stage 1
Stage 2
Stage 3
Moles of elements / mole fractions in system:
C 0.14201993E-07 / 0.47339753E-05
CR 0.82015821E-03 / 0.27338478
NI 0.21798418E-02 / 0.72661049

Time-step converged t0= 0.100000000E-06 dt= 0.200000000E-06
-----
Starting time-step t0= 0.300000000E-06 dt= 0.400000000E-06
Stage 1
Evaluating Jacobian
Iteration # 1 sum residual **2: 0.85928988E-03
Stage 2
Stage 3
Moles of elements / mole fractions in system:
C 0.14201996E-07 / 0.47339762E-05
CR 0.82015821E-03 / 0.27338478
NI 0.21798418E-02 / 0.72661049

Time-step converged t0= 0.300000000E-06 dt= 0.400000000E-06
-----
Starting time-step t0= 0.700000000E-06 dt= 0.800000000E-06
Stage 1
Iteration # 1 sum residual **2: 0.14356446E-03
Stage 2
Stage 3
Moles of elements / mole fractions in system:
C 0.14202001E-07 / 0.47339780E-05
CR 0.82015821E-03 / 0.27338478
NI 0.21798418E-02 / 0.72661049

Time-step converged t0= 0.700000000E-06 dt= 0.800000000E-06
-----
Starting time-step t0= 0.150000000E-05 dt= 0.160000000E-05
Stage 1
Iteration # 1 sum residual **2: 0.61865070E-04
Stage 2
Stage 3
Moles of elements / mole fractions in system:
C 0.14202012E-07 / 0.47339817E-05
CR 0.82015821E-03 / 0.27338478
NI 0.21798418E-02 / 0.72661049

Time-step converged t0= 0.150000000E-05 dt= 0.160000000E-05
-----
Starting time-step t0= 0.310000000E-05 dt= 0.320000000E-05
Stage 1
Iteration # 1 sum residual **2: 0.42610973E-04
Stage 2
Stage 3
Moles of elements / mole fractions in system:
C 0.14202034E-07 / 0.47339891E-05
CR 0.82015821E-03 / 0.27338478
NI 0.21798418E-02 / 0.72661049

Time-step converged t0= 0.310000000E-05 dt= 0.320000000E-05
-----
Starting time-step t0= 0.630000000E-05 dt= 0.640000000E-05
Stage 1
Iteration # 1 sum residual **2: 0.35739934E-04
Stage 2
Stage 3
Moles of elements / mole fractions in system:
C 0.14202079E-07 / 0.47340038E-05
CR 0.82015821E-03 / 0.27338478
NI 0.21798418E-02 / 0.72661049
```

Time-step converged t0= 0.63000000E-05 dt= 0.64000000E-05

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

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

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

output ignored...

... output resumed

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

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

KEEPING TIME-RECORD FOR TIME 3598786.9
AND FOR TIME 3600000.0
WORKSPACE RECLAIMED

INTERPOLATION SCHEME USED THIS FRACTION OF
THE ALLOCATED MEMORY: 0.817338868519136
EFFICIENCY FACTOR: 92.8870231802691

DEALLOCATING

TIMESTEP AT 3600000.00 SELECTED

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

exd1b-plot

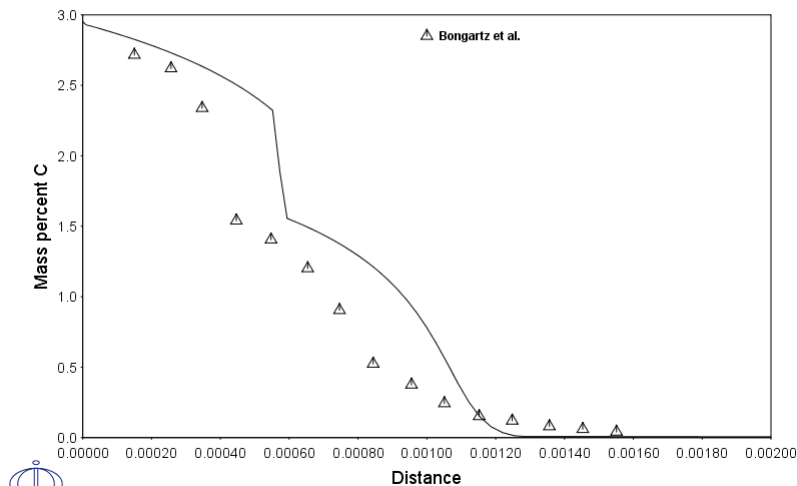
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exd1b\plot.DCM"DIC>
DIC>
DIC> @@ exd1_plot.DCM
DIC>
DIC> @@
DIC> @@ FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE exd1b
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 3.60000E+06
*** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
*** ENTERING M3C2 AS A DIFFUSION NONE PHASE
*** ENTERING M7C3 AS A DIFFUSION NONE PHASE
DIC> read exd1
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post

POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
```

```
POST-1:
POST-1: @@
POST-1: @@ PLOT THE TOTAL CARBON CONCENTRATION PROFILE
POST-1: @@
POST-1: s-d-a y w-p c
POST-1: s-d-a x distance global
INFO: Distance is set as independent variable
POST-1: s-s-s x n 0 2e-3
POST-1: s-p-c time 3600000
POST-1:
POST-1: app y exd1.exp
PROLOGUE NUMBER: /0/: 1
DATASET NUMBER(s): /-1/: 1
POST-1:
POST-1: @@
POST-1: @@ SET A TITLE ON THE PLOT
POST-1: @@
POST-1: set-tit d1.1
POST-1:
POST-1: plot
```

d1.1

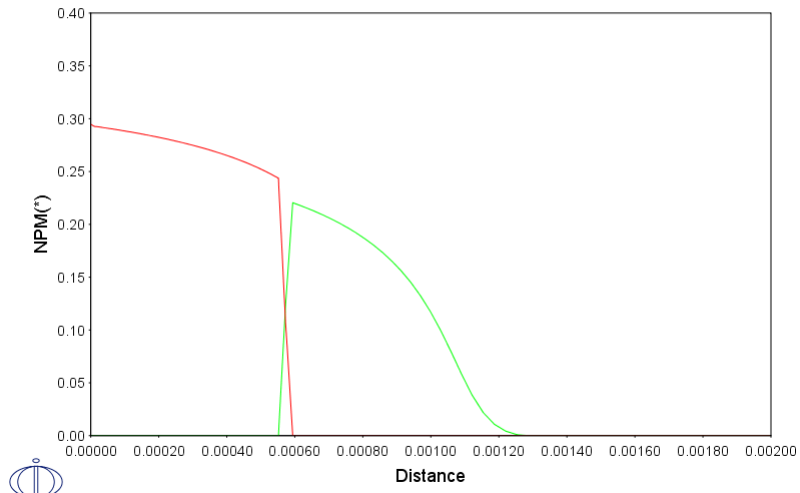
2018.02.18.22.03.40
Time=3600000
CELL#1



```
POST-1:
POST-1:
POST-1:
POST-1: @?<_hit_return_to_continue_>
POST-1:
POST-1: @@
POST-1: @@ PLOT THE AMOUNT OF CARBIDES FORMED
POST-1: @@
POST-1: s-d-a y npm(*)
POST-1: s-s-s y n 0 0.4
POST-1: app n
POST-1:
POST-1: set-tit d1.2
POST-1: plot
```

d1.2

2018.02.18.22.03.46
Time = 3600000
CELL #1



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

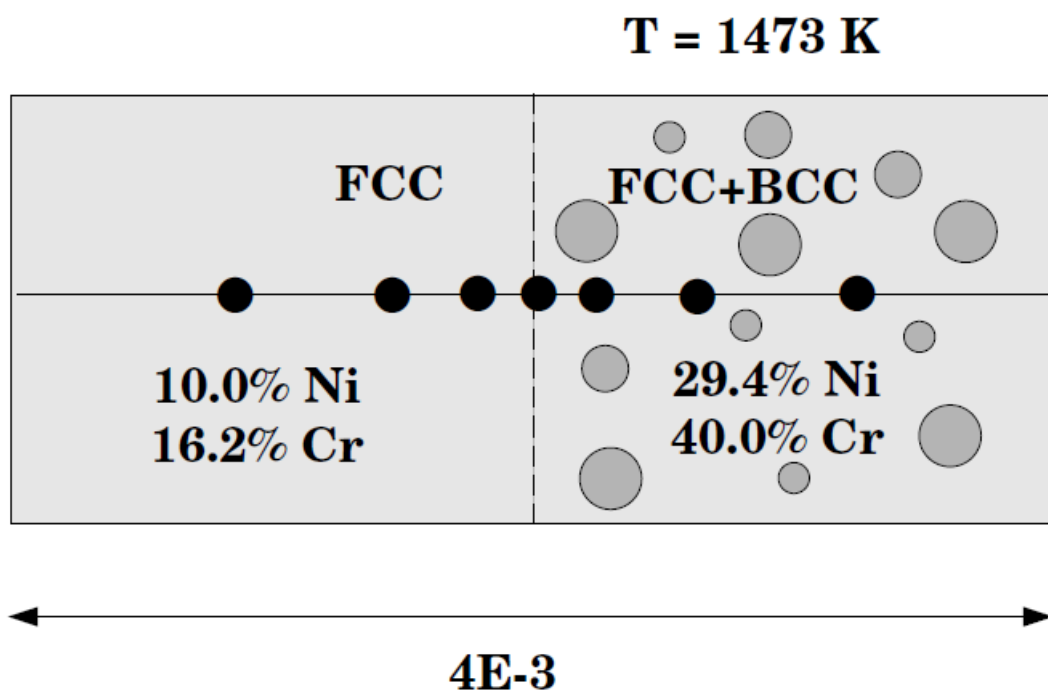


Example exd2a

Diffusion couple of Fe-Ni-Cr alloys: Step-profile

This example calculates the interdiffusion in a diffusion couple between a two-phase (FCC+BCC) and a single-phase (FCC) Fe-Ni-Cr alloy. Initially it uses a step profile. This simulation can be run with either the DISPERSED SYSTEM MODEL or the HOMOGENIZATION MODEL. In this example the DISPERSED SYSTEM MODEL is used.

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



exd2a-setup

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

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

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

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

List of references for assessed data

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

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

List of references for assessed data

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

```

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

DIC>
DIC> @@
DIC> @@ ENTER THE REGION fer
DIC> @@
DIC> enter-region fer
DIC>
DIC>
DIC> @@
DIC> @@ ENTER A DOUBLE GEOMETRICAL GRID INTO THE REGION
DIC> @@ THIS GIVES A SHORT DISTANCE BETWEEN THE GRIDPOINTS
DIC> @@ IN THE MIDDLE OF THE REGION WHERE THE INITIAL INTERFACE IS
DIC> @@
DIC> enter-grid fer
WIDTH OF REGION /1/: 4e-3
TYPE /LINEAR/: double
NUMBER OF POINTS /50/: 200
VALUE OF R IN THE GEOMETRICAL SERIE FOR LOWER PART OF REGION: 0.97
VALUE OF R IN THE GEOMETRICAL SERIE FOR UPPER PART OF REGION: 1.03093
DIC>
DIC> @@
DIC> @@ ENTER A MATRIX PHASE IN THE REGION
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act fer matrix fcc
DIC>
DIC> @@
DIC> @@ ENTER THE START COMPOSITION FOR THE MATRIX PHASE FROM FILES
DIC> @@
DIC> enter-composition
REGION NAME : /FER/: fer
PHASE NAME: /FCC_A1/: fcc
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /CR/: cr
TYPE /LINEAR/: read d2cr.dat
PROFILE FOR /NI/: ni
TYPE /LINEAR/: read d2ni.dat
DIC>
DIC> @@
DIC> @@ ENTER FERRITE AS THE SPHEROIDAL PHASE IN THE REGION.
DIC> @@ SINCE THE FRACTION OF FERRITE IS SMALL, AND THESE APPEAR
DIC> @@ AS ISOLATED PARTICLES, FERRITE IS ENTERED AS A SPHEROIDAL PHASE
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /FER/: fer
PHASE TYPE /MATRIX/: sph
PHASE NAME: /NONE/: bcc
DIC>
DIC> @@
DIC> @@ ENTER A COMPOSITION FOR THE SPHEROIDAL PHASE
DIC> @@ USE THE EQUILIBRIUM VALUE
DIC> @@
DIC> enter-composition
REGION NAME : /FER/: fer
PHASE NAME: /FCC_A1/: bcc
USE EQUILIBRIUM VALUE /Y/: y
DIC>
DIC>
DIC> @@
DIC> @@ ENTER A LABYRINTH FACTOR
DIC> @@ IN THIS CASE THE LOW DIFFUSIVITY PHASE IS THE MATRIX AND THE
DIC> @@ "EFFECTIVE" DIFFUSIVITY IN THE AUSTENITE+FERRITE TWO-PHASE
DIC> @@ REGION IS EXPECTED TO BE HIGHER THAN THE DIFFUSIVITY IN THE
DIC> @@ AUSTENITE.
DIC> enter-lab
REGION NAME : fer
f(T,P,VOLFR,X)= 1+3*(1-volfr)/volfr;
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME AND OTHER SIMULATION PARAMETERS
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 720000
AUTOMATIC TIMESTEP CONTROL /YES/: YES
MAX TIMESTEP DURING INTEGRATION /72000/: 5000
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC> set-simulation-condition
NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDF: /2/:
CHECK INTERFACE POSITION /NO/:
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/: 99
DEGREE OF IMPLICIT WHEN INTEGRATING PDEs (0 -> 0.5 -> 1): /.5/:
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /NO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDF /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> go d-m
TIME STEP AT TIME 0.00000E+00
DIC> read exd2
OK
DIC> sim
U-FRACTION IN SYSTEM: CR = .297842647391914 FE = .517227320517284
NI = .184930032090802
TOTAL SIZE OF SYSTEM: .004 [m]
WARNING:BCC_A2 HAS NO VOLUME FRACTION, CREATING ONE
```

```
U-FRACTION IN SYSTEM: CR = .297842647391914 FE = .517227320517284
NI = .184930032090802
TOTAL SIZE OF SYSTEM: .004 [m]
TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297842647356821 FE = .517227320600573
NI = .184930032042606
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep 0 seconds
TIME = 0.10010000E-03 DT = 0.10000000E-03 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297842648005432 FE = .517227319061159
NI = .18493003293341
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep 0 seconds
TIME = 0.40010010 DT = 0.400000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297842676377595 FE = .517227251840507
NI = .184930071781899
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep 0 seconds
TIME = 281.72200 DT = 281.32190 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .29784776027007 FE = .517216317308823
NI = .184935922421107
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep 0 seconds
TIME = 844.36579 DT = .562.64380 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297849615184738 FE = .517212946633455
NI = .184937438181807
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep 0 seconds
TIME = 1969.6534 DT = 1125.2876 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297850550731969 FE = .517211426818701
NI = .18493802244933
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep 0 seconds
TIME = 4220.2286 DT = 2250.5752 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .29785119000635 FE = .517210569323814
NI = .18493831167555
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep 0 seconds
TIME = 8721.3789 DT = 4501.1504 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297851494954329 FE = .517210020163945
NI = .184938484881725
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep 1 seconds
TIME = 13721.379 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297851732113685 FE = .517209740277055
NI = .184938527609259
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep 0 seconds
TIME = 18721.379 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297851883453499 FE = .517209584045538
NI = .184938532500963
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep 0 seconds
TIME = 23721.379 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297851977657541 FE = .517209483265981
NI = .184938539076478
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep 0 seconds
TIME = 28721.379 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297852029985815 FE = .517209412426198
NI = .184938557587987
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep 0 seconds
TIME = 33721.379 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297852049765999 FE = .517209361691084
NI = .184938588542917
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep 0 seconds
TIME = 38721.379 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297852045015463 FE = .517209326359902
NI = .184938628624635
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep 1 seconds
TIME = 43721.379 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .29785205230068 FE = .517209299378176
NI = .184938648321145
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep 0 seconds
TIME = 48721.379 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297852064900627 FE = .517209276184267
NI = .184938658915106
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep 0 seconds
TIME = 53721.379 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297852069935234 FE = .517209260646735
```

```

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

output ignored...

... output resumed

```

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

```
TIME = 693721.38 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297852035106901 FE = .517209102778509
NI = .184938862114591
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep 1 seconds
TIME = 698721.38 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297852041265549 FE = .517209100862487
NI = .184938857871964
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep 0 seconds
TIME = 703721.38 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297852048238891 FE = .517209099115038
NI = .184938852646072
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep 0 seconds
TIME = 708721.38 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297852055131586 FE = .517209097666857
NI = .184938847201557
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep 0 seconds
TIME = 713721.38 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297852061470614 FE = .517209096580512
NI = .184938841948874
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep 1 seconds
TIME = 718721.38 DT = 5000.0000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .297852066979841 FE = .517209095891422
NI = .184938837128738
TOTAL SIZE OF SYSTEM: .004 [m]
CPU time used in timestep 0 seconds
TIME = 720000.00 DT = 1278.6211 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: CR = .2978520717672 FE = .517209095429389
NI = .184938832803411
TOTAL SIZE OF SYSTEM: .004 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 0.0000000
DELETING TIME-RECORD FOR TIME 0.10000000E-06
DELETING TIME-RECORD FOR TIME 0.10010000E-03
DELETING TIME-RECORD FOR TIME 468721.38
DELETING TIME-RECORD FOR TIME 708721.38
DELETING TIME-RECORD FOR TIME 713721.38

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

TIMESTEP AT 720000.000 SELECTED
```

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

exd2a-plot

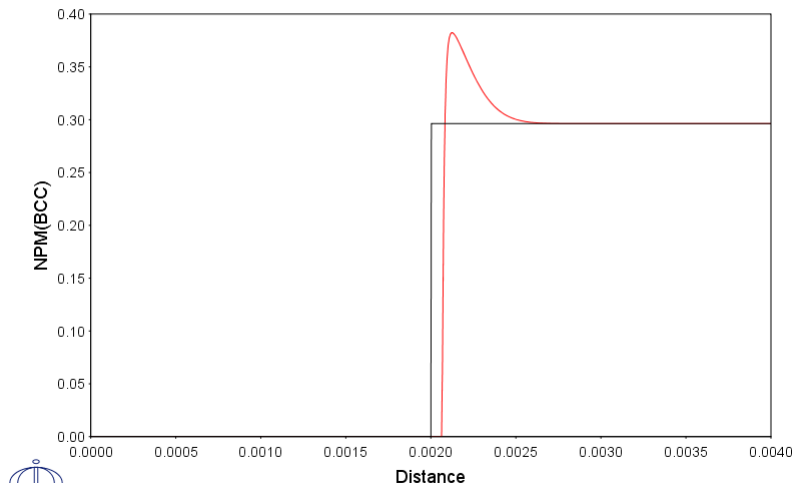
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exd2a\plot.DCM"DIC>
DIC>
DIC> @@ exd2_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE D2
DIC> @@
DIC> @@ ENTER THE DICTRA MODULE AND SPECIFY THE STORE-RESULT FILE
DIC> @@
DIC>
DIC> go d-m
      TIME STEP AT TIME 7.20000E+05
DIC> read exd2
      OK
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA POST PROCESSOR
DIC> @@
DIC> post

      POST PROCESSOR VERSION 1.7
      Implemented by Bjorn Jonsson
```

```
POST-1:
POST-1:
POST-1: @@
POST-1: @@ LET US SEE HOW THE FRACTION OF FERRITE HAS CHANGED
POST-1: @@ AS A RESULT OF THE DIFFUSION
POST-1: @@
POST-1: s-d-a y npm(bcc)
POST-1: s-d-a x distance global
      INFO: Distance is set as independent variable
POST-1: s-p-c time 0.720000
POST-1: set-tit Figure D2.1
POST-1: pl
```

Figure D2.1

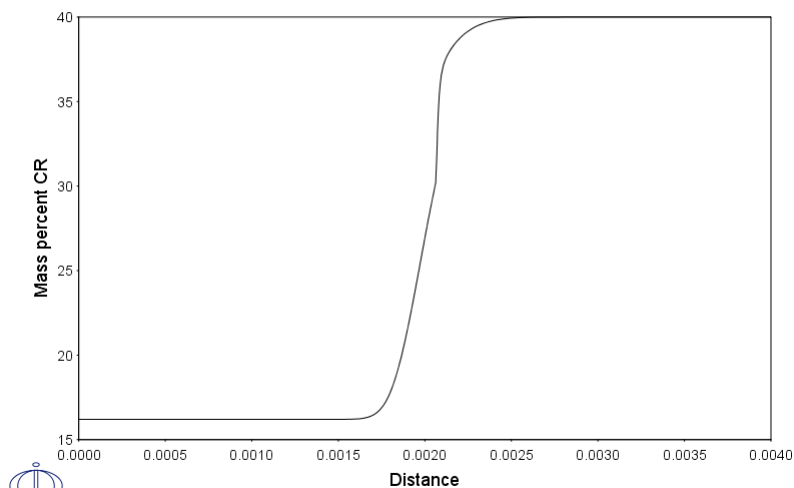
2018.02.18.22.07.13
Time=0.720000
CELL#1



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

Figure D2.2

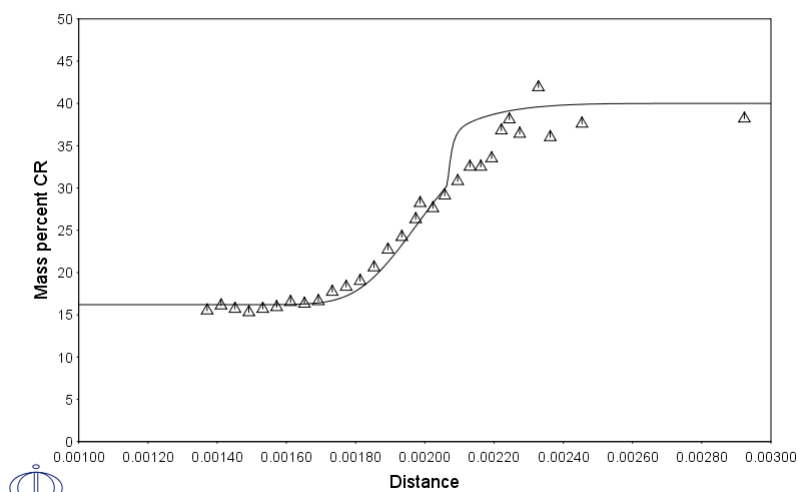
2018.02.18.22.07.14
Time = 720000
CELL #1



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

Figure D2.3

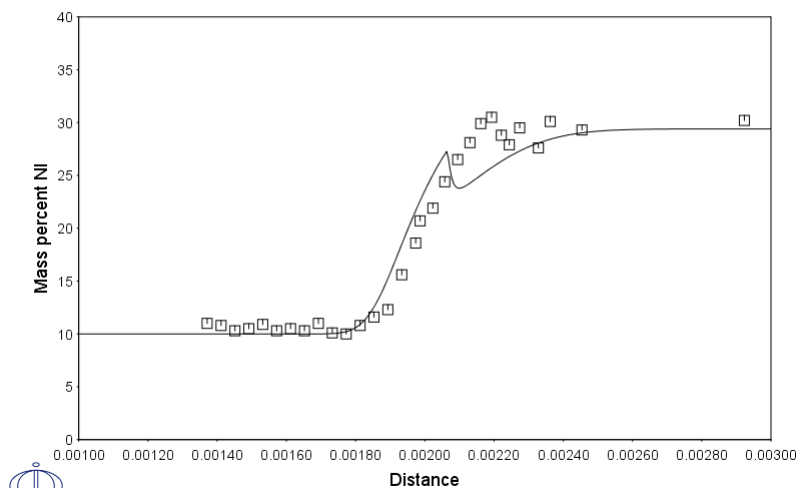
2018.02.18.22.07.14
Time = 720000
CELL #1



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

Figure D2.4

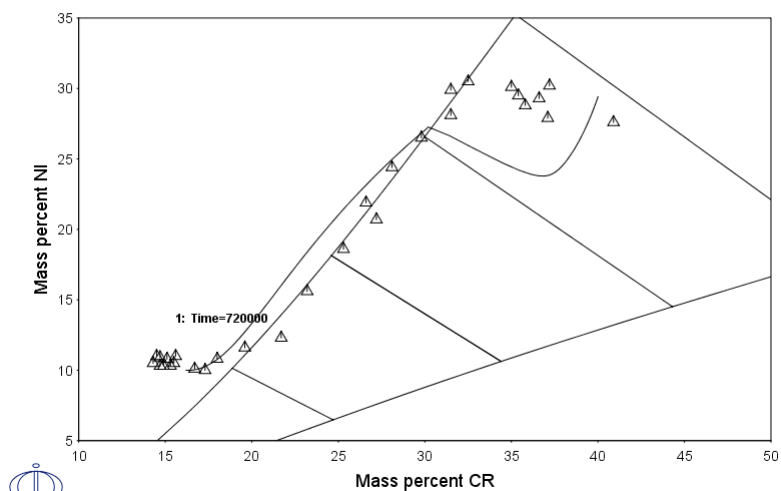
2018.02.18.22.07.15
Time = 720000
CELL #1



```
POST-1:
POST-1:
POST-1:
POST-1: @?<_hit_return_to_continue_>
POST-1: @@
POST-1: @@ LET US PLOT THE DIFFUSION PATH FOR THE COUPLE.
POST-1: @@ WE APPEND THE TERNARY PHASE-DIAGRAM CALCULATED IN THERMO-CALC
POST-1: @@ AND THE EXPERIMENTAL DATA
POST-1: @@
POST-1: s-d-a x w-p cr
POST-1: s-d-a y w-p ni
POST-1: s-i-v dis ql
POST-1: s-p-c time last
POST-1:
POST-1: app y exd2.exp
PROLOGUE NUMBER: /1/: 1
DATASET NUMBER(s): /-1/: 6 7 8
POST-1:
POST-1: s-s-s x n 10 50
POST-1: s-s-s y n 5 35
POST-1:
POST-1: set-tit Figure D2.5
POST-1: pl
```

Figure D2.5

2018.02.18.22.07.15
Time = 720000
CELL #1



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

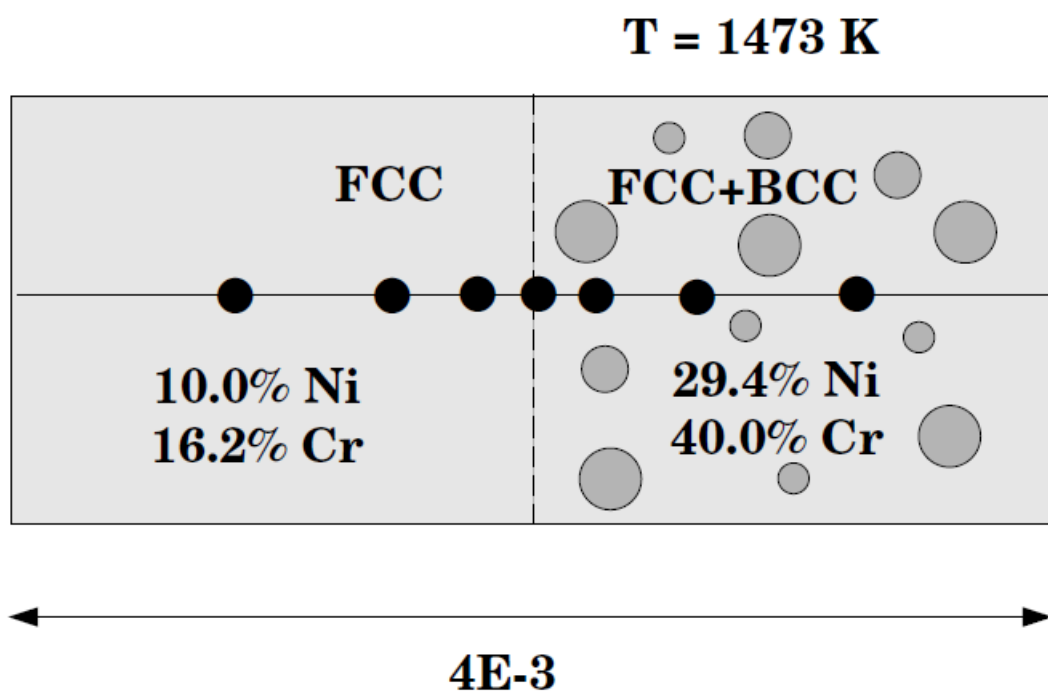


Example exd2b

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

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

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



exd2b-setup

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

```
SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exd2b\setup.DCM" ?@@
NO SUCH COMMAND, USE HELP
SYS: @@ Diffusion in dispersed systems.
SYS: @@ Diffusion couple of Fe-Cr-Ni alloys: Homogenization model
SYS: @@ This example calculates the interdiffusion in a diffusion
SYS: @@ couple between a two-phase (FCC+BCC) and a single-phase (FCC)
SYS: @@ Fe-Ni-Cr alloy. This case is from A. Engström: Scand. J. Met.,
SYS: @@ v. 24, 1995, pp.12-20. This simulation can be run with either
SYS: @@ the DISPERSED SYSTEM MODEL or the HOMOGENIZATION MODEL.
SYS: @@ Here the default HOMOGENIZATION MODEL is used and then
SYS: @@ ENTER_HOMOGENIZATION_FUNCTION should be used instead of
SYS: @@ ENTER_LABYRINTH_FUNCTION.
SYS: -----
NO SUCH COMMAND, USE HELP
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASE
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Current database: Steels/Fe-Alloys v9.0

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

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

List of references for assessed data

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

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

List of references for assessed data

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

```

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

DIC>
DIC> @@
DIC> @@ ENTER THE REGION fer
DIC> @@
DIC> enter-region fer
DIC>
DIC>
DIC> @@
DIC> @@ ENTER A DOUBLE-GEOMETRICAL GRID INTO THE REGION
DIC> @@ THIS GIVES A SHORT DISTANCE BETWEEN THE GRIDPOINTS
DIC> @@ IN THE MIDDLE OF THE REGION WHERE THE INITIAL INTERFACE IS
DIC> @@
DIC> enter-grid fer
WIDTH OF REGION /1/: 4e-3
TYPE /LINEAR/: double
NUMBER OF POINTS /50/: 200
VALUE OF R IN THE GEOMETRICAL SERIE FOR LOWER PART OF REGION: 0.97
VALUE OF R IN THE GEOMETRICAL SERIE FOR UPPER PART OF REGION: 1.03093
DIC>
DIC> @@
DIC> @@ ENTER A MATRIX PHASE IN THE REGION
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act fer matrix fcc
DIC>
DIC> @@
DIC> @@ ENTER THE START COMPOSITION FOR THE MATRIX PHASE FROM FILES
DIC> @@
DIC> enter-composition
REGION NAME : /FER/: fer
PHASE NAME: /FCC_A1/: fcc
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /CR/: cr
TYPE /LINEAR/: read d2cr.dat
PROFILE FOR /NI/: ni
TYPE /LINEAR/: read d2ni.dat
DIC>
DIC> @@
DIC> @@ ENTER FERRITE AS THE SPHEROIDAL PHASE IN THE REGION
DIC> @@ SINCE THE FRACTION OF FERRITE IS SMALL, AND THESE APPEAR
DIC> @@ AS ISOLATED PARTICLES, FERRITE IS ENTERED AS A SPHEROIDAL PHASE
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /FER/: fer
PHASE TYPE /MATRIX/: sph
PHASE NAME: /NONE/: bcc
DIC>
DIC> @@
DIC> @@ ENTER THE COMPOSITION FOR THE SPHEROIDAL PHASE
DIC> @@ USE THE EQUILIBRIUM VALUE
DIC> @@
DIC> enter-composition
REGION NAME : /FER/: fer
PHASE NAME: /FCC_A1/: bcc
USE EQUILIBRIUM VALUE /Y/: y
DIC>
DIC> @@ SELECT A HOMOGENIZATION FUNCTION
DIC> @@ IN THIS CASE THE LOWER HASHIN-SHTRIKMAN BOUND
DIC> en-ho 1
SELECTED FUNCTION IS HASHIN-SHTRIKMAN BOUND: GENERAL LOWER
DIC>
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME AND OTHER SIMULATION PARAMETERS
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 720000
AUTOMATIC TIMESTEP CONTROL /YES/: YES
MAX TIMESTEP DURING INTEGRATION /72000/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC> set-simulation-condition
NS01A PRINT CONTROL : /0/: 0
FLUX CORRECTION FACTOR : /1/: 1
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/: 2
CHECK INTERFACE POSITION /NO/: n
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/: act
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/: y
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/: 99
DEGREE OF IMPLICIT WHEN INTEGRATING PDEs (0 -> 0.5 -> 1): /.5/: 1
MAX TIMESTEP CHANGE PER TIMESTEP : /2/: 2
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /NO/: n
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/: y
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/: n
DIC>
DIC>
DIC> @@
DIC> @@ SAVE THE SETUP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC>
DIC> save exd2 y
DIC>
DIC> set-inter
--OK--
DIC>

```

exd2b-run

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exd2b\run.DCM"DIC>
DIC>
DIC> @@ exd2_run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING THE SIMULATION OF EXAMPLE D2
DIC> @@
DIC>
DIC> @@
DIC> @@ READ THE SETUP FROM FILE AND START THE SIMULATION
DIC> @@
DIC>
DIC> go d-m
TIME STEP AT TIME 0.000000E+00
DIC> read exd2
OK
DIC> sim
STARTING SIMULATION USING HOMOGENIZATION MODEL
-----
Saving results
-----
WARNING:BCC_A2 HAS NO VOLUME FRACTION, CREATING ONE
Starting time-step t0= 0.0000000 dt= 0.10000000E-06
Stage 1
Stage 2
Stage 3
Moles of elements / mole fractions in system:
CR 0.11913706E-02 / 0.29784265
FE 0.20689093E-02 / 0.51722732
NI 0.73972013E-03 / 0.18493003

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

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

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

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

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

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

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

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

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

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

output ignored...

... output resumed

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

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

```
Time-step converged t0= 683382.98 dt= 36617.016
-----
Saving results
-----
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 0.0000000
DELETING TIME-RECORD FOR TIME 0.10000000E-06
DELETING TIME-RECORD FOR TIME 805.30637
DELETING TIME-RECORD FOR TIME 1556.9256
DELETING TIME-RECORD FOR TIME 2415.9191
DELETING TIME-RECORD FOR TIME 3489.6609
DELETING TIME-RECORD FOR TIME 4348.6544
DELETING TIME-RECORD FOR TIME 5207.6478
DELETING TIME-RECORD FOR TIME 6496.1380
DELETING TIME-RECORD FOR TIME 7355.1315
DELETING TIME-RECORD FOR TIME 8214.1250
DELETING TIME-RECORD FOR TIME 9073.1184
DELETING TIME-RECORD FOR TIME 9932.1119
DELETING TIME-RECORD FOR TIME 10791.105
DELETING TIME-RECORD FOR TIME 11650.099
DELETING TIME-RECORD FOR TIME 13368.086
DELETING TIME-RECORD FOR TIME 15086.073
DELETING TIME-RECORD FOR TIME 16804.060
DELETING TIME-RECORD FOR TIME 18522.046
DELETING TIME-RECORD FOR TIME 20240.033
DELETING TIME-RECORD FOR TIME 21958.020
DELETING TIME-RECORD FOR TIME 25393.994
DELETING TIME-RECORD FOR TIME 28829.968
DELETING TIME-RECORD FOR TIME 30547.955
DELETING TIME-RECORD FOR TIME 33983.929
DELETING TIME-RECORD FOR TIME 37419.903
DELETING TIME-RECORD FOR TIME 40855.876
DELETING TIME-RECORD FOR TIME 44291.850
DELETING TIME-RECORD FOR TIME 51163.798
DELETING TIME-RECORD FOR TIME 58035.746
DELETING TIME-RECORD FOR TIME 64907.693
DELETING TIME-RECORD FOR TIME 71779.641
DELETING TIME-RECORD FOR TIME 78651.589
DELETING TIME-RECORD FOR TIME 85523.536
DELETING TIME-RECORD FOR TIME 88959.510
DELETING TIME-RECORD FOR TIME 95831.458
```

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

KEEPING TIME-RECORD FOR TIME 683382.98
AND FOR TIME 720000.00
WORKSPACE RECLAIMED

INTERPOLATION SCHEME USED THIS FRACTION OF
THE ALLOCATED MEMORY: 0.565747808406386
EFFICIENCY FACTOR: 36.6497967359925

DEALLOCATING

TIMESTEP AT 720000.000 SELECTED

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

exd2b-plot

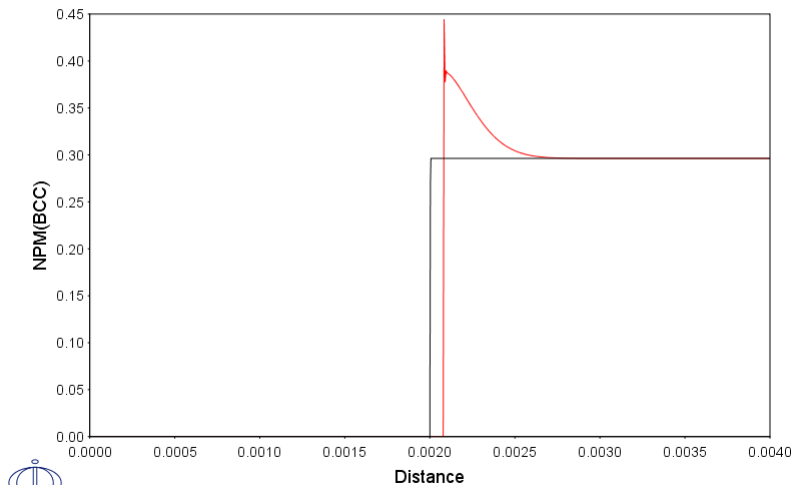
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exd2b\plot.DCM"DIC>
DIC>
DIC> @@ exd2_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE D2
DIC> @@
DIC> @@ ENTER THE DICTRA MODULE AND SPECIFY THE STORE-RESULT FILE
DIC> @@
DIC>
DIC> go d-m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

      POST PROCESSOR VERSION 1.7
      Implemented by Bjorn Jonsson

POST-1:
POST-1:
POST-1: @@
POST-1: @@ LET US FIRST SEE HOW THE FRACTION OF FERRITE HAS CHANGED
POST-1: @@ AS A RESULT OF THE DIFFUSION
POST-1: @@
POST-1: s-d-a y npm(bcc)
POST-1: s-d-a x distance global
      INFO: Distance is set as independent variable
POST-1: s-p-c time 0.720000
POST-1: set-tit Figure D2.1
POST-1: pl
```

Figure D2.1

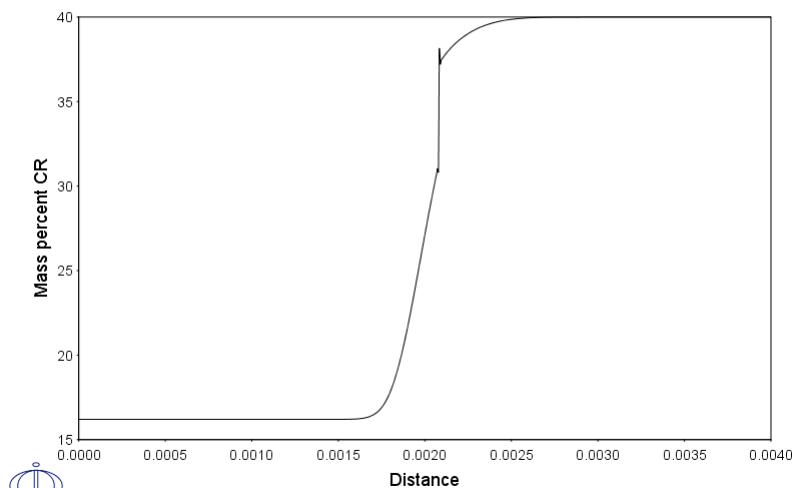
2018.02.18.22.10.24
Time=0.720000
CELL#1



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

Figure D2.2

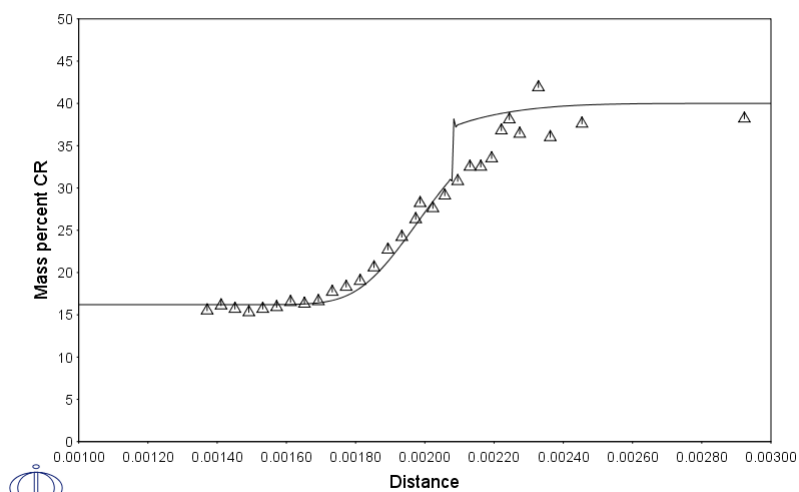
2018.02.18.22.10.26
Time = 720000
CELL #1



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

Figure D2.3

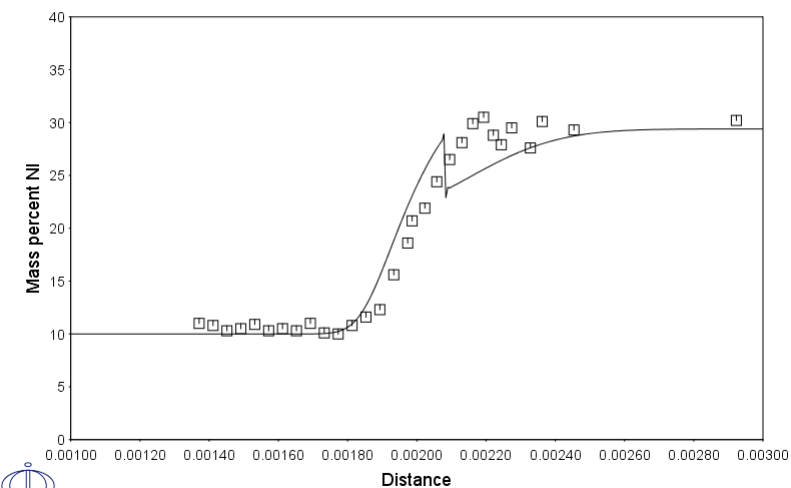
2018.02.18.22.10.27
Time = 720000
CELL #1



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

Figure D2.4

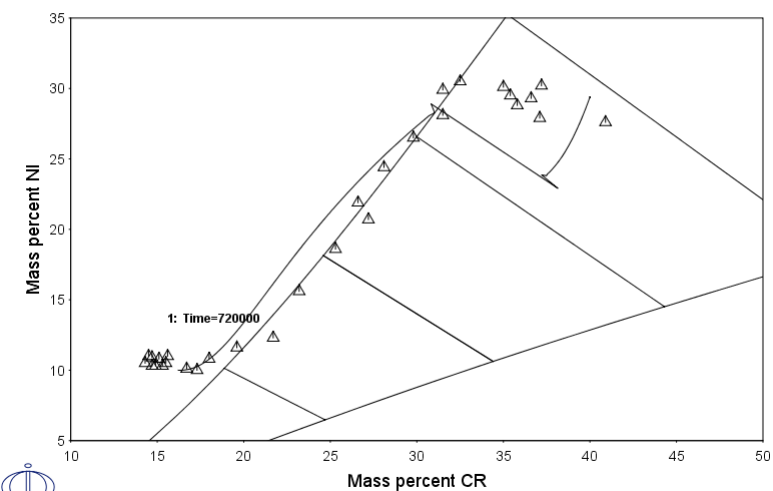
2018.02.18.22.10.29
Time = 720000
CELL #1



```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1: @@
POST-1: @@ LET US PLOT THE DIFFUSION PATH FOR THE COUPLE
POST-1: @@ WE APPEND THE TERNARY PHASE-DIAGRAM CALCULATED IN THERMO-CALC
POST-1: @@ AND THE EXPERIMENTAL DATA
POST-1: @@
POST-1: s-d-a x w-p cr
POST-1: s-d-a y w-p ni
POST-1: s-i-v dis ql
POST-1: s-p-c time last
POST-1:
POST-1: app y exd2.exp
PROLOGUE NUMBER: /1/: 1
DATASET NUMBER(s): /-1/: 6 7 8
POST-1:
POST-1: s-s-s x n 10 50
POST-1: s-s-s y n 5 35
POST-1:
POST-1: set-tit Figure D2.5
POST-1: pl
```

Figure D2.5

2018.02.18.22.10.30
Time = 720000
CELL #1



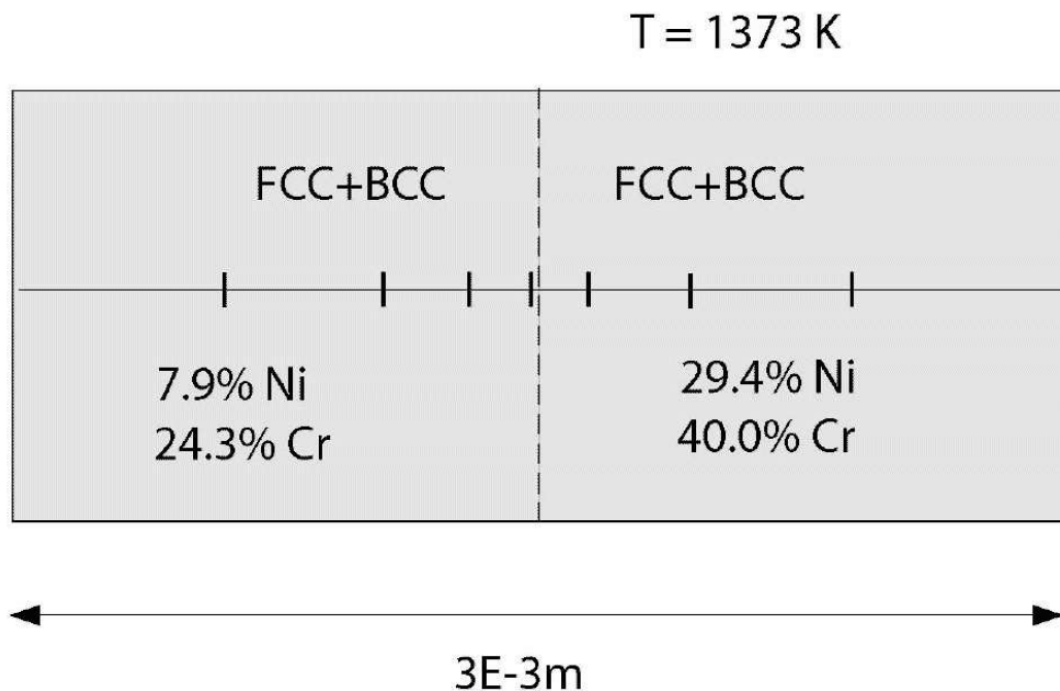
```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1: set-interactive
--OK--
POST-1:
```




Example exd3

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

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



exd3-setup

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

```
SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exd3\setup.DCM"SYS: ?@@
NO SUCH COMMAND, USE HELP
SYS: @@ Diffusion in dispersed systems.
SYS: @@ Diffusion couple of Fe-Cr-Ni alloys: Homogenization model
SYS: @@ This example uses the homogenization model. It is taken from
SYS: @@ H. Larsson and A. Engström, Acta. Mater. v.54 (2006), pp. 2431-2439.
SYS: @@ Experimental data from A. Engström, Scand J Metall, v.243 (1995), p.12.
SYS: @@ The homogenization model can be used for multiphase simulations
SYS: @@ like the dispersed system model, but unlike the dispersed system model
SYS: @@ there is no need to have a single continuous matrix phase and, furthermore,
SYS: @@ there is no need to limit the size of time-steps.
SYS: @@ The set-up is performed in the same manner as for the dispersed system
SYS: @@ model, which means that a certain phase is entered as the matrix phase
SYS: @@ and the other phases are entered as spheroidal, but the choice of matrix
SYS: @@ phase will not affect the simulation.
SYS: -----
NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exd3_setup.DCM
SYS:
SYS:
SYS: go da
THERMODYNAMIC DATABASE module
Current database: Steels/Fe-Alloys v9.0

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

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

List of references for assessed data

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

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

List of references for assessed data

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

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

```

DIC> ent-reg
REGION NAME : fecrni
DIC>
DIC> ent-grid
REGION NAME : /FECRNI/: fecrni
WIDTH OF REGION /1/: 3e-3
TYPE /LINEAR/: double
NUMBER OF POINTS /50/: 60
VALUE OF R IN THE GEOMETRICAL SERIE FOR LOWER PART OF REGION: 0.85
VALUE OF R IN THE GEOMETRICAL SERIE FOR UPPER PART OF REGION: 1.15
DIC>
DIC> ent-ph
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /FECRNI/: fecrni
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC> ent-ph
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /FECRNI/: fecrni
PHASE TYPE /MATRIX/: sph
PHASE NAME: /NONE/: bcc
DIC>
DIC> ent-comp
REGION NAME : /FECRNI/: fecrni
PHASE NAME: /FCC_A1/: fcc#1
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: m-f
PROFILE FOR /CR/: cr
TYPE /LINEAR/: read cr.dat
PROFILE FOR /NI/: ni
TYPE /LINEAR/: read ni.dat
DIC>
DIC> ent-comp
REGION NAME : /FECRNI/: fecrni
PHASE NAME: /FCC_A1/: bcc
USE EQUILIBRIUM VALUE /Y/: y
DIC>
DIC> se-si-ti
END TIME FOR INTEGRATION /.1/: 3.6e5
AUTOMATIC TIMESTEP CONTROL /YES/: yes
MAX TIMESTEP DURING INTEGRATION /36000/: 3.6e4
INITIAL TIMESTEP : /1E-07/: 1
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/: 1e-7
DIC>
DIC> @@ SIMULATIONS ARE FASTER WHEN THE RESULTS ARE NOT SAVED
DIC> @@ FOR EVERY TIME STEP
DIC> s-s-c
NS01A PRINT CONTROL : /0/: 0
FLUX CORRECTION FACTOR : /1/: 1
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIFF: /2/: 2
CHECK INTERFACE POSITION /NO/: n
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/: act
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/: y
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/: 99
DEGREE OF IMPLICITY WHEN INTEGRATING PDES (0 -> 0.5 -> 1): /.5/: .5
MAX TIMESTEP CHANGE PER TIMESTEP : /2/: 2
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /NO/: n
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIFF /YES/: y
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/:
DIC>
DIC> @@ There are a several options available for the homogenization
DIC> @@ model. There is also an interpolation scheme that may reduce
DIC> @@ simulation times. However, for this example, the default settings
DIC> @@ are kept and the interpolation scheme is turned off.
DIC> @@
DIC> homogen yes yes
INFO: HOMOGENIZATION MODEL ENABLED
DIC>
DIC> @@ There are a large number of homogenization functions
DIC> @@ available. These determine how the average kinetics
DIC> @@ of the multiphase mixture is evaluated. For this example
DIC> @@ the General lower Hashin-Shtrikman bound is a good choice.
DIC> en-ho
ENTER HOMOGENIZATION FUNCTION # /5/: 1
SELECTED FUNCTION IS HASHIN-SHTRIKMAN BOUND: GENERAL LOWER
DIC>
DIC>
DIC>
DIC> save exd3 Y
DIC>
DIC>
DIC> set-inter
--OK--
DIC>

```

exd3-run

DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exd3\run.DCM"DIC>

DIC>

DIC> @@ exd3_run.DCM

DIC>

DIC> @@

DIC> @@ READ THE SETUP FROM FILE AND START THE SIMULATION

DIC> @@

DIC>

DIC> go d-m

TIME STEP AT TIME 0.00000E+00

DIC> read exd3

OK

DIC>

DIC> sim

STARTING SIMULATION USING HOMOGENIZATION MODEL

Saving results

WARNING:BCC_A2 HAS NO VOLUME FRACTION, CREATING ONE

Starting time-step t0= 0.0000000 dt= 1.0000000

Stage 1

Evaluating Jacobian

Iteration # 1 sum residual **2: 0.91200732E-03

Stage 2

Stage 3

Moles of elements / mole fractions in system:

CR 0.10202298E-02 / 0.34007660

FE 0.14697902E-02 / 0.48993007

NI 0.50997997E-03 / 0.16999332

Time-step converged t0= 0.0000000 dt= 1.0000000

Saving results

Starting time-step t0= 1.0000000 dt= 2.0000000

Stage 1

Iteration # 1 sum residual **2: 0.49065622E-03

Stage 2

Stage 3

Moles of elements / mole fractions in system:

CR 0.10202298E-02 / 0.34007660

FE 0.14697902E-02 / 0.48993007

NI 0.50997997E-03 / 0.16999332

Time-step converged t0= 1.0000000 dt= 2.0000000

Starting time-step t0= 3.0000000 dt= 4.0000000

Stage 1

Iteration # 1 sum residual **2: 0.35181588E-03

Stage 2

Stage 3

Moles of elements / mole fractions in system:

CR 0.10202298E-02 / 0.34007660

FE 0.14697902E-02 / 0.48993007

NI 0.50997997E-03 / 0.16999332

Time-step converged t0= 3.0000000 dt= 4.0000000

Starting time-step t0= 7.0000000 dt= 8.0000000

Stage 1

Iteration # 1 sum residual **2: 0.32271218E-02

Stage 2

Stage 3

Moles of elements / mole fractions in system:

CR 0.10202298E-02 / 0.34007660

FE 0.14697902E-02 / 0.48993007

NI 0.50997997E-03 / 0.16999332

Time-step converged t0= 7.0000000 dt= 8.0000000

Starting time-step t0= 15.000000 dt= 16.000000

Stage 1

Iteration # 1 sum residual **2: 0.82413380

Stage 2

Stage 3

Moles of elements / mole fractions in system:

CR 0.10202298E-02 / 0.34007660

FE 0.14697902E-02 / 0.48993007

NI 0.50997997E-03 / 0.16999332

Time-step converged t0= 15.000000 dt= 16.000000

Starting time-step t0= 31.000000 dt= 32.000000

Stage 1

Iteration # 1 sum residual **2: 22.492550

Iteration # 2 sum residual **2: 0.41246053E-02

Stage 2

Iteration # 1 sum residual **2: 0.24687442E-02

Stage 3

Moles of elements / mole fractions in system:

CR 0.10202298E-02 / 0.34007660

FE 0.14697902E-02 / 0.48993007

NI 0.50997997E-03 / 0.16999332

Time-step converged t0= 31.000000 dt= 32.000000

Starting time-step t0= 63.000000 dt= 64.000000

Stage 1

Iteration # 1 sum residual **2: 318.00997

Iteration # 2 sum residual **2: 0.11435874E-01

Stage 2

Iteration # 1 sum residual **2: 0.11990052E-02

Stage 3

Moles of elements / mole fractions in system:

CR 0.10202298E-02 / 0.34007660

FE 0.14697902E-02 / 0.48993007

NI 0.50997997E-03 / 0.16999332

Time-step converged t0= 63.000000 dt= 64.000000

Starting time-step t0= 127.00000 dt= 128.00000

Stage 1

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

```
Time-step converged t0= 127.00000 dt= 128.00000
```

```
-----
Starting time-step t0= 255.00000 dt= 256.00000
```

```
Stage 1
Iteration # 1 sum residual **2: 24933.971
Iteration # 2 sum residual **2: 200.02314
Iteration # 3 sum residual **2: 2.7825925
Iteration # 4 sum residual **2: 0.14360047E-02
Stage 2
Iteration # 1 sum residual **2: 6.6165731
```

output ignored...

... output resumed

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

```
Time-step converged t0= 311295.00 dt= 16384.000
```

```
-----
Saving results
```

```
-----
Starting time-step t0= 327679.00 dt= 16384.000
```

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

```
Time-step converged t0= 327679.00 dt= 16384.000
```

```
-----
Saving results
```

```
-----
Starting time-step t0= 344063.00 dt= 15937.000
```

```
Stage 1
Iteration # 1 sum residual **2: 10895.376
Iteration # 2 sum residual **2: 147.96473
Iteration # 3 sum residual **2: 1.3594067
Iteration # 4 sum residual **2: 0.92703049E-02
Stage 2
Iteration # 1 sum residual **2: 7306.4604
Iteration # 2 sum residual **2: 1629.4028
Iteration # 3 sum residual **2: 366.42901
Iteration # 4 sum residual **2: 82.096557
Iteration # 5 sum residual **2: 18.503682
Iteration # 6 sum residual **2: 3.9577610
Iteration # 7 sum residual **2: 0.37067955
Stage 3
Iteration # 1 sum residual **2: 22370.989
Iteration # 2 sum residual **2: 4974.7263
Iteration # 3 sum residual **2: 1104.1227
Iteration # 4 sum residual **2: 243.11191
Iteration # 5 sum residual **2: 52.266894
Iteration # 6 sum residual **2: 10.405947
Iteration # 7 sum residual **2: 1.5400717
Moles of elements / mole fractions in system:
CR 0.10202298E-02 / 0.34007660
FE 0.14697902E-02 / 0.48993007
```

NI 0.50997997E-03 / 0.16999332

Time-step converged t0= 344063.00 dt= 15937.000

Saving results

MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE

DELETING TIME-RECORD FOR TIME	0.0000000
DELETING TIME-RECORD FOR TIME	1.0000000
DELETING TIME-RECORD FOR TIME	511.00000
DELETING TIME-RECORD FOR TIME	1023.0000
DELETING TIME-RECORD FOR TIME	1535.0000
DELETING TIME-RECORD FOR TIME	2047.0000
DELETING TIME-RECORD FOR TIME	3071.0000
DELETING TIME-RECORD FOR TIME	4095.0000
DELETING TIME-RECORD FOR TIME	6143.0000
DELETING TIME-RECORD FOR TIME	8191.0000
DELETING TIME-RECORD FOR TIME	10239.000
DELETING TIME-RECORD FOR TIME	12287.000
DELETING TIME-RECORD FOR TIME	16383.000
DELETING TIME-RECORD FOR TIME	24575.000
DELETING TIME-RECORD FOR TIME	32767.000
DELETING TIME-RECORD FOR TIME	40959.000
DELETING TIME-RECORD FOR TIME	49151.000
DELETING TIME-RECORD FOR TIME	65535.000
DELETING TIME-RECORD FOR TIME	81919.000
DELETING TIME-RECORD FOR TIME	98303.000
DELETING TIME-RECORD FOR TIME	114687.00
DELETING TIME-RECORD FOR TIME	131071.00
DELETING TIME-RECORD FOR TIME	147455.00
DELETING TIME-RECORD FOR TIME	163839.00
DELETING TIME-RECORD FOR TIME	180223.00
DELETING TIME-RECORD FOR TIME	196607.00
DELETING TIME-RECORD FOR TIME	212991.00
DELETING TIME-RECORD FOR TIME	229375.00
DELETING TIME-RECORD FOR TIME	245759.00
DELETING TIME-RECORD FOR TIME	262143.00
DELETING TIME-RECORD FOR TIME	278527.00
DELETING TIME-RECORD FOR TIME	294911.00
DELETING TIME-RECORD FOR TIME	311295.00
DELETING TIME-RECORD FOR TIME	327679.00

KEEPING TIME-RECORD FOR TIME 344063.00
AND FOR TIME 360000.00
WORKSPACE RECLAIMED

INTERPOLATION SCHEME USED THIS FRACTION OF
THE ALLOCATED MEMORY: 0.381320622645912
EFFICIENCY FACTOR: 7.09082167832168

DEALLOCATING

TIMESTEP AT 360000.000 SELECTED

DIC>

DIC>

DIC> set-inter

--OK--

DIC>

exd3-plot

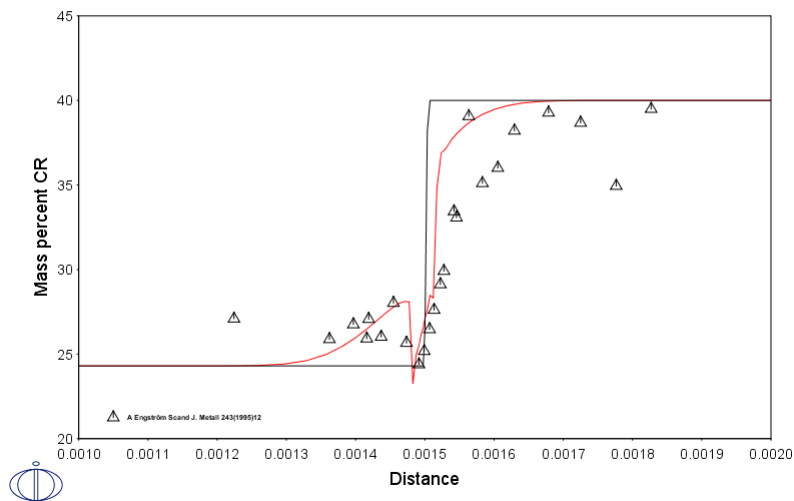
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exd3\plot.DCM"DIC>
DIC>
DIC> @@ exd3_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE d3
DIC> @@
DIC> @@ ENTER THE DICTRA MODULE AND SPECIFY THE STORE-RESULT FILE
DIC> @@
DIC>
DIC> go d-m
      TIME STEP AT TIME 3.60000E+05
DIC> read exd3
      OK
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA POST PROCESSOR
DIC> @@
DIC> post

      POST PROCESSOR VERSION 1.7
      Implemented by Bjorn Jonsson
```

```
POST-1:
POST-1:
POST-1: @@
POST-1: @@ First study the composition profiles of Cr and Ni
POST-1: @@
POST-1: s-d-a x distance global
      INFO: Distance is set as independent variable
POST-1: s-d-a y w-p Cr
POST-1: s-p-c time 0.360000
POST-1: set-tit Figure D3.1
POST-1:
POST-1: app yes k5k7cr.exp 0; 1
POST-1:
POST-1: s-s-s x n 1e-3 2e-3
POST-1:
POST-1: s-s-s y n 20 45
POST-1:
POST-1: plot
```

Figure D3.1

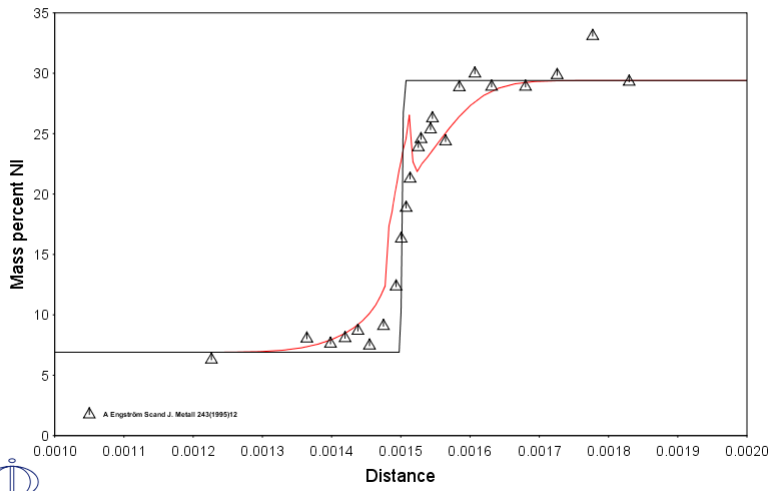
2018.02.18.22.13.34
Time = 0.360000
CELL #1



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

Figure D3.2

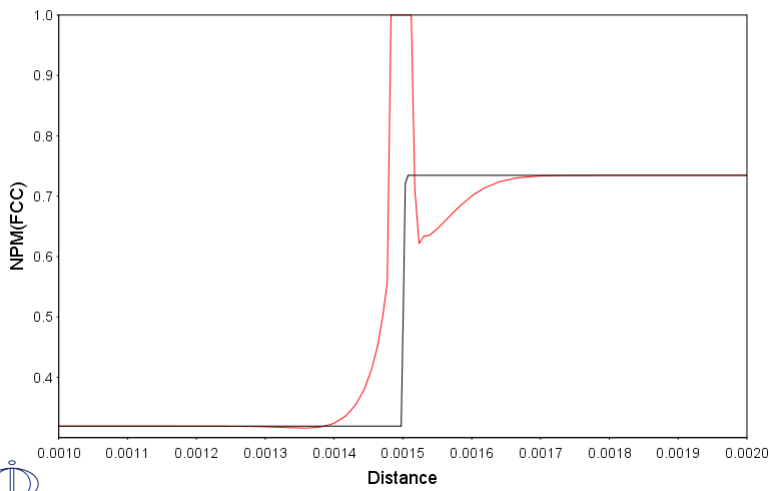
2018.02.18.22.13.35
Time = 0.360000
CELL #1



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

Figure D3.3

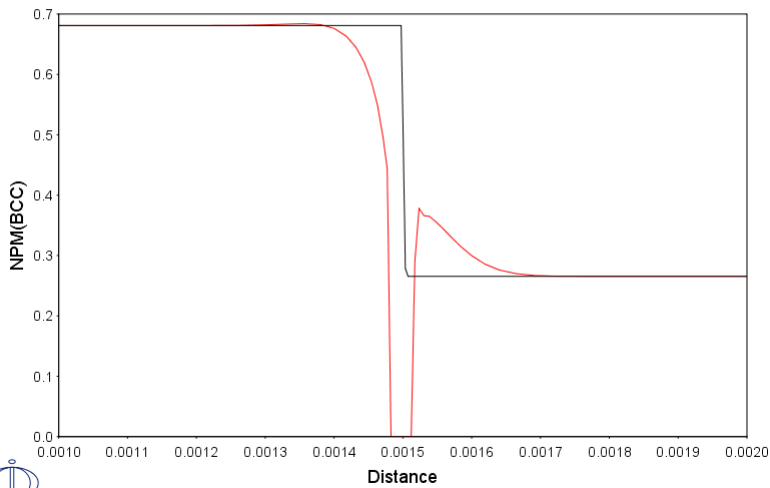
2018.02.18.22.13.35
Time = 0.360000
CELL #1



POST-1:
POST-1: @?<_hit_return_to_continue_>
POST-1: s-d-a y npm(bcc)
POST-1: set-tit Figure D3.4
POST-1: plot

Figure D3.4

2018.02.18.22.13.36
Time = 0.360000
CELL #1

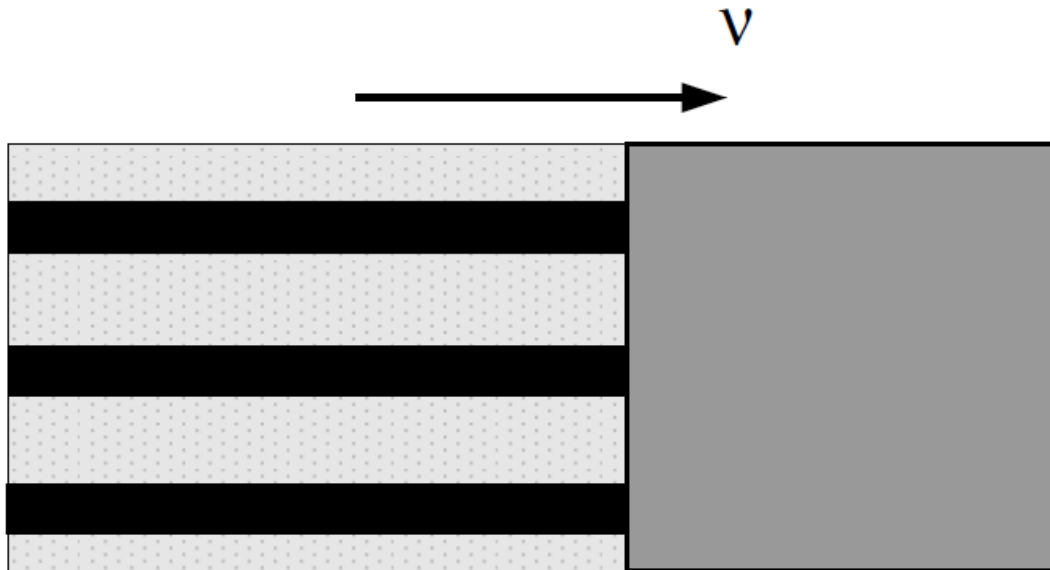


POST-1:


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



Cooperative Growth

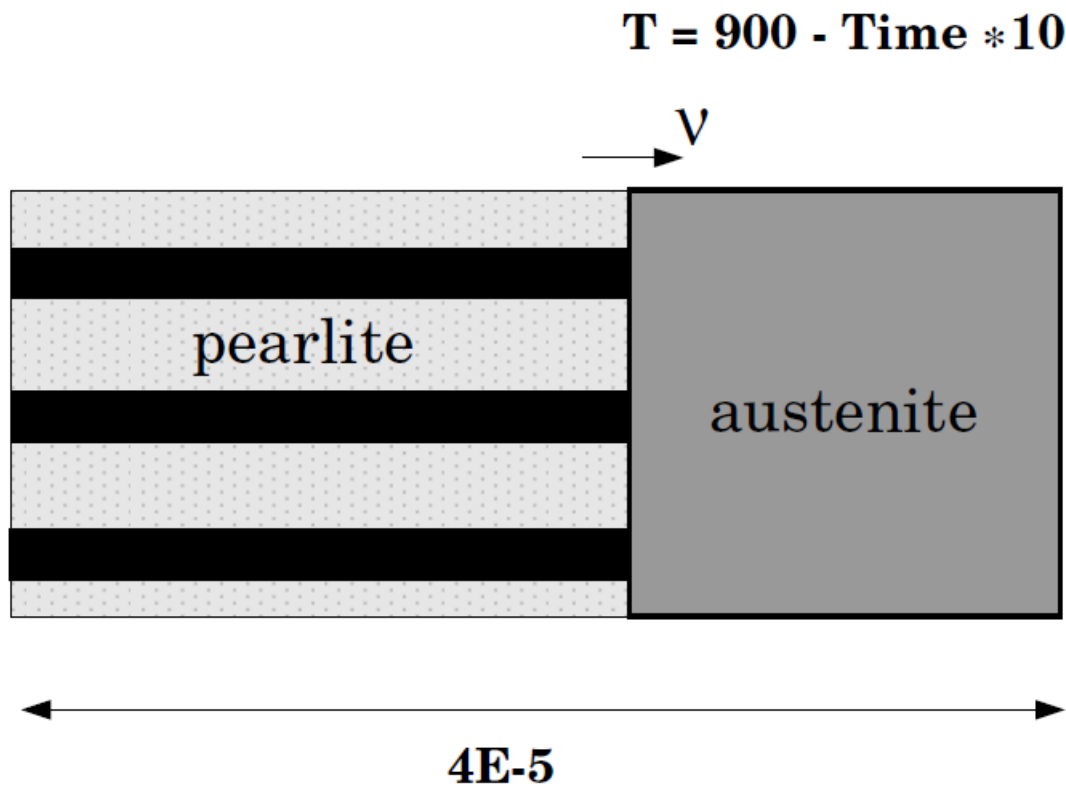




Example exe1

Growth of pearlite in an Fe-Mn-C alloy

This is an example of pearlite growth in an Fe-0.50wt%C - 0.91wt%Mn steel.



exel-setup

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

```
SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exel\setup.DCM" ?@@
NO SUCH COMMAND, USE HELP
SYS: @@ Cooperative growth.
SYS: @@ Growth of pearlite in an Fe-Mn-C alloy
SYS: @@ An example of pearlite growth in an Fe-0.50wt%C-0.91wt%Mn steel.
SYS: -----
NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exel_setup.DCM
SYS:
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASE
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Current database: Steels/Fe-Alloys v9.0

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

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

List of references for assessed data

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

VA  DEFINED
APP: def-sys fe c mn
FE          C          MN
DEFINED
APP: rej-ph /all
BCC_A2      CEMENTITE      FCC_A1
FE4N_LP1    HCP_A3        LIQUID:L
REJECTED
APP: rest-ph bcc,fcc,cem
BCC_A2      FCC_A1        CEMENTITE
RESTORED
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

List of references for assessed data

'This parameter has not been assessed'
```

```

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

DIC>
DIC> @@
DIC> @@ ENTER A REGION
DIC> @@
DIC> enter-reg pearlite
DIC>
DIC> @@
DIC> @@ ENTER A SMALL INITIAL SIZE OF THE GRID IN THE 'PEARLITE' REGION
DIC> @@
DIC> enter-grid pearlite 5e-10 lin 5
DIC>
DIC> @@
DIC> @@ ENTER INTO THE 'PEARLITE' REGION THE PHASES 'BCC' AND 'CEM' AND SPECIFY
DIC> @@ THAT ARE PRESENT IN THE FORM OF A 'LAMELLAR AGGREGATE. SET THE STATUS
DIC> @@ TO 'ACTIVE'. SEVERAL PROMPTS FOLLOW ABOUT THE VALUES OF THE PARAMETERS
DIC> @@ IN THE PEARLITE GROWTH MODEL, FOR EXAMPLE AS SURFACE TENSION, OPTIMUM
DIC> @@ GROWTH RATE FACTOR, AND BOUNDARY DIFFUSION COEFFICIENTS.
DIC> @@
DIC> @@ CARBON(C) IS TREATED IN A SPECIAL WAY. IF 'AUTOMATIC' IS ENTERED
DIC> @@ THE DIFFUSION OF C IS CALCULATED ACCORDING TO AN EQUATION FOR
DIC> @@ MIXED BOUNDARY AND VOLUME DIFFUSION. YOU CAN CHOOSE BETWEEN
DIC> @@ MANUAL OR AUTOMATIC START VALUES FOR ALL VARIABLES EXCEPT THE GROWTH
DIC> @@ RATE. IN THIS EXAMPLE WE WILL TRY 1E-6
DIC> @@
DIC> @@ FOR MORE INFORMATION ABOUT THE PEARLITE GROWTH MODEL SEE
DIC> @@ B. JONSSON: TRITA-MAC-0478, 1992 (ROYAL INSTITUTE OF TECHNOLOGY)
DIC> @@ STOCKHOLM, SWEDEN, 1992.
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /PEARLITE/: pearlite
PHASE TYPE /MATRIX/: lam

Eutectiod reaction is "GAMMA" ==> "ALPHA" + "BETA"

Enter name of "ALPHA" phase /BCC_A2/: bcc_a2
Enter name of "BETA" phase /CEMENTITE/: cementite
Enter name of "GAMMA" phase /FCC_A1/: fcc_a1
Enter "ALPHA"/"BETA" surface tension
LOW TIME LIMIT /0/: 0
Surface tension(T,P,TIME)= 1;
HIGH TIME LIMIT /*/: 1000
ANY MORE RANGES /N/: N
Enter "ALPHA"/"GAMMA" surface tension
LOW TIME LIMIT /0/: 0
Surface tension(T,P,TIME)= 1;
HIGH TIME LIMIT /*/: 1000
ANY MORE RANGES /N/: N
Enter "BETA"/"GAMMA" surface tension
LOW TIME LIMIT /0/: 0
Surface tension(T,P,TIME)= 1;
HIGH TIME LIMIT /*/: 1000
ANY MORE RANGES /N/: N
Optimum growth condition factor /2/: 2
Name of dependent element /FE/: fe
INPUT OF DIFFUSION DATA
Growth model (VOLUME/BOUNDARY/KIRKALDY) for element C /BOUNDARY/: boundary
DF(C) = /value/AUTOMATIC/MIXED/: auto
Growth model (VOLUME/BOUNDARY/KIRKALDY) for element MN /BOUNDARY/: boundary
DF(MN) = /value/MIXED/: 5.4e-14
DQ(MN): 155000
Automatic start values for the S0 determination /Y/: Y
Growth rate V: 1E-6
Automatic start values on other variables /Y/: Y
DIC>
DIC> @@
DIC> @@ INITIATE THE COMPOSITION RECORDS FOR THE 'PEARLITE'
DIC> @@
DIC> enter-composition
REGION NAME : /PEARLITE/: pearlite
DIC>
DIC> @@
DIC> @@ NOW CONTINUE BY DEFINING A MATRIX PHASE INTO WHICH THE PEARLITE
DIC> @@ WILL GROW. START BY ENTERING A REGION NAME, 'AUSTENITE'
DIC> @@
DIC> enter-region austenite
ATTACH TO REGION NAMED /PEARLITE/:
ATTACHED TO THE RIGHT OF PEARLITE /YES/:
DIC> @@
DIC> @@ SPECIFY WHAT PHASE 'FCC' WILL BE PRESENT IN THE 'AUSTENITE' REGION
DIC> @@ AND WHAT TYPE OF PHASE 'MATRIX' IT IS AND ITS INITIAL STATE 'ACTIVE'
DIC> @@
DIC> enter-phase act austenite matrix fcc
DIC>
DIC> @@
DIC> @@ WE ALSO NEED TO HAVE A SPATIAL GRID IN THE 'AUSTENITE' REGION.

```

```

DIC> @@ CHOSE SIZE '4E-5' GRIDTYPE 'GEOMETRICAL', '30' GRIDPOINTS AND '1.5'
DIC> @@ AS VALUES FOR THE GEOMETRICAL FACTOR OF THE GRID.
DIC> @@
DIC> enter-grid austenite 4e-5 geo 30 1.5
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL CONCENTRATION PROFILES IN THE 'FCC' PHASE OF THE
DIC> @@ 'AUSTENITE' REGION. CONCENTRATIONS MUST BE GIVEN IN Y-FRACTIONS.
DIC> @@
DIC> enter-composition
REGION NAME : /AUSTENITE/: austenite
PHASE NAME: /FCC_A1/: fcc
DEPENDENT COMPONENT ? /MN/: fe
COMPOSITION TYPE /MOLE_FRACTION/: site-fraction
PROFILE FOR MN
TYPE /LINEAR/: lin 9.29232973E-3 9.29232973E-3
PROFILE FOR C
TYPE /LINEAR/: lin 2.3384332E-2 2.3384332E-2
DIC>
DIC> @@
DIC> @@ THE MATRIX PHASE IS NOW COMPLETE.
DIC> @@
DIC>
DIC> @@
DIC> @@ SPECIFY A SPHERICAL '2' GEOMETRY
DIC> @@
DIC> enter-geo 2
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 5
AUTOMATIC TIMESTEP CONTROL /YES/: YES
MAX TIMESTEP DURING INTEGRATION /.5/: 0.1
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exel Y
DIC>
DIC> set-inter
--OK--
DIC>

```

exel-run

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exel\run.DCM"DIC>
DIC>
DIC> @@ exel_run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING EXAMPLE e1
DIC> @@
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA MONITOR
DIC> @@
DIC> go d-m
TIME STEP AT TIME 0.00000E+00
DIC>
DIC> @@
DIC> @@ READ SETUP FROM FILE
DIC> @@
DIC> read exel
OK
DIC>
DIC> @@
DIC> @@ START THE SIMULATION
DIC> @@
DIC> simulate
Trying old scheme
U-FRACTION IN SYSTEM: C = .0233843320030518 FE = .990707670399293
MN = .0092923297312127
TOTAL SIZE OF SYSTEM: 2.68092626329E-13 [m^3]
U-FRACTION IN SYSTEM: C = .0233843320030518 FE = .990707670399293
MN = .0092923297312127
TOTAL SIZE OF SYSTEM: 2.68092626329E-13 [m^3]
17 GRIDPOINT(S) ADDED TO CELL #1 REGION: AUSTENITE
TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.0000000
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.76465982E-05 AND 0.76465982E-05
POSITION OF INTERFACE PEARLITE / AUSTENITE IS 0.50076466E-09
U-FRACTION IN SYSTEM: C = .0233843320030518 FE = .990707670399294
MN = .00929232973121271
TOTAL SIZE OF SYSTEM: 2.68092626329E-13 [m^3]
10 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: AUSTENITE

CPU time used in timestep 0 seconds
4 GRIDPOINT(S) ADDED TO CELL #1 REGION: AUSTENITE
TIME = 0.10010000E-03 DT = 0.10000000E-03 SUM OF SQUARES = 0.0000000
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.76468335E-05 AND 0.76468335E-05
POSITION OF INTERFACE PEARLITE / AUSTENITE IS 0.12654480E-08
U-FRACTION IN SYSTEM: C = .0233843320030518 FE = .990707670399295
MN = .00929232973121271
TOTAL SIZE OF SYSTEM: 2.68092626329E-13 [m^3]
CPU time used in timestep 0 seconds
1 GRIDPOINT(S) REMOVED FROM CELL# 1 REGION # 1
TIME = 0.13026424E-02 DT = 0.12025424E-02 SUM OF SQUARES = 0.0000000
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.76496630E-05 AND 0.76496630E-05
POSITION OF INTERFACE PEARLITE / AUSTENITE IS 0.10464492E-07
U-FRACTION IN SYSTEM: C = .0233843320030518 FE = .990707670399295
MN = .00929232973121271
TOTAL SIZE OF SYSTEM: 2.68092626329E-13 [m^3]
CPU time used in timestep 0 seconds
2 GRIDPOINT(S) REMOVED FROM CELL# 1 REGION # 1
TIME = 0.37077272E-02 DT = 0.24050848E-02 SUM OF SQUARES = 0.0000000
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.76553232E-05 AND 0.76553232E-05
POSITION OF INTERFACE PEARLITE / AUSTENITE IS 0.28876193E-07
U-FRACTION IN SYSTEM: C = .0233843320030517 FE = .990707670399294
MN = .0092923297312127
TOTAL SIZE OF SYSTEM: 2.68092626329E-13 [m^3]
CPU time used in timestep 0 seconds
1 GRIDPOINT(S) REMOVED FROM CELL# 1 REGION # 1
TIME = 0.85178967E-02 DT = 0.48101695E-02 SUM OF SQUARES = 0.0000000
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.76666480E-05 AND 0.76666480E-05
POSITION OF INTERFACE PEARLITE / AUSTENITE IS 0.65754070E-07
U-FRACTION IN SYSTEM: C = .0233843320030517 FE = .990707670399295
MN = .0092923297312127
TOTAL SIZE OF SYSTEM: 2.68092626329E-13 [m^3]
CPU time used in timestep 0 seconds
1 GRIDPOINT(S) REMOVED FROM CELL# 1 REGION # 1
TIME = 0.18138236E-01 DT = 0.96203391E-02 SUM OF SQUARES = 0.0000000
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.76893156E-05 AND 0.76893156E-05
POSITION OF INTERFACE PEARLITE / AUSTENITE IS 0.13972789E-06
U-FRACTION IN SYSTEM: C = .0233843320030517 FE = .990707670399294
MN = .00929232973121269
TOTAL SIZE OF SYSTEM: 2.68092626329E-13 [m^3]
CPU time used in timestep 0 seconds
1 GRIDPOINT(S) REMOVED FROM CELL# 1 REGION # 1
TIME = 0.37378914E-01 DT = 0.19240678E-01 SUM OF SQUARES = 0.0000000
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.77347217E-05 AND 0.77347217E-05
POSITION OF INTERFACE PEARLITE / AUSTENITE IS 0.28854918E-06
U-FRACTION IN SYSTEM: C = .0233843320030516 FE = .990707670399294
MN = .00929232973121269
TOTAL SIZE OF SYSTEM: 2.68092626329E-13 [m^3]
CPU time used in timestep 0 seconds
1 GRIDPOINT(S) REMOVED FROM CELL# 1 REGION # 1
TIME = 0.75860270E-01 DT = 0.38481356E-01 SUM OF SQUARES = 0.0000000
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.78258159E-05 AND 0.78258159E-05
POSITION OF INTERFACE PEARLITE / AUSTENITE IS 0.58969719E-06
U-FRACTION IN SYSTEM: C = .0233843320030516 FE = .990707670399294
MN = .00929232973121268
TOTAL SIZE OF SYSTEM: 2.68092626329E-13 [m^3]
CPU time used in timestep 0 seconds
1 GRIDPOINT(S) REMOVED FROM CELL# 1 REGION # 1
TIME = 0.15282298 DT = 0.76962713E-01 SUM OF SQUARES = 0.0000000
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.80091146E-05 AND 0.80091146E-05
POSITION OF INTERFACE PEARLITE / AUSTENITE IS 0.12061004E-05
U-FRACTION IN SYSTEM: C = .0233843320030516 FE = .990707670399294
MN = .00929232973121267
TOTAL SIZE OF SYSTEM: 2.68092626329E-13 [m^3]
CPU time used in timestep 0 seconds
TIME = 0.25282298 DT = 0.10000000 SUM OF SQUARES = 0.0000000
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.82494350E-05 AND 0.82494350E-05
POSITION OF INTERFACE PEARLITE / AUSTENITE IS 0.20310439E-05
U-FRACTION IN SYSTEM: C = .0233843320030516 FE = .990707670399294
MN = .00929232973121267
TOTAL SIZE OF SYSTEM: 2.68092626329E-13 [m^3]
CPU time used in timestep 0 seconds
1 GRIDPOINT(S) REMOVED FROM CELL# 1 REGION # 1
```

```
TIME = 0.35282298 DT = 0.10000000 SUM OF SQUARES = 0.0000000
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.84921077E-05 AND 0.84921077E-05
POSITION OF INTERFACE PEARLITE / AUSTENITE IS 0.28802546E-05
U-FRACTION IN SYSTEM: C = .0233843320030515 FE = .990707670399295
MN = .00929232973121269
TOTAL SIZE OF SYSTEM: 2.68092626329E-13 [m^3]
CPU time used in timestep 0 seconds
TIME = 0.45282298 DT = 0.10000000 SUM OF SQUARES = 0.0000000
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.87370419E-05 AND 0.87370419E-05
POSITION OF INTERFACE PEARLITE / AUSTENITE IS 0.37539588E-05
U-FRACTION IN SYSTEM: C = .0233843320030515 FE = .990707670399294
MN = .00929232973121275
TOTAL SIZE OF SYSTEM: 2.68092626329E-13 [m^3]
```

output ignored...

... output resumed

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

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



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

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

TIMESTEP AT      5.0000000      SELECTED

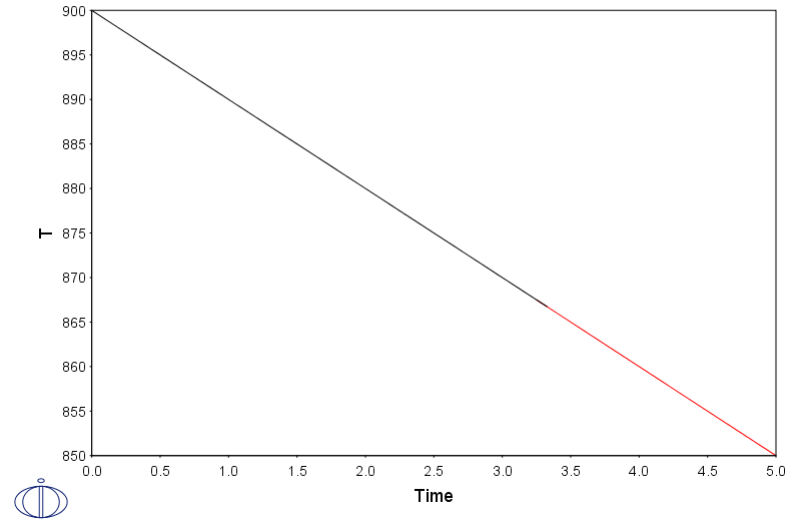
DIC>
DIC> @@
DIC> @@ THE SIMULATION IS FINISHED
DIC> @@
DIC>
DIC> set-inter
--OK--
DIC>
```

exel-plot

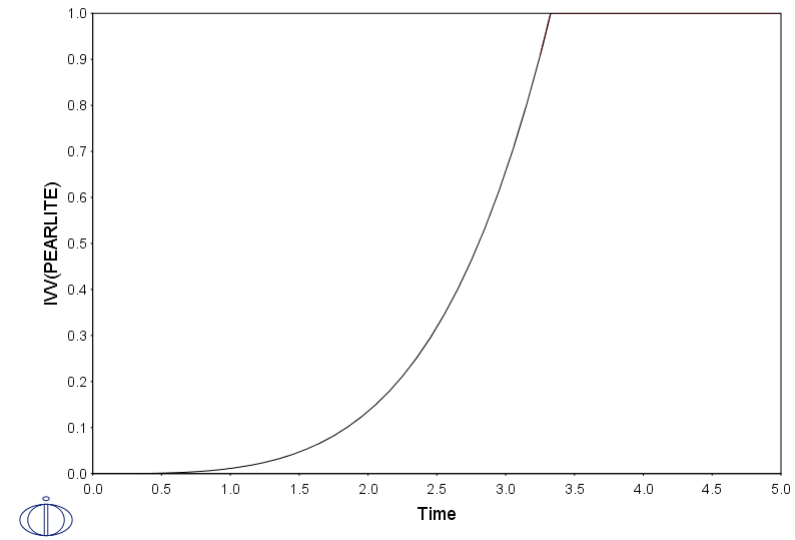
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exel\plot.DCM"DIC>
DIC>
DIC> @@ exel_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE e1
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
    TIME STEP AT TIME 5.00000E+00
DIC> read exel
    OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post

    POST PROCESSOR VERSION 1.7
    Implemented by Bjorn Jonsson
```

```
POST-1:
POST-1: @@
POST-1: @@ PLOT THE TEMPERATURE AS A FUNCTION OF TIME
POST-1: @@
POST-1: s-d-a x time
    INFO: Time is set as independent variable
POST-1: s-d-a y t
POST-1: s-p-c interface first
POST-1:
POST-1: plot
    20180218221640
    "FIRST" INTERFACE OF SYSTEM
    CELL#1
```



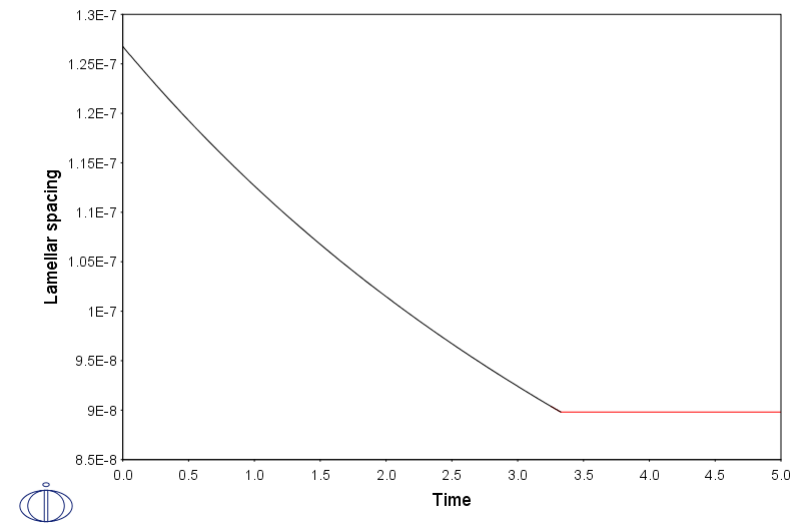
```
POST-1:
POST-1:
POST-1: Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ NOW PLOT THE FRACTION OF PEARLITE VS. TIME
POST-1: @@
POST-1: s-d-a y ivv(pearlite)
POST-1:
POST-1: plot
```



```

POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ PLOT THE LAMELLAR SPACING AS A FUNCTION OF TIME
POST-1: @@
POST-1: s-d-a
POST-1: AXIS (X, Y OR Z) : y
POST-1: VARIABLE : lamellar-sp
POST-1: IN REGION: /*/: pearlite
POST-1:
POST-1: s-p-c
POST-1: CONDITION /INTEGRAL/: interface
POST-1: INTERFACE : pearlite
POST-1: UPPER OR LOWER INTERFACE OF REGION PEARLITE#1 /LOWER/: upper
POST-1:
POST-1: plot
2018.02.18.22.16.41
UPPER INTERFACE OF REGION "PEARLITE#1"
CELL#1

```

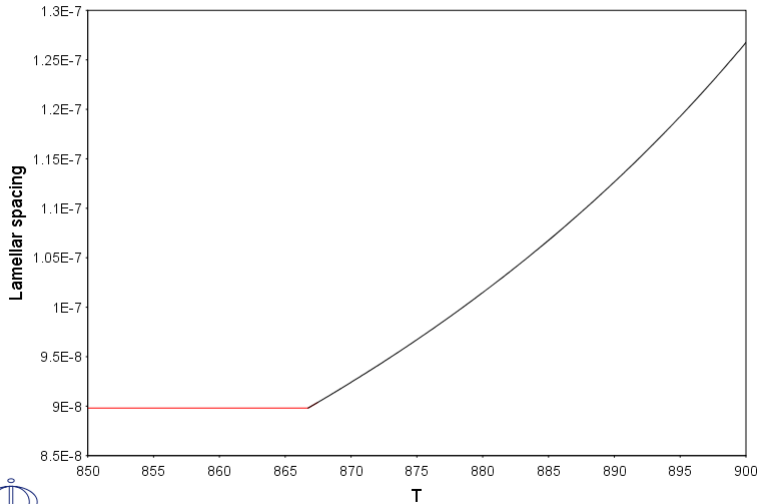


```

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

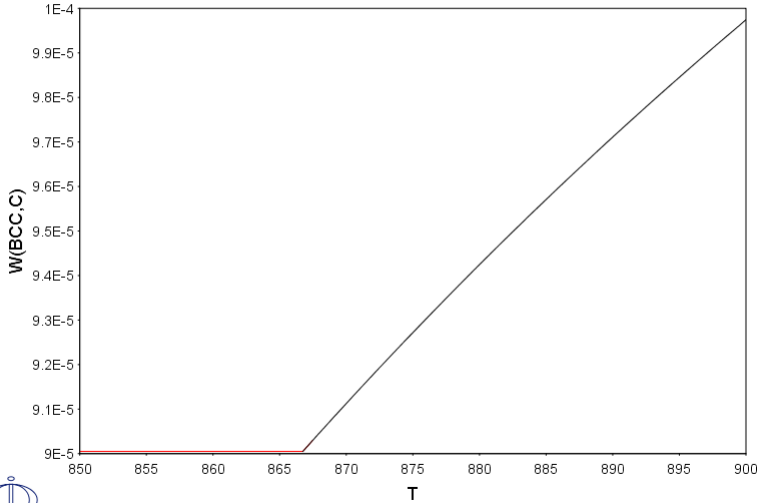
```

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



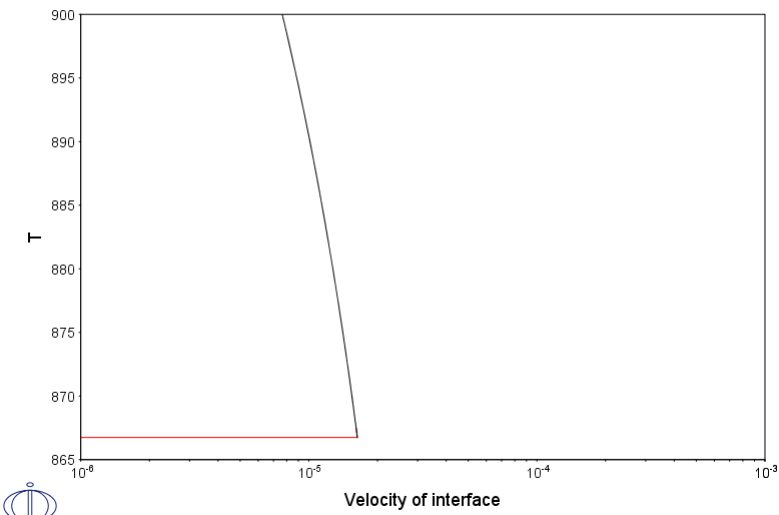
```
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ AND THE C COMPOSITION IN THE FERRITE VS. TEMP
POST-1: @@
POST-1: s-d-a y w(bcc,c)
POST-1:
POST-1:
POST-1: plot
```

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



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

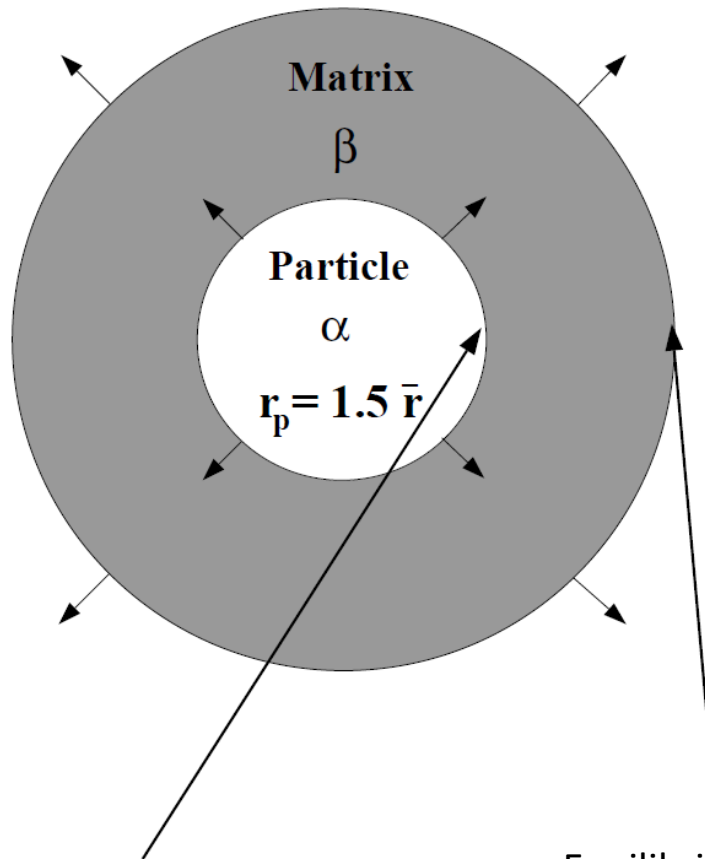
2018.02.18.22.16.43
UPPER INTERFACE OF REGION "PEARLITE#1"
CELL #1



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



Coarsening



Moving phase interface
with α and β in local
equilibrium.

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

Equilibrium as defined by
the average composition
in the system.

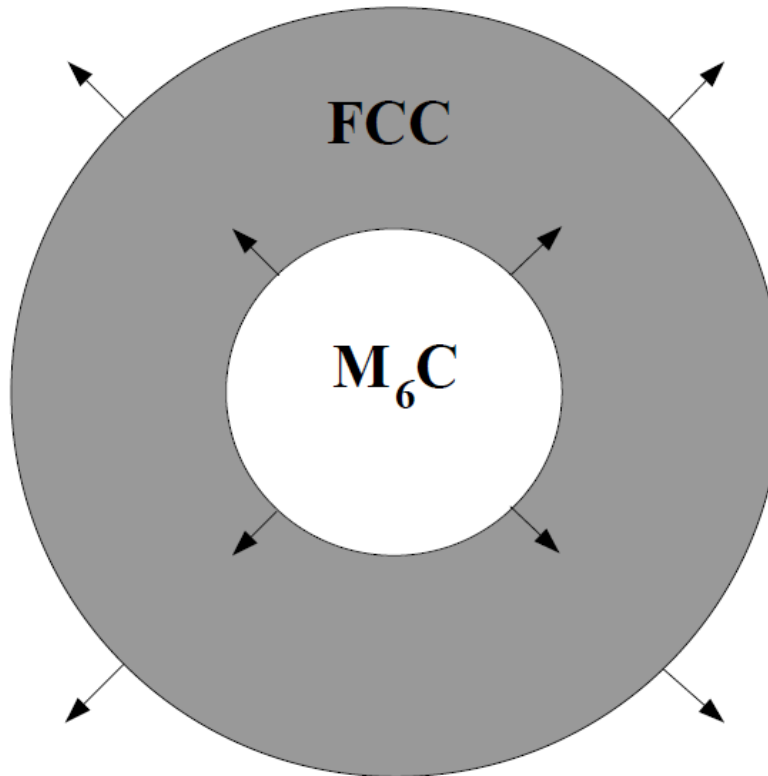
$\frac{2\sigma V_m}{r_p}$ Interfacial energy
contribution for α phase



Example exf1

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

This example calculates the Ostwald-ripening of a spherical M_6C carbide in an austenite matrix.



$$T = 1173K$$

$$r_p = 0.228 \mu m$$

exf1-setup

About Stockholm, Sweden

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

SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exf1\setup.DCM"SYS: @@

SYS: @@ Coarsening problem.

SYS: @@ Coarsening of M6C precipitate in an Fe-Mo-C alloy

SYS: @@ This example calculates the Ostwald-ripening of a spherical

SYS: @@ M6C carbide in an austenite matrix.

SYS: -----

NO SUCH COMMAND, USE HELP

SYS: @@

SYS: @@ RETRIEVE DATA FROM THE DATABASES

SYS: @@

SYS: go da

THERMODYNAMIC DATABASE module

Current database: Steels/Fe-Alloys v9.0

VA /- DEFINED
L12_FCC B2_BCC DICTRA_FCC_A1
REJECTED

TDB_TCFE9: switch tcfe7

Current database: Steels/Fe-Alloys v7.0

VA DEFINED
L12_FCC B2_BCC B2_VACANCY
HIGH_SIGMA DICTRA_FCC_A1 REJECTED

TDB_TCFE7: def-sys fe mo c

FE MO C

DEFINED

TDB_TCFE7: rej ph * all

GAS:G LIQUID:L BCC_A2
FCC_A1 HCP_A3 DIAMOND_FCC_A4
GRAPHITE CEMENTITE M23C6
M7C3 M6C M5C2
M3C2 MC_ETA MC_SHP
KSI_CARBIDE A1_KAPPA KAPPA
Z_PHASE FE4N_LP1 FECN_CHI
SIGMA MU_PHASE P_PHASE
R_PHASE CHI_A12 LAVES_PHASE_C14
REJECTED

TDB_TCFE7: res ph fcc m6c

FCC_A1 M6C RESTORED

TDB_TCFE7: get

REINITIATING GES

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

FUNCTIONS

List of references for assessed data

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

-OK-

TDB_TCFE7:

TDB_TCFE7: @@

TDB_TCFE7: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE MOBILITY DATA

TDB_TCFE7: @@

TDB_TCFE7: app

Use one of these databases

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

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

DATABASE NAME /TCFE7/: mobfe2

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

VA DEFINED

APP: def-sys fe mo c

FE MO C

DEFINED

APP: rej ph * all

BCC_A2 CEMENTITE FCC_A1
FE4N_LP1 HCP_A3 LIQUID:L

REJECTED

APP: res ph fcc m6c

*** M6C INPUT IGNORED

FCC_A1 RESTORED

APP: get

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

FUNCTIONS

List of references for assessed data

'This parameter has not been assessed'

'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'

'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe-Ni'

'H. Oikawa, Tech. Rept. Tohoku Univ., 48(1983)7.; Impurity diffusion of Mo in fcc Fe.'

-OK-

APP:

```

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

DIC>
DIC> @@
DIC> @@ ENTER REGIONS part AND aus
DIC> @@
DIC> enter-region
REGION NAME : part
DIC> enter-region aus
ATTACH TO REGION NAMED /PART/:
ATTACHED TO THE RIGHT OF PART /YES/:
DIC> @@
DIC> @@ ENTER GEOMETRICAL GRIDS INTO THE REGIONS
DIC> @@
DIC> @@
DIC> @@ THE INITIAL SIZE OF THE CARBIDE PARTICLE IS ASSUMED TO BE KNOWN
DIC> @@ (IN THIS CASE THE VALUE IS FROM NISHIZAWA ET. AL.). THE
DIC> @@ AVERAGE PARTICLE SIZE IS ASSUMED TO BE 0.152E-6 METERS. HOWEVER, THE
DIC> @@ CALCULATIONS ARE PERFORMED ON A MAXIMUM SIZE PARTICLE, WHICH IS ASSUMED
DIC> @@ TO BE 1.5 TIMES THE AVERAGE SIZE. THE SURROUNDING AUSTENITIC MATRIX
DIC> @@ SIZE IS CHOSEN TO MAINTAIN THE AVERAGE COMPOSITION.
DIC> @@
DIC> enter-grid
REGION NAME : /PART/: part
WIDTH OF REGION /1/: 0.228E-6
TYPE /LINEAR/: AUTO
DIC>
DIC> enter-grid
REGION NAME : /AUS/: aus
WIDTH OF REGION /1/: 4.53147041E-7
TYPE /LINEAR/: AUTO
DIC>
DIC> @@
DIC> @@ ENTER PHASES INTO REGIONS
DIC> @@
DIC> enter-phase active part matrix m6c
DIC>
DIC> enter-phase active aus matrix fcc#1
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITIONS IN THE PHASES
DIC> @@
DIC> enter-composition
REGION NAME : /PART/: part
PHASE NAME: /M6C/: m6c
DEPENDENT COMPONENT ? /MO/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-f
PROFILE FOR /MO/: mo lin 6.20117E-01 6.20117E-01
DIC>
DIC> enter-composition
REGION NAME : /AUS/: aus
PHASE NAME: /FCC_A1/: fcc#1
DEPENDENT COMPONENT ? /MO/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-f
PROFILE FOR /C/: mo lin 1.82099E-02 1.82099E-02
PROFILE FOR /MO/: c lin 2.83351E-03 2.83351E-03
DIC>
DIC>
DIC> @@
DIC> @@ SET A SPHERICAL GEOMETRY
DIC> @@
DIC> ent-geo 2
DIC>
DIC> @@
DIC> @@ ENTER THE SURFACE TENSION ENERGY CONTRIBUTION AS A FUNCTION OF
DIC> @@ THE INTERFACE POSITION (THE RADIUS OF THE PARTICLE).
DIC> @@ ALSO ENTER THE MOLAR VOLUME OF THE PHASE CORRECTED TO BE THE
DIC> @@ MOLAR VOLUME PER SUBSTITUTIONAL ATOM.
DIC> @@
DIC> @@ THE SURFACE TENSION IS 0.7, THE MOLAR VOLUME IS 0.71 AND THE
DIC> @@ TRANSFORMATION TO MOLAR VOLUME PER SUBSTITUTIONAL ATOM IS 7/6.
DIC> @@
DIC> set-surf 2*0.7*0.71*(7/6)/X;
ENTERED FUNCTION :2*.7*.71*7/6/X FOR CELL #1
DIC>
DIC>
DIC> @@
DIC> @@ ENABLE THE SIMPLIFIED MODEL FOR THE COARSENING (OSTWALD-RIPENING)
DIC> @@
DIC> coarse YES
DIC>
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME AND OTHER SIMULATION PARAMETERS
DIC> @@
DIC> set-simulation-time 1E6
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /100000/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exfl Y
DIC>
DIC> set-inter

```


exfl-run

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exfl\run.DCM"DIC> @@ exfl_run.DCM
DIC>
DIC> @@
DIC> @@ READ THE SETUP FROM FILE AND START THE SIMULATION
DIC> @@
DIC>
DIC> go d-m
TIME STEP AT TIME 0.00000E+00
*** ENTERING M6C AS A DIFFUSION NONE PHASE
DIC> read exfl
OK
DIC> sim
Region: PART
single geometric dense at 0.22800E-06
0.80000 64
Region: AUS
single geometric dense at 0.0000
1.0060 63
Trying old scheme 4
GENERATING STARTING VALUES FOR CELL # 1 INTERFACE # 2
DETERMINING INITIAL EQUILIBRIUM VALUES
CALCULATING STARTING VALUES: 9 EQUILIBRIUM CALCULATIONS DONE 6 OUT OF 9

U-FRACTION IN SYSTEM: C = .0190652843033664 FE = .970761291162784
MO = .0292387089677228
TOTAL SIZE OF SYSTEM: 1.32376603026E-18 [m^3]
U-FRACTION IN SYSTEM: C = .0190652843033664 FE = .970761291162784
MO = .0292387089677228
TOTAL SIZE OF SYSTEM: 1.32376603026E-18 [m^3]
0.610222970497725 0.610391048253450 0.610222911134997 2.564830791787979E-002 2.191933775022290E-
003 1.266865136119346E-004 1.096501638371350E-003 1.278319034558927E-004 4.432656719961518E-
007 1.566395510936704E-009 1.947833880265816E-009 3.659995728395455E-009 1.418022229672293E-
009 1.309139620588423E-009 1.103985036086987E-009 3.800021162887927E-009 7.446660865207878E-
010 2.344009117646817E-010 1.080152646799767E-013 1.867047643211421E-018 TIME = 0.10000000E-06 DT = 0.10000000E-
06 SUM OF SQUARES = 0.18670476E-17
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.50349420E-05 AND -0.50349420E-05
POSITION OF INTERFACE PART / AUS IS 0.22799950E-06
U-FRACTION IN SYSTEM: C = .0190659317665459 FE = .970759487634635
MO = .0292405124958722
TOTAL SIZE OF SYSTEM: 1.32375726043E-18 [m^3]
6 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: PART

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

TIME = 0.25446963E-05 DT = 0.24446963E-05 SUM OF SQUARES = 0.80253037E-19
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.39311816E-08 AND -0.39311816E-08
POSITION OF INTERFACE PART / AUS IS 0.22799949E-06
U-FRACTION IN SYSTEM: C = .0190664790765648 FE = .970759484142024
MO = .0292405159884825
TOTAL SIZE OF SYSTEM: 1.32375709303E-18 [m^3]
CPU time used in timestep 0 seconds
2.515003169879022E-008 2.515606839736259E-008 2.499418773175797E-008 2.005402508809647E-008 1.975188680744917E-
008 1.916893094188025E-008 1.798098166063758E-008 1.797987078560134E-008 1.576162116879742E-
008 1.172706230484645E-008 5.463976248626018E-009 5.470072379592426E-009 2.575739208186408E-
011 1.050353544654548E-019 TIME = 0.74340890E-05 DT = 0.48893927E-05 SUM OF SQUARES = 0.10503535E-18
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.56316592E-09 AND -0.56316592E-09
POSITION OF INTERFACE PART / AUS IS 0.22799948E-06
U-FRACTION IN SYSTEM: C = .0190671017667952 FE = .970759483934874
MO = .0292405161956331
TOTAL SIZE OF SYSTEM: 1.32375704507E-18 [m^3]
CPU time used in timestep 0 seconds
4.33251967282598E-010 4.333461945146029E-010 4.418343369955179E-010 4.025620070840790E-010 4.017875831196053E-
010 4.002414387371992E-010 3.971401167325227E-010 3.975914295836094E-010 3.909910643665908E-
010 3.788198544736429E-010 3.550709191441153E-010 3.557264804400251E-010 3.098645677267985E-
010 2.286943575027542E-010 1.032590621477480E-010 1.037482117905484E-010 5.751503861739746E-
014 2.763822793450989E-024 TIME = 0.17212874E-04 DT = 0.97787853E-05 SUM OF SQUARES = 0.27638228E-23
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.11628456E-09 AND -0.11628456E-09
POSITION OF INTERFACE PART / AUS IS 0.22799948E-06
U-FRACTION IN SYSTEM: C = .0190679130625397 FE = .970759484400328
MO = .0292405157301795
TOTAL SIZE OF SYSTEM: 1.32375702526E-18 [m^3]
CPU time used in timestep 1 seconds
2.076847912747820E-011 2.077191339162079E-011 2.354369667011284E-011

output ignored...

... output resumed

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

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

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

```

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

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

CPU time used in timestep 0 seconds
7.325232698426969E-010 7.226212817693013E-010 6.940725678957351E-010 1.243095839897094E-013 8.495379236702611E-
021 TIME = 1000000.0 DT = 32001.747 SUM OF SQUARES = 0.84953792E-20
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.39032951E-13 AND 0.39032951E-13
POSITION OF INTERFACE PART / AUS IS 0.27417834E-06
U-FRACTION IN SYSTEM: C = .0195446957121146 FE = .970707245727071
MO = .0292927544034362
TOTAL SIZE OF SYSTEM: 2.30200418971E-18 [m^3]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 0.0000000
DELETING TIME-RECORD FOR TIME 0.10000000E-06
DELETING TIME-RECORD FOR TIME 0.25446963E-05
DELETING TIME-RECORD FOR TIME 0.74340890E-05
DELETING TIME-RECORD FOR TIME 0.17212874E-04
DELETING TIME-RECORD FOR TIME 0.36770445E-04
DELETING TIME-RECORD FOR TIME 0.75885586E-04
DELETING TIME-RECORD FOR TIME 0.15411587E-03
DELETING TIME-RECORD FOR TIME 0.31057643E-03
DELETING TIME-RECORD FOR TIME 0.62349756E-03
DELETING TIME-RECORD FOR TIME 0.12493398E-02
DELETING TIME-RECORD FOR TIME 0.25010243E-02
DELETING TIME-RECORD FOR TIME 0.50043934E-02
DELETING TIME-RECORD FOR TIME 0.10011131E-01
DELETING TIME-RECORD FOR TIME 0.20024608E-01
DELETING TIME-RECORD FOR TIME 0.40051560E-01
DELETING TIME-RECORD FOR TIME 0.80105465E-01
DELETING TIME-RECORD FOR TIME 0.16021327
DELETING TIME-RECORD FOR TIME 0.32042889
DELETING TIME-RECORD FOR TIME 0.64086013
DELETING TIME-RECORD FOR TIME 1.2817226
DELETING TIME-RECORD FOR TIME 2.5634476
DELETING TIME-RECORD FOR TIME 5.1268975
DELETING TIME-RECORD FOR TIME 10.253797
DELETING TIME-RECORD FOR TIME 20.507597
DELETING TIME-RECORD FOR TIME 41.015196
DELETING TIME-RECORD FOR TIME 82.030394
DELETING TIME-RECORD FOR TIME 164.06079
DELETING TIME-RECORD FOR TIME 328.12158
DELETING TIME-RECORD FOR TIME 656.24317
DELETING TIME-RECORD FOR TIME 1312.4863
DELETING TIME-RECORD FOR TIME 2624.9727
DELETING TIME-RECORD FOR TIME 5249.9454
DELETING TIME-RECORD FOR TIME 10499.891
DELETING TIME-RECORD FOR TIME 20999.782
DELETING TIME-RECORD FOR TIME 41999.563
DELETING TIME-RECORD FOR TIME 83999.126
DELETING TIME-RECORD FOR TIME 167998.25
DELETING TIME-RECORD FOR TIME 267998.25
DELETING TIME-RECORD FOR TIME 367998.25
DELETING TIME-RECORD FOR TIME 467998.25
DELETING TIME-RECORD FOR TIME 567998.25
DELETING TIME-RECORD FOR TIME 667998.25
DELETING TIME-RECORD FOR TIME 767998.25
DELETING TIME-RECORD FOR TIME 867998.25

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

TIMESTEP AT 1000000.00 SELECTED

```

```

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

```

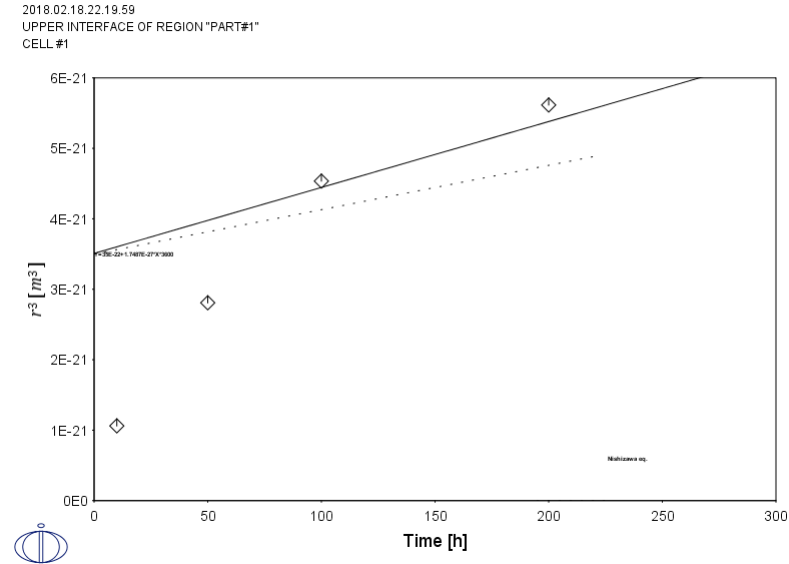
exf1-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exf1\plot.DCM"DIC> @@ exf1_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE f1
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 1.00000E+06
*** ENTERING M6C AS A DIFFUSION NONE PHASE
DIC> read exf1
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post

POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson

POST-1:
POST-1: @@
POST-1: @@ PLOT THE AVERAGE PARTICLE SIZE (CUBED) AS THIS ASSUMED TO
POST-1: @@ SCALE LINEARLY WITH TIME. THEN A FUNCTION IS ENTERED SO
POST-1: @@ THIS QUANTITY CAN BE ACCESSED. WE ALSO WANT TO PLOT THIS
POST-1: @@ QUANTITY VERSUS TIME (IN HOURS) SO A FUNCTION IS ENTERED.
POST-1: @@
POST-1: enter-symbol func rr3=(poi(part,u)/1.5)**3;
POST-1: enter-symbol func hours=time/3600;
POST-1: s-d-a x hours
POST-1: s-d-a y rr3
POST-1:
POST-1: @@
POST-1: @@ AS WE ARE PLOTTING FUNCTIONS ON BOTH AXES WE MUST EXPLICITLY
POST-1: @@ DEFINE THE INDEPENDENT VARIABLE AND THE PLOT CONDITION
POST-1: @@
POST-1: s-ind time
POST-1: s-p-c inter
INTERFACE : part upper
POST-1:
POST-1:
POST-1: set-axis-text-status x n
AXIS TEXT : Time [h]
POST-1:
POST-1: @@
POST-1: @@ WHEN THIS IS PLOTTED, THIS AXIS TEXT NOTATION WORKS WELL FOR
POST-1: @@ THE AVERAGE RADIUS CUBED. FOR MORE INFORMATION ABOUT HOW TO
POST-1: @@ ADJUST TEXT IN THE POST PROCESSOR USING THE DATAPLOT LANGUAGE,
POST-1: @@ SEARCH THE ONLINE HELP (FROM THE MAIN MENU -> HELP > ONLINE HELP)
POST-1:
POST-1:
POST-1: set-axis-text-status y n
AXIS TEXT : \latex r^3\, [m^3]
POST-1:
POST-1:
POST-1: @@
POST-1: @@ COMPARE WITH EXPERIMENTAL DATA FROM NISHIZAWA ET AL.
POST-1: @@ TRANS. JPN. INST. MET. VOL. 22 1981 PP. 733-742.
POST-1: @@
POST-1:
POST-1: app y exf1
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 1
POST-1:
POST-1: s-s-s y n 0 6e-21
POST-1:
POST-1: @@
POST-1: @@ SET A TITLE ON THE PLOT
POST-1: @@
POST-1: set-title Figure f1.1
POST-1:
POST-1: plot
```

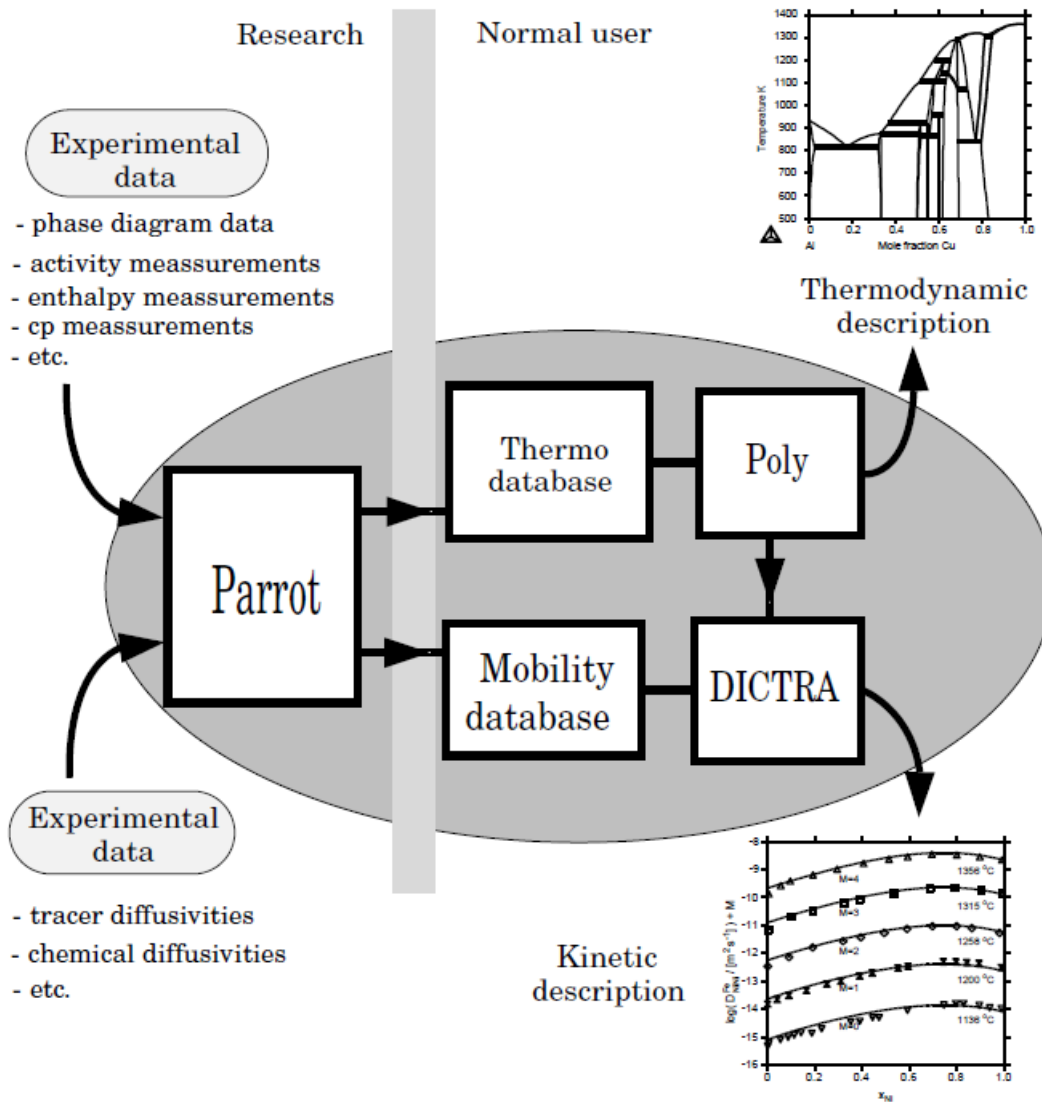
Figure f1.1



```
POST-1:
POST-1:??<_hit_return_to_continue_>
POST-1: @@
POST-1: @@ THE DIFFENCE BETWEEN THE CALCULATION AND THE EQUATION USED BY
POST-1: @@ NISHIZAWA ET AL. IS MAINLY DUE TO DIFFERENT THERMODYNAMIC
POST-1: @@ DESCRIPTIONS AND DIFFUSIVITIES.
POST-1: @@
POST-1:
POST-1: set-inter
--OK--
POST-1:
```



Kinetic Data

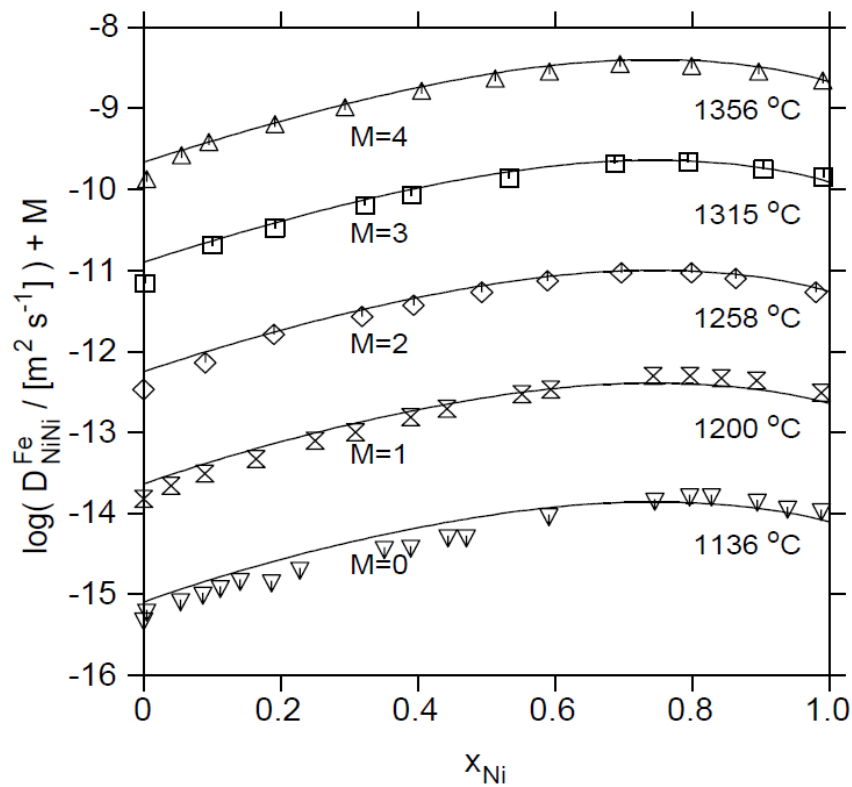




Example exg1

Checking diffusivities in an Fe-Ni alloy

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



exg1-setup

About Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

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

SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exg1\setup.DCM" @@

SYS: @@ Kinetic data example.

SYS: @@ Checking mobilities and diffusivities in an Fe-Ni alloy

SYS: @@ This is an example file to check the mobilities and diffusivities

SYS: @@ in an Fe-Ni alloy.

SYS: -----

NO SUCH COMMAND, USE HELP

SYS:

SYS: @@ exg1_setup.DCM

SYS:

SYS: @@

SYS: @@ START BY GOING TO THE DATABASE MODULE

SYS: @@

SYS: go da

THERMODYNAMIC DATABASE module

Current database: Steels/Fe-Alloys v9.0

VA /- DEFINED

L12_FCC B2_BCC DICTRA_FCC_A1

REJECTED

TDB_TCFE9:

TDB_TCFE9: @@

TDB_TCFE9: @@ SELECT A DATABASE FOR THERMODYNAMIC DATA

TDB_TCFE9: @@

TDB_TCFE9: sw tcf7

Current database: Steels/Fe-Alloys v7.0

VA DEFINED

L12_FCC B2_BCC B2_VACANCY

HIGH_SIGMA DICTRA_FCC_A1 REJECTED

TDB_TCFE7:

TDB_TCFE7: @@

TDB_TCFE7: @@ DEFINE THE SYSTEM TO WORK WITH

TDB_TCFE7: @@

TDB_TCFE7: def-sys fe ni

FE NI DEFINED

TDB_TCFE7:

TDB_TCFE7: @@

TDB_TCFE7: @@ EXCLUDE THE THERMODYNAMIC DATA FOR THE PHASES THAT ARE NOT NEEDED

TDB_TCFE7: @@

TDB_TCFE7: rej ph * all

LIQUID:L BCC_A2 FCC_A1

HCP_A3 A1_KAPPA KAPPA

LAVES_PHASE_C14 NBNi3 Ni3Ti

REJECTED

TDB_TCFE7: res ph fcc

FCC_A1 RESTORED

TDB_TCFE7:

TDB_TCFE7: @@

TDB_TCFE7: @@ RETRIEVE DATA FROM THE DATABASE FILE

TDB_TCFE7: @@

TDB_TCFE7: get

REINITIATING GES

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

FUNCTIONS

List of references for assessed data

'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'

'A. Dinsdale, T. Chart, MTDS NPL, unpublished work (1986); FE-NI'

'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;

Molar volumes'

'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'

-OK-

TDB_TCFE7:

TDB_TCFE7: @@

TDB_TCFE7: @@ MOBILITY/DIFFUSIVITY DATA ARE STORED IN A SEPARATE DATABASE FILE.

TDB_TCFE7: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE DATA

TDB_TCFE7: @@

TDB_TCFE7: app

Use one of these databases

TCFE9 = Steels/Fe-Alloys v9.0

TCFE10 = Steels/Fe-Alloys v10.0 SNAPSHOT

TCFE8 = Steels/Fe-Alloys v8.1

FROST1 = FROST database v1.0

TCFE7 = Steels/Fe-Alloys v7.0

TCFE6 = Steels/Fe-Alloys v6.2

TCFE5 = Steels/Fe-Alloys v5.0

TCFE4 = Steels/Fe-Alloys v4.1

TCFE3 = Steels/Fe-Alloys v3.1

TCFE2 = Steels/Fe-Alloys v2.1

TCFE1 = Steels/Fe-Alloys v1.0

TCNi9 = Ni-Alloys v9.0 SNAPSHOT

NI25 = NI25 database

TCNi8 = Ni-Alloys v8.1

TCNi7 = Ni-Alloys v7.1

TCNi6 = Ni-Alloys v6.0

TCNi5 = Ni-Alloys v5.1

TCNi4 = Ni-Alloys v4.0

TCNi1 = Ni-Alloys v1.3

TCAL5 = Al-Alloys v5.0

TCAL4 = Al-Alloys v4.0

TCAL3 = Al-Alloys v3.0

TCAL2 = Al-Alloys v2.1

TCAL1 = Al-Alloys v1.2

TCMG4 = Mg-Alloys v4.0

TCMG3 = Mg-Alloys v3.0

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

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

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

List of references for assessed data

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

```

APP: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP
APP: @@
APP: go d-m
      NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ LIST MOBILITY DATA
DIC> @@
DIC> list-mob-data
      Sorry, LIST-DATA disabled for this database
DIC>
DIC>
DIC>
DIC> @?<Hit_return_to_continue>
DIC>
DIC> @@
DIC> @@ CHECK THE DIFFUSIVITIES
DIC> @@
DIC> check
      AMBIGUOUS COMMAND, USE HELP
DIC>
DIC> fcc
      NO SUCH COMMAND, USE HELP
DIC> fe
      NO SUCH COMMAND, USE HELP
DIC> 0.3
      NO SUCH COMMAND, USE HELP
DIC> 101325
      NO SUCH COMMAND, USE HELP
DIC> 1409
      NO SUCH COMMAND, USE HELP
DIC> dl
      NO SUCH COMMAND, USE HELP
DIC>
DIC>
DIC> @?<Hit_return_to_continue>
DIC>
DIC> @@
DIC> @@ USE STEPPING IN POLY-3 TO CALCULATE THE DIFFUSIVITIES VS. COMPOSITION
DIC> @@
DIC> go p-3
POLY_3: s-c t=1409,p=101325,n=1,x(ni)=0.3
POLY_3: c-e
      Using global minimization procedure
      Calculated          209 grid points in          0 s
      Found the set of lowest grid points in          0 s
      Calculated POLY solution          0 s, total time    0 s
POLY_3:
POLY_3: s-a-v
Axis number: /1/: 1
Condition /NONE/: x(ni)
Min value /0/: 0
Max value /1/: 1
Increment /.025/: 1e-3
POLY_3:
POLY_3: step
Option? /NORMAL/: normal
      No initial equilibrium, using default
      Step will start from axis value    0.300000
...OK

```

```

Phase Region from    0.300000    for:
      FCC_A1

```

```

Global test at 3.08000E-01 .... OK
Global test at 3.18000E-01 .... OK
Global test at 3.28000E-01 .... OK
Global test at 3.38000E-01 .... OK
Global test at 3.48000E-01 .... OK
Global test at 3.58000E-01 .... OK
Global test at 3.68000E-01 .... OK
Global test at 3.78000E-01 .... OK
Global test at 3.88000E-01 .... OK
Global test at 3.98000E-01 .... OK
Global test at 4.08000E-01 .... OK
Global test at 4.18000E-01 .... OK
Global test at 4.28000E-01 .... OK
Global test at 4.38000E-01 .... OK
Global test at 4.48000E-01 .... OK
Global test at 4.58000E-01 .... OK
Global test at 4.68000E-01 .... OK
Global test at 4.78000E-01 .... OK
Global test at 4.88000E-01 .... OK
Global test at 4.98000E-01 .... OK
Global test at 5.08000E-01 .... OK
Global test at 5.18000E-01 .... OK
Global test at 5.28000E-01 .... OK
Global test at 5.38000E-01 .... OK
Global test at 5.48000E-01 .... OK
Global test at 5.58000E-01 .... OK
Global test at 5.68000E-01 .... OK
Global test at 5.78000E-01 .... OK
Global test at 5.88000E-01 .... OK
Global test at 5.98000E-01 .... OK
Global test at 6.08000E-01 .... OK
Global test at 6.18000E-01 .... OK
Global test at 6.28000E-01 .... OK
Global test at 6.38000E-01 .... OK
Global test at 6.48000E-01 .... OK
Global test at 6.58000E-01 .... OK
Global test at 6.68000E-01 .... OK
Global test at 6.78000E-01 .... OK
Global test at 6.88000E-01 .... OK
Global test at 6.98000E-01 .... OK
Global test at 7.08000E-01 .... OK
Global test at 7.18000E-01 .... OK
Global test at 7.28000E-01 .... OK
Global test at 7.38000E-01 .... OK
Global test at 7.48000E-01 .... OK
Global test at 7.58000E-01 .... OK
Global test at 7.68000E-01 .... OK
Global test at 7.78000E-01 .... OK
Global test at 7.88000E-01 .... OK

```

```

Global test at 7.98000E-01 .... OK
Global test at 8.08000E-01 .... OK
Global test at 8.18000E-01 .... OK
Global test at 8.28000E-01 .... OK
Global test at 8.38000E-01 .... OK
Global test at 8.48000E-01 .... OK
Global test at 8.58000E-01 .... OK
Global test at 8.68000E-01 .... OK
Global test at 8.78000E-01 .... OK
Global test at 8.88000E-01 .... OK
Global test at 8.98000E-01 .... OK
Global test at 9.08000E-01 .... OK
Global test at 9.18000E-01 .... OK
Global test at 9.28000E-01 .... OK
Global test at 9.38000E-01 .... OK
Global test at 9.48000E-01 .... OK
Global test at 9.58000E-01 .... OK
Global test at 9.68000E-01 .... OK
Global test at 9.78000E-01 .... OK
Global test at 9.88000E-01 .... OK
Global test at 9.98000E-01 .... OK
Terminating at 1.00000
Calculated 703 equilibria

```

```

Phase Region from 0.300000 for:
FCC_A1

```

```

Global test at 2.92000E-01 .... OK
Global test at 2.82000E-01 .... OK
Global test at 2.72000E-01 .... OK
Global test at 2.62000E-01 .... OK
Global test at 2.52000E-01 .... OK
Global test at 2.42000E-01 .... OK
Global test at 2.32000E-01 .... OK
Global test at 2.22000E-01 .... OK
Global test at 2.12000E-01 .... OK
Global test at 2.02000E-01 .... OK
Global test at 1.92000E-01 .... OK
Global test at 1.82000E-01 .... OK
Global test at 1.72000E-01 .... OK
Global test at 1.62000E-01 .... OK
Global test at 1.52000E-01 .... OK
Global test at 1.42000E-01 .... OK
Global test at 1.32000E-01 .... OK
Global test at 1.22000E-01 .... OK
Global test at 1.12000E-01 .... OK
Global test at 1.02000E-01 .... OK
Global test at 9.20000E-02 .... OK
Global test at 8.20000E-02 .... OK
Global test at 7.20000E-02 .... OK
Global test at 6.20000E-02 .... OK
Global test at 5.20000E-02 .... OK
Global test at 4.20000E-02 .... OK
Global test at 3.20000E-02 .... OK
Global test at 2.20000E-02 .... OK
Global test at 1.20000E-02 .... OK
Global test at 2.00000E-03 .... OK
Terminating at 0.100000E-11
Calculated 303 equilibria
*** Buffer saved on file: C:\Users\developer\Documents\RESULT_002.POLY3

```

```

POLY_3:
POLY_3: @@
POLY_3: @@ ENTER THE POST PROCESSOR AND PLOT THE RESULT
POLY_3: @@
POLY_3: post

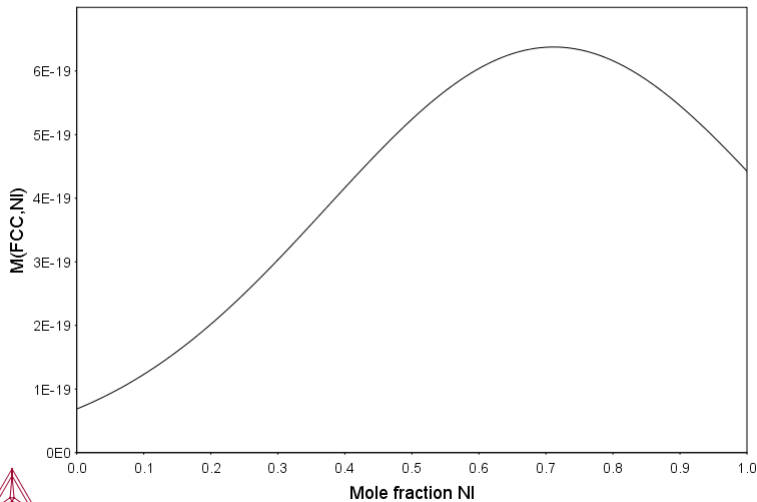
```

POLY-3 POSTPROCESSOR VERSION 3.2

```

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

```

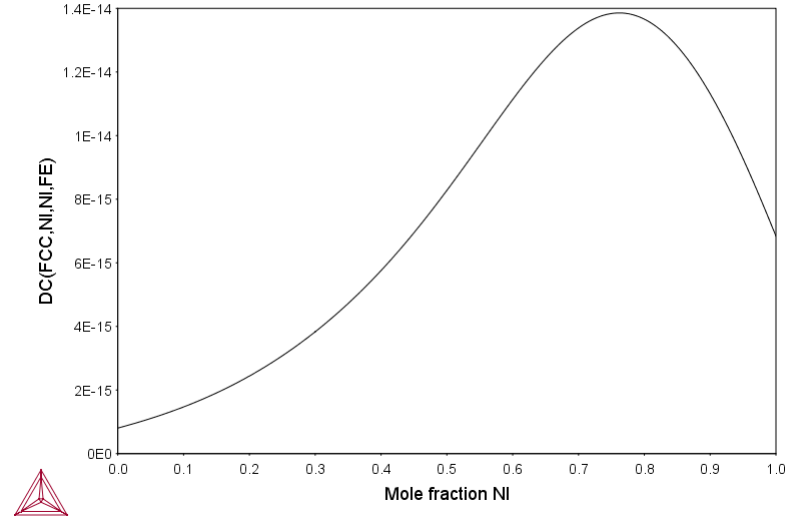


```

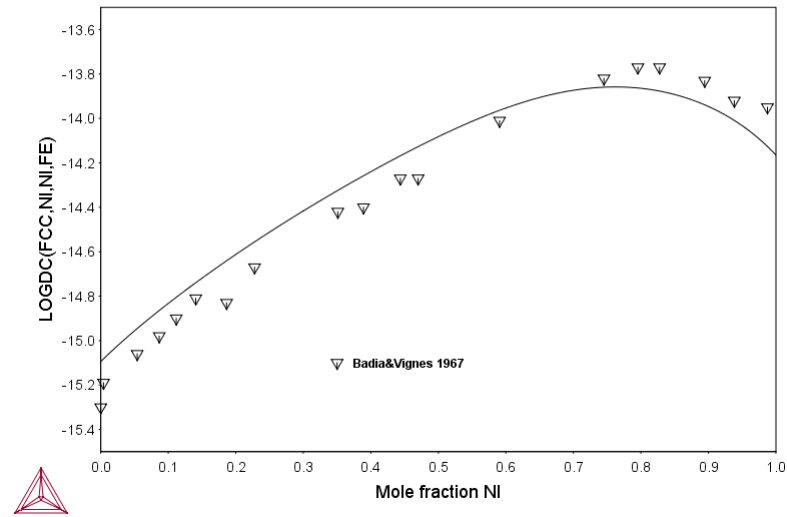
POST:
POST:
POST:
POST: @?<Hit_return_to_continue>

```

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



```
POST:
POST:
POST: @?<Hit_return_to_continue>
POST:
POST: @@
POST: @@ PLOT THE LOGARITHM OF DC AND APPEND THE EXPERIMENTAL DATA
POST: @@
POST: s-d-a y logdc(fcc,ni,ni,fe)
POST:
POST: app y feni.exp
PROLOGUE NUMBER: /0/: 1
DATASET NUMBER(s): /-1/: 1
POST:
POST: s-s-s y n -15.5 -13.5
POST:
POST: plot
2018.02.18.22.21.24
MOBFE2: FE, NI
T=1409, P=1.01325E5, N=1
```



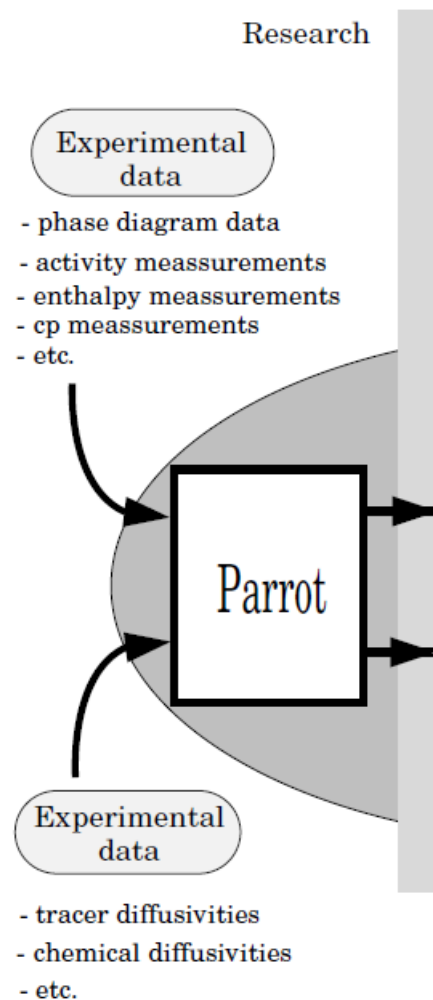
```
POST:
POST:
POST: @?<Hit_return_to_continue>
POST:
POST: set-inter
POST:
```



Example exg2

Optimization of mobilities in Ni-Al fcc alloys

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



exg2-setup

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

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

VA /- DEFINED
LI2_FCC B2_BCC DICTRA_FCC_A1
REJECTED
TDB_TCFE9: sw us tdata
Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

VA DEFINED
TDB_USER: def-sys el
ELEMENTS: al ni
AL NI DEFINED
TDB_USER: rej ph *
LIQUID B2_BCC BCC_A2
FCC_A1 GAMMA_PRIME REJECTED
TDB_USER: rest ph fcc_al
FCC_A1 RESTORED
TDB_USER: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....
-OK-
TDB_USER:
TDB_USER: @@
TDB_USER: @@ APPEND THE KINETIC DATA FROM THE MOBILITY DATABASE IN ORDER TO
TDB_USER: @@ HAVE SOME DUMMY PARAMETERS.
TDB_USER: @@
TDB_USER: app mob2
Current database: Alloys Mobility v2.7

VA DEFINED
GAS:G REJECTED
APP: def-sys
ELEMENTS: al ni
AL NI DEFINED
APP: rej ph *
BCC_A2 FCC_A1 M4N
HCP_A3 LIQUID:L REJECTED
APP: res ph fcc_al
FCC_A1 RESTORED
APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

List of references for assessed data

'This parameter has not been assessed'
'A. Engstrom and J. Agren: Z. Metallkunde 87(1996)92-97;
Al, Cr and Ni diffusion in fcc Al-Cr-Ni'
'B. Jonsson: Scand. J. Metall. 24(1995)21-27;
Ni self-diffusion'

-OK-
APP:
APP: @@
APP: @@ GO TO THE DICTRA MODULE AND DEFINE THE KINETIC PARAMETERS. THE
APP: @@ VARIABLES V1,V2,V3 AND V4 ARE TO BE OPTIMIZED. NOTE THAT IF
APP: @@ YOU ARE OPTIMIZING PARAMETERS FOR A PHASE WITH MAGNETIC
APP: @@ CONTRIBUTION. I.E. USING BOTH MF- AND MQ-PARAMETERS, YOU
APP: @@ MIGHT HAVE TO ENTER THE PARROT MODULE AND GO BACK BEFORE
APP: @@ ENTERING PARAMETERS CONTAINING VARIABLES.
APP: @@
APP: go dic_par

PARROT VERSION 5.3d RUNNING ON PC/WINDOWS NT

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

PARROT:
PARROT:
PARROT: go d-m
NO TIME STEP DEFINED
DIC>
DIC> @@ MOBILITY OF Al IN Al
DIC> ENTER-MOB-DATA
PARAMETER: MQ(FCC_A1&AL,AL:VA) 298.15 -142000+R*T*LN(1.71E-4); 6000 N
MQ(FCC_A1&AL#1,AL:VA;0)
DIC>
DIC> @@ MOBILITY OF Al IN Ni
DIC> ENTER-MOB-DATA
```



```
PARAMETER: MQ(FCC_A1&AL,NI:VA) 298.15 -284000+R*T*LN(7.5E-4); 6000 N
MQ(FCC_A1&AL#1,NI:VA;0)
DIC>
DIC> @@ MOBILITY OF Al INTERACTION BETWEEN Al AND Ni
DIC> ENTER-MOB-DATA
PARAMETER: MQ(FCC_A1&AL,AL,NI:VA;0) 298.15 V1+V2*T; 6000 N
MQ(FCC_A1&AL#1,AL,NI:VA;0)
DIC>
DIC> @@ MOBILITY OF Ni IN Al
DIC> ENTER-MOB-DATA
PARAMETER: MQ(FCC_A1&NI,AL:VA) 298.15 -145900+R*T*LN(4.4E-4); 6000 N
MQ(FCC_A1&NI#1,AL:VA;0)
DIC>
DIC> @@ MOBILITY OF Ni IN Ni
DIC> ENTER-MOB-DATA
PARAMETER: MQ(FCC_A1&NI,NI:VA) 298.15 -287000-69.8*T; 6000 N
MQ(FCC_A1&NI#1,NI:VA;0)
DIC>
DIC> @@ MOBILITY OF Ni INTERACTION BETWEEN Ni AND Al
DIC> ENTER-MOB-DATA
PARAMETER: MQ(FCC_A1&NI,NI,AL:VA;0) 298.15 V3+V4*T; 6000 N
MQ(FCC_A1&NI#1,AL,NI:VA;0)
DIC>
DIC> @@
DIC> @@ GO TO PARROT AND SAVE THE SET UP TO FILE
DIC> @@
DIC> go dic_parrot
```

PARROT VERSION 5.3d RUNNING ON PC/WINDOWS NT

PARROT: create-new-store-file opt

PARROT:

PARROT: set-inter

--OK--

PARROT:

exg2-run

```
PARROT>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exg2\run.DCM"PARROT: @@ exg2_run.DCM
PARROT:
PARROT: @@-----
PARROT: @@ FILE FOR DOING THE OPTIMIZATION IN PARROT
PARROT: @@-----
PARROT:
PARROT: @@
PARROT: @@ GO TO PARROT AND READ THE SETUP
PARROT: @@
PARROT: go dic_parrot

PARROT VERSION 5.3d RUNNING ON PC/WINDOWS NT

PARROT: set-store-file opt
PARROT:
PARROT:
PARROT: @@
PARROT: @@ COMPILE THE EXPERIMENTAL DATA IN exp.DOP INTO STRUCTURED BINARY DATA.
PARROT: @@
PARROT: compile-experiments exp
OUTPUT TO SCREEN OR FILE /SCREEN/:
INITIATE STORE FILE: /Y/:

$-----
$ DOP-FILE CONTAINING EXPERIMENTAL INFORMATION USED DURING THE
$ OTIMIZATION IN PARROT (COMPARE WITH POP-FILE USED WHEN EVALUATING
$ THERMODYNAMIC DATA). THE EXPERIMENTAL DATA HERE STEAM FROM A STUDY BY
$ YAMAMOTO ET AL. TRANS. JPN. INST. MET. VOL. 21,NO. 9 (1980), P. 601.
$
$ CONSULT THE THERMO-CALC USER'S GUIDE TO LEARN MORE ABOUT SYNTAXES
$ FOR OPTIMIZATION OF THERMODYNAMIC DATA.
$-----

ENTER CONST P0=101325

TABLE_HEAD 10
CREATE_NEW 0010,1
C-S PH FCC=ENT 1
S-C T=1573,N=1,P=P0
S-C X(AL)=-.01055
EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.6:.1
CREATE_NEW 0011,1
C-S PH FCC=ENT 1
S-C T=1573,N=1,P=P0
S-C X(AL)=-.02032
EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.56:.1
CREATE_NEW 0012,1
C-S PH FCC=ENT 1
S-C T=1573,N=1,P=P0
S-C X(AL)=-.02957
EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.65:.1
CREATE_NEW 0013,1
C-S PH FCC=ENT 1
S-C T=1573,N=1,P=P0
S-C X(AL)=-.03884
EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.52:.1
CREATE_NEW 0014,1
C-S PH FCC=ENT 1
S-C T=1573,N=1,P=P0
S-C X(AL)=-.03884
EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.52:.1
CREATE_NEW 0015,1
C-S PH FCC=ENT 1
S-C T=1573,N=1,P=P0
S-C X(AL)=-.04927
EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.48:.1
CREATE_NEW 0016,1
C-S PH FCC=ENT 1
S-C T=1573,N=1,P=P0
S-C X(AL)=-.06062
EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.43:.1
CREATE_NEW 0017,1
C-S PH FCC=ENT 1
S-C T=1573,N=1,P=P0
S-C X(AL)=-.07029
EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.41:.1
CREATE_NEW 0018,1
C-S PH FCC=ENT 1
S-C T=1573,N=1,P=P0
S-C X(AL)=-.08113
EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.37:.1
CREATE_NEW 0019,1
C-S PH FCC=ENT 1
S-C T=1573,N=1,P=P0
S-C X(AL)=-.09166
EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.32:.1
CREATE_NEW 0020,1
C-S PH FCC=ENT 1
S-C T=1573,N=1,P=P0
S-C X(AL)=-.09945
EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.28:.1
CREATE_NEW 0021,1
C-S PH FCC=ENT 1
S-C T=1573,N=1,P=P0
S-C X(AL)=-.1099
EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.24:.1
CREATE_NEW 0022,1
C-S PH FCC=ENT 1
S-C T=1573,N=1,P=P0
S-C X(AL)=-.1207
EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.2:.1
CREATE_NEW 0023,1
C-S PH FCC=ENT 1
S-C T=1573,N=1,P=P0
S-C X(AL)=-.129
EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.18:.1
CREATE_NEW 0024,1
C-S PH FCC=ENT 1
S-C T=1573,N=1,P=P0
S-C X(AL)=-.1392
EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.16:.1
CREATE_NEW 0025,1
```

```
C-S PH FCC=ENT 1
S-C T=1573,N=1,P=P0
S-C X(AL)=.1503
EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.1:.1
CREATE_NEW 0026,1
C-S PH FCC=ENT 1
S-C T=1573,N=1,P=P0
S-C X(AL)=.1589
EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.08:.1
CREATE_NEW 0027,1
C-S PH FCC=ENT 1
S-C T=1573,N=1,P=P0
S-C X(AL)=.1716
EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.02:.1
CREATE_NEW 0028,1
```

output ignored...

... output resumed

```
V3      -1.32972463E+05  -1.32959167E+05  -1.32959167E+05   3.97449919E+00   3.97449919E+00
      3.97449919E+00   3.97449919E+00   3.97449919E+00   3.97449919E+00   3.97449919E+00
      3.97449919E+00   3.97449919E+00   3.97449919E+00   3.97449919E+00   3.97449919E+00
      3.97449919E+00   3.97449919E+00   3.97449919E+00   3.97449919E+00   3.97449919E+00
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
```

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

Sorry, LIST-DATA disabled for this database

===== BLOCK NUMBER 1

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

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

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

exg2-plot

```
PARROT>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exg2\plot.DCM"PARROT: @@ exg2_plot.DCM
PARROT:
PARROT: @@-----
PARROT: @@ FILE FOR PLOTTING THE RESULT AFTER THE OPTIMIZATION. HERE
PARROT: @@ DIFFUSIVITIES CALCULATED FROM THE OPTIMIZED VARIABLES ARE
PARROT: @@ COMPARED WITH EXPERIMENTALLY MEASURED ONES.
PARROT: @@-----
PARROT:
PARROT: @@
PARROT: @@ GO TO PARROT AND READ THE FILE CONTAINING THE RESULT FROM
PARROT: @@ THE OPTIMIZATION.
PARROT: @@
PARROT: go dic_parrot

PARROT VERSION 5.3d RUNNING ON PC/WINDOWS NT

PARROT: set-store-file opt
PARROT:
PARROT: @@
PARROT: @@ GO TO POLY3 AND STEP IN X(AL)
PARROT: @@
PARROT: go p-3
POLY_3: s-c n=1,p=101325,t=1573
POLY_3: s-c x(al)=.1
POLY_3: c-e,,,,
Using global minimization procedure
Calculated          209 grid points in          0 s
Found the set of lowest grid points in          0 s
Calculated POLY solution          0 s, total time    0 s
POLY_3: add,,
POLY_3:
POLY_3: s-a-v 1 x(al) 0.0001 .20 0.001,,,,
POLY_3: step
Option? /NORMAL/:
Step will start from axis value    0.100000
...OK

Phase Region from    0.100000    for:
FCC_A1
Global test at    1.08000E-01 .... OK
Global test at    1.18000E-01 .... OK
Global test at    1.28000E-01 .... OK
Global test at    1.38000E-01 .... OK
Global test at    1.48000E-01 .... OK
Global test at    1.58000E-01 .... OK
Global test at    1.68000E-01 .... OK
Global test at    1.78000E-01 .... OK
Global test at    1.88000E-01 .... OK
Global test at    1.98000E-01 .... OK
Terminating at    0.200000
Calculated    103 equilibria

Phase Region from    0.100000    for:
FCC_A1
Global test at    9.20000E-02 .... OK
Global test at    8.20000E-02 .... OK
Global test at    7.20000E-02 .... OK
Global test at    6.20000E-02 .... OK
Global test at    5.20000E-02 .... OK
Global test at    4.20000E-02 .... OK
Global test at    3.20000E-02 .... OK
Global test at    2.20000E-02 .... OK
Global test at    1.20000E-02 .... OK
Global test at    2.00000E-03 .... OK
Terminating at    0.100000E-03
Calculated    103 equilibria
*** Buffer saved on file: C:\Users\developer\Documents\RESULT_002.POLY3
POLY_3: @@
POLY_3: @@ REPEATE THE PROCEDURE FOR SOME OTHER TEMPERATURES
POLY_3: @@
POLY_3: s-c t=1523,x(al)=.1
POLY_3: c-e,,,,,,
Using global minimization procedure
Calculated          209 grid points in          0 s
Found the set of lowest grid points in          0 s
Calculated POLY solution          0 s, total time    0 s
POLY_3: s-a-v 1 x(al) 0.0001 .20 0.001,,,,
POLY_3: step
Option? /NORMAL/:
Step will start from axis value    0.100000
...OK

Phase Region from    0.100000    for:
FCC_A1
Global test at    1.08000E-01 .... OK
Global test at    1.18000E-01 .... OK
Global test at    1.28000E-01 .... OK
Global test at    1.38000E-01 .... OK
Global test at    1.48000E-01 .... OK
Global test at    1.58000E-01 .... OK
Global test at    1.68000E-01 .... OK
Global test at    1.78000E-01 .... OK
Global test at    1.88000E-01 .... OK
Global test at    1.98000E-01 .... OK
Terminating at    0.200000
Calculated    103 equilibria

Phase Region from    0.100000    for:
FCC_A1
Global test at    9.20000E-02 .... OK
Global test at    8.20000E-02 .... OK
Global test at    7.20000E-02 .... OK
Global test at    6.20000E-02 .... OK
Global test at    5.20000E-02 .... OK
Global test at    4.20000E-02 .... OK
Global test at    3.20000E-02 .... OK
Global test at    2.20000E-02 .... OK
Global test at    1.20000E-02 .... OK
Global test at    2.00000E-03 .... OK
Terminating at    0.100000E-03
Calculated    103 equilibria
```

```

*** Buffer saved on file: C:\Users\developer\Documents\RESULT_002.POLY3
POLY_3: s-c t=1473,x(al)=.1
POLY_3: c-e,,,,,,,,
Using global minimization procedure
Calculated          209 grid points in          0 s
Found the set of lowest grid points in          0 s
Calculated POLY solution          0 s, total time  0 s
POLY_3: s-a-v 1 x(al) 0.0001 .20 0.001,,,,
POLY_3: step
Option? /NORMAL/:
Step will start from axis value    0.100000
...OK

Phase Region from    0.100000    for:
FCC_A1
Global test at    1.08000E-01 .... OK
Global test at    1.18000E-01 .... OK
Global test at    1.28000E-01 .... OK
Global test at    1.38000E-01 .... OK
Global test at    1.48000E-01 .... OK
Global test at    1.58000E-01 .... OK
Global test at    1.68000E-01 .... OK
Global test at    1.78000E-01 .... OK
Global test at    1.88000E-01 .... OK
Global test at    1.98000E-01 .... OK
Terminating at    0.200000
Calculated    103 equilibria

Phase Region from    0.100000    for:
FCC_A1
Global test at    9.20000E-02 .... OK
Global test at    8.20000E-02 .... OK
Global test at    7.20000E-02 .... OK
Global test at    6.20000E-02 .... OK
Global test at    5.20000E-02 .... OK
Global test at    4.20000E-02 .... OK
Global test at    3.20000E-02 .... OK
Global test at    2.20000E-02 .... OK
Global test at    1.20000E-02 .... OK
Global test at    2.00000E-03 .... OK
Terminating at    0.100000E-03
Calculated    103 equilibria
*** Buffer saved on file: C:\Users\developer\Documents\RESULT_002.POLY3
POLY_3: s-c t=1423,x(al)=.1
POLY_3: c-e,,,,,,,,
Using global minimization procedure
Calculated          209 grid points in          0 s
Found the set of lowest grid points in          0 s
Calculated POLY solution          0 s, total time  0 s
POLY_3: s-a-v 1 x(al) 0.0001 .20 0.001,,,,
POLY_3: step
Option? /NORMAL/:
Step will start from axis value    0.100000
...OK

Phase Region from    0.100000    for:
FCC_A1
Global test at    1.08000E-01 .... OK
Global test at    1.18000E-01 .... OK
Global test at    1.28000E-01 .... OK
Global test at    1.38000E-01 .... OK
Global test at    1.48000E-01 .... OK
Global test at    1.58000E-01 .... OK
Global test at    1.68000E-01 .... OK
Global test at    1.78000E-01 .... OK
Global test at    1.88000E-01 .... OK
Global test at    1.98000E-01 .... OK
Terminating at    0.200000
Calculated    103 equilibria

Phase Region from    0.100000    for:
FCC_A1
Global test at    9.20000E-02 .... OK
Global test at    8.20000E-02 .... OK
Global test at    7.20000E-02 .... OK
Global test at    6.20000E-02 .... OK
Global test at    5.20000E-02 .... OK
Global test at    4.20000E-02 .... OK
Global test at    3.20000E-02 .... OK
Global test at    2.20000E-02 .... OK
Global test at    1.20000E-02 .... OK
Global test at    2.00000E-03 .... OK
Terminating at    0.100000E-03
Calculated    103 equilibria
*** Buffer saved on file: C:\Users\developer\Documents\RESULT_002.POLY3
POLY_3: s-c t=1373,x(al)=.1
POLY_3: c-e,,,,,,,,
Using global minimization procedure
Calculated          209 grid points in          0 s
Found the set of lowest grid points in          0 s
Calculated POLY solution          0 s, total time  0 s
POLY_3: s-a-v 1 x(al) 0.0001 .20 0.001,,,,
POLY_3: step
Option? /NORMAL/:
Step will start from axis value    0.100000
...OK

Phase Region from    0.100000    for:
FCC_A1
Global test at    1.08000E-01 .... OK
Global test at    1.18000E-01 .... OK
Global test at    1.28000E-01 .... OK
Global test at    1.38000E-01 .... OK
Global test at    1.48000E-01 .... OK
Global test at    1.58000E-01 .... OK
Global test at    1.68000E-01 .... OK
Global test at    1.78000E-01 .... OK
Global test at    1.88000E-01 .... OK
Global test at    1.98000E-01 .... OK
Terminating at    0.200000
Calculated    103 equilibria

Phase Region from    0.100000    for:
FCC_A1
Global test at    9.20000E-02 .... OK

```

```

Global test at 8.20000E-02 .... OK
Global test at 7.20000E-02 .... OK
Global test at 6.20000E-02 .... OK
Global test at 5.20000E-02 .... OK
Global test at 4.20000E-02 .... OK
Global test at 3.20000E-02 .... OK
Global test at 2.20000E-02 .... OK
Global test at 1.20000E-02 .... OK
Global test at 2.00000E-03 .... OK
Terminating at 0.100000E-03
Calculated 103 equilibria
*** Buffer saved on file: C:\Users\developer\Documents\RESULT_002.POLY3
POLY_3: s-c t=1323,x(al)=.1
POLY_3: c-e,,,,,,,,
Using global minimization procedure
Calculated 209 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY_3: s-a-v 1 x(al) 0.0001 .20 0.001,,,,
POLY_3: step
Option? /NORMAL/:
Step will start from axis value 0.100000
...OK

Phase Region from 0.100000 for:
FCC_A1
Global test at 1.08000E-01 .... OK
Global test at 1.18000E-01 .... OK
Global test at 1.28000E-01 .... OK
Global test at 1.38000E-01 .... OK
Global test at 1.48000E-01 .... OK
Global test at 1.58000E-01 .... OK
Global test at 1.68000E-01 .... OK
Global test at 1.78000E-01 .... OK
Global test at 1.88000E-01 .... OK
Global test at 1.98000E-01 .... OK
Terminating at 0.200000
Calculated 103 equilibria

Phase Region from 0.100000 for:
FCC_A1
Global test at 9.20000E-02 .... OK
Global test at 8.20000E-02 .... OK
Global test at 7.20000E-02 .... OK
Global test at 6.20000E-02 .... OK
Global test at 5.20000E-02 .... OK
Global test at 4.20000E-02 .... OK
Global test at 3.20000E-02 .... OK
Global test at 2.20000E-02 .... OK
Global test at 1.20000E-02 .... OK
Global test at 2.00000E-03 .... OK
Terminating at 0.100000E-03
Calculated 103 equilibria
*** Buffer saved on file: C:\Users\developer\Documents\RESULT_002.POLY3
POLY_3: s-c t=1273,x(al)=.1
POLY_3: c-e,,,,,,,,
Using global minimization procedure
Calculated 209 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY_3: s-a-v 1 x(al) 0.0001 .20 0.001,,,,
POLY_3: step
Option? /NORMAL/:
Step will start from axis value 0.100000
...OK

Phase Region from 0.100000 for:
FCC_A1
Global test at 1.08000E-01 .... OK
Global test at 1.18000E-01 .... OK
Global test at 1.28000E-01 .... OK
Global test at 1.38000E-01 .... OK
Global test at 1.48000E-01 .... OK
Global test at 1.58000E-01 .... OK
Global test at 1.68000E-01 .... OK
Global test at 1.78000E-01 .... OK
Global test at 1.88000E-01 .... OK
Global test at 1.98000E-01 .... OK
Terminating at 0.200000
Calculated 103 equilibria

Phase Region from 0.100000 for:
FCC_A1
Global test at 9.20000E-02 .... OK
Global test at 8.20000E-02 .... OK
Global test at 7.20000E-02 .... OK
Global test at 6.20000E-02 .... OK
Global test at 5.20000E-02 .... OK
Global test at 4.20000E-02 .... OK
Global test at 3.20000E-02 .... OK
Global test at 2.20000E-02 .... OK
Global test at 1.20000E-02 .... OK
Global test at 2.00000E-03 .... OK
Terminating at 0.100000E-03
Calculated 103 equilibria
*** Buffer saved on file: C:\Users\developer\Documents\RESULT_002.POLY3
POLY_3: @@
POLY_3: @@ ENTER THE POST MODULE, PLOT THE DIFFUSIVITY ON THE Y-AXIS
POLY_3: @@ AND MOLE-FRACTION AL ON THE X-AXIS.
POLY_3: @@
POLY_3: post

POLY-3 POSTPROCESSOR VERSION 3.2

POST:
POST: s-d-a x m-f al
POST: s-d-a y logdc(fcc,al,al,ni)
POST:
POST: app y yama.exp
PROLOGUE NUMBER: /0/: 1
DATASET NUMBER(s): /-1/: 1 2 3 4 5 6 7
POST:
POST:
POST: s-t-m-s y

```

COMMAND NOT SUPPORTED IN THIS PLOT DRIVER

POST: s-s-s y n -15 -11.7

POST: s-t-m-s y

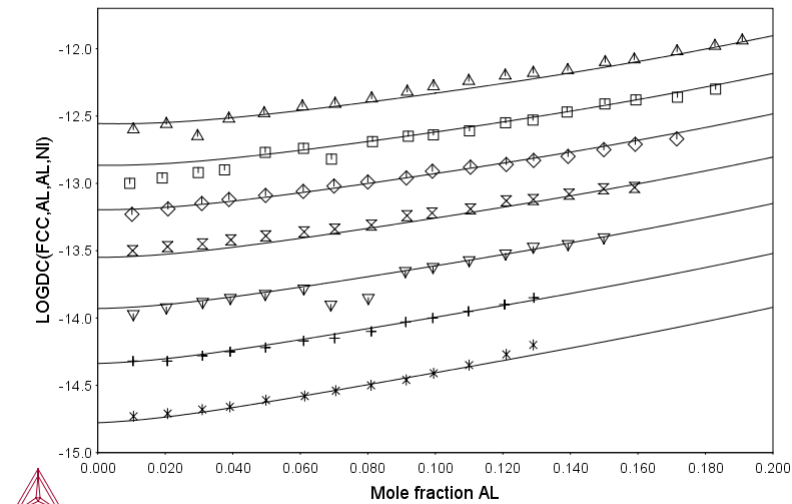
COMMAND NOT SUPPORTED IN THIS PLOT DRIVER

POST: plo

2018.02.18.22.24.24

MOB2: AL, NI

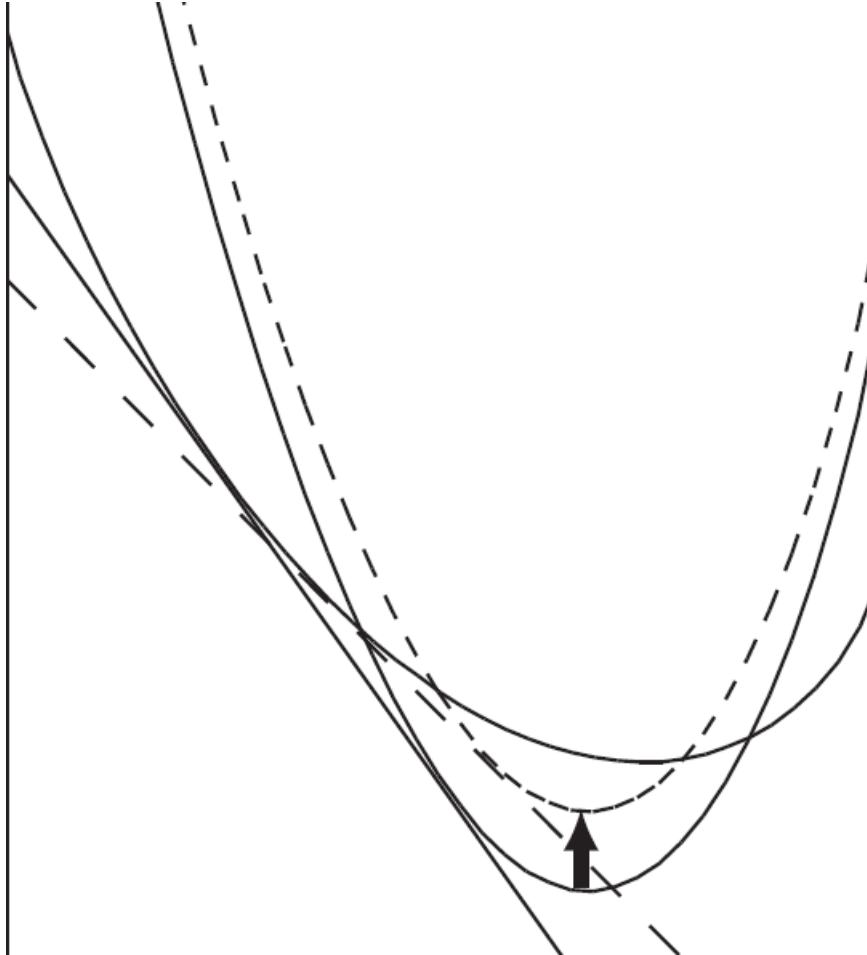
T=1273, N=1., P=1.01325E5



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



Deviation From Local Equilibrium

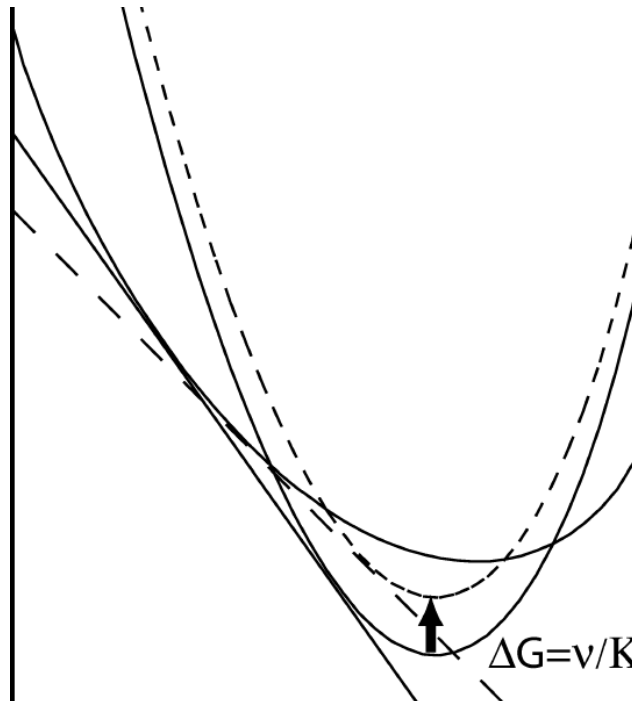




Example exh1

σ/γ diffusion couple with limited interface mobility

This example calculates the growth of ferrite (α) into austenite (γ) with a limited interface mobility. This is achieved by adding a Gibbs-energy contribution to the ferrite using the SET-SURFACE-ENERGY command.



exh1-setup

About

```
SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exh1\setup.DCM"SYS: @@
SYS: @@ Deviation from local equilibrium.
SYS: @@ Ferrite/austenite diffusion couple with interface mobility
SYS: @@ This example calculates the growth of ferrite into austenite with
SYS: @@ a limited interface mobility. this is done by adding a Gibbs-energy
SYS: @@ contribution to the ferrite using the SET-SURFACE-ENERGY command.
SYS: -----
NO SUCH COMMAND, USE HELP
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASE
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Current database: Steels/Fe-Alloys v9.0

VA          /-  DEFINED
L12_FCC     B2_BCC          DICTRA_FCC_A1
REJECTED

TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE THE DATA
TDB_TCFE9: @@
TDB_TCFE9: sw FEDEMO
Current database: Iron Demo Database v2.0

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

List of references for assessed data

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

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

List of references for assessed data

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

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

```

DIC> enter-region
REGION NAME : austenite
ATTACH TO REGION NAMED /FERRITE/:
ATTACHED TO THE RIGHT OF FERRITE /YES/:
DIC>
DIC> @@
DIC> @@ ENTER GRIDS INTO THE REGIONS
DIC> @@
DIC> enter-grid
REGION NAME : /FERRITE/: ferrite
WIDTH OF REGION /1/: 1e-9
TYPE /LINEAR/: AUTO
DIC>
DIC> enter-grid austenite
WIDTH OF REGION /1/: 0.999e-6
TYPE /LINEAR/: AUTO
DIC>
DIC> @@
DIC> @@ ENTER THE active PHASES INTO THE REGIONS
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /FERRITE/: ferrite
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: bcc
DIC>
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /AUSTENITE/: austenite
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITION INTO BCC
DIC> @@
DIC> enter-composition
REGION NAME : /FERRITE/: ferrite
PHASE NAME: /BCC_A2/: bcc
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: C
TYPE /LINEAR/: linear
VALUE OF FIRST POINT : 0.019091893
VALUE OF LAST POINT : /1.9091893E-2/: 0.019091893
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITION INTO FCC
DIC> @@
DIC> enter-composition
REGION NAME : /AUSTENITE/: austenite
PHASE NAME: /FCC_A1/: fcc#1
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: C
TYPE /LINEAR/: linear
VALUE OF FIRST POINT : 0.0191
VALUE OF LAST POINT : /1.91E-2/: 0.0191
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exhl y
DIC>
DIC> set-inter
--OK--
DIC>

```

exh1-run

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exh1\run.DCM"DIC>
DIC>
DIC> @@
DIC> @@ READ THE SETUP FROM FILE AND START THE SIMULATION
DIC> @@
DIC>
DIC> go d-m
TIME STEP AT TIME 0.00000E+00
DIC>
DIC> read exh1
OK
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-sim-time
END TIME FOR INTEGRATION /.1/: 2.5E-3
AUTOMATIC TIMESTEP CONTROL /YES/: YES
MAX TIMESTEP DURING INTEGRATION /2.5E-04/:
INITIAL TIMESTEP : /1E-07/: 1E-7
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/: 1E-7
DIC>
DIC>
DIC> @@
DIC> @@ START THE SIMULATION
DIC> @@
DIC> sim
Region: FERRITE
single geometric dense at 0.10000E-08
0.99998 24
Region: AUSTENITE
single geometric dense at 0.0000
1.0666 84
Trying old scheme 3
U-FRACTION IN SYSTEM: C = 8.88253285685629E-04 FE = 1
TOTAL SIZE OF SYSTEM: 1E-06 [m]
U-FRACTION IN SYSTEM: C = 8.88253285685629E-04 FE = 1
TOTAL SIZE OF SYSTEM: 1E-06 [m]
2.137709938668809E-004 2.137625593908550E-004 13.8289495127833 2.120998911211383E-004 2.112667987639259E-
004 2.108508673392353E-004 2.106430553153946E-004 2.104353457505012E-004 2.101948160083122E-
004 2.097141691516830E-004 2.087545259495225E-004 2.068418415894586E-004 2.030428810465509E-
004 1.955505926692782E-004 1.809885467492963E-004 1.535545782472665E-004 1.054471345952774E-
004 3.627422069935879E-005 13.8289494178875 3.615700697463181E-005 3.609847124386777E-
005 3.606922116142028E-005 3.605460056591150E-005 3.603998293423047E-005 3.602477904360235E-
005 3.599438088533936E-005 3.593362306058377E-005 3.581226137811151E-005 3.557015388125908E-
005 3.508840236026233E-005 3.413475320871956E-005 3.226687046760648E-005 2.868876723327018E-
005 2.216320975615694E-005 1.163469076818617E-005 7.48347199232498 1.161266684728771E-
005 1.160166271119065E-005 1.159616259921805E-005 1.159341303224015E-005 1.159066379128802E-
005 1.158790570211405E-005 1.158239050832246E-005 1.157136405908550E-005 1.154932691389981E-
005 1.150531563662104E-005 1.141754513473569E-005 1.124301234138844E-005 1.089797959650757E-
005 1.022404547389298E-005 1.490118083345267E-002 1.019021771314144E-005 1.017332485335765E-
005 1.016488367857833E-005 1.016066440497390E-005 1.015644600723762E-005 1.015204959594981E-
005 1.014325962855260E-005 1.012569111466427E-005 1.009059977048929E-005 1.002059981643303E-
005 9.881330845574529E-006 4.762707187234291E-006 4.438313610609329E-003 2.058831409609227E-
006 2.181365147016879E-007 6.215863080991705E-009 1.005966849204609E-011 2.807707691965722E-
008 1.740878263349759E-015 2.916483860250238E-008 3.123181243512367E-019 TIME = 0.10000000E-06 DT = 0.10000000E-
06 SUM OF SQUARES = 0.31231812E-18
CELL # 1 VELOCITY AT INTERFACE # 2 IS 4.9961063 AND 4.9961063
POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.50061063E-06
U-FRACTION IN SYSTEM: C = 9.00101592838844E-04 FE = 1
TOTAL SIZE OF SYSTEM: 1E-06 [m]
19 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: FERRITE
3 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: AUSTENITE

CPU time used in timestep 0 seconds

output ignored...

... output resumed

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

CPU time used in timestep 0 seconds
1.224778860998174E-007 1.223249305229064E-007 2.395848834555112E-010 6.518470747369290E-013 4.308904388595452E-
018 TIME = 0.24993550E-02 DT = 0.73586367E-06 SUM OF SQUARES = 0.43089044E-17
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.10897992E-02 AND 0.10897992E-02
POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.93871144E-06
U-FRACTION IN SYSTEM: C = 8.98994454594015E-04 FE = 1
TOTAL SIZE OF SYSTEM: 1E-06 [m]
CPU time used in timestep 0 seconds
3.060424563913232E-007 3.057378465845341E-007 3.253009099214644E-010 5.404686073474901E-013 1.316128993548938E-
018 TIME = 0.24997404E-02 DT = 0.38538368E-06 SUM OF SQUARES = 0.13161290E-17
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.12900930E-02 AND 0.12900930E-02
POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.93920862E-06
U-FRACTION IN SYSTEM: C = 8.9905213314465E-04 FE = 1
TOTAL SIZE OF SYSTEM: 1E-06 [m]
1 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: FERRITE

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

```
1.382362431546073E-006      1.381359929145516E-006      1.794347463483156E-010      9.495490590523165E-015      3.811431082021190E-
022      TIME = 0.25000000E-02 DT = 0.62515089E-07 SUM OF SQUARES = 0.38114311E-21
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.18529405E-02 AND 0.18529405E-02
POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.93961729E-06
U-FRACTION IN SYSTEM: C = 8.99171776165061E-04 FE = 1
TOTAL SIZE OF SYSTEM: 1E-06 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 0.00000000
DELETING TIME-RECORD FOR TIME 0.10000000E-06
DELETING TIME-RECORD FOR TIME 0.30000000E-06
DELETING TIME-RECORD FOR TIME 0.70000000E-06
DELETING TIME-RECORD FOR TIME 0.15000000E-05
DELETING TIME-RECORD FOR TIME 0.28565340E-05
DELETING TIME-RECORD FOR TIME 0.52015355E-05
DELETING TIME-RECORD FOR TIME 0.98915385E-05
DELETING TIME-RECORD FOR TIME 0.19271544E-04
DELETING TIME-RECORD FOR TIME 0.33687180E-04
DELETING TIME-RECORD FOR TIME 0.53417475E-04
DELETING TIME-RECORD FOR TIME 0.78654357E-04
DELETING TIME-RECORD FOR TIME 0.10952898E-03
DELETING TIME-RECORD FOR TIME 0.14613093E-03
DELETING TIME-RECORD FOR TIME 0.18853080E-03
DELETING TIME-RECORD FOR TIME 0.23679894E-03
DELETING TIME-RECORD FOR TIME 0.29104868E-03
DELETING TIME-RECORD FOR TIME 0.35145422E-03
DELETING TIME-RECORD FOR TIME 0.41823577E-03
DELETING TIME-RECORD FOR TIME 0.48723333E-03
DELETING TIME-RECORD FOR TIME 0.55628734E-03
DELETING TIME-RECORD FOR TIME 0.62546243E-03
DELETING TIME-RECORD FOR TIME 0.69481214E-03
DELETING TIME-RECORD FOR TIME 0.76438006E-03
DELETING TIME-RECORD FOR TIME 0.83419596E-03
DELETING TIME-RECORD FOR TIME 0.90425844E-03
DELETING TIME-RECORD FOR TIME 0.97473720E-03
DELETING TIME-RECORD FOR TIME 0.10456577E-02
DELETING TIME-RECORD FOR TIME 0.11169996E-02
DELETING TIME-RECORD FOR TIME 0.11887867E-02
DELETING TIME-RECORD FOR TIME 0.12609691E-02
DELETING TIME-RECORD FOR TIME 0.13331751E-02
DELETING TIME-RECORD FOR TIME 0.14056136E-02
DELETING TIME-RECORD FOR TIME 0.14782826E-02
DELETING TIME-RECORD FOR TIME 0.15511175E-02
DELETING TIME-RECORD FOR TIME 0.16239994E-02
DELETING TIME-RECORD FOR TIME 0.16973709E-02
DELETING TIME-RECORD FOR TIME 0.17714236E-02
DELETING TIME-RECORD FOR TIME 0.18459453E-02
DELETING TIME-RECORD FOR TIME 0.19208358E-02
DELETING TIME-RECORD FOR TIME 0.19960898E-02
DELETING TIME-RECORD FOR TIME 0.20715732E-02
DELETING TIME-RECORD FOR TIME 0.21477958E-02
DELETING TIME-RECORD FOR TIME 0.22245450E-02
DELETING TIME-RECORD FOR TIME 0.23020845E-02
DELETING TIME-RECORD FOR TIME 0.23637495E-02
DELETING TIME-RECORD FOR TIME 0.24066138E-02
DELETING TIME-RECORD FOR TIME 0.24364991E-02
DELETING TIME-RECORD FOR TIME 0.24572377E-02
DELETING TIME-RECORD FOR TIME 0.24715984E-02
DELETING TIME-RECORD FOR TIME 0.24814555E-02
DELETING TIME-RECORD FOR TIME 0.24881136E-02
DELETING TIME-RECORD FOR TIME 0.24925865E-02
DELETING TIME-RECORD FOR TIME 0.24955318E-02
DELETING TIME-RECORD FOR TIME 0.24974221E-02
DELETING TIME-RECORD FOR TIME 0.24986191E-02
DELETING TIME-RECORD FOR TIME 0.24993550E-02
DELETING TIME-RECORD FOR TIME 0.24997404E-02

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

TIMESTEP AT 0.25000000E-02 SELECTED

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

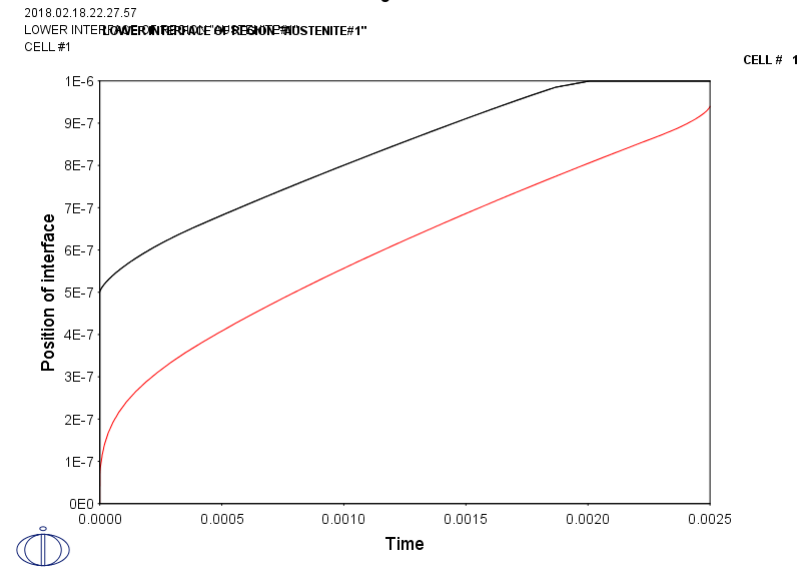
exh1-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exh1\plot.DCM"DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 2.50000E-03
DIC>
DIC> read exh1
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post

POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
```

```
POST-1:
POST-1: @@
POST-1: @@ SET THE DATA APPENDED FROM THE "EXP" FILE TO BE READ
POST-1: @@
POST-1: set-col for for red
COMMAND NOT SUPPORTED IN THIS PLOT DRIVER
POST-1:
POST-1: @@
POST-1: @@ COMPARE THE POSITION OF THE INTERFACE AS A FUNCTION OF TIME
POST-1: @@
POST-1: s-d-a x time
INFO: Time is set as independent variable
POST-1: s-d-a y posi aus low
POST-1:
POST-1: @@
POST-1: @@ APPEND THE SIMULATION (WITHOUT THE ENERGY CONTRIBUTION) FROM FILE
POST-1: @@
POST-1: app y noadd.exp 1; 1
POST-1:
POST-1: @@
POST-1: @@ SET A TITLE ON THE PLOT
POST-1: @@
POST-1: set-title Figure h1
POST-1:
POST-1: @@
POST-1: @@ PLOT THE RESULTS
POST-1: @@
POST-1: plot
```

Figure h1



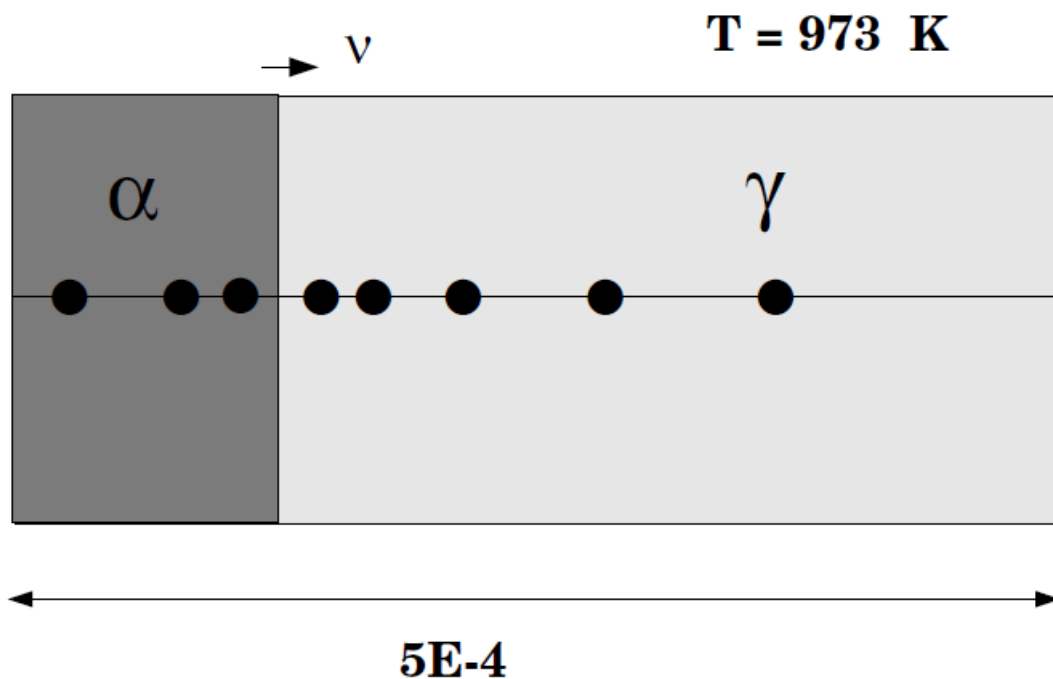
```
POST-1:
POST-1:
POST-1: set-inter
--OK--
POST-1:
```



Example exh2

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

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



exh2-setup

```
AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exh2\setup.DCM"SYS: @@
SYS: @@ Deviation from local equilibrium.
SYS: @@ Ferrite/austenite para-equilibrium in an Fe-Ni-C alloy
SYS: @@ This example calculates the growth of ferrite into austenite
SYS: @@ in an Fe-2.02%Ni-0.0885%C alloy using the para-equilibrium model.
SYS: @@ The results are compared with experimental information from
SYS: @@ Hutchinson, C. R., A. Fuchsmann, and Yves Brechet. "The diffusional
SYS: @@ formation of ferrite from austenite in Fe-C-Ni alloys." Metall.
SYS: @@ Mat. Trans. A 35.4 (2004): 1211-1221.
SYS: -----
NO SUCH COMMAND, USE HELP
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASE
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Current database: Steels/Fe-Alloys v9.0

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

VA          /- DEFINED
TDB_FEDEMO: def-sys fe ni c
FE          NI          C
DEFINED
TDB_FEDEMO: rej ph * all
GAS:G      LIQUID:L      BCC_A2
CEMENTITE   DIAMOND_FCC_A4 FCC_A1
GRAPHITE    HCP_A3      KSI_CARBIDE
LAVES_PHASE_C14 M23C6      M5C2
M7C3_REJECTED
TDB_FEDEMO: res ph bcc fcc
BCC_A2      FCC_A1 RESTORED
TDB_FEDEMO: get
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

List of references for assessed data

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

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

List of references for assessed data

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

```

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

DIC>
DIC> @@
DIC> @@ START BY ENTERING THE REGIONS ferrite AND austenite WHERE THE
DIC> @@ BCC AND FCC PHASES ARE PUT, RESPECTIVELY. THE FERRITE REGION IS
DIC> @@ ASSUMED INITIALLY TO BE VERY THIN, 1E-9 METERS.
DIC> @@
DIC> enter-region
REGION NAME : ferrite
DIC>
DIC> enter-region
REGION NAME : austenite
ATTACH TO REGION NAMED /FERRITE/:
ATTACHED TO THE RIGHT OF FERRITE /YES/:
DIC>
DIC> @@
DIC> @@ ENTER GRIDS INTO THE REGIONS
DIC> @@
DIC> enter-grid
REGION NAME : /FERRITE/: ferrite
WIDTH OF REGION /1/: 1e-9
TYPE /LINEAR/: AUTO
DIC>
DIC> enter-grid austenite
WIDTH OF REGION /1/: 50e-6
TYPE /LINEAR/: AUTO
DIC>
DIC> @@
DIC> @@ ENTER active PHASES INTO THE REGIONS
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /FERRITE/: ferrite
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: bcc
DIC>
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /AUSTENITE/: austenite
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITION INTO BCC
DIC> @@
DIC> enter-composition
REGION NAME : /FERRITE/: ferrite
PHASE NAME: /BCC_A2/: bcc
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: c
TYPE /LINEAR/: linear
VALUE OF FIRST POINT : 0.0885
VALUE OF LAST POINT : /8.85E-2/: 0.0885
PROFILE FOR /NI/: ni
TYPE /LINEAR/: linear
VALUE OF FIRST POINT : 2.02
VALUE OF LAST POINT : /2.02/: 2.02
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITION INTO FCC
DIC> @@
DIC> enter-composition
REGION NAME : /AUSTENITE/: austenite
PHASE NAME: /FCC_A1/: fcc#1
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: c
TYPE /LINEAR/: linear
VALUE OF FIRST POINT : 0.0885
VALUE OF LAST POINT : /8.85E-2/: 0.0885
PROFILE FOR /NI/: ni
TYPE /LINEAR/: linear
VALUE OF FIRST POINT : 2.02
VALUE OF LAST POINT : /2.02/: 2.02
DIC>
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exh2 y
DIC>
DIC> set-inter
--OK--
DIC>

```

exh2-run

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exh2\run.DCM"DIC>
DIC>
DIC>
DIC> @@
DIC> @@ FILE TO RUN EXAMPLE exh2
DIC> @@
DIC>
DIC> @@
DIC> @@ READ THE SETUP FROM FILE
DIC> @@
DIC>
DIC> go d-m
TIME STEP AT TIME 0.00000E+00
DIC>
DIC> read exh2
OK
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-sim-time 50,,,,,,,,,
DIC>
DIC>
DIC> @@
DIC> @@ ENABLE THE PARA-EQUILIBRIUM MODEL
DIC> @@
DIC> para
ENABLE PARAEQ : /NO/: YES
U-FRACTION OF COMPONENT FE /AUTO/: AUTO
U-FRACTION OF COMPONENT NI /AUTO/: AUTO
DIC>
DIC> @@
DIC> @@ START THE SIMULATION
DIC> @@
DIC> sim
Region: FERRITE
single geometric dense at 0.10000E-08
0.99997 24
Region: AUSTENITE
single geometric dense at 0.0000
1.1602 98
Trying old scheme 4
GENERATING STARTING VALUES FOR CELL # 1 INTERFACE # 2
DETERMINING INITIAL EQUILIBRIUM VALUES
CALCULATING STARTING VALUES: 9 EQUILIBRIUM CALCULATIONS DONE 6 OUT OF 9

U-FRACTION IN SYSTEM: C = .00412262676333 FE = .980742621143594
NI = .0192573788564064
TOTAL SIZE OF SYSTEM: 5.0001E-05 [m]
U-FRACTION IN SYSTEM: C = .00412262676333 FE = .980742621143594
NI = .0192573788564064
TOTAL SIZE OF SYSTEM: 5.0001E-05 [m]
13403.6958745548 13403.6958745560 13396.6824657623 181.652814770282 1.24966106488886 3.83383219646144
003 1.422760580718459E-005 4.522508972366437E-007 2.881050295641052E-014 TIME = 0.10000000E-06 DT = 0.10000000E-
06 SUM OF SQUARES = 0.28810503E-13
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.20145484E-01 AND 0.20145484E-01
POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.30145484E-08
U-FRACTION IN SYSTEM: C = .00412273714809213 FE = .980742621143594
NI = .0192573788564064
TOTAL SIZE OF SYSTEM: 5.0001E-05 [m]
11 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: AUSTENITE

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

output ignored...

... output resumed

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

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

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

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

```
CPU time used in timestep                2 seconds
5794.90030702191      5794.90030702416      5789.28666554113      21.1377744513434      5.223026175570823E-
002      1.429845859724257E-002      3.466078132925075E-005      1.478441856462062E-007      1.640219090103663E-
003      7.286653961560384E-018      TIME = 50.000000      DT = 0.99808403      SUM OF SQUARES = 0.72866540E-17
CELL # 1 VELOCITY AT INTERFACE # 2 IS 0.23051013E-06 AND 0.23051013E-06
POSITION OF INTERFACE FERRITE / AUSTENITE IS 0.15151336E-04
U-FRACTION IN SYSTEM: C = .0041309481336738 FE = .980742621143594
NI = .0192573788564067
```

TOTAL SIZE OF SYSTEM: 5.0001E-05 [m]

MUST SAVE WORKSPACE ON FILE

WORKSPACE SAVED ON FILE

RECLAIMING WORKSPACE

DELETING TIME-RECORD FOR TIME 0.0000000

DELETING TIME-RECORD FOR TIME 0.10000000E-06

DELETING TIME-RECORD FOR TIME 0.20000000E-06

DELETING TIME-RECORD FOR TIME 0.35656740E-06

DELETING TIME-RECORD FOR TIME 0.63794974E-06

DELETING TIME-RECORD FOR TIME 0.11506591E-05

DELETING TIME-RECORD FOR TIME 0.21687314E-05

DELETING TIME-RECORD FOR TIME 0.42048761E-05

DELETING TIME-RECORD FOR TIME 0.82771656E-05

DELETING TIME-RECORD FOR TIME 0.15887371E-04

DELETING TIME-RECORD FOR TIME 0.25918565E-04

DELETING TIME-RECORD FOR TIME 0.39472933E-04

DELETING TIME-RECORD FOR TIME 0.59571679E-04

DELETING TIME-RECORD FOR TIME 0.95661762E-04

DELETING TIME-RECORD FOR TIME 0.16784193E-03

DELETING TIME-RECORD FOR TIME 0.31220226E-03

DELETING TIME-RECORD FOR TIME 0.60092292E-03

DELETING TIME-RECORD FOR TIME 0.11783643E-02

DELETING TIME-RECORD FOR TIME 0.20786157E-02

DELETING TIME-RECORD FOR TIME 0.34937926E-02

DELETING TIME-RECORD FOR TIME 0.60665663E-02

DELETING TIME-RECORD FOR TIME 0.11212114E-01

DELETING TIME-RECORD FOR TIME 0.21503208E-01

DELETING TIME-RECORD FOR TIME 0.40842356E-01

DELETING TIME-RECORD FOR TIME 0.75054322E-01

DELETING TIME-RECORD FOR TIME 0.13545785

DELETING TIME-RECORD FOR TIME 0.24516935

DELETING TIME-RECORD FOR TIME 0.44180830

DELETING TIME-RECORD FOR TIME 0.79606820

DELETING TIME-RECORD FOR TIME 1.4337573

DELETING TIME-RECORD FOR TIME 2.5843697

DELETING TIME-RECORD FOR TIME 4.6661977

DELETING TIME-RECORD FOR TIME 6.9580953

DELETING TIME-RECORD FOR TIME 9.4344356

DELETING TIME-RECORD FOR TIME 12.083242

DELETING TIME-RECORD FOR TIME 14.887008

DELETING TIME-RECORD FOR TIME 17.833560

DELETING TIME-RECORD FOR TIME 20.908984

DELETING TIME-RECORD FOR TIME 24.107288

DELETING TIME-RECORD FOR TIME 27.422352

DELETING TIME-RECORD FOR TIME 30.849994

DELETING TIME-RECORD FOR TIME 34.377834

DELETING TIME-RECORD FOR TIME 38.001764

DELETING TIME-RECORD FOR TIME 41.718584

DELETING TIME-RECORD FOR TIME 45.525738

KEEPING TIME-RECORD FOR TIME 49.001916

AND FOR TIME 50.000000

WORKSPACE RECLAIMED

TIMESTEP AT 50.0000000 SELECTED

DIC>

DIC>

DIC> set-inter

OK---

DIC>

exh2-plot

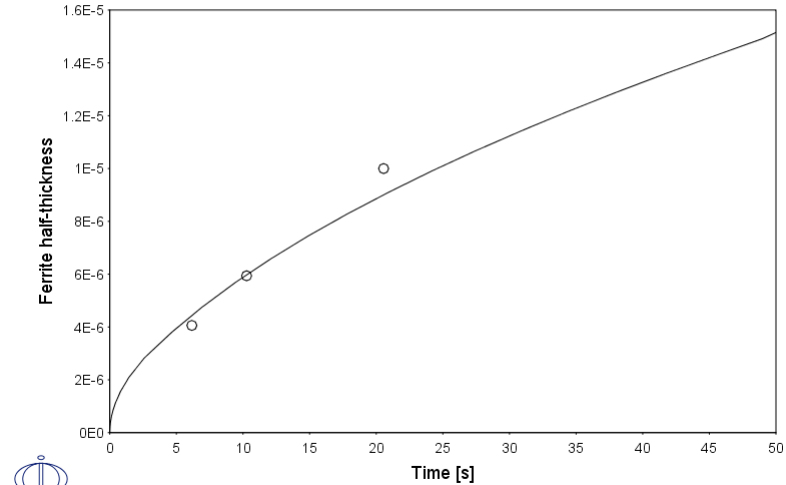
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exh2\plot.DCM"DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 5.00000E+01
DIC>
DIC> read exh2
OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post

POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
```

```
POST-1:
POST-1:
POST-1: @@
POST-1: @@ WE WANT TO PLOT THE POSITION OF THE INTERFACE AS A FUNCTION OF TIME
POST-1: @@ I.E. THE FERRITE HALF-THICKNESS
POST-1: @@
POST-1: s-d-a x time
INFO: Time is set as independent variable
POST-1: s-d-a y posi aus low
POST-1:
POST-1: @@
POST-1: @@ APPEND THE EXPERIMENTAL INFORMATION
POST-1: @@
POST-1: app y exh2.exp 1; 1
POST-1:
POST-1: @@
POST-1: @@ SET A TITLE ON THE PLOT
POST-1: @@
POST-1: set-title Figure h2
POST-1:
POST-1: @@
POST-1: @@ RENAME THE AXIS LABELS
POST-1: @@
POST-1: set-axis-text-status
AXIS (X, Y OR Z) : x
AUTOMATIC AXIS TEXT (Y OR N) /N/: NO
AXIS TEXT : Time [s]
POST-1:
POST-1: set-axis-text-status
AXIS (X, Y OR Z) : y
AUTOMATIC AXIS TEXT (Y OR N) /N/: NO
AXIS TEXT : Ferrite half-thickness
POST-1:
POST-1: @@
POST-1: @@ PLOT THE RESULTS
POST-1: @@
POST-1: plot
```

Figure h2

2018.02.18.22.32.07
LOWER INTERFACE OF REGION "AUSTENITE#1"
CELL #1



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

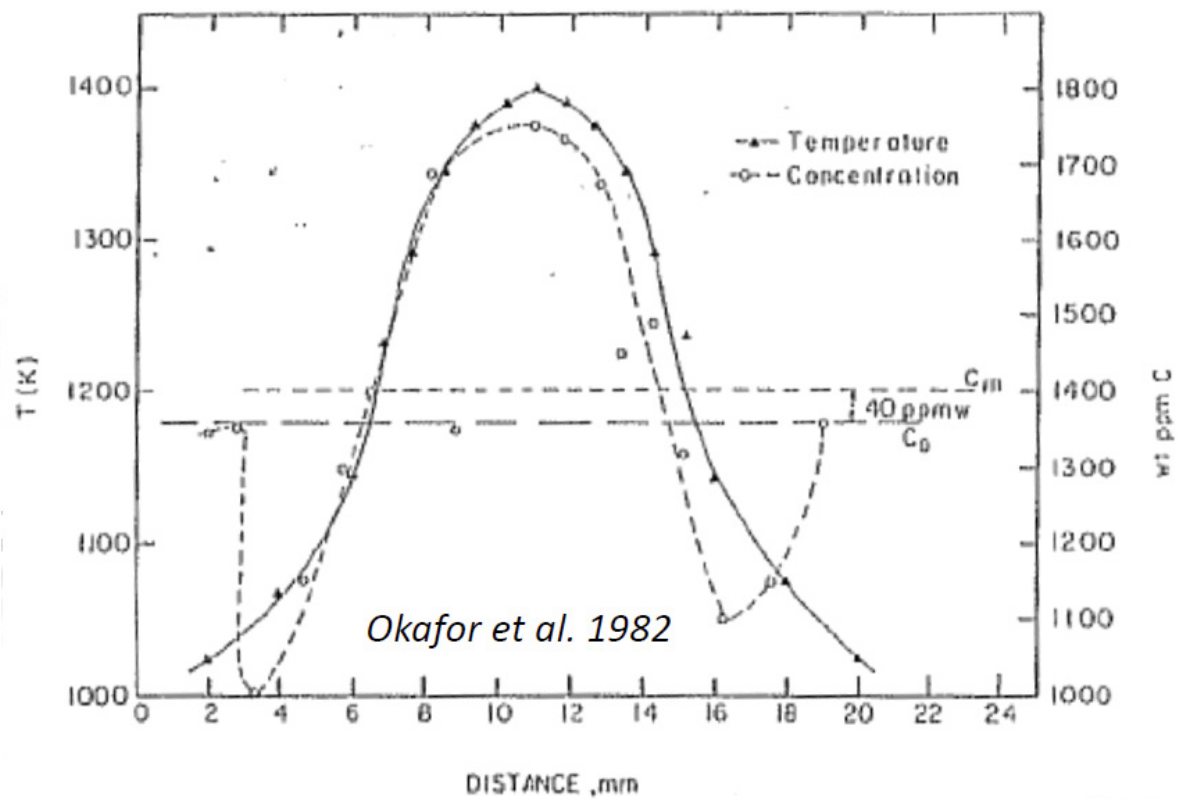


Example exh3

Diffusion induced by a temperature gradient (thermomigration)

This calculation shows how a temperature gradient induces diffusion.

$$J_C = -\frac{u_C}{V_s} y_{Va} M_{CVa} \left(\frac{\partial \mu_C}{\partial x} + \frac{Q_C^*}{T} \frac{\partial T}{\partial x} \right)$$



exh3-setup

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

```
SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exh3\setup.DCM"SYS: @@
SYS: @@ Deviation from local equilibrium.
SYS: @@ Diffusion induced by a temperature gradient (thermomigration)
SYS: @@ This calculation shows how a temperature gradient induces
SYS: @@ diffusion.
SYS: -----
NO SUCH COMMAND, USE HELP
SYS:
SYS: go da
THERMODYNAMIC DATABASE module
Current database: Steels/Fe-Alloys v9.0

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

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

List of references for assessed data

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

-OK-
TDB_FEDEMO: app mfedemo
Current database: Fe-Alloys Mobility demo database v2.0

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

List of references for assessed data

'This parameter has not been assessed'
'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'
'B. Jonsson: Z. Metallkunde 85(1994)502-509; C diffusion in fcc Cr-Fe-Ni'
'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
-Ni'
'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Ni self-diffusion'

-OK-
APP:
APP: go d-m
NO TIME STEP DEFINED
*** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
DIC>
DIC> @@ ENTER A GAUSSIAN-SHAPED TEMPERATURE GRADIENT
DIC> set-cond glob T 0 1000+400*exp(-3.35074E4*(x-11e-3)**2); * N

DIC>
DIC> set-ref C grap,,,,,,,,,
DIC>
DIC> ent-reg aus,,,,,
DIC>
DIC> ent-grid aus 25e-3 auto
DIC>
DIC> ent-pha act aus matrix fcc#1
DIC>
DIC> ent-comp aus fcc#1 fe w-p
PROFILE FOR /C/: c lin 0.14 0.14
PROFILE FOR /NI/: ni lin 32.5 32.5
DIC>
DIC> s-s-time 5E7,,,,,,,,,
DIC>
```

```
DIC> @@ ENTER THE HEAT OF TRANSFER PARAMETER FOR CARBON
DIC> ent-heat-tra-p
HEAT TRANSFER PARAMETER FOR PHASE: fcc
ELEMENT: C
PARAMETER /0/: -42000
DIC>
DIC>
DIC> save exh3 y
DIC>
DIC> set-inter
--OK--
DIC>
```


exh3-run

DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exh3\run.DCM"DIC>

DIC> go d-m

TIME STEP AT TIME 0.00000E+00

*** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE

DIC>

DIC> read exh3

OK

DIC>

DIC> sim

Region: AUS

linear grid 75

U-FRACTION IN SYSTEM: C = .00662305741857947 FE = .68534915460493
NI = .31465084539507

TOTAL SIZE OF SYSTEM: .025 [m]

U-FRACTION IN SYSTEM: C = .00662305741857947 FE = .68534915460493
NI = .31465084539507

TOTAL SIZE OF SYSTEM: .025 [m]

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

U-FRACTION IN SYSTEM: C = .00662305741857946 FE = .68534915460493
NI = .31465084539507

TOTAL SIZE OF SYSTEM: .025 [m]

CPU time used in timestep 0 seconds

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

U-FRACTION IN SYSTEM: C = .00662305741857947 FE = .68534915460493
NI = .31465084539507

TOTAL SIZE OF SYSTEM: .025 [m]

CPU time used in timestep 0 seconds

TIME = 0.40010010 DT = 0.40000000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00662305741857947 FE = .68534915460493
NI = .31465084539507

TOTAL SIZE OF SYSTEM: .025 [m]

CPU time used in timestep 0 seconds

TIME = 1600.4001 DT = 1600.0000 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .0066230574185794 FE = .68534915460493
NI = .31465084539507

TOTAL SIZE OF SYSTEM: .025 [m]

CPU time used in timestep 0 seconds

TIME = 75752.427 DT = 74152.027 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00662305741850892 FE = .68534915460493
NI = .31465084539507

TOTAL SIZE OF SYSTEM: .025 [m]

CPU time used in timestep 1 seconds

TIME = 224056.48 DT = 148304.05 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00662305741822253 FE = .68534915460493
NI = .31465084539507

TOTAL SIZE OF SYSTEM: .025 [m]

CPU time used in timestep 0 seconds

TIME = 520664.59 DT = 296608.11 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00662305741822208 FE = .68534915460493
NI = .31465084539507

TOTAL SIZE OF SYSTEM: .025 [m]

CPU time used in timestep 0 seconds

TIME = 1113880.8 DT = 593216.22 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00662305741822194 FE = .68534915460493
NI = .31465084539507

TOTAL SIZE OF SYSTEM: .025 [m]

CPU time used in timestep 1 seconds

TIME = 2300313.2 DT = 1186432.4 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00662305741819878 FE = .68534915460493
NI = .31465084539507

TOTAL SIZE OF SYSTEM: .025 [m]

CPU time used in timestep 0 seconds

TIME = 4673178.1 DT = 2372864.9 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00662305741817995 FE = .68534915460493
NI = .31465084539507

TOTAL SIZE OF SYSTEM: .025 [m]

CPU time used in timestep 1 seconds

TIME = 7599334.5 DT = 2926156.3 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00662305741819184 FE = .68534915460493
NI = .31465084539507

TOTAL SIZE OF SYSTEM: .025 [m]

CPU time used in timestep 0 seconds

TIME = 10079984. DT = 2480649.1 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00662305741819794 FE = .68534915460493
NI = .31465084539507

TOTAL SIZE OF SYSTEM: .025 [m]

CPU time used in timestep 0 seconds

TIME = 12348045. DT = 2268061.6 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00662305741820075 FE = .68534915460493
NI = .31465084539507

TOTAL SIZE OF SYSTEM: .025 [m]

CPU time used in timestep 1 seconds

TIME = 14506749. DT = 2158703.9 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00662305741820244 FE = .68534915460493
NI = .31465084539507

TOTAL SIZE OF SYSTEM: .025 [m]

CPU time used in timestep 0 seconds

TIME = 16599481. DT = 2092732.2 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00662305741820524 FE = .68534915460493
NI = .31465084539507

TOTAL SIZE OF SYSTEM: .025 [m]

CPU time used in timestep 1 seconds

TIME = 18648923. DT = 2049441.3 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00662305741790953 FE = .685349154604931
NI = .31465084539507

TOTAL SIZE OF SYSTEM: .025 [m]

CPU time used in timestep 0 seconds

TIME = 20668354. DT = 2019431.3 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00662305741737831 FE = .685349154604931
NI = .31465084539507

TOTAL SIZE OF SYSTEM: .025 [m]

CPU time used in timestep 0 seconds

TIME = 22666114. DT = 1997759.7 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00662305741692653 FE = .68534915460493
NI = .31465084539507

TOTAL SIZE OF SYSTEM: .025 [m]

CPU time used in timestep 1 seconds

TIME = 24647703. DT = 1981589.3 SUM OF SQUARES = 0.0000000

U-FRACTION IN SYSTEM: C = .00662305741653748 FE = .68534915460493
NI = .31465084539507

TOTAL SIZE OF SYSTEM: .025 [m]

CPU time used in timestep 0 seconds

```

TIME = 26616876. DT = 1969173.4 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .0066230574162012 FE = .685349154604931
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep 0 seconds
TIME = 28576276. DT = 1959399.6 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741590643 FE = .68534915460493
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep 1 seconds
TIME = 30527808. DT = 1951532.4 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741564765 FE = .68534915460493
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep 0 seconds
TIME = 32472884. DT = 1945075.6 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741542058 FE = .68534915460493
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep 0 seconds
TIME = 34412572. DT = 1939688.3 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741522016 FE = .68534915460493
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep 1 seconds
TIME = 36347704. DT = 1935131.5 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741504403 FE = .68534915460493
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep 0 seconds
TIME = 38278937. DT = 1931233.7 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741488843 FE = .68534915460493
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep 0 seconds
TIME = 40206807. DT = 1927869.8 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741474968 FE = .68534915460493
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep 1 seconds
TIME = 42131753. DT = 1924946.2 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741462626 FE = .68534915460493
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep 0 seconds
TIME = 44054144. DT = 1922391.1 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741451708 FE = .68534915460493
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep 0 seconds
TIME = 45974292. DT = 1920148.0 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741441852 FE = .68534915460493
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep 1 seconds
TIME = 47614300. DT = 1640007.6 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741434809 FE = .685349154604931
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep 0 seconds
TIME = 48910464. DT = 1296163.5 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741430267 FE = .68534915460493
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep 0 seconds
TIME = 49749384. DT = 838920.23 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741428061 FE = .68534915460493
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
CPU time used in timestep 1 seconds
TIME = 50000000. DT = 250616.21 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: C = .00662305741428022 FE = .68534915460493
NI = .31465084539507
TOTAL SIZE OF SYSTEM: .025 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 0.0000000
DELETING TIME-RECORD FOR TIME 0.10000000E-06
DELETING TIME-RECORD FOR TIME 0.10010000E-03
DELETING TIME-RECORD FOR TIME 0.40010010
DELETING TIME-RECORD FOR TIME 1600.4001
DELETING TIME-RECORD FOR TIME 75752.427
DELETING TIME-RECORD FOR TIME 224056.48
DELETING TIME-RECORD FOR TIME 520664.59
DELETING TIME-RECORD FOR TIME 1113880.8
DELETING TIME-RECORD FOR TIME 2300313.2
DELETING TIME-RECORD FOR TIME 4673178.1
DELETING TIME-RECORD FOR TIME 7599334.5
DELETING TIME-RECORD FOR TIME 10079984.
DELETING TIME-RECORD FOR TIME 12348045.
DELETING TIME-RECORD FOR TIME 14506749.
DELETING TIME-RECORD FOR TIME 16599481.
DELETING TIME-RECORD FOR TIME 18648923.
DELETING TIME-RECORD FOR TIME 20668354.
DELETING TIME-RECORD FOR TIME 22666114.
DELETING TIME-RECORD FOR TIME 24647703.
DELETING TIME-RECORD FOR TIME 26616876.
DELETING TIME-RECORD FOR TIME 28576276.
DELETING TIME-RECORD FOR TIME 30527808.
DELETING TIME-RECORD FOR TIME 32472884.
DELETING TIME-RECORD FOR TIME 34412572.
DELETING TIME-RECORD FOR TIME 36347704.
DELETING TIME-RECORD FOR TIME 38278937.
DELETING TIME-RECORD FOR TIME 40206807.
DELETING TIME-RECORD FOR TIME 42131753.
DELETING TIME-RECORD FOR TIME 44054144.
DELETING TIME-RECORD FOR TIME 45974292.
DELETING TIME-RECORD FOR TIME 47614300.
DELETING TIME-RECORD FOR TIME 48910464.
KEEPING TIME-RECORD FOR TIME 49749384.
AND FOR TIME 50000000.
WORKSPACE RECLAIMED
TIMESTEP AT 50000000.0 SELECTED

```

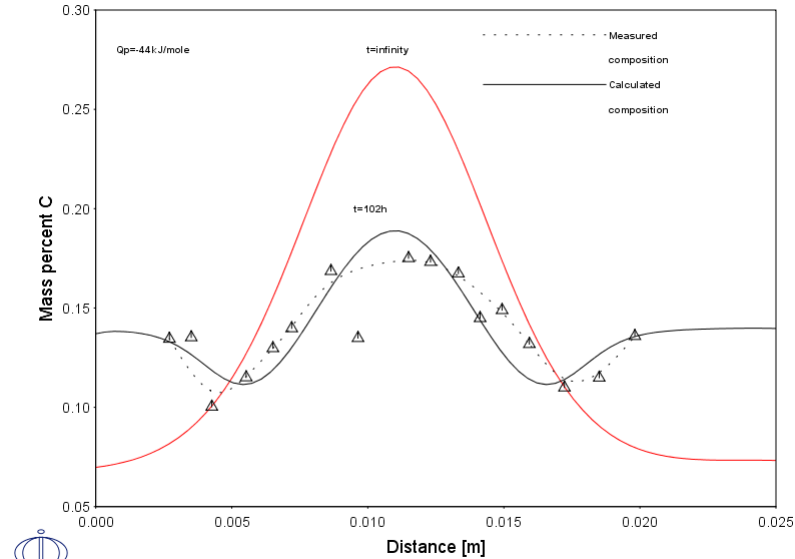
```
DIC>  
DIC> set-inter  
--OK--  
DIC>
```

exh3-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exh3\plot.DCM"DIC> go d-m
TIME STEP AT TIME 5.00000E+07
*** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
DIC>
DIC>
DIC> read exh3
OK
DIC>
DIC> post

POST PROCESSOR VERSION 1.7
Implemented by Bjorn Jonsson
```

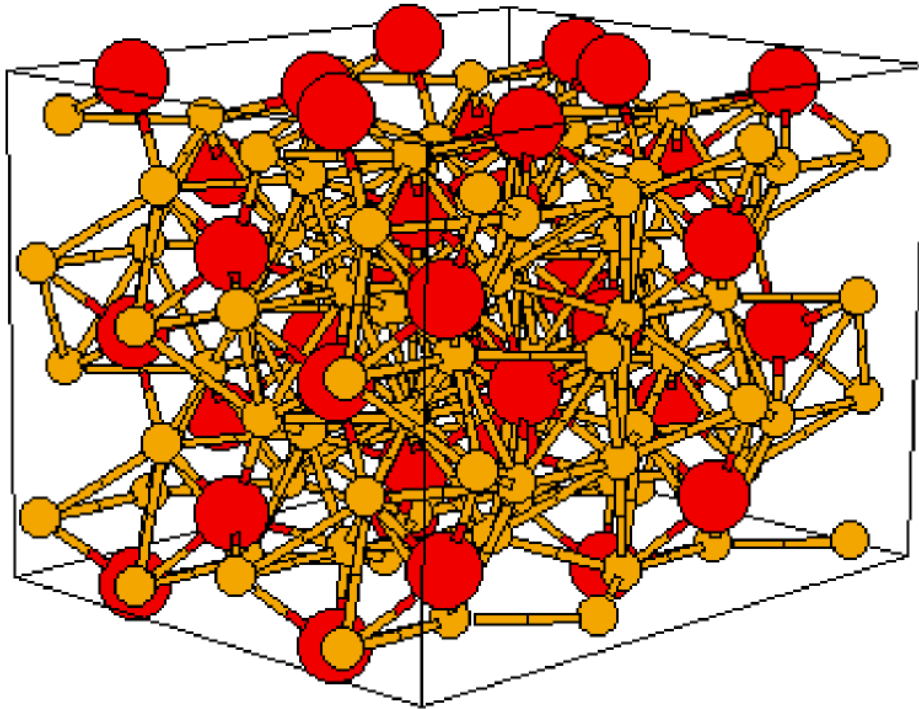
```
POST-1: s-d-a x dist glob
INFO: Distance is set as independent variable
POST-1: s-d-a y w-p c
POST-1: s-p-c time 367200 5E7
POST-1: s-s-s y n 0.1 0.18
POST-1: s-s-s y y
POST-1: app y exh3.exp 0; 1 3;
POST-1: s-p-o n y y n y n n,,,,,,,,,
POST-1:
POST-1: set-ax-text-st x
AUTOMATIC AXIS TEXT (Y OR N) /N/: n
AXIS TEXT : Distance [m]
POST-1:
POST-1: set-ax-text-st y
AUTOMATIC AXIS TEXT (Y OR N) /N/: n
AXIS TEXT : Mass percent C
POST-1:
POST-1: plot
```



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



Diffusion in Complex Phases

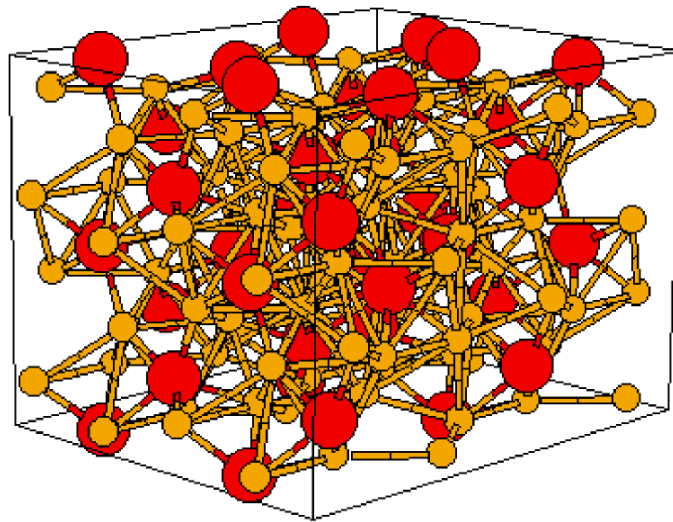




Example exi1

Diffusion in system with B2 ordering

Diffusion 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.



[illegible]

exil-run

DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exil\run.DCM"DIC>

DIC>

DIC> @@ exil_run.DCM

DIC>

DIC> @@

DIC> @@ FILE FOR RUNNING EXAMPLE i1

DIC> @@

DIC>

DIC> @@

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

DIC> @@

DIC> go d-m

TIME STEP AT TIME 0.00000E+00

DIC> read exil

OK

DIC>

DIC> @@

DIC> @@ START THE SIMULATION

DIC> @@

DIC> sim

U-FRACTION IN SYSTEM: AL = .429499345639258 FE = .290517917020317
NI = .279982737340425
TOTAL SIZE OF SYSTEM: .002 [m]
U-FRACTION IN SYSTEM: AL = .429499345639258 FE = .290517917020317
NI = .279982737340425
TOTAL SIZE OF SYSTEM: .002 [m]
6 GRIDPOINT(S) ADDED TO CELL #1 REGION: BETA
TIME = 0.10000000E-06 DT = 0.10000000E-06 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: AL = .429499345639258 FE = .290517917020317
NI = .279982737340425
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 1 seconds
TIME = 0.10010000E-03 DT = 0.10000000E-03 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: AL = .429499345639258 FE = .290517917020317
NI = .279982737340425
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 0 seconds
TIME = 0.40010010 DT = 0.40000000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: AL = .429499345639258 FE = .290517917020317
NI = .279982737340426
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 0 seconds
TIME = 513.08856 DT = 512.68846 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: AL = .429499345639248 FE = .290517917020326
NI = .279982737340426
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 1 seconds
TIME = 1538.4655 DT = 1025.3769 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: AL = .429499345639233 FE = .290517917020342
NI = .279982737340425
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 1 seconds
TIME = 3589.2193 DT = 2050.7538 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: AL = .429499345639231 FE = .290517917020344
NI = .279982737340425
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 1 seconds
TIME = 7690.7270 DT = 4101.5077 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: AL = .429499345639227 FE = .290517917020345
NI = .279982737340428
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 2 seconds
TIME = 15893.742 DT = 8203.0154 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: AL = .429499345639233 FE = .290517917020341
NI = .279982737340426
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 1 seconds
TIME = 32299.773 DT = 16406.031 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: AL = .42949934563921 FE = .290517917020362
NI = .279982737340428
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 2 seconds
TIME = 65111.835 DT = 32812.062 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: AL = .429499345639174 FE = .290517917020382
NI = .279982737340444
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 2 seconds
TIME = 99671.835 DT = 34560.000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: AL = .429499345639089 FE = .290517917020496
NI = .279982737340415
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 2 seconds
TIME = 134231.83 DT = 34560.000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: AL = .429499345639132 FE = .290517917020483
NI = .279982737340386
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 2 seconds
TIME = 168791.83 DT = 34560.000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: AL = .429499345639167 FE = .290517917020446
NI = .279982737340387
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 2 seconds
TIME = 203351.83 DT = 34560.000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: AL = .429499345639157 FE = .290517917020456
NI = .279982737340388
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 1 seconds
TIME = 237911.83 DT = 34560.000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: AL = .429499345639151 FE = .290517917020441
NI = .279982737340408
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 2 seconds
TIME = 272471.83 DT = 34560.000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: AL = .429499345639151 FE = .290517917020425
NI = .279982737340423
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 2 seconds
TIME = 307031.83 DT = 34560.000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: AL = .42949934563916 FE = .290517917020412
NI = .279982737340428
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 1 seconds

```
TIME = 341591.83 DT = 34560.000 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: AL = .429499345639173 FE = .290517917020402
NI = .279982737340426
TOTAL SIZE OF SYSTEM: .002 [m]
CPU time used in timestep 2 seconds
TIME = 345600.00 DT = 4008.1652 SUM OF SQUARES = 0.0000000
U-FRACTION IN SYSTEM: AL = .429499345639173 FE = .290517917020401
NI = .279982737340426
TOTAL SIZE OF SYSTEM: .002 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 0.0000000
DELETING TIME-RECORD FOR TIME 0.10000000E-06
DELETING TIME-RECORD FOR TIME 0.10010000E-03
DELETING TIME-RECORD FOR TIME 0.40010010
DELETING TIME-RECORD FOR TIME 513.08856
DELETING TIME-RECORD FOR TIME 1538.4655
DELETING TIME-RECORD FOR TIME 3589.2193
DELETING TIME-RECORD FOR TIME 7690.7270
DELETING TIME-RECORD FOR TIME 15893.742
DELETING TIME-RECORD FOR TIME 32299.773
DELETING TIME-RECORD FOR TIME 65111.835
DELETING TIME-RECORD FOR TIME 99671.835
DELETING TIME-RECORD FOR TIME 134231.83
DELETING TIME-RECORD FOR TIME 168791.83
DELETING TIME-RECORD FOR TIME 203351.83
DELETING TIME-RECORD FOR TIME 237911.83
DELETING TIME-RECORD FOR TIME 272471.83
DELETING TIME-RECORD FOR TIME 307031.83

KEEPING TIME-RECORD FOR TIME 341591.83
AND FOR TIME 345600.00
WORKSPACE RECLAIMED

TIMESTEP AT 345600.000 SELECTED
```

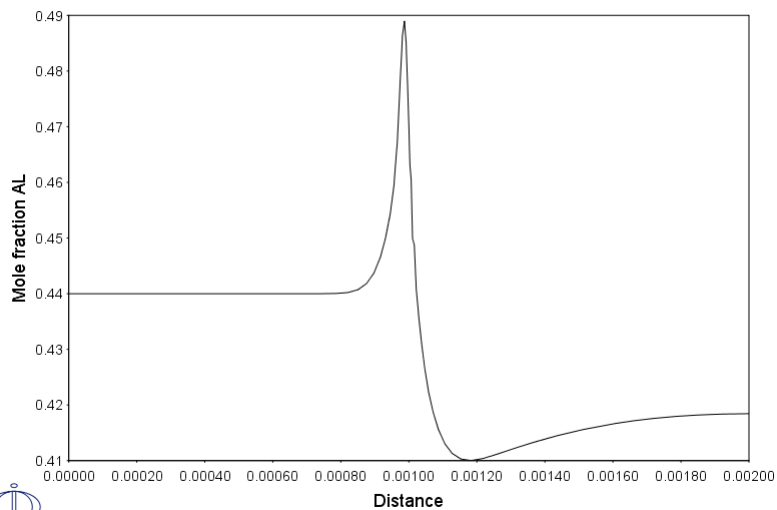
```
DIC>
DIC> set-inter
--OK--
DIC>
```

exil-plot

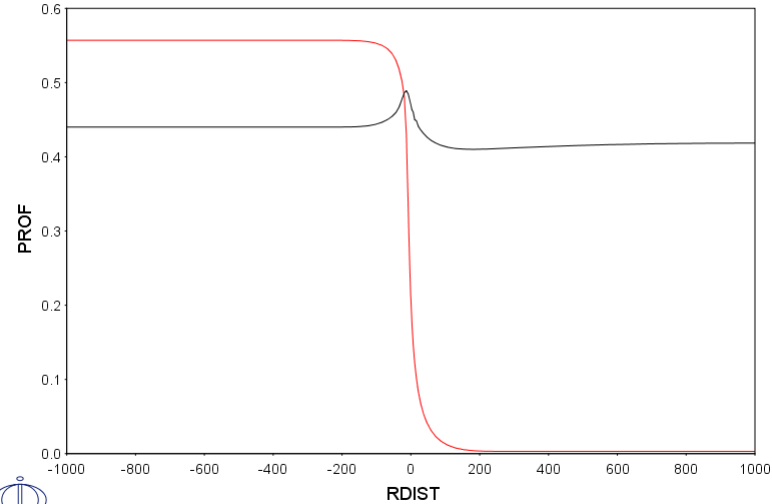
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exil\plot.DCM"DIC>
DIC> @@ exil_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE i1
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
      TIME STEP AT TIME 3.45600E+05
DIC> read exil
      OK
DIC>
DIC> @@
DIC> @@ ENTER THE POST PROCESSOR
DIC> @@
DIC> post

      POST PROCESSOR VERSION 1.7
      Implemented by Bjorn Jonsson
```

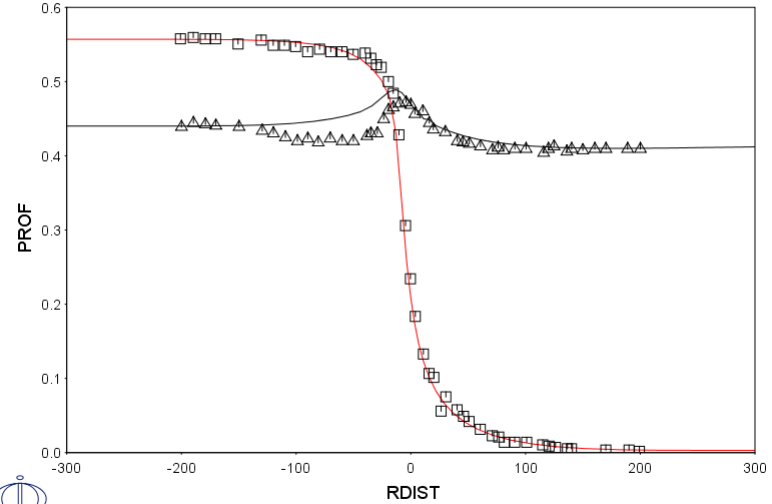
```
POST-1:
POST-1: s-d-a x dist glob
      INFO: Distance is set as independent variable
POST-1:
POST-1: s-d-a y m-f al
POST-1:
POST-1: s-p-c time last
POST-1:
POST-1: plot
      2018.02.18.22.38.40
      Time=345600
      CELL#1
```



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



```
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: app y exil.exp
PROLOGUE NUMBER: /0/: 1
DATASET NUMBER(s): /-1/: 1
POST-1:
POST-1: s-s-s x n -300 300
POST-1:
POST-1: plot
2018.02.18.22.38.41
Time = 345600
CELL #1
```



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



Example exi2

Diffusion of carbon in cementite

This example demonstrates the use of the model for calculation of diffusion through a stoichiometric phase. The flux of a component in the stoichiometric phase is assumed to be proportional to the difference in chemical potential at each side of the stoichiometric phase multiplied with the mobility for the component in the phase. The mobility is assessed from experimental information and is basically the tracer diffusivity for the component. This calculation is compared with experimental data where a sample of pure iron has been exposed to a gas atmosphere with a certain carbon activity. The weight gain is then measured as a function of time. The experimental data is obtained from Ozturk B., Fearing V. L., Ruth A. Jr. and Simkovich G., Met. Trans A, vol 13A (1982), pp. 1871-1873.

$$J \sim \Delta\mu$$

exi2-setup

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

```
SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exi2\setup.DCM" @@
SYS: @@ Diffusion in complex phases.
SYS: @@ Diffusion of carbon in cementite
SYS: @@ This example demonstrates the use of the model for calculation of
SYS: @@ diffusion through a stoichiometric phase. The flux of a component in
SYS: @@ the stoichiometric phase is assumed to be proportional to the
SYS: @@ difference in chemical potential at each side of the stoichiometric
SYS: @@ phase multiplied with the mobility for the component in the phase. The
SYS: @@ mobility is assessed from experimental information and is basically
SYS: @@ the tracer diffusivity for the component.
SYS: @@
SYS: @@ This calculation is compared with experimental data where a sample of
SYS: @@ pure iron has been exposed to a gas atmosphere with a certain carbon
SYS: @@ activity. The weight gain is then measured as a function of time.
SYS: @@ The experimental data is obtained from Ozturk B., Fearing V. L.,
SYS: @@ Ruth A. Jr. and Simkovich G., Met. Trans A, vol 13A (1982), pp. 1871-1873.
SYS: -----
NO SUCH COMMAND, USE HELP
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASES
SYS: @@
SYS: go da
THERMODYNAMIC DATABASE module
Current database: Steels/Fe-Alloys v9.0

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

VA                /- DEFINED
TDB_FEDEMO: def-sys fe c
FE                C DEFINED
TDB_FEDEMO: rej ph * all
GAS:G             LIQUID:L             BCC_A2
CEMENTITE         DIAMOND_FCC_A4       FCC_A1
GRAPHITE          HCP_A3              KSI_CARBIDE
LAVES_PHASE_C14   M23C6              MSC2
M7C3 REJECTED
TDB_FEDEMO: res ph bcc fcc cementite grap
BCC_A2            FCC_A1              CEMENTITE
GRAPHITE RESTORED
TDB_FEDEMO: get
REINITIATING GES .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

List of references for assessed data

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

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

List of references for assessed data

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

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

```

TDB_APP: go d-m
NO TIME STEP DEFINED
*** ENTERING FCC_A1 AS A DIFFUSION NONE PHASE
*** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
DIC>
DIC> set-ref c grap,,,,,,,,,
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob t 0 723; * n

DIC>
DIC> @@
DIC> @@ ENTER THE REGIONS carb AND fer
DIC> @@
DIC> enter-region
REGION NAME : fer
DIC>
DIC> enter-region
REGION NAME : carb
ATTACH TO REGION NAMED /FER/:
ATTACHED TO THE RIGHT OF FER /YES/:
DIC> @@
DIC> @@ ENTER LINEAR GRIDS INTO THE REGIONS
DIC> @@
DIC>
DIC> @@
DIC> @@ ENTER A SIZE FOR THE FERRITE
DIC> @@
DIC> enter-grid
REGION NAME : /FER/: fer
WIDTH OF REGION /1/: 3.3E-6
TYPE /LINEAR/: AUTO
DIC>
DIC> @@
DIC> @@ ENTER A SIZE (VERY SMALL) FOR THE CEMENTITE LAYER
DIC> @@
DIC> @@
DIC> enter-grid
REGION NAME : /CARB/: carb
WIDTH OF REGION /1/: 1E-12
TYPE /LINEAR/: AUTO
DIC>
DIC>
DIC> @@
DIC> @@ ENTER PHASES INTO THE REGIONS
DIC> @@
DIC> enter-phase act carb matrix cementite
COMPOSITION RECORD FOR STOICHIOMETRIC PHASE CEMENTITE IN REGION CARB CREATED
DIC> enter-phase act fer matrix bcc#1
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITIONS IN THE PHASES
DIC> @@
DIC> enter-composition
REGION NAME : /FER/: carb
PHASE NAME: /CEMENTITE/: cementite
DIC>
DIC> enter-composition
REGION NAME : /FER/: fer
PHASE NAME: /BCC_A2/: bcc#1
COMPOSITION TYPE /MOLE FRACTION/: weig-fraction
PROFILE FOR /C/: C lin 1E-5 1E-5
DIC>
DIC> set-cond bound upp

CONDITION TYPE /CLOSED_SYSTEM/: mix
Dependent substitutional element:FE
Dependent interstitial element:VA
LOW TIME LIMIT /0/: 0
ACR(C)(TIME)= 9;
HIGH TIME LIMIT /*/: *
ANY MORE RANGES /N/: N
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ SIMULATE FOR 150 MINUTES
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 9000
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /900/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exi2 Y
DIC>
DIC> set-inter
--OK--
DIC>

```

exi2-run

DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exi2\run.DCM"DIC>

DIC>

DIC> @@ exi2_run.DCM

DIC>

DIC> @@

DIC> @@ FILE FOR RUNNING EXAMPLE i2

DIC> @@

DIC>

DIC> @@

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

DIC> @@

DIC> go d-m

TIME STEP AT TIME 0.00000E+00

*** ENTERING FCC_A1 AS A DIFFUSION NONE PHASE

*** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE

DIC> read exi2

OK

DIC>

DIC> @@

DIC> @@ START THE SIMULATION

DIC> @@

DIC> sim

Region: FER

single geometric dense at 0.33000E-05

0.91945 87

Region: CARB

double geometric

dense at outer boundaries, coarse at 0.50000E-12

lower part 1.2500 9

upper part 0.80000 9

Trying old scheme 3

U-FRACTION IN SYSTEM: C = 4.6598005784384E-05 FE = 1

TOTAL SIZE OF SYSTEM: 3.300001E-06 [m]

U-FRACTION IN SYSTEM: C = 4.6598005784384E-05 FE = 1

TOTAL SIZE OF SYSTEM: 3.300001E-06 [m]

0.111094107740055 0.111116327660160 1.168933545308438E-022 TIME = 0.10000000E-06 DT = 0.10000000E-

06 SUM OF SQUARES = 0.11689335E-21

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.55732855E-06 AND -0.55732855E-06

POSITION OF INTERFACE FER / CARB IS 0.32999999E-05

U-FRACTION IN SYSTEM: C = 4.65969237107415E-05 FE = 1

TOTAL SIZE OF SYSTEM: 3.300001E-06 [m]

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

CPU time used in timestep 0 seconds

1.985503622653894E-006 1.986016682715920E-006 8.569005889170424E-023 TIME = 0.25999666E-05 DT = 0.24999666E-

05 SUM OF SQUARES = 0.85690059E-22

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.12341808E-06 AND -0.12341808E-06

POSITION OF INTERFACE FER / CARB IS 0.32999996E-05

U-FRACTION IN SYSTEM: C = 4.66223850218017E-05 FE = 1

TOTAL SIZE OF SYSTEM: 3.300001E-06 [m]

CPU time used in timestep 0 seconds

9.632817666940026E-007 9.640732404382950E-007 1.188374989701993E-025 TIME = 0.75998999E-05 DT = 0.49999333E-

05 SUM OF SQUARES = 0.11883750E-24

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.91502734E-07 AND -0.91502734E-07

POSITION OF INTERFACE FER / CARB IS 0.32999992E-05

U-FRACTION IN SYSTEM: C = 4.66617913784151E-05 FE = 1

TOTAL SIZE OF SYSTEM: 3.300001E-06 [m]

CPU time used in timestep 0 seconds

5.520598281728834E-007 5.525040595679586E-007 1.288882881968142E-026 TIME = 0.17599767E-04 DT = 0.99998666E-

05 SUM OF SQUARES = 0.12888829E-25

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.67380405E-07 AND -0.67380405E-07

POSITION OF INTERFACE FER / CARB IS 0.32999985E-05

U-FRACTION IN SYSTEM: C = 4.67208116371187E-05 FE = 1

TOTAL SIZE OF SYSTEM: 3.300001E-06 [m]

CPU time used in timestep 0 seconds

3.294904029785897E-007 3.297431202262137E-007 1.269811257175113E-026 TIME = 0.37599500E-04 DT = 0.19999733E-

04 SUM OF SQUARES = 0.12698113E-25

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.48810906E-07 AND -0.48810906E-07

POSITION OF INTERFACE FER / CARB IS 0.32999975E-05

U-FRACTION IN SYSTEM: C = 4.68069809139129E-05 FE = 1

TOTAL SIZE OF SYSTEM: 3.300001E-06 [m]

CPU time used in timestep 0 seconds

1.842051604935253E-007 1.843420424813243E-007 3.758018249556124E-025 TIME = 0.77598966E-04 DT = 0.39999466E-

04 SUM OF SQUARES = 0.37580182E-24

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.34957854E-07 AND -0.34957854E-07

POSITION OF INTERFACE FER / CARB IS 0.32999961E-05

U-FRACTION IN SYSTEM: C = 4.69308608646658E-05 FE = 1

TOTAL SIZE OF SYSTEM: 3.300001E-06 [m]

14 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: CARB

CPU time used in timestep 0 seconds

9.778279830287753E-008 9.785422392329824E-008 1.355451665779685E-025 TIME = 0.15759790E-03 DT = 0.79998933E-

04 SUM OF SQUARES = 0.13554517E-24

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.24876846E-07 AND -0.24876846E-07

POSITION OF INTERFACE FER / CARB IS 0.32999941E-05

U-FRACTION IN SYSTEM: C = 4.71074840882462E-05 FE = 1

TOTAL SIZE OF SYSTEM: 3.300001E-06 [m]

49 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: CARB

CPU time used in timestep 0 seconds

5.038045599773962E-006 5.041694015305950E-006 4.707624364821560E-025 TIME = 0.31759576E-03 DT = 0.15999787E-

03 SUM OF SQUARES = 0.47076244E-24

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.17645081E-07 AND -0.17645081E-07

POSITION OF INTERFACE FER / CARB IS 0.32999913E-05

U-FRACTION IN SYSTEM: C = 4.73582549999065E-05 FE = 1

TOTAL SIZE OF SYSTEM: 3.300001E-06 [m]

55 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: CARB

output ignored...

... output resumed

TIME = 3142.1594 DT = 900.00000 SUM OF SQUARES = 0.30225501E-26

CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.44854482E-11 AND -0.44854482E-11

POSITION OF INTERFACE FER / CARB IS 0.32722305E-05

U-FRACTION IN SYSTEM: C = .00283057618776405 FE = 1

TOTAL SIZE OF SYSTEM: 3.300001E-06 [m]

55 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: CARB

CPU time used in timestep 1 seconds


```

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

CPU time used in timestep      0 seconds
1.337273690876802E-008      1.340171249585930E-008      1.438406288208647E-
026    TIME =      4942.1594    DT =      900.00000    SUM OF SQUARES =      0.14384063E-25
CELL # 1 VELOCITY AT INTERFACE # 2 IS      -0.34097971E-11 AND      -0.34097971E-11
POSITION OF INTERFACE FER / CARB IS      0.32657116E-05
U-FRACTION IN SYSTEM:  C = .00348899893656266  FE = 1
TOTAL SIZE OF SYSTEM:  3.300001E-06 [m]
  9  GRIDPOINT(S) REMOVED FROM CELL #1  REGION: CARB

CPU time used in timestep      0 seconds
6.238597393059804E-009      6.256204153119521E-009      5.571054466188241E-
030    TIME =      5842.1594    DT =      900.00000    SUM OF SQUARES =      0.55710545E-29
CELL # 1 VELOCITY AT INTERFACE # 2 IS      -0.31046285E-11 AND      -0.31046285E-11
POSITION OF INTERFACE FER / CARB IS      0.32629174E-05
U-FRACTION IN SYSTEM:  C = .00377121604704412  FE = 1
TOTAL SIZE OF SYSTEM:  3.300001E-06 [m]
 20  GRIDPOINT(S) REMOVED FROM CELL #1  REGION: CARB

CPU time used in timestep      0 seconds
3.280281446289517E-009      3.291907995765650E-009      1.610509839104679E-
030    TIME =      6742.1594    DT =      900.00000    SUM OF SQUARES =      0.16105098E-29
CELL # 1 VELOCITY AT INTERFACE # 2 IS      -0.28707015E-11 AND      -0.28707015E-11
POSITION OF INTERFACE FER / CARB IS      0.32603338E-05
U-FRACTION IN SYSTEM:  C = .00403216870914912  FE = 1
TOTAL SIZE OF SYSTEM:  3.300001E-06 [m]
  6  GRIDPOINT(S) REMOVED FROM CELL #1  REGION: CARB

CPU time used in timestep      0 seconds
1.864873578096803E-007      1.872981047449765E-007      1.864276412969093E-
029    TIME =      7642.1594    DT =      900.00000    SUM OF SQUARES =      0.18642764E-28
CELL # 1 VELOCITY AT INTERFACE # 2 IS      -0.26837249E-11 AND      -0.26837249E-11
POSITION OF INTERFACE FER / CARB IS      0.32579185E-05
U-FRACTION IN SYSTEM:  C = .00427612481768502  FE = 1
TOTAL SIZE OF SYSTEM:  3.300001E-06 [m]
  7  GRIDPOINT(S) REMOVED FROM CELL #1  REGION: CARB

CPU time used in timestep      0 seconds
1.118941665788623E-007      1.124814013240834E-007      7.257773708191617E-
030    TIME =      8542.1594    DT =      900.00000    SUM OF SQUARES =      0.72577737E-29
CELL # 1 VELOCITY AT INTERFACE # 2 IS      -0.25296909E-11 AND      -0.25296909E-11
POSITION OF INTERFACE FER / CARB IS      0.32556417E-05
U-FRACTION IN SYSTEM:  C = .00450607892012097  FE = 1
TOTAL SIZE OF SYSTEM:  3.300001E-06 [m]
  6  GRIDPOINT(S) REMOVED FROM CELL #1  REGION: CARB

CPU time used in timestep      0 seconds
6.975845435923255E-008      7.019562001951880E-008      7.183192071095221E-
030    TIME =      9000.0000    DT =      457.84063    SUM OF SQUARES =      0.71831921E-29
CELL # 1 VELOCITY AT INTERFACE # 2 IS      -0.23998555E-11 AND      -0.23998555E-11
POSITION OF INTERFACE FER / CARB IS      0.32545430E-05
U-FRACTION IN SYSTEM:  C = .00461705531635601  FE = 1
TOTAL SIZE OF SYSTEM:  3.300001E-06 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME      0.00000000
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      7642.1594
DELETING TIME-RECORD FOR TIME      7642.1594

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

TIMESTEP AT      9000.00000    SELECTED

```

```

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

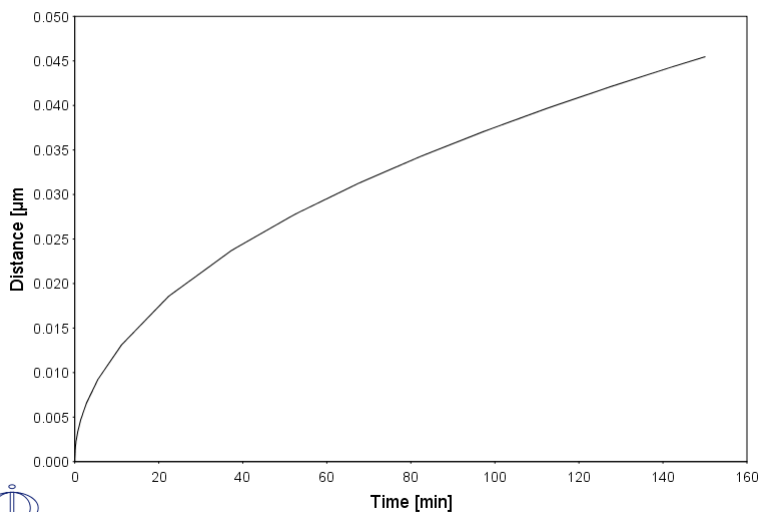
```

exi2-plot

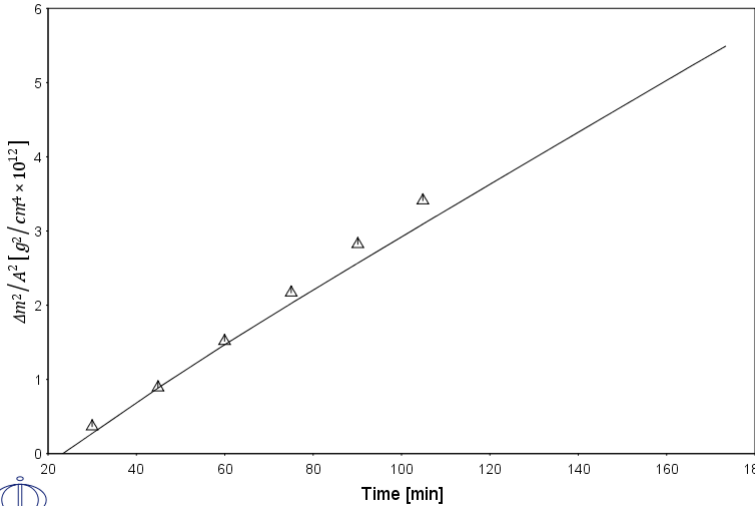
```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exi2\plot.DCM"DIC>
DIC> @@ exi2_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE i2
DIC> @@
DIC> @@
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
      TIME STEP AT TIME 9.00000E+03
      *** ENTERING FCC_A1 AS A DIFFUSION NONE PHASE
      *** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
DIC>
DIC>
DIC> read exi2 Y
      OK
DIC>
DIC> @@
DIC> @@ PLOT THE SIZE OF THE CEMENTITE LAYER AS A FUNCTION OF TIME
DIC> @@
DIC> post

      POST PROCESSOR VERSION 1.7
      Implemented by Bjorn Jonsson
```

```
POST-1:
POST-1: ent-symb func csize
FUNCTION: 1e6*(poi(car,u)-poi(car,l));
POST-1:
POST-1: ent-symb func minutes
FUNCTION: time/60;
POST-1:
POST-1: s-d-a x minutes
POST-1: s-d-a y csize
POST-1:
POST-1: s-p-c inter first
POST-1:
POST-1: s-a-t-s x n Time [min]
POST-1: s-a-t-s y n Distance [m]
POST-1:
POST-1: plot
      2018.02.18.22.41.40
      "FIRST" INTERFACE OF SYSTEM
      CELL #1
```



```
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: @@
POST-1: @@ ASSUME A CERTAIN TIME FOR NUCLEATION OF THE CEMENTITE LAYER
POST-1: @@
POST-1: ent-symb func cortim
FUNCTION: (time+1400)/60;
POST-1:
POST-1: @@
POST-1: @@ PLOT THE WEIGHT GAIN AS A FUNCTION OF TIME
POST-1: @@
POST-1: ent-symb func cwei
FUNCTION: 1e12*((poi(car,u)-poi(car,l))-1E-12)*12.01/2.33E-5*1e-4)**2;
POST-1:
POST-1: s-d-a x cortim
POST-1: s-d-a y cwei
POST-1:
POST-1: @@
POST-1: @@ COMPARE WITH EXPERIMENTAL DATA
POST-1: @@
POST-1: app y exi2.exp 0; 1
POST-1:
POST-1:
POST-1: s-a-t-s x n Time [min]
POST-1: s-a-t-s y n \latex \Delta m^2/A^2\, [g^2/cm^4\times 10^{12}]
POST-1:
POST-1: plot
```



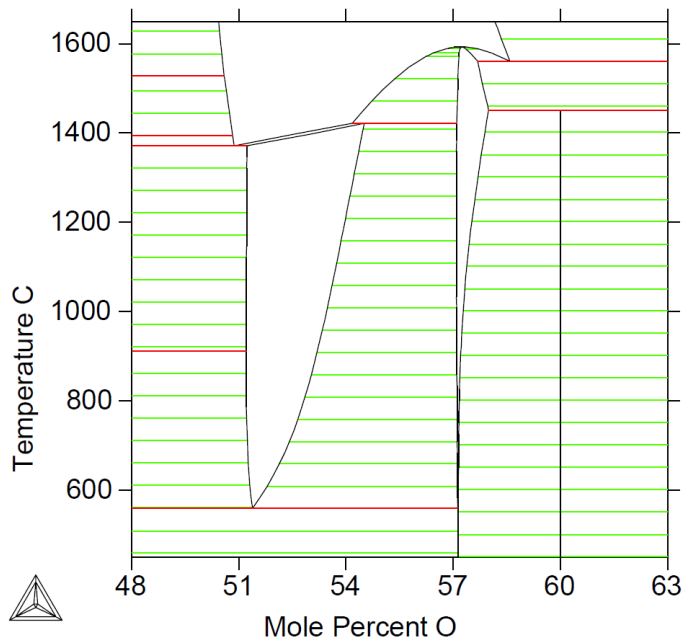
POST-1:
POST-1:
POST-1: set-inter
--OK--
POST-1:



Example exi3a

Diffusion in iron oxide (FeO)

This example shows the oxidation of an iron sample and the consequent growth of an oxide layer using the grain boundary diffusion contribution model.



exi3a-setup

About Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

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

SYS:SYS:MACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exi3a\setup.DCM"SYS: @@

SYS: @@ Diffusion in complex phases.

SYS: @@ Diffusion in iron oxide (FeO)

SYS: @@ This example shows the oxidation of an iron sample and the

SYS: @@ consequent growth of an oxide layer.

SYS: -----

NO SUCH COMMAND, USE HELP

SYS:

SYS: @@ exi3_setup.DCM

SYS:

SYS: @@

SYS: @@ START BY GOING TO THE DATABASE MODULE

SYS: @@

SYS: go da

THERMODYNAMIC DATABASE module

Current database: Steels/Fe-Alloys v9.0

VA /- DEFINED

L12_FCC B2_BCC DICTRA_FCC_A1

REJECTED

TDB_TCFE9:

TDB_TCFE9: @@

TDB_TCFE9: @@ SELECT A USER DATABASE FOR READING THE THERMODYNAMIC DATA

TDB_TCFE9: @@

TDB_TCFE9: sw user FeO.TDB

Current database: User defined Database

This database does not support the DATABASE_INFORMATION command

VA /- DEFINED

TDB_USER: def-sys fe o

FE O DEFINED

TDB_USER: rej sp *

/- VA FE

O FE+2 FE+3

FE+4 FE2O3 FEO

FE03/2 O-2 O2

REJECTED

TDB_USER: res sp fe fe+2 fe+3 o o2 o-2 va

FE FE+2 FE+3

O O2 O-2

VA RESTORED

TDB_USER: rej ph * all

GAS:G BCC_A2 SPINEL:I

REJECTED

TDB_USER: res ph bcc spinel gas

BCC_A2 SPINEL:I GAS:G

RESTORED

TDB_USER:

TDB_USER: get

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

Reference REF368 missing close to line 55

Reference REF304 missing close to line 63

Reference REF420 missing close to line 65

Reference REF420 missing close to line 67

Reference REF368 missing close to line 69

Reference REF368 missing close to line 70

Reference REF368 missing close to line 72

Reference REF418 missing close to line 74

Reference REF418 missing close to line 76

Reference REF304 missing close to line 78

Reference REF30 missing close to line 86

Reference REF30 missing close to line 88

Reference REF30 missing close to line 90

Reference REF420 missing close to line 92

Reference REF420 missing close to line 94

Reference REF30 missing close to line 96

Reference REF30 missing close to line 98

Reference REF30 missing close to line 100

Reference REF420 missing close to line 102

Reference REF420 missing close to line 104

Reference REF30 missing close to line 106

Reference REF30 missing close to line 108

Reference REF30 missing close to line 110

Reference REF420 missing close to line 112

Reference REF420 missing close to line 114

Reference REF30 missing close to line 116

Reference REF30 missing close to line 118

Reference REF30 missing close to line 120

Reference REF420 missing close to line 122

Reference REF420 missing close to line 124

Reference REF30 missing close to line 126

Reference REF30 missing close to line 128

Reference REF30 missing close to line 130

Reference REF420 missing close to line 132

Reference REF420 missing close to line 134

Reference REF30 missing close to line 136

Reference REF30 missing close to line 138

Reference REF30 missing close to line 140

Reference REF420 missing close to line 142

Reference REF420 missing close to line 144

Reference REF30 missing close to line 146

Reference REF30 missing close to line 148

Reference REF30 missing close to line 150

Reference REF420 missing close to line 152

Reference REF420 missing close to line 154

Reference REF30 missing close to line 156

Reference REF30 missing close to line 158

Reference REF30 missing close to line 160

Reference REF420 missing close to line 162

```

Reference REF420      missing close to line      164
Reference REF30       missing close to line      166
Reference REF30       missing close to line      168
Reference REF30       missing close to line      170
Reference REF420      missing close to line      172
Reference REF420      missing close to line      174
Reference REF30       missing close to line      176
Reference REF30       missing close to line      178
Reference REF30       missing close to line      180
Reference REF420      missing close to line      182
Reference REF420      missing close to line      184
Reference REF30       missing close to line      186
Reference REF30       missing close to line      188
Reference REF30       missing close to line      190
Reference REF420      missing close to line      192
Reference REF420      missing close to line      194
Reference REF30       missing close to line      196
Reference REF30       missing close to line      198
Reference REF30       missing close to line      200
Reference REF420      missing close to line      202
Reference REF420      missing close to line      204
FUNCTIONS ....
-OK-
TDB_USER:
TDB_USER: @@
TDB_USER: @@ SWITCH TO A USER-DEFINED MOBILITY DATABASE TO RETRIEVE MOBILITY DATA
TDB_USER: @@
TDB_USER: app user Fe0mob.TDB
Current database: User defined Database
test database

VA                      /-                      O
DEFINED
TDB_APP: def-sys fe o
FE_DEFINED
TDB_APP: rej sp *
/-                      VA                      FE
O                      FE+2                    FE+3
FE2O3                  FEO                      FEO3/2
O-2                    O2 REJECTED
TDB_APP: res sp fe fe+2 fe+3 o o2 o-2 va
FE                      FE+2                    FE+3
O                      O2                      O-2
VA RESTORED
TDB_APP: rej ph * all
SPINEL:I                GAS:G                    BCC_A2
REJECTED
TDB_APP: res ph bcc spinel gas
BCC_A2                  SPINEL:I                GAS:G
RESTORED
TDB_APP:
TDB_APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

List of references for assessed data

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

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

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

```

```

DIC> @@
DIC> @@ ENTER A THIN INITIAL SIZE FOR THE OXIDE
DIC> @@
DIC> @@
DIC> ent-grid sp 1.00e-10 AUTO
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITIONS IN BCC
DIC> @@
DIC> ent-comp fer bcc#1 m-f
PROFILE FOR /O/: o lin 1e-9 1e-9
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITIONS IN THE OXIDE
DIC> @@
DIC> ent-comp sp spinel m-f
    this is a phase with charged species
    with more than 2 sublattices
PROFILE FOR /FE/: FE lin 4.28771E-01 4.28549E-01
DIC>
DIC>
DIC> @@
DIC> @@ ENTER A BOUNDARY CONDITION "GAS" ON THE UPPER (RIGHT-MOST) INTERFACE
DIC> @@ OF THE OXIDE. THIS ALLOWS THE SYSTEM TO EXPAND AND THE OXIDE LAYER
DIC> @@ TO GROW EXTERNALLY. FOR THIS EXAMPLE AN OXYGEN ACTIVITY IS SPECIFIED
DIC> @@ THAT IS LOW ENOUGH NOT TO FORM CORUNDUM (FE2O3). WE ALSO SPECIFY
DIC> @@ THAT THERE IS NO FLUX OF Fe ACROSS THIS INTERFACE, I.E. NO Fe
DIC> @@ IS ALLOWED TO ENTER OR LEAVE THE SYSTEM.
DIC> @@
DIC> set-cond boundary upper gas

TYPE OF CONDITION FOR COMPONENT FE /ZERO_FLUX/: zero-flux
TYPE OF CONDITION FOR COMPONENT O /ZERO_FLUX/: act
LOW TIME LIMIT /O/: 0 4.5e-4; * N
DIC>
DIC>
DIC> @@
DIC> @@ ENTER START VALUES FOR THE INITIAL INTERFACE VELOCITIES
DIC> @@
DIC> s-a-s-v -1e-5 1e-5 yes
    STARTING VALUES WILL BE TAKEN FROM PROFILES
DIC>
DIC>
DIC> @@
DIC> @@ SIMULATE FOR 24 HOURS
DIC> @@
DIC> s-s-time 86400,,,
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC> @@
DIC> @@ SPECIFY THAT POTENTIALS AND NOT ACTIVITIES ARE VARIED AT THE PHASE
DIC> @@ INTERFACE. ALSO USE A FULLY IMPLICIT SCHEME FOR TIME INTEGRATION.
DIC> @@
DIC> s-s-c 0 1 1 YES POT YES YES 1 2,,,,,,,,,
    RELEASING OLD STARTING VALUES
DIC>
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exi3.DIC Y
DIC>
DIC> set-inter
--OK--
DIC>

```

exi3a-run

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exi3a\run.DCM"DIC>
DIC>
DIC> @@ exi3_run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING EXAMPLE i3
DIC> @@
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 0.00000E+00
DIC> read exi3
OK
DIC>
DIC> @@
DIC> @@ START THE SIMULATION
DIC> @@
DIC> sim y
Region: FER
single geometric dense at 0.50000E-02
0.87386 95
Region: SP
double geometric
dense at outer boundaries, coarse at 0.50000E-10
lower part 1.2500 9
upper part 0.80000 9
Trying old scheme 3
U-FRACTION IN SYSTEM: FE = 0.99999999500542 O = 2.10000395011622E-08
TOTAL SIZE OF SYSTEM: .0049999901 [m]
U-FRACTION IN SYSTEM: FE = 0.99999999500542 O = 2.10000395011622E-08
TOTAL SIZE OF SYSTEM: .0049999901 [m]
0.347387301619340 0.347386528699253 0.347386701354488 4.618089872755317E-002 1.115577003344626E-
022 TIME = 0.100000000E-06 DT = 0.100000000E-06 SUM OF SQUARES = 0.11155770E-21
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.39646054E-03 AND 0.00000000
POSITION OF INTERFACE FER / SP IS 0.49999900E-02
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.66982674E-03 AND 0.00000000
POSITION OF INTERFACE SP / gas interface IS 0.49999901E-02
U-FRACTION IN SYSTEM: FE = 0.99999998954903 O = 3.44015229571833E-08
TOTAL SIZE OF SYSTEM: .00499999012734 [m]
10 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: FER

CPU time used in timestep 0 seconds
1.507552605990936E-005 1.507739146467480E-005 1.507822847287634E-005 2.226308397782723E-007 2.476318028538286E-
031 TIME = 0.300000000E-06 DT = 0.200000000E-06 SUM OF SQUARES = 0.24763180E-30
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.14849229E-03 AND 0.00000000
POSITION OF INTERFACE FER / SP IS 0.49999899E-02
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.20393047E-03 AND 0.00000000
POSITION OF INTERFACE SP / gas interface IS 0.49999901E-02
U-FRACTION IN SYSTEM: FE = 0.99999998713864 O = 4.25584032292646E-08
TOTAL SIZE OF SYSTEM: .00499999013842 [m]

CPU time used in timestep 1 seconds
1.398975101859364E-008 1.397926494961065E-008 1.395940586724563E-008 3.137487096517389E-011 7.276780229330289E-
034 TIME = 0.700000000E-06 DT = 0.400000000E-06 SUM OF SQUARES = 0.72767802E-33
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.14913262E-03 AND 0.00000000
POSITION OF INTERFACE FER / SP IS 0.49999899E-02
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.21655229E-03 AND 0.00000000
POSITION OF INTERFACE SP / gas interface IS 0.49999902E-02
U-FRACTION IN SYSTEM: FE = 0.99999998167656 O = 5.9883649440439E-08
TOTAL SIZE OF SYSTEM: .00499999016539 [m]

CPU time used in timestep 0 seconds
5.609742547589773E-007 5.611284846250793E-007 5.611264634536804E-007 2.444637655298936E-010 1.128709675659560E-
034 TIME = 0.150000000E-05 DT = 0.800000000E-06 SUM OF SQUARES = 0.11287097E-33
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.93393028E-04 AND 0.00000000
POSITION OF INTERFACE FER / SP IS 0.49999898E-02
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.13339356E-03 AND 0.00000000
POSITION OF INTERFACE SP / gas interface IS 0.49999902E-02
U-FRACTION IN SYSTEM: FE = 0.99999997507588 O = 8.12291255492651E-08
TOTAL SIZE OF SYSTEM: .00499999019739 [m]
23 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: SP

CPU time used in timestep 0 seconds
8.108701239277702E-006 8.112502967450534E-006 8.112138099848266E-006 1.121067578002317E-008 3.531749267158546E-
032 TIME = 0.310000000E-05 DT = 0.160000000E-05 SUM OF SQUARES = 0.35317493E-31
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.70760985E-04 AND 0.00000000
POSITION OF INTERFACE FER / SP IS 0.49999897E-02
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.10183290E-03 AND 0.00000000
POSITION OF INTERFACE SP / gas interface IS 0.49999902E-02
U-FRACTION IN SYSTEM: FE = 0.99999996490465 O = 1.13820151455531E-07
TOTAL SIZE OF SYSTEM: .00499999024711 [m]
35 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: SP

CPU time used in timestep 0 seconds
8.100481734301132E-006 8.103302413441165E-006 8.103162850361541E-006 7.195354227408064E-009 8.335665540551005E-
033 TIME = 0.630000000E-05 DT = 0.320000000E-05 SUM OF SQUARES = 0.83356655E-32
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.49011444E-04 AND 0.00000000
POSITION OF INTERFACE FER / SP IS 0.49999895E-02
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.70269554E-04 AND 0.00000000
POSITION OF INTERFACE SP / gas interface IS 0.49999903E-02
U-FRACTION IN SYSTEM: FE = 0.99999995092491 O = 1.5879999799066E-07
TOTAL SIZE OF SYSTEM: .00499999031513 [m]

output ignored...

... output resumed

POSITION OF INTERFACE FER / SP IS 0.49497263E-02
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.85406534E-09 AND 0.00000000
POSITION OF INTERFACE SP / gas interface IS 0.50216007E-02
U-FRACTION IN SYSTEM: FE = .995601423066401 O = .0143132204538531
TOTAL SIZE OF SYSTEM: .005021600735 [m]
23 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: SP

CPU time used in timestep 1 seconds
2.789556769619959E-007 2.794057581865568E-007 2.793655764673843E-007 3.800585456559765E-010 3.352321809449032E-
033 TIME = 56943.895 DT = 8640.0000 SUM OF SQUARES = 0.33523218E-32
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.54743813E-09 AND 0.00000000
POSITION OF INTERFACE FER / SP IS 0.49449965E-02
```



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

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

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

CPU time used in timestep 0 seconds
9.562030960084013E-008 5.978502100270548E-008 5.977212458826642E-008 6.869420014653385E-011 2.456312995478252E-
033 TIME = 82863.895 DT = 8640.0000 SUM OF SQUARES = 0.24563130E-32
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.44778107E-09 AND 0.0000000
POSITION OF INTERFACE FER / SP IS 0.49326392E-02
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.64203085E-09 AND 0.0000000
POSITION OF INTERFACE SP / gas interface IS 0.50289875E-02
U-FRACTION IN SYSTEM: FE = .994130359456937 O = .0191587681410625
TOTAL SIZE OF SYSTEM: .00502898750134 [m]
8 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: SP

CPU time used in timestep 0 seconds
9.162180973319777E-009 9.108164931689858E-009 9.224421743565125E-009 1.011580316905061E-011 2.783570622747177E-
034 TIME = 86400.000 DT = 3536.1047 SUM OF SQUARES = 0.27835706E-33
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.44500201E-09 AND 0.0000000
POSITION OF INTERFACE FER / SP IS 0.49310656E-02
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.61834793E-09 AND 0.0000000
POSITION OF INTERFACE SP / gas interface IS 0.50296005E-02
U-FRACTION IN SYSTEM: FE = .994008758985575 O = .0195911680901775
TOTAL SIZE OF SYSTEM: .00502960047066 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 0.0000000
DELETING TIME-RECORD FOR TIME 0.10000000E-06
DELETING TIME-RECORD FOR TIME 0.30000000E-06
DELETING TIME-RECORD FOR TIME 0.70000000E-06
DELETING TIME-RECORD FOR TIME 0.15000000E-05
DELETING TIME-RECORD FOR TIME 0.31000000E-05
DELETING TIME-RECORD FOR TIME 0.63000000E-05
DELETING TIME-RECORD FOR TIME 0.12700000E-04
DELETING TIME-RECORD FOR TIME 0.25500000E-04
DELETING TIME-RECORD FOR TIME 0.51100000E-04
DELETING TIME-RECORD FOR TIME 0.10230000E-03
DELETING TIME-RECORD FOR TIME 0.20470000E-03
DELETING TIME-RECORD FOR TIME 0.40950000E-03
DELETING TIME-RECORD FOR TIME 0.81910000E-03
DELETING TIME-RECORD FOR TIME 0.16383000E-02
DELETING TIME-RECORD FOR TIME 0.32767000E-02
DELETING TIME-RECORD FOR TIME 0.65535000E-02
DELETING TIME-RECORD FOR TIME 0.13107100E-01
DELETING TIME-RECORD FOR TIME 0.26214300E-01
DELETING TIME-RECORD FOR TIME 0.52428700E-01
DELETING TIME-RECORD FOR TIME 0.10485750
DELETING TIME-RECORD FOR TIME 0.20971510
DELETING TIME-RECORD FOR TIME 0.41943030
DELETING TIME-RECORD FOR TIME 0.83886070
DELETING TIME-RECORD FOR TIME 1.6777215
DELETING TIME-RECORD FOR TIME 3.3554431
DELETING TIME-RECORD FOR TIME 6.7108863
DELETING TIME-RECORD FOR TIME 13.421773
DELETING TIME-RECORD FOR TIME 26.843545
DELETING TIME-RECORD FOR TIME 53.687091
DELETING TIME-RECORD FOR TIME 107.37418
DELETING TIME-RECORD FOR TIME 214.74836
DELETING TIME-RECORD FOR TIME 429.49673
DELETING TIME-RECORD FOR TIME 858.99346
DELETING TIME-RECORD FOR TIME 1717.9869
DELETING TIME-RECORD FOR TIME 3435.9738
DELETING TIME-RECORD FOR TIME 6871.9477
DELETING TIME-RECORD FOR TIME 13743.895
DELETING TIME-RECORD FOR TIME 22383.895
DELETING TIME-RECORD FOR TIME 31023.895
DELETING TIME-RECORD FOR TIME 39663.895
DELETING TIME-RECORD FOR TIME 48303.895
DELETING TIME-RECORD FOR TIME 56943.895
DELETING TIME-RECORD FOR TIME 65583.895
DELETING TIME-RECORD FOR TIME 74223.895

KEEPING TIME-RECORD FOR TIME 82863.895
AND FOR TIME 86400.000
WORKSPACE RECLAIMED

TIMESTEP AT 86400.0000 SELECTED
```

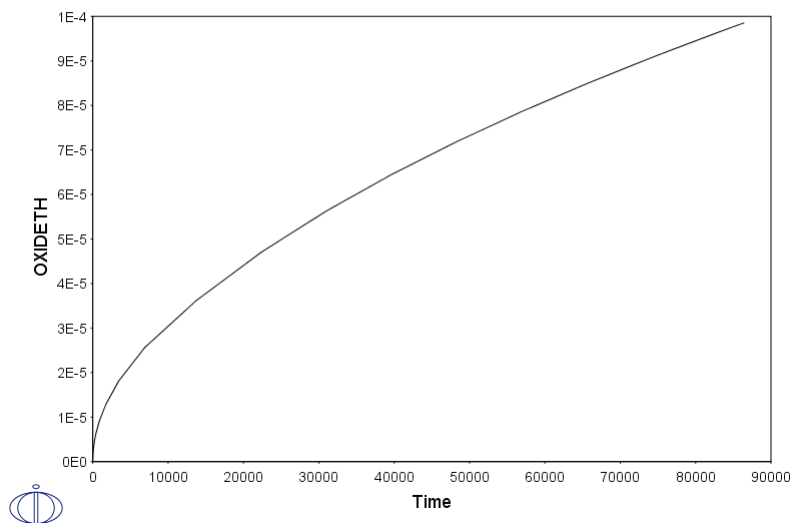
```
DIC>
DIC> set-inter
--OK--
DIC>
```

exi3a-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exi3a\plot.DCM"DIC>
DIC> @@ exi3_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE i3
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
      TIME STEP AT TIME 8.64000E+04
DIC> read exi3
      OK
DIC>
DIC> @@
DIC> @@ ENTER THE POST PROCESSOR
DIC> @@
DIC> post

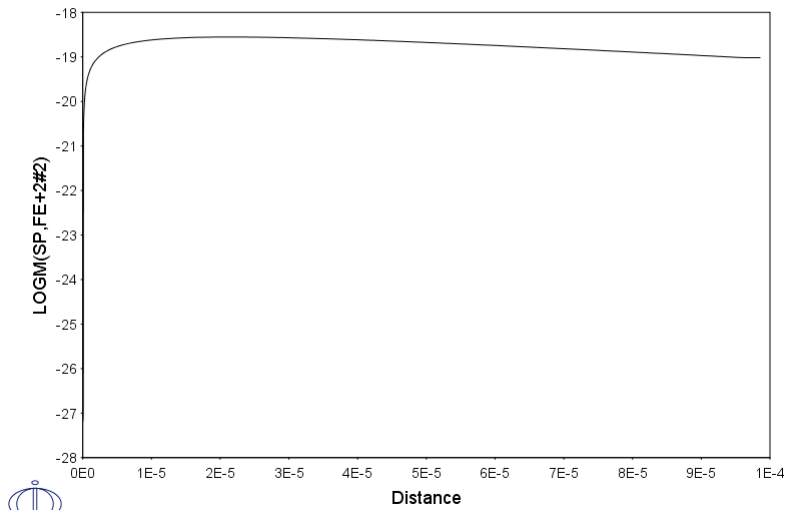
      POST PROCESSOR VERSION 1.7
      Implemented by Bjorn Jonsson
```

```
POST-1:
POST-1: @@
POST-1: @@ PLOT THE THICKNESS OF THE OXIDE LAYER GROWING AT THE SURFACE.
POST-1: @@ FOR THIS WE NEED TO ENTER A FUNCTION ACCORDING TO THE FOLLOWING.
POST-1: ent func oxideth
FUNCTION: poi(sp,upper)-poi(sp,lower)
&
POST-1: @@
POST-1: @@ PUT THIS FUNCTION ON THE Y-AXIS
POST-1: @@
POST-1: s-d-a y oxideth
POST-1:
POST-1: @@
POST-1: @@ AND PLOT THE OXIDE THICKNESS VERSUS TIME
POST-1: @@
POST-1: s-d-a x time
      INFO: Time is set as independent variable
POST-1:
POST-1: @@
POST-1: @@ SINCE WE ARE PLOTTING A FUNCTION, SPECIFY A PLOT CONDITION
POST-1: @@
POST-1: s-p-c interface sp upper
POST-1:
POST-1: plot
      2018.02.18.22.44.49
      UPPER INTERFACE OF REGION "SP#1"
      CELL #1
```

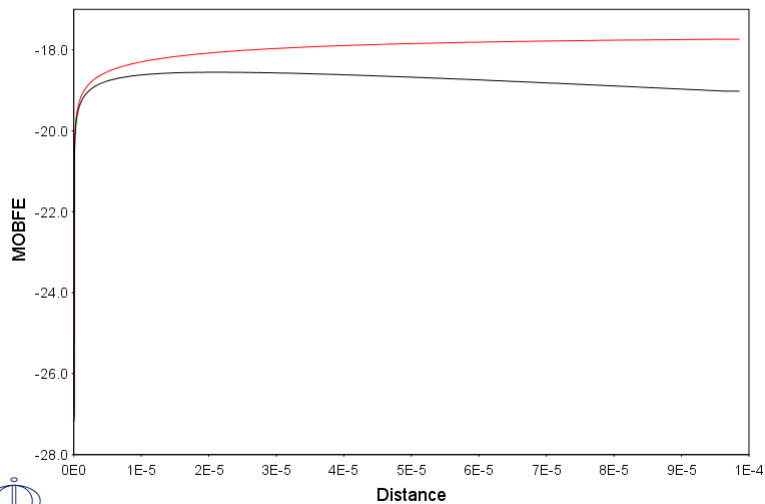


```
POST-1:
POST-1: @@<Hit_return_to_continue>
POST-1:
POST-1: @@
POST-1: @@ NOW PLOT THE MOBILITY IN A SPINEL FOR Fe+2 ON THE SECOND SUBLATTICE
POST-1: @@
POST-1: s-d-a y logm(sp,fe+2#2)
POST-1:
POST-1: @@
POST-1: @@ LIMIT THE PLOT TO THE SPINEL PHASE
POST-1: @@
POST-1: s-d-a x dis local sp
      INFO: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

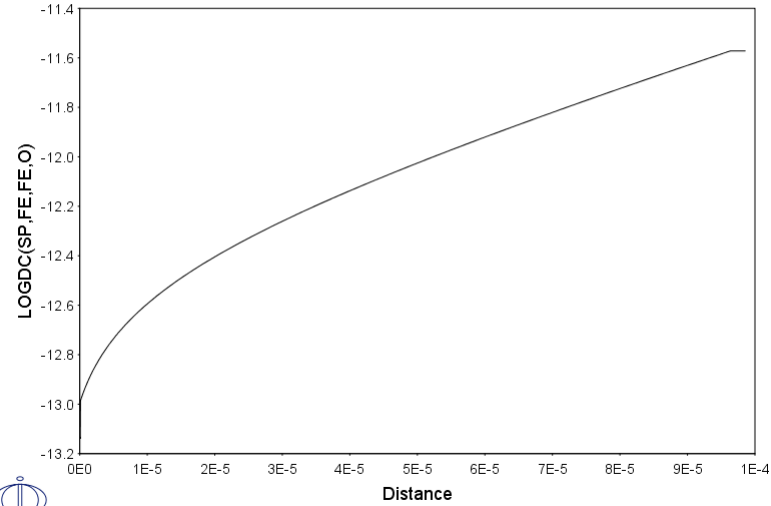
2018.02.18.22.44.50
Time = 86400
CELL #1



```
POST-1:
POST-1:
POST-1: @?<Hit_return_to_continue>
POST-1:
POST-1: @@
POST-1: @@ COMPARE MOBILITIES IN A SPINEL FOR Fe+2 AND Fe+3 SPECIES PRESENT ON THE
POST-1: @@ SECOND SUBLATTICE. FOR THIS WE NEED TO ENTER A TABLE.
POST-1: @@
POST-1: ent table mobfe
Variable(s) logm(sp,fe+2#2) logm(sp,fe+3#2)
POST-1:
POST-1: s-d-a y mobfe
COLUMN NUMBER /*/:
POST-1:
POST-1: plot
2018.02.18.22.44.51
Time = 86400
CELL #1
```



```
POST-1:
POST-1:
POST-1: @?<Hit_return_to_continue>
POST-1: @@
POST-1: @@ NOW PLOT THE INTERDIFFUSION COEFFICIENT OF Fe IN A SPINEL
POST-1: @@
POST-1: s-d-a y logdc(sp,fe,fe,o)
POST-1:
POST-1: plot
```



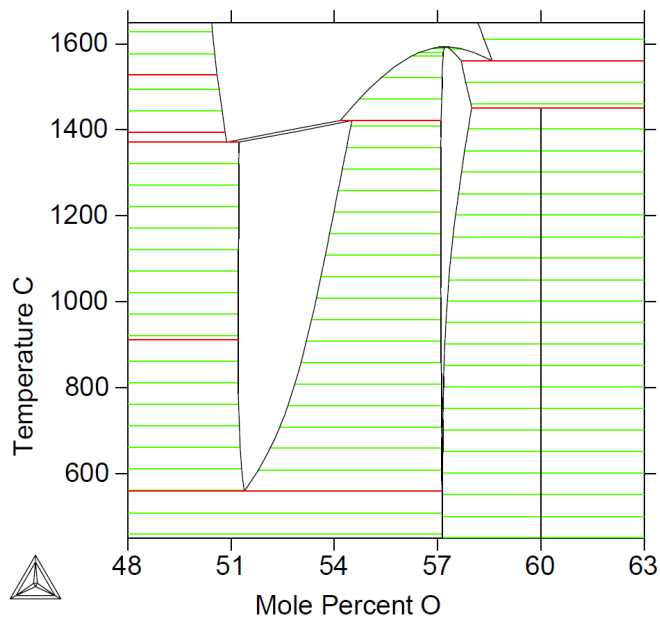
POST-1:
POST-1:
POST-1: set-inter
--OK--
POST-1:



Example i3b

Diffusion in iron oxide (FeO) with grain boundary contribution

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



exi3b-setup

About simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,
Stockholm, Sweden

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

SYS: **SYS:** **MACRO** "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exi3b\setup.DCM" @@

SYS: @@ Diffusion in complex phases.

SYS: @@ Diffusion in iron oxide (FeO) with a grain boundary contribution

SYS: @@ This example shows the oxidation of an iron sample and consequent

SYS: @@ growth of an oxide layer using the grain boundary diffusion

SYS: @@ contribution model.

SYS: -----

NO SUCH COMMAND, USE HELP

SYS:

SYS: @@ exi3_setup.DCM

SYS:

SYS: @@

SYS: @@ START BY GOING TO THE DATABASE MODULE

SYS: @@

SYS: go da

THERMODYNAMIC DATABASE module

Current database: Steels/Fe-Alloys v9.0

VA /- DEFINED
L12_FCC B2_BCC DICTRA_FCC_A1
REJECTED

TDB_TCFE9:

TDB_TCFE9: @@

TDB_TCFE9: @@ SELECT A USER DATABASE TO READ THE THERMODYNAMIC DATA

TDB_TCFE9: @@

TDB_TCFE9: sw user FeO.TDB

Current database: User defined Database

This database does not support the DATABASE_INFORMATION command

VA /- DEFINED

TDB_USER: def-sys fe o

FE O DEFINED

TDB_USER: rej sp *

VA FE
/- FE+2 FE+3
O FE+2
FE+4 FE2O3 FEO
FEO3/2 O-2 O2
REJECTED

TDB_USER: res sp fe fe+2 fe+3 o o2 o-2 va

FE FE+2 FE+3
O O2 O-2

VA RESTORED

TDB_USER: rej ph * all

GAS:G BCC_A2 SPINEL:I

REJECTED

TDB_USER: res ph bcc spinel gas

BCC_A2 SPINEL:I GAS:G

RESTORED

TDB_USER:

TDB_USER: get

ELEMENTS

SPECIES

PHASES

PARAMETERS ...

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

```

Reference REF30      missing close to line      158
Reference REF30      missing close to line      160
Reference REF420     missing close to line      162
Reference REF420     missing close to line      164
Reference REF30      missing close to line      166
Reference REF30      missing close to line      168
Reference REF30      missing close to line      170
Reference REF420     missing close to line      172
Reference REF420     missing close to line      174
Reference REF30      missing close to line      176
Reference REF30      missing close to line      178
Reference REF30      missing close to line      180
Reference REF420     missing close to line      182
Reference REF420     missing close to line      184
Reference REF30      missing close to line      186
Reference REF30      missing close to line      188
Reference REF30      missing close to line      190
Reference REF420     missing close to line      192
Reference REF420     missing close to line      194
Reference REF30      missing close to line      196
Reference REF30      missing close to line      198
Reference REF30      missing close to line      200
Reference REF420     missing close to line      202
Reference REF420     missing close to line      204
FUNCTIONS ....
-OK-
TDB_USER:
TDB_USER: @@
TDB_USER: @@ SWITCH TO A USER-DEFINED MOBILITY DATABASE TO RETRIEVE MOBILITY DATA
TDB_USER: @@
TDB_USER: app user Fe0mob.TDB
Current database: User defined Database
test database

VA              /-              O
DEFINED
TDB_APP: def-sys fe o
FE DEFINED
TDB_APP: rej sp *
/-              VA              FE
O              FE+2            FE+3
FE2O3         FEO             FEO3/2
O-2           O2 REJECTED
TDB_APP: res sp fe fe+2 fe+3 o o2 o-2 va
FE              FE+2            FE+3
O              O2              O-2
VA RESTORED
TDB_APP: rej ph * all
SPINEL:I              GAS:G              BCC_A2
REJECTED
TDB_APP: res ph bcc spinel gas
BCC_A2              SPINEL:I              GAS:G
RESTORED
TDB_APP:
TDB_APP: get
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

List of references for assessed data

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

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

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

```

```

DIC> @@
DIC> ent-grid fer 4.99999e-3 AUTO
DIC>
DIC> @@
DIC> @@ ENTER A THIN INITIAL SIZE FOR THE OXIDE
DIC> @@
DIC> @@
DIC> ent-grid sp 1.00e-10 AUTO
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITIONS IN BCC
DIC> @@
DIC> ent-comp fer bcc#1 m-f
PROFILE FOR /O/: o lin 1e-9 1e-9
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITIONS IN THE OXIDE
DIC> @@
DIC> ent-comp sp spinel m-f
    this is a phase with charged species
    with more than 2 sublattices
PROFILE FOR /FE/: FE lin 4.28771E-01 4.28549E-01
DIC>
DIC>
DIC> @@
DIC> @@ ENTER A BOUNDARY CONDITION "GAS" ON THE UPPER (RIGHT-MOST) INTERFACE
DIC> @@ OF THE OXIDE. THIS ALLOWS THE SYSTEM TO EXPAND AND THE OXIDE LAYER
DIC> @@ TO GROW EXTERNALLY. FOR THIS EXAMPLE AN OXYGEN ACTIVITY IS SPECIFIED
DIC> @@ THAT IS LOW ENOUGH NOT TO FORM CORUNDUM (FE2O3). ALSO SPECIFY THAT
DIC> @@ THERE IS NO FLUX OF Fe ACROSS THIS INTERFACE, I.E. NO Fe IS
DIC> @@ ALLOWED TO ENTER OR LEAVE THE SYSTEM.
DIC> @@
DIC> set-cond boundary upper gas

TYPE OF CONDITION FOR COMPONENT FE /ZERO_FLUX/: zero-flux
TYPE OF CONDITION FOR COMPONENT O /ZERO_FLUX/: act
LOW TIME LIMIT /O/: 0 4.5e-4; * N
DIC>
DIC>
DIC> @@
DIC> @@ ENTER START VALUES FOR THE INITIAL INTERFACE VELOCITIES
DIC> @@
DIC> s-a-s-v -1e-5 1e-5 yes
    STARTING VALUES WILL BE TAKEN FROM PROFILES
DIC>
DIC>
DIC> @@
DIC> @@ SIMULATE FOR 24 HOURS
DIC> @@
DIC> s-s-time 86400,,,,
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC> @@
DIC> @@ SPECIFY THAT POTENTIALS AND NOT ACTIVITIES ARE VARIED AT THE PHASE
DIC> @@ INTERFACE. ALSO USE A FULLY IMPLICIT SCHEME FOR TIME INTEGRATION.
DIC> @@
DIC> s-s-c 0 1 1 YES POT YES YES 1 2,,,,,,,,,
    RELEASING OLD STARTING VALUES
DIC>
DIC>
DIC> @@ ENABLE THE GRAIN BOUNDARY DIFFUSION CONTRIBUTION MODEL
DIC> GB
REGION NAME : /SP/: SP
PHASE NAME: /SPINEL/: SPINEL
Enable model for grainboundary contribution to diffusion /YES/: YES
Grainboundary thickness /5E-10/: 5e-10
Grainsize(T,P,TIME)= 10.0e-6;
Bulkdiffusion activation energy multiplier /.5/: 0.333333
Enable model for dislocation contribution to diffusion /YES/: NO
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exi3b.DIC Y
DIC>
DIC>
DIC>
DIC> set-inter
--OK--
DIC>

```


exi3b-run

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exi3b\run.DCM"DIC>
DIC>
DIC> @@ exi3_run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING EXAMPLE i3
DIC> @@
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
TIME STEP AT TIME 0.00000E+00
DIC> read exi3b
OK
DIC>
DIC> @@
DIC> @@ START THE SIMULATION
DIC> @@
DIC> sim y
Region: FER
single geometric dense at 0.50000E-02
0.87386 95
Region: SP
double geometric
dense at outer boundaries, coarse at 0.50000E-10
lower part 1.2500 9
upper part 0.80000 9
Trying old scheme 3
U-FRACTION IN SYSTEM: FE = 0.99999999500542 O = 2.10000395011622E-08
TOTAL SIZE OF SYSTEM: .0049999901 [m]
U-FRACTION IN SYSTEM: FE = 0.99999999500542 O = 2.10000395011622E-08
TOTAL SIZE OF SYSTEM: .0049999901 [m]
6.141047161402763E-002 6.141016485504380E-002 6.141020906836839E-002 8.444643043596949E-003 1.457879775798498E-
024 TIME = 0.100000000E-06 DT = 0.100000000E-06 SUM OF SQUARES = 0.14578798E-23
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.16337999E-03 AND 0.0000000
POSITION OF INTERFACE FER / SP IS 0.49999900E-02
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.29859730E-03 AND 0.0000000
POSITION OF INTERFACE SP / gas interface IS 0.49999901E-02
U-FRACTION IN SYSTEM: FE = 0.99999999230859 O = 2.69769194565743E-08
TOTAL SIZE OF SYSTEM: .00499999011352 [m]
10 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: FER

CPU time used in timestep 0 seconds
8.109452882793873E-006 8.108765481852460E-006 8.108714358263970E-006 3.429203689632118E-007 3.460921124583648E-
030 TIME = 0.300000000E-06 DT = 0.200000000E-06 SUM OF SQUARES = 0.34609211E-29
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.37478240E-03 AND 0.0000000
POSITION OF INTERFACE FER / SP IS 0.49999899E-02
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.57006118E-03 AND 0.0000000
POSITION OF INTERFACE SP / gas interface IS 0.49999902E-02
U-FRACTION IN SYSTEM: FE = 0.99999998461782 O = 4.97790566167421E-08
TOTAL SIZE OF SYSTEM: .00499999015258 [m]

CPU time used in timestep 0 seconds
8.244220084356107E-006 8.245624820001861E-006 8.245834323740700E-006 5.265259157283041E-009 3.040545442780437E-
031 TIME = 0.700000000E-06 DT = 0.400000000E-06 SUM OF SQUARES = 0.30405454E-30
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.17607366E-03 AND 0.0000000
POSITION OF INTERFACE FER / SP IS 0.49999898E-02
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.24106846E-03 AND 0.0000000
POSITION OF INTERFACE SP / gas interface IS 0.49999902E-02
U-FRACTION IN SYSTEM: FE = 0.99999997890226 O = 6.90656000538019E-08
TOTAL SIZE OF SYSTEM: .00499999017858 [m]

CPU time used in timestep 0 seconds
1.134920301888734E-007 1.135894804039261E-007 1.135506444176019E-007 5.608707817274067E-010 5.589428618385944E-
033 TIME = 0.150000000E-05 DT = 0.800000000E-06 SUM OF SQUARES = 0.55894286E-32
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.14432292E-03 AND 0.0000000
POSITION OF INTERFACE FER / SP IS 0.49999897E-02
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.20898651E-03 AND 0.0000000
POSITION OF INTERFACE SP / gas interface IS 0.49999902E-02
U-FRACTION IN SYSTEM: FE = 0.99999996836327 O = 1.02505972099334E-07
TOTAL SIZE OF SYSTEM: .00499999023031 [m]
8 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: SP

CPU time used in timestep 1 seconds
4.495117154993389E-007 4.496453319495406E-007 4.496431998391493E-007 2.514741666006164E-010 2.513206922058051E-
034 TIME = 0.310000000E-05 DT = 0.160000000E-05 SUM OF SQUARES = 0.25132069E-33
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.94208025E-04 AND 0.0000000
POSITION OF INTERFACE FER / SP IS 0.49999896E-02
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.13424763E-03 AND 0.0000000
POSITION OF INTERFACE SP / gas interface IS 0.49999903E-02
U-FRACTION IN SYSTEM: FE = 0.99999995509026 O = 1.45469731183719E-07
TOTAL SIZE OF SYSTEM: .00499999029437 [m]
32 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: SP

CPU time used in timestep 0 seconds
1.153179467205265E-005 1.153635784462131E-005 1.153592952376297E-005 1.797713989031012E-008 1.284911245787787E-
030 TIME = 0.630000000E-05 DT = 0.320000000E-05 SUM OF SQUARES = 0.12849112E-29
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.67615626E-04 AND 0.0000000
POSITION OF INTERFACE FER / SP IS 0.49999894E-02
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.97021972E-04 AND 0.0000000
POSITION OF INTERFACE SP / gas interface IS 0.49999904E-02
U-FRACTION IN SYSTEM: FE = 0.99999993575642 O = 2.07571156029763E-07
TOTAL SIZE OF SYSTEM: .00499999038847 [m]

output ignored...

... output resumed

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

CPU time used in timestep 1 seconds
5.273117098378293E-007 5.281046129101103E-007 5.280427494561641E-007 7.076339562288592E-010 1.841670509320294E-
032 TIME = 56943.895 DT = 8640.0000 SUM OF SQUARES = 0.18416705E-31
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.70247282E-09 AND 0.0000000
POSITION OF INTERFACE FER / SP IS 0.49272776E-02
```

CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.10045406E-08 AND 0.0000000
POSITION OF INTERFACE SP / gas interface IS 0.50312191E-02
U-FRACTION IN SYSTEM: FE = .99366131709631 O = .020659486569886
TOTAL SIZE OF SYSTEM: .00503121911345 [m]
9 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: SP

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

CPU time used in timestep 1 seconds
1.646046081816719E-007 1.649792107009017E-007 1.649481519432754E-007 1.988144432406818E-010 1.123208362097712E-
033 TIME = 74223.895 DT = 8640.0000 SUM OF SQUARES = 0.11232084E-32
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.60654812E-09 AND 0.0000000
POSITION OF INTERFACE FER / SP IS 0.49164301E-02
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.86919604E-09 AND 0.0000000
POSITION OF INTERFACE SP / gas interface IS 0.50359098E-02
U-FRACTION IN SYSTEM: FE = .992730593159095 O = .0237257189757379
TOTAL SIZE OF SYSTEM: .00503590981819 [m]
11 GRIDPOINT(S) REMOVED FROM CELL #1 REGION: SP

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

CPU time used in timestep 0 seconds
1.518627609602451E-008 1.512781289831391E-008 1.530717153876908E-008 1.085155039390110E-011 1.301507345230437E-
034 TIME = 86400.0000 DT = 3536.1047 SUM OF SQUARES = 0.13015073E-33
CELL # 1 VELOCITY AT INTERFACE # 2 IS -0.56483678E-09 AND 0.0000000
POSITION OF INTERFACE FER / SP IS 0.49094993E-02
CELL # 1 VELOCITY AT INTERFACE # 3 IS 0.78548555E-09 AND 0.0000000
POSITION OF INTERFACE SP / gas interface IS 0.50388274E-02
U-FRACTION IN SYSTEM: FE = .992153350362077 O = .0256664807148033
TOTAL SIZE OF SYSTEM: .00503882739841 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME 0.0000000
DELETING TIME-RECORD FOR TIME 0.10000000E-06
DELETING TIME-RECORD FOR TIME 0.30000000E-06
DELETING TIME-RECORD FOR TIME 0.70000000E-06
DELETING TIME-RECORD FOR TIME 0.15000000E-05
DELETING TIME-RECORD FOR TIME 0.31000000E-05
DELETING TIME-RECORD FOR TIME 0.63000000E-05
DELETING TIME-RECORD FOR TIME 0.12700000E-04
DELETING TIME-RECORD FOR TIME 0.25500000E-04
DELETING TIME-RECORD FOR TIME 0.51100000E-04
DELETING TIME-RECORD FOR TIME 0.10230000E-03
DELETING TIME-RECORD FOR TIME 0.20470000E-03
DELETING TIME-RECORD FOR TIME 0.40950000E-03
DELETING TIME-RECORD FOR TIME 0.81910000E-03
DELETING TIME-RECORD FOR TIME 0.16383000E-02
DELETING TIME-RECORD FOR TIME 0.32767000E-02
DELETING TIME-RECORD FOR TIME 0.65535000E-02
DELETING TIME-RECORD FOR TIME 0.13107100E-01
DELETING TIME-RECORD FOR TIME 0.26214300E-01
DELETING TIME-RECORD FOR TIME 0.52428700E-01
DELETING TIME-RECORD FOR TIME 0.10485750
DELETING TIME-RECORD FOR TIME 0.20971510
DELETING TIME-RECORD FOR TIME 0.41943030
DELETING TIME-RECORD FOR TIME 0.83886070
DELETING TIME-RECORD FOR TIME 1.6777215
DELETING TIME-RECORD FOR TIME 3.3554431
DELETING TIME-RECORD FOR TIME 6.7108863
DELETING TIME-RECORD FOR TIME 13.421773
DELETING TIME-RECORD FOR TIME 26.843545
DELETING TIME-RECORD FOR TIME 53.687091
DELETING TIME-RECORD FOR TIME 107.37418
DELETING TIME-RECORD FOR TIME 214.74836
DELETING TIME-RECORD FOR TIME 429.49673
DELETING TIME-RECORD FOR TIME 858.99346
DELETING TIME-RECORD FOR TIME 1717.9869
DELETING TIME-RECORD FOR TIME 3435.9738
DELETING TIME-RECORD FOR TIME 6871.9477
DELETING TIME-RECORD FOR TIME 13743.895
DELETING TIME-RECORD FOR TIME 22383.895
DELETING TIME-RECORD FOR TIME 31023.895
DELETING TIME-RECORD FOR TIME 39663.895
DELETING TIME-RECORD FOR TIME 48303.895
DELETING TIME-RECORD FOR TIME 56943.895
DELETING TIME-RECORD FOR TIME 65583.895
DELETING TIME-RECORD FOR TIME 74223.895

KEEPING TIME-RECORD FOR TIME 82863.895
AND FOR TIME 86400.000
WORKSPACE RECLAIMED

TIMESTEP AT 86400.0000 SELECTED

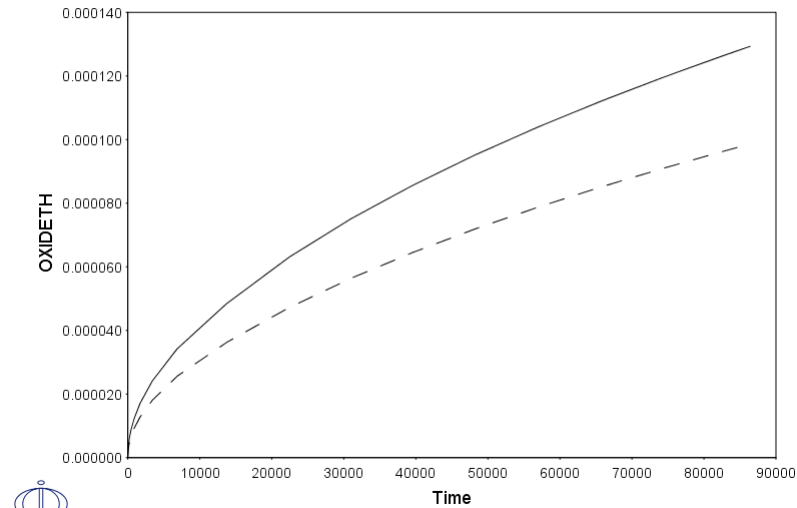
DIC>
DIC> set-inter
--OK--
DIC>

exi3b-plot

```
DIC>AboutMACRO "c:\jenkins\workspace\DICTRA-Generate-Console-Examples\examples\exi3b\plot.DCM"DIC>
DIC> @@ exi3_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE i3
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
      TIME STEP AT TIME    8.64000E+04
DIC> read exi3b
      OK
DIC>
DIC> @@
DIC> @@ ENTER THE POST PROCESSOR
DIC> @@
DIC> post

      POST PROCESSOR VERSION    1.7
      Implemented by Bjorn Jonsson
```

```
POST-1:
POST-1: @@
POST-1: @@ PLOT THE THICKNESS OF THE OXIDE LAYER GROWING AT THE SURFACE.
POST-1: @@ FOR THIS WE NEED TO ENTER A FUNCTION ACCORDING TO THE FOLLOWING.
POST-1: ent func oxideth
FUNCTION: poi(sp,upper)-poi(sp,lower)
&
POST-1: @@
POST-1: @@ PUT THIS FUNCTION ON THE Y-AXIS
POST-1: @@
POST-1: s-d-a y oxideth
POST-1:
POST-1: @@
POST-1: @@ AND PLOT THE OXIDE THICKNESS VERSUS TIME
POST-1: @@
POST-1: s-d-a x time
      INFO: Time is set as independent variable
POST-1:
POST-1: @@
POST-1: @@ SINCE WE ARE PLOTTING A FUNCTION, SPECIFY A PLOT CONDITION
POST-1: @@
POST-1: s-p-c interface sp upper
POST-1:
POST-1: app y exi3a.exp 0; 1;
POST-1:
POST-1: plot
2018.02.18.22.48.16
UPPER INTERFACE OF REGION"SP#1"
CELL #1
```



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

