# Diffusion Module (DICTRA) Example Macros

**Thermo-Calc Version 2020b**

Thermo-Calc Software

Copyright 2020 Thermo-Calc Software AB. All rights reserved.

Information in this document is subject to change without notice. The software described in this document is furnished under a license agreement or nondisclosure agreement. The software may be used or copied only in accordance with the terms of those agreements.

Thermo-Calc Software AB

Råsundavägen 18, SE-169 67 Solna, Sweden

+46 8 545 959 30

documentation@thermocalc.com

www.thermocalc.com

**exa1**

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

**exa2a**

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

**exa2b**

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

**exa3**

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

**exa4**

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

**exa5**

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

**exa6**

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

**exa7**

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

**exb1a**

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

**exb1b**

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

**exb1c**

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

**exb2**

Moving boundary problem. Cementite dissolution in an Fe-Cr-C alloy This example calculates the dissolution of a spherical cementite particle in an austenite matrix. This case is from Z.-K. Liu, L. Höglund, B. Jönsson and J. Ågren: Metall. Trans.A, v.22A (1991), pp. 1745-1752.

**exb3**

Moving boundary example. Dissolution of 23-carbide in an austenitic matrix This example calculates the dissolution of an M23C6 particle in an austenite matrix. A film of ferrite is allowed to nucleate around the carbide during the precipitation.

**exb4a**

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

**exb4b**

Moving boundary problem. Solidification path of an Fe-18%Cr-8%Ni alloy: Peritectic reaction This example is the same as exb4a but now a peritectic reaction is assumed: LIQUID + BCC -> FCC. Hence the FCC region should appear in between the LIQUID and the BCC. Comparison is made with both a Scheil-Gulliver simulation and equilibrium solidification conditions, both done in Thermo-Calc.

**exb4c**

Moving boundary problem. Solidification path of an Fe-18%Cr-8%Ni alloy This example is the same as exb4b but now the diffusivity data is amended for the LIQUID and a high value for the diffusivity is used to simulate a case where it is assumed that the composition in the LIQUID is always homogeneous. This example is less realistic than exb4b. Comparison is made with both a Scheil-Gulliver simulation and equilibrium solidification conditions, both done in Thermo-Calc.

**exb4d**

Moving boundary problem. Solidification path of an Fe-18%Cr-8%Ni alloy This example is the same as exb4b but instead of controlling the temperature the amount of heat extracted is given. Comparison is made with both a Scheil-Gulliver simulation and equilibrium solidification conditions, both done in Thermo-Calc.

**exb5**

Moving boundary problem. Ternary diffusion couple of Fe-Ni-Cr alloys This example demonstrates the evaluation of a ternary Fe-Cr-Ni diffusion couple. A thin slice of alpha phase (38%Cr, 0%Ni) is clamped between two thicker slices of gamma phase (27%Cr, 20%Ni). The assembly is subsequently heat treated at 1373 K. This example corresponds to diffusion couple A in M. Kajihara, C.-B. Lim and M. Kikuchi: ISIJ International 33 (1993), pp. 498-507. See also M. Kajihara and M. Kikichi: Acta Metall.Mater. 41 (1993), pp.2045-2059.

**exb6**

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

**exb7**

This example modifies the database interactively, which is not yet supported by GES6. Therefore, we enforce the use of GES5.

**exc1**

Cell calculation. Carbon cannon in ferrite/austenite: Fe-C system, 2-cell calculation This example simulates what happens to a ferrite plate that has inherited the carbon content of its parent austenite. The ferrite plate formed is embedded in an austenite matrix. This setup corresponds to a proposed mechanism for formation of Widmannstätten ferrite or for the ferrite phase of the bainite structure. It is assumed that the phase boundary between ferrite and austenite is immobile, this is achieved in the simulation by putting the ferrite and the austenite in two different cells. See also M. Hillert, L. Höglund and J. Ågren: Acta Metall. Mater. 41 (1993), pp.1951-1957.

**exc2**

Cell calculation. Cementite dissolution in an Fe-Cr-C alloy: Three particle sizes and three different cells This example calculates the dissolution of cementite particles in an austenite matrix. This example is the same as exc1 but instead there are three particle sizes. A total of six particles are considered using three different cells. This is to represent some size distribution among the cementite particles. See also Z.-K. Liu, L. Höglund, B. Jönsson and J. Ågren: Metall.Trans.A, v. 22A (1991), pp. 1745-1752.

**exd1a**

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

**exd1b**

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

**exd2a**

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

**exd2b**

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

**exd3**

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

**exe1**

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

**exf1**

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

**exg1**

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

**exg2**

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

**exh1**

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

**exh2**

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

**exh3**

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

**exi1**

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

**exi2**

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

**exi3a**

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

**exi3b**

# 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.

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

## Results

### exa1-setup

```
SYS:About

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

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 21012) 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: Mon Nov 11 11:13:13 2019


SYS:SYS:MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exa1\setup.DCM.test"
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  v10.0

 VA                       /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10:
TDB_TCFE10: @@
TDB_TCFE10: @@ USE THERMODYNAMIC DATABASE TO RETRIEVE DATA
TDB_TCFE10: @@
TDB_TCFE10: switch_database
 Use one of these databases

 TCFE10  =  Steels/Fe-Alloys  v10.0
 TCFE9   =  Steels/Fe-Alloys  v9.1
 TCFE8   =  Steels/Fe-Alloys  v8.1
 TCFE7   =  Steels/Fe-Alloys  v7.0
 TCFE6   =  Steels/Fe-Alloys  v6.2
 TCFE5   =  Steels/Fe-Alloys  v5.0
 TCFE4   =  Steels/Fe-Alloys  v4.1
 TCFE3   =  Steels/Fe-Alloys  v3.1
 TCFE2   =  Steels/Fe-Alloys  v2.1
 TCFE1   =  Steels/Fe-Alloys  v1.0
 FROST1  =  FROST database v1.2
 FEDAT   =  TCS/TT Steels Database v1.0
 TCNI10  =  Ni-Alloys  v10.0 SNAPSHOT
 TCNI9   =  Ni-Alloys  v9.1
 TCNI8   =  Ni-Alloys  v8.2
 TCNI7   =  Ni-Alloys  v7.2
 TCNI6   =  Ni-Alloys  v6.1
 TCNI5   =  Ni-Alloys  v5.1
 TCNI4   =  Ni-Alloys  v4.0
 TCNI1   =  Ni-Alloys  v1.3
 TCAL6   =  Al-Alloys  v6.0
 TCAL5   =  Al-Alloys  v5.1
 TCAL4   =  Al-Alloys  v4.0
 TCAL3   =  Al-Alloys  v3.0
 TCAL2   =  Al-Alloys  v2.1
 TCAL1   =  Al-Alloys  v1.2
 TCMG5   =  Mg-Alloys  v5.1
 TCMG4   =  Mg-Alloys  v4.0
 TCMG3   =  Mg-Alloys  v3.0
 TCMG2   =  Mg-Alloys  v2.0
 TCMG1   =  Mg-Alloys  v1.1
 TCTI2   =  Ti-Alloys  v2.1
 TCTI1   =  Ti-Alloys  v1.0
 TCCU3   =  Cu-Alloys  v3.1
 TCCU2   =  Cu-Alloys  v2.0
 TCCU1   =  Cu-Alloys  v1.0
 TCCC1   =  Cemented carbide  v1.0
 TCHEA4  =  High Entropy Alloy  v4.0
 TCHEA3  =  High Entropy Alloy  v3.1
 TCHEA2  =  High Entropy Alloy  v2.1.1
 TCHEA1  =  High Entropy Alloy  v1.0
 SSOL7   =  SGTE Alloy Solutions Database v7.0
 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
 TCOX10  =  Metal Oxide Solutions  v10.0 SNAPSHOT
```

```
 TCOX9   =  Metal Oxide Solutions  v9.0
 TCOX8   =  Metal Oxide Solutions  v8.0
 TCOX7   =  Metal Oxide Solutions  v7.0
 TCOX6   =  Metal Oxide Solutions  v6.0
 TCOX5   =  Metal Oxide Solutions  v5.1
 TCOX4   =  Metal Oxide Solutions  v4.1
 ION3    =  Ionic Solutions  v3.0
 ION2    =  Ionic Solutions  v2.6
 ION1    =  Ionic Solutions  v1.5
 NOX2    =  NPL Oxide Solutions Database v2.1
 TCNOBL2 =  Noble Metals Alloys v2.0 SNAPSHOT
 TCNOBL1 =  Noble Metals Alloys v1.0
 TCSLD3  =  Solder Alloys  v3.2
 TCSLD2  =  Solder Alloys  v2.0
 TCSLD1  =  Solder Alloys  v1.1
 TCSI1   =  Ultrapure Silicon  v1.2
 TCMP2   =  Materials Processing  v2.5
 TCES1   =  Combustion/Sintering  v1.1
 TCSC1   =  Super Conductor  v1.0
 TCFC1   =  SOFC Database v1.0
 TCNF2   =  Nuclear Fuels  v2.1b
 NUMT2   =  Nuclear Materials  v2.1
 NUOX4   =  Nuclear Oxides  v4.2
 NUCL15  =  IRSN NUCLEA-15_4
 NUCL10  =  ThermoData NUCLEA Alloys-oxides TDB v10.2
 MEPH15  =  IRSN Mephista-15_1
 MEPH11  =  ThermoData MEPHISTA Nuclear Fuels TDB v11.2
 TCAQ3   =  Aqueous Solution  v3.0
 TCAQ2   =  Aqueous Solution  v2.7
 AQS2    =  TGG Aqueous Solution Database v2.6
 GCE2    =  TGG Geochemical/Environmental TDB v2.3
 FEDEMO  =  Iron Demo Database v2.1
 ALDEMO  =  Aluminum Demo Database v3.0
 NIDEMO  =  Nickel Demo Database v1.1
 CUDEMO  =  Copper Demo Database v1.0
 SLDEMO  =  Solder Demo Database v1.0
 OXDEMO  =  Oxide Demo Database v1.0
 SUBDEMO =  Substance Demo Database v1.0
 PTERN   =  Public Ternary Alloys TDB v1.3
 PAQ2    =  Public Aqueous Soln (SIT) TDB v2.4
 PG35    =  G35 Binary Semi-Conductors TDB v1.2
 PURE5   =  SGTE Unary (Pure Elements) TDB v5.1
 MOB2    =  Alloys Mobility  v2.7
 MOB1    =  Alloys Mobility  v1.3
 MOBFE1  =  Steels/Fe-Alloys Mobility  v1.1
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBFE5  =  Steels/Fe-Alloys Mobility  v5.0
 MOBNI5  =  Ni-Alloys Mobility  v5.1
 MOBNI4  =  Ni-Alloys Mobility  v4.1
 MOBNI3  =  Ni-Alloys Mobility  v3.2
 MOBNI2  =  Ni-Alloys Mobility  v2.4
 MOBNI1  =  Ni-Alloys Mobility  v1.10
 MOBAL5  =  Al-Alloys Mobility  v5.0
 MOBAL4  =  Al-Alloys Mobility  v4.0
 MOBAL3  =  Al-Alloys Mobility  v3.0
 MOBAL2  =  Al-Alloys Mobility  v2.0
 MOBAL1  =  Al-Alloys Mobility  v1.0
 MOBCU1  =  Cu-Alloys Mobility  v1.0
 MOBCU2  =  Cu-Alloys Mobility  v2.0
 MOBCU3  =  Cu-Alloys Mobility  v3.0
 MOBHEA1 =  High Entropy Alloys Mobility  v1.0
 MOBHEA2 =  High Entropy Alloys Mobility  v2.0
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBSLD1 =  Solder-Alloys Mobility  v1.1
 MOBTI3  =  Ti-Alloys Mobility  v3.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v2.0
 MFEDEMO =  Fe-Alloys Mobility demo database v2.0
 MNIDEMO =  Ni-Alloys Mobility demo database v1.0
 MCUDEMO =  Cu-Alloys Mobility demo database v1.0
 USER    =  User defined Database

DATABASE NAME /TCFE10/: fedemo
 Current database: Iron Demo Database v2.1

 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                  CBCC_A12
 CUB_A13                 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
14:19:22,929 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
```

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

 List of references for assessed data

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

 TCFE10  =  Steels/Fe-Alloys  v10.0
 TCFE9   =  Steels/Fe-Alloys  v9.1
 TCFE8   =  Steels/Fe-Alloys  v8.1
 TCFE7   =  Steels/Fe-Alloys  v7.0
 TCFE6   =  Steels/Fe-Alloys  v6.2
 TCFE5   =  Steels/Fe-Alloys  v5.0
 TCFE4   =  Steels/Fe-Alloys  v4.1
 TCFE3   =  Steels/Fe-Alloys  v3.1
 TCFE2   =  Steels/Fe-Alloys  v2.1
 TCFE1   =  Steels/Fe-Alloys  v1.0
 FROST1  =  FROST database v1.2
 FEDAT   =  TCS/TT Steels Database v1.0
 TCNI10  =  Ni-Alloys  v10.0 SNAPSHOT
 TCNI9   =  Ni-Alloys  v9.1
 TCNI8   =  Ni-Alloys  v8.2
 TCNI7   =  Ni-Alloys  v7.2
 TCNI6   =  Ni-Alloys  v6.1
 TCNI5   =  Ni-Alloys  v5.1
 TCNI4   =  Ni-Alloys  v4.0
 TCNI1   =  Ni-Alloys  v1.3
 TCAL6   =  Al-Alloys  v6.0
 TCAL5   =  Al-Alloys  v5.1
 TCAL4   =  Al-Alloys  v4.0
 TCAL3   =  Al-Alloys  v3.0
 TCAL2   =  Al-Alloys  v2.1
 TCAL1   =  Al-Alloys  v1.2
 TCMG5   =  Mg-Alloys  v5.1
 TCMG4   =  Mg-Alloys  v4.0
 TCMG3   =  Mg-Alloys  v3.0
 TCMG2   =  Mg-Alloys  v2.0
 TCMG1   =  Mg-Alloys  v1.1
 TCTI2   =  Ti-Alloys  v2.1
 TCTI1   =  Ti-Alloys  v1.0
 TCCU3   =  Cu-Alloys  v3.1
 TCCU2   =  Cu-Alloys  v2.0
 TCCU1   =  Cu-Alloys  v1.0
 TCCC1   =  Cemented carbide  v1.0
 TCHEA4  =  High Entropy Alloy  v4.0
 TCHEA3  =  High Entropy Alloy  v3.1
 TCHEA2  =  High Entropy Alloy  v2.1.1
 TCHEA1  =  High Entropy Alloy  v1.0
 SSOL7   =  SGTE Alloy Solutions Database v7.0
 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
 TCOX10  =  Metal Oxide Solutions  v10.0 SNAPSHOT
 TCOX9   =  Metal Oxide Solutions  v9.0
 TCOX8   =  Metal Oxide Solutions  v8.0
 TCOX7   =  Metal Oxide Solutions  v7.0
 TCOX6   =  Metal Oxide Solutions  v6.0
 TCOX5   =  Metal Oxide Solutions  v5.1
 TCOX4   =  Metal Oxide Solutions  v4.1
 ION3    =  Ionic Solutions  v3.0
 ION2    =  Ionic Solutions  v2.6
 ION1    =  Ionic Solutions  v1.5
 NOX2    =  NPL Oxide Solutions Database v2.1
 TCNOBL2 =  Noble Metals Alloys v2.0 SNAPSHOT
 TCNOBL1 =  Noble Metals Alloys v1.0
 TCSLD3  =  Solder Alloys  v3.2
 TCSLD2  =  Solder Alloys  v2.0
 TCSLD1  =  Solder Alloys  v1.1
 TCSI1   =  Ultrapure Silicon  v1.2
 TCMP2   =  Materials Processing  v2.5
 TCES1   =  Combustion/Sintering  v1.1
 TCSC1   =  Super Conductor  v1.0
 TCFC1   =  SOFC Database v1.0
 TCNF2   =  Nuclear Fuels  v2.1b
 NUMT2   =  Nuclear Materials  v2.1
 NUOX4   =  Nuclear Oxides  v4.2
 NUCL15  =  IRSN NUCLEA-15_4
 NUCL10  =  ThermoData NUCLEA Alloys-oxides TDB v10.2
 MEPH15  =  IRSN Mephista-15_1
 MEPH11  =  ThermoData MEPHISTA Nuclear Fuels TDB v11.2
 TCAQ3   =  Aqueous Solution  v3.0
 TCAQ2   =  Aqueous Solution  v2.7
 AQS2    =  TGG Aqueous Solution Database v2.6
 GCE2    =  TGG Geochemical/Environmental TDB v2.3
 FEDEMO  =  Iron Demo Database v2.1
 ALDEMO  =  Aluminum Demo Database v3.0
 NIDEMO  =  Nickel Demo Database v1.1
 CUDEMO  =  Copper Demo Database v1.0
```

```
 SLDEMO  =  Solder Demo Database v1.0
 OXDEMO  =  Oxide Demo Database v1.0
 SUBDEMO =  Substance Demo Database v1.0
 PTERN   =  Public Ternary Alloys TDB v1.3
 PAQ2    =  Public Aqueous Soln (SIT) TDB v2.4
 PG35    =  G35 Binary Semi-Conductors TDB v1.2
 PURE5   =  SGTE Unary (Pure Elements) TDB v5.1
 MOB2    =  Alloys Mobility  v2.7
 MOB1    =  Alloys Mobility  v1.3
 MOBFE1  =  Steels/Fe-Alloys Mobility  v1.1
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBFE5  =  Steels/Fe-Alloys Mobility  v5.0
 MOBNI5  =  Ni-Alloys Mobility  v5.1
 MOBNI4  =  Ni-Alloys Mobility  v4.1
 MOBNI3  =  Ni-Alloys Mobility  v3.2
 MOBNI2  =  Ni-Alloys Mobility  v2.4
 MOBNI1  =  Ni-Alloys Mobility  v1.10
 MOBAL5  =  Al-Alloys Mobility  v5.0
 MOBAL4  =  Al-Alloys Mobility  v4.0
 MOBAL3  =  Al-Alloys Mobility  v3.0
 MOBAL2  =  Al-Alloys Mobility  v2.0
 MOBAL1  =  Al-Alloys Mobility  v1.0
 MOBCU1  =  Cu-Alloys Mobility  v1.0
 MOBCU2  =  Cu-Alloys Mobility  v2.0
 MOBCU3  =  Cu-Alloys Mobility  v3.0
 MOBHEA1 =  High Entropy Alloys Mobility  v1.0
 MOBHEA2 =  High Entropy Alloys Mobility  v2.0
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBSLD1 =  Solder-Alloys Mobility  v1.1
 MOBTI3  =  Ti-Alloys Mobility  v3.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v2.0
 MFEDEMO =  Fe-Alloys Mobility demo database v2.0
 MNIDEMO =  Ni-Alloys Mobility demo database v1.0
 MCUDEMO =  Cu-Alloys Mobility demo database v1.0
 USER    =  User defined Database

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

 VA  DEFINED
APP: define_system
ELEMENTS: fe ni
 FE                    NI  DEFINED
APP: reject
ELEMENTS, SPECIES, PHASES, CONSTITUENT OR SYSTEM: /PHASES/: phase
PHASES: *
 BCC_A2                FCC_A1  REJECTED
APP:
APP: restore
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /ELEMENTS/: phase
PHASES: fcc
 FCC_A1  RESTORED
APP:
APP: get_data
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'This parameter has not been assessed'
  'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
      -Ni'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Ni self-diffusion'
 -OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP
APP: @@
APP: goto_module
MODULE NAME: dictra_monitor
 NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set_condition
GLOBAL OR BOUNDARY CONDITION /GLOBAL/: global
VARIABLE : T
LOW TIME LIMIT /0/: 0
T(TIME,X)= 1400;
HIGH TIME LIMIT /*/: *
ANY MORE RANGES /N/: N
DIC>
DIC> @@
DIC> @@ START BY ENTERING A REGION
DIC> @@
DIC> enter_region
REGION NAME : austenite
DIC>
DIC> @@
DIC> @@ ENTER A GRID INTO THE REGION
DIC> @@
DIC> @@ FOR SIMPLICITY, AN EQUIDISTANT GRID IS USED
DIC> @@
DIC> enter_grid_coordinates
REGION NAME : /AUSTENITE/: austenite
WIDTH OF REGION /1/: 1e-4
TYPE /LINEAR/: AUTO
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE active PHASE INTO THE REGION
DIC> @@
DIC> enter_phase_in_region
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
```

```
REGION NAME : /AUSTENITE/: austenite
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC> @@
DIC> @@ ENTER AN INITIAL Ni COMPOSITION INTO THE PHASE. A LINEAR
DIC> @@ VARIATION IN THE REGION IS ASSUMED.
DIC> @@
DIC> enter_compositions
REGION NAME : /AUSTENITE/: austenite
PHASE NAME: /FCC_A1/: fcc#1
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: weight_percent
PROFILE FOR /NI/: ni
TYPE /LINEAR/: linear
VALUE OF FIRST POINT : 10
VALUE OF LAST POINT : /10/: 50
DIC>
DIC> @@
DIC> @@ THE BOUNDARY CONDITION IS A CLOSED SYSTEM AS WE DO NOT SPECIFY
DIC> @@ ANYTHING ELSE
DIC> @@
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set_simulation_time
END TIME FOR INTEGRATION /.1/: 1E6
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /100000/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO FILE AND EXIT
DIC> @@
DIC> save_workspaces exa1 Y
DIC>
DIC> set_interactive
 --OK---
DIC>
```

**exa1-run**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exa1\run.DCM.test"
DIC>
DIC>
DIC> @@ exa1_run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING EXAMPLE a1
DIC> @@
DIC> goto_module
MODULE NAME: dictra_monitor
 TIME STEP AT TIME  0.00000E+00
DIC>
DIC> read_workspaces exa1
 OK
DIC>
DIC> @@
DIC> @@ Start the simulation
DIC> @@
DIC> simulate_reaction
 Region: AUSTENITE
 linear grid   75
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
 U-FRACTION IN SYSTEM:  FE = .709680136600384  NI = .290319863399616
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 U-FRACTION IN SYSTEM:  FE = .709680136600384  NI = .290319863399616
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .709680136600384  NI = .290319863399616
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.10010000E-03 DT =  0.10000000E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .709680136600384  NI = .290319863399616
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.40010010     DT =  0.40000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .709680136600384  NI = .290319863399616
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   241.69569     DT =   241.29559     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .709680136600384  NI = .290319863399616
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    1 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 = .709680136600384  NI = .290319863399617
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   223302.44     DT =   100000.00     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .709680136600384  NI = .290319863399616
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   323302.44     DT =   100000.00     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .709680136600384  NI = .290319863399616
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   423302.44     DT =   100000.00     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .709680136600385  NI = .290319863399616
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   523302.44     DT =   100000.00     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .709680136600384  NI = .290319863399616
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   623302.44     DT =   100000.00     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .709680136600385  NI = .290319863399615
 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 = .709680136600384  NI = .290319863399616
 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 = .709680136600384  NI = .290319863399616
 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 = .709680136600385  NI = .290319863399615
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   1000000.0     DT =   76697.555     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .709680136600385  NI = .290319863399615
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 MUST SAVE WORKSPACE ON FILE
```

```
 WORKSPACE SAVED ON FILE
 RECLAIMING WORKSPACE
 DELETING TIME-RECORD FOR TIME    0.0000000
 DELETING TIME-RECORD FOR TIME   0.10000000E-06
 DELETING TIME-RECORD FOR TIME   0.10010000E-03
 DELETING TIME-RECORD FOR TIME   0.40010010
 DELETING TIME-RECORD FOR TIME    241.69569
 DELETING TIME-RECORD FOR TIME    724.28686
 DELETING TIME-RECORD FOR TIME    1689.4692
 DELETING TIME-RECORD FOR TIME    3619.8339
 DELETING TIME-RECORD FOR TIME    7480.5633
 DELETING TIME-RECORD FOR TIME    15202.022
 DELETING TIME-RECORD FOR TIME    30644.940
 DELETING TIME-RECORD FOR TIME    61530.775
 DELETING TIME-RECORD FOR TIME    123302.44
 DELETING TIME-RECORD FOR TIME    223302.44
 DELETING TIME-RECORD FOR TIME    323302.44
 DELETING TIME-RECORD FOR TIME    423302.44
 DELETING TIME-RECORD FOR TIME    523302.44
 DELETING TIME-RECORD FOR TIME    623302.44
 DELETING TIME-RECORD FOR TIME    723302.44
 DELETING TIME-RECORD FOR TIME    823302.44

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

 TIMESTEP AT     1000000.00     SELECTED

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

**exa1-plot**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exa1\plot.DCM.test"
DIC>
DIC>
DIC> @@ exa1_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE a1
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> goto_module
MODULE NAME: dictra_monitor
 TIME STEP AT TIME  1.00000E+06
DIC> read_workspaces exa1
 OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post_processor
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:
POST-1: @@
POST-1: @@ PLOT SOME CONCENTRATION PROFILES
POST-1: @@
POST-1: set_diagram_axis
AXIS (X, Y OR Z) : x
VARIABLE : distance
  INFO: Distance is set as independent variable
DISTANCE : /GLOBAL/: global
POST-1:
POST-1: set_diagram_axis
AXIS (X, Y OR Z) : y
VARIABLE : weight-percent
FOR COMPONENT : ni
POST-1:
POST-1: set_plot_condition
CONDITION /TIME/: time
VALUE(S) /LAST/: 0 1e5 3e5 1e6
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot_diagram
```

2019.11.11.14.21.33
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**

```
SYS:About

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

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 21012) 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: Mon Nov 11 11:13:13 2019


SYS:SYS:MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exa2a\setup.DCM.test"
SYS: @@
SYS: @@ One-phase problem.
SYS: @@ Homogenization of a binary Fe-Ni alloy.
SYS: @@ A Ni rich and a Ni lean alloy are put together and initially
SYS: @@ there is a step profile.
SYS: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exa2a_setup.DCM
SYS:
SYS: @@
SYS: @@ IN exa1 ALL THE COMMANDS WERE WRITTEN IN FULL BUT NOW ABBREVIATED
SYS: @@ COMMANDS ARE USED
SYS: @@
SYS:
SYS: @@
SYS: @@ FIRST DEFINE A LOG-FILE FOR THIS EXAMPLE
SYS: @@
SYS: set_log_file setup
Heading:
SYS: @@
SYS: @@ NOW GO TO THE DATABASE MODULE
SYS: @@
SYS: go da
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v10.0

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10:
TDB_TCFE10: @@
TDB_TCFE10: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA
TDB_TCFE10: @@
TDB_TCFE10: sw FEDEMO
   ... the command in full is SWITCH_DATABASE
 Current database: Iron Demo Database v2.1

 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                  CBCC_A12
 CUB_A13                 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
14:23:30,216 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

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

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

```
TCFE5   =  Steels/Fe-Alloys  v5.0
TCFE4   =  Steels/Fe-Alloys  v4.1
TCFE3   =  Steels/Fe-Alloys  v3.1
TCFE2   =  Steels/Fe-Alloys  v2.1
TCFE1   =  Steels/Fe-Alloys  v1.0
FROST1  =  FROST database v1.2
FEDAT   =  TCS/TT Steels Database v1.0
TCNI10  =  Ni-Alloys  v10.0 SNAPSHOT
TCNI9   =  Ni-Alloys  v9.1
TCNI8   =  Ni-Alloys  v8.2
TCNI7   =  Ni-Alloys  v7.2
TCNI6   =  Ni-Alloys  v6.1
TCNI5   =  Ni-Alloys  v5.1
TCNI4   =  Ni-Alloys  v4.0
TCNI1   =  Ni-Alloys  v1.3
TCAL6   =  Al-Alloys  v6.0
TCAL5   =  Al-Alloys  v5.1
TCAL4   =  Al-Alloys  v4.0
TCAL3   =  Al-Alloys  v3.0
TCAL2   =  Al-Alloys  v2.1
TCAL1   =  Al-Alloys  v1.2
TCMG5   =  Mg-Alloys  v5.1
TCMG4   =  Mg-Alloys  v4.0
TCMG3   =  Mg-Alloys  v3.0
TCMG2   =  Mg-Alloys  v2.0
TCMG1   =  Mg-Alloys  v1.1
TCTI2   =  Ti-Alloys  v2.1
TCTI1   =  Ti-Alloys  v1.0
TCCU3   =  Cu-Alloys  v3.1
TCCU2   =  Cu-Alloys  v2.0
TCCU1   =  Cu-Alloys  v1.0
TCCC1   =  Cemented carbide  v1.0
TCHEA4  =  High Entropy Alloy  v4.0
TCHEA3  =  High Entropy Alloy  v3.1
TCHEA2  =  High Entropy Alloy  v2.1.1
TCHEA1  =  High Entropy Alloy  v1.0
SSOL7   =  SGTE Alloy Solutions Database v7.0
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
TCOX10  =  Metal Oxide Solutions  v10.0 SNAPSHOT
TCOX9   =  Metal Oxide Solutions  v9.0
TCOX8   =  Metal Oxide Solutions  v8.0
TCOX7   =  Metal Oxide Solutions  v7.0
TCOX6   =  Metal Oxide Solutions  v6.0
TCOX5   =  Metal Oxide Solutions  v5.1
TCOX4   =  Metal Oxide Solutions  v4.1
ION3    =  Ionic Solutions  v3.0
ION2    =  Ionic Solutions  v2.6
ION1    =  Ionic Solutions  v1.5
NOX2    =  NPL Oxide Solutions Database v2.1
TCNOBL2 =  Noble Metals Alloys v2.0 SNAPSHOT
TCNOBL1 =  Noble Metals Alloys v1.0
TCSLD3  =  Solder Alloys  v3.2
TCSLD2  =  Solder Alloys  v2.0
TCSLD1  =  Solder Alloys  v1.1
TCSI1   =  Ultrapure Silicon  v1.2
TCMP2   =  Materials Processing  v2.5
TCES1   =  Combustion/Sintering  v1.1
TCSC1   =  Super Conductor  v1.0
TCFC1   =  SOFC Database v1.0
TCNF2   =  Nuclear Fuels  v2.1b
NUMT2   =  Nuclear Materials  v2.1
NUOX4   =  Nuclear Oxides  v4.2
NUCL15  =  IRSN NUCLEA-15_4
NUCL10  =  ThermoData NUCLEA Alloys-oxides TDB v10.2
MEPH15  =  IRSN Mephista-15_1
MEPH11  =  ThermoData MEPHISTA Nuclear Fuels TDB v11.2
TCAQ3   =  Aqueous Solution  v3.0
TCAQ2   =  Aqueous Solution  v2.7
AQS2    =  TGG Aqueous Solution Database v2.6
GCE2    =  TGG Geochemical/Environmental TDB v2.3
FEDEMO  =  Iron Demo Database v2.1
ALDEMO  =  Aluminum Demo Database v3.0
NIDEMO  =  Nickel Demo Database v1.1
CUDEMO  =  Copper Demo Database v1.0
SLDEMO  =  Solder Demo Database v1.0
OXDEMO  =  Oxide Demo Database v1.0
SUBDEMO =  Substance Demo Database v1.0
PTERN   =  Public Ternary Alloys TDB v1.3
PAQ2    =  Public Aqueous Soln (SIT) TDB v2.4
PG35    =  G35 Binary Semi-Conductors TDB v1.2
PURE5   =  SGTE Unary (Pure Elements) TDB v5.1
MOB2    =  Alloys Mobility  v2.7
MOB1    =  Alloys Mobility  v1.3
MOBFE1  =  Steels/Fe-Alloys Mobility  v1.1
MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
MOBFE5  =  Steels/Fe-Alloys Mobility  v5.0
MOBNI5  =  Ni-Alloys Mobility  v5.1
MOBNI4  =  Ni-Alloys Mobility  v4.1
MOBNI3  =  Ni-Alloys Mobility  v3.2
MOBNI2  =  Ni-Alloys Mobility  v2.4
MOBNI1  =  Ni-Alloys Mobility  v1.10
MOBAL5  =  Al-Alloys Mobility  v5.0
MOBAL4  =  Al-Alloys Mobility  v4.0
MOBAL3  =  Al-Alloys Mobility  v3.0
MOBAL2  =  Al-Alloys Mobility  v2.0
MOBAL1  =  Al-Alloys Mobility  v1.0
MOBCU1  =  Cu-Alloys Mobility  v1.0
```

```
 MOBCU2  =  Cu-Alloys Mobility  v2.0
 MOBCU3  =  Cu-Alloys Mobility  v3.0
 MOBHEA1 =  High Entropy Alloys Mobility  v1.0
 MOBHEA2 =  High Entropy Alloys Mobility  v2.0
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBSLD1 =  Solder-Alloys Mobility  v1.1
 MOBTI3  =  Ti-Alloys Mobility  v3.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v2.0
 MFEDEMO =  Fe-Alloys Mobility demo database v2.0
 MNIDEMO =  Ni-Alloys Mobility demo database v1.0
 MCUDEMO =  Cu-Alloys Mobility demo database v1.0
 USER    =  User defined Database

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

 VA  DEFINED
APP: def-sys fe ni
   ... the command in full is DEFINE_SYSTEM
 FE                      NI  DEFINED
APP: rej ph * all
   ... the command in full is REJECT
 BCC_A2                  FCC_A1  REJECTED
APP: res ph fcc
   ... the command in full is RESTORE
 FCC_A1  RESTORED
APP: get
   ... the command in full is GET_DATA
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'This parameter has not been assessed'
  'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
      -Ni'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Ni self-diffusion'
 -OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP
APP: @@
APP: go d-m
   ... the command in full is GOTO_MODULE
 NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond
   ... the command in full is SET_CONDITION
GLOBAL OR BOUNDARY CONDITION /GLOBAL/: glob
VARIABLE : T
LOW TIME LIMIT /0/: 0
T(TIME,X)= 1400;
HIGH TIME LIMIT /*/: *
ANY MORE RANGES /N/: N
DIC>
DIC> @@
DIC> @@ ENTER A REGION
DIC> @@
DIC> enter-region
REGION NAME : austenite
DIC>
DIC> @@
DIC> @@ ENTER A GRID INTO THE REGION.
DIC> @@ IN THIS CASE WE WANT SEVERAL POINTS IN THE MIDDLE OF THE REGION,
DIC> @@ SO A DOUBLE GEOMETRIC GRID IS CONSTRUCTED.
DIC> @@
DIC> enter-grid
   ... the command in full is ENTER_GRID_COORDINATES
REGION NAME : /AUSTENITE/: austenite
WIDTH OF REGION /1/: 1e-4
TYPE /LINEAR/: double
NUMBER OF POINTS /50/: 60
VALUE OF R IN THE GEOMETRICAL SERIE FOR LOWER PART OF REGION: 0.9
VALUE OF R IN THE GEOMETRICAL SERIE FOR UPPER PART OF REGION: 1.11
DIC>
DIC> @@
DIC> @@ ENTER THE active PHASES INTO THE REGIONS
DIC> @@
DIC> enter-phase
   ... the command in full is ENTER_PHASE_IN_REGION
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /AUSTENITE/: austenite
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL Ni COMPOSITION INTO THE PHASE. READ DATA FROM
DIC> @@ THE FILE ni.dat WHICH CONTAINS THE Ni-PROFILE.
DIC> @@
DIC> enter-composition
   ... the command in full is ENTER_COMPOSITIONS
REGION NAME : /AUSTENITE/: austenite
PHASE NAME: /FCC_A1/: fcc#1
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /NI/: ni
TYPE /LINEAR/: read a2ani.dat
   ... the command in full is CREATE_NEW_EQUILIBRIUM
   ... the command in full is COMPUTE_EQUILIBRIUM
   ... the command in full is COMPUTE_EQUILIBRIUM
   ... the command in full is COMPUTE_EQUILIBRIUM
   ... the command in full is COMPUTE_EQUILIBRIUM
   ... the command in full is COMPUTE_EQUILIBRIUM
```

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

```
DIC> @@
DIC> @@ THE BOUNDARY CONDITION IS A CLOSED SYSTEM AS WE DO NOT SPECIFY
DIC> @@ ANYTHING ELSE
DIC> @@
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 1E6
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /100000/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO FILE AND EXIT
DIC> @@
DIC> save exa2a Y
   ... the command in full is SAVE_WORKSPACES
DIC>
DIC> set-inter
   ... the command in full is SET_INTERACTIVE
 --OK---
DIC>
```

**exa2a-run**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exa2a\run.DCM.test"
   ... the command in full is MACRO_FILE_OPEN
DIC>
DIC>
DIC> @@ exa2a_run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING EXAMPLE a2a
DIC> @@
DIC>
DIC> @@
DIC> @@ LET US DEFINE A LOG-FILE FOR THIS EXAMPLE
DIC> @@
DIC> @@set-log-file run
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA MONITOR AN READ SETUP FROM FILE
DIC> @@
DIC> go d-m
   ... the command in full is GOTO_MODULE
 TIME STEP AT TIME  0.00000E+00
DIC>
DIC> read exa2a
   ... the command in full is READ_WORKSPACES
   ... the command in full is DEFINE_COMPONENTS
   ... the command in full is SELECT_EQUILIBRIUM
 OK
DIC>
DIC> @@
DIC> @@ START THE SIMULATION
DIC> @@
DIC> simulate
   ... the command in full is SIMULATE_REACTION
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
   ... the command in full is SET_NUMERICAL_LIMITS
 U-FRACTION IN SYSTEM:  FE = .708888245406169  NI = .29111175459383
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 U-FRACTION IN SYSTEM:  FE = .708888245406169  NI = .29111175459383
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  2  GRIDPOINT(S) ADDED   TO   CELL #1   REGION: AUSTENITE
 TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .708888245406169  NI = .29111175459383
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.10010000E-03 DT =  0.10000000E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .708888245406169  NI = .29111175459383
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.40010010     DT =  0.40000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .708888245406169  NI = .29111175459383
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   10.408313     DT =   10.008213     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .708888245406169  NI = .29111175459383
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   30.424739     DT =   20.016426     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .70888824540617  NI = .29111175459383
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   70.457590     DT =   40.032851     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .70888824540617  NI = .29111175459383
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   150.52329     DT =   80.065703     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .70888824540617  NI = .29111175459383
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   310.65470     DT =   160.13141     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .70888824540617  NI = .29111175459383
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   630.91751     DT =   320.26281     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .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 = .70888824540617  NI = .29111175459383
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   10238.802     DT =   5124.2050     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .70888824540617  NI = .29111175459383
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   20487.212     DT =   10248.410     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .70888824540617  NI = .29111175459383
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   40984.032     DT =   20496.820     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .70888824540617  NI = .29111175459383
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   81977.671     DT =   40993.640     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .708888245406169  NI = .29111175459383
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   163964.95     DT =   81987.280     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .708888245406168  NI = .291111754593832
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   263964.95     DT =   100000.00     SUM OF SQUARES =   0.0000000
```

```
 U-FRACTION IN SYSTEM:  FE = .708888245406169  NI = .29111175459383
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    1 seconds
 TIME =   363964.95     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 =   463964.95     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 =   563964.95     DT =   100000.00     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .708888245406169  NI = .291111754593831
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   663964.95     DT =   100000.00     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .708888245406168  NI = .291111754593833
 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 = .708888245406167  NI = .291111754593833
 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 = .708888245406167  NI = .291111754593833
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   963964.95     DT =   100000.00     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .708888245406168  NI = .291111754593832
 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 = .708888245406168  NI = .291111754593832
 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>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exa2a\plot.DCM.test"
   ... the command in full is MACRO_FILE_OPEN
DIC>
DIC>
DIC> @@ exa2a_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE a2a
DIC> @@
DIC>
DIC> @@
DIC> @@ LET US DEFINE A LOG-FILE FOR THIS EXAMPLE
DIC> @@
DIC> set-log-file plot
 AMBIGUOUS COMMAND, USE HELP
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
   ... the command in full is GOTO_MODULE
 TIME STEP AT TIME  1.00000E+06
DIC>
DIC> read exa2a
   ... the command in full is READ_WORKSPACES
   ... the command in full is DEFINE_COMPONENTS
   ... the command in full is SELECT_EQUILIBRIUM
 OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
   ... the command in full is POST_PROCESSOR
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:
POST-1: @@
POST-1: @@ PLOT SOME NI-CONCENTRATION PROFILES
POST-1: @@
POST-1: s-d-a
   ... the command in full is SET_DIAGRAM_AXIS
AXIS (X, Y OR Z) : x
VARIABLE : dist
  INFO: Distance is set as independent variable
   ... the command in full is SET_INDEPENDENT_VARIABLE
DISTANCE : /GLOBAL/: glo
POST-1:
POST-1: s-d-a
   ... the command in full is SET_DIAGRAM_AXIS
AXIS (X, Y OR Z) : y
VARIABLE : weight-percent
FOR COMPONENT : ni
POST-1:
POST-1: s-p-c
   ... the command in full is SET_PLOT_CONDITION
CONDITION /TIME/: time
VALUE(S) /LAST/: 0 1e5 3e5 1e6
POST-1:
POST-1: @@
POST-1: @@ SET SCALING ON Y-AXIS BEFORE PLOTTING
POST-1: @@
POST-1: s-s-s
   ... the command in full is SET_SCALING_STATUS
AXIS (X, Y OR Z) : y
AUTOMATIC SCALING  (Y OR N) /N/: n
MIN VALUE : 0
MAX VALUE : 60
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFILE
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
   ... the command in full is PLOT_DIAGRAM
```

2019.11.11.14.25.41
Time = 0,100000,300000,1000000
CELL #1

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

# Example exa2b

## Homogenization of a binary Fe-Ni alloy

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

**exa2b-setup**

```
SYS:About

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

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 21012) 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: Mon Nov 11 11:13:13 2019


SYS:SYS:MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exa2b\setup.DCM.test"
SYS: @@
SYS: @@ One-phase problem.
SYS: @@ Homogenization of a binary Fe-Ni alloy.
SYS: @@ This example is identical to a2a  but instead it uses implicit time
SYS: @@ integration instead of the trapezoidal method for solving the PDEs.
SYS: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exa2b_setup.DCM
SYS:
SYS: @@
SYS: @@ FIRST DEFINE A LOG-FILE FOR THIS EXAMPLE
SYS: @@
SYS: set_log_file setup
Heading:
SYS: @@
SYS: @@ THEN GO TO THE DATABASE MODULE
SYS: @@
SYS: go da
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v10.0

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10:
TDB_TCFE10: @@
TDB_TCFE10: @@ USE THE TCFE DATABASE FOR THERMODYNAMIC DATA
TDB_TCFE10: @@
TDB_TCFE10: sw fedemo
   ... the command in full is SWITCH_DATABASE
 Current database: Iron Demo Database v2.1

 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                  CBCC_A12
 CUB_A13                 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
14:27:02,936 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

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

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

```
FROST1  =  FROST database v1.2
FEDAT   =  TCS/TT Steels Database v1.0
TCNI10  =  Ni-Alloys  v10.0 SNAPSHOT
TCNI9   =  Ni-Alloys  v9.1
TCNI8   =  Ni-Alloys  v8.2
TCNI7   =  Ni-Alloys  v7.2
TCNI6   =  Ni-Alloys  v6.1
TCNI5   =  Ni-Alloys  v5.1
TCNI4   =  Ni-Alloys  v4.0
TCNI1   =  Ni-Alloys  v1.3
TCAL6   =  Al-Alloys  v6.0
TCAL5   =  Al-Alloys  v5.1
TCAL4   =  Al-Alloys  v4.0
TCAL3   =  Al-Alloys  v3.0
TCAL2   =  Al-Alloys  v2.1
TCAL1   =  Al-Alloys  v1.2
TCMG5   =  Mg-Alloys  v5.1
TCMG4   =  Mg-Alloys  v4.0
TCMG3   =  Mg-Alloys  v3.0
TCMG2   =  Mg-Alloys  v2.0
TCMG1   =  Mg-Alloys  v1.1
TCTI2   =  Ti-Alloys  v2.1
TCTI1   =  Ti-Alloys  v1.0
TCCU3   =  Cu-Alloys  v3.1
TCCU2   =  Cu-Alloys  v2.0
TCCU1   =  Cu-Alloys  v1.0
TCCC1   =  Cemented carbide  v1.0
TCHEA4  =  High Entropy Alloy  v4.0
TCHEA3  =  High Entropy Alloy  v3.1
TCHEA2  =  High Entropy Alloy  v2.1.1
TCHEA1  =  High Entropy Alloy  v1.0
SSOL7   =  SGTE Alloy Solutions Database v7.0
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
TCOX10  =  Metal Oxide Solutions  v10.0 SNAPSHOT
TCOX9   =  Metal Oxide Solutions  v9.0
TCOX8   =  Metal Oxide Solutions  v8.0
TCOX7   =  Metal Oxide Solutions  v7.0
TCOX6   =  Metal Oxide Solutions  v6.0
TCOX5   =  Metal Oxide Solutions  v5.1
TCOX4   =  Metal Oxide Solutions  v4.1
ION3    =  Ionic Solutions  v3.0
ION2    =  Ionic Solutions  v2.6
ION1    =  Ionic Solutions  v1.5
NOX2    =  NPL Oxide Solutions Database v2.1
TCNOBL2 =  Noble Metals Alloys v2.0 SNAPSHOT
TCNOBL1 =  Noble Metals Alloys v1.0
TCSLD3  =  Solder Alloys  v3.2
TCSLD2  =  Solder Alloys  v2.0
TCSLD1  =  Solder Alloys  v1.1
TCSI1   =  Ultrapure Silicon  v1.2
TCMP2   =  Materials Processing  v2.5
TCES1   =  Combustion/Sintering  v1.1
TCSC1   =  Super Conductor  v1.0
TCFC1   =  SOFC Database v1.0
TCNF2   =  Nuclear Fuels  v2.1b
NUMT2   =  Nuclear Materials  v2.1
NUOX4   =  Nuclear Oxides  v4.2
NUCL15  =  IRSN NUCLEA-15_4
NUCL10  =  ThermoData NUCLEA Alloys-oxides TDB v10.2
MEPH15  =  IRSN Mephista-15_1
MEPH11  =  ThermoData MEPHISTA Nuclear Fuels TDB v11.2
TCAQ3   =  Aqueous Solution  v3.0
TCAQ2   =  Aqueous Solution  v2.7
AQS2    =  TGG Aqueous Solution Database v2.6
GCE2    =  TGG Geochemical/Environmental TDB v2.3
FEDEMO  =  Iron Demo Database v2.1
ALDEMO  =  Aluminum Demo Database v3.0
NIDEMO  =  Nickel Demo Database v1.1
CUDEMO  =  Copper Demo Database v1.0
SLDEMO  =  Solder Demo Database v1.0
OXDEMO  =  Oxide Demo Database v1.0
SUBDEMO =  Substance Demo Database v1.0
PTERN   =  Public Ternary Alloys TDB v1.3
PAQ2    =  Public Aqueous Soln (SIT) TDB v2.4
PG35    =  G35 Binary Semi-Conductors TDB v1.2
PURE5   =  SGTE Unary (Pure Elements) TDB v5.1
MOB2    =  Alloys Mobility  v2.7
MOB1    =  Alloys Mobility  v1.3
MOBFE1  =  Steels/Fe-Alloys Mobility  v1.1
MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
MOBFE5  =  Steels/Fe-Alloys Mobility  v5.0
MOBNI5  =  Ni-Alloys Mobility  v5.1
MOBNI4  =  Ni-Alloys Mobility  v4.1
MOBNI3  =  Ni-Alloys Mobility  v3.2
MOBNI2  =  Ni-Alloys Mobility  v2.4
MOBNI1  =  Ni-Alloys Mobility  v1.10
MOBAL5  =  Al-Alloys Mobility  v5.0
MOBAL4  =  Al-Alloys Mobility  v4.0
MOBAL3  =  Al-Alloys Mobility  v3.0
MOBAL2  =  Al-Alloys Mobility  v2.0
MOBAL1  =  Al-Alloys Mobility  v1.0
MOBCU1  =  Cu-Alloys Mobility  v1.0
MOBCU2  =  Cu-Alloys Mobility  v2.0
MOBCU3  =  Cu-Alloys Mobility  v3.0
MOBHEA1 =  High Entropy Alloys Mobility  v1.0
MOBHEA2 =  High Entropy Alloys Mobility  v2.0
MOBMG1  =  Mg-Alloys Mobility  v1.0
```

```
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBSLD1 =  Solder-Alloys Mobility  v1.1
 MOBTI3  =  Ti-Alloys Mobility  v3.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v2.0
 MFEDEMO =  Fe-Alloys Mobility demo database v2.0
 MNIDEMO =  Ni-Alloys Mobility demo database v1.0
 MCUDEMO =  Cu-Alloys Mobility demo database v1.0
 USER    =  User defined Database

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

 VA  DEFINED
APP: def-sys fe ni
   ... the command in full is DEFINE_SYSTEM
 FE                      NI  DEFINED
APP: rej ph * all
   ... the command in full is REJECT
 BCC_A2                  FCC_A1  REJECTED
APP: res ph fcc
   ... the command in full is RESTORE
 FCC_A1  RESTORED
APP: get
   ... the command in full is GET_DATA
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'This parameter has not been assessed'
  'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
      -Ni'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Ni self-diffusion'
 -OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP
APP: @@
APP: go d-m
   ... the command in full is GOTO_MODULE
 NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond
   ... the command in full is SET_CONDITION
GLOBAL OR BOUNDARY CONDITION /GLOBAL/: glob
VARIABLE : T
LOW TIME LIMIT /0/: 0
T(TIME,X)= 1400;
HIGH TIME LIMIT /*/: *
ANY MORE RANGES /N/: N
DIC>
DIC> @@
DIC> @@ ENTER A REGION
DIC> @@
DIC> enter-region
REGION NAME : austenite
DIC>
DIC> @@
DIC> @@ ENTER A GRID INTO THE REGION.
DIC> @@ AS IN EXAMPLE a2a WE WANT SEVERAL POINTS IN THE MIDDLE OF THE REGION,
DIC> @@ SO A DOUBLE GEOMETRIC GRID IS ALSO CONSTRUCTED IN THIS EXAMPLE.
DIC> @@
DIC> enter-grid
   ... the command in full is ENTER_GRID_COORDINATES
REGION NAME : /AUSTENITE/: austenite
WIDTH OF REGION /1/: 1e-4
TYPE /LINEAR/: double
NUMBER OF POINTS /50/: 60
VALUE OF R IN THE GEOMETRICAL SERIE FOR LOWER PART OF REGION: 0.9
VALUE OF R IN THE GEOMETRICAL SERIE FOR UPPER PART OF REGION: 1.11
DIC>
DIC> @@
DIC> @@ ENTER ACTIVE PHASES INTO THE REGIONS
DIC> @@
DIC> enter-phase
   ... the command in full is ENTER_PHASE_IN_REGION
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /AUSTENITE/: austenite
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL Ni COMPOSITION INTO THE PHASE. READ DATA FROM
DIC> @@ THE FILE ni.dat WHICH CONTAINS THE Ni-PROFILE.
DIC> @@
DIC> enter-composition
   ... the command in full is ENTER_COMPOSITIONS
REGION NAME : /AUSTENITE/: austenite
PHASE NAME: /FCC_A1/: fcc#1
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /NI/: ni
TYPE /LINEAR/: read a2bni.dat
   ... the command in full is CREATE_NEW_EQUILIBRIUM
   ... the command in full is COMPUTE_EQUILIBRIUM
   ... the command in full is COMPUTE_EQUILIBRIUM
   ... the command in full is COMPUTE_EQUILIBRIUM
   ... the command in full is COMPUTE_EQUILIBRIUM
   ... the command in full is COMPUTE_EQUILIBRIUM
   ... the command in full is COMPUTE_EQUILIBRIUM
   ... the command in full is COMPUTE_EQUILIBRIUM
   ... the command in full is COMPUTE_EQUILIBRIUM
   ... the command in full is COMPUTE_EQUILIBRIUM
   ... the command in full is COMPUTE_EQUILIBRIUM
```

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

```
DIC> @@
DIC> @@ AFTER THE SIMULATION IN exa2a THE PROFILES HAVE SOME FLUCTUATIONS. WE
DIC> @@ NOW TRY TO GET RID OF THESE USING IMPLICIT (1) TIME INTEGRATION
DIC> @@ INSTEAD OF THE MORE ACCURATE (BUT LESS STABLE) TRAPETZOIDAL METHOD
DIC> @@ (THE DEFAULT).
DIC> @@
DIC> s-s-c
   ... the command in full is SET_SIMULATION_CONDITION
NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /AUTO/:
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -> 1): /AUTO/: 1.0
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/: @@
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/: @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 1E6
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /100000/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO FILE AND EXIT
DIC> @@
DIC> save exa2b Y
   ... the command in full is SAVE_WORKSPACES
DIC>
DIC> set-inter
   ... the command in full is SET_INTERACTIVE
 --OK---
DIC>
```

**exa2b-run**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exa2b\run.DCM.test"
   ... the command in full is MACRO_FILE_OPEN
DIC>
DIC>
DIC> @@ exa2b_run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING EXAMPLE a2b
DIC> @@
DIC>
DIC> @@
DIC> @@ LET US DEFINE A LOG-FILE FOR THIS EXAMPLE
DIC> @@
DIC> set-log-file run
 AMBIGUOUS COMMAND, USE HELP
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA MONITOR AN READ SETUP FROM FILE
DIC> @@
DIC> go d-m
   ... the command in full is GOTO_MODULE
 TIME STEP AT TIME  0.00000E+00
DIC> read exa2b
   ... the command in full is READ_WORKSPACES
   ... the command in full is DEFINE_COMPONENTS
   ... the command in full is SELECT_EQUILIBRIUM
 OK
DIC>
DIC> @@
DIC> @@ Start the simulation
DIC> @@
DIC> simulate
   ... the command in full is SIMULATE_REACTION
   ... the command in full is SET_NUMERICAL_LIMITS
 U-FRACTION IN SYSTEM:  FE = .708888245406169  NI = .29111175459383
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 U-FRACTION IN SYSTEM:  FE = .708888245406169  NI = .29111175459383
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  2  GRIDPOINT(S) ADDED   TO   CELL #1   REGION: AUSTENITE
 TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .708888245406169  NI = .29111175459383
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.10010000E-03 DT =  0.10000000E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .708888245406169  NI = .29111175459383
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.40010010     DT =  0.40000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  FE = .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 = .708888245406169  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 = .70888824540617  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 = .70888824540617  NI = .29111175459383
 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 = .708888245406171  NI = .291111754593829
 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 = .708888245406172  NI = .291111754593828
 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 = .708888245406173  NI = .291111754593827
 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 = .708888245406169  NI = .291111754593831
```

```
 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 = .708888245406171  NI = .291111754593829
 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 = .708888245406166  NI = .291111754593834
 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 = .708888245406164  NI = .291111754593836
 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 = .708888245406165  NI = .291111754593835
 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 = .708888245406162  NI = .291111754593838
 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 = .708888245406163  NI = .291111754593836
 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 = .708888245406167  NI = .291111754593833
 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 = .708888245406166  NI = .291111754593833
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 MUST SAVE WORKSPACE ON FILE
 WORKSPACE SAVED ON FILE
 RECLAIMING WORKSPACE
 DELETING TIME-RECORD FOR TIME    0.0000000
 DELETING TIME-RECORD FOR TIME   0.10000000E-06
 DELETING TIME-RECORD FOR TIME   0.10010000E-03
 DELETING TIME-RECORD FOR TIME   0.40010010
 DELETING TIME-RECORD FOR TIME    10.403455
 DELETING TIME-RECORD FOR TIME    30.410165
 DELETING TIME-RECORD FOR TIME    70.423585
 DELETING TIME-RECORD FOR TIME    150.45043
 DELETING TIME-RECORD FOR TIME    310.50411
 DELETING TIME-RECORD FOR TIME    630.61147
 DELETING TIME-RECORD FOR TIME    1270.8262
 DELETING TIME-RECORD FOR TIME    2551.2556
 DELETING TIME-RECORD FOR TIME    5112.1145
 DELETING TIME-RECORD FOR TIME    10233.832
 DELETING TIME-RECORD FOR TIME    20477.268
 DELETING TIME-RECORD FOR TIME    40964.139
 DELETING TIME-RECORD FOR TIME    81937.881
 DELETING TIME-RECORD FOR TIME    163885.37
 DELETING TIME-RECORD FOR TIME    263885.37
 DELETING TIME-RECORD FOR TIME    363885.37
 DELETING TIME-RECORD FOR TIME    463885.37
 DELETING TIME-RECORD FOR TIME    563885.37
 DELETING TIME-RECORD FOR TIME    663885.37
 DELETING TIME-RECORD FOR TIME    763885.37
 DELETING TIME-RECORD FOR TIME    863885.37

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

 TIMESTEP AT     1000000.00     SELECTED

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

**exa2b-plot**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exa2b\plot.DCM.test"
   ... the command in full is MACRO_FILE_OPEN
DIC>
DIC>
DIC> @@ exa2b_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE a2b
DIC> @@
DIC>
DIC> @@
DIC> @@ LET US DEFINE A LOG-FILE FOR THIS EXAMPLE
DIC> @@
DIC> set-log-file plot
 AMBIGUOUS COMMAND, USE HELP
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
   ... the command in full is GOTO_MODULE
 TIME STEP AT TIME  1.00000E+06
DIC> read exa2b
   ... the command in full is READ_WORKSPACES
   ... the command in full is DEFINE_COMPONENTS
   ... the command in full is SELECT_EQUILIBRIUM
 OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
   ... the command in full is POST_PROCESSOR
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:
POST-1: @@
POST-1: @@ PLOT SOME CONCENTRATION PROFILES
POST-1: @@
POST-1: s-d-a
   ... the command in full is SET_DIAGRAM_AXIS
AXIS (X, Y OR Z) : x
VARIABLE : dist
  INFO: Distance is set as independent variable
   ... the command in full is SET_INDEPENDENT_VARIABLE
DISTANCE : /GLOBAL/: glo
POST-1:
POST-1: s-d-a
   ... the command in full is SET_DIAGRAM_AXIS
AXIS (X, Y OR Z) : y
VARIABLE : w-p
FOR COMPONENT : ni
POST-1:
POST-1: s-p-c
   ... the command in full is SET_PLOT_CONDITION
CONDITION /TIME/: time
VALUE(S) /LAST/: 0 1e5 3e5 1e6
POST-1:
POST-1: @@
POST-1: @@ SET SCALING ON Y-AXIS BEFORE PLOTTING
POST-1: @@
POST-1: s-s-s
   ... the command in full is SET_SCALING_STATUS
AXIS (X, Y OR Z) : y
AUTOMATIC SCALING  (Y OR N) /N/: n
MIN VALUE : 0
MAX VALUE : 60
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFILE
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
   ... the command in full is PLOT_DIAGRAM
```

2019.11.11.14.29.16
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**

```
SYS:About

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

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 21012) 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: Mon Nov 11 11:13:13 2019


SYS:SYS:MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exa3\setup.DCM.test"
SYS: @@
SYS: @@ One-phase problem.
SYS: @@ Uphill diffusion in an Fe-Si-C alloy
SYS: @@ This is an example to simulate uphill diffusion in a ternary single
SYS: @@ phase austenite matrix due to the classical Darken experiment published
SYS: @@ by L.S. Darken: Trans. Aime, v.180 (1949), pp. 430-438.
SYS: @@
SYS: @@ In this example two pieces of austenite (3.80 wt%Si, 0.49 wt%C) and
SYS: @@ (0.05 wt%Si, 0.45 wt%C) are put together and are subsequently annealed
SYS: @@ at 1050C for 13 days. As both pieces are austenite they must be entered
SYS: @@ into the same region. This is done by individually giving the compositions
SYS: @@ of Si and C in each grid point. These data are then stored to file.
SYS: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ darken_setup.DCM
SYS:
SYS: @@
SYS: @@ Note that LOG-FILES used previously in examples a2a and a2b are
SYS: @@ no longer used.
SYS: @@
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASE
SYS: @@
SYS: go da
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v10.0

 VA                       /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10:
TDB_TCFE10: @@
TDB_TCFE10: @@ USE A TCFE DATABASE FOR THE THERMODYNAMIC DATA
TDB_TCFE10: @@
TDB_TCFE10: sw tcfe9
 Current database: Steels/Fe-Alloys  v9.1

 VA                       /-  DEFINED
 L12_FCC                  B2_BCC                   DICTRA_FCC_A1
   REJECTED
TDB_TCFE9: def-sys fe si c
 FE                       SI                       C
   DEFINED
TDB_TCFE9: rej ph * all
 GAS:G                    LIQUID:L                 BCC_A2
 FCC_A1                   HCP_A3                   CBCC_A12
 CUB_A13                  DIAMOND_FCC_A4           GRAPHITE
 CEMENTITE                M23C6                    M7C3
 M5C2                     KSI_CARBIDE              FE4N_LP1
 FECN_CHI                 LAVES_PHASE_C14          M3SI
 CR3SI                    FE2SI                    FESI2_H
 FESI2_L                  MSI                      M5SI3
 AL4C3                    FE8SI2C                  SIC
 AL5FE4                   MP_B31                   M2P_C22
 M2O3C:I  REJECTED
TDB_TCFE9: res ph fcc
 FCC_A1  RESTORED
TDB_TCFE9: get
14:30:43,739 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
  'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
  'J. Lacaze and B. Sundman, Metall. Mater. Trans. A, 22A (1991) 2211-2223;
      Fe-Si and Fe-Si-C'
  'J. Miettinen and B. Hallstedt, CALPHAD, 22 (1998) 231-256; Fe-Si and Fe
      -Si-C'
 -OK-
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE MOBILITY DATA
TDB_TCFE9: @@
TDB_TCFE9: app mobfe4
 Current database: Steels/Fe-Alloys Mobility  v4.0

 VA  DEFINED
 B2_BCC  REJECTED
APP: def-sys  fe si c
 FE                       SI                       C
   DEFINED
APP: rej ph * all
 BCC_A2                   CEMENTITE                FCC_A1
```

```
 FE4N_LP1                HCP_A3                  LIQUID:L
   REJECTED
APP: res ph fcc
 FCC_A1  RESTORED
APP: get
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 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>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exa3\run.DCM.test"
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
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
 U-FRACTION IN SYSTEM:  C = .0215351122808224  FE = .96291921367461
                        SI = .0370807863253901
 TOTAL SIZE OF SYSTEM:  .05 [m]
 U-FRACTION IN SYSTEM:  C = .0215351122808224  FE = .96291921367461
                        SI = .0370807863253901
 TOTAL SIZE OF SYSTEM:  .05 [m]
 TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351122808224  FE = .96291921367461
                        SI = .0370807863253901
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.10010000E-03 DT =  0.10000000E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351122808224  FE = .96291921367461
                        SI = .0370807863253901
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.40010010     DT =  0.40000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351122808224  FE = .96291921367461
                        SI = .0370807863253901
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    0 seconds
 TIME =   21.165600     DT =   20.765500     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351122808224  FE = .96291921367461
                        SI = .0370807863253901
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    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                    1 seconds
 TIME =   2637.6186     DT =   1328.9920     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .021535112280823  FE = .96291921367461
                        SI = .03708078632539
 TOTAL SIZE OF SYSTEM:  .05 [m]
  CPU time used in timestep                    0 seconds
 TIME =   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 = .0370807863253901
 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                    1 seconds
 TIME =   170090.61     DT =   85055.489     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215351122808123  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 = .0215351122809501  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                    0 seconds
TIME =   2721755.3     DT =   1360887.8     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0215351122812752  FE = .96291921367461
                       SI = .03708078632539
TOTAL SIZE OF SYSTEM:  .05 [m]
 CPU time used in timestep                    0 seconds
TIME =   5443530.9     DT =   2721775.6     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0215351122811047  FE = .96291921367461
                       SI = .03708078632539
TOTAL SIZE OF SYSTEM:  .05 [m]
 CPU time used in timestep                    1 seconds
TIME =   10887082.     DT =   5443551.3     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0215351122807851  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 = .0215351122805233  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 = .0215351122804133  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 = .0215351122803482  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 = .0215351122803353  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 = .021535112280406  FE = .96291921367461
                       SI = .0370807863253899
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 = .021535112280591  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 = .0215351122806838  FE = .96291921367461
                       SI = .03708078632539
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 = .0215351122809351  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 = .021535112281113  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 = .0215351122816696  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 = .0215351122822483  FE = .96291921367461
                       SI = .03708078632539
TOTAL SIZE OF SYSTEM:  .05 [m]
 CPU time used in timestep                    1 seconds
TIME =  0.63935491E+10 DT =  0.10000000E+10 SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0215351122828043  FE = .96291921367461
                       SI = .0370807863253901
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 = .0215351122833152  FE = .96291921367461
                       SI = .0370807863253901
TOTAL SIZE OF SYSTEM:  .05 [m]
 CPU time used in timestep                    0 seconds
TIME =  0.83935491E+10 DT =  0.10000000E+10 SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0215351122836845  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 = .0215351122841004  FE = .96291921367461
                       SI = .0370807863253901
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 = .0215351122842448  FE = .96291921367461
                       SI = .03708078632539
TOTAL SIZE OF SYSTEM:  .05 [m]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME    0.0000000
DELETING TIME-RECORD FOR TIME   0.10000000E-06
DELETING TIME-RECORD FOR TIME   0.10010000E-03
DELETING TIME-RECORD FOR TIME   0.40010010
```

```
 DELETING TIME-RECORD FOR TIME    21.165600
 DELETING TIME-RECORD FOR TIME    62.696601
 DELETING TIME-RECORD FOR TIME    145.75860
 DELETING TIME-RECORD FOR TIME    311.88260
 DELETING TIME-RECORD FOR TIME    644.13060
 DELETING TIME-RECORD FOR TIME    1308.6266
 DELETING TIME-RECORD FOR TIME    2637.6186
 DELETING TIME-RECORD FOR TIME    5295.6026
 DELETING TIME-RECORD FOR TIME    10611.571
 DELETING TIME-RECORD FOR TIME    21243.507
 DELETING TIME-RECORD FOR TIME    42507.379
 DELETING TIME-RECORD FOR TIME    85035.123
 DELETING TIME-RECORD FOR TIME    170090.61
 DELETING TIME-RECORD FOR TIME    340201.59
 DELETING TIME-RECORD FOR TIME    680423.54
 DELETING TIME-RECORD FOR TIME    1360867.5
 DELETING TIME-RECORD FOR TIME    2721755.3
 DELETING TIME-RECORD FOR TIME    5443530.9
 DELETING TIME-RECORD FOR TIME    10887082.
 DELETING TIME-RECORD FOR TIME    21774185.
 DELETING TIME-RECORD FOR TIME    43548390.
 DELETING TIME-RECORD FOR TIME    87096800.
 DELETING TIME-RECORD FOR TIME   0.17419362E+09
 DELETING TIME-RECORD FOR TIME   0.34838726E+09
 DELETING TIME-RECORD FOR TIME   0.69677454E+09
 DELETING TIME-RECORD FOR TIME   0.13935491E+10
 DELETING TIME-RECORD FOR TIME   0.23935491E+10
 DELETING TIME-RECORD FOR TIME   0.33935491E+10
 DELETING TIME-RECORD FOR TIME   0.43935491E+10
 DELETING TIME-RECORD FOR TIME   0.53935491E+10
 DELETING TIME-RECORD FOR TIME   0.63935491E+10
 DELETING TIME-RECORD FOR TIME   0.73935491E+10
 DELETING TIME-RECORD FOR TIME   0.83935491E+10

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

 TIMESTEP AT    0.100000000E+11 SELECTED

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

**exa3-plot**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exa3\plot.DCM.test"
DIC>
DIC>
DIC> @@ darken_plot.DCM
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA MODULE AND SPECIFY THE STORE-RESULT FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  1.00000E+10
DIC> read exa3
 OK
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA POST PROCESSOR
DIC> @@
DIC> post
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1: @@
POST-1: @@ PLOT THE CONCENTRATION PROFILE FOR Si AT TIMES 0, 1E5, 1123200, 1E7,
POST-1: @@ 1E8, 1E9 AND 1E10 S
POST-1: @@
POST-1: @@ SET DISTANCE IN SYSTEM AS X-AXIS, WEIGHT-% SI ON Y-AXIS AND SPECIFY
POST-1: @@ FOR WHICH SIMULATION TIMES TO PLOT THE PROFILES.
POST-1: @@
POST-1: set-diagram-axis x distance global
  INFO: Distance is set as independent variable
POST-1: set-diagram-axis y weight-percent si
POST-1: set-plot-condition time 0 1E5 1123200 1e7 1E8 1E9 1E10
POST-1:
POST-1: @@
POST-1: @@ PLOT THE DIAGRAM
POST-1: @@
POST-1: set-title
TITLE : Figure a3.1
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

Figure a3.1

```
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1: @@
POST-1: @@ PLOT THE CONCENTRATION PROFILES FOR C
POST-1: @@
POST-1: @@ WE ONLY NEED TO CHANGE THE Y-AXIS
POST-1: @@
POST-1: set-diagram-axis y w-p c
POST-1: set-title Figure a3.2
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

Figure a3.2

```
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1: @@
POST-1: @@ COMPARE WITH DARKEN'S EXPERIMENTS
POST-1: @@
POST-1: append_experimental_data  yes exa3.exp 0; 1
POST-1:
POST-1: set-plot-condition time 1123200
POST-1:
POST-1: s-s-s
AXIS (X, Y OR Z) : y
AUTOMATIC SCALING  (Y OR N) /N/: n
MIN VALUE : 0.25
MAX VALUE : 0.75
POST-1:
POST-1: set-title Figure a3.3
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

Figure a3.3

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

# Example exa4

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

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

**exa4-setup**

```
SYS:About

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

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 21012) 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: Mon Nov 11 11:13:13 2019


SYS:SYS:MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exa4\setup.DCM.test"
SYS: @@
SYS: @@ One-phase problem.
SYS: @@ Carburization of binary Fe-C alloy: Comparison to an analytical erf solution
SYS: @@ This is a simple binary simulation with a single phase region.
SYS: @@ The numerical simulation is compared with an analytical erf solution.
SYS: @@ For this reason a special database erf.tdb is created where the
SYS: @@ diffusion coefficient is set to a concentration independent value.
SYS: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exa4_setup.DCM
SYS:
SYS:
SYS: @@
SYS: @@ READ THE DATA FROM THE DATABASES
SYS: @@
SYS: go da
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v10.0

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10: sw FEDEMO
 Current database: Iron Demo Database v2.1

 VA                      /-  DEFINED
TDB_FEDEMO: def-system fe,c
 FE                      C  DEFINED
TDB_FEDEMO: rej-ph *
 GAS:G                   LIQUID:L                BCC_A2
 CBCC_A12                CEMENTITE               CUB_A13
 DIAMOND_FCC_A4          FCC_A1                  GRAPHITE
 HCP_A3                  KSI_CARBIDE             LAVES_PHASE_C14
 M23C6                   M5C2                    M7C3
   REJECTED
TDB_FEDEMO: rest-ph fcc
 FCC_A1  RESTORED
TDB_FEDEMO: get
14:34:30,308 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
 -OK-
TDB_FEDEMO:
TDB_FEDEMO: append user exa4.TDB
 Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

 VA  DEFINED
14:34:31,598 INFO  USER_790547025_7, number of lines read: 29
14:34:31,727 INFO  Parsing of USER_790547025_7 completed in 182 ms
TDB_APP: def-system fe,c
 FE                      C  DEFINED
TDB_APP: rej-ph *
 FCC_A1  REJECTED
TDB_APP: rest-ph fcc
 FCC_A1  RESTORED
TDB_APP: get
 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
14:34:32,123 INFO  Preparing system for use: USER_790547025_7
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
14:34:33,525 INFO  Preparing phase for use: FCC_A1
DIC>
DIC>
DIC> @@
DIC> @@ SET A FIXED COMPOSITION AS THE BOUNDARY VALUE
DIC> @@
DIC> set-condition
GLOBAL OR BOUNDARY CONDITION /GLOBAL/: boundary
BOUNDARY /LOWER/: lower
CONDITION TYPE /CLOSED_SYSTEM/: state-variable-value
State variable expression #1 : /N=1/: n=1
State variable expression #2 : x(c)=0.03
DIC>
DIC>
DIC> @@
DIC> @@ SET A SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 100
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /10/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC>
DIC> save exa4 Y
DIC>
DIC> set-inter
 --OK---
DIC>
```

**exa4-run**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exa4\run.DCM.test"
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
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
 U-FRACTION IN SYSTEM:  C = .0050251256281407  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 U-FRACTION IN SYSTEM:  C = .0050251256281407  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00502599895421297  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.26001020E-05 DT =  0.25001020E-05 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00502674234772398  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.76003060E-05 DT =  0.50002040E-05 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00502762855271361  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.17600714E-04 DT =  0.10000408E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00502880490898696  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.37601530E-04 DT =  0.20000816E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00503042289514107  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.77603162E-04 DT =  0.40001632E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00503268130112881  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.15760643E-03 DT =  0.80003264E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00503585491527872  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.31761295E-03 DT =  0.16000653E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00504032903043467  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.63762601E-03 DT =  0.32001306E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00504664654067874  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.12776521E-02 DT =  0.64002611E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00505557392100181  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.25577043E-02 DT =  0.12800522E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00506819425567398  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.51178088E-02 DT =  0.25601044E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00508603865206295  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.10238018E-01 DT =  0.51202089E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00511127199989312  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.20478435E-01 DT =  0.10240418E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0051469556180961  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.40959271E-01 DT =  0.20480836E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00519741865567008  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.81920942E-01 DT =  0.40961671E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00526878330573381  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.16384428     DT =  0.81923342E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00536970755217346  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.32769097     DT =  0.16384668     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00551243555924854  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.65538434     DT =  0.32769337     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00571428313781583  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   1.3107711     DT =  0.65538674     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00599973850521004  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   2.6215446     DT =   1.3107735     SUM OF SQUARES =   0.0000000
```

```
 U-FRACTION IN SYSTEM:  C = .00640343298842195  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   5.2430915     DT =   2.6215470     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00697433052866847  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    1 seconds
 TIME =   10.486185     DT =   5.2430939     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00778159421638383  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 = .00887736257293564  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 = .00972196664325369  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   40.486185     DT =   10.000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .010436351986536  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   50.486185     DT =   10.000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0110669328932657  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   60.486185     DT =   10.000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0116377078880251  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   70.486185     DT =   10.000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0121630223717782  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   80.486185     DT =   10.000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0126522650845277  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   90.486185     DT =   10.000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0131119785059757  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   100.00000     DT =   9.5138146     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .013526298212787  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 MUST SAVE WORKSPACE ON FILE
 WORKSPACE SAVED ON FILE
 RECLAIMING WORKSPACE
 DELETING TIME-RECORD FOR TIME    0.0000000
 DELETING TIME-RECORD FOR TIME   0.10000000E-06
 DELETING TIME-RECORD FOR TIME   0.26001020E-05
 DELETING TIME-RECORD FOR TIME   0.76003060E-05
 DELETING TIME-RECORD FOR TIME   0.17600714E-04
 DELETING TIME-RECORD FOR TIME   0.37601530E-04
 DELETING TIME-RECORD FOR TIME   0.77603162E-04
 DELETING TIME-RECORD FOR TIME   0.15760643E-03
 DELETING TIME-RECORD FOR TIME   0.31761295E-03
 DELETING TIME-RECORD FOR TIME   0.63762601E-03
 DELETING TIME-RECORD FOR TIME   0.12776521E-02
 DELETING TIME-RECORD FOR TIME   0.25577043E-02
 DELETING TIME-RECORD FOR TIME   0.51178088E-02
 DELETING TIME-RECORD FOR TIME   0.10238018E-01
 DELETING TIME-RECORD FOR TIME   0.20478435E-01
 DELETING TIME-RECORD FOR TIME   0.40959271E-01
 DELETING TIME-RECORD FOR TIME   0.81920942E-01
 DELETING TIME-RECORD FOR TIME   0.16384428
 DELETING TIME-RECORD FOR TIME   0.32769097
 DELETING TIME-RECORD FOR TIME   0.65538434
 DELETING TIME-RECORD FOR TIME    1.3107711
 DELETING TIME-RECORD FOR TIME    2.6215446
 DELETING TIME-RECORD FOR TIME    5.2430915
 DELETING TIME-RECORD FOR TIME    10.486185
 DELETING TIME-RECORD FOR TIME    20.486185
 DELETING TIME-RECORD FOR TIME    30.486185
 DELETING TIME-RECORD FOR TIME    40.486185
 DELETING TIME-RECORD FOR TIME    50.486185
 DELETING TIME-RECORD FOR TIME    60.486185
 DELETING TIME-RECORD FOR TIME    70.486185
 DELETING TIME-RECORD FOR TIME    80.486185

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

 TIMESTEP AT     100.000000     SELECTED

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

**exa4-plot**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exa4\plot.DCM.test"
DIC>
DIC>
DIC> @@ exa4_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE exa4
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  1.00000E+02
DIC> read exa4
 OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1: @@
POST-1: @@ PLOT A COMPOSITION PROFILE
POST-1: @@
POST-1: s-d-a x distance global
  INFO: Distance is set as independent variable
POST-1: s-d-a y x(c)
POST-1: s-p-c time 25
POST-1:
POST-1: @@
POST-1: @@ ENTER THE ANALYTICAL SOLUTION, CALLED ERFSOL
POST-1: @@
POST-1: enter-symbol
Function or table /FUNCTION/: function
NAME: erfsol
FUNCTION: 0.03-0.025*erf(gd/sqrt(4*dc(fcc,c,c,fe)*25));
POST-1:
POST-1: @@
POST-1: @@ COMPARE THE ANALYTICAL AND NUMERICAL SOLUTIONS
POST-1: @@
POST-1: enter-symbol
Function or table /FUNCTION/: table
NAME: aaa
Variable(s) x(c) erfsol
POST-1:
POST-1: s-d-a y aaa
COLUMN NUMBER /*/: 1 2
POST-1:
POST-1: set-axis-text
AXIS (X, Y OR Z) : y
AUTOMATIC AXIS TEXT  (Y OR N) /N/: n
AXIS TEXT : Mole fraction C
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

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

```
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

2019.11.11.14.36.32
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**

```
SYS:About

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

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 21012) 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: Mon Nov 11 11:13:13 2019


SYS:SYS:MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exa5\setup.DCM.test"
SYS: ?@@
 NO SUCH COMMAND, USE HELP
SYS: @@ One-phase problem.
SYS: @@ Carburization of a binary Fe-0.15 wt% C alloy.
SYS: @@ A mixture of 40% N2 and 60% cracked methanol is used as carrier gas.
SYS: @@ The carburizing "carbon potential" in the gas is 0.85 wt%.
SYS: @@ A surface reaction controls the flux of C at the surface.
SYS: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exa5_setup.DCM
SYS:
SYS: @@
SYS: @@ GO TO THE DATABASES AND READ THE THERMODYNAMIC AND KINETIC DATA
SYS: @@
SYS: go da
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v10.0

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10: sw FEDEMO
 Current database: Iron Demo Database v2.1

 VA                      /-  DEFINED
TDB_FEDEMO: def-sys fe,c
 FE                      C  DEFINED
TDB_FEDEMO: rej-ph *
 GAS:G                   LIQUID:L                BCC_A2
 CBCC_A12                CEMENTITE               CUB_A13
 DIAMOND_FCC_A4          FCC_A1                  GRAPHITE
 HCP_A3                  KSI_CARBIDE             LAVES_PHASE_C14
 M23C6                   M5C2                    M7C3
   REJECTED
TDB_FEDEMO: rest-ph fcc graphite
 FCC_A1                  GRAPHITE  RESTORED
TDB_FEDEMO: get
14:37:51,366 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
  'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121 -127; Molar
      volumes'
 -OK-
TDB_FEDEMO:@?
TDB_FEDEMO: append
 Use one of these databases

 TCFE10  =  Steels/Fe-Alloys  v10.0
 TCFE9   =  Steels/Fe-Alloys  v9.1
 TCFE8   =  Steels/Fe-Alloys  v8.1
 TCFE7   =  Steels/Fe-Alloys  v7.0
 TCFE6   =  Steels/Fe-Alloys  v6.2
 TCFE5   =  Steels/Fe-Alloys  v5.0
 TCFE4   =  Steels/Fe-Alloys  v4.1
 TCFE3   =  Steels/Fe-Alloys  v3.1
 TCFE2   =  Steels/Fe-Alloys  v2.1
 TCFE1   =  Steels/Fe-Alloys  v1.0
 FROST1  =  FROST database v1.2
 FEDAT   =  TCS/TT Steels Database v1.0
 TCNI10  =  Ni-Alloys  v10.0 SNAPSHOT
 TCNI9   =  Ni-Alloys  v9.1
 TCNI8   =  Ni-Alloys  v8.2
 TCNI7   =  Ni-Alloys  v7.2
 TCNI6   =  Ni-Alloys  v6.1
 TCNI5   =  Ni-Alloys  v5.1
 TCNI4   =  Ni-Alloys  v4.0
 TCNI1   =  Ni-Alloys  v1.3
 TCAL6   =  Al-Alloys  v6.0
 TCAL5   =  Al-Alloys  v5.1
 TCAL4   =  Al-Alloys  v4.0
 TCAL3   =  Al-Alloys  v3.0
 TCAL2   =  Al-Alloys  v2.1
 TCAL1   =  Al-Alloys  v1.2
 TCMG5   =  Mg-Alloys  v5.1
 TCMG4   =  Mg-Alloys  v4.0
 TCMG3   =  Mg-Alloys  v3.0
 TCMG2   =  Mg-Alloys  v2.0
 TCMG1   =  Mg-Alloys  v1.1
 TCTI2   =  Ti-Alloys  v2.1
 TCTI1   =  Ti-Alloys  v1.0
 TCCU3   =  Cu-Alloys  v3.1
 TCCU2   =  Cu-Alloys  v2.0
 TCCU1   =  Cu-Alloys  v1.0
 TCCC1   =  Cemented carbide  v1.0
```

```
 TCHEA4  =  High Entropy Alloy  v4.0
 TCHEA3  =  High Entropy Alloy  v3.1
 TCHEA2  =  High Entropy Alloy  v2.1.1
 TCHEA1  =  High Entropy Alloy  v1.0
 SSOL7   =  SGTE Alloy Solutions Database v7.0
 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
 TCOX10  =  Metal Oxide Solutions  v10.0 SNAPSHOT
 TCOX9   =  Metal Oxide Solutions  v9.0
 TCOX8   =  Metal Oxide Solutions  v8.0
 TCOX7   =  Metal Oxide Solutions  v7.0
 TCOX6   =  Metal Oxide Solutions  v6.0
 TCOX5   =  Metal Oxide Solutions  v5.1
 TCOX4   =  Metal Oxide Solutions  v4.1
 ION3    =  Ionic Solutions  v3.0
 ION2    =  Ionic Solutions  v2.6
 ION1    =  Ionic Solutions  v1.5
 NOX2    =  NPL Oxide Solutions Database v2.1
 TCNOBL2 =  Noble Metals Alloys v2.0 SNAPSHOT
 TCNOBL1 =  Noble Metals Alloys v1.0
 TCSLD3  =  Solder Alloys  v3.2
 TCSLD2  =  Solder Alloys  v2.0
 TCSLD1  =  Solder Alloys  v1.1
 TCSI1   =  Ultrapure Silicon  v1.2
 TCMP2   =  Materials Processing  v2.5
 TCES1   =  Combustion/Sintering  v1.1
 TCSC1   =  Super Conductor  v1.0
 TCFC1   =  SOFC Database v1.0
 TCNF2   =  Nuclear Fuels  v2.1b
 NUMT2   =  Nuclear Materials  v2.1
 NUOX4   =  Nuclear Oxides  v4.2
 NUCL15  =  IRSN NUCLEA-15_4
 NUCL10  =  ThermoData NUCLEA Alloys-oxides TDB v10.2
 MEPH15  =  IRSN Mephista-15_1
 MEPH11  =  ThermoData MEPHISTA Nuclear Fuels TDB v11.2
 TCAQ3   =  Aqueous Solution  v3.0
 TCAQ2   =  Aqueous Solution  v2.7
 AQS2    =  TGG Aqueous Solution Database v2.6
 GCE2    =  TGG Geochemical/Environmental TDB v2.3
 FEDEMO  =  Iron Demo Database v2.1
 ALDEMO  =  Aluminum Demo Database v3.0
 NIDEMO  =  Nickel Demo Database v1.1
 CUDEMO  =  Copper Demo Database v1.0
 SLDEMO  =  Solder Demo Database v1.0
 OXDEMO  =  Oxide Demo Database v1.0
 SUBDEMO =  Substance Demo Database v1.0
 PTERN   =  Public Ternary Alloys TDB v1.3
 PAQ2    =  Public Aqueous Soln (SIT) TDB v2.4
 PG35    =  G35 Binary Semi-Conductors TDB v1.2
 PURE5   =  SGTE Unary (Pure Elements) TDB v5.1
 MOB2    =  Alloys Mobility  v2.7
 MOB1    =  Alloys Mobility  v1.3
 MOBFE1  =  Steels/Fe-Alloys Mobility  v1.1
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBFE5  =  Steels/Fe-Alloys Mobility  v5.0
 MOBNI5  =  Ni-Alloys Mobility  v5.1
 MOBNI4  =  Ni-Alloys Mobility  v4.1
 MOBNI3  =  Ni-Alloys Mobility  v3.2
 MOBNI2  =  Ni-Alloys Mobility  v2.4
 MOBNI1  =  Ni-Alloys Mobility  v1.10
 MOBAL5  =  Al-Alloys Mobility  v5.0
 MOBAL4  =  Al-Alloys Mobility  v4.0
 MOBAL3  =  Al-Alloys Mobility  v3.0
 MOBAL2  =  Al-Alloys Mobility  v2.0
 MOBAL1  =  Al-Alloys Mobility  v1.0
 MOBCU1  =  Cu-Alloys Mobility  v1.0
 MOBCU2  =  Cu-Alloys Mobility  v2.0
 MOBCU3  =  Cu-Alloys Mobility  v3.0
 MOBHEA1 =  High Entropy Alloys Mobility  v1.0
 MOBHEA2 =  High Entropy Alloys Mobility  v2.0
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBSLD1 =  Solder-Alloys Mobility  v1.1
 MOBTI3  =  Ti-Alloys Mobility  v3.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v2.0
 MFEDEMO =  Fe-Alloys Mobility demo database v2.0
 MNIDEMO =  Ni-Alloys Mobility demo database v1.0
 MCUDEMO =  Cu-Alloys Mobility demo database v1.0
 USER    =  User defined Database

DATABASE NAME /FEDEMO/: 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>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exa5\run.DCM.test"
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
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
 U-FRACTION IN SYSTEM:  C = .00698495916383109  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
 U-FRACTION IN SYSTEM:  C = .00698495916383109  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
 TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698495916398349  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1 seconds
 TIME =  0.24659766E-05 DT =  0.23659766E-05 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698495916758908  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.71979297E-05 DT =  0.47319532E-05 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698495917479988  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.16661836E-04 DT =  0.94639063E-05 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .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 = .00698495939106305  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 = .0069849600827771  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.12091140E-02 DT =  0.60569000E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698496100461467  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.24204940E-02 DT =  0.12113800E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698496284726693  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1 seconds
 TIME =  0.48432541E-02 DT =  0.24227600E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698496652968263  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.96887741E-02 DT =  0.48455200E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698497388635673  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.19379814E-01 DT =  0.96910401E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0069849885766828  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.38761894E-01 DT =  0.19382080E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698501789240893  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.77526054E-01 DT =  0.38764160E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .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 = .00698519272377668  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 = .00698588265674895  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1 seconds
 TIME =   1.2404509     DT =  0.62022656     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698678864751835  FE = 1
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
```

```
TIME =   2.4809040     DT =   1.2404531     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00698856957978377  FE = 1
TOTAL SIZE OF SYSTEM:  .003 [m]
 CPU time used in timestep                    0 seconds
TIME =   4.9618102     DT =   2.4809063     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0069920463860113  FE = 1
TOTAL SIZE OF SYSTEM:  .003 [m]
 CPU time used in timestep                    0 seconds
TIME =   9.9236228     DT =   4.9618125     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00699876996632461  FE = 1
TOTAL SIZE OF SYSTEM:  .003 [m]
 CPU time used in timestep                    0 seconds
TIME =   19.847248     DT =   9.9236250     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00701160601590709  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 = .00703569376361482  FE = 1
TOTAL SIZE OF SYSTEM:  .003 [m]
 CPU time used in timestep                    1 seconds
TIME =   79.388998     DT =   39.694500     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00707989462116305  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 = .00729474138750391  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 = .00752054375503578  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 = .00788106518443627  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 = .00843611780537715  FE = 1
TOTAL SIZE OF SYSTEM:  .003 [m]
 CPU time used in timestep                    1 seconds
TIME =   4340.4480     DT =   1800.0000     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00904710226999661  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 = .00955134567261153  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 = .00999113675765143  FE = 1
TOTAL SIZE OF SYSTEM:  .003 [m]
 CPU time used in timestep                    0 seconds
TIME =   9740.4480     DT =   1800.0000     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0103863764716784  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 = .0107484090267332  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 = .0110844421240413  FE = 1
TOTAL SIZE OF SYSTEM:  .003 [m]
 CPU time used in timestep                    1 seconds
TIME =   15140.448     DT =   1800.0000     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0113993948509895  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 = .011696805029564  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 = .0118647499013452  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>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exa5\plot.DCM.test"
DIC>
DIC>
DIC> @@ exa5_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE a5
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  1.80000E+04
 *** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
DIC> read exa5
 OK
DIC>
DIC> @@
DIC> @@ ENTER THE POST PROCESSOR
DIC> @@
DIC> post
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1: @@
POST-1: @@ PLOT SOME DIFFERENT CONCENTRATION PROFILES
POST-1: @@
POST-1: s-d-a x dist glo
  INFO: Distance is set as independent variable
POST-1: s-d-a y w-p c
POST-1: s-p-c time 100 1000 5000 18000
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

```
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: @@
POST-1: @@ PLOT THE VARIATION OF THE C ACTIVITY AT THE SURFACE
POST-1: @@
POST-1: s-d-a y acr(c)
POST-1:
POST-1: s-d-a x time
  INFO: Time is set as independent variable
POST-1:
POST-1: s-p-c
CONDITION /TIME/: interface
INTERFACE : first
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

2019.11.11.14.39.54
"FIRST" INTERFACE OF SYSTEM
CELL #1

```
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: @@
POST-1: @@ USE A LOGARITHMIC SCALE ON THE X-AXIS
POST-1: @@
POST-1: set-axis-type
AXIS (X, Y OR Z) : x
AXIS TYPE /LINEAR/: logarithmic
POST-1:
POST-1: s-s-s x n 0.001 2e4
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

2019.11.11.14.39.54
"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:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

2019.11.11.14.39.55
CELL #1

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

# Example exa6

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

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

**exa6-setup**

```
SYS:About

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

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 21012) 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: Mon Nov 11 11:13:13 2019


SYS:SYS:MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exa6\setup.DCM.test"
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  v10.0

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10:
TDB_TCFE10: @@
TDB_TCFE10: @@ USE THE TCFE DATABASE FOR THERMODYNAMIC DATA
TDB_TCFE10: @@
TDB_TCFE10: sw tcfe9
 Current database: Steels/Fe-Alloys  v9.1

 VA                      /-  DEFINED
 L12_FCC                 B2_BCC                  DICTRA_FCC_A1
   REJECTED
TDB_TCFE9: def-sys fe si mn c
 FE                      SI                      MN
 C  DEFINED
TDB_TCFE9: rej ph * all
 GAS:G                   LIQUID:L                BCC_A2
 FCC_A1                  HCP_A3                  CBCC_A12
 CUB_A13                 DIAMOND_FCC_A4          GRAPHITE
 CEMENTITE               M23C6                   M7C3
 M5C2                    KSI_CARBIDE             FE4N_LP1
 FECN_CHI                LAVES_PHASE_C14         M3SI
 MN9SI2                  MN11SI19                MN6SI
 G_PHASE                 CR3SI                   FE2SI
 FESI2_H                 FESI2_L                 MSI
 M5SI3                   AL4C3                   FE8SI2C
 SIC                     MN5SIC                  CUZN_EPSILON
 AL5FE4                  MP_B31                  M2P_C22
 FLUORITE_C1:I           ZRO2_TETR:I             M2O3C:I
 M2O3H:I  REJECTED
TDB_TCFE9: res ph fcc,grap
 FCC_A1                  GRAPHITE  RESTORED
TDB_TCFE9: get
14:41:15,912 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121-127; Molar
      volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
  'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
  'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, CALPHAD, 34, 279
      -85(2010); Mn-C'
  'J. Lacaze and B. Sundman, Metall. Mater. Trans. A, 22A (1991) 2211-2223;
      Fe-Si and Fe-Si-C'
  'W. Huang, CALPHAD, 13 (1989) 243-252; TRITA-MAC 388 (rev 1989); FE-MN'
  'W. Zheng, J. Alloys Compd., 632 (2015) 661-675'
  'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, CALPHAD,
      submitted, 2011; Fe-Mn-C'
  'J. Miettinen and B. Hallstedt, CALPHAD, 22 (1998) 231-256; Fe-Si and Fe
      -Si-C'
  'A. Forsberg and J. Agren, J. Phase Equilib., 14 (1993) 354-363; Fe-Mn-Si'
 -OK-
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ SWITCH TO A MOBILITY DATABASE TO RETRIVE KINETIC DATA
TDB_TCFE9: @@
TDB_TCFE9: app
 Use one of these databases

 TCFE10  =  Steels/Fe-Alloys  v10.0
 TCFE9   =  Steels/Fe-Alloys  v9.1
 TCFE8   =  Steels/Fe-Alloys  v8.1
```

```
TCFE7   =  Steels/Fe-Alloys  v7.0
TCFE6   =  Steels/Fe-Alloys  v6.2
TCFE5   =  Steels/Fe-Alloys  v5.0
TCFE4   =  Steels/Fe-Alloys  v4.1
TCFE3   =  Steels/Fe-Alloys  v3.1
TCFE2   =  Steels/Fe-Alloys  v2.1
TCFE1   =  Steels/Fe-Alloys  v1.0
FROST1  =  FROST database v1.2
FEDAT   =  TCS/TT Steels Database v1.0
TCNI10  =  Ni-Alloys  v10.0 SNAPSHOT
TCNI9   =  Ni-Alloys  v9.1
TCNI8   =  Ni-Alloys  v8.2
TCNI7   =  Ni-Alloys  v7.2
TCNI6   =  Ni-Alloys  v6.1
TCNI5   =  Ni-Alloys  v5.1
TCNI4   =  Ni-Alloys  v4.0
TCNI1   =  Ni-Alloys  v1.3
TCAL6   =  Al-Alloys  v6.0
TCAL5   =  Al-Alloys  v5.1
TCAL4   =  Al-Alloys  v4.0
TCAL3   =  Al-Alloys  v3.0
TCAL2   =  Al-Alloys  v2.1
TCAL1   =  Al-Alloys  v1.2
TCMG5   =  Mg-Alloys  v5.1
TCMG4   =  Mg-Alloys  v4.0
TCMG3   =  Mg-Alloys  v3.0
TCMG2   =  Mg-Alloys  v2.0
TCMG1   =  Mg-Alloys  v1.1
TCTI2   =  Ti-Alloys  v2.1
TCTI1   =  Ti-Alloys  v1.0
TCCU3   =  Cu-Alloys  v3.1
TCCU2   =  Cu-Alloys  v2.0
TCCU1   =  Cu-Alloys  v1.0
TCCC1   =  Cemented carbide  v1.0
TCHEA4  =  High Entropy Alloy  v4.0
TCHEA3  =  High Entropy Alloy  v3.1
TCHEA2  =  High Entropy Alloy  v2.1.1
TCHEA1  =  High Entropy Alloy  v1.0
SSOL7   =  SGTE Alloy Solutions Database v7.0
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
TCOX10  =  Metal Oxide Solutions  v10.0 SNAPSHOT
TCOX9   =  Metal Oxide Solutions  v9.0
TCOX8   =  Metal Oxide Solutions  v8.0
TCOX7   =  Metal Oxide Solutions  v7.0
TCOX6   =  Metal Oxide Solutions  v6.0
TCOX5   =  Metal Oxide Solutions  v5.1
TCOX4   =  Metal Oxide Solutions  v4.1
ION3    =  Ionic Solutions  v3.0
ION2    =  Ionic Solutions  v2.6
ION1    =  Ionic Solutions  v1.5
NOX2    =  NPL Oxide Solutions Database v2.1
TCNOBL2 =  Noble Metals Alloys v2.0 SNAPSHOT
TCNOBL1 =  Noble Metals Alloys v1.0
TCSLD3  =  Solder Alloys  v3.2
TCSLD2  =  Solder Alloys  v2.0
TCSLD1  =  Solder Alloys  v1.1
TCSI1   =  Ultrapure Silicon  v1.2
TCMP2   =  Materials Processing  v2.5
TCES1   =  Combustion/Sintering  v1.1
TCSC1   =  Super Conductor  v1.0
TCFC1   =  SOFC Database v1.0
TCNF2   =  Nuclear Fuels  v2.1b
NUMT2   =  Nuclear Materials  v2.1
NUOX4   =  Nuclear Oxides  v4.2
NUCL15  =  IRSN NUCLEA-15_4
NUCL10  =  ThermoData NUCLEA Alloys-oxides TDB v10.2
MEPH15  =  IRSN Mephista-15_1
MEPH11  =  ThermoData MEPHISTA Nuclear Fuels TDB v11.2
TCAQ3   =  Aqueous Solution  v3.0
TCAQ2   =  Aqueous Solution  v2.7
AQS2    =  TGG Aqueous Solution Database v2.6
GCE2    =  TGG Geochemical/Environmental TDB v2.3
FEDEMO  =  Iron Demo Database v2.1
ALDEMO  =  Aluminum Demo Database v3.0
NIDEMO  =  Nickel Demo Database v1.1
CUDEMO  =  Copper Demo Database v1.0
SLDEMO  =  Solder Demo Database v1.0
OXDEMO  =  Oxide Demo Database v1.0
SUBDEMO =  Substance Demo Database v1.0
PTERN   =  Public Ternary Alloys TDB v1.3
PAQ2    =  Public Aqueous Soln (SIT) TDB v2.4
PG35    =  G35 Binary Semi-Conductors TDB v1.2
PURE5   =  SGTE Unary (Pure Elements) TDB v5.1
MOB2    =  Alloys Mobility  v2.7
MOB1    =  Alloys Mobility  v1.3
MOBFE1  =  Steels/Fe-Alloys Mobility  v1.1
MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
MOBFE5  =  Steels/Fe-Alloys Mobility  v5.0
MOBNI5  =  Ni-Alloys Mobility  v5.1
MOBNI4  =  Ni-Alloys Mobility  v4.1
MOBNI3  =  Ni-Alloys Mobility  v3.2
MOBNI2  =  Ni-Alloys Mobility  v2.4
MOBNI1  =  Ni-Alloys Mobility  v1.10
MOBAL5  =  Al-Alloys Mobility  v5.0
MOBAL4  =  Al-Alloys Mobility  v4.0
MOBAL3  =  Al-Alloys Mobility  v3.0
MOBAL2  =  Al-Alloys Mobility  v2.0
```

```
 MOBAL1  =  Al-Alloys Mobility  v1.0
 MOBCU1  =  Cu-Alloys Mobility  v1.0
 MOBCU2  =  Cu-Alloys Mobility  v2.0
 MOBCU3  =  Cu-Alloys Mobility  v3.0
 MOBHEA1 =  High Entropy Alloys Mobility  v1.0
 MOBHEA2 =  High Entropy Alloys Mobility  v2.0
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBSLD1 =  Solder-Alloys Mobility  v1.1
 MOBTI3  =  Ti-Alloys Mobility  v3.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v2.0
 MFEDEMO =  Fe-Alloys Mobility demo database v2.0
 MNIDEMO =  Ni-Alloys Mobility demo database v1.0
 MCUDEMO =  Cu-Alloys Mobility demo database v1.0
 USER    =  User defined Database

DATABASE NAME /TCFE9/: mobfe4
 Current database: Steels/Fe-Alloys Mobility  v4.0

 VA  DEFINED
 B2_BCC  REJECTED
APP: def-sys fe si mn c
 FE                      SI                      MN
 C  DEFINED
APP: rej ph * all
 BCC_A2                  CEMENTITE               FCC_A1
 FE4N_LP1                HCP_A3                  LIQUID:L
   REJECTED
APP: res ph fcc
 FCC_A1  RESTORED
APP: get
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'This parameter has not been assessed'
  'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'
  'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
      -Ni'
  'Y. Liu, L. Zhang, et al. CALPHAD 33(2009)614-23; Fe-Mn-C (fcc)'
  'M. Yin, et al. (2010) unpublished work.'
  'W. Zheng, et al., J. Alloys and Compounds, 632 (2015) 661-675; Fe-Mn-Si
      (fcc)'
  'D. Bergner et al., Defect and Diffusion Forum 66-69(1989)409. Impurity
      diffusion of Si in fcc Fe.'
 -OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE PROBLEM IS SET UP
APP: @@
APP: go d-m
 NO TIME STEP DEFINED
 *** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
DIC>
DIC> @@
DIC> @@ ENTER GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 1273; * N
DIC>
DIC> @@
DIC> @@ SET THE REFERENCE STATE FOR CARBON
DIC> @@
DIC> set-ref C grap * 101325
DIC>
DIC> @@
DIC> @@ ENTER A REGION
DIC> @@
DIC> enter-region aus
DIC>
DIC> @@
DIC> @@ ENTER A DOUBLE GEOMETRIC GRID INTO THE REGION
DIC> @@
DIC> enter-grid
REGION NAME : /AUS/: aus
WIDTH OF REGION /1/: 1e-2
TYPE /LINEAR/: AUTO
DIC>
DIC> @@
DIC> @@ SET THE GEOMETRY (1 = CYLINDER)
DIC> @@
DIC> enter-geo
GEOMETRICAL EXPONENT /0/: 1
DIC>
DIC> @@
DIC> @@ SET THE FIRST INTERFACE => TUBE
DIC> @@
DIC> set-first-interface
COORDINATE FOR FIRST INTERFACE /0/: 2e-2
DIC>
DIC> @@
DIC> @@ ENTER AN active PHASE IN THE REGION
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /AUS/: aus
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc_a1#1
DIC>
DIC> @@
DIC> @@ ENTER INITIAL COMPOSITIONS INTO THE PHASE
DIC> @@
DIC> enter-composition
REGION NAME : /AUS/: aus
PHASE NAME: /FCC_A1/: fcc#1
DEPENDENT COMPONENT ? /SI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
```

```
PROFILE FOR /C/: si lin 0.7 0.7
PROFILE FOR /MN/: mn lin 0.6 0.6
PROFILE FOR /SI/: c lin 5e-2 5e-2
DIC>
DIC> @@
DIC> @@ SET THE BOUNDARY CONDITIONS ON BOTH THE LOWER AND UPPER PART OF THE REGION
DIC> @@
DIC> @@ USE MIXED CONDITIONS: AN ACTIVITY CONDITION FOR C AND CLOSED
DIC> @@ SYSTEMS FOR MN AND SI.
DIC> @@
DIC> set-cond
GLOBAL OR BOUNDARY CONDITION /GLOBAL/: boundary
BOUNDARY /LOWER/: lower
CONDITION TYPE /CLOSED_SYSTEM/: mixed
Dependent substitutional element:FE
Dependent interstitial element:VA
TYPE OF CONDITION FOR COMPONENT C /ZERO_FLUX/: activity
LOW TIME LIMIT /0/: 0
ACR(C)(TIME)= 0.9;
HIGH TIME LIMIT /*/: *
ANY MORE RANGES /N/: N
TYPE OF CONDITION FOR COMPONENT MN /ZERO_FLUX/: zero_flux
TYPE OF CONDITION FOR COMPONENT SI /ZERO_FLUX/: zero_flux
DIC>
DIC> set-cond
GLOBAL OR BOUNDARY CONDITION /GLOBAL/: boundary
BOUNDARY /UPPER/: upper
CONDITION TYPE /CLOSED_SYSTEM/: mixed
Dependent substitutional element:FE
Dependent interstitial element:VA
TYPE OF CONDITION FOR COMPONENT C /ZERO_FLUX/: activity
LOW TIME LIMIT /0/: 0
ACR(C)(TIME)= 1e-5;
HIGH TIME LIMIT /*/: *
ANY MORE RANGES /N/: N
TYPE OF CONDITION FOR COMPONENT MN /ZERO_FLUX/: zero_flux
TYPE OF CONDITION FOR COMPONENT SI /ZERO_FLUX/: zero_flux
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 1e9
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /100000000/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC> @@
DIC> @@ SAVE TO FILE
DIC> @@
DIC> save exa6 y
DIC>
DIC> set-inter
 --OK---
DIC>
```

**exa6-run**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exa6\run.DCM.test"
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
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
 U-FRACTION IN SYSTEM:  C = .00115488575879621  FE = .490055682684517
                        MN = .00302988813183616  SI = .00691442924890042
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
 U-FRACTION IN SYSTEM:  C = .00115488575879621  FE = .490055682684517
                        MN = .00302988813183616  SI = .00691442924890042
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
 TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00116822817821891  FE = .490055682684517
                        MN = .00302988813183616  SI = .00691442924890042
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0 seconds
 TIME =  0.10010000E-03 DT =  0.10000000E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00116829188694328  FE = .490055682684517
                        MN = .00302988813183616  SI = .00691442924890042
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0 seconds
 TIME =   3.0557610     DT =   3.0556609     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00118959189435653  FE = .490055682684521
                        MN = .00302988813183664  SI = .00691442924889593
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    1 seconds
 TIME =   9.1670828     DT =   6.1113218     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00121111672154579  FE = .490055682684524
                        MN = .00302988813183702  SI = .00691442924889251
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0 seconds
 TIME =   21.389726     DT =   12.222644     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00123890626455181  FE = .490055682684528
                        MN = .00302988813183746  SI = .00691442924888853
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0 seconds
 TIME =   45.835013     DT =   24.445287     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00127670303015352  FE = .490055682684532
                        MN = .00302988813183797  SI = .00691442924888392
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    1 seconds
 TIME =   94.725588     DT =   48.890574     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00132921753226138  FE = .490055682684536
                        MN = .00302988813183855  SI = .00691442924887889
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0 seconds
 TIME =   192.50674     DT =   97.781148     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00140291029963708  FE = .49005568268454
                        MN = .00302988813183909  SI = .00691442924887446
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0 seconds
 TIME =   388.06903     DT =   195.56230     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00150683893865951  FE = .490055682684541
                        MN = .00302988813183934  SI = .00691442924887331
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0 seconds
 TIME =   779.19363     DT =   391.12459     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00165382101622263  FE = .490055682684533
                        MN = .00302988813183861  SI = .00691442924888217
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    1 seconds
 TIME =   1561.4428     DT =   782.24919     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00186208912002594  FE = .49005568268452
                        MN = .00302988813183733  SI = .00691442924889648
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0 seconds
 TIME =   3125.9412     DT =   1564.4984     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00215763950853838  FE = .490055682684545
                        MN = .00302988813184034  SI = .00691442924886802
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0 seconds
 TIME =   6254.9379     DT =   3128.9967     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00257762247234064  FE = .490055682684614
                        MN = .00302988813184873  SI = .00691442924879131
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    1 seconds
 TIME =   12512.931     DT =   6257.9935     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00317612553687888  FE = .490055682684701
                        MN = .00302988813186053  SI = .00691442924869196
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0 seconds
 TIME =   25028.918     DT =   12515.987     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00403212708748457  FE = .490055682684788
                        MN = .00302988813187388  SI = .00691442924859185
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    1 seconds
 TIME =   50060.892     DT =   25031.974     SUM OF SQUARES =   0.0000000
```

```
 U-FRACTION IN SYSTEM:  C = .0052618594638577  FE = .490055682684867
                        MN = .00302988813188714  SI = .00691442924849985
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0 seconds
 TIME =   100124.84     DT =   50063.948     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00703878462392716  FE = .490055682684956
                        MN = .00302988813189985  SI = .00691442924839735
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    1 seconds
 TIME =   200252.74     DT =   100127.90     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00961468135205796  FE = .490055682685084
                        MN = .0030298881319146  SI = .00691442924825484
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0 seconds


output ignored...



... output resumed

  CPU time used in timestep                    1 seconds
 TIME =   1602043.3     DT =   801023.17     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165165842674942  FE = .490055682687091
                        MN = .00302988813214933  SI = .00691442924601361
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0 seconds
 TIME =   3071117.5     DT =   1469074.2     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165253458723486  FE = .490055682689399
                        MN = .00302988813240262  SI = .00691442924345169
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    1 seconds
 TIME =   5521426.5     DT =   2450309.1     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165254570895428  FE = .490055682693946
                        MN = .00302988813287881  SI = .00691442923842824
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0 seconds
 TIME =   9715746.1     DT =   4194319.5     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165253215591163  FE = .490055682703382
                        MN = .00302988813383215  SI = .00691442922803932
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    1 seconds
 TIME =   17813876.     DT =   8098130.0     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165250052909423  FE = .490055682726195
                        MN = .00302988813607049  SI = .00691442920298777
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0 seconds
 TIME =   34010136.     DT =   16196260.     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165246276464081  FE = .490055682784398
                        MN = .00302988814169422  SI = .00691442913916063
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    1 seconds
 TIME =   66402656.     DT =   32392520.     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165243580713319  FE = .490055682920989
                        MN = .00302988815540702  SI = .00691442898885753
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0 seconds
 TIME =  0.13118770E+09 DT =   64785040.     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165244582014691  FE = .490055683192306
                        MN = .00302988818558275  SI = .00691442868736454
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    1 seconds
 TIME =  0.23061023E+09 DT =   99422537.     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165263917143574  FE = .490055683555767
                        MN = .00302988823056496  SI = .00691442827892098
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    1 seconds
 TIME =  0.33012543E+09 DT =   99515198.     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165303267851656  FE = .49005568386721
                        MN = .00302988827178368  SI = .0069144279262599
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0 seconds
 TIME =  0.42970616E+09 DT =   99580728.     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165336326908911  FE = .490055684142115
                        MN = .00302988830951066  SI = .00691442761362775
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    1 seconds
 TIME =  0.52934108E+09 DT =   99634921.     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165366300962678  FE = .490055684390274
                        MN = .00302988834435611  SI = .00691442733062356
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0 seconds
 TIME =  0.62902222E+09 DT =   99681143.     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165394384249259  FE = .490055684617852
                        MN = .00302988837682077  SI = .00691442707058051
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    1 seconds
 TIME =  0.72874408E+09 DT =   99721854.     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165421143527837  FE = .490055684829008
                        MN = .00302988840729343  SI = .00691442682895181
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    1 seconds
 TIME =  0.82850228E+09 DT =   99758206.     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165446894756978  FE = .490055685026688
                        MN = .00302988843607474  SI = .0069144266024909
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0 seconds
 TIME =  0.92829328E+09 DT =   99791002.     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165471833610485  FE = .490055685213062
                        MN = .00302988846340021  SI = .00691442638879089
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    1 seconds
 TIME =  0.98979354E+09 DT =   61500257.     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .016549869431163  FE = .490055685322987
                        MN = .00302988847959188  SI = .00691442626267452
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
  CPU time used in timestep                    0 seconds
 TIME =  0.10000000E+10 DT =   10206459.     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0165516055116171  FE = .490055685340902
                        MN = .00302988848223566  SI = .00691442624211591
 TOTAL SIZE OF SYSTEM:  .00314159265359 [m^2]
 MUST SAVE WORKSPACE ON FILE
 WORKSPACE SAVED ON FILE
 RECLAIMING WORKSPACE
 DELETING TIME-RECORD FOR TIME    0.0000000
```

```
 DELETING TIME-RECORD FOR TIME   0.10000000E-06
 DELETING TIME-RECORD FOR TIME   0.10010000E-03
 DELETING TIME-RECORD FOR TIME    3.0557610
 DELETING TIME-RECORD FOR TIME    9.1670828
 DELETING TIME-RECORD FOR TIME    21.389726
 DELETING TIME-RECORD FOR TIME    45.835013
 DELETING TIME-RECORD FOR TIME    94.725588
 DELETING TIME-RECORD FOR TIME    192.50674
 DELETING TIME-RECORD FOR TIME    388.06903
 DELETING TIME-RECORD FOR TIME    779.19363
 DELETING TIME-RECORD FOR TIME    1561.4428
 DELETING TIME-RECORD FOR TIME    3125.9412
 DELETING TIME-RECORD FOR TIME    6254.9379
 DELETING TIME-RECORD FOR TIME    12512.931
 DELETING TIME-RECORD FOR TIME    25028.918
 DELETING TIME-RECORD FOR TIME    50060.892
 DELETING TIME-RECORD FOR TIME    100124.84
 DELETING TIME-RECORD FOR TIME    200252.74
 DELETING TIME-RECORD FOR TIME    400508.53
 DELETING TIME-RECORD FOR TIME    801020.11
 DELETING TIME-RECORD FOR TIME    1602043.3
 DELETING TIME-RECORD FOR TIME    3071117.5
 DELETING TIME-RECORD FOR TIME    5521426.5
 DELETING TIME-RECORD FOR TIME    9715746.1
 DELETING TIME-RECORD FOR TIME    17813876.
 DELETING TIME-RECORD FOR TIME    34010136.
 DELETING TIME-RECORD FOR TIME    66402656.
 DELETING TIME-RECORD FOR TIME   0.13118770E+09
 DELETING TIME-RECORD FOR TIME   0.23061023E+09
 DELETING TIME-RECORD FOR TIME   0.33012543E+09
 DELETING TIME-RECORD FOR TIME   0.42970616E+09
 DELETING TIME-RECORD FOR TIME   0.52934108E+09
 DELETING TIME-RECORD FOR TIME   0.62902222E+09
 DELETING TIME-RECORD FOR TIME   0.72874408E+09
 DELETING TIME-RECORD FOR TIME   0.82850228E+09
 DELETING TIME-RECORD FOR TIME   0.92829328E+09

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

 TIMESTEP AT    0.100000000E+10 SELECTED

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

**exa6-plot**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exa6\plot.DCM.test"
DIC>
DIC>
DIC> @@ exa6_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE exa6
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  1.00000E+09
 *** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
DIC> read exa6
 OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:
POST-1: @@
POST-1: @@ PLOT THE CONCENTRATION OF C AT DIFFERENT TIMES
POST-1: @@
POST-1: s-d-a x distance global
  INFO: Distance is set as independent variable
POST-1: s-d-a y w-p c
POST-1: s-p-c time 0,1e4,2e5,1e7,1e9
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

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

2019.11.11.14.43.44
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:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

2019.11.11.14.43.45
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:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

2019.11.11.14.43.46
Time = 0,10000,200000,1E+07,1E+09
CELL #1

```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ FINALLY, LOOK AT THE ACTIVITY PROFILES OF SI
POST-1: @@
POST-1: s-d-a y ac(si)
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

2019.11.11.14.43.49
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**

```
SYS:About

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

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 21012) 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: Mon Nov 11 11:13:13 2019


SYS:SYS:MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exa7\setup.DCM.test"
SYS: @@ One phase example.
SYS: @@ Homogenization heat treatment
SYS: @@ The initial segregation profile is created from a Scheil
SYS: @@ calculation (see macro create_initial_profile.TCM). The command
SYS: @@ INPUT_SCHEIL_PROFILE in the DICTRA MONITOR performs most of the
SYS: @@ set up. Only time and temperature must  be entered after the
SYS: @@ INPUT_SCHEIL_PROFILE command is executed.
SYS: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ In this example only a single phase, ferrite, is entered in the simulation
SYS: go da
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v10.0

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10: sw FEDEMO
 Current database: Iron Demo Database v2.1

 VA                      /-  DEFINED
TDB_FEDEMO: def-sys fe cr ni mn
 FE                      CR                      NI
 MN  DEFINED
TDB_FEDEMO: rej ph *
 LIQUID:L                BCC_A2                  CBCC_A12
 CHI_A12                 CUB_A13                 DIAMOND_FCC_A4
 FCC_A1                  HCP_A3                  LAVES_PHASE_C14
 SIGMA  REJECTED
TDB_FEDEMO: rest ph bcc
 BCC_A2  RESTORED
TDB_FEDEMO: get
14:45:11,322 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270
      (1986); CR-FE'
  'B.-J. Lee, Metall. Trans. A, 24A (1993) 1919-1933; Cr-Mn, Fe-Cr -Mn'
  'B.-J. Lee, CALPHAD, 17 (1993) 251-268; revision of Fe-Cr and Fe -Ni liquid'
  'B.-J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
  'A. Dinsdale and T. Chart, MTDS NPL, Unpublished work (1986); CR -NI'
  'W. Huang, CALPHAD, 13 (1989) 243-252; TRITA-MAC 388 (rev 1989); FE-MN'
  'L. Zhang, Y. Du, H. Xu, S. Liu, Y. Liu, F. Zheng, et al., Int. J. Mater.
      Res. 100 (2009) 160-175; Fe-Mn-Ni'
  'A. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); FE-NI'
  'S. Liu, Unpublished work (2010); Mn-Ni'
 -OK-
TDB_FEDEMO:
TDB_FEDEMO: 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>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exa7\run.DCM.test"
DIC> go dict-mon
 TIME STEP AT TIME  0.00000E+00
DIC>
DIC> read exa7
 OK
DIC>
DIC> sim
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
 U-FRACTION IN SYSTEM:  CR = .180420497424242  FE = .796498787878788
                        MN = .00999016878282828  NI = .0130905459141414
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 U-FRACTION IN SYSTEM:  CR = .180420497424242  FE = .796498787878788
                        MN = .00999016878282828  NI = .0130905459141414
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .180420497424242  FE = .796498787878788
                        MN = .00999016878282828  NI = .0130905459141414
 TOTAL SIZE OF SYSTEM:  1E-04 [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:  CR = .180420497424243  FE = .796498787878788
                        MN = .00999016878282828  NI = .0130905459141414
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     0 seconds
 TIME =  0.41908397     DT =  0.41898387     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .180420497424242  FE = .796498787878788
                        MN = .00999016878282789  NI = .0130905459141418
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     0 seconds
 TIME =   1.2570517     DT =  0.83796774     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .180420497424242  FE = .796498787878788
                        MN = .0099901687828279  NI = .0130905459141418
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     1 seconds
 TIME =   2.9329872     DT =   1.6759355     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .180420497424243  FE = .796498787878788
                        MN = .00999016878282889  NI = .0130905459141397
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     0 seconds
 TIME =   6.2848581     DT =   3.3518710     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .180420497424257  FE = .796498787878809
                        MN = .00999016878284567  NI = .0130905459140889
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     0 seconds
 TIME =   12.988600     DT =   6.7037419     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .180420497424302  FE = .796498787878887
                        MN = .0099901687828762  NI = .0130905459139341
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     1 seconds
 TIME =   26.396084     DT =   13.407484     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .180420497424318  FE = .796498787878861
                        MN = .00999016878290129  NI = .0130905459139196
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     0 seconds
 TIME =   53.211052     DT =   26.814968     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .180420497424435  FE = .796498787878771
                        MN = .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 = .180420497424574  FE = .796498787878386
                        MN = .00999016878336976  NI = .0130905459136696
 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 = .7964987878782
                        MN = .00999016878339539  NI = .0130905459139731
 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 = .79649878787776
                        MN = .0099901687835091  NI = .0130905459146418
 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 = .796498787877897
                        MN = .00999016878346275  NI = .0130905459145564
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     1 seconds
 TIME =   1148.6206     DT =   360.00000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .180420497423612  FE = .796498787877388
                        MN = .0099901687833258  NI = .0130905459156742
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     0 seconds
 TIME =   1508.6206     DT =   360.00000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .180420497423264  FE = .796498787877025
                        MN = .0099901687831708  NI = .0130905459165403
 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 = .180420497422964  FE = .796498787875229
                        MN = .00999016878345041  NI = .0130905459183568
 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 = .180420497422684  FE = .796498787872687
                        MN = .00999016878399131  NI = .0130905459206371
 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 = .180420497422471  FE = .796498787870924
                        MN = .00999016878437158  NI = .0130905459222343
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     1 seconds
 TIME =   2948.6206     DT =   360.00000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .180420497422315  FE = .796498787869698
                        MN = .00999016878464259  NI = .0130905459233444
 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 = .180420497422201  FE = .796498787868845
                        MN = .00999016878483191  NI = .013090545924121
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3600.0000     DT =   291.37940     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .180420497422136  FE = .796498787868424
                        MN = .00999016878491989  NI = .0130905459245201
 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>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exa7\plot.DCM.test"
DIC> go dict-mon
 TIME STEP AT TIME  3.60000E+03
DIC>
DIC> read exa7
 OK
DIC>
DIC> post
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1: s-p-c time 0,3600
POST-1: s-d-a x d g
  INFO: Distance is set as independent variable
POST-1: s-d-a y w-p mn
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

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

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

# Moving Boundary Problems

# Example exb1a

## γ to α transformation in a binary Fe-C alloy

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

***Fe - C Phase diagram***

**exb1a-setup**

```
SYS:About

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

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 21012) 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: Mon Nov 11 11:13:13 2019


SYS:SYS:MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exb1a\setup.DCM.test"
SYS: @@
SYS: @@ Moving boundary problem.
SYS: @@  Austenite to ferrite transformation in a binary Fe-C alloy
SYS: @@ This example calculates a ferrite(BCC)/austenite(FCC)transformation
SYS: @@ in a binary Fe-C alloy.  The initial state is an austenite of 2mm
SYS: @@ thickness. The composition of the austenite is Fe-0.15wt%C.
SYS: @@
SYS: @@ After austenitization the specimen is quenched down to 1050K.
SYS: @@ The system is assumed closed, so no boundary conditions are set
SYS: @@ (a closed system is the default). Ferrite is expected to grow
SYS: @@ into the austenite, which is why we start with a thin
SYS: @@ region with ferrite adjacent to the austenite.
SYS: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exb1a_setup.DCM
SYS:
SYS:
SYS: @@
SYS: @@ START BY GOING TO THE DATABASE MODULE
SYS: @@
SYS: go da
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v10.0

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10:
TDB_TCFE10: @@
TDB_TCFE10: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE THE DATA
TDB_TCFE10: @@
TDB_TCFE10: sw FEDEMO
 Current database: Iron Demo Database v2.1

 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
 CBCC_A12                CEMENTITE               CUB_A13
 DIAMOND_FCC_A4          FCC_A1                  GRAPHITE
 HCP_A3                  KSI_CARBIDE             LAVES_PHASE_C14
 M23C6                   M5C2                    M7C3
   REJECTED
TDB_FEDEMO: res ph fcc bcc
 FCC_A1                  BCC_A2  RESTORED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ RETRIEVE DATA FROM THE DATABASE FILE
TDB_FEDEMO: @@
TDB_FEDEMO: get
14:48:49,215 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'P. Franke, Estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
  'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
 -OK-
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ 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

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

```
FROST1  =  FROST database v1.2
FEDAT   =  TCS/TT Steels Database v1.0
TCNI10  =  Ni-Alloys  v10.0 SNAPSHOT
TCNI9   =  Ni-Alloys  v9.1
TCNI8   =  Ni-Alloys  v8.2
TCNI7   =  Ni-Alloys  v7.2
TCNI6   =  Ni-Alloys  v6.1
TCNI5   =  Ni-Alloys  v5.1
TCNI4   =  Ni-Alloys  v4.0
TCNI1   =  Ni-Alloys  v1.3
TCAL6   =  Al-Alloys  v6.0
TCAL5   =  Al-Alloys  v5.1
TCAL4   =  Al-Alloys  v4.0
TCAL3   =  Al-Alloys  v3.0
TCAL2   =  Al-Alloys  v2.1
TCAL1   =  Al-Alloys  v1.2
TCMG5   =  Mg-Alloys  v5.1
TCMG4   =  Mg-Alloys  v4.0
TCMG3   =  Mg-Alloys  v3.0
TCMG2   =  Mg-Alloys  v2.0
TCMG1   =  Mg-Alloys  v1.1
TCTI2   =  Ti-Alloys  v2.1
TCTI1   =  Ti-Alloys  v1.0
TCCU3   =  Cu-Alloys  v3.1
TCCU2   =  Cu-Alloys  v2.0
TCCU1   =  Cu-Alloys  v1.0
TCCC1   =  Cemented carbide  v1.0
TCHEA4  =  High Entropy Alloy  v4.0
TCHEA3  =  High Entropy Alloy  v3.1
TCHEA2  =  High Entropy Alloy  v2.1.1
TCHEA1  =  High Entropy Alloy  v1.0
SSOL7   =  SGTE Alloy Solutions Database v7.0
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
TCOX10  =  Metal Oxide Solutions  v10.0 SNAPSHOT
TCOX9   =  Metal Oxide Solutions  v9.0
TCOX8   =  Metal Oxide Solutions  v8.0
TCOX7   =  Metal Oxide Solutions  v7.0
TCOX6   =  Metal Oxide Solutions  v6.0
TCOX5   =  Metal Oxide Solutions  v5.1
TCOX4   =  Metal Oxide Solutions  v4.1
ION3    =  Ionic Solutions  v3.0
ION2    =  Ionic Solutions  v2.6
ION1    =  Ionic Solutions  v1.5
NOX2    =  NPL Oxide Solutions Database v2.1
TCNOBL2 =  Noble Metals Alloys v2.0 SNAPSHOT
TCNOBL1 =  Noble Metals Alloys v1.0
TCSLD3  =  Solder Alloys  v3.2
TCSLD2  =  Solder Alloys  v2.0
TCSLD1  =  Solder Alloys  v1.1
TCSI1   =  Ultrapure Silicon  v1.2
TCMP2   =  Materials Processing  v2.5
TCES1   =  Combustion/Sintering  v1.1
TCSC1   =  Super Conductor  v1.0
TCFC1   =  SOFC Database v1.0
TCNF2   =  Nuclear Fuels  v2.1b
NUMT2   =  Nuclear Materials  v2.1
NUOX4   =  Nuclear Oxides  v4.2
NUCL15  =  IRSN NUCLEA-15_4
NUCL10  =  ThermoData NUCLEA Alloys-oxides TDB v10.2
MEPH15  =  IRSN Mephista-15_1
MEPH11  =  ThermoData MEPHISTA Nuclear Fuels TDB v11.2
TCAQ3   =  Aqueous Solution  v3.0
TCAQ2   =  Aqueous Solution  v2.7
AQS2    =  TGG Aqueous Solution Database v2.6
GCE2    =  TGG Geochemical/Environmental TDB v2.3
FEDEMO  =  Iron Demo Database v2.1
ALDEMO  =  Aluminum Demo Database v3.0
NIDEMO  =  Nickel Demo Database v1.1
CUDEMO  =  Copper Demo Database v1.0
SLDEMO  =  Solder Demo Database v1.0
OXDEMO  =  Oxide Demo Database v1.0
SUBDEMO =  Substance Demo Database v1.0
PTERN   =  Public Ternary Alloys TDB v1.3
PAQ2    =  Public Aqueous Soln (SIT) TDB v2.4
PG35    =  G35 Binary Semi-Conductors TDB v1.2
PURE5   =  SGTE Unary (Pure Elements) TDB v5.1
MOB2    =  Alloys Mobility  v2.7
MOB1    =  Alloys Mobility  v1.3
MOBFE1  =  Steels/Fe-Alloys Mobility  v1.1
MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
MOBFE5  =  Steels/Fe-Alloys Mobility  v5.0
MOBNI5  =  Ni-Alloys Mobility  v5.1
MOBNI4  =  Ni-Alloys Mobility  v4.1
MOBNI3  =  Ni-Alloys Mobility  v3.2
MOBNI2  =  Ni-Alloys Mobility  v2.4
MOBNI1  =  Ni-Alloys Mobility  v1.10
MOBAL5  =  Al-Alloys Mobility  v5.0
MOBAL4  =  Al-Alloys Mobility  v4.0
MOBAL3  =  Al-Alloys Mobility  v3.0
MOBAL2  =  Al-Alloys Mobility  v2.0
MOBAL1  =  Al-Alloys Mobility  v1.0
MOBCU1  =  Cu-Alloys Mobility  v1.0
MOBCU2  =  Cu-Alloys Mobility  v2.0
MOBCU3  =  Cu-Alloys Mobility  v3.0
MOBHEA1 =  High Entropy Alloys Mobility  v1.0
MOBHEA2 =  High Entropy Alloys Mobility  v2.0
MOBMG1  =  Mg-Alloys Mobility  v1.0
```

```
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBSLD1 =  Solder-Alloys Mobility  v1.1
 MOBTI3  =  Ti-Alloys Mobility  v3.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v2.0
 MFEDEMO =  Fe-Alloys Mobility demo database v2.0
 MNIDEMO =  Ni-Alloys Mobility demo database v1.0
 MCUDEMO =  Cu-Alloys Mobility demo database v1.0
 USER    =  User defined Database

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

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

 List of references for assessed data

  'This parameter has not been assessed'
  'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'
  'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
      -Ni'
  'B. Jonsson: Z. Metallkunde 85(1994)498-501; C and N diffusion in bcc Cr
      -Fe-Ni'
  'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
      in bcc Fe'
 -OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP
APP: @@
APP: go d-m
 NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER GLOBAL CONDITION T
DIC> @@
DIC> set-condition global T 0 1050; * N
DIC>
DIC> @@
DIC> @@ START BY ENTERING THE REGIONS ferrite AND austenite WHERE WE
DIC> @@ PUT THE BCC AND FCC PHASE, RESPECTIVELY. THE FERRITE REGION IS
DIC> @@ ASSUMED INITIALLY TO BE VERY THIN, 1E-9 METERS.
DIC> @@
DIC> enter-region
REGION NAME : ferrite
DIC>
DIC> enter-region
REGION NAME : austenite
ATTACH TO REGION NAMED /FERRITE/:
ATTACHED TO THE RIGHT OF FERRITE /YES/:
DIC>
DIC> @@
DIC> @@ ENTER GRIDS INTO THE REGIONS
DIC> @@
DIC> enter-grid
REGION NAME : /FERRITE/: ferrite
WIDTH OF REGION /1/: 1e-9
TYPE /LINEAR/: AUTO
DIC>
DIC> enter-grid austenite
WIDTH OF REGION /1/: 20e-4
TYPE /LINEAR/: AUTO
DIC>
DIC> @@
DIC> @@ ENTER active PHASES INTO THE REGIONS
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /FERRITE/: ferrite
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: bcc
DIC>
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /AUSTENITE/: austenite
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ ENTER AN INITIAL COMPOSITION INTO BCC
DIC> @@
DIC> enter-composition
REGION NAME : /FERRITE/: ferrite
PHASE NAME: /BCC_A2/: bcc
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: C
TYPE /LINEAR/: linear
VALUE OF FIRST POINT : 0.01
VALUE OF LAST POINT : /1E-2/: 0.01
DIC>
DIC> @@
DIC> @@ ENTER AN INITIAL COMPOSITION INTO FCC
DIC> @@
DIC> enter-composition
REGION NAME : /AUSTENITE/: austenite
PHASE NAME: /FCC_A1/: fcc#1
COMPOSITION TYPE /MOLE_FRACTION/: w-p
```

```
PROFILE FOR /C/: C
TYPE /LINEAR/: linear
VALUE OF FIRST POINT : 0.15
VALUE OF LAST POINT : /0.15/: 0.15
DIC>
DIC> @@
DIC> @@ THE BOUNDARY CONDITION IS A CLOSED SYSTEM AS WE DO NOT SPECIFY
DIC> @@ ANYTHING ELSE
DIC> @@
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 1e9
AUTOMATIC TIMESTEP CONTROL /YES/: YES
MAX TIMESTEP DURING INTEGRATION /100000000/: 1e8
INITIAL TIMESTEP : /1E-07/: 1E-5
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/: 1E-5
DIC>
DIC>
DIC> @@
DIC> @@ IMPLICIT (1) TIME INTEGRATION IS USED INSTEAD OF THE MORE ACCURATE
DIC> @@ (BUT LESS STABLE) TRAPETZOIDAL METHOD WHICH IS THE DEFAULT.
DIC> @@
DIC> s-s-c
NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /AUTO/:
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -> 1): /AUTO/: 1.0
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/:
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exb1a Y
DIC>
DIC> set-inter
 --OK---
DIC>
```

**exb1a-run**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exb1a\run.DCM.test"
DIC>
DIC>
DIC> @@ exb1a_run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING EXAMPLE b1a
DIC> @@
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  0.00000E+00
DIC> read exb1a
 OK
DIC>
DIC> @@
DIC> @@ START THE SIMULATION
DIC> @@
DIC> simulate
 Region: FERRITE
 single geometric dense at  0.10000E-08
  1.0000       24
 Region: AUSTENITE
 single geometric dense at   0.0000
  1.1762       99
  Trying old scheme                       3
 U-FRACTION IN SYSTEM:  C = .00698495590385911  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]
 U-FRACTION IN SYSTEM:  C = .00698495590385911  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]
 3.981486698395194E-005        3.982285206223790E-005        1.590378050717499E-012        8.422113835746911E-020       TIME =  0.10000000E-
04 DT =  0.10000000E-04 SUM OF SQUARES =  0.84221138E-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 = .00698495590212123  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]
  13  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUSTENITE

  CPU time used in timestep                    0 seconds
 3.499840016754033E-006        3.500511904249956E-006        1.189295167153537E-007        4.111386278498581E-008        2.962711489812290E-
009        2.530748984847927E-012        1.388215646533131E-016        6.302028868602742E-024       TIME =  0.30000000E-04 DT =  0.20000000E-
04 SUM OF SQUARES =  0.63020289E-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 = .00698495800112155  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]
  CPU time used in timestep                    0 seconds
 8.791374341914706E-008        8.798286131288386E-008        8.680197148511708E-012        8.237998777204505E-016        5.570658332104316E-
024       TIME =  0.70000000E-04 DT =  0.40000000E-04 SUM OF SQUARES =  0.55706583E-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 = .00698495800112151  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]
  CPU time used in timestep                    0 seconds
 3.282053178498482E-006        3.283518217738399E-006        3.522797165763882E-006        1.817586682189996E-007        4.865296022642763E-
008        3.905763819835909E-011        5.263908083351613E-015        6.537906182240236E-022       TIME =  0.15000000E-03 DT =  0.80000000E-
04 SUM OF SQUARES =  0.65379062E-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 = .00698495794642423  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]
  CPU time used in timestep                    0 seconds
  2  GRIDPOINT(S) ADDED   TO   CELL #1   REGION: FERRITE
 4.713654652390555E-007        4.723390763359801E-007        4.586676384660827E-012        4.399046976856031E-017       TIME =  0.31000000E-
03 DT =  0.16000000E-03 SUM OF SQUARES =  0.43990470E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.51923334E-04 AND   0.51923334E-04
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.48655891E-07
 U-FRACTION IN SYSTEM:  C = .00698495386454072  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]
  CPU time used in timestep                    0 seconds
 4.378612637278334E-006        4.381488086560821E-006        1.153721994970485E-009        2.848526252439885E-013        1.743908466437677E-
020       TIME =  0.63000000E-03 DT =  0.32000000E-03 SUM OF SQUARES =  0.17439085E-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 = .006984948587741  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]
  CPU time used in timestep                    0 seconds
 2.098301746880194E-006        2.099772516707655E-006        6.174131548456762E-010        1.696049180678346E-013        1.285332330763806E-
020       TIME =  0.12700000E-02 DT =  0.64000000E-03 SUM OF SQUARES =  0.12853323E-19

output ignored...



... output resumed

TIME =  0.57592186E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.15364008E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.19926141E-15 AND  -0.19926141E-15
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.13794590E-02
 U-FRACTION IN SYSTEM:  C = .00698584273647938  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUSTENITE

  CPU time used in timestep                    0 seconds
 4.535237501308182E-005        4.535773928372776E-005        6.377119607700181E-
022       TIME =  0.67592186E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.63771196E-21
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.13492716E-15 AND   0.13492716E-15
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.13794725E-02
 U-FRACTION IN SYSTEM:  C = .00698570514621074  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]
  20  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: FERRITE

  CPU time used in timestep                    0 seconds
 1.970327668730446E-005        1.970567086562696E-005        5.024070003177980E-
019       TIME =  0.77592186E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.50240700E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.85417341E-16 AND  -0.85417341E-16
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.13794639E-02
 U-FRACTION IN SYSTEM:  C = .00698579224946741  FE = 1
```

```
 TOTAL SIZE OF SYSTEM:  .002000001 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUSTENITE

  CPU time used in timestep                    0 seconds
 9.869293459165407E-006        9.870366152308391E-006        1.893331983544551E-
022       TIME =  0.87592186E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.18933320E-21
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.70327802E-16 AND   0.70327802E-16
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.13794710E-02
 U-FRACTION IN SYSTEM:  C = .00698572053357829  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]
  10  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: FERRITE

  CPU time used in timestep                    0 seconds
 1.668288167588449E-005        1.668402994762454E-005        2.250176276744608E-
028       TIME =  0.97592186E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.22501763E-27
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.13134925E-15 AND  -0.13134925E-15
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.13794578E-02
 U-FRACTION IN SYSTEM:  C = .00698585447532275  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUSTENITE

  CPU time used in timestep                    0 seconds
 4.795129124478679E-005        4.795492713364641E-005        1.073766223439627E-
019       TIME =  0.10000000E+10 DT =   24078140.     SUM OF SQUARES =  0.10737662E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.21081044E-15 AND   0.21081044E-15
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.13794629E-02
 U-FRACTION IN SYSTEM:  C = .00698580271423688  FE = 1
 TOTAL SIZE OF SYSTEM:  .002000001 [m]
 MUST SAVE WORKSPACE ON FILE
 WORKSPACE SAVED ON FILE
 RECLAIMING WORKSPACE
 DELETING TIME-RECORD FOR TIME    0.0000000
 DELETING TIME-RECORD FOR TIME   0.10000000E-04
 DELETING TIME-RECORD FOR TIME   0.30000000E-04
 DELETING TIME-RECORD FOR TIME   0.70000000E-04
 DELETING TIME-RECORD FOR TIME   0.15000000E-03
 DELETING TIME-RECORD FOR TIME   0.31000000E-03
 DELETING TIME-RECORD FOR TIME   0.63000000E-03
 DELETING TIME-RECORD FOR TIME   0.12700000E-02
 DELETING TIME-RECORD FOR TIME   0.25500000E-02
 DELETING TIME-RECORD FOR TIME   0.51100000E-02
 DELETING TIME-RECORD FOR TIME   0.10230000E-01
 DELETING TIME-RECORD FOR TIME   0.20470000E-01
 DELETING TIME-RECORD FOR TIME   0.40950000E-01
 DELETING TIME-RECORD FOR TIME   0.81910000E-01
 DELETING TIME-RECORD FOR TIME   0.16383000
 DELETING TIME-RECORD FOR TIME   0.32767000
 DELETING TIME-RECORD FOR TIME   0.65535000
 DELETING TIME-RECORD FOR TIME    1.3107100
 DELETING TIME-RECORD FOR TIME    2.6214300
 DELETING TIME-RECORD FOR TIME    5.2428700
 DELETING TIME-RECORD FOR TIME    10.485750
 DELETING TIME-RECORD FOR TIME    20.971510
 DELETING TIME-RECORD FOR TIME    41.943030
 DELETING TIME-RECORD FOR TIME    83.886070
 DELETING TIME-RECORD FOR TIME    167.77215
 DELETING TIME-RECORD FOR TIME    335.54431
 DELETING TIME-RECORD FOR TIME    671.08863
 DELETING TIME-RECORD FOR TIME    1342.1773
 DELETING TIME-RECORD FOR TIME    2684.3546
 DELETING TIME-RECORD FOR TIME    5368.7091
 DELETING TIME-RECORD FOR TIME    10737.418
 DELETING TIME-RECORD FOR TIME    21474.836
 DELETING TIME-RECORD FOR TIME    42949.673
 DELETING TIME-RECORD FOR TIME    85899.346
 DELETING TIME-RECORD FOR TIME    171798.69
 DELETING TIME-RECORD FOR TIME    343597.38
 DELETING TIME-RECORD FOR TIME    687194.77
 DELETING TIME-RECORD FOR TIME    1374389.5
 DELETING TIME-RECORD FOR TIME    2748779.1
 DELETING TIME-RECORD FOR TIME    5497558.1
 DELETING TIME-RECORD FOR TIME    10995116.
 DELETING TIME-RECORD FOR TIME    21990233.
 DELETING TIME-RECORD FOR TIME    43980465.
 DELETING TIME-RECORD FOR TIME    87960930.
 DELETING TIME-RECORD FOR TIME   0.17592186E+09
 DELETING TIME-RECORD FOR TIME   0.27592186E+09
 DELETING TIME-RECORD FOR TIME   0.37592186E+09
 DELETING TIME-RECORD FOR TIME   0.47592186E+09
 DELETING TIME-RECORD FOR TIME   0.57592186E+09
 DELETING TIME-RECORD FOR TIME   0.67592186E+09
 DELETING TIME-RECORD FOR TIME   0.77592186E+09
 DELETING TIME-RECORD FOR TIME   0.87592186E+09

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

 TIMESTEP AT    0.100000000E+10 SELECTED

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

**exb1a-plot**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exb1a\plot.DCM.test"
DIC>
DIC>
DIC> @@ exb1a_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE b1a
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  1.00000E+09
DIC> read exb1a
 OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:
POST-1: @@
POST-1: @@ PLOT THE CARBON CONCENTRATIONS AT DIFFERENT TIMES
POST-1: @@
POST-1: s-d-a x distance global
  INFO: Distance is set as independent variable
POST-1: s-d-a y w-p c
POST-1: s-p-c time 1e3,1e5,1e9
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ PLOT THE POSITION OF THE BCC/FCC INTERPHASE
POST-1: @@
POST-1: s-d-a x time
  INFO: Time is set as independent variable
POST-1: s-d-a y
VARIABLE : pos
INTERFACE : aus
UPPER OR LOWER INTERFACE OF REGION AUSTENITE#1 /LOWER/: lower
POST-1:
POST-1: set_axis_type
AXIS (X, Y OR Z) : x
AXIS TYPE /LINEAR/: log
POST-1:
POST-1: s-s-s
AXIS (X, Y OR Z) : x
AUTOMATIC SCALING  (Y OR N) /N/: n
MIN VALUE : 10
MAX VALUE : 1e9
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

2019.11.11.14.50.58
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:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

2019.11.11.14.50.59
LOWER INTERFACE OF REGION "AUSTENITE#1"
CELL #1

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

# Example exb1b

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

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

**exb1b-setup**

```
SYS:About

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

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 21012) 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: Mon Nov 11 11:13:13 2019


SYS:SYS:MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exb1b\setup.DCM.test"
SYS: @@
SYS: @@ Moving boundary problem.
SYS: @@ Austenite to ferrite transformation in a binary Fe-C alloy
SYS: @@ This is the same example as in exb1a but now the problem is with
SYS: @@ ferrite as an inactive phase adjacent to the initial austenite.
SYS: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exb1b_setup.DCM
SYS:
SYS: @@
SYS: @@ START BY GOING TO THE DATABASE MODULE
SYS: @@
SYS: go da
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v10.0

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10:
TDB_TCFE10: @@
TDB_TCFE10: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA
TDB_TCFE10: @@
TDB_TCFE10: sw FEDEMO
 Current database: Iron Demo Database v2.1

 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
 CBCC_A12                CEMENTITE               CUB_A13
 DIAMOND_FCC_A4          FCC_A1                  GRAPHITE
 HCP_A3                  KSI_CARBIDE             LAVES_PHASE_C14
 M23C6                   M5C2                    M7C3
   REJECTED
TDB_FEDEMO: res ph fcc bcc
 FCC_A1                  BCC_A2  RESTORED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ RETRIEVE DATA FROM THE DATABASE FILE
TDB_FEDEMO: @@
TDB_FEDEMO: get
14:52:21,618 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'P. Franke, Estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
  'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
 -OK-
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ 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

 TCFE10  =  Steels/Fe-Alloys  v10.0
 TCFE9   =  Steels/Fe-Alloys  v9.1
 TCFE8   =  Steels/Fe-Alloys  v8.1
 TCFE7   =  Steels/Fe-Alloys  v7.0
 TCFE6   =  Steels/Fe-Alloys  v6.2
 TCFE5   =  Steels/Fe-Alloys  v5.0
 TCFE4   =  Steels/Fe-Alloys  v4.1
 TCFE3   =  Steels/Fe-Alloys  v3.1
 TCFE2   =  Steels/Fe-Alloys  v2.1
 TCFE1   =  Steels/Fe-Alloys  v1.0
 FROST1  =  FROST database v1.2
 FEDAT   =  TCS/TT Steels Database v1.0
 TCNI10  =  Ni-Alloys  v10.0 SNAPSHOT
 TCNI9   =  Ni-Alloys  v9.1
 TCNI8   =  Ni-Alloys  v8.2
 TCNI7   =  Ni-Alloys  v7.2
 TCNI6   =  Ni-Alloys  v6.1
 TCNI5   =  Ni-Alloys  v5.1
```

```
TCNI4   =  Ni-Alloys  v4.0
TCNI1   =  Ni-Alloys  v1.3
TCAL6   =  Al-Alloys  v6.0
TCAL5   =  Al-Alloys  v5.1
TCAL4   =  Al-Alloys  v4.0
TCAL3   =  Al-Alloys  v3.0
TCAL2   =  Al-Alloys  v2.1
TCAL1   =  Al-Alloys  v1.2
TCMG5   =  Mg-Alloys  v5.1
TCMG4   =  Mg-Alloys  v4.0
TCMG3   =  Mg-Alloys  v3.0
TCMG2   =  Mg-Alloys  v2.0
TCMG1   =  Mg-Alloys  v1.1
TCTI2   =  Ti-Alloys  v2.1
TCTI1   =  Ti-Alloys  v1.0
TCCU3   =  Cu-Alloys  v3.1
TCCU2   =  Cu-Alloys  v2.0
TCCU1   =  Cu-Alloys  v1.0
TCCC1   =  Cemented carbide  v1.0
TCHEA4  =  High Entropy Alloy  v4.0
TCHEA3  =  High Entropy Alloy  v3.1
TCHEA2  =  High Entropy Alloy  v2.1.1
TCHEA1  =  High Entropy Alloy  v1.0
SSOL7   =  SGTE Alloy Solutions Database v7.0
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
TCOX10  =  Metal Oxide Solutions  v10.0 SNAPSHOT
TCOX9   =  Metal Oxide Solutions  v9.0
TCOX8   =  Metal Oxide Solutions  v8.0
TCOX7   =  Metal Oxide Solutions  v7.0
TCOX6   =  Metal Oxide Solutions  v6.0
TCOX5   =  Metal Oxide Solutions  v5.1
TCOX4   =  Metal Oxide Solutions  v4.1
ION3    =  Ionic Solutions  v3.0
ION2    =  Ionic Solutions  v2.6
ION1    =  Ionic Solutions  v1.5
NOX2    =  NPL Oxide Solutions Database v2.1
TCNOBL2 =  Noble Metals Alloys v2.0 SNAPSHOT
TCNOBL1 =  Noble Metals Alloys v1.0
TCSLD3  =  Solder Alloys  v3.2
TCSLD2  =  Solder Alloys  v2.0
TCSLD1  =  Solder Alloys  v1.1
TCSI1   =  Ultrapure Silicon  v1.2
TCMP2   =  Materials Processing  v2.5
TCES1   =  Combustion/Sintering  v1.1
TCSC1   =  Super Conductor  v1.0
TCFC1   =  SOFC Database v1.0
TCNF2   =  Nuclear Fuels  v2.1b
NUMT2   =  Nuclear Materials  v2.1
NUOX4   =  Nuclear Oxides  v4.2
NUCL15  =  IRSN NUCLEA-15_4
NUCL10  =  ThermoData NUCLEA Alloys-oxides TDB v10.2
MEPH15  =  IRSN Mephista-15_1
MEPH11  =  ThermoData MEPHISTA Nuclear Fuels TDB v11.2
TCAQ3   =  Aqueous Solution  v3.0
TCAQ2   =  Aqueous Solution  v2.7
AQS2    =  TGG Aqueous Solution Database v2.6
GCE2    =  TGG Geochemical/Environmental TDB v2.3
FEDEMO  =  Iron Demo Database v2.1
ALDEMO  =  Aluminum Demo Database v3.0
NIDEMO  =  Nickel Demo Database v1.1
CUDEMO  =  Copper Demo Database v1.0
SLDEMO  =  Solder Demo Database v1.0
OXDEMO  =  Oxide Demo Database v1.0
SUBDEMO =  Substance Demo Database v1.0
PTERN   =  Public Ternary Alloys TDB v1.3
PAQ2    =  Public Aqueous Soln (SIT) TDB v2.4
PG35    =  G35 Binary Semi-Conductors TDB v1.2
PURE5   =  SGTE Unary (Pure Elements) TDB v5.1
MOB2    =  Alloys Mobility  v2.7
MOB1    =  Alloys Mobility  v1.3
MOBFE1  =  Steels/Fe-Alloys Mobility  v1.1
MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
MOBFE5  =  Steels/Fe-Alloys Mobility  v5.0
MOBNI5  =  Ni-Alloys Mobility  v5.1
MOBNI4  =  Ni-Alloys Mobility  v4.1
MOBNI3  =  Ni-Alloys Mobility  v3.2
MOBNI2  =  Ni-Alloys Mobility  v2.4
MOBNI1  =  Ni-Alloys Mobility  v1.10
MOBAL5  =  Al-Alloys Mobility  v5.0
MOBAL4  =  Al-Alloys Mobility  v4.0
MOBAL3  =  Al-Alloys Mobility  v3.0
MOBAL2  =  Al-Alloys Mobility  v2.0
MOBAL1  =  Al-Alloys Mobility  v1.0
MOBCU1  =  Cu-Alloys Mobility  v1.0
MOBCU2  =  Cu-Alloys Mobility  v2.0
MOBCU3  =  Cu-Alloys Mobility  v3.0
MOBHEA1 =  High Entropy Alloys Mobility  v1.0
MOBHEA2 =  High Entropy Alloys Mobility  v2.0
MOBMG1  =  Mg-Alloys Mobility  v1.0
MOBSI1  =  Si-Alloys Mobility  v1.0
MOBSLD1 =  Solder-Alloys Mobility  v1.1
MOBTI3  =  Ti-Alloys Mobility  v3.0
MOBTI2  =  Ti-Alloys Mobility  v2.0
MOBTI1  =  Ti-Alloys Mobility  v1.0
MALDEMO =  Al-Alloys Mobility demo database v2.0
MFEDEMO =  Fe-Alloys Mobility demo database v2.0
MNIDEMO =  Ni-Alloys Mobility demo database v1.0
```

```
 MCUDEMO =  Cu-Alloys Mobility demo database v1.0
 USER    =  User defined Database

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

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

 List of references for assessed data

  'This parameter has not been assessed'
  'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'
  'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
      -Ni'
  'B. Jonsson: Z. Metallkunde 85(1994)498-501; C and N diffusion in bcc Cr
      -Fe-Ni'
  'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
      in bcc Fe'
 -OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP
APP: @@
APP: go d-m
 NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 1050; * N
DIC>
DIC> @@
DIC> @@ START BY ENTERING THE REGION austenite WHERE WE PUT THE fcc PHASE
DIC> @@
DIC> enter-region
REGION NAME : austenite
DIC>
DIC> @@
DIC> @@ ENTER THE GRID INTO THE REGION
DIC> @@
DIC> enter-grid
REGION NAME : /AUSTENITE/: austenite
WIDTH OF REGION /1/: 20e-4
TYPE /LINEAR/: AUTO
DIC>
DIC> @@
DIC> @@ ENTER THE active PHASES INTO THE REGIONS
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /AUSTENITE/: austenite
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC> @@
DIC> @@ ENTER THE inactive PHASES INTO THE REGIONS
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inactive
ATTACH TO REGION NAMED /AUSTENITE/: austenite
ATTACHED TO THE RIGHT OF AUSTENITE /YES/: no
PHASE NAME: /NONE/: bcc
 REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-5
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITION FOR FCC
DIC> @@
DIC> enter-composition
REGION NAME : /AUSTENITE/: austenite
PHASE NAME: /FCC_A1/: fcc#1
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: C
TYPE /LINEAR/: lin
VALUE OF FIRST POINT : 0.15
VALUE OF LAST POINT : /0.15/: 0.15
DIC>
DIC> @@
DIC> @@ THE BOUNDARY CONDITION IS A CLOSED SYSTEM AS WE DO NOT SPECIFY
DIC> @@ ANYTHING ELSE
DIC> @@
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 1e9
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /100000000/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ IMPLICIT (1) TIME INTEGRATION IS USED INSTEAD OF THE MORE ACCURATE
DIC> @@ (BUT LESS STABLE) TRAPETZOIDAL METHOD WHICH IS THE DEFAULT.
DIC> @@
DIC> s-s-c
```

```
NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /AUTO/:
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -> 1): /AUTO/: 1.0
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/:
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exb1b Y

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

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

**exb1b-run**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exb1b\run.DCM.test"
DIC>
DIC>
DIC> @@ exb1b_run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING EXAMPLE b1b
DIC> @@
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  0.00000E+00
DIC> read exb1b
 OK
DIC>
DIC> @@
DIC> @@ START THE SIMULATION
DIC> @@
DIC> sim
 Region: AUSTENITE
 single geometric dense at   0.0000
  1.2284      102
 U-FRACTION IN SYSTEM:  C = .00698495916383108  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
 U-FRACTION IN SYSTEM:  C = .00698495916383108  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
 INFO: PHASE BCC_A2 IS SCHEDULED TO APPEAR
   REGION STATUS CHANGE, ITERATING: TIME=  0.50000000E-07
   REGION STATUS CHANGE, ITERATING: TIME=  0.25000000E-07
 TIME =  0.25000000E-07 DT =  0.25000000E-07
 U-FRACTION IN SYSTEM:  C = .00698495916383108  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
 MUST SAVE WORKSPACE ON FILE
 WORKSPACE SAVED ON FILE
 RECLAIMING WORKSPACE

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

  Trying old scheme                    3
 U-FRACTION IN SYSTEM:  C = .00698156310125388  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
 U-FRACTION IN SYSTEM:  C = .00698156310125388  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  1  GRIDPOINT(S) ADDED   TO   CELL #1   REGION: R_BCC_A2
 2.641796457615056E-003        2.641820164613401E-003        0.237813210027546        2.896595830854927E-003        2.863309993054893E-
003        2.465854445577573E-003        3.038053080121225E-003        2.558808984270720E-003        2.415833955535861E-
003        2.363564686115593E-003        3.038053080121225E-003        2.415833955535861E-003        2.496303890482957E-
003        2.376837928709497E-003        2.369135059341974E-003        2.366895698823924E-003        2.361896017028972E-
003        2.360225243301796E-003        2.369135059341974E-003        2.361896017028972E-003        2.359389068072184E-
003        2.358662180339569E-003        2.369135059341974E-003        2.359389068072184E-003        2.361278860714089E-
003        2.358761592036592E-003        2.358656983976153E-003        2.358709289015734E-003        2.358624346087840E-
003        2.358591707433402E-003        2.358824346542741E-003        2.358624346087840E-003        2.358620293471447E-
003        2.358624346087840E-003        2.358620293471447E-003        2.358624346087840E-003


     ERROR RETURN FROM NS01A BECAUSE    5 CALLS OF CALFUN FAILED TO IMPROVE THE RESIDUALS
 *** ERROR  1890 IN DCNS01: ERROR RETURN FROM NS01A
 2.641796457615056E-003        2.641796461150068E-003        2.641796457615056E-003        0.237508579819959        2.641796457615056E-
003        2.896591057258121E-003        2.641796461150068E-003        2.641796457615056E-
003        0.237508579819959        2.641796457615056E-003        2.896591057258121E-003        2.641796457615056E-
003        3.038163915825988E-003        2.641796457615056E-003        2.775733791491543E-003        2.641796457615056E-
003        2.558805763213206E-003        2.558805763213206E-003        2.363552975740587E-003        2.363552975740587E-
003        5.738025859324140E-003        2.363552975740587E-003        2.558805763213206E-003        2.363552975817769E-
003        2.363552975740587E-003

output ignored...



... output resumed

 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.62828906E-16 AND   0.62828906E-16
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13796467E-02
 U-FRACTION IN SYSTEM:  C = .00698392110790924  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  5  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_BCC_A2

  CPU time used in timestep                    0 seconds
 2.334103381700427E-006        2.334487099558977E-006        4.999449696713977E-
029       TIME =  0.60500275E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.49994497E-28
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.13337965E-16 AND  -0.13337965E-16
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13796454E-02
 U-FRACTION IN SYSTEM:  C = .00698393470913857  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUSTENITE

  CPU time used in timestep                    0 seconds
 4.150258752341024E-005        4.150602239630179E-005        1.600696493093292E-
018       TIME =  0.70500275E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.16006965E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.18516576E-16 AND   0.18516576E-16
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13796473E-02
 U-FRACTION IN SYSTEM:  C = .00698391582708524  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_BCC_A2

  CPU time used in timestep                    0 seconds
 2.685801124862139E-005        2.686184732485364E-005        3.633434088767752E-
017       TIME =  0.80500275E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.36334341E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.72645873E-17 AND  -0.72645873E-17
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13796465E-02
```

```
 U-FRACTION IN SYSTEM:  C = .00698392323505816  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUSTENITE

  CPU time used in timestep                    1 seconds
 6.865812362918548E-005        6.866052985034949E-005        1.475550048511266E-
017       TIME =  0.90500275E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.14755500E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.33508870E-16 AND   0.33508870E-16
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13796499E-02
 U-FRACTION IN SYSTEM:  C = .006983889064794  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
 1.236458183132819E-005        1.236929231472599E-005        2.095296479852855E-
025       TIME =  0.10000000E+10 DT =   94997254.     SUM OF SQUARES =  0.20952965E-24
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.15597347E-16 AND   0.15597347E-16
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13796514E-02
 U-FRACTION IN SYSTEM:  C = .00698387395528536  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   0.60937151E-05
 DELETING TIME-RECORD FOR TIME   0.18031145E-04
 DELETING TIME-RECORD FOR TIME   0.41906006E-04
 DELETING TIME-RECORD FOR TIME   0.89655726E-04
 DELETING TIME-RECORD FOR TIME   0.18515517E-03
 DELETING TIME-RECORD FOR TIME   0.37615405E-03
 DELETING TIME-RECORD FOR TIME   0.75815182E-03
 DELETING TIME-RECORD FOR TIME   0.15221473E-02
 DELETING TIME-RECORD FOR TIME   0.30501384E-02
 DELETING TIME-RECORD FOR TIME   0.61061205E-02
 DELETING TIME-RECORD FOR TIME   0.12218085E-01
 DELETING TIME-RECORD FOR TIME   0.24442013E-01
 DELETING TIME-RECORD FOR TIME   0.48889870E-01
 DELETING TIME-RECORD FOR TIME   0.97785584E-01
 DELETING TIME-RECORD FOR TIME   0.19557701
 DELETING TIME-RECORD FOR TIME   0.39115987
 DELETING TIME-RECORD FOR TIME   0.78232558
 DELETING TIME-RECORD FOR TIME    1.5646570
 DELETING TIME-RECORD FOR TIME    3.1293199
 DELETING TIME-RECORD FOR TIME    6.2586455
 DELETING TIME-RECORD FOR TIME    12.517297
 DELETING TIME-RECORD FOR TIME    25.034600
 DELETING TIME-RECORD FOR TIME    50.069205
 DELETING TIME-RECORD FOR TIME    100.13842
 DELETING TIME-RECORD FOR TIME    200.27684
 DELETING TIME-RECORD FOR TIME    400.55368
 DELETING TIME-RECORD FOR TIME    801.10737
 DELETING TIME-RECORD FOR TIME    1602.2148
 DELETING TIME-RECORD FOR TIME    3204.4295
 DELETING TIME-RECORD FOR TIME    6408.8590
 DELETING TIME-RECORD FOR TIME    12817.718
 DELETING TIME-RECORD FOR TIME    25635.436
 DELETING TIME-RECORD FOR TIME    51270.872
 DELETING TIME-RECORD FOR TIME    102541.74
 DELETING TIME-RECORD FOR TIME    205083.49
 DELETING TIME-RECORD FOR TIME    410166.98
 DELETING TIME-RECORD FOR TIME    820333.96
 DELETING TIME-RECORD FOR TIME    1640667.9
 DELETING TIME-RECORD FOR TIME    3281335.8
 DELETING TIME-RECORD FOR TIME    6562671.6
 DELETING TIME-RECORD FOR TIME    13125343.
 DELETING TIME-RECORD FOR TIME    26250687.
 DELETING TIME-RECORD FOR TIME    52501373.
 DELETING TIME-RECORD FOR TIME   0.10500275E+09
 DELETING TIME-RECORD FOR TIME   0.20500275E+09
 DELETING TIME-RECORD FOR TIME   0.30500275E+09
 DELETING TIME-RECORD FOR TIME   0.40500275E+09
 DELETING TIME-RECORD FOR TIME   0.50500275E+09
 DELETING TIME-RECORD FOR TIME   0.60500275E+09
 DELETING TIME-RECORD FOR TIME   0.70500275E+09
 DELETING TIME-RECORD FOR TIME   0.80500275E+09

 KEEPING TIME-RECORD FOR TIME   0.90500275E+09
 AND FOR TIME                   0.10000000E+10
 WORKSPACE RECLAIMED

 TIMESTEP AT    0.100000000E+10 SELECTED

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

**exb1b-plot**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exb1b\plot.DCM.test"
DIC>
DIC>
DIC> @@ exb1b_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE b1b
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  1.00000E+09
DIC> read exb1b
 OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:
POST-1: @@
POST-1: @@ PLOT THE CARBON CONCENTRATIONS AT DIFFERENT TIMES
POST-1: @@
POST-1: s-d-a y w-p c
POST-1: s-d-a x dist glob
  INFO: Distance is set as independent variable
POST-1: s-p-c time 1e3,1e5,1e9
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ PLOT THE POSITION OF THE BCC/FCC INTERPHASE
POST-1: @@
POST-1: s-d-a x time
  INFO: Time is set as independent variable
POST-1: s-d-a y
VARIABLE : pos
INTERFACE : aus
UPPER OR LOWER INTERFACE OF REGION AUSTENITE#1 /LOWER/: lower
POST-1:
POST-1: set_axis_type
AXIS (X, Y OR Z) : x
AXIS TYPE /LINEAR/: log
POST-1:
POST-1: s-s-s
AXIS (X, Y OR Z) : x
AUTOMATIC SCALING  (Y OR N) /N/: n
MIN VALUE : 10
MAX VALUE : 1e9
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
ORKING ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

2019.11.11.14.54.39
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:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
ORKING ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

2019.11.11.14.54.40
LOWER INTERFACE OF REGION "AUSTENITE#1"
CELL #1

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

# Example exb1c

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

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

**exb1c-setup**

```
SYS:About

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

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 21012) 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: Mon Nov 11 11:13:13 2019


SYS:SYS:MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exb1c\setup.DCM.test"
SYS: @@
SYS: @@ Moving boundary problem.
SYS: @@ Austenite to ferrite transformation in a binary Fe-C alloy
SYS: @@ This is the same example as in exb1a and exb1b but now the
SYS: @@ simulation starts at a higher temperature and assumes a gradual cooling
SYS: @@ down to 1050 K.
SYS: @@
SYS: @@ When 1050 K is reached, the temperature is kept constant and thus has an
SYS: @@ isothermal transformation. As in exb1b ferrite is an inactive
SYS: @@ phase adjacent to the initial austenite.
SYS: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exb1c_setup.DCM
SYS:
SYS: @@
SYS: @@ START BY GOING TO THE DATABASE MODULE
SYS: @@
SYS: go da
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v10.0

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10:
TDB_TCFE10: @@
TDB_TCFE10: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA
TDB_TCFE10: @@
TDB_TCFE10: sw FEDEMO
 Current database: Iron Demo Database v2.1

 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
 CBCC_A12                CEMENTITE               CUB_A13
 DIAMOND_FCC_A4          FCC_A1                  GRAPHITE
 HCP_A3                  KSI_CARBIDE             LAVES_PHASE_C14
 M23C6                   M5C2                    M7C3
   REJECTED
TDB_FEDEMO: res ph fcc bcc
 FCC_A1                  BCC_A2  RESTORED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ RETRIEVE DATA FROM THE DATABASE FILE
TDB_FEDEMO: @@
TDB_FEDEMO: get
14:56:03,930 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'P. Franke, Estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
  'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
 -OK-
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ 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

 TCFE10  =  Steels/Fe-Alloys  v10.0
 TCFE9   =  Steels/Fe-Alloys  v9.1
 TCFE8   =  Steels/Fe-Alloys  v8.1
 TCFE7   =  Steels/Fe-Alloys  v7.0
 TCFE6   =  Steels/Fe-Alloys  v6.2
 TCFE5   =  Steels/Fe-Alloys  v5.0
 TCFE4   =  Steels/Fe-Alloys  v4.1
 TCFE3   =  Steels/Fe-Alloys  v3.1
 TCFE2   =  Steels/Fe-Alloys  v2.1
 TCFE1   =  Steels/Fe-Alloys  v1.0
 FROST1  =  FROST database v1.2
 FEDAT   =  TCS/TT Steels Database v1.0
 TCNI10  =  Ni-Alloys  v10.0 SNAPSHOT
```

```
TCNI9   =  Ni-Alloys  v9.1
TCNI8   =  Ni-Alloys  v8.2
TCNI7   =  Ni-Alloys  v7.2
TCNI6   =  Ni-Alloys  v6.1
TCNI5   =  Ni-Alloys  v5.1
TCNI4   =  Ni-Alloys  v4.0
TCNI1   =  Ni-Alloys  v1.3
TCAL6   =  Al-Alloys  v6.0
TCAL5   =  Al-Alloys  v5.1
TCAL4   =  Al-Alloys  v4.0
TCAL3   =  Al-Alloys  v3.0
TCAL2   =  Al-Alloys  v2.1
TCAL1   =  Al-Alloys  v1.2
TCMG5   =  Mg-Alloys  v5.1
TCMG4   =  Mg-Alloys  v4.0
TCMG3   =  Mg-Alloys  v3.0
TCMG2   =  Mg-Alloys  v2.0
TCMG1   =  Mg-Alloys  v1.1
TCTI2   =  Ti-Alloys  v2.1
TCTI1   =  Ti-Alloys  v1.0
TCCU3   =  Cu-Alloys  v3.1
TCCU2   =  Cu-Alloys  v2.0
TCCU1   =  Cu-Alloys  v1.0
TCCC1   =  Cemented carbide  v1.0
TCHEA4  =  High Entropy Alloy  v4.0
TCHEA3  =  High Entropy Alloy  v3.1
TCHEA2  =  High Entropy Alloy  v2.1.1
TCHEA1  =  High Entropy Alloy  v1.0
SSOL7   =  SGTE Alloy Solutions Database v7.0
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
TCOX10  =  Metal Oxide Solutions  v10.0 SNAPSHOT
TCOX9   =  Metal Oxide Solutions  v9.0
TCOX8   =  Metal Oxide Solutions  v8.0
TCOX7   =  Metal Oxide Solutions  v7.0
TCOX6   =  Metal Oxide Solutions  v6.0
TCOX5   =  Metal Oxide Solutions  v5.1
TCOX4   =  Metal Oxide Solutions  v4.1
ION3    =  Ionic Solutions  v3.0
ION2    =  Ionic Solutions  v2.6
ION1    =  Ionic Solutions  v1.5
NOX2    =  NPL Oxide Solutions Database v2.1
TCNOBL2 =  Noble Metals Alloys v2.0 SNAPSHOT
TCNOBL1 =  Noble Metals Alloys v1.0
TCSLD3  =  Solder Alloys  v3.2
TCSLD2  =  Solder Alloys  v2.0
TCSLD1  =  Solder Alloys  v1.1
TCSI1   =  Ultrapure Silicon  v1.2
TCMP2   =  Materials Processing  v2.5
TCES1   =  Combustion/Sintering  v1.1
TCSC1   =  Super Conductor  v1.0
TCFC1   =  SOFC Database v1.0
TCNF2   =  Nuclear Fuels  v2.1b
NUMT2   =  Nuclear Materials  v2.1
NUOX4   =  Nuclear Oxides  v4.2
NUCL15  =  IRSN NUCLEA-15_4
NUCL10  =  ThermoData NUCLEA Alloys-oxides TDB v10.2
MEPH15  =  IRSN Mephista-15_1
MEPH11  =  ThermoData MEPHISTA Nuclear Fuels TDB v11.2
TCAQ3   =  Aqueous Solution  v3.0
TCAQ2   =  Aqueous Solution  v2.7
AQS2    =  TGG Aqueous Solution Database v2.6
GCE2    =  TGG Geochemical/Environmental TDB v2.3
FEDEMO  =  Iron Demo Database v2.1
ALDEMO  =  Aluminum Demo Database v3.0
NIDEMO  =  Nickel Demo Database v1.1
CUDEMO  =  Copper Demo Database v1.0
SLDEMO  =  Solder Demo Database v1.0
OXDEMO  =  Oxide Demo Database v1.0
SUBDEMO =  Substance Demo Database v1.0
PTERN   =  Public Ternary Alloys TDB v1.3
PAQ2    =  Public Aqueous Soln (SIT) TDB v2.4
PG35    =  G35 Binary Semi-Conductors TDB v1.2
PURE5   =  SGTE Unary (Pure Elements) TDB v5.1
MOB2    =  Alloys Mobility  v2.7
MOB1    =  Alloys Mobility  v1.3
MOBFE1  =  Steels/Fe-Alloys Mobility  v1.1
MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
MOBFE5  =  Steels/Fe-Alloys Mobility  v5.0
MOBNI5  =  Ni-Alloys Mobility  v5.1
MOBNI4  =  Ni-Alloys Mobility  v4.1
MOBNI3  =  Ni-Alloys Mobility  v3.2
MOBNI2  =  Ni-Alloys Mobility  v2.4
MOBNI1  =  Ni-Alloys Mobility  v1.10
MOBAL5  =  Al-Alloys Mobility  v5.0
MOBAL4  =  Al-Alloys Mobility  v4.0
MOBAL3  =  Al-Alloys Mobility  v3.0
MOBAL2  =  Al-Alloys Mobility  v2.0
MOBAL1  =  Al-Alloys Mobility  v1.0
MOBCU1  =  Cu-Alloys Mobility  v1.0
MOBCU2  =  Cu-Alloys Mobility  v2.0
MOBCU3  =  Cu-Alloys Mobility  v3.0
MOBHEA1 =  High Entropy Alloys Mobility  v1.0
MOBHEA2 =  High Entropy Alloys Mobility  v2.0
MOBMG1  =  Mg-Alloys Mobility  v1.0
MOBSI1  =  Si-Alloys Mobility  v1.0
MOBSLD1 =  Solder-Alloys Mobility  v1.1
MOBTI3  =  Ti-Alloys Mobility  v3.0
```

```
 MOBTI2  =  Ti-Alloys Mobility  v2.0
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v2.0
 MFEDEMO =  Fe-Alloys Mobility demo database v2.0
 MNIDEMO =  Ni-Alloys Mobility demo database v1.0
 MCUDEMO =  Cu-Alloys Mobility demo database v1.0
 USER    =  User defined Database

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

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

 List of references for assessed data

  'This parameter has not been assessed'
  'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'
  'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
      -Ni'
  'B. Jonsson: Z. Metallkunde 85(1994)498-501; C and N diffusion in bcc Cr
      -Fe-Ni'
  'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
      in bcc Fe'
 -OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP
APP: @@
APP: go d-m
 NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER GLOBAL CONDITION T
DIC> @@
DIC> @@ ASSUME THAT THE COOLING RATE IS 10K/MINUTE DOWN TO 1050K
DIC> @@
DIC> set-cond
GLOBAL OR BOUNDARY CONDITION /GLOBAL/: glob
VARIABLE : T
LOW TIME LIMIT /0/: 0
T(TIME,X)= 1173-time*0.1667;
HIGH TIME LIMIT /*/: 738
ANY MORE RANGES /N/: y
T(TIME,X)= 1050;
HIGH TIME LIMIT /*/: *
ANY MORE RANGES /N/: N
DIC>
DIC> @@
DIC> @@ START BY ENTERING THE REGION austenite WHERE WE PUT THE fcc PHASE
DIC> @@
DIC> enter-region
REGION NAME : austenite
DIC>
DIC> @@
DIC> @@ ENTER THE GRID INTO THE REGION
DIC> @@
DIC> enter-grid
REGION NAME : /AUSTENITE/: austenite
WIDTH OF REGION /1/: 20e-4
TYPE /LINEAR/: AUTO
DIC>
DIC> @@
DIC> @@ ENTER THE active PHASES INTO THE REGIONS
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /AUSTENITE/: austenite
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC> @@
DIC> @@ ENTER THE inactive PHASES INTO THE REGIONS
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inact
ATTACH TO REGION NAMED /AUSTENITE/: austenite
ATTACHED TO THE RIGHT OF AUSTENITE /YES/: no
PHASE NAME: /NONE/: bcc
 REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-5
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITION FOR FCC
DIC> @@
DIC> enter-composition
REGION NAME : /AUSTENITE/: austenite
PHASE NAME: /FCC_A1/: fcc#1
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: C
TYPE /LINEAR/: lin
VALUE OF FIRST POINT : 0.15
VALUE OF LAST POINT : /0.15/: 0.15
DIC>
DIC> @@
DIC> @@ THE BOUNDARY CONDITION IS A CLOSED SYSTEM AS WE DO NOT SPECIFY
DIC> @@ ANYTHING ELSE.
DIC> @@
DIC>
DIC> @@
```

```
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 738
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /73.8/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC> @@
DIC> @@ IMPLICIT (1) TIME INTEGRATION IS USED INSTEAD OF THE MORE ACCURATE
DIC> @@ (BUT LESS STABLE) TRAPETZOIDAL METHOD WHICH IS THE DEFAULT.
DIC> @@
DIC> s-s-c
NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /AUTO/:
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -> 1): /AUTO/: 1.0
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/:
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exb1c Y
DIC>
DIC> set-inter
 --OK---
DIC>
```

**exb1c-run**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exb1c\run.DCM.test"
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 = .00698495916383108  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
 U-FRACTION IN SYSTEM:  C = .00698495916383108  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
 TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698495916383108  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    1 seconds
 TIME =  0.24660033E-05 DT =  0.23660033E-05 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698495916383108  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.71980098E-05 DT =  0.47320065E-05 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698495916383108  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.16662023E-04 DT =  0.94640131E-05 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698495916383108  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.35590049E-04 DT =  0.18928026E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698495916383108  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.73446101E-04 DT =  0.37856052E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698495916383108  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.14915821E-03 DT =  0.75712105E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698495916383108  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.30058242E-03 DT =  0.15142421E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698495916383108  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.60343083E-03 DT =  0.30284842E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698495916383108  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.12091277E-02 DT =  0.60569684E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698495916383108  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.24205213E-02 DT =  0.12113937E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698495916383108  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.48433087E-02 DT =  0.24227873E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698495916383108  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.96888834E-02 DT =  0.48455747E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698495916383108  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.19380033E-01 DT =  0.96911494E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698495916383108  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.38762332E-01 DT =  0.19382299E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698495916383108  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.77526929E-01 DT =  0.38764598E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00698495916383109  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    1 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 = .00698495916383109  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 = .00698495916383109  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 = .0069849591638311  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 = .00698495916383107  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 = .00698495916383105  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 = .00698495916383098  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    0 seconds


output ignored...



... output resumed

 3.603227678061542E-005        3.604114340896829E-005        5.596528604264911E-
033       TIME =  0.43290458E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.55965286E-32
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.67782292E-16 AND   0.67782292E-16
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13794411E-02
 U-FRACTION IN SYSTEM:  C = .00698601770553276  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  5  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_BCC_A2

  CPU time used in timestep                    0 seconds
 1.346741670350485E-005        1.346841105784895E-005        1.360472343084249E-
018       TIME =  0.53290458E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.13604723E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.11351159E-15 AND  -0.11351159E-15
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13794298E-02
 U-FRACTION IN SYSTEM:  C = .00698613345760261  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUSTENITE

  CPU time used in timestep                    0 seconds
 1.337421555810630E-005        1.337587500157234E-005        1.528234819010838E-
027       TIME =  0.63290458E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.15282348E-26
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.68073223E-16 AND   0.68073223E-16
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13794366E-02
 U-FRACTION IN SYSTEM:  C = .00698606404075852  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  4  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_BCC_A2

  CPU time used in timestep                    0 seconds
 7.843152332779303E-006        7.843914423743844E-006        5.293114704408065E-
032       TIME =  0.73290458E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.52931147E-31
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.70606021E-16 AND  -0.70606021E-16
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13794295E-02
 U-FRACTION IN SYSTEM:  C = .00698613604039153  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    0 seconds
 4.483924980437298E-006        4.484522648424397E-006        1.136218712246799E-
021       TIME =  0.83290458E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.11362187E-20
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.34633176E-16 AND   0.34633176E-16
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13794330E-02
 U-FRACTION IN SYSTEM:  C = .00698610072363056  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
 2.726925031826145E-006        2.724639367223028E-006        2.225652791982499E-
030       TIME =  0.93290458E+09 DT =  0.10000000E+09 SUM OF SQUARES =  0.22256528E-29
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.42037398E-16 AND   0.42037398E-16
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13794372E-02
 U-FRACTION IN SYSTEM:  C = .00698605785650249  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
 3.315675851048835E-004        3.315981840536485E-004        3.966614047191010E-
028       TIME =  0.10000000E+10 DT =   67095423.     SUM OF SQUARES =  0.39666140E-27
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.48086084E-16 AND  -0.48086084E-16
 POSITION OF INTERFACE R_BCC_A2 / AUSTENITE IS   0.13794340E-02
 U-FRACTION IN SYSTEM:  C = .00698609075687852  FE = 1
 TOTAL SIZE OF SYSTEM:  .002 [m]
 MUST SAVE WORKSPACE ON FILE
 WORKSPACE SAVED ON FILE
 RECLAIMING WORKSPACE
 DELETING TIME-RECORD FOR TIME    738.00000
 DELETING TIME-RECORD FOR TIME    769.68675
 DELETING TIME-RECORD FOR TIME    833.06026
 DELETING TIME-RECORD FOR TIME    959.80726
 DELETING TIME-RECORD FOR TIME    1213.3013
 DELETING TIME-RECORD FOR TIME    1720.2893
 DELETING TIME-RECORD FOR TIME    2734.2654
 DELETING TIME-RECORD FOR TIME    4762.2175
 DELETING TIME-RECORD FOR TIME    8818.1217
 DELETING TIME-RECORD FOR TIME    16929.930
 DELETING TIME-RECORD FOR TIME    33153.547
 DELETING TIME-RECORD FOR TIME    65600.781
 DELETING TIME-RECORD FOR TIME    130495.25
 DELETING TIME-RECORD FOR TIME    260284.19
 DELETING TIME-RECORD FOR TIME    519862.06
 DELETING TIME-RECORD FOR TIME    1039017.8
 DELETING TIME-RECORD FOR TIME    2077329.3
 DELETING TIME-RECORD FOR TIME    4153952.3
 DELETING TIME-RECORD FOR TIME    8307198.2
 DELETING TIME-RECORD FOR TIME    16613690.
 DELETING TIME-RECORD FOR TIME    33226674.
 DELETING TIME-RECORD FOR TIME    66452642.
 DELETING TIME-RECORD FOR TIME   0.13290458E+09
 DELETING TIME-RECORD FOR TIME   0.23290458E+09
 DELETING TIME-RECORD FOR TIME   0.33290458E+09
 DELETING TIME-RECORD FOR TIME   0.43290458E+09
 DELETING TIME-RECORD FOR TIME   0.53290458E+09
 DELETING TIME-RECORD FOR TIME   0.63290458E+09
 DELETING TIME-RECORD FOR TIME   0.73290458E+09
```

```
 DELETING TIME-RECORD FOR TIME   0.83290458E+09

 KEEPING TIME-RECORD FOR TIME   0.93290458E+09
 AND FOR TIME                   0.10000000E+10
 WORKSPACE RECLAIMED

 TIMESTEP AT    0.100000000E+10 SELECTED

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

**exb1c-plot**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exb1c\plot.DCM.test"
DIC>
DIC>
DIC> @@ exb1c_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE b1c
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  1.00000E+09
DIC> read exb1c
 OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:
POST-1: @@
POST-1: @@ PLOT TEMPERATURE VS. TIME
POST-1: @@
POST-1: s-d-a y t
POST-1: s-d-a x time
  INFO: Time is set as independent variable
POST-1: s-p-c
CONDITION /TIME/: interface
INTERFACE : austenite
UPPER OR LOWER INTERFACE OF REGION AUSTENITE#1 /LOWER/: lower
POST-1: s-s-s x n 0 1000
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
ORKING ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

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

2019.11.11.14.58.33
LOWER INTERFACE OF REGION "AUSTENITE#1"
CELL #1

```
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: @@
POST-1: @@ PLOT THE POSITION OF THE BCC/FCC INTERPHASE
POST-1: @@
POST-1: s-d-a
AXIS (X, Y OR Z) : y
VARIABLE : position
INTERFACE : austenite
UPPER OR LOWER INTERFACE OF REGION AUSTENITE#1 /LOWER/: lower
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
ORKING ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

2019.11.11.14.58.34
LOWER INTERFACE OF REGION "AUSTENITE#1"
CELL #1

```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: @@
POST-1: @@ PLOT THE CARBON CONCENTRATION VS. DISTANCE
POST-1: @@
POST-1: s-d-a y w-p c
POST-1: s-d-a x dis glob
  INFO: Distance is set as independent variable
POST-1: s-p-c time 500,700,1200,2000
POST-1: set-axis-type x lin
POST-1: s-s-s x n 0 3e-4
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
ORKING ...OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

2019.11.11.14.58.35
Time = 500,700,1200,2000
CELL #1

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

# Example exb2

## Cementite dissolution in an Fe-Cr-C alloy

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

**exb2-setup**

```
SYS:About

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

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 21012) 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: Mon Nov 11 11:13:13 2019


SYS:SYS:MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exb2\setup.DCM.test"
SYS: ?@@
 NO SUCH COMMAND, USE HELP
SYS: @@ Moving boundary problem.
SYS: @@ Cementite dissolution in an Fe-Cr-C alloy
SYS: @@ This example calculates the dissolution of a spherical cementite
SYS: @@ particle in an austenite matrix.
SYS: @@ This case is from Z.-K. Liu, L. Höglund, B. Jönsson and J. Ågren:
SYS: @@ Metall. Trans.A, v.22A (1991), pp. 1745-1752.
SYS: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS: @@
SYS: @@ In order to achieve the correct average composition in the calculation
SYS: @@ it is necessary to take into account that the calculation is set up
SYS: @@ using the volume fraction of the phases. To calculate the initial
SYS: @@ state at the heat treatment temperature we first need to determine
SYS: @@ the state at the normalizing temperature. To calculate the volume
SYS: @@ fraction of the phases we need to enter a number of functions
SYS: @@ that calculate these quantities. NOTE: The volume fractions are
SYS: @@ determined by assuming that only the substitutional components
SYS: @@ contribute to the volume of a system, whereas the interstitial
SYS: @@ components do not.
SYS: @@
SYS: @@ The total radius of the system can be calculated from the relation:
SYS: @@
SYS: @@    3
SYS: @@   R       V
SYS: @@    cem     cem    f
SYS: @@   ----  = ---- = V
SYS: @@    3              cem
SYS: @@   R       V
SYS: @@    tot     tot
SYS: @@
SYS: @@
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASES
SYS: @@
SYS: go da
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v10.0

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10:
TDB_TCFE10: @@
TDB_TCFE10: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE THE DATA
TDB_TCFE10: @@
TDB_TCFE10: sw FEDEMO
 Current database: Iron Demo Database v2.1

 VA                      /-  DEFINED
TDB_FEDEMO: def-sys fe cr c
 FE                      CR                      C
   DEFINED
TDB_FEDEMO: rej ph * all
 GAS:G                   LIQUID:L                BCC_A2
 CBCC_A12                CEMENTITE               CHI_A12
 CUB_A13                 DIAMOND_FCC_A4          FCC_A1
 GRAPHITE                HCP_A3                  KSI_CARBIDE
 LAVES_PHASE_C14         M23C6                   M3C2
 M5C2                    M7C3                    SIGMA
   REJECTED
TDB_FEDEMO: res ph fcc bcc cem
 FCC_A1                  BCC_A2                  CEMENTITE
   RESTORED
TDB_FEDEMO: get
14:59:57,802 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 Creating a new composition set FCC_A1#2
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

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

```
  'J. Bratberg, Z. Metallkd., 96 (2005) 335-344; Fe-Cr-Mo-C'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, 2016; FCC Fe-Cr-C and C-Cr-Ni'
  'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
 -OK-
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE THE MOBILITY DATA
TDB_FEDEMO: @@
TDB_FEDEMO: app mobfe4
 Current database: Steels/Fe-Alloys Mobility  v4.0

 VA  DEFINED
 B2_BCC  REJECTED
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:

POLY: @@
POLY: @@ SET THE CONDITIONS AT THE NORMALIZING TEMPERATURE
POLY: @@
POLY: set-cond T=1008,P=101325,N=1
POLY: set-cond X(CR)=0.0206,X(C)=0.0391
POLY:
POLY:
POLY: @@
POLY: @@ ENTER FUNCTIONS TO DETERMINE THE VOLUME-FRACTIONS
POLY: @@
POLY:
POLY: @@ Radius of the cementite particle
POLY: ent-symb var rcem=0.5255e-6;
POLY:
POLY: @@ total number of moles of substitutional components
POLY: ent-symb func nstot=n(fe)+n(cr);
POLY:
POLY: @@ number of moles of substitutional components in cementite
POLY: ent-symb func nscem=n(cem,fe)+n(cem,cr);
POLY:
POLY: @@ volume fraction (U-fraction) of cementite
POLY: ent-symb func vfcem=nscem/nstot;
POLY:
POLY: @@ total radius of the system
POLY: ent-symb func rtot=rcem/vfcem**(1/3);
POLY:
POLY: @@ radius of the surrounding austenite matrix
POLY: ent-symb func rmat=rtot-rcem;
POLY:
POLY:
POLY: @@
POLY: @@ COMPUTE THE EQUILIBRIUM
POLY: @@
POLY: compute-eq
 Using global minimization procedure
Calculated          4113 grid points in             1 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     1  s
POLY:
POLY:
POLY: @@
POLY: @@ SHOW THE COMPUTED VALUES TO BE USED IN THE DICTRA CALCULATION
POLY: @@
POLY: show rmat
 RMAT=5.3924863E-7
POLY: show w(cem,cr),w(bcc,cr),w(bcc,c)
 W(CEMENTITE,CR)=0.12581645
 W(BCC_A2,CR)=4.4332285E-3
 W(BCC_A2,C)=1.510215E-4
POLY:
POLY: ent var wmatcr=w(bcc,cr);
POLY: ent var wmatc=w(bcc,c);
POLY: ent var wcemcr=w(cem,cr);
POLY:
POLY:
POLY: @@
POLY: @@ ENTER THE DICTRA MONITOR
POLY: @@
POLY: go d-m
 NO TIME STEP DEFINED
 *** ENTERING BCC_A2 AS A DIFFUSION NONE PHASE
DIC>
DIC> @@
```

```
DIC> @@ ENTER GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob t 0 1183; * n
DIC>
DIC> @@
DIC> @@ ENTER THE REGIONS carb AND aus
DIC> @@
DIC> enter-region
REGION NAME : carb
DIC>
DIC> enter-region
REGION NAME : aus
ATTACH TO REGION NAMED /CARB/:
ATTACHED TO THE RIGHT OF CARB /YES/:
DIC> @@
DIC> @@ ENTER GEOMTRICAL GRIDS INTO THE REGIONS
DIC> @@
DIC>
DIC> @@
DIC> @@ THE INITIAL SIZE OF THE CEMENTITE PARTICLE IS ASSUMED TO BE KNOWN
DIC> @@ (IN THIS CASE THE VALUE IS TAKEN FROM LIU ET AL. WHO ESTIMATED THE
DIC> @@ AVERAGE INITIAL DIAMETER OF THE PARTICLES TO 1.051E-6 METERS).
DIC> @@
DIC> enter-grid
REGION NAME : /CARB/: carb
WIDTH OF REGION /1/: rcem
TYPE /LINEAR/: AUTO
DIC>
DIC> @@
DIC> @@ THE SIZE OF THE FCC REGION CAN BE CALCULATED FROM A MASS BALANCE
DIC> @@ AFTER ESTIMATING THE INITIAL COMPOSITIONS IN THE TWO PHASES
DIC> @@
DIC> enter-grid
REGION NAME : /AUS/: aus
WIDTH OF REGION /1/: rmat
TYPE /LINEAR/: AUTO
DIC>
DIC> @@
DIC> @@ ENTER PHASES INTO REGIONS
DIC> @@
DIC> enter-phase act carb  matrix   cementite
DIC> enter-phase act aus   matrix   fcc#1
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITIONS IN THE PHASES
DIC> @@
DIC> enter-composition
REGION NAME : /CARB/: carb
PHASE NAME: /CEMENTITE/: cementite
COMPOSITION TYPE /MOLE_FRACTION/: weig-fraction
PROFILE FOR /CR/: cr lin wcemcr wcemcr
DIC>
DIC> enter-composition
REGION NAME : /AUS/: aus
PHASE NAME: /FCC_A1#1/: fcc#1
DEPENDENT COMPONENT ? /FE/: fe
COMPOSITION TYPE /MOLE_FRACTION/: weig-fraction
PROFILE FOR /C/: CR lin wmatcr wmatcr
PROFILE FOR /CR/: C  lin wmatc wmatc
DIC>
DIC> @@
DIC> @@ SET TO A SPHERICAL GEOMETRY
DIC> @@
DIC> enter-geo
GEOMETRICAL EXPONENT /0/: 2
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME AND OTHER SIMULATION PARAMETERS
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 10000
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /1000/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exb2 Y
DIC>
DIC> set-inter
 --OK---
DIC>
```

**exb2-run**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exb2\run.DCM.test"
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
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
  Trying old scheme                      4
 GENERATING STARTING VALUES FOR CELL #  1 INTERFACE #  2
 DETERMINING INITIAL EQUILIBRIUM VALUES
CALCULATING STARTING VALUES:       9   EQUILIBRIUM CALCULATIONS               DONE     6 OUT OF     9
04
 U-FRACTION IN SYSTEM:  C = .0406910188418179  CR = .0214382349908298
                        FE = .978561765139677
 TOTAL SIZE OF SYSTEM:  5.0562655986E-18 [m^3]
 U-FRACTION IN SYSTEM:  C = .0406910188418179  CR = .0214382349908298
                        FE = .978561765139677
 TOTAL SIZE OF SYSTEM:  5.0562655986E-18 [m^3]
 0.175650510569693        0.175691773365776        0.175650565704887        2.957532598262705E-003        7.754437973954904E-
005        5.789560069630489E-006        8.570927935873340E-007        3.747773447018736E-007        3.453239600660704E-
007        1.349945520946721E-007        1.350781378780822E-007        1.346761780051463E-007        1.361219741582676E-
007        1.343486158194617E-007        1.340757896503063E-007        1.335307279090488E-007        1.344901657992158E-
007        1.324431149504957E-007        1.302779707747475E-007        1.259882989075563E-007        1.269270676223991E-
007        1.175749112099342E-007        1.014430318537531E-007        7.217953336273408E-008        7.299680974519162E-
008        2.728135257885179E-008        7.241610548617600E-011        4.089073963496126E-014        7.514683382235863E-
019       TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =  0.75146834E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.39436721E-02 AND  -0.39436721E-02
 POSITION OF INTERFACE CARB / AUS IS   0.52510563E-06
 U-FRACTION IN SYSTEM:  C = .040729015482772  CR = .0214383281162587
                        FE = .978561672014248
 TOTAL SIZE OF SYSTEM:  5.0562655986E-18 [m^3]
  15  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: CARB

  CPU time used in timestep                    1 seconds
 2.248325209321603E-005        2.248775172894691E-005        2.248323619912327E-005        1.887682070920329E-009        1.633889154953991E-
009        1.019554313744803E-009        6.882194693841950E-010        6.885274143371537E-010        2.216753869789131E-
010        6.151368346632002E-014        2.128398194024441E-017       TIME =  0.30000000E-06 DT =  0.20000000E-
06 SUM OF SQUARES =  0.21283982E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.22443437E-04 AND  -0.22443437E-04
 POSITION OF INTERFACE CARB / AUS IS   0.52510114E-06
 U-FRACTION IN SYSTEM:  C = .04072976539935  CR = .0214383291134799
                        FE = .978561671017027
 TOTAL SIZE OF SYSTEM:  5.0562655986E-18 [m^3]
  CPU time used in timestep                    1 seconds
 6.026886170825013E-004        6.026583061555723E-004        6.026723276184566E-004        8.498836109403279E-005        3.515899392378279E-
005        2.728068988264678E-007        4.049299892501169E-010        6.350509499750248E-015        2.881397662001674E-
018       TIME =  0.70000000E-06 DT =  0.40000000E-06 SUM OF SQUARES =  0.28813977E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.46375286E-05 AND  -0.46375286E-05
 POSITION OF INTERFACE CARB / AUS IS   0.52509929E-06
 U-FRACTION IN SYSTEM:  C = .0407315536943019  CR = .0214383294273154
                        FE = .978561670703191
 TOTAL SIZE OF SYSTEM:  5.0562655986E-18 [m^3]
  CPU time used in timestep                    0 seconds
 2.365053655012762E-004        2.365034011209155E-004        2.364987464533052E-004        7.190707366893964E-005        1.444187969352898E-
007        4.667902972828912E-011        2.104088520712535E-014        2.043530358251172E-017       TIME =  0.15000000E-05 DT =  0.80000000E-
06 SUM OF SQUARES =  0.20435304E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.40628788E-05 AND  -0.40628788E-05
 POSITION OF INTERFACE CARB / AUS IS   0.52509604E-06
 U-FRACTION IN SYSTEM:  C = .0407314707249635  CR = .0214383297893152
                        FE = .978561670341192
 TOTAL SIZE OF SYSTEM:  5.0562655986E-18 [m^3]


output ignored...



... output resumed

 2.580869394261902E-009        5.015415040680126E-014        1.091155062739396E-
018       TIME =   8322.3726     DT =   1000.0000     SUM OF SQUARES =  0.10911551E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.10698859E-10 AND  -0.10698859E-10
 POSITION OF INTERFACE CARB / AUS IS   0.24609437E-06
 U-FRACTION IN SYSTEM:  C = .0407634558563499  CR = .0214383888189068
                        FE = .9785616113116
 TOTAL SIZE OF SYSTEM:  5.0562655986E-18 [m^3]
  CPU time used in timestep                    1 seconds
 7.781486142655097E-009        7.835745516537438E-009        7.798361379053343E-009        2.589058562767993E-009        8.888444995778480E-
010        5.326033085355878E-015        4.852987386598771E-
018       TIME =   9322.3726     DT =   1000.0000     SUM OF SQUARES =  0.48529874E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.10110968E-10 AND  -0.10110968E-10
 POSITION OF INTERFACE CARB / AUS IS   0.23598340E-06
 U-FRACTION IN SYSTEM:  C = .0407634735489172  CR = .0214383876988838
                        FE = .978561612431669
 TOTAL SIZE OF SYSTEM:  5.0562655986E-18 [m^3]
  CPU time used in timestep                    2 seconds
 9.389970214480779E-007        9.385364140151186E-007        9.381662915696209E-007        7.531848103874387E-008        1.299658492831811E-
012        1.611056716035278E-018       TIME =   10000.000     DT =   677.62736     SUM OF SQUARES =  0.16110567E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.95523071E-11 AND  -0.95523071E-11
 POSITION OF INTERFACE CARB / AUS IS   0.22951050E-06
 U-FRACTION IN SYSTEM:  C = .04076347223984  CR = .0214383869711002
                        FE = .978561613159406
 TOTAL SIZE OF SYSTEM:  5.0562655986E-18 [m^3]
 MUST SAVE WORKSPACE ON FILE
 WORKSPACE SAVED ON FILE
```

```
 RECLAIMING WORKSPACE
 DELETING TIME-RECORD FOR TIME    0.0000000
 DELETING TIME-RECORD FOR TIME   0.10000000E-06
 DELETING TIME-RECORD FOR TIME   0.30000000E-06
 DELETING TIME-RECORD FOR TIME   0.70000000E-06
 DELETING TIME-RECORD FOR TIME   0.15000000E-05
 DELETING TIME-RECORD FOR TIME   0.31000000E-05
 DELETING TIME-RECORD FOR TIME   0.63000000E-05
 DELETING TIME-RECORD FOR TIME   0.12700000E-04
 DELETING TIME-RECORD FOR TIME   0.25500000E-04
 DELETING TIME-RECORD FOR TIME   0.51100000E-04
 DELETING TIME-RECORD FOR TIME   0.99418841E-04
 DELETING TIME-RECORD FOR TIME   0.17900385E-03
 DELETING TIME-RECORD FOR TIME   0.30071417E-03
 DELETING TIME-RECORD FOR TIME   0.47831765E-03
 DELETING TIME-RECORD FOR TIME   0.72934329E-03
 DELETING TIME-RECORD FOR TIME   0.10758312E-02
 DELETING TIME-RECORD FOR TIME   0.15428938E-02
 DELETING TIME-RECORD FOR TIME   0.21467122E-02
 DELETING TIME-RECORD FOR TIME   0.29017145E-02
 DELETING TIME-RECORD FOR TIME   0.38194470E-02
 DELETING TIME-RECORD FOR TIME   0.49085220E-02
 DELETING TIME-RECORD FOR TIME   0.61737172E-02
 DELETING TIME-RECORD FOR TIME   0.76140704E-02
 DELETING TIME-RECORD FOR TIME   0.92225530E-02
 DELETING TIME-RECORD FOR TIME   0.10986205E-01
 DELETING TIME-RECORD FOR TIME   0.12887621E-01
 DELETING TIME-RECORD FOR TIME   0.14913721E-01
 DELETING TIME-RECORD FOR TIME   0.17051346E-01
 DELETING TIME-RECORD FOR TIME   0.19290988E-01
 DELETING TIME-RECORD FOR TIME   0.21633640E-01
 DELETING TIME-RECORD FOR TIME   0.24076629E-01
 DELETING TIME-RECORD FOR TIME   0.26619724E-01
 DELETING TIME-RECORD FOR TIME   0.29264997E-01
 DELETING TIME-RECORD FOR TIME   0.32010611E-01
 DELETING TIME-RECORD FOR TIME   0.34862598E-01
 DELETING TIME-RECORD FOR TIME   0.37829873E-01
 DELETING TIME-RECORD FOR TIME   0.40921693E-01
 DELETING TIME-RECORD FOR TIME   0.44136483E-01
 DELETING TIME-RECORD FOR TIME   0.47480849E-01
 DELETING TIME-RECORD FOR TIME   0.50961527E-01
 DELETING TIME-RECORD FOR TIME   0.54593384E-01
 DELETING TIME-RECORD FOR TIME   0.58383853E-01
 DELETING TIME-RECORD FOR TIME   0.62357656E-01
 DELETING TIME-RECORD FOR TIME   0.66521873E-01
 DELETING TIME-RECORD FOR TIME   0.68802708E-01
 DELETING TIME-RECORD FOR TIME   0.71497059E-01
 DELETING TIME-RECORD FOR TIME   0.74612522E-01
 DELETING TIME-RECORD FOR TIME   0.78159054E-01
 DELETING TIME-RECORD FOR TIME   0.82115298E-01
 DELETING TIME-RECORD FOR TIME   0.86491020E-01
 DELETING TIME-RECORD FOR TIME   0.91276780E-01
 DELETING TIME-RECORD FOR TIME   0.96473166E-01
 DELETING TIME-RECORD FOR TIME   0.10206052
 DELETING TIME-RECORD FOR TIME   0.10804860
 DELETING TIME-RECORD FOR TIME   0.11445063
 DELETING TIME-RECORD FOR TIME   0.12133071
 DELETING TIME-RECORD FOR TIME   0.12873462
 DELETING TIME-RECORD FOR TIME   0.13674928
 DELETING TIME-RECORD FOR TIME   0.14543690
 DELETING TIME-RECORD FOR TIME   0.15494720
 DELETING TIME-RECORD FOR TIME   0.16561157
 DELETING TIME-RECORD FOR TIME   0.17786478
 DELETING TIME-RECORD FOR TIME   0.19239402
 DELETING TIME-RECORD FOR TIME   0.21034788
 DELETING TIME-RECORD FOR TIME   0.23440524
 DELETING TIME-RECORD FOR TIME   0.27065630
 DELETING TIME-RECORD FOR TIME   0.33538860
 DELETING TIME-RECORD FOR TIME   0.41264653
 DELETING TIME-RECORD FOR TIME   0.50846372
 DELETING TIME-RECORD FOR TIME   0.63474294
 DELETING TIME-RECORD FOR TIME   0.81581355
 DELETING TIME-RECORD FOR TIME   0.91499001
 DELETING TIME-RECORD FOR TIME    1.0985361
 DELETING TIME-RECORD FOR TIME    1.4398813
 DELETING TIME-RECORD FOR TIME    1.6508783
 DELETING TIME-RECORD FOR TIME    2.0594177
 DELETING TIME-RECORD FOR TIME    2.8475130
 DELETING TIME-RECORD FOR TIME    4.3514103
 DELETING TIME-RECORD FOR TIME    7.2050126
 DELETING TIME-RECORD FOR TIME    12.704359
 DELETING TIME-RECORD FOR TIME    23.586131
 DELETING TIME-RECORD FOR TIME    45.349675
 DELETING TIME-RECORD FOR TIME    88.876763
 DELETING TIME-RECORD FOR TIME    175.93094
 DELETING TIME-RECORD FOR TIME    350.03929
 DELETING TIME-RECORD FOR TIME    698.25599
 DELETING TIME-RECORD FOR TIME    1394.6894
 DELETING TIME-RECORD FOR TIME    2322.3726
 DELETING TIME-RECORD FOR TIME    3322.3726
 DELETING TIME-RECORD FOR TIME    4322.3726
 DELETING TIME-RECORD FOR TIME    5322.3726
 DELETING TIME-RECORD FOR TIME    6322.3726
 DELETING TIME-RECORD FOR TIME    7322.3726
 DELETING TIME-RECORD FOR TIME    8322.3726

 KEEPING TIME-RECORD FOR TIME    9322.3726
 AND FOR TIME                    10000.000
 WORKSPACE RECLAIMED

 TIMESTEP AT     10000.0000     SELECTED

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

**exb2-plot**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exb2\plot.DCM.test"
DIC>
DIC>
DIC> @@ exb2_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE b2
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  1.00000E+04
 *** ENTERING BCC_A2 AS A DIFFUSION NONE PHASE
DIC> read exb2
 OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1: @@
POST-1: @@ LET US PLOT CHROMIUM CONCENTRATION PROFILES
POST-1: @@ WE THEN SET THE DISTANCE AS X-AXIS (NOTE THAT DISTANCE IS AUTOMATICALLY
POST-1: @@ SET AS THE INDEPENDENT VARIABLE) AND U-FRACTION CARBON AS Y-AXIS
POST-1: @@ REMEMBER THAT THE PLOT CONDITION ALSO MUST BE SET.
POST-1: @@
POST-1: @@ NOTICE THAT ALL DISTANCES IN THE DATA FILE ARE GIVEN RELATIVE TO THE
POST-1: @@ CEM/FCC INTERFACE. FOR THIS REASON AN OFFSET MUST BE GIVEN TO THE
POST-1: @@ DATA ACCORDING TO THE ACTUAL PARTICLE RADIUS AT THE SPECIFIED TIME.
POST-1: @@
POST-1: enter-symb
Function or table /FUNCTION/: func
NAME: rdist
FUNCTION: gd-poi(carb,u);
POST-1:
POST-1: s-d-a x rdist
POST-1:
POST-1: s-i-v
VARIABLE /TIME/: dist
DISTANCE : /GLOBAL/: glo
POST-1:
POST-1: s-d-a y uf(cr)
POST-1:
POST-1: s-p-c time 10
POST-1:
POST-1: @@
POST-1: @@ SET THE TITLE ON THE PLOT
POST-1: @@
POST-1: set-title Figure b2.1
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

Figure b2.1

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

```
DATASET NUMBER(s): /-1/: -1
 DATASET 1 CONCENTRATION PROFILE T=10S
 DATASET 2 CONCENTRATION PROFILE T=100S
 DATASET 3 CONCENTRATION PROFILE T=1000S
 DATASET 4 CONCENTRATION PROFILE T=10000S
 DATASET 5 VOLUME FRACTION CEMENTITE VS. TIME
 DATASET 6 MEAN PARTICLE DIAMETER VS. TIME
POST-1:
POST-1: @@
POST-1: @@ SELECT THE PROPER DATASET
POST-1: @@
POST-1: app y exb2.exp
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 1
POST-1:
POST-1: set-title Figure b2.2
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

Figure b2.2

```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: @@
POST-1: @@ PLOT ALSO FOR 100, 1000 AND 10000 seconds
POST-1: @@
POST-1:
POST-1: s-p-c time 100
POST-1:
POST-1: app y exb2.exp
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 2
POST-1:
POST-1: set-title Figure b2.3
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

Figure b2.3

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

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

Figure b2.4

```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: s-p-c time 10000
POST-1:
POST-1: app y exb2.exp
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 4
POST-1:
POST-1: set-title Figure b2.5
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

Figure b2.5

```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: @@
POST-1: @@ ALSO PLOT HOW THE VOLUME FRACTION OF CEMENTITE VARIES
POST-1: @@ WITH TIME
POST-1: @@
```

```
POST-1: s-d-a y ivv(cem)
POST-1: s-s-s y n 0 .15
POST-1:
POST-1: s-d-a x time
  INFO: Time is set as independent variable
POST-1: set-axis-type x log
POST-1: s-s-s x n .01 10000
POST-1:
POST-1: s-p-c integral
POST-1:
POST-1: app y exb2.exp
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 5
POST-1:
POST-1: set-title Figure b2.6
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

**Figure b2.6**

```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: @@
POST-1: @@ ALSO PLOT HOW THE DIAMETER OF CEMENTITE VARIES WITH TIME
POST-1: @@
POST-1: enter func diam=2*poi(carb,u);
POST-1: s-d-a y diam
POST-1:
POST-1: s-p-c interface carb upper
POST-1:
POST-1: app y exb2.exp
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 6
POST-1:
POST-1: set-title Figure b2.7
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

**Figure b2.7**

```
POST-1:
```

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

# Example exb3

## Dissolution of 23-carbide in an austenitic matrix

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

**exb3-setup**

```
SYS:About

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

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 21012) 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: Mon Nov 11 11:13:13 2019


SYS:SYS:MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exb3\setup.DCM.test"
SYS:
SYS: @@ Moving boundary example.
SYS: @@ Dissolution of 23-carbide in an austenitic matrix
SYS: @@ This example calculates the dissolution of an M23C6 particle in an
SYS: @@ austenite matrix. A film of ferrite is allowed to nucleate around the
SYS: @@ carbide during the precipitation.
SYS: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASES
SYS: @@
SYS: go da
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v10.0

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10:
TDB_TCFE10: @@
TDB_TCFE10: @@ USE A DATABASE FOR THERMODYNAMIC DATA
TDB_TCFE10: @@
TDB_TCFE10: sw fedemo
 Current database: Iron Demo Database v2.1

 VA                      /-  DEFINED
TDB_FEDEMO: def-sys fe c cr
 FE                      C                       CR
   DEFINED
TDB_FEDEMO: rej ph *
 GAS:G                   LIQUID:L                BCC_A2
 CBCC_A12                CEMENTITE               CHI_A12
 CUB_A13                 DIAMOND_FCC_A4          FCC_A1
 GRAPHITE                HCP_A3                  KSI_CARBIDE
 LAVES_PHASE_C14         M23C6                   M3C2
 M5C2                    M7C3                    SIGMA
   REJECTED
TDB_FEDEMO: res ph fcc bcc m23
 FCC_A1                  BCC_A2                  M23C6
   RESTORED
TDB_FEDEMO: get
15:09:01,395 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 Creating a new composition set FCC_A1#2
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'J-O. Andersson, CALPHAD, 11 (1987) 271-276; TRITA 0314; C-CR'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'P. Franke, Estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
  'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'A.V. Khvan, B. Hallstedt, C. Broeckmann, CALPHAD, 46, 24 -33(2014); Cr-Fe
      -C'
  'J-O. Andersson, Metall. Trans. A, 19A (1988) 627-636 TRITA 0207 (1986); C
      -CR-FE'
  'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270
      (1986); CR-FE'
  'J. Bratberg, Z. Metallkd., 96 (2005) 335-344; Fe-Cr-Mo-C'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, 2016; FCC Fe-Cr-C and C-Cr-Ni'
  'B.-J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
  'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
  'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, CALPHAD,
      submitted, 2011; Fe-Mn-C'
 -OK-
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ 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 .......
 Creating a new composition set FCC_A1#3
 PARAMETERS ...
 FUNCTIONS ....
```

```
 List of references for assessed data

  'This parameter has not been assessed'
  'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'
  'B. Jonsson: Z. Metallkunde 85(1994)502-509; C diffusion in fcc Cr-Fe-Ni'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Fe diffusion fcc Cr-Fe'
  'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
      -Ni'
  'B. Jonsson: Z. Metallkunde 85(1994)498-501; C and N diffusion in bcc Cr
      -Fe-Ni'
  'B. Jonsson: ISIJ International, 35(1995)1415-1421; Cr, Fe and Ni
      diffusion bcc Cr-Fe-Ni'
  'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
      in bcc Fe'
 -OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR
APP: @@
APP: go d-m
 NO TIME STEP DEFINED
 *** ENTERING M23C6 AS A DIFFUSION NONE PHASE
DIC>
DIC>
DIC> @@ THE MOBILITY DATABASE LACKS KINETIC DATA FOR THE M23-CARBIDE
DIC> @@ SO AN ESTIMATE FOR THE MOBILITIES IN THIS PHASE ARE ENTERED.
DIC> ent-mob-est M23 c
M[M23,C](T)= 0;
DIC>
DIC> ent-mob-est M23 cr
M[M23,CR](T)= 3e-11*exp(-278000/8.3145/T);
DIC>
DIC> ent-mob-est M23 fe
M[M23,FE](T)= 1e-11*exp(-275000/8.3145/T);
DIC>
DIC> @@
DIC> @@ ENTER GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 1273;   * N
DIC>
DIC> @@
DIC> @@ ENTER THE REGIONS carbide AND matrix
DIC> @@
DIC> enter-region  carbide
DIC> enter-region  matrix
ATTACH TO REGION NAMED /CARBIDE/:
ATTACHED TO THE RIGHT OF CARBIDE /YES/:
DIC> @@
DIC> @@ ASSUME SOME REASONABLE SIZE OF THE CARBIDE PARTICLE
DIC> @@
DIC> enter-grid  carbide  5.00000000E-7 AUTO
DIC> @@
DIC> @@ THE SIZE OF THE FCC REGION WE CAN CALCULATE FROM A MASS BALANCE
DIC> @@ AFTER ESTIMATING THE INITIAL COMPOSITIONS IN THE TWO PHASES.
DIC> @@
DIC> enter-grid  matrix  5.55859755E-7 AUTO
DIC> @@
DIC> @@ ENTER PHASES INTO THE REGION MATRIX. BOUNDARY CONDITIONS ARE GIVEN
DIC> @@ IF THE INACTIVE PHASE bcc IS NUCLEATED
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /CARBIDE/: matrix
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inact
ATTACH TO REGION NAMED /MATRIX/: matrix
ATTACHED TO THE RIGHT OF MATRIX /YES/: no
PHASE NAME: /NONE/: bcc#1
DEPENDENT COMPONENT ? /FE/: fe
 REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/:
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> @@
DIC> @@ ENTER THE PHASE INTO THE REGION carbide
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /CARBIDE/: carbide
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: m23c6
DIC>
DIC> @@
DIC> @@ ENTER COMPOSITIONS INTO THE PHASES
DIC> @@
DIC> enter-composition
REGION NAME : /CARBIDE/: carbide
PHASE NAME: /M23C6/: m23c6
DEPENDENT COMPONENT ? /FE/: fe
COMPOSITION TYPE /MOLE_FRACTION/: mole-fraction
PROFILE FOR /CR/: cr lin 0.55079807 0.55079807
DIC>
DIC>
DIC> enter-composition
REGION NAME : /MATRIX/: matrix
PHASE NAME: /FCC_A1#1/: fcc#1
DEPENDENT COMPONENT ? /FE/: fe
COMPOSITION TYPE /MOLE_FRACTION/: mole-fraction
PROFILE FOR /C/: cr lin 8.5203899E-2 8.5203899E-2
PROFILE FOR /CR/: c lin 1.8072433E-4  1.8072433E-4
DIC>
DIC> @@
DIC> @@ SET TO A SPHERICAL GEOMETRY
DIC> @@
DIC> enter-geo
GEOMETRICAL EXPONENT /0/: 2
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME AND OTHER SIMULATION PARAMETERS
```

```
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 8000
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /800/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exb3 Y
DIC>
DIC>
DIC>
DIC> set-inter
 --OK---
DIC>
```

**exb3-run**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exb3\run.DCM.test"
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
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
  Trying old scheme                          4
 GENERATING STARTING VALUES FOR CELL #  1 INTERFACE #  2
 DETERMINING INITIAL EQUILIBRIUM VALUES
CALCULATING STARTING VALUES:       9   EQUILIBRIUM CALCULATIONS               DONE     6 OUT OF     9
 U-FRACTION IN SYSTEM:  C = .0278637912207471  CR = .149918318671311
                        FE = .850081681459196
 TOTAL SIZE OF SYSTEM:  4.93068569406E-18 [m^3]
 U-FRACTION IN SYSTEM:  C = .0278637912207471  CR = .149918318671311
                        FE = .850081681459196
 TOTAL SIZE OF SYSTEM:  4.93068569406E-18 [m^3]
 0.565663007975140        0.565797019192574        0.565663812089353        1.015925208844388E-002        3.012654895338404E-
004        4.777345255083737E-005        2.965739035927175E-006        7.215362066518790E-007        8.262638042925529E-
007        4.246506052337524E-008        4.119324775683631E-008        3.974271203568553E-008        4.355497133468889E-
008        3.870625294938786E-008        3.673410109131649E-008        3.294771044661376E-008        3.668595705502996E-
008        2.600355362298377E-008        1.460917535833680E-008        1.658190586881922E-009        4.335933783142457E-
012        1.279149061210870E-015        2.899183757917577E-017       TIME =  0.10000000E-06 DT =  0.10000000E-
06 SUM OF SQUARES =  0.28991838E-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 = .850081500378045
 TOTAL SIZE OF SYSTEM:  4.93068569406E-18 [m^3]
  16  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: CARBIDE

  CPU time used in timestep                    4 seconds
 1.096405342625200E-004        1.096626445881131E-004        1.096405350852025E-004        5.301312524141611E-008        2.238795451060536E-
008        6.726062442981646E-011        8.232621768236381E-014        3.182690117220420E-019       TIME =  0.30000000E-06 DT =  0.20000000E-
06 SUM OF SQUARES =  0.31826901E-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                    0 seconds
 1.217834959636711E-004        1.217822143858938E-004        1.217736602728491E-004        6.952194466350004E-007        2.897691706994565E-
009        5.944767570801350E-012        3.496665643790705E-016        2.031659036000881E-022       TIME =  0.70000000E-06 DT =  0.40000000E-
06 SUM OF SQUARES =  0.20316590E-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]


output ignored...



... output resumed

 7.842659452247582E-012        6.520881344490448E-017       TIME =   5409.7851     DT =   800.00000     SUM OF SQUARES =  0.65208813E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.72308869E-12 AND  -0.72308869E-12
 POSITION OF INTERFACE CARBIDE / MATRIX IS   0.39304432E-06
 U-FRACTION IN SYSTEM:  C = .02783499678338  CR = .149835754383248
                        FE = .850164245747259
 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
 7.262619945355082E-008        7.264687381257723E-008        7.255535488579354E-008        4.641230084750455E-008        3.661593273579005E-
008        1.942209635845363E-008        1.000538093885446E-009        1.803648993904889E-015        3.646685955428781E-
020       TIME =   6209.7851     DT =   800.00000     SUM OF SQUARES =  0.36466860E-19
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.28844466E-12 AND  -0.28844466E-12
 POSITION OF INTERFACE CARBIDE / MATRIX IS   0.39281357E-06
 U-FRACTION IN SYSTEM:  C = .0278349981532123  CR = .149835754877017
                        FE = .85016424525349
 TOTAL SIZE OF SYSTEM:  4.93068569406E-18 [m^3]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: MATRIX

  CPU time used in timestep                    1 seconds
 2.499408544210097E-008        2.499891510914368E-008        2.495149549230841E-008        1.653438796056412E-008        1.510498316357031E-
008        1.236875418274282E-008        7.651024711867039E-009        7.648821162555544E-009        1.612785941721711E-
009        3.398271330582563E-015        1.408630067826926E-
```

```
020       TIME =   7009.7851     DT =   800.00000     SUM OF SQUARES =  0.14086301E-19
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.39184175E-13 AND  -0.39184175E-13
 POSITION OF INTERFACE CARBIDE / MATRIX IS   0.39278222E-06
 U-FRACTION IN SYSTEM:  C = .0278350007342459  CR = .149835755259257
                        FE = .85016424487125
 TOTAL SIZE OF SYSTEM:  4.93068569406E-18 [m^3]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: MATRIX

  CPU time used in timestep                    2 seconds
 8.504197975767985E-009        8.504579725774189E-009        8.478713689719143E-009        5.537068891238242E-009        5.466922614992864E-
009        5.330122284556945E-009        5.054509117912391E-009        5.054463016691719E-009        4.532425520148021E-
009        3.566389377159551E-009        2.002743734955091E-009        2.003328010359017E-009        2.257018246195875E-
010        4.626375824113882E-017       TIME =   7809.7851     DT =   800.00000     SUM OF SQUARES =  0.46263758E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.10374557E-12 AND   0.10374557E-12
 POSITION OF INTERFACE CARBIDE / MATRIX IS   0.39286522E-06
 U-FRACTION IN SYSTEM:  C = .0278350032487749  CR = .149835755274631
                        FE = .850164244855876
 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
 7.350065550855383E-008        7.349852284487402E-008        7.383438410434848E-008        2.885866109238800E-008        2.849461323285014E-
008        2.736210879806945E-008        2.552219813437210E-008        2.550744713061817E-008        2.177027968603356E-
008        1.535778088165292E-008        5.786330784629844E-009        7.289677930847106E-
017       TIME =   8000.0000     DT =   190.21494     SUM OF SQUARES =  0.72896779E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.41239119E-12 AND   0.41239119E-12
 POSITION OF INTERFACE CARBIDE / MATRIX IS   0.39294366E-06
 U-FRACTION IN SYSTEM:  C = .0278350037691698  CR = .14983575527978
                        FE = .850164244850728
 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    45.315565
 DELETING TIME-RECORD FOR TIME    67.607791
 DELETING TIME-RECORD FOR TIME    67.607801
 DELETING TIME-RECORD FOR TIME    67.607821
 DELETING TIME-RECORD FOR TIME    67.607861
 DELETING TIME-RECORD FOR TIME    67.607941
 DELETING TIME-RECORD FOR TIME    67.608101
 DELETING TIME-RECORD FOR TIME    67.608421
 DELETING TIME-RECORD FOR TIME    67.609061
 DELETING TIME-RECORD FOR TIME    67.610341
 DELETING TIME-RECORD FOR TIME    67.612901
 DELETING TIME-RECORD FOR TIME    67.618021
 DELETING TIME-RECORD FOR TIME    67.628261
 DELETING TIME-RECORD FOR TIME    67.648741
 DELETING TIME-RECORD FOR TIME    67.689701
 DELETING TIME-RECORD FOR TIME    67.771621
 DELETING TIME-RECORD FOR TIME    67.935461
 DELETING TIME-RECORD FOR TIME    68.263141
 DELETING TIME-RECORD FOR TIME    68.918501
 DELETING TIME-RECORD FOR TIME    70.229221
 DELETING TIME-RECORD FOR TIME    72.850661
 DELETING TIME-RECORD FOR TIME    78.093541
 DELETING TIME-RECORD FOR TIME    88.579301
 DELETING TIME-RECORD FOR TIME    109.55082
 DELETING TIME-RECORD FOR TIME    151.49386
 DELETING TIME-RECORD FOR TIME    235.37994
 DELETING TIME-RECORD FOR TIME    403.15210
 DELETING TIME-RECORD FOR TIME    738.69642
 DELETING TIME-RECORD FOR TIME    1409.7851
 DELETING TIME-RECORD FOR TIME    2209.7851
 DELETING TIME-RECORD FOR TIME    3009.7851
 DELETING TIME-RECORD FOR TIME    3809.7851
 DELETING TIME-RECORD FOR TIME    4609.7851
 DELETING TIME-RECORD FOR TIME    5409.7851
 DELETING TIME-RECORD FOR TIME    6209.7851
 DELETING TIME-RECORD FOR TIME    7009.7851

 KEEPING TIME-RECORD FOR TIME    7809.7851
 AND FOR TIME                    8000.0000
 WORKSPACE RECLAIMED

 TIMESTEP AT     8000.00000     SELECTED

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

**exb3-plot**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exb3\plot.DCM.test"
DIC>
DIC>
DIC> @@ exb3_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE b3
DIC> @@
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA MODULE AND SPECIFY THE STORE RESULT FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  8.00000E+03
DIC> read exb3
 OK
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA POST PROCESSOR
DIC> @@
DIC> post
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1: @@
POST-1: @@ LET US SEE HOW THE AMOUNT OF FERRITE VARIED DURING THE
POST-1: @@ SIMULATION
POST-1: @@
POST-1: s-d-a y iww(bcc)
POST-1: s-d-a x time
  INFO: Time is set as independent variable
POST-1: s-ax-typ x log
POST-1: s-s-s x n 1E-5 1E3
POST-1: s-s-s y n 0 0.1
POST-1:
POST-1: set-tit Figure b3.1
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
ORKING ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

Figure b3.1

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

Figure b3.2

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

Figure b3.3

```
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: @@
POST-1: @@ AND FINALLY LOOK AT THE CHANGE OF RADIUS OF THE M23-CARBIDE
POST-1: @@
POST-1: s-d-a y position carbide upper
POST-1: s-s-s x n 1E-4 1E4
POST-1:
POST-1: set-tit Figure b3.4
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
ORKING ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

Figure b3.4

2019.11.11.15.19.22
UPPER INTERFACE OF REGION "CARBIDE#1"
CELL #1

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

# Example exb4a

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

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

**exb4a-setup**

```
SYS:About

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

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 21012) 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: Mon Nov 11 11:13:13 2019


SYS:SYS:MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exb4a\setup.DCM.test"
SYS: @@
SYS: @@ Moving boundary problem.
SYS: @@ Solidification path of an Fe-18%Cr-8%Ni alloy: Eutectic reaction
SYS: @@ This example demonstrates the solidification path of an Fe-18%Cr-8%Ni
SYS: @@ alloy. A eutectic reaction is assumed, LIQUID -> BCC + FCC. Hence the
SYS: @@ BCC and FCC regions should be on separate sides of the liquid region.
SYS: @@ Comparison is made with both a Scheil-Gulliver simulation and equilibrium
SYS: @@ solidification conditions, both done in Thermo-Calc.
SYS: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exb4a_setup.DCM
SYS:
SYS:
SYS: @@
SYS: @@ START BY GOING TO THE DATABASE MODULE
SYS: @@
SYS: go da
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v10.0

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10:
TDB_TCFE10: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA
TDB_TCFE10: sw tcfe9
 Current database: Steels/Fe-Alloys  v9.1

 VA                      /-  DEFINED
 L12_FCC                 B2_BCC                  DICTRA_FCC_A1
   REJECTED
TDB_TCFE9:
TDB_TCFE9: @@ DEFINE THE SYSTEM TO WORK WITH
TDB_TCFE9: def-sys fe ni cr
 FE                      NI                      CR
   DEFINED
TDB_TCFE9:
TDB_TCFE9: @@ EXCLUDE THE THERMODYNAMIC DATA FOR THE PHASES THAT ARE NOT NEEDED
TDB_TCFE9: rej ph /all
 LIQUID:L                BCC_A2                  FCC_A1
 HCP_A3                  CBCC_A12                CUB_A13
 SIGMA                   CHI_A12                 LAVES_PHASE_C14
 CR3SI                   NBNI3                   NI3TI
 CRZN17                  BETA1                   GAMMA
 AL5FE4                  FLUORITE_C1:I           ZRO2_TETR:I
 M2O3C:I                 CENI2                   CENI5
   REJECTED
TDB_TCFE9: res ph fcc liq bcc
 FCC_A1                  LIQUID:L                BCC_A2
   RESTORED
TDB_TCFE9:
TDB_TCFE9: @@ RETRIEVE DATA FROM THE DATABASE FILE
TDB_TCFE9: get
15:20:43,718 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'J. Brillo and I. Egry, Int. J. Thermophysics, 24, 1155-1170'
  'B.-J. Lee, CALPHAD, 17 (1993) 251-268; revision of Fe-Cr and Fe-Ni liquid'
  'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270
      (1986); CR-FE'
  'B.-J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
  'A. Dinsdale and T. Chart, MTDS NPL, Unpublished work (1986); CR-NI'
  'A. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); FE-NI'
 -OK-
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ MOBILITY/DIFFUSIVITY DATA ARE STORED IN A SEPARATE DATABASE FILE.
TDB_TCFE9: @@ SWITCH TO A MOBILITY DATABASE AND APPEND THE DATA
TDB_TCFE9: @@
TDB_TCFE9: app
 Use one of these databases

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

```
TCNI10  =  Ni-Alloys  v10.0 SNAPSHOT
TCNI9   =  Ni-Alloys  v9.1
TCNI8   =  Ni-Alloys  v8.2
TCNI7   =  Ni-Alloys  v7.2
TCNI6   =  Ni-Alloys  v6.1
TCNI5   =  Ni-Alloys  v5.1
TCNI4   =  Ni-Alloys  v4.0
TCNI1   =  Ni-Alloys  v1.3
TCAL6   =  Al-Alloys  v6.0
TCAL5   =  Al-Alloys  v5.1
TCAL4   =  Al-Alloys  v4.0
TCAL3   =  Al-Alloys  v3.0
TCAL2   =  Al-Alloys  v2.1
TCAL1   =  Al-Alloys  v1.2
TCMG5   =  Mg-Alloys  v5.1
TCMG4   =  Mg-Alloys  v4.0
TCMG3   =  Mg-Alloys  v3.0
TCMG2   =  Mg-Alloys  v2.0
TCMG1   =  Mg-Alloys  v1.1
TCTI2   =  Ti-Alloys  v2.1
TCTI1   =  Ti-Alloys  v1.0
TCCU3   =  Cu-Alloys  v3.1
TCCU2   =  Cu-Alloys  v2.0
TCCU1   =  Cu-Alloys  v1.0
TCCC1   =  Cemented carbide  v1.0
TCHEA4  =  High Entropy Alloy  v4.0
TCHEA3  =  High Entropy Alloy  v3.1
TCHEA2  =  High Entropy Alloy  v2.1.1
TCHEA1  =  High Entropy Alloy  v1.0
SSOL7   =  SGTE Alloy Solutions Database v7.0
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
TCOX10  =  Metal Oxide Solutions  v10.0 SNAPSHOT
TCOX9   =  Metal Oxide Solutions  v9.0
TCOX8   =  Metal Oxide Solutions  v8.0
TCOX7   =  Metal Oxide Solutions  v7.0
TCOX6   =  Metal Oxide Solutions  v6.0
TCOX5   =  Metal Oxide Solutions  v5.1
TCOX4   =  Metal Oxide Solutions  v4.1
ION3    =  Ionic Solutions  v3.0
ION2    =  Ionic Solutions  v2.6
ION1    =  Ionic Solutions  v1.5
NOX2    =  NPL Oxide Solutions Database v2.1
TCNOBL2 =  Noble Metals Alloys v2.0 SNAPSHOT
TCNOBL1 =  Noble Metals Alloys v1.0
TCSLD3  =  Solder Alloys  v3.2
TCSLD2  =  Solder Alloys  v2.0
TCSLD1  =  Solder Alloys  v1.1
TCSI1   =  Ultrapure Silicon  v1.2
TCMP2   =  Materials Processing  v2.5
TCES1   =  Combustion/Sintering  v1.1
TCSC1   =  Super Conductor  v1.0
TCFC1   =  SOFC Database v1.0
TCNF2   =  Nuclear Fuels  v2.1b
NUMT2   =  Nuclear Materials  v2.1
NUOX4   =  Nuclear Oxides  v4.2
NUCL15  =  IRSN NUCLEA-15_4
NUCL10  =  ThermoData NUCLEA Alloys-oxides TDB v10.2
MEPH15  =  IRSN Mephista-15_1
MEPH11  =  ThermoData MEPHISTA Nuclear Fuels TDB v11.2
TCAQ3   =  Aqueous Solution  v3.0
TCAQ2   =  Aqueous Solution  v2.7
AQS2    =  TGG Aqueous Solution Database v2.6
GCE2    =  TGG Geochemical/Environmental TDB v2.3
FEDEMO  =  Iron Demo Database v2.1
ALDEMO  =  Aluminum Demo Database v3.0
NIDEMO  =  Nickel Demo Database v1.1
CUDEMO  =  Copper Demo Database v1.0
SLDEMO  =  Solder Demo Database v1.0
OXDEMO  =  Oxide Demo Database v1.0
SUBDEMO =  Substance Demo Database v1.0
PTERN   =  Public Ternary Alloys TDB v1.3
PAQ2    =  Public Aqueous Soln (SIT) TDB v2.4
PG35    =  G35 Binary Semi-Conductors TDB v1.2
PURE5   =  SGTE Unary (Pure Elements) TDB v5.1
MOB2    =  Alloys Mobility  v2.7
MOB1    =  Alloys Mobility  v1.3
MOBFE1  =  Steels/Fe-Alloys Mobility  v1.1
MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
MOBFE5  =  Steels/Fe-Alloys Mobility  v5.0
MOBNI5  =  Ni-Alloys Mobility  v5.1
MOBNI4  =  Ni-Alloys Mobility  v4.1
MOBNI3  =  Ni-Alloys Mobility  v3.2
MOBNI2  =  Ni-Alloys Mobility  v2.4
MOBNI1  =  Ni-Alloys Mobility  v1.10
MOBAL5  =  Al-Alloys Mobility  v5.0
MOBAL4  =  Al-Alloys Mobility  v4.0
MOBAL3  =  Al-Alloys Mobility  v3.0
MOBAL2  =  Al-Alloys Mobility  v2.0
MOBAL1  =  Al-Alloys Mobility  v1.0
MOBCU1  =  Cu-Alloys Mobility  v1.0
MOBCU2  =  Cu-Alloys Mobility  v2.0
MOBCU3  =  Cu-Alloys Mobility  v3.0
MOBHEA1 =  High Entropy Alloys Mobility  v1.0
MOBHEA2 =  High Entropy Alloys Mobility  v2.0
MOBMG1  =  Mg-Alloys Mobility  v1.0
MOBSI1  =  Si-Alloys Mobility  v1.0
MOBSLD1 =  Solder-Alloys Mobility  v1.1
```

```
 MOBTI3  =  Ti-Alloys Mobility  v3.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v2.0
 MFEDEMO =  Fe-Alloys Mobility demo database v2.0
 MNIDEMO =  Ni-Alloys Mobility demo database v1.0
 MCUDEMO =  Cu-Alloys Mobility demo database v1.0
 USER    =  User defined Database

DATABASE NAME /TCFE9/: mobfe4
 Current database: Steels/Fe-Alloys Mobility  v4.0

 VA  DEFINED
 B2_BCC  REJECTED
APP: def-sys fe ni cr
 FE                      NI                      CR
   DEFINED
APP: rej ph /all
 BCC_A2                  FCC_A1                  HCP_A3
 LIQUID:L  REJECTED
APP: res ph fcc liq bcc
 FCC_A1                  LIQUID:L                BCC_A2
   RESTORED
APP: get
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'This parameter has not been assessed'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Fe diffusion fcc Cr-Fe'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Ni diffusion fcc Cr-Ni'
  'B. Jonsson: Z. Metallkunde 86(1995)686-692; Cr, Fe and Ni diffusion fcc
      Cr-Fe-Ni'
  'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
      -Ni'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Ni self-diffusion'
  'B. Jonsson: ISIJ International, 35(1995)1415-1421; Cr, Fe and Ni
      diffusion bcc Cr-Fe-Ni'
  'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
      in bcc Fe'
  'No assessed or estimated parameters'
  'Estimation by using the modified Sutherland equation from Chen et al.,
      Phil. Magazine 94 (2014) 1552.'
  'L. Zhang et al., Acta Mater., 58(2010)3664.'
 -OK-
APP:
APP: @@
APP: @@ 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
DIC>
DIC> @@
DIC> @@ ENTER inactive PHASES INTO THE REGION: ONE PHASE ON EACH SIDE OF THE LIQUID
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inact
ATTACH TO REGION NAMED /SMALTA/: smalta
ATTACHED TO THE RIGHT OF SMALTA /YES/: no
PHASE NAME: /NONE/: fcc#1
DEPENDENT COMPONENT ? /NI/: fe
 REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-5
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inact
ATTACH TO REGION NAMED /SMALTA/: smalta
ATTACHED TO THE RIGHT OF SMALTA /YES/: yes
PHASE NAME: /NONE/: bcc#1
DEPENDENT COMPONENT ? /NI/: fe
 REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-5
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> @@
DIC> @@ ENTER A START COMPOSITION FOR THE LIQUID
DIC> @@
DIC> enter-composition
REGION NAME : /SMALTA/: smalta
```

```
PHASE NAME: /LIQUID/: liq
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /CR/: cr lin 18 18
PROFILE FOR /NI/: ni lin  8  8
DIC>
DIC> @@
DIC> @@ THE BOUNDARY CONDITION IS A CLOSED SYSTEM (THE DEFAULT) AS WE DO NOT SPECIFY
DIC> @@ ANYTHING ELSE.
DIC> @@
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 200
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /20/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC> @@
DIC> @@ CHECK THE INTERFACE POSITION. THIS IS TO MAKE SURE THAT THE
DIC> @@ LIQUID REGION DOES NOT SHRINK TOO MUCH DURING A TIMESTEP.
DIC> @@ IN ADDITION THE TIMESTEP IS CONTROLLED BY THE PHASE INTERFACE
DIC> @@ DISPLACEMENT DURING THE SIMULATION.
DIC> @@
DIC> s-s-c
NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /AUTO/: AUTO
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -> 1): /AUTO/:
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/:
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exb4a Y
DIC>
DIC> set-inter
 --OK---
DIC>
```

**exb4a-run**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exb4a\run.DCM.test"
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   1.2275       22
upper part  0.81465       22
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
 INFO: TIMESTEP IS CONTROLLED BY INTERFACE POSITION
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .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 = .733068011219291
                        NI = .0754116207882254
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     0 seconds
 TIME =  0.26028659E-05 DT =  0.25028659E-05 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                        NI = .0754116207882254
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     1 seconds
 TIME =  0.76085978E-05 DT =  0.50057319E-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 =  0.17620062E-04 DT =  0.10011464E-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 =  0.37642989E-04 DT =  0.20022928E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     0 seconds
 TIME =  0.77688844E-04 DT =  0.40045855E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     0 seconds
 TIME =  0.15778055E-03 DT =  0.80091710E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     0 seconds
 TIME =  0.31796397E-03 DT =  0.16018342E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     0 seconds
 TIME =  0.63833082E-03 DT =  0.32036684E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     1 seconds
 TIME =  0.12790645E-02 DT =  0.64073368E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     0 seconds
 TIME =  0.25605319E-02 DT =  0.12814674E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     0 seconds
 TIME =  0.51234666E-02 DT =  0.25629347E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     0 seconds
 TIME =  0.10249336E-01 DT =  0.51258694E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     0 seconds
 TIME =  0.20501075E-01 DT =  0.10251739E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     0 seconds
 TIME =  0.41004553E-01 DT =  0.20503478E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                        NI = .0754116207882257
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     0 seconds
 TIME =  0.82011508E-01 DT =  0.41006956E-01 SUM OF SQUARES =   0.0000000
```

```
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                        NI = .0754116207882258
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.16402542     DT =  0.82013911E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                        NI = .0754116207882258
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.32805324     DT =  0.16402782     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882253
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds


output ignored...



... output resumed

 5.542934333783168E-006        5.543835346474996E-006        5.539195393409994E-006        7.175837208877064E-010        4.399029530767442E-
013        4.451028544431255E-018       TIME =   178.38332     DT =   1.3107200     SUM OF SQUARES =  0.44510285E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.59985783E-07 AND  -0.59985783E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.70798178E-05
 U-FRACTION IN SYSTEM:  CR = .191500837979822  FE = .733100607964596
                        NI = .0753985540555812
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_BCC_A2

  CPU time used in timestep                    3 seconds
 1.087065304378251E-005        1.087060101713879E-005        1.086454111694428E-005        3.773770956572133E-007        3.512348972155006E-
011        3.747131556972127E-016        6.340638018029198E-
021       TIME =   181.00476     DT =   2.6214400     SUM OF SQUARES =  0.63406380E-20
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.43957893E-07 AND  -0.43957893E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.69645848E-05
 U-FRACTION IN SYSTEM:  CR = .191500837897805  FE = .733100608151871
                        NI = .0753985539503245
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  2  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_BCC_A2

  CPU time used in timestep                    2 seconds
 7.968408693824177E-006        7.968557460424453E-006        7.965070185661955E-006        9.965449641189200E-007        1.848627215926160E-
007        1.454557047497034E-012        9.973812413524481E-
017       TIME =   186.24764     DT =   5.2428800     SUM OF SQUARES =  0.99738124E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.17721359E-07 AND  -0.17721359E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.68716738E-05
 U-FRACTION IN SYSTEM:  CR = .191500837821298  FE = .733100608392575
                        NI = .0753985537861273
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_BCC_A2

  CPU time used in timestep                    3 seconds
 5.760481817011469E-006        5.760635919222245E-006        5.758981491136858E-006        2.368950875121988E-006        1.576724032131475E-
006        3.735113243933488E-007        4.317225825391490E-011        4.720036528407242E-015        6.408552293150036E-
019       TIME =   196.73340     DT =   10.485760     SUM OF SQUARES =  0.64085523E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.21802019E-07 AND   0.21802019E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.71002846E-05
 U-FRACTION IN SYSTEM:  CR = .191500837818841  FE = .733100608438356
                        NI = .075398553742803
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    4 seconds
 1.322182341558138E-005        1.322203876929120E-005        1.321670022007051E-005        7.855625357604408E-008        2.238353908333859E-
011        5.880045551000630E-017       TIME =   200.00000     DT =   3.2666019     SUM OF SQUARES =  0.58800456E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.13886077E-07 AND   0.13886077E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.71456448E-05
 U-FRACTION IN SYSTEM:  CR = .191500837812953  FE = .733100608467317
                        NI = .0753985537197298
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 MUST SAVE WORKSPACE ON FILE
 WORKSPACE SAVED ON FILE
 RECLAIMING WORKSPACE
 DELETING TIME-RECORD FOR TIME    175.56749
 DELETING TIME-RECORD FOR TIME    175.76189
 DELETING TIME-RECORD FOR TIME    175.76190
 DELETING TIME-RECORD FOR TIME    175.76192
 DELETING TIME-RECORD FOR TIME    175.76196
 DELETING TIME-RECORD FOR TIME    175.76204
 DELETING TIME-RECORD FOR TIME    175.76220
 DELETING TIME-RECORD FOR TIME    175.76252
 DELETING TIME-RECORD FOR TIME    175.76316
 DELETING TIME-RECORD FOR TIME    175.76444
 DELETING TIME-RECORD FOR TIME    175.76700
 DELETING TIME-RECORD FOR TIME    175.77212
 DELETING TIME-RECORD FOR TIME    175.78236
 DELETING TIME-RECORD FOR TIME    175.80284
 DELETING TIME-RECORD FOR TIME    175.84380
 DELETING TIME-RECORD FOR TIME    175.92572
 DELETING TIME-RECORD FOR TIME    176.08956
 DELETING TIME-RECORD FOR TIME    176.41724
 DELETING TIME-RECORD FOR TIME    177.07260
 DELETING TIME-RECORD FOR TIME    178.38332
 DELETING TIME-RECORD FOR TIME    181.00476
 DELETING TIME-RECORD FOR TIME    186.24764

 KEEPING TIME-RECORD FOR TIME    196.73340
 AND FOR TIME                    200.00000
 WORKSPACE RECLAIMED

 TIMESTEP AT     200.000000     SELECTED

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

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

**exb4a-plot**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exb4a\plot.DCM.test"
DIC>
DIC>
DIC> @@ exb4a_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE b4a
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  2.00000E+02
DIC> read exb4a
 OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1: set-title Fe-18%Cr-8%Ni
POST-1:
POST-1: @@
POST-1: @@ PLOT THE FRACTION OF SOLID AND COMPARE WITH A SCHEIL-GULLIVER SIMULATION
POST-1: @@ AND EQUILIBRIUM SOLIDIFICATION (DATA ON FILE exb4.exp)
POST-1: @@
POST-1: enter function fs=1-ivv(liquid);
POST-1: s-d-a x fs
POST-1: s-s-s x n 0 1
POST-1: set-axis-text
AXIS (X, Y OR Z) : x
AUTOMATIC AXIS TEXT  (Y OR N) /N/: n
AXIS TEXT : Fraction Solid
POST-1:
POST-1: s-d-a y t-c
POST-1: s-s-s y n 1420 1480
POST-1:
POST-1: s-p-c interface smalta lower
POST-1:
POST-1: app y exb4a.exp 0; 1
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
ORKING ...orking ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

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

# Example exb4b

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

This example is the same as exb4a but now a peritectic reaction is assumed, LIQUID + BCC -> FCC. Hence the FCC region should appear in between the LIQUID and the BCC. Comparison is made with both a Scheil-Gulliver simulation and equilibrium solidification conditions, both made with Thermo-Calc.

**exb4b-setup**

```
SYS:About

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

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 21012) 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: Mon Nov 11 11:13:13 2019


SYS:SYS:MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exb4b\setup.DCM.test"
SYS: @@
SYS: @@ Moving boundary problem.
SYS: @@ Solidification path of an Fe-18%Cr-8%Ni alloy: Peritectic reaction
SYS: @@ This example is the same as exb4a but now a peritectic reaction is assumed:
SYS: @@ LIQUID + BCC -> FCC. Hence the FCC region should appear in between the LIQUID
SYS: @@ and the BCC. Comparison is made with both a Scheil-Gulliver simulation and
SYS: @@ equilibrium solidification conditions, both done in Thermo-Calc.
SYS: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exb4b_setup.DCM
SYS:
SYS:
SYS: @@
SYS: @@ START BY GOING TO THE DATABASE MODULE
SYS: @@
SYS: go da
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v10.0

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10:
TDB_TCFE10: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA
TDB_TCFE10: sw fedemo
 Current database: Iron Demo Database v2.1

 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                  CBCC_A12
 CHI_A12                 CUB_A13                 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
15:31:03,973 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

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

 TCFE10  =  Steels/Fe-Alloys  v10.0
 TCFE9   =  Steels/Fe-Alloys  v9.1
 TCFE8   =  Steels/Fe-Alloys  v8.1
 TCFE7   =  Steels/Fe-Alloys  v7.0
 TCFE6   =  Steels/Fe-Alloys  v6.2
 TCFE5   =  Steels/Fe-Alloys  v5.0
 TCFE4   =  Steels/Fe-Alloys  v4.1
 TCFE3   =  Steels/Fe-Alloys  v3.1
 TCFE2   =  Steels/Fe-Alloys  v2.1
 TCFE1   =  Steels/Fe-Alloys  v1.0
 FROST1  =  FROST database v1.2
 FEDAT   =  TCS/TT Steels Database v1.0
 TCNI10  =  Ni-Alloys  v10.0 SNAPSHOT
 TCNI9   =  Ni-Alloys  v9.1
 TCNI8   =  Ni-Alloys  v8.2
 TCNI7   =  Ni-Alloys  v7.2
 TCNI6   =  Ni-Alloys  v6.1
 TCNI5   =  Ni-Alloys  v5.1
 TCNI4   =  Ni-Alloys  v4.0
```

```
TCNI1   =  Ni-Alloys  v1.3
TCAL6   =  Al-Alloys  v6.0
TCAL5   =  Al-Alloys  v5.1
TCAL4   =  Al-Alloys  v4.0
TCAL3   =  Al-Alloys  v3.0
TCAL2   =  Al-Alloys  v2.1
TCAL1   =  Al-Alloys  v1.2
TCMG5   =  Mg-Alloys  v5.1
TCMG4   =  Mg-Alloys  v4.0
TCMG3   =  Mg-Alloys  v3.0
TCMG2   =  Mg-Alloys  v2.0
TCMG1   =  Mg-Alloys  v1.1
TCTI2   =  Ti-Alloys  v2.1
TCTI1   =  Ti-Alloys  v1.0
TCCU3   =  Cu-Alloys  v3.1
TCCU2   =  Cu-Alloys  v2.0
TCCU1   =  Cu-Alloys  v1.0
TCCC1   =  Cemented carbide  v1.0
TCHEA4  =  High Entropy Alloy  v4.0
TCHEA3  =  High Entropy Alloy  v3.1
TCHEA2  =  High Entropy Alloy  v2.1.1
TCHEA1  =  High Entropy Alloy  v1.0
SSOL7   =  SGTE Alloy Solutions Database v7.0
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
TCOX10  =  Metal Oxide Solutions  v10.0 SNAPSHOT
TCOX9   =  Metal Oxide Solutions  v9.0
TCOX8   =  Metal Oxide Solutions  v8.0
TCOX7   =  Metal Oxide Solutions  v7.0
TCOX6   =  Metal Oxide Solutions  v6.0
TCOX5   =  Metal Oxide Solutions  v5.1
TCOX4   =  Metal Oxide Solutions  v4.1
ION3    =  Ionic Solutions  v3.0
ION2    =  Ionic Solutions  v2.6
ION1    =  Ionic Solutions  v1.5
NOX2    =  NPL Oxide Solutions Database v2.1
TCNOBL2 =  Noble Metals Alloys v2.0 SNAPSHOT
TCNOBL1 =  Noble Metals Alloys v1.0
TCSLD3  =  Solder Alloys  v3.2
TCSLD2  =  Solder Alloys  v2.0
TCSLD1  =  Solder Alloys  v1.1
TCSI1   =  Ultrapure Silicon  v1.2
TCMP2   =  Materials Processing  v2.5
TCES1   =  Combustion/Sintering  v1.1
TCSC1   =  Super Conductor  v1.0
TCFC1   =  SOFC Database v1.0
TCNF2   =  Nuclear Fuels  v2.1b
NUMT2   =  Nuclear Materials  v2.1
NUOX4   =  Nuclear Oxides  v4.2
NUCL15  =  IRSN NUCLEA-15_4
NUCL10  =  ThermoData NUCLEA Alloys-oxides TDB v10.2
MEPH15  =  IRSN Mephista-15_1
MEPH11  =  ThermoData MEPHISTA Nuclear Fuels TDB v11.2
TCAQ3   =  Aqueous Solution  v3.0
TCAQ2   =  Aqueous Solution  v2.7
AQS2    =  TGG Aqueous Solution Database v2.6
GCE2    =  TGG Geochemical/Environmental TDB v2.3
FEDEMO  =  Iron Demo Database v2.1
ALDEMO  =  Aluminum Demo Database v3.0
NIDEMO  =  Nickel Demo Database v1.1
CUDEMO  =  Copper Demo Database v1.0
SLDEMO  =  Solder Demo Database v1.0
OXDEMO  =  Oxide Demo Database v1.0
SUBDEMO =  Substance Demo Database v1.0
PTERN   =  Public Ternary Alloys TDB v1.3
PAQ2    =  Public Aqueous Soln (SIT) TDB v2.4
PG35    =  G35 Binary Semi-Conductors TDB v1.2
PURE5   =  SGTE Unary (Pure Elements) TDB v5.1
MOB2    =  Alloys Mobility  v2.7
MOB1    =  Alloys Mobility  v1.3
MOBFE1  =  Steels/Fe-Alloys Mobility  v1.1
MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
MOBFE5  =  Steels/Fe-Alloys Mobility  v5.0
MOBNI5  =  Ni-Alloys Mobility  v5.1
MOBNI4  =  Ni-Alloys Mobility  v4.1
MOBNI3  =  Ni-Alloys Mobility  v3.2
MOBNI2  =  Ni-Alloys Mobility  v2.4
MOBNI1  =  Ni-Alloys Mobility  v1.10
MOBAL5  =  Al-Alloys Mobility  v5.0
MOBAL4  =  Al-Alloys Mobility  v4.0
MOBAL3  =  Al-Alloys Mobility  v3.0
MOBAL2  =  Al-Alloys Mobility  v2.0
MOBAL1  =  Al-Alloys Mobility  v1.0
MOBCU1  =  Cu-Alloys Mobility  v1.0
MOBCU2  =  Cu-Alloys Mobility  v2.0
MOBCU3  =  Cu-Alloys Mobility  v3.0
MOBHEA1 =  High Entropy Alloys Mobility  v1.0
MOBHEA2 =  High Entropy Alloys Mobility  v2.0
MOBMG1  =  Mg-Alloys Mobility  v1.0
MOBSI1  =  Si-Alloys Mobility  v1.0
MOBSLD1 =  Solder-Alloys Mobility  v1.1
MOBTI3  =  Ti-Alloys Mobility  v3.0
MOBTI2  =  Ti-Alloys Mobility  v2.0
MOBTI1  =  Ti-Alloys Mobility  v1.0
MALDEMO =  Al-Alloys Mobility demo database v2.0
MFEDEMO =  Fe-Alloys Mobility demo database v2.0
MNIDEMO =  Ni-Alloys Mobility demo database v1.0
MCUDEMO =  Cu-Alloys Mobility demo database v1.0
```

```
 USER    =  User defined Database

DATABASE NAME /FEDEMO/: mobfe4
 Current database: Steels/Fe-Alloys Mobility  v4.0

 VA  DEFINED
 B2_BCC  REJECTED
APP: def-sys fe ni cr
 FE                      NI                      CR
   DEFINED
APP: rej ph /all
 BCC_A2                  FCC_A1                  HCP_A3
 LIQUID:L  REJECTED
APP: res ph fcc liq bcc
 FCC_A1                  LIQUID:L                BCC_A2
   RESTORED
APP: get
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'This parameter has not been assessed'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Fe diffusion fcc Cr-Fe'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Ni diffusion fcc Cr-Ni'
  'B. Jonsson: Z. Metallkunde 86(1995)686-692; Cr, Fe and Ni diffusion fcc
      Cr-Fe-Ni'
  'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
      -Ni'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Ni self-diffusion'
  'B. Jonsson: ISIJ International, 35(1995)1415-1421; Cr, Fe and Ni
      diffusion bcc Cr-Fe-Ni'
  'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
      in bcc Fe'
  'No assessed or estimated parameters'
  'Estimation by using the modified Sutherland equation from Chen et al.,
      Phil. Magazine 94 (2014) 1552.'
  'L. Zhang et al., Acta Mater., 58(2010)3664.'
 -OK-
APP:
APP: @@
APP: @@ 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
DIC>
DIC> @@
DIC> @@ ENTER inactive PHASES INTO THE REGION, WITH BOTH PHASES ON THE SAME
DIC> @@ SIDE OF THE LIQUID REGION IN ORDER TO GET A PERITECTIC REACTION.
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inact
ATTACH TO REGION NAMED /SMALTA/: smalta
ATTACHED TO THE RIGHT OF SMALTA /YES/: yes
PHASE NAME: /NONE/: fcc#1
DEPENDENT COMPONENT ? /NI/: fe
 REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-5
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inact
ATTACH TO REGION NAMED /SMALTA/: smalta
ATTACHED TO THE RIGHT OF SMALTA /YES/: yes
PHASE NAME: /NONE/: bcc#1
DEPENDENT COMPONENT ? /NI/: fe
 REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-5
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> @@
DIC> @@ ENTER THE START COMPOSITION FOR THE LIQUID
DIC> @@
DIC> enter-composition
REGION NAME : /SMALTA/: smalta
PHASE NAME: /LIQUID/: liq
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /CR/: cr lin 18 18
PROFILE FOR /NI/: ni lin  8  8
DIC>
DIC> @@
```

```
DIC> @@ THE BOUNDARY CONDITION IS A CLOSED SYSTEM (DEFAULT) AS WE DO NOT SPECIFY
DIC> @@ ANYTHING ELSE.
DIC> @@
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 200
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /20/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ CHECK THE INTERFACE POSITION. THIS IS TO MAKE SURE THAT THE LIQUID REGION
DIC> @@ DOES NOT SHRINK TOO MUCH DURING A TIMESTEP. IN ADDITION, THE TIMESTEP IS
DIC> @@ CONTROLLED BY THE PHASE INTERFACE DISPLACEMENT DURING THE SIMULATION.
DIC> @@
DIC> s-s-c
NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /AUTO/: yes
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -> 1): /AUTO/:
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/: @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exb4b Y
DIC>
DIC> set-inter
 --OK---
DIC>
```

**exb4b-run**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exb4b\run.DCM.test"
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
 0.93810       83
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
 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                     1 seconds
 TIME =  0.27420944E-05 DT =  0.26420944E-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 =  0.80262833E-05 DT =  0.52841888E-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 =  0.18594661E-04 DT =  0.10568378E-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 =  0.39731416E-04 DT =  0.21136755E-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 =  0.82004927E-04 DT =  0.42273511E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882254
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     0 seconds
 TIME =  0.16655195E-03 DT =  0.84547022E-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 =  0.33564599E-03 DT =  0.16909404E-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 =  0.67383408E-03 DT =  0.33818809E-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 =  0.13502102E-02 DT =  0.67637617E-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 =  0.27029626E-02 DT =  0.13527523E-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                     1 seconds
 TIME =  0.54084673E-02 DT =  0.27055047E-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 =  0.10819477E-01 DT =  0.54110094E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219291
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     0 seconds
 TIME =  0.21641495E-01 DT =  0.10822019E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882253
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     0 seconds
 TIME =  0.43285533E-01 DT =  0.21644038E-01 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 =  0.86573608E-01 DT =  0.43288075E-01 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 =  0.17314976     DT =  0.86576150E-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 =  0.34630206     DT =  0.17315230     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992485  FE = .73306801121929
                        NI = .0754116207882249
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.69260666     DT =  0.34630460     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992481  FE = .733068011219295
                        NI = .075411620788224
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds


output ignored...



... output resumed

 6.775753779219018E-015        3.048582722925273E-022       TIME =   192.47835     DT =  0.65536000     SUM OF SQUARES =  0.30485827E-21
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.34384207E-07 AND  -0.34384207E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.10512412E-04
 U-FRACTION IN SYSTEM:  CR = .190992128354091  FE = .733624292238162
                        NI = .0753835794077466
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_BCC_A2

  CPU time used in timestep                    3 seconds
 1.271276426789546E-007        1.271900313145755E-007        1.266742511753762E-007        6.715444428789370E-009        5.045569058952233E-
009        2.173985527556019E-009        2.876738952432043E-014        1.047107700103497E-
021       TIME =   193.78907     DT =   1.3107200     SUM OF SQUARES =  0.10471077E-20
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.21224567E-07 AND  -0.21224567E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.10484592E-04
 U-FRACTION IN SYSTEM:  CR = .190992128353888  FE = .733624292238256
                        NI = .0753835794078568
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    3 seconds
 3.673224989202575E-007        3.674218643028170E-007        3.675333590934570E-007        3.422572672746983E-007        3.255319510096666E-
007        2.924995790244669E-007        2.213488902704164E-007        1.125397895793485E-007        1.124694772506478E-
007        3.563047144937056E-009        3.623320984829895E-015        2.301929753548040E-
021       TIME =   196.41051     DT =   2.6214400     SUM OF SQUARES =  0.23019298E-20
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.52820526E-08 AND  -0.52820526E-08
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.10470746E-04
 U-FRACTION IN SYSTEM:  CR = .190992128353654  FE = .733624292238312
                        NI = .0753835794080336
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_BCC_A2

  CPU time used in timestep                    4 seconds
 3.343036110597140E-007        3.343273662626317E-007        3.345162746466100E-007        3.083825276799892E-007        3.032546105936810E-
007        2.931057537093564E-007        2.724460315002981E-007        2.724296058861459E-007        2.340689386814265E-
007        1.653938406023987E-007        6.422807697217936E-008        4.303388598016980E-013        2.019317446542121E-
018       TIME =   200.00000     DT =   3.5894936     SUM OF SQUARES =  0.20193174E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.93527344E-08 AND   0.93527344E-08
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.10504317E-04
 U-FRACTION IN SYSTEM:  CR = .190992128357782  FE = .733624292238012
                        NI = .0753835794042062
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 MUST SAVE WORKSPACE ON FILE
 WORKSPACE SAVED ON FILE
 RECLAIMING WORKSPACE
 DELETING TIME-RECORD FOR TIME    183.93246
 DELETING TIME-RECORD FOR TIME    191.16764
 DELETING TIME-RECORD FOR TIME    191.16765
 DELETING TIME-RECORD FOR TIME    191.16767
 DELETING TIME-RECORD FOR TIME    191.16771
 DELETING TIME-RECORD FOR TIME    191.16779
 DELETING TIME-RECORD FOR TIME    191.16795
 DELETING TIME-RECORD FOR TIME    191.16827
 DELETING TIME-RECORD FOR TIME    191.16891
 DELETING TIME-RECORD FOR TIME    191.17019
 DELETING TIME-RECORD FOR TIME    191.17275
 DELETING TIME-RECORD FOR TIME    191.17787
 DELETING TIME-RECORD FOR TIME    191.18811
 DELETING TIME-RECORD FOR TIME    191.20859
 DELETING TIME-RECORD FOR TIME    191.24955
 DELETING TIME-RECORD FOR TIME    191.33147
 DELETING TIME-RECORD FOR TIME    191.49531
 DELETING TIME-RECORD FOR TIME    191.82299
 DELETING TIME-RECORD FOR TIME    192.47835
 DELETING TIME-RECORD FOR TIME    193.78907

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

 TIMESTEP AT     200.000000     SELECTED

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

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

**exb4b-plot**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exb4b\plot.DCM.test"
DIC>
DIC>
DIC> @@ exb4b_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE b4b
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  2.00000E+02
DIC> read exb4b
 OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1: set-title Fe-18%Cr-8%Ni
POST-1:
POST-1: @@
POST-1: @@ PLOT THE FRACTION OF SOLID AND COMPARE WITH A SCHEIL-GULLIVER
POST-1: @@ SIMULATION AND EQUILIBRIUM SOLIDIFICATION (DATA ON FILE exb4.exp)
POST-1: @@
POST-1: enter func fs=1-ivv(liquid);
POST-1: s-d-a x fs
POST-1: s-s-s x n 0 1
POST-1: s-ax-te x n Fraction Solid
POST-1:
POST-1: s-d-a y t-c
POST-1: s-s-s y n 1420 1480
POST-1:
POST-1: s-p-c interf smalta lower
POST-1:
POST-1: app y exb4b.exp 0; 1
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
ORKING ...orking ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

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

# Example exb4c

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

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

**exb4c-setup**

```
SYS:About

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

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 21012) 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: Mon Nov 11 11:13:13 2019


SYS:SYS:MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exb4c\setup.DCM.test"
SYS: @@
SYS: @@ Moving boundary problem.
SYS: @@ Solidification path of an Fe-18%Cr-8%Ni alloy
SYS: @@ This example is the same as exb4b but now the diffusivity data is amended
SYS: @@ for the LIQUID and a high value for the diffusivity is used to simulate a
SYS: @@ case where it is assumed that the composition in the LIQUID is always
SYS: @@ homogeneous. This example is less realistic than exb4b.
SYS: @@ Comparison is made with both a Scheil-Gulliver simulation and equilibrium
SYS: @@ solidification conditions, both done in Thermo-Calc.
SYS: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exb4c_setup.DCM
SYS:
SYS: @@
SYS: @@ START BY GOING TO THE DATABASE MODULE
SYS: @@
SYS: go da
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v10.0

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10:
TDB_TCFE10: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA
TDB_TCFE10: sw tcfe9
 Current database: Steels/Fe-Alloys  v9.1

 VA                      /-  DEFINED
 L12_FCC                 B2_BCC                  DICTRA_FCC_A1
   REJECTED
TDB_TCFE9:
TDB_TCFE9: @@ DEFINE THE SYSTEM TO WORK WITH
TDB_TCFE9: def-sys fe ni cr
 FE                      NI                      CR
   DEFINED
TDB_TCFE9:
TDB_TCFE9: @@ EXCLUDE THE THERMODYNAMIC DATA FOR THE PHASES THAT ARE NOT NEEDED
TDB_TCFE9: rej ph /all
 LIQUID:L                BCC_A2                  FCC_A1
 HCP_A3                  CBCC_A12                CUB_A13
 SIGMA                   CHI_A12                 LAVES_PHASE_C14
 CR3SI                   NBNI3                   NI3TI
 CRZN17                  BETA1                   GAMMA
 AL5FE4                  FLUORITE_C1:I           ZRO2_TETR:I
 M2O3C:I                 CENI2                   CENI5
   REJECTED
TDB_TCFE9: res ph fcc liq bcc
 FCC_A1                  LIQUID:L                BCC_A2
   RESTORED
TDB_TCFE9:
TDB_TCFE9: @@ RETRIEVE DATA FROM THE DATABASE FILE
TDB_TCFE9: get
15:41:17,874 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'J. Brillo and I. Egry, Int. J. Thermophysics, 24, 1155-1170'
  'B.-J. Lee, CALPHAD, 17 (1993) 251-268; revision of Fe-Cr and Fe-Ni liquid'
  'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270
      (1986); CR-FE'
  'B.-J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
  'A. Dinsdale and T. Chart, MTDS NPL, Unpublished work (1986); CR-NI'
  'A. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); FE-NI'
 -OK-
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ MOBILITY/DIFFUSIVITY DATA ARE STORED IN A SEPARATE DATABASE FILE.
TDB_TCFE9: @@ SWITCH TO A MOBILITY DATABASE AND APPEND THE DATA.
TDB_TCFE9: @@
TDB_TCFE9: app
 Use one of these databases

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

```
TCNI10  =  Ni-Alloys  v10.0 SNAPSHOT
TCNI9   =  Ni-Alloys  v9.1
TCNI8   =  Ni-Alloys  v8.2
TCNI7   =  Ni-Alloys  v7.2
TCNI6   =  Ni-Alloys  v6.1
TCNI5   =  Ni-Alloys  v5.1
TCNI4   =  Ni-Alloys  v4.0
TCNI1   =  Ni-Alloys  v1.3
TCAL6   =  Al-Alloys  v6.0
TCAL5   =  Al-Alloys  v5.1
TCAL4   =  Al-Alloys  v4.0
TCAL3   =  Al-Alloys  v3.0
TCAL2   =  Al-Alloys  v2.1
TCAL1   =  Al-Alloys  v1.2
TCMG5   =  Mg-Alloys  v5.1
TCMG4   =  Mg-Alloys  v4.0
TCMG3   =  Mg-Alloys  v3.0
TCMG2   =  Mg-Alloys  v2.0
TCMG1   =  Mg-Alloys  v1.1
TCTI2   =  Ti-Alloys  v2.1
TCTI1   =  Ti-Alloys  v1.0
TCCU3   =  Cu-Alloys  v3.1
TCCU2   =  Cu-Alloys  v2.0
TCCU1   =  Cu-Alloys  v1.0
TCCC1   =  Cemented carbide  v1.0
TCHEA4  =  High Entropy Alloy  v4.0
TCHEA3  =  High Entropy Alloy  v3.1
TCHEA2  =  High Entropy Alloy  v2.1.1
TCHEA1  =  High Entropy Alloy  v1.0
SSOL7   =  SGTE Alloy Solutions Database v7.0
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
TCOX10  =  Metal Oxide Solutions  v10.0 SNAPSHOT
TCOX9   =  Metal Oxide Solutions  v9.0
TCOX8   =  Metal Oxide Solutions  v8.0
TCOX7   =  Metal Oxide Solutions  v7.0
TCOX6   =  Metal Oxide Solutions  v6.0
TCOX5   =  Metal Oxide Solutions  v5.1
TCOX4   =  Metal Oxide Solutions  v4.1
ION3    =  Ionic Solutions  v3.0
ION2    =  Ionic Solutions  v2.6
ION1    =  Ionic Solutions  v1.5
NOX2    =  NPL Oxide Solutions Database v2.1
TCNOBL2 =  Noble Metals Alloys v2.0 SNAPSHOT
TCNOBL1 =  Noble Metals Alloys v1.0
TCSLD3  =  Solder Alloys  v3.2
TCSLD2  =  Solder Alloys  v2.0
TCSLD1  =  Solder Alloys  v1.1
TCSI1   =  Ultrapure Silicon  v1.2
TCMP2   =  Materials Processing  v2.5
TCES1   =  Combustion/Sintering  v1.1
TCSC1   =  Super Conductor  v1.0
TCFC1   =  SOFC Database v1.0
TCNF2   =  Nuclear Fuels  v2.1b
NUMT2   =  Nuclear Materials  v2.1
NUOX4   =  Nuclear Oxides  v4.2
NUCL15  =  IRSN NUCLEA-15_4
NUCL10  =  ThermoData NUCLEA Alloys-oxides TDB v10.2
MEPH15  =  IRSN Mephista-15_1
MEPH11  =  ThermoData MEPHISTA Nuclear Fuels TDB v11.2
TCAQ3   =  Aqueous Solution  v3.0
TCAQ2   =  Aqueous Solution  v2.7
AQS2    =  TGG Aqueous Solution Database v2.6
GCE2    =  TGG Geochemical/Environmental TDB v2.3
FEDEMO  =  Iron Demo Database v2.1
ALDEMO  =  Aluminum Demo Database v3.0
NIDEMO  =  Nickel Demo Database v1.1
CUDEMO  =  Copper Demo Database v1.0
SLDEMO  =  Solder Demo Database v1.0
OXDEMO  =  Oxide Demo Database v1.0
SUBDEMO =  Substance Demo Database v1.0
PTERN   =  Public Ternary Alloys TDB v1.3
PAQ2    =  Public Aqueous Soln (SIT) TDB v2.4
PG35    =  G35 Binary Semi-Conductors TDB v1.2
PURE5   =  SGTE Unary (Pure Elements) TDB v5.1
MOB2    =  Alloys Mobility  v2.7
MOB1    =  Alloys Mobility  v1.3
MOBFE1  =  Steels/Fe-Alloys Mobility  v1.1
MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
MOBFE5  =  Steels/Fe-Alloys Mobility  v5.0
MOBNI5  =  Ni-Alloys Mobility  v5.1
MOBNI4  =  Ni-Alloys Mobility  v4.1
MOBNI3  =  Ni-Alloys Mobility  v3.2
MOBNI2  =  Ni-Alloys Mobility  v2.4
MOBNI1  =  Ni-Alloys Mobility  v1.10
MOBAL5  =  Al-Alloys Mobility  v5.0
MOBAL4  =  Al-Alloys Mobility  v4.0
MOBAL3  =  Al-Alloys Mobility  v3.0
MOBAL2  =  Al-Alloys Mobility  v2.0
MOBAL1  =  Al-Alloys Mobility  v1.0
MOBCU1  =  Cu-Alloys Mobility  v1.0
MOBCU2  =  Cu-Alloys Mobility  v2.0
MOBCU3  =  Cu-Alloys Mobility  v3.0
MOBHEA1 =  High Entropy Alloys Mobility  v1.0
MOBHEA2 =  High Entropy Alloys Mobility  v2.0
MOBMG1  =  Mg-Alloys Mobility  v1.0
MOBSI1  =  Si-Alloys Mobility  v1.0
MOBSLD1 =  Solder-Alloys Mobility  v1.1
```

```
 MOBTI3  =  Ti-Alloys Mobility  v3.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v2.0
 MFEDEMO =  Fe-Alloys Mobility demo database v2.0
 MNIDEMO =  Ni-Alloys Mobility demo database v1.0
 MCUDEMO =  Cu-Alloys Mobility demo database v1.0
 USER    =  User defined Database

DATABASE NAME /TCFE9/: mobfe4
 Current database: Steels/Fe-Alloys Mobility  v4.0

 VA  DEFINED
 B2_BCC  REJECTED
APP: def-sys fe ni cr
 FE                      NI                      CR
   DEFINED
APP: rej ph /all
 BCC_A2                  FCC_A1                  HCP_A3
 LIQUID:L  REJECTED
APP: res ph fcc liq bcc
 FCC_A1                  LIQUID:L                BCC_A2
   RESTORED
APP: get
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'This parameter has not been assessed'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Fe diffusion fcc Cr-Fe'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Ni diffusion fcc Cr-Ni'
  'B. Jonsson: Z. Metallkunde 86(1995)686-692; Cr, Fe and Ni diffusion fcc
      Cr-Fe-Ni'
  'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
      -Ni'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Ni self-diffusion'
  'B. Jonsson: ISIJ International, 35(1995)1415-1421; Cr, Fe and Ni
      diffusion bcc Cr-Fe-Ni'
  'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
      in bcc Fe'
  'No assessed or estimated parameters'
  'Estimation by using the modified Sutherland equation from Chen et al.,
      Phil. Magazine 94 (2014) 1552.'
  'L. Zhang et al., Acta Mater., 58(2010)3664.'
 -OK-
APP:
APP: @@
APP: @@ 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
DIC>
DIC> @@
DIC> @@ ENTER inactive PHASES INTO THE REGION, BOTH PHASES ON THE SAME SIDE
DIC> @@ OF THE LIQUID REGION IN ORDER TO GET A PERITECTIC REACTION.
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inact
ATTACH TO REGION NAMED /SMALTA/: smalta
ATTACHED TO THE RIGHT OF SMALTA /YES/: yes
PHASE NAME: /NONE/: fcc#1
DEPENDENT COMPONENT ? /NI/: fe
 REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-5
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inact
ATTACH TO REGION NAMED /SMALTA/: smalta
ATTACHED TO THE RIGHT OF SMALTA /YES/: yes
PHASE NAME: /NONE/: bcc#1
DEPENDENT COMPONENT ? /NI/: fe
 REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-5
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> @@
DIC> @@ ENTER THE START COMPOSITION FOR THE LIQUID
DIC> @@
DIC> enter-composition
REGION NAME : /SMALTA/: smalta
PHASE NAME: /LIQUID/: liq
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /CR/: cr lin 18 18
PROFILE FOR /NI/: ni lin  8  8
DIC>
DIC> @@
DIC> @@ THE BOUNDARY CONDITION IS A CLOSED SYSTEM (DEFAULT) AS WE DO NOT SPECIFY
DIC> @@ ANYTHING ELSE
DIC> @@
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
```

```
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 200
AUTOMATIC TIMESTEP CONTROL /YES/: yes
MAX TIMESTEP DURING INTEGRATION /20/: 1
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ CHECK THE INTERFACE POSITION. THIS IS TO MAKE SURE THAT THE LIQUID
DIC> @@ REGION DOES NOT SHRINK TOO MUCH DURING A TIMESTEP.  IN ADDITION THE TIMESTEP
DIC> @@ IS CONTROLLED BY THE PHASE INTERFACE DISPLACEMENT DURING THE SIMULATION.
DIC> @@
DIC> s-s-c
NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /AUTO/: yes
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -> 1): /AUTO/:
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/: @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exb4c Y
DIC>
DIC> set-inter
 --OK---
DIC>
```

**exb4c-run**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exb4c\run.DCM.test"
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
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
 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                     1 seconds
 TIME =  0.10773101E-05 DT =  0.97731005E-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 =  0.30319302E-05 DT =  0.19546201E-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 =  0.69411704E-05 DT =  0.39092402E-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 =  0.14759651E-04 DT =  0.78184804E-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 =  0.30396612E-04 DT =  0.15636961E-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 =  0.61670533E-04 DT =  0.31273922E-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 =  0.12421838E-03 DT =  0.62547843E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     0 seconds
 TIME =  0.24931406E-03 DT =  0.12509569E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     0 seconds
 TIME =  0.49950544E-03 DT =  0.25019137E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     0 seconds
 TIME =  0.99988818E-03 DT =  0.50038275E-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 =  0.20006537E-02 DT =  0.10007655E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992482  FE = .733068011219293
                        NI = .0754116207882257
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     0 seconds
 TIME =  0.40021847E-02 DT =  0.20015310E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992482  FE = .733068011219293
                        NI = .0754116207882259
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     0 seconds
 TIME =  0.80052466E-02 DT =  0.40030620E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992478  FE = .733068011219298
                        NI = .0754116207882241
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     0 seconds
 TIME =  0.16011371E-01 DT =  0.80061240E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992479  FE = .733068011219296
                        NI = .0754116207882251
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     0 seconds
 TIME =  0.32023619E-01 DT =  0.16012248E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992493  FE = .733068011219288
                        NI = .0754116207882191
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                     0 seconds
```

```
 TIME =  0.64048114E-01 DT =  0.32024496E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992497  FE = .733068011219264
                        NI = .0754116207882391
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.12809711     DT =  0.64048992E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992473  FE = .733068011219282
                        NI = .0754116207882449
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.25619509     DT =  0.12809798     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .191520367992311  FE = .733068011219435
                        NI = .0754116207882534
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds


output ignored...



... output resumed

  RESCALING AND SWITCHING OFF FLUX CORRECTION
 1.224378523822907E-007        1.225008963325901E-007        1.224335220640407E-007        1.225778963781896E-007        1.223233147665263E-
007        8.673238722526615E-008        5.134158656473326E-008        1.773615735598941E-008        1.311191698765730E-
012        9.104752655308351E-015        1.983364854504793E-015        1.159299879105780E-013        3.742136004295150E-
016        SWITCHING ON FLUX CORRECTION
 3.255005269782696E-007        3.259625305719853E-007        3.255005685945684E-007        3.255766652380911E-007        3.255020236510350E-
007        4.845113099980688E-008        8.954428646635762E-010        3.323329576667625E-013        2.643213540012078E-
015        3.160822728721250E-016       TIME =   200.00000     DT =  0.83999467     SUM OF SQUARES =  0.31608227E-15
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.85595141E-07 AND  -0.85595141E-07
 POSITION OF INTERFACE SMALTA / R_FCC_A1 IS   0.39444098E-06
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.13575623E-07 AND   0.13575623E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.10985707E-04
 U-FRACTION IN SYSTEM:  CR = .191209945892415  FE = .733434891799682
                        NI = .0753551623079026
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 MUST SAVE WORKSPACE ON FILE
 WORKSPACE SAVED ON FILE
 RECLAIMING WORKSPACE
 DELETING TIME-RECORD FOR TIME    170.32213
 DELETING TIME-RECORD FOR TIME    170.48228
 DELETING TIME-RECORD FOR TIME    170.48228
 DELETING TIME-RECORD FOR TIME    170.48228
 DELETING TIME-RECORD FOR TIME    170.48228
 DELETING TIME-RECORD FOR TIME    170.48229
 DELETING TIME-RECORD FOR TIME    170.48229
 DELETING TIME-RECORD FOR TIME    170.48229
 DELETING TIME-RECORD FOR TIME    170.48230
 DELETING TIME-RECORD FOR TIME    170.48231
 DELETING TIME-RECORD FOR TIME    170.48233
 DELETING TIME-RECORD FOR TIME    170.48239
 DELETING TIME-RECORD FOR TIME    170.48249
 DELETING TIME-RECORD FOR TIME    170.48269
 DELETING TIME-RECORD FOR TIME    170.48310
 DELETING TIME-RECORD FOR TIME    170.48392
 DELETING TIME-RECORD FOR TIME    170.48556
 DELETING TIME-RECORD FOR TIME    170.48884
 DELETING TIME-RECORD FOR TIME    170.49539
 DELETING TIME-RECORD FOR TIME    170.50850
 DELETING TIME-RECORD FOR TIME    170.53471
 DELETING TIME-RECORD FOR TIME    170.58714
 DELETING TIME-RECORD FOR TIME    170.69200
 DELETING TIME-RECORD FOR TIME    170.90171
 DELETING TIME-RECORD FOR TIME    171.32114
 DELETING TIME-RECORD FOR TIME    172.16001
 DELETING TIME-RECORD FOR TIME    173.16001
 DELETING TIME-RECORD FOR TIME    174.16001
 DELETING TIME-RECORD FOR TIME    175.16001
 DELETING TIME-RECORD FOR TIME    176.16001
 DELETING TIME-RECORD FOR TIME    177.16001
 DELETING TIME-RECORD FOR TIME    178.16001
 DELETING TIME-RECORD FOR TIME    179.16001
 DELETING TIME-RECORD FOR TIME    180.16001
 DELETING TIME-RECORD FOR TIME    181.16001
 DELETING TIME-RECORD FOR TIME    182.16001
 DELETING TIME-RECORD FOR TIME    183.16001
 DELETING TIME-RECORD FOR TIME    184.16001
 DELETING TIME-RECORD FOR TIME    185.16001
 DELETING TIME-RECORD FOR TIME    186.16001
 DELETING TIME-RECORD FOR TIME    187.16001
 DELETING TIME-RECORD FOR TIME    188.16001
 DELETING TIME-RECORD FOR TIME    189.16001
 DELETING TIME-RECORD FOR TIME    190.16001
 DELETING TIME-RECORD FOR TIME    191.16001
 DELETING TIME-RECORD FOR TIME    192.16001
 DELETING TIME-RECORD FOR TIME    193.16001
 DELETING TIME-RECORD FOR TIME    194.16001
 DELETING TIME-RECORD FOR TIME    195.16001
 DELETING TIME-RECORD FOR TIME    196.16001
 DELETING TIME-RECORD FOR TIME    197.16001
 DELETING TIME-RECORD FOR TIME    198.16001

 KEEPING TIME-RECORD FOR TIME    199.16001
 AND FOR TIME                    200.00000
 WORKSPACE RECLAIMED

 TIMESTEP AT     200.000000     SELECTED

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

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

**exb4c-plot**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exb4c\plot.DCM.test"
DIC>
DIC>
DIC> @@ exb4c_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE b4c
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  2.00000E+02
DIC> read exb4c
 OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1: set-title Fe-18%Cr-8%Ni
POST-1:
POST-1: @@
POST-1: @@ PLOT THE FRACTION OF SOLID AND COMPARE WITH A SCHEIL-GULLIVER
POST-1: @@ SIMULATION AND EQUILIBRIUM SOLIDIFICATION (DATA ON FILE exb4.exp).
POST-1: @@ IN THIS CASE WE CAN SEE THAT ALL THREE LINES INITIALLY FALL
POST-1: @@ ON THE SAME LINE.
POST-1: @@
POST-1: enter func fs=1-ivv(liquid);
POST-1: s-d-a x fs
POST-1: s-s-s x n 0 1
POST-1: s-ax-te x n Fraction solid
POST-1:
POST-1: s-d-a y t-c
POST-1: s-s-s y n 1420 1480
POST-1:
POST-1: s-p-c interf smalta lower
POST-1:
POST-1: app y exb4c.exp 0; 1
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
ORKING ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

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

# Example exb4d

## Solidification path of an Fe-18%Cr-8%Ni alloy: Peritectic reaction, heat-flux controls the temperature

This example is the same as exb4b but instead of controlling the temperature the amount heat extracted is given. Comparison is made with both a Scheil-Gulliver simulation and equilibrium solidification conditions, both made with Thermo-Calc.

**exb4d-setup**

```
SYS:About

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

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 21012) 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: Mon Nov 11 11:13:13 2019


SYS:SYS:MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exb4d\setup.DCM.test"
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  v10.0

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10:
TDB_TCFE10: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA
TDB_TCFE10: sw fedemo
 Current database: Iron Demo Database v2.1

 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                  CBCC_A12
 CHI_A12                 CUB_A13                 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
15:54:50,007 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

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

 TCFE10  =  Steels/Fe-Alloys  v10.0
 TCFE9   =  Steels/Fe-Alloys  v9.1
 TCFE8   =  Steels/Fe-Alloys  v8.1
 TCFE7   =  Steels/Fe-Alloys  v7.0
 TCFE6   =  Steels/Fe-Alloys  v6.2
 TCFE5   =  Steels/Fe-Alloys  v5.0
 TCFE4   =  Steels/Fe-Alloys  v4.1
 TCFE3   =  Steels/Fe-Alloys  v3.1
 TCFE2   =  Steels/Fe-Alloys  v2.1
 TCFE1   =  Steels/Fe-Alloys  v1.0
 FROST1  =  FROST database v1.2
 FEDAT   =  TCS/TT Steels Database v1.0
 TCNI10  =  Ni-Alloys  v10.0 SNAPSHOT
 TCNI9   =  Ni-Alloys  v9.1
 TCNI8   =  Ni-Alloys  v8.2
 TCNI7   =  Ni-Alloys  v7.2
 TCNI6   =  Ni-Alloys  v6.1
 TCNI5   =  Ni-Alloys  v5.1
 TCNI4   =  Ni-Alloys  v4.0
 TCNI1   =  Ni-Alloys  v1.3
```

```
TCAL6   =  Al-Alloys  v6.0
TCAL5   =  Al-Alloys  v5.1
TCAL4   =  Al-Alloys  v4.0
TCAL3   =  Al-Alloys  v3.0
TCAL2   =  Al-Alloys  v2.1
TCAL1   =  Al-Alloys  v1.2
TCMG5   =  Mg-Alloys  v5.1
TCMG4   =  Mg-Alloys  v4.0
TCMG3   =  Mg-Alloys  v3.0
TCMG2   =  Mg-Alloys  v2.0
TCMG1   =  Mg-Alloys  v1.1
TCTI2   =  Ti-Alloys  v2.1
TCTI1   =  Ti-Alloys  v1.0
TCCU3   =  Cu-Alloys  v3.1
TCCU2   =  Cu-Alloys  v2.0
TCCU1   =  Cu-Alloys  v1.0
TCCC1   =  Cemented carbide  v1.0
TCHEA4  =  High Entropy Alloy  v4.0
TCHEA3  =  High Entropy Alloy  v3.1
TCHEA2  =  High Entropy Alloy  v2.1.1
TCHEA1  =  High Entropy Alloy  v1.0
SSOL7   =  SGTE Alloy Solutions Database v7.0
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
TCOX10  =  Metal Oxide Solutions  v10.0 SNAPSHOT
TCOX9   =  Metal Oxide Solutions  v9.0
TCOX8   =  Metal Oxide Solutions  v8.0
TCOX7   =  Metal Oxide Solutions  v7.0
TCOX6   =  Metal Oxide Solutions  v6.0
TCOX5   =  Metal Oxide Solutions  v5.1
TCOX4   =  Metal Oxide Solutions  v4.1
ION3    =  Ionic Solutions  v3.0
ION2    =  Ionic Solutions  v2.6
ION1    =  Ionic Solutions  v1.5
NOX2    =  NPL Oxide Solutions Database v2.1
TCNOBL2 =  Noble Metals Alloys v2.0 SNAPSHOT
TCNOBL1 =  Noble Metals Alloys v1.0
TCSLD3  =  Solder Alloys  v3.2
TCSLD2  =  Solder Alloys  v2.0
TCSLD1  =  Solder Alloys  v1.1
TCSI1   =  Ultrapure Silicon  v1.2
TCMP2   =  Materials Processing  v2.5
TCES1   =  Combustion/Sintering  v1.1
TCSC1   =  Super Conductor  v1.0
TCFC1   =  SOFC Database v1.0
TCNF2   =  Nuclear Fuels  v2.1b
NUMT2   =  Nuclear Materials  v2.1
NUOX4   =  Nuclear Oxides  v4.2
NUCL15  =  IRSN NUCLEA-15_4
NUCL10  =  ThermoData NUCLEA Alloys-oxides TDB v10.2
MEPH15  =  IRSN Mephista-15_1
MEPH11  =  ThermoData MEPHISTA Nuclear Fuels TDB v11.2
TCAQ3   =  Aqueous Solution  v3.0
TCAQ2   =  Aqueous Solution  v2.7
AQS2    =  TGG Aqueous Solution Database v2.6
GCE2    =  TGG Geochemical/Environmental TDB v2.3
FEDEMO  =  Iron Demo Database v2.1
ALDEMO  =  Aluminum Demo Database v3.0
NIDEMO  =  Nickel Demo Database v1.1
CUDEMO  =  Copper Demo Database v1.0
SLDEMO  =  Solder Demo Database v1.0
OXDEMO  =  Oxide Demo Database v1.0
SUBDEMO =  Substance Demo Database v1.0
PTERN   =  Public Ternary Alloys TDB v1.3
PAQ2    =  Public Aqueous Soln (SIT) TDB v2.4
PG35    =  G35 Binary Semi-Conductors TDB v1.2
PURE5   =  SGTE Unary (Pure Elements) TDB v5.1
MOB2    =  Alloys Mobility  v2.7
MOB1    =  Alloys Mobility  v1.3
MOBFE1  =  Steels/Fe-Alloys Mobility  v1.1
MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
MOBFE5  =  Steels/Fe-Alloys Mobility  v5.0
MOBNI5  =  Ni-Alloys Mobility  v5.1
MOBNI4  =  Ni-Alloys Mobility  v4.1
MOBNI3  =  Ni-Alloys Mobility  v3.2
MOBNI2  =  Ni-Alloys Mobility  v2.4
MOBNI1  =  Ni-Alloys Mobility  v1.10
MOBAL5  =  Al-Alloys Mobility  v5.0
MOBAL4  =  Al-Alloys Mobility  v4.0
MOBAL3  =  Al-Alloys Mobility  v3.0
MOBAL2  =  Al-Alloys Mobility  v2.0
MOBAL1  =  Al-Alloys Mobility  v1.0
MOBCU1  =  Cu-Alloys Mobility  v1.0
MOBCU2  =  Cu-Alloys Mobility  v2.0
MOBCU3  =  Cu-Alloys Mobility  v3.0
MOBHEA1 =  High Entropy Alloys Mobility  v1.0
MOBHEA2 =  High Entropy Alloys Mobility  v2.0
MOBMG1  =  Mg-Alloys Mobility  v1.0
MOBSI1  =  Si-Alloys Mobility  v1.0
MOBSLD1 =  Solder-Alloys Mobility  v1.1
MOBTI3  =  Ti-Alloys Mobility  v3.0
MOBTI2  =  Ti-Alloys Mobility  v2.0
MOBTI1  =  Ti-Alloys Mobility  v1.0
MALDEMO =  Al-Alloys Mobility demo database v2.0
MFEDEMO =  Fe-Alloys Mobility demo database v2.0
MNIDEMO =  Ni-Alloys Mobility demo database v1.0
MCUDEMO =  Cu-Alloys Mobility demo database v1.0
USER    =  User defined Database
```

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

 VA  DEFINED

 *** WARNING: This database cannot be used with GES6, temporarily reverting to G
 ES5

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

 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
DIC>
DIC> @@
DIC> @@ ENTER inactive PHASES INTO THE REGION, BOTH PHASES ON THE
DIC> @@ SAME SIDE OF THE LIQUID REGION TO GET A PERITECTIC REACTION.
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inact
ATTACH TO REGION NAMED /SMALTA/: smalta
ATTACHED TO THE RIGHT OF SMALTA /YES/: yes
PHASE NAME: /NONE/: fcc#1
DEPENDENT COMPONENT ? /NI/: fe
 REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-3
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inact
ATTACH TO REGION NAMED /SMALTA/: smalta
ATTACHED TO THE RIGHT OF SMALTA /YES/: yes
PHASE NAME: /NONE/: bcc#1
DEPENDENT COMPONENT ? /NI/: fe
 REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-3
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> @@
DIC> @@ ENTER A START COMPOSITION FOR THE LIQUID
DIC> @@
DIC> enter-composition
REGION NAME : /SMALTA/: smalta
PHASE NAME: /LIQUID/: liq
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /CR/: cr lin 18 18
```

```
PROFILE FOR /NI/: ni lin  8  8
DIC>
DIC> @@
DIC> @@ THE BOUNDARY CONDITION IS A CLOSED SYSTEM (DEFAULT) AS WE DO NOT SPECIFY
DIC> @@ ANYTHING ELSE
DIC> @@
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 200
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /20/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ CHECK THE INTERFACE POSITION. THIS IS TO MAKE SURE THAT THE LIQUID REGION
DIC> @@ DOES NOT SHRINK TOO MUCH DURING A TIMESTEP. IN ADDITION THE TIMESTEP IS
DIC> @@ CONTROLLED BY THE PHASE INTERFACE DISPLACEMENT DURING THE SIMULATION.
DIC> @@
DIC> s-s-c
NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /AUTO/: yes
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/: no
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -> 1): /AUTO/:
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/: @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exb4d Y
DIC>
DIC> set-inter
 --OK---
DIC>
```

**exb4d-run**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exb4d\run.DCM.test"
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
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
 TEMPERATURE:   1900.     ENTHALPY:  0.7394E+05
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882254
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 TEMPERATURE:   1900.     ENTHALPY:  0.7394E+05
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882254
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 3.863918610051234E-007        3.864691456616007E-007        3.837208091757153E-016        3.821106605297053E-025       TIME =  0.10000000E-
06 DT =  0.10000000E-06 SUM OF SQUARES =  0.38211066E-24
 TEMPERATURE:   1900.     ENTHALPY:  0.7394E+05
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882254
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 9.508205000173971E-018       TIME =  0.26002472E-05 DT =  0.25002472E-05 SUM OF SQUARES =  0.95082050E-17
 TEMPERATURE:   1900.     ENTHALPY:  0.7394E+05
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882255
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 3.803283213789877E-017       TIME =  0.76007416E-05 DT =  0.50004944E-05 SUM OF SQUARES =  0.38032832E-16
 TEMPERATURE:   1900.     ENTHALPY:  0.7394E+05
 U-FRACTION IN SYSTEM:  CR = .191520367992483  FE = .733068011219292
                        NI = .0754116207882254
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 1.521313188418321E-016        1.521313188418321E-016


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


     ERROR RETURN FROM NS01A BECAUSE A NEARBY STATIONARY POINT OF F(X) IS PREDICTED
 *** ERROR  1890 IN DCNS01: ERROR RETURN FROM NS01A
 1.666578045201216E-016        1.666578045201216E-016        1.666578045201216E-016        1.352478211635110E-012        1.666578045201216E-
016        7.573827019817665E-030        7.573827019817665E-030        7.573827019817665E-030        7.573827019817665E-
030        1.666578045201216E-016        5.562266575976920E-030        5.562266575976920E-030        5.562266575976920E-
030        5.562266575976920E-030        5.562266575976920E-030        5.562266575976920E-030        1.041609024951602E-
017        1.546768164561797E-029       TIME =  0.37603708E-04 DT =  0.20001978E-04 SUM OF SQUARES =  0.15467682E-28


output ignored...



... output resumed

 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  6  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_FCC_A1

  CPU time used in timestep                    2 seconds
 1.010611839641213E-007        1.010624112174118E-007        1.010620821966687E-007        1.010407815978725E-007        7.802524850104379E-
009        1.010731516713628E-013        8.491417896581680E-
019       TIME =   197.90144     DT =  0.39375000     SUM OF SQUARES =  0.84914179E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.80357395E-07 AND   0.80357395E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.53376600E-05
 TEMPERATURE:   1702.     ENTHALPY:  0.5587E+05
 U-FRACTION IN SYSTEM:  CR = .19142649256958  FE = .73317849065027
                        NI = .0753950167801494
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  14  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_FCC_A1

  CPU time used in timestep                    1 seconds
 5.895191095916032E-007        5.896964303258992E-007        5.902402434406712E-007        5.893737193956263E-007        3.967197178262157E-
007        3.583238933502586E-007        2.901878750191593E-007        2.902122464542427E-007        1.672868017032316E-
007        2.285303868088257E-008        1.345973070721034E-014        6.746593624445023E-
018       TIME =   198.68894     DT =  0.78750000     SUM OF SQUARES =  0.67465936E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.89888651E-07 AND   0.89888651E-07
 POSITION OF INTERFACE R_FCC_A1 / R_BCC_A2 IS   0.54084473E-05
 TEMPERATURE:   1701.     ENTHALPY:  0.5580E+05
 U-FRACTION IN SYSTEM:  CR = .191426492569597  FE = .733178490650262
                        NI = .0753950167801402
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
```

```
  26  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: R_FCC_A1

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

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

 TIMESTEP AT     200.000000     SELECTED

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

**exb4d-plot**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exb4d\plot.DCM.test"
DIC>
DIC>
DIC> @@ exb4d_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE b4b
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  2.00000E+02
DIC> read exb4d
 OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1: set-title Fe-18%Cr-8%Ni
POST-1:
POST-1: @@
POST-1: @@ PLOT THE FRACTION OF SOLID AND COMPARE WITH SCHEIL-GULLIVER
POST-1: @@ SIMULATION AND EQUILIBRIUM SOLIDIFICATION (DATA ON FILE exb4.exp)
POST-1: @@
POST-1: s-d-a x time
  INFO: Time is set as independent variable
POST-1: s-d-a y T
POST-1: s-p-c inter first
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
ORKING ...orking ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

```
POST-1:
POST-1:Hit RETURN to continue
POST-1: enter func fs=1-ivv(liquid);
POST-1: s-d-a x fs
POST-1: s-s-s x n 0 1
POST-1: s-ax-te x n Fraction solid
POST-1:
POST-1: s-d-a y t-c
POST-1: s-s-s y n 1420 1480
POST-1:
POST-1: s-p-c interf smalta lower
POST-1:
POST-1: app y exb4d.exp 0; 1
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
ORKING ...orking ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

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

# Example exb5

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

This example demonstrates the evaluation of a ternary Fe-Cr-Ni diffusion couple. A thin slice of α phase (38%Cr, 0%Ni) is clamped between two thicker slices of γ phase (27%Cr, 20%Ni). The assembly is subsequently heat treated at 1373K. This setup corresponds to diffusion couple A in M. Kajihara, C.-B. Lim and M. Kikuchi: ISIJ International 33 (1993), pp. 498-507. See also M. Kajihara and M. Kikichi: Acta Metall.Mater. 41 (1993), pp.2045-2059.

**exb5-setup**

```
SYS:About

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

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 21012) 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: Mon Nov 11 11:13:13 2019


SYS:SYS:MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exb5\setup.DCM.test"
SYS: @@
SYS: @@ Moving boundary problem.
SYS: @@ Ternary diffusion couple of Fe-Ni-Cr alloys
SYS: @@ This example demonstrates the evaluation of a ternary Fe-Cr-Ni diffusion
SYS: @@ couple. A thin slice of alpha phase (38%Cr, 0%Ni) is clamped between
SYS: @@ two thicker slices of gamma phase (27%Cr, 20%Ni). The assembly is
SYS: @@ subsequently heat treated at 1373 K. This example corresponds to diffusion
SYS: @@ couple A in M. Kajihara, C.-B. Lim and M. Kikuchi: ISIJ International
SYS: @@ 33 (1993), pp. 498-507. See also M. Kajihara and M. Kikichi: Acta Metall.Mater.
SYS: @@ 41 (1993), pp.2045-2059.
SYS: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exb5_setup.DCM
SYS:
SYS: @@
SYS: @@ GO TO A DATABASE AND READ THE THERMODYNAMIC AND KINETIC DATA
SYS: @@
SYS: go da
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v10.0

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10: sw fedemo
 Current database: Iron Demo Database v2.1

 VA                      /-  DEFINED
TDB_FEDEMO: def-sys cr fe ni
 CR                      FE                      NI
   DEFINED
TDB_FEDEMO: rej-ph /all
 LIQUID:L                BCC_A2                  CBCC_A12
 CHI_A12                 CUB_A13                 FCC_A1
 HCP_A3                  LAVES_PHASE_C14         SIGMA
   REJECTED
TDB_FEDEMO: res-ph bcc,fcc
 BCC_A2                  FCC_A1  RESTORED
TDB_FEDEMO: get
16:03:06,364 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

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

 TCFE10  =  Steels/Fe-Alloys  v10.0
 TCFE9   =  Steels/Fe-Alloys  v9.1
 TCFE8   =  Steels/Fe-Alloys  v8.1
 TCFE7   =  Steels/Fe-Alloys  v7.0
 TCFE6   =  Steels/Fe-Alloys  v6.2
 TCFE5   =  Steels/Fe-Alloys  v5.0
 TCFE4   =  Steels/Fe-Alloys  v4.1
 TCFE3   =  Steels/Fe-Alloys  v3.1
 TCFE2   =  Steels/Fe-Alloys  v2.1
 TCFE1   =  Steels/Fe-Alloys  v1.0
 FROST1  =  FROST database v1.2
 FEDAT   =  TCS/TT Steels Database v1.0
 TCNI10  =  Ni-Alloys  v10.0 SNAPSHOT
 TCNI9   =  Ni-Alloys  v9.1
 TCNI8   =  Ni-Alloys  v8.2
 TCNI7   =  Ni-Alloys  v7.2
 TCNI6   =  Ni-Alloys  v6.1
 TCNI5   =  Ni-Alloys  v5.1
 TCNI4   =  Ni-Alloys  v4.0
 TCNI1   =  Ni-Alloys  v1.3
 TCAL6   =  Al-Alloys  v6.0
 TCAL5   =  Al-Alloys  v5.1
 TCAL4   =  Al-Alloys  v4.0
 TCAL3   =  Al-Alloys  v3.0
 TCAL2   =  Al-Alloys  v2.1
 TCAL1   =  Al-Alloys  v1.2
 TCMG5   =  Mg-Alloys  v5.1
 TCMG4   =  Mg-Alloys  v4.0
 TCMG3   =  Mg-Alloys  v3.0
 TCMG2   =  Mg-Alloys  v2.0
 TCMG1   =  Mg-Alloys  v1.1
 TCTI2   =  Ti-Alloys  v2.1
```

```
 TCTI1   =  Ti-Alloys  v1.0
 TCCU3   =  Cu-Alloys  v3.1
 TCCU2   =  Cu-Alloys  v2.0
 TCCU1   =  Cu-Alloys  v1.0
 TCCC1   =  Cemented carbide  v1.0
 TCHEA4  =  High Entropy Alloy  v4.0
 TCHEA3  =  High Entropy Alloy  v3.1
 TCHEA2  =  High Entropy Alloy  v2.1.1
 TCHEA1  =  High Entropy Alloy  v1.0
 SSOL7   =  SGTE Alloy Solutions Database v7.0
 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
 TCOX10  =  Metal Oxide Solutions  v10.0 SNAPSHOT
 TCOX9   =  Metal Oxide Solutions  v9.0
 TCOX8   =  Metal Oxide Solutions  v8.0
 TCOX7   =  Metal Oxide Solutions  v7.0
 TCOX6   =  Metal Oxide Solutions  v6.0
 TCOX5   =  Metal Oxide Solutions  v5.1
 TCOX4   =  Metal Oxide Solutions  v4.1
 ION3    =  Ionic Solutions  v3.0
 ION2    =  Ionic Solutions  v2.6
 ION1    =  Ionic Solutions  v1.5
 NOX2    =  NPL Oxide Solutions Database v2.1
 TCNOBL2 =  Noble Metals Alloys v2.0 SNAPSHOT
 TCNOBL1 =  Noble Metals Alloys v1.0
 TCSLD3  =  Solder Alloys  v3.2
 TCSLD2  =  Solder Alloys  v2.0
 TCSLD1  =  Solder Alloys  v1.1
 TCSI1   =  Ultrapure Silicon  v1.2
 TCMP2   =  Materials Processing  v2.5
 TCES1   =  Combustion/Sintering  v1.1
 TCSC1   =  Super Conductor  v1.0
 TCFC1   =  SOFC Database v1.0
 TCNF2   =  Nuclear Fuels  v2.1b
 NUMT2   =  Nuclear Materials  v2.1
 NUOX4   =  Nuclear Oxides  v4.2
 NUCL15  =  IRSN NUCLEA-15_4
 NUCL10  =  ThermoData NUCLEA Alloys-oxides TDB v10.2
 MEPH15  =  IRSN Mephista-15_1
 MEPH11  =  ThermoData MEPHISTA Nuclear Fuels TDB v11.2
 TCAQ3   =  Aqueous Solution  v3.0
 TCAQ2   =  Aqueous Solution  v2.7
 AQS2    =  TGG Aqueous Solution Database v2.6
 GCE2    =  TGG Geochemical/Environmental TDB v2.3
 FEDEMO  =  Iron Demo Database v2.1
 ALDEMO  =  Aluminum Demo Database v3.0
 NIDEMO  =  Nickel Demo Database v1.1
 CUDEMO  =  Copper Demo Database v1.0
 SLDEMO  =  Solder Demo Database v1.0
 OXDEMO  =  Oxide Demo Database v1.0
 SUBDEMO =  Substance Demo Database v1.0
 PTERN   =  Public Ternary Alloys TDB v1.3
 PAQ2    =  Public Aqueous Soln (SIT) TDB v2.4
 PG35    =  G35 Binary Semi-Conductors TDB v1.2
 PURE5   =  SGTE Unary (Pure Elements) TDB v5.1
 MOB2    =  Alloys Mobility  v2.7
 MOB1    =  Alloys Mobility  v1.3
 MOBFE1  =  Steels/Fe-Alloys Mobility  v1.1
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBFE5  =  Steels/Fe-Alloys Mobility  v5.0
 MOBNI5  =  Ni-Alloys Mobility  v5.1
 MOBNI4  =  Ni-Alloys Mobility  v4.1
 MOBNI3  =  Ni-Alloys Mobility  v3.2
 MOBNI2  =  Ni-Alloys Mobility  v2.4
 MOBNI1  =  Ni-Alloys Mobility  v1.10
 MOBAL5  =  Al-Alloys Mobility  v5.0
 MOBAL4  =  Al-Alloys Mobility  v4.0
 MOBAL3  =  Al-Alloys Mobility  v3.0
 MOBAL2  =  Al-Alloys Mobility  v2.0
 MOBAL1  =  Al-Alloys Mobility  v1.0
 MOBCU1  =  Cu-Alloys Mobility  v1.0
 MOBCU2  =  Cu-Alloys Mobility  v2.0
 MOBCU3  =  Cu-Alloys Mobility  v3.0
 MOBHEA1 =  High Entropy Alloys Mobility  v1.0
 MOBHEA2 =  High Entropy Alloys Mobility  v2.0
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBSLD1 =  Solder-Alloys Mobility  v1.1
 MOBTI3  =  Ti-Alloys Mobility  v3.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v2.0
 MFEDEMO =  Fe-Alloys Mobility demo database v2.0
 MNIDEMO =  Ni-Alloys Mobility demo database v1.0
 MCUDEMO =  Cu-Alloys Mobility demo database v1.0
 USER    =  User defined Database

DATABASE NAME /FEDEMO/: 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>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exb5\run.DCM.test"
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
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
  Trying old scheme                    4
 GENERATING STARTING VALUES FOR CELL #  1 INTERFACE #  2
 DETERMINING INITIAL EQUILIBRIUM VALUES
CALCULATING STARTING VALUES:       9   EQUILIBRIUM CALCULATIONS              *** ERROR  1611 IN QTHISS: TOO MANY ITERATIONS
 Give the command INFO TROUBLE for help
 DONE     6 OUT OF     9                                                     *** 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]
 3.503057562886359E-002        3.503838978365914E-002        3.503070722821699E-002        6.010860849728436E-004        4.996097709884086E-
004        3.843186467579116E-004        2.950169743173567E-004        2.951542157074272E-004        1.282237850461803E-
004        1.381556889258480E-007        1.911573577860582E-009        4.796670199127128E-011        2.303329573479827E-
015        9.076446564795043E-022       TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =  0.90764466E-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
 9.795982825923318E-004        9.797942120145652E-004        9.795987026603873E-004        1.691347619213920E-012        1.336248725813137E-
012        1.296755508755182E-012        1.534999389686798E-012        6.680078113294400E-012        1.211461410126802E-
012        1.208868038883532E-012        1.209218294227699E-012        6.030069421951742E-012        1.204231833024221E-
012        1.202965670449502E-012        1.202807770706800E-012        5.949304371358198E-012        1.202017608479717E-
012        1.201382005677497E-012        1.200629566641394E-012        5.941375535485801E-012        1.199444110338236E-
012        1.197808658376458E-012        1.194411670664971E-012        5.934987258752826E-012        1.188089753613608E-
012        1.175555861730537E-012        1.150438012336459E-012

output ignored...



... output resumed

 5.903159413548798E-012        5.623263617602902E-018       TIME =   2202011.6     DT =   360000.00     SUM OF SQUARES =  0.56232636E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.76087575E-11 AND  -0.76087575E-11
 POSITION OF INTERFACE ALPHA / GAMMA IS   0.95399425E-04
 U-FRACTION IN SYSTEM:  CR = .305280444969116  FE = .471672025958576
                        NI = .223047529072309
 TOTAL SIZE OF SYSTEM:  5.9345E-04 [m]
  7  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: GAMMA

  CPU time used in timestep                    2 seconds
 1.857518189654954E-006        1.860331047100623E-006        1.852885298908214E-006        1.312200324210213E-008        2.817259646342437E-
009        2.721415225819412E-013        5.566163328280860E-
022       TIME =   2562011.6     DT =   360000.00     SUM OF SQUARES =  0.55661633E-21
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.64452717E-11 AND  -0.64452717E-11
 POSITION OF INTERFACE ALPHA / GAMMA IS   0.93079127E-04
 U-FRACTION IN SYSTEM:  CR = .305280445340828  FE = .471672025304567
                        NI = .223047529354604
 TOTAL SIZE OF SYSTEM:  5.9345E-04 [m]
  6  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: GAMMA

  CPU time used in timestep                    2 seconds
 6.450183719788725E-007        6.464359949913071E-007        6.423189734736494E-007        3.408084210502422E-009        6.612816617269455E-
010        3.282384775077124E-015        2.598461744996450E-
023       TIME =   2922011.6     DT =   360000.00     SUM OF SQUARES =  0.25984617E-22
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.58181916E-11 AND  -0.58181916E-11
 POSITION OF INTERFACE ALPHA / GAMMA IS   0.90984578E-04
 U-FRACTION IN SYSTEM:  CR = .305280445518342  FE = .471672025224071
                        NI = .223047529257587
 TOTAL SIZE OF SYSTEM:  5.9345E-04 [m]
  7  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: GAMMA

  CPU time used in timestep                    2 seconds
 3.680117157702362E-007        3.689844214837353E-007        3.659976376876573E-007        1.727063392771554E-009        3.115314300000561E-
```

```
010        1.472819943068062E-015        7.399676411167170E-
025       TIME =   3282011.6     DT =   360000.00     SUM OF SQUARES =  0.73996764E-24
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.53569961E-11 AND  -0.53569961E-11
 POSITION OF INTERFACE ALPHA / GAMMA IS   0.89056060E-04
 U-FRACTION IN SYSTEM:  CR = .305280446098281  FE = .471672023538559
                        NI = .22304753036316
 TOTAL SIZE OF SYSTEM:  5.9345E-04 [m]
  5  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: GAMMA

  CPU time used in timestep                    1 seconds
 4.266420757950378E-009        4.268962376840457E-009        4.285278128027233E-009        1.878548996070811E-009        8.600583530051114E-
010        4.296047628313606E-016        3.057801091211827E-
024       TIME =   3600000.0     DT =   317988.44     SUM OF SQUARES =  0.30578011E-23
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.49339125E-11 AND  -0.49339125E-11
 POSITION OF INTERFACE ALPHA / GAMMA IS   0.87487133E-04
 U-FRACTION IN SYSTEM:  CR = .305280446350432  FE = .47167202291035
                        NI = .223047530739217
 TOTAL SIZE OF SYSTEM:  5.9345E-04 [m]
 MUST SAVE WORKSPACE ON FILE
 WORKSPACE SAVED ON FILE
 RECLAIMING WORKSPACE
 DELETING TIME-RECORD FOR TIME    0.0000000
 DELETING TIME-RECORD FOR TIME   0.10000000E-06
 DELETING TIME-RECORD FOR TIME   0.93355784E-05
 DELETING TIME-RECORD FOR TIME   0.27806735E-04
 DELETING TIME-RECORD FOR TIME   0.64749049E-04
 DELETING TIME-RECORD FOR TIME   0.13863368E-03
 DELETING TIME-RECORD FOR TIME   0.28640293E-03
 DELETING TIME-RECORD FOR TIME   0.58194144E-03
 DELETING TIME-RECORD FOR TIME   0.11730185E-02
 DELETING TIME-RECORD FOR TIME   0.23551725E-02
 DELETING TIME-RECORD FOR TIME   0.47194806E-02
 DELETING TIME-RECORD FOR TIME   0.94480967E-02
 DELETING TIME-RECORD FOR TIME   0.18905329E-01
 DELETING TIME-RECORD FOR TIME   0.37819794E-01
 DELETING TIME-RECORD FOR TIME   0.75648723E-01
 DELETING TIME-RECORD FOR TIME   0.15130658
 DELETING TIME-RECORD FOR TIME   0.19274610
 DELETING TIME-RECORD FOR TIME   0.21544345
 DELETING TIME-RECORD FOR TIME   0.26083817
 DELETING TIME-RECORD FOR TIME   0.35162760
 DELETING TIME-RECORD FOR TIME   0.40135502
 DELETING TIME-RECORD FOR TIME   0.50080986
 DELETING TIME-RECORD FOR TIME   0.69971953
 DELETING TIME-RECORD FOR TIME   0.91386552
 DELETING TIME-RECORD FOR TIME    1.3421575
 DELETING TIME-RECORD FOR TIME    2.0765292
 DELETING TIME-RECORD FOR TIME    3.2890531
 DELETING TIME-RECORD FOR TIME    5.5909634
 DELETING TIME-RECORD FOR TIME    10.194784
 DELETING TIME-RECORD FOR TIME    13.853758
 DELETING TIME-RECORD FOR TIME    21.171706
 DELETING TIME-RECORD FOR TIME    35.807602
 DELETING TIME-RECORD FOR TIME    65.079394
 DELETING TIME-RECORD FOR TIME    89.577418
 DELETING TIME-RECORD FOR TIME    138.57347
 DELETING TIME-RECORD FOR TIME    236.56556
 DELETING TIME-RECORD FOR TIME    319.77937
 DELETING TIME-RECORD FOR TIME    486.20699
 DELETING TIME-RECORD FOR TIME    761.28228
 DELETING TIME-RECORD FOR TIME    1232.2012
 DELETING TIME-RECORD FOR TIME    2093.8577
 DELETING TIME-RECORD FOR TIME    3662.1624
 DELETING TIME-RECORD FOR TIME    6798.7718
 DELETING TIME-RECORD FOR TIME    13071.991
 DELETING TIME-RECORD FOR TIME    25618.429
 DELETING TIME-RECORD FOR TIME    50711.304
 DELETING TIME-RECORD FOR TIME    100897.06
 DELETING TIME-RECORD FOR TIME    201268.56
 DELETING TIME-RECORD FOR TIME    402011.56
 DELETING TIME-RECORD FOR TIME    762011.56
 DELETING TIME-RECORD FOR TIME    1122011.6
 DELETING TIME-RECORD FOR TIME    1482011.6
 DELETING TIME-RECORD FOR TIME    1842011.6
 DELETING TIME-RECORD FOR TIME    2202011.6
 DELETING TIME-RECORD FOR TIME    2562011.6
 DELETING TIME-RECORD FOR TIME    2922011.6

 KEEPING TIME-RECORD FOR TIME    3282011.6
 AND FOR TIME                    3600000.0
 WORKSPACE RECLAIMED

 TIMESTEP AT     3600000.00     SELECTED

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

**exb5-plot**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exb5\plot.DCM.test"
DIC>
DIC>
DIC> @@ exb5_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE b5
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  3.60000E+06
DIC> read exb5
 OK
DIC>
DIC> @@
DIC> @@ ENTER THE POST PROCESSOR, PLOT SOME QUANTITIES AND COMPARE WITH EXPERIMENTS
DIC> @@
DIC> post
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1: set-title Diffusion Couple A
POST-1:
POST-1: @@
POST-1: @@ WE ARE INTERESTED IN THE POSITION OF THE UPPER INTERFACE OF REGION ALPHA
POST-1: @@
POST-1: s-p-c interf alpha upper
POST-1:
POST-1: @@
POST-1: @@ l0 IS THE INITIAL THICKNESS USED FOR NORMALIZATION
POST-1: @@
POST-1: enter func l0=186.9e-6;
POST-1: enter func aa=2*poi(alpha,u)/l0;
POST-1: enter func ab=time/l0**2;
POST-1: s-i-v time
POST-1:
POST-1: s-d-a x ab
POST-1: s-s-s x n 1e10 1e15
POST-1: s-ax-ty x log
POST-1:
POST-1: s-d-a y aa
POST-1: s-s-s y n 0 2
POST-1:
POST-1: app y exb5.exp
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 7
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

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

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

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

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

```
POST-1:
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: s-p-c time 3600000
POST-1: app y exb5.exp 0; 4
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

```
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ FINALLY PLOT DIFFERENT DIFFUSION PATHS.
POST-1: @@
POST-1: s-d-a x w(ni)
POST-1: s-s-s x n .00 .40
POST-1:
POST-1: s-d-a y w(cr)
POST-1: s-s-s y n .20 .45
POST-1:
POST-1: s-i-v dist glob
POST-1:
POST-1: s-p-c time 3600,36000,360000,3600000
POST-1:
POST-1: app y exb5.exp 0; 5 6
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

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

# Example exb6

## Micro-segregation of phosphorus

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

**exb6-setup**

```
SYS:About

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

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 21012) 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: Mon Nov 11 11:13:13 2019


SYS:SYS:MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exb6\setup.DCM.test"
SYS: @@
SYS: @@ Moving boundary problem.
SYS: @@ Microsegregation of phosphorus
SYS: @@ This example illustrates the effect of microsegregation
SYS: @@ of phosphorus during peritectic solidification in steel.
SYS: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@
SYS: @@ START BY GOING TO THE DATABASE MODULE
SYS: @@
SYS: go da
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v10.0

 VA                       /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10:
TDB_TCFE10: @@ USE A TCFE DATABASE FOR THERMODYNAMIC DATA
TDB_TCFE10: sw tcfe9
 Current database: Steels/Fe-Alloys  v9.1

 VA                       /-  DEFINED
 L12_FCC                  B2_BCC                   DICTRA_FCC_A1
   REJECTED
TDB_TCFE9:
TDB_TCFE9: @@ DEFINE THE SYSTEM TO WORK WITH
TDB_TCFE9: def-sys fe c si mn p
 FE                       C                        SI
 MN                       P  DEFINED
TDB_TCFE9:
TDB_TCFE9: @@ EXCLUDE THE THERMODYNAMIC DATA FOR THE PHASES THAT ARE NOT NEEDED
TDB_TCFE9: rej ph /all
 GAS:G                    LIQUID:L                 BCC_A2
 FCC_A1                   HCP_A3                   CBCC_A12
 CUB_A13                  DIAMOND_FCC_A4           RED_P
 WHITE_P                  GRAPHITE                 CEMENTITE
 M23C6                    M7C3                     M5C2
 KSI_CARBIDE              FE4N_LP1                 FECN_CHI
 LAVES_PHASE_C14          M3SI                     MN9SI2
 MN11SI19                 MN6SI                    G_PHASE
 CR3SI                    FE2SI                    FESI2_H
 FESI2_L                  MSI                      M5SI3
 AL4C3                    FE8SI2C                  SIC
 MN5SIC                   CUZN_EPSILON             AL5FE4
 MP_B31                   CU3P_D021                M2P_C22
 M3P_D0E                  MN3P_D0E                 FENBP
 FESI4P4                  SIP                      SIP2
 FLUORITE_C1:I            ZRO2_TETR:I              M2O3C:I
 M2O3H:I  REJECTED
TDB_TCFE9: res ph fcc liq bcc
 FCC_A1                   LIQUID:L                 BCC_A2
   RESTORED
TDB_TCFE9:
TDB_TCFE9: @@ RETRIEVE DATA FROM THE DATABASE FILE
TDB_TCFE9: get
16:08:05,677 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121-127; Molar
      volumes'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2012; Molar volumes'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  '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'
  'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
  'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, CALPHAD, 34, 279
      -85(2010); Mn-C'
  'W. Huang, Metall. Trans. A, 21A (1990) 2115-2123; TRITA-MAC 411 (Rev
      1989); C-FE-MN'
  'J.-H. Shim, C.-S. Oh, and D.N. Lee, Z. Metallkd., 2000, 91, p 114-120; Fe
      -C-P'
  'J. Grobner, H.L. Lukas and F. Aldinger, CALPHAD, 20 (1996) 247-254; Si-C
      and Al-Si-C'
  'J. Lacaze and B. Sundman, Metall. Mater. Trans. A, 22A (1991) 2211-2223;
      Fe-Si and Fe-Si-C'
  'W. Huang, CALPHAD, 13 (1989) 243-252; TRITA-MAC 388 (rev 1989); FE-MN'
  'J.-H. Shim, C.-S. Oh and D.N. Lee, J. Korean Inst. Met. Mater., 34 (1996)
      1385-1393; Fe-P'
  'J. Miettinen, G. Vassilev, J. Phase Equilib. Diffus. 59 (2014) 601-607;
      Cr-Fe-P'
  'J. Miettinen and B. Hallstedt, CALPHAD, 22 (1998) 231-256; Fe-Si and Fe
      -Si-C'
  'J. Miettinen, G. Vassilev, J. Phase Equilib. Diffus, 35(5), 2014, 587-594;
      . Mn-P and Fe-Mn-P'
```

```
  'W. Zheng, J. Alloys Compd., 632 (2015) 661-675'
  'S.-M. Liang and R. Schmid-Fetzer, J. Phase Equilib., 2014, 35, 24-35'
  'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, CALPHAD,
      submitted, 2011; Fe-Mn-C'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, 2014; Revision of the liquid
      C-Fe-Si description'
  'W. Zheng et al., J. Iron Steel Res. Int. 24(2)(2017) 190-197'
  'A. Forsberg and J. Agren, J. Phase Equilib., 14 (1993) 354-363; Fe-Mn-Si'
  'J. Miettinen, G. Vassilev, J. Phase Equilib. Diffus, 37(5) 2016, 283-290;
      Fe-P-Si'
 -OK-
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ MOBILITY/DIFFUSIVITY DATA ARE STORED IN A SEPARATE DATABASE FILE.
TDB_TCFE9: @@ SWITCH TO A MOBILITY DATABASE AND APPEND THE DATA.
TDB_TCFE9: @@
TDB_TCFE9: app
 Use one of these databases

 TCFE10  =  Steels/Fe-Alloys  v10.0
 TCFE9   =  Steels/Fe-Alloys  v9.1
 TCFE8   =  Steels/Fe-Alloys  v8.1
 TCFE7   =  Steels/Fe-Alloys  v7.0
 TCFE6   =  Steels/Fe-Alloys  v6.2
 TCFE5   =  Steels/Fe-Alloys  v5.0
 TCFE4   =  Steels/Fe-Alloys  v4.1
 TCFE3   =  Steels/Fe-Alloys  v3.1
 TCFE2   =  Steels/Fe-Alloys  v2.1
 TCFE1   =  Steels/Fe-Alloys  v1.0
 FROST1  =  FROST database v1.2
 FEDAT   =  TCS/TT Steels Database v1.0
 TCNI10  =  Ni-Alloys  v10.0 SNAPSHOT
 TCNI9   =  Ni-Alloys  v9.1
 TCNI8   =  Ni-Alloys  v8.2
 TCNI7   =  Ni-Alloys  v7.2
 TCNI6   =  Ni-Alloys  v6.1
 TCNI5   =  Ni-Alloys  v5.1
 TCNI4   =  Ni-Alloys  v4.0
 TCNI1   =  Ni-Alloys  v1.3
 TCAL6   =  Al-Alloys  v6.0
 TCAL5   =  Al-Alloys  v5.1
 TCAL4   =  Al-Alloys  v4.0
 TCAL3   =  Al-Alloys  v3.0
 TCAL2   =  Al-Alloys  v2.1
 TCAL1   =  Al-Alloys  v1.2
 TCMG5   =  Mg-Alloys  v5.1
 TCMG4   =  Mg-Alloys  v4.0
 TCMG3   =  Mg-Alloys  v3.0
 TCMG2   =  Mg-Alloys  v2.0
 TCMG1   =  Mg-Alloys  v1.1
 TCTI2   =  Ti-Alloys  v2.1
 TCTI1   =  Ti-Alloys  v1.0
 TCCU3   =  Cu-Alloys  v3.1
 TCCU2   =  Cu-Alloys  v2.0
 TCCU1   =  Cu-Alloys  v1.0
 TCCC1   =  Cemented carbide  v1.0
 TCHEA4  =  High Entropy Alloy  v4.0
 TCHEA3  =  High Entropy Alloy  v3.1
 TCHEA2  =  High Entropy Alloy  v2.1.1
 TCHEA1  =  High Entropy Alloy  v1.0
 SSOL7   =  SGTE Alloy Solutions Database v7.0
 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
 TCOX10  =  Metal Oxide Solutions  v10.0 SNAPSHOT
 TCOX9   =  Metal Oxide Solutions  v9.0
 TCOX8   =  Metal Oxide Solutions  v8.0
 TCOX7   =  Metal Oxide Solutions  v7.0
 TCOX6   =  Metal Oxide Solutions  v6.0
 TCOX5   =  Metal Oxide Solutions  v5.1
 TCOX4   =  Metal Oxide Solutions  v4.1
 ION3    =  Ionic Solutions  v3.0
 ION2    =  Ionic Solutions  v2.6
 ION1    =  Ionic Solutions  v1.5
 NOX2    =  NPL Oxide Solutions Database v2.1
 TCNOBL2 =  Noble Metals Alloys v2.0 SNAPSHOT
 TCNOBL1 =  Noble Metals Alloys v1.0
 TCSLD3  =  Solder Alloys  v3.2
 TCSLD2  =  Solder Alloys  v2.0
 TCSLD1  =  Solder Alloys  v1.1
 TCSI1   =  Ultrapure Silicon  v1.2
 TCMP2   =  Materials Processing  v2.5
 TCES1   =  Combustion/Sintering  v1.1
 TCSC1   =  Super Conductor  v1.0
 TCFC1   =  SOFC Database v1.0
 TCNF2   =  Nuclear Fuels  v2.1b
 NUMT2   =  Nuclear Materials  v2.1
 NUOX4   =  Nuclear Oxides  v4.2
 NUCL15  =  IRSN NUCLEA-15_4
 NUCL10  =  ThermoData NUCLEA Alloys-oxides TDB v10.2
 MEPH15  =  IRSN Mephista-15_1
 MEPH11  =  ThermoData MEPHISTA Nuclear Fuels TDB v11.2
 TCAQ3   =  Aqueous Solution  v3.0
 TCAQ2   =  Aqueous Solution  v2.7
 AQS2    =  TGG Aqueous Solution Database v2.6
 GCE2    =  TGG Geochemical/Environmental TDB v2.3
 FEDEMO  =  Iron Demo Database v2.1
 ALDEMO  =  Aluminum Demo Database v3.0
 NIDEMO  =  Nickel Demo Database v1.1
 CUDEMO  =  Copper Demo Database v1.0
 SLDEMO  =  Solder Demo Database v1.0
```

```
 OXDEMO  =  Oxide Demo Database v1.0
 SUBDEMO =  Substance Demo Database v1.0
 PTERN   =  Public Ternary Alloys TDB v1.3
 PAQ2    =  Public Aqueous Soln (SIT) TDB v2.4
 PG35    =  G35 Binary Semi-Conductors TDB v1.2
 PURE5   =  SGTE Unary (Pure Elements) TDB v5.1
 MOB2    =  Alloys Mobility  v2.7
 MOB1    =  Alloys Mobility  v1.3
 MOBFE1  =  Steels/Fe-Alloys Mobility  v1.1
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBFE5  =  Steels/Fe-Alloys Mobility  v5.0
 MOBNI5  =  Ni-Alloys Mobility  v5.1
 MOBNI4  =  Ni-Alloys Mobility  v4.1
 MOBNI3  =  Ni-Alloys Mobility  v3.2
 MOBNI2  =  Ni-Alloys Mobility  v2.4
 MOBNI1  =  Ni-Alloys Mobility  v1.10
 MOBAL5  =  Al-Alloys Mobility  v5.0
 MOBAL4  =  Al-Alloys Mobility  v4.0
 MOBAL3  =  Al-Alloys Mobility  v3.0
 MOBAL2  =  Al-Alloys Mobility  v2.0
 MOBAL1  =  Al-Alloys Mobility  v1.0
 MOBCU1  =  Cu-Alloys Mobility  v1.0
 MOBCU2  =  Cu-Alloys Mobility  v2.0
 MOBCU3  =  Cu-Alloys Mobility  v3.0
 MOBHEA1 =  High Entropy Alloys Mobility  v1.0
 MOBHEA2 =  High Entropy Alloys Mobility  v2.0
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBSLD1 =  Solder-Alloys Mobility  v1.1
 MOBTI3  =  Ti-Alloys Mobility  v3.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v2.0
 MFEDEMO =  Fe-Alloys Mobility demo database v2.0
 MNIDEMO =  Ni-Alloys Mobility demo database v1.0
 MCUDEMO =  Cu-Alloys Mobility demo database v1.0
 USER    =  User defined Database

DATABASE NAME /TCFE9/: mobfe4
 Current database: Steels/Fe-Alloys Mobility  v4.0

 VA  DEFINED
 B2_BCC  REJECTED
APP: def-sys fe c si mn p
 FE                      C                       SI
 MN                      P  DEFINED
APP: rej ph /all
 BCC_A2                  CEMENTITE               FCC_A1
 FE4N_LP1                HCP_A3                  LIQUID:L
   REJECTED
APP: res ph fcc liq bcc
 FCC_A1                  LIQUID:L                BCC_A2
   RESTORED
APP: get
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'This parameter has not been assessed'
  'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'
  'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
      -Ni'
  'Y. Liu, L. Zhang, et al. CALPHAD 33(2009)614-23; Fe-Mn-C (fcc)'
  'M. Yin, et al. (2010) unpublished work.'
  'W. Zheng, et al., J. Alloys and Compounds, 632 (2015) 661-675; Fe-Mn-Si
      (fcc)'
  'V. V. Mural and P. L. Gruzin, Phys. Met. Metallogr. (English Transl.) 17
      (5) (1964)154.; Impurity diff of P in fcc Fe.'
  'D. Bergner et al., Defect and Diffusion Forum 66-69(1989)409. Impurity
      diffusion of Si in fcc Fe.'
  'B. Jonsson: Z. Metallkunde 85(1994)498-501; C and N diffusion in bcc Cr
      -Fe-Ni'
  'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
      in bcc Fe'
  'S. Deng, et al., CALPHAD, 56 (2017) 230-240.'
  'B. Jonsson: Unpublished research bcc Fe-Si 1994'
  'Assessed from data presented in Landholt-Bornstein, Vol. 26, ed. H.
      Mehrer, springer (1990); Impurity diff of Mn in bcc Fe.'
  'Assessed from data presented in Landholt-Bornstein, Vol. 26, ed. H.
      Mehrer, springer (1990); Impurity diff of P in bcc Fe.'
  'No assessed or estimated parameters'
  'Estimation by using the modified Sutherland equation from Chen et al.,
      Phil. Magazine 94 (2014) 1552.'
  'L. Zhang et al., Acta Mater., 58(2010)3664.'
  'S.Q. Wang et al., Int J Mater Res, 104 (2013) 721-735. '
  'G. Barreau et al., C. R. Acad. Sci. (Paris) C 272(1971)618.; Impurity
      diffusion of Cr in fcc Cu.'
  'Y. Tang et al., CALPHAD, 49(2015)58.'
 -OK-
APP:
APP: @@
APP: @@ 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
DIC>
DIC> @@
DIC> @@ ENTER inactive PHASES INTO THE REGION, BOTH PHASES ON THE SAME SIDE
DIC> @@ OF THE LIQUID REGION TO GET A PERITECTIC REACTION.
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inact
ATTACH TO REGION NAMED /SMALTA/: smalta
ATTACHED TO THE RIGHT OF SMALTA /YES/: no
PHASE NAME: /NONE/: fcc#1
DEPENDENT COMPONENT ? /SI/: fe
 REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-5
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: inact
ATTACH TO REGION NAMED /SMALTA/: smalta
ATTACHED TO THE RIGHT OF SMALTA /YES/: no
PHASE NAME: /NONE/: bcc#1
DEPENDENT COMPONENT ? /SI/: fe
 REQUIRED DRIVING FORCE FOR PRECIPITATION: /1E-05/: 1e-5
CONDITION TYPE /CLOSED_SYSTEM/: closed
DIC>
DIC> @@
DIC> @@ ENTER A START COMPOSITION FOR THE LIQUID
DIC> @@
DIC> enter-composition
REGION NAME : /SMALTA/: smalta
PHASE NAME: /LIQUID/: liq
DEPENDENT COMPONENT ? /SI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: c lin 0.4 0.4
PROFILE FOR /MN/: si lin 0.7 0.7
PROFILE FOR /P/: mn lin 0.8 0.8
PROFILE FOR /SI/: p lin 0.03 0.03
DIC>
DIC> @@
DIC> @@ THE BOUNDARY CONDITION IS A CLOSED SYSTEM (DEFAULT) AS WE DO NOT SPECIFY
DIC> @@ ANYTHING ELSE
DIC> @@
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 3000
AUTOMATIC TIMESTEP CONTROL /YES/: yes
MAX TIMESTEP DURING INTEGRATION /300/: 15
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC>
DIC>
DIC>
DIC> @@ CHECK THE INTERFACE POSITION. THIS IS TO MAKE SURE THAT THE LIQUID REGION
DIC> @@ DOES NOT SHRINK TOO MUCH DURING A TIMESTEP. IN ADDITION THE TIMESTEP IS
DIC> @@ CONTROLLED BY THE PHASE INTERFACE DISPLACEMENT DURING THE SIMULATION.
DIC> @@
DIC> s-s-c
NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /AUTO/: yes
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -> 1): /AUTO/:
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/:
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exb6 Y
DIC>
DIC> set-inter
 --OK---
DIC>
```

**exb6-run**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exb6\run.DCM.test"
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
  1.0649       83
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
 U-FRACTION IN SYSTEM:  C = .0185375871047351  FE = .977481861209078
                        MN = .00810568126669963  P = 5.39133528237328E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 U-FRACTION IN SYSTEM:  C = .0185375871047351  FE = .977481861209078
                        MN = .00810568126669963  P = 5.39133528237328E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
 TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .018537587104735  FE = .977481861209078
                        MN = .00810568126669963  P = 5.39133528237328E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.22705714E-05 DT =  0.21705714E-05 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .018537587104735  FE = .977481861209078
                        MN = .00810568126669963  P = 5.39133528237328E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    1 seconds
 TIME =  0.66117143E-05 DT =  0.43411429E-05 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0185375871047351  FE = .977481861209078
                        MN = .00810568126669963  P = 5.39133528237328E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.15294000E-04 DT =  0.86822858E-05 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0185375871047351  FE = .977481861209078
                        MN = .00810568126669963  P = 5.39133528237328E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    1 seconds
 TIME =  0.32658572E-04 DT =  0.17364572E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .018537587104735  FE = .977481861209078
                        MN = .00810568126669963  P = 5.39133528237328E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.67387715E-04 DT =  0.34729143E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .018537587104735  FE = .977481861209078
                        MN = .00810568126669963  P = 5.39133528237327E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.13684600E-03 DT =  0.69458286E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .018537587104735  FE = .977481861209078
                        MN = .00810568126669963  P = 5.39133528237328E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    1 seconds
 TIME =  0.27576257E-03 DT =  0.13891657E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .018537587104735  FE = .977481861209078
                        MN = .00810568126669963  P = 5.39133528237328E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.55359572E-03 DT =  0.27783314E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .018537587104735  FE = .977481861209078
                        MN = .00810568126669964  P = 5.39133528237328E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.11092620E-02 DT =  0.55566629E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .018537587104735  FE = .977481861209078
                        MN = .00810568126669963  P = 5.39133528237328E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    1 seconds
 TIME =  0.22205946E-02 DT =  0.11113326E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .018537587104735  FE = .977481861209078
                        MN = .00810568126669964  P = 5.39133528237327E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.44432597E-02 DT =  0.22226652E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .018537587104735  FE = .977481861209078
                        MN = .00810568126669964  P = 5.39133528237327E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.88885901E-02 DT =  0.44453303E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .018537587104735  FE = .977481861209078
                        MN = .00810568126669964  P = 5.39133528237327E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.17779251E-01 DT =  0.88906606E-02 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .018537587104735  FE = .977481861209078
                        MN = .00810568126669963  P = 5.39133528237327E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
```

```
 TIME =  0.35560572E-01 DT =  0.17781321E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .018537587104735  FE = .977481861209078
                        MN = .00810568126669962  P = 5.39133528237327E-04
                        SI = .0138733239959838
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    1 seconds
 TIME =  0.71123215E-01 DT =  0.35562643E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .018537587104735  FE = .977481861209078
                        MN = .00810568126669963  P = 5.39133528237328E-04
                        SI = .0138733239959839
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.14224850     DT =  0.71125285E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0185375871047351  FE = .977481861209078
                        MN = .00810568126669965  P = 5.39133528237335E-04
                        SI = .0138733239959839
 TOTAL SIZE OF SYSTEM:  1E-04 [m]
  CPU time used in timestep                    0 seconds
 TIME =  0.28449907     DT =  0.14225057     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0185375871047352  FE = .977481861209078
                        MN = .0081056812666997  P = 5.39133528237319E-04


output ignored...



... output resumed

 DELETING TIME-RECORD FOR TIME    925.71866
 DELETING TIME-RECORD FOR TIME    940.71866
 DELETING TIME-RECORD FOR TIME    955.71866
 DELETING TIME-RECORD FOR TIME    970.71866
 DELETING TIME-RECORD FOR TIME    985.71866
 DELETING TIME-RECORD FOR TIME    1000.7187
 DELETING TIME-RECORD FOR TIME    1015.7187
 DELETING TIME-RECORD FOR TIME    1030.7187
 DELETING TIME-RECORD FOR TIME    1045.7187
 DELETING TIME-RECORD FOR TIME    1060.7187
 DELETING TIME-RECORD FOR TIME    1075.7187
 DELETING TIME-RECORD FOR TIME    1090.7187
 DELETING TIME-RECORD FOR TIME    1105.7187
 DELETING TIME-RECORD FOR TIME    1120.7187
 DELETING TIME-RECORD FOR TIME    1135.7187
 DELETING TIME-RECORD FOR TIME    1150.7187
 DELETING TIME-RECORD FOR TIME    1165.7187
 DELETING TIME-RECORD FOR TIME    1180.7187
 DELETING TIME-RECORD FOR TIME    1195.7187
 DELETING TIME-RECORD FOR TIME    1210.7187
 DELETING TIME-RECORD FOR TIME    1225.7187
 DELETING TIME-RECORD FOR TIME    1240.7187
 DELETING TIME-RECORD FOR TIME    1255.7187
 DELETING TIME-RECORD FOR TIME    1270.7187
 DELETING TIME-RECORD FOR TIME    1285.7187
 DELETING TIME-RECORD FOR TIME    1300.7187
 DELETING TIME-RECORD FOR TIME    1315.7187
 DELETING TIME-RECORD FOR TIME    1330.7187
 DELETING TIME-RECORD FOR TIME    1345.7187
 DELETING TIME-RECORD FOR TIME    1360.7187
 DELETING TIME-RECORD FOR TIME    1375.7187
 DELETING TIME-RECORD FOR TIME    1390.7187
 DELETING TIME-RECORD FOR TIME    1405.7187
 DELETING TIME-RECORD FOR TIME    1420.7187
 DELETING TIME-RECORD FOR TIME    1435.7187
 DELETING TIME-RECORD FOR TIME    1450.7187
 DELETING TIME-RECORD FOR TIME    1465.7187
 DELETING TIME-RECORD FOR TIME    1480.7187
 DELETING TIME-RECORD FOR TIME    1495.7187
 DELETING TIME-RECORD FOR TIME    1510.7187
 DELETING TIME-RECORD FOR TIME    1525.7187
 DELETING TIME-RECORD FOR TIME    1540.7187
 DELETING TIME-RECORD FOR TIME    1555.7187
 DELETING TIME-RECORD FOR TIME    1570.7187
 DELETING TIME-RECORD FOR TIME    1585.7187
 DELETING TIME-RECORD FOR TIME    1600.7187
 DELETING TIME-RECORD FOR TIME    1615.7187
 DELETING TIME-RECORD FOR TIME    1630.7187
 DELETING TIME-RECORD FOR TIME    1645.7187
 DELETING TIME-RECORD FOR TIME    1660.7187
 DELETING TIME-RECORD FOR TIME    1675.7187
 DELETING TIME-RECORD FOR TIME    1690.7187
 DELETING TIME-RECORD FOR TIME    1705.7187
 DELETING TIME-RECORD FOR TIME    1720.7187
 DELETING TIME-RECORD FOR TIME    1735.7187
 DELETING TIME-RECORD FOR TIME    1750.7187
 DELETING TIME-RECORD FOR TIME    1765.7187
 DELETING TIME-RECORD FOR TIME    1780.7187
 DELETING TIME-RECORD FOR TIME    1795.7187
 DELETING TIME-RECORD FOR TIME    1810.7187
 DELETING TIME-RECORD FOR TIME    1825.7187
 DELETING TIME-RECORD FOR TIME    1840.7187
 DELETING TIME-RECORD FOR TIME    1855.7187
 DELETING TIME-RECORD FOR TIME    1870.7187
 DELETING TIME-RECORD FOR TIME    1885.7187
 DELETING TIME-RECORD FOR TIME    1900.7187
 DELETING TIME-RECORD FOR TIME    1915.7187
 DELETING TIME-RECORD FOR TIME    1930.7187
 DELETING TIME-RECORD FOR TIME    1945.7187
 DELETING TIME-RECORD FOR TIME    1960.7187
 DELETING TIME-RECORD FOR TIME    1975.7187
 DELETING TIME-RECORD FOR TIME    1990.7187
 DELETING TIME-RECORD FOR TIME    2005.7187
 DELETING TIME-RECORD FOR TIME    2020.7187
 DELETING TIME-RECORD FOR TIME    2035.7187
 DELETING TIME-RECORD FOR TIME    2050.7187
 DELETING TIME-RECORD FOR TIME    2065.7187
 DELETING TIME-RECORD FOR TIME    2080.7187
 DELETING TIME-RECORD FOR TIME    2095.7187
 DELETING TIME-RECORD FOR TIME    2110.7187
 DELETING TIME-RECORD FOR TIME    2125.7187
 DELETING TIME-RECORD FOR TIME    2140.7187
 DELETING TIME-RECORD FOR TIME    2155.7187
 DELETING TIME-RECORD FOR TIME    2170.7187
 DELETING TIME-RECORD FOR TIME    2185.7187
 DELETING TIME-RECORD FOR TIME    2200.7187
 DELETING TIME-RECORD FOR TIME    2215.7187
```

```
 DELETING TIME-RECORD FOR TIME    2230.7187
 DELETING TIME-RECORD FOR TIME    2245.7187
 DELETING TIME-RECORD FOR TIME    2260.7187
 DELETING TIME-RECORD FOR TIME    2275.7187
 DELETING TIME-RECORD FOR TIME    2290.7187
 DELETING TIME-RECORD FOR TIME    2305.7187
 DELETING TIME-RECORD FOR TIME    2320.7187
 DELETING TIME-RECORD FOR TIME    2335.7187
 DELETING TIME-RECORD FOR TIME    2350.7187
 DELETING TIME-RECORD FOR TIME    2365.7187
 DELETING TIME-RECORD FOR TIME    2380.7187
 DELETING TIME-RECORD FOR TIME    2395.7187
 DELETING TIME-RECORD FOR TIME    2410.7187
 DELETING TIME-RECORD FOR TIME    2425.7187
 DELETING TIME-RECORD FOR TIME    2440.7187
 DELETING TIME-RECORD FOR TIME    2455.7187
 DELETING TIME-RECORD FOR TIME    2470.7187
 DELETING TIME-RECORD FOR TIME    2485.7187
 DELETING TIME-RECORD FOR TIME    2500.7187
 DELETING TIME-RECORD FOR TIME    2515.7187
 DELETING TIME-RECORD FOR TIME    2530.7187
 DELETING TIME-RECORD FOR TIME    2545.7187
 DELETING TIME-RECORD FOR TIME    2560.7187
 DELETING TIME-RECORD FOR TIME    2575.7187
 DELETING TIME-RECORD FOR TIME    2590.7187
 DELETING TIME-RECORD FOR TIME    2605.7187
 DELETING TIME-RECORD FOR TIME    2620.7187
 DELETING TIME-RECORD FOR TIME    2635.7187
 DELETING TIME-RECORD FOR TIME    2650.7187
 DELETING TIME-RECORD FOR TIME    2665.7187
 DELETING TIME-RECORD FOR TIME    2680.7187
 DELETING TIME-RECORD FOR TIME    2695.7187
 DELETING TIME-RECORD FOR TIME    2710.7187
 DELETING TIME-RECORD FOR TIME    2725.7187
 DELETING TIME-RECORD FOR TIME    2740.7187
 DELETING TIME-RECORD FOR TIME    2755.7187
 DELETING TIME-RECORD FOR TIME    2770.7187
 DELETING TIME-RECORD FOR TIME    2785.7187
 DELETING TIME-RECORD FOR TIME    2800.7187
 DELETING TIME-RECORD FOR TIME    2815.7187
 DELETING TIME-RECORD FOR TIME    2830.7187
 DELETING TIME-RECORD FOR TIME    2845.7187
 DELETING TIME-RECORD FOR TIME    2860.7187
 DELETING TIME-RECORD FOR TIME    2875.7187
 DELETING TIME-RECORD FOR TIME    2890.7187
 DELETING TIME-RECORD FOR TIME    2905.7187
 DELETING TIME-RECORD FOR TIME    2920.7187
 DELETING TIME-RECORD FOR TIME    2935.7187
 DELETING TIME-RECORD FOR TIME    2950.7187
 DELETING TIME-RECORD FOR TIME    2965.7187
 DELETING TIME-RECORD FOR TIME    2980.7187

 KEEPING TIME-RECORD FOR TIME    2995.7187
 AND FOR TIME                    3000.0000
 WORKSPACE RECLAIMED

 TIMESTEP AT     3000.00000     SELECTED

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

**exb6-plot**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exb6\plot.DCM.test"
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  3.00000E+03
DIC> read exb6
 OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1: set-title Fe-0.4%C-0.7%Si-0.8%Mn-0.03%P
POST-1:
POST-1: s-d-a y t-c
POST-1: s-d-a x time
  INFO: Time is set as independent variable
POST-1: s-p-c interf first
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
ORKING ...orking ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

```
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ PLOT THE FRACTION OF SOLID
POST-1: @@
POST-1: enter func fs=1-ivv(liq);
POST-1: s-d-a x fs
POST-1: s-s-s x n 0 1
POST-1: s-ax-te x n Fraction solid
POST-1:
POST-1: s-d-a y t-c
POST-1:
POST-1:
POST-1: s-p-c interf smalta lower
POST-1:
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
ORKING ...orking ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

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

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

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

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

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

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

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

```
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: ent function mnn
FUNCTION: w(mn)/0.008
&
POST-1: ent function sin
FUNCTION: w(si)/0.007
&
POST-1: ent function pn
FUNCTION: w(p)/0.0003
&
POST-1: ent function cn
FUNCTION: w(c)/0.004
&
POST-1: ent tabel segregation
Variable(s) mnn sin pn cn
POST-1:
POST-1:
POST-1: s-d-a y segregation
COLUMN NUMBER /*/:
POST-1:
POST-1:
POST-1: s-p-c time 610
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

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

```
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: s-p-c time 1500
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

```
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: s-p-c time 3000
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

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

# Example exb7

## Moving boundary problem with multiple phases on each side of the boundary

This example shows how to enter dispersed phases on either side of a phase interface. The particular case shows how the kinetics of a ferrite to austenite transformation is affected by simultaneous precipitation of niobium carbide. The transformation is caused by carburization.

**exb7-setup**

```
SYS:About

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

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 21012) 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: Mon Nov 11 11:13:13 2019


SYS:SYS:MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exb7\setup.DCM"
SYS: @@ This example modifies the database interactively, which is not
SYS: @@ yet supported by GES6. Therefore, we enforce the use of GES5.
SYS: set-ges-version 5
SYS:
SYS: @@
SYS: @@ Moving boundary problem.
SYS: @@ Moving boundary problem with multiple phases on each side
SYS: @@ This example shows how to enter dispersed phases on either side
SYS: @@ of a phase interface. The particular case shows how
SYS: @@ the kinetics of a ferrite to austenite transformation is
SYS: @@ affected by simultaneous precipitation of niobium carbide.
SYS: @@ The transformation is caused by carburization.
SYS: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASE
SYS: @@
SYS: go da
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v10.0

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10:
TDB_TCFE10: @@
TDB_TCFE10: @@ USE A TCFE DATABASE FOR THERMODYNAMIC DATA
TDB_TCFE10: @@
TDB_TCFE10: sw tcfe9
 Current database: Steels/Fe-Alloys  v9.1

 VA                      /-  DEFINED
 L12_FCC                 B2_BCC                  DICTRA_FCC_A1
   REJECTED
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ DEFINE THE SYSTEM TO WORK WITH
TDB_TCFE9: @@
TDB_TCFE9: def-species fe c nb
 FE                      C                       NB
   DEFINED
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ EXCLUDE THE THERMODYNAMIC DATA FOR THE PHASES THAT ARE NOT NEEDED
TDB_TCFE9: @@
TDB_TCFE9: rej ph * all
 GAS:G                   LIQUID:L                BCC_A2
 FCC_A1                  HCP_A3                  CBCC_A12
 CUB_A13                 DIAMOND_FCC_A4          GRAPHITE
 CEMENTITE               M23C6                   M7C3
 M6C                     M5C2                    KSI_CARBIDE
 Z_PHASE                 FE4N_LP1                FECN_CHI
 SIGMA                   MU_PHASE                LAVES_PHASE_C14
 G_PHASE                 CR3SI                   NBNI3
 AL5FE4  REJECTED
TDB_TCFE9: res ph fcc bcc grap
 FCC_A1                  BCC_A2                  GRAPHITE
   RESTORED
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ RETRIEVE DATA FROM THE DATABASE FILE
TDB_TCFE9: @@
TDB_TCFE9: get
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 Creating a new composition set FCC_A1#2
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121-127; Molar
      volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'P. Franke, Estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
  'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
  'A.V. Khvan, B. Hallstedt, CALPHAD, 40, 10-15(2013); Fe-Nb, Nb-C, Nb-N, Fe
      -Mn-Nb, Fe-Nb-C, Fe-Nb-N, Nb-C-N, Fe-Mn-Nb-C, Fe-Mn-Nb-N'
  'B.-J. Lee, Metall. Mater. Trans. A, 32A (2001) 2423-39'
  'S. Canderyd, Report IM-2005-109, Stockholm, Sweden; Fe-Nb-C'
  'W. Huang, Z. Metallkd., 6 (1990) 397-404; Fe-Nb-C'
 -OK-
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ NOW APPEND A SSUB DATABASE FROM WHICH WE READ THE THERMODYNAMIC
TDB_TCFE9: @@ DESCRIPTION OF NIOBIUM CARBIDE
TDB_TCFE9: @@
TDB_TCFE9:
```

```
TDB_TCFE9: app SSUB6
 Current database: SGTE Substances Database v6.0

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

 List of references for assessed data

   C1NB1 I. BARIN 3rd. Edition
      C1NB1
      Data taken from BARIN 3rd. Ed. (1995)
 -OK-
APP:
APP:
APP: @@
APP: @@ MOBILITY/DIFFUSIVITY DATA ARE STORED IN A SEPARATE DATABASE FILE.
APP: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE THE DATA
APP: @@
APP: app mobfe4
 Current database: Steels/Fe-Alloys Mobility  v4.0

 VA  DEFINED
 B2_BCC  REJECTED
APP: def-sys fe c nb
 FE                      C                       NB
   DEFINED
APP: rej ph * all
 BCC_A2                  CEMENTITE               FCC_A1
 FE4N_LP1                HCP_A3                  LIQUID:L
   REJECTED
APP: res ph fcc bcc
 FCC_A1                  BCC_A2  RESTORED
APP: get
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'This parameter has not been assessed'
  'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'
  'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
      -Ni'
  'J. Geise and Ch. Herzig, Z. Metallkd. 76(1985)622.; Impurity diffusion of
      Nb in fcc Fe.'
  'Assessed from data presented by B. B. Yu and R. F. Davis J. Phys. Chem.
      Solids 40(1979)997.; C Self-Diff in NbC.'
  'B. Jonsson: Z. Metallkunde 85(1994)498-501; C and N diffusion in bcc Cr
      -Fe-Ni'
  'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
      in bcc Fe'
  'R. F. Peart, Acta Metall. 10(1962)519.; Impurity diffusion of Fe in bcc
      Nb.'
  'Assessed from data presented in Landholt-Bornstein, Vol. 26, ed. H.
      Mehrer, springer (1990); Impurity diff of Nb in bcc Fe.'
  'R. E. Einziger et al., Phys. Rev. B 17(1978)440.; self-diffusion of Nb in
      bcc Nb.'
 -OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR WHERE THE SYSTEM IS SET UP
APP: @@
APP: go d-m
 NO TIME STEP DEFINED
 *** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
 *** ENTERING C1NB1_S AS A DIFFUSION NONE PHASE
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 1073.15; * N
DIC>
DIC> @@
DIC> @@ ENTER REGIONS ferr AND aus
DIC> @@
DIC> enter-region
REGION NAME : ferr
DIC>
DIC> ent-reg
REGION NAME : aus
ATTACH TO REGION NAMED /FERR/: ferr
ATTACHED TO THE RIGHT OF FERR /YES/: n
DIC>
DIC> @@
DIC> @@ ENTER GRIDS INTO REGIONS
DIC> @@
DIC> enter-grid
REGION NAME : /AUS/: ferr
WIDTH OF REGION /1/: 2.499999e-3
TYPE /LINEAR/: AUTO
DIC>
DIC>
DIC> enter-grid
```

```
REGION NAME : /AUS/: aus
WIDTH OF REGION /1/: 1e-9
TYPE /LINEAR/: AUTO
DIC>
DIC>
DIC> @@
DIC> @@ ENTER active PHASES INTO REGIONS
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /AUS/: ferr
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: bcc
DIC>
DIC>
DIC> en-ph
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /AUS/: ferr
PHASE TYPE /MATRIX/: sph
PHASE NAME: /NONE/: c1nb1_s
 INFO: EQUILIBRIUM COMPOSITION AND FRACTION OF SPHEROID PHASES USED AS DEFAULT
DIC>
DIC>
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /AUS/: aus
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC>
DIC> en-ph
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /AUS/: aus
PHASE TYPE /MATRIX/: sph
PHASE NAME: /NONE/: c1nb1_s
 INFO: EQUILIBRIUM COMPOSITION AND FRACTION OF SPHEROID PHASES USED AS DEFAULT
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITIONS OF THE PHASES
DIC> @@
DIC> enter-composition
REGION NAME : /AUS/: ferr
PHASE NAME: /BCC_A2/: bcc
DEPENDENT COMPONENT ? /NB/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: C
TYPE /LINEAR/: lin
VALUE OF FIRST POINT : 1e-3
VALUE OF LAST POINT : /1E-3/: 1e-3
PROFILE FOR /NB/: nb
TYPE /LINEAR/: lin
VALUE OF FIRST POINT : 0.28
VALUE OF LAST POINT : /0.28/: 0.28
DIC>
DIC> en-co
REGION NAME : /AUS/: ferr
PHASE NAME: /BCC_A2/: c1nb1_s
USE EQUILIBRIUM VALUE /Y/: y
DIC>
DIC> enter-composition
REGION NAME : /AUS/: aus
PHASE NAME: /FCC_A1#1/: fcc#1
DEPENDENT COMPONENT ? /NB/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: C
TYPE /LINEAR/: lin
VALUE OF FIRST POINT : 0.89
VALUE OF LAST POINT : /0.89/: 0.89
PROFILE FOR /NB/: nb
TYPE /LINEAR/: lin
VALUE OF FIRST POINT : 0.28
VALUE OF LAST POINT : /0.28/: 0.28
DIC>
DIC> en-co
REGION NAME : /AUS/: aus
PHASE NAME: /FCC_A1#1/: c1nb1_s
USE EQUILIBRIUM VALUE /Y/: y
DIC>
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 32400
AUTOMATIC TIMESTEP CONTROL /YES/: y
MAX TIMESTEP DURING INTEGRATION /3240/: 3240
INITIAL TIMESTEP : /1E-07/: 1e-8
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/: 1e-15
DIC>
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ SET THE REFERENCE PHASE OF CARBON AS GRAPHITE
DIC> @@
DIC> s-ref
Component: c
Reference state: grap
Temperature /*/: *
Pressure /100000/: 1e5
DIC>
DIC> @@
DIC> @@ SET THE BOUNDARY CONDITION.
DIC> @@ THE CARBON ACTIVITY IS THE ONE ON THE BOUNDARY
DIC> @@
DIC> s-cond
GLOBAL OR BOUNDARY CONDITION /GLOBAL/: bound
BOUNDARY /LOWER/: low
CONDITION TYPE /CLOSED_SYSTEM/: mix
Dependent substitutional element:FE
```

```
Dependent interstitial element:VA
TYPE OF CONDITION FOR COMPONENT C /ZERO_FLUX/: act
LOW TIME LIMIT /0/: 0
ACR(C)(TIME)= 1.0;
HIGH TIME LIMIT /*/: *
ANY MORE RANGES /N/: N
TYPE OF CONDITION FOR COMPONENT NB /ZERO_FLUX/: zero
DIC>
DIC> @@
DIC> @@ ENABLE THE HOMOGENIZATION MODEL
DIC> @@
DIC> ho y y
 INFO: HOMOGENIZATION MODEL ENABLED
DIC>
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exb7 Y
DIC>
DIC>
DIC> set-inter
 --OK---
DIC>
```

**exb7-run**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exb7\run.DCM"
DIC> @@
DIC> @@ READ THE SET UP FROM FILE AND START THE SIMULATION
DIC> @@
DIC>
DIC> go d-m
 TIME STEP AT TIME  0.00000E+00
 *** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
 *** ENTERING C1NB1_S AS A DIFFUSION NONE PHASE
DIC> read exb7
 OK
DIC> sim yes
 Region: AUS
 double geometric
 dense at outer boundaries, coarse at  0.50000E-09
lower part   1.0800       16
upper part  0.92593       16
 Region: FERR
 single geometric dense at   0.0000
  1.0800      114
 DEGREE OF IMPLICITY SET TO EULER BACKWARD
 STARTING SIMULATION USING HOMOGENIZATION MODEL
 ----------------------------------------------
 WARNING: ELEMENT C
 IS BOTH INTERSTITIAL AND SUBSTITUTIONAL
 AND RESULTS MUST BE INTERPRETED WITH CARE
 INFO: PHASE WITH LIMITED SOLUBILITY OF ELEMENT(S) EXIST
 A FALLBACK PHASE ZZDICTRA_GHOST WILL BE DEFINED
 ALONG WITH THE FOLLOWING PARAMETERS:
 G(ZZDICTRA_GHOST,C;0)-H298(GRAPHITE,C;0)
 G(ZZDICTRA_GHOST,FE;0)-H298(BCC_A2,FE;0)
 G(ZZDICTRA_GHOST,NB;0)-H298(BCC_A2,NB;0)
 L(ZZDICTRA_GHOST,C,FE;0)
 L(ZZDICTRA_GHOST,C,NB;0)
 L(ZZDICTRA_GHOST,FE,NB;0)
 INFO: FCC_A1#2 is stable but not entered in the simulation
  WARNING:C1NB1_S HAS NO VOLUME FRACTION, CREATING ONE
  WARNING:C1NB1_S HAS NO VOLUME FRACTION, CREATING ONE
Starting time-step t0=   0.0000000     dt=  0.10000000E-07
 Error                     408
 Error                     408
Starting time-step t0=  0.48828125E-11 dt=  0.48828125E-11
Starting time-step t0=  0.97656250E-11 dt=  0.97656250E-11
Starting time-step t0=  0.19531250E-10 dt=  0.19531250E-10
Starting time-step t0=  0.39062500E-10 dt=  0.39062500E-10
Starting time-step t0=  0.78125000E-10 dt=  0.78125000E-10
Starting time-step t0=  0.15625000E-09 dt=  0.15625000E-09
Starting time-step t0=  0.31250000E-09 dt=  0.15625000E-09
Starting time-step t0=  0.46875000E-09 dt=  0.31250000E-09
Starting time-step t0=  0.78125000E-09 dt=  0.31250000E-09
Starting time-step t0=  0.10937500E-08 dt=  0.31250000E-09
Starting time-step t0=  0.14062500E-08 dt=  0.31250000E-09
Starting time-step t0=  0.17187500E-08 dt=  0.62500000E-09
Starting time-step t0=  0.23437500E-08 dt=  0.62500000E-09
Starting time-step t0=  0.29687500E-08 dt=  0.12500000E-08
Starting time-step t0=  0.42187500E-08 dt=  0.25000000E-08
Starting time-step t0=  0.67187500E-08 dt=  0.50000000E-08
Starting time-step t0=  0.11718750E-07 dt=  0.10000000E-07
Starting time-step t0=  0.21718750E-07 dt=  0.10000000E-07
Starting time-step t0=  0.31718750E-07 dt=  0.10000000E-07
Starting time-step t0=  0.41718750E-07 dt=  0.10000000E-07
Starting time-step t0=  0.51718750E-07 dt=  0.20000000E-07
Starting time-step t0=  0.71718750E-07 dt=  0.20000000E-07
Starting time-step t0=  0.91718750E-07 dt=  0.20000000E-07
Starting time-step t0=  0.11171875E-06 dt=  0.40000000E-07
Starting time-step t0=  0.15171875E-06 dt=  0.40000000E-07
Starting time-step t0=  0.19171875E-06 dt=  0.80000000E-07
Starting time-step t0=  0.27171875E-06 dt=  0.80000000E-07
Starting time-step t0=  0.35171875E-06 dt=  0.16000000E-06
Starting time-step t0=  0.51171875E-06 dt=  0.32000000E-06
Starting time-step t0=  0.83171875E-06 dt=  0.64000000E-06
Starting time-step t0=  0.14717187E-05 dt=  0.12800000E-05
Starting time-step t0=  0.27517187E-05 dt=  0.25600000E-05
Starting time-step t0=  0.53117187E-05 dt=  0.51200000E-05
Starting time-step t0=  0.10431719E-04 dt=  0.10240000E-04
Starting time-step t0=  0.20671719E-04 dt=  0.20480000E-04
Starting time-step t0=  0.41151719E-04 dt=  0.40960000E-04
Starting time-step t0=  0.82111719E-04 dt=  0.81920000E-04
Starting time-step t0=  0.16403172E-03 dt=  0.16384000E-03
Starting time-step t0=  0.32787172E-03 dt=  0.32768000E-03
Starting time-step t0=  0.65555172E-03 dt=  0.65536000E-03
Starting time-step t0=  0.13109117E-02 dt=  0.13107200E-02
Starting time-step t0=  0.26216317E-02 dt=  0.26214400E-02
Starting time-step t0=  0.52430717E-02 dt=  0.52428800E-02
Starting time-step t0=  0.10485952E-01 dt=  0.10485760E-01
Starting time-step t0=  0.20971712E-01 dt=  0.20971520E-01
Starting time-step t0=  0.41943232E-01 dt=  0.41943040E-01
Starting time-step t0=  0.83886272E-01 dt=  0.41943040E-01
Starting time-step t0=  0.12582931     dt=  0.41943040E-01
Starting time-step t0=  0.16777235     dt=  0.83886080E-01
Starting time-step t0=  0.18874387     dt=  0.20971520E-01
 Error                     408
 Error                     408
Starting time-step t0=  0.18907155     dt=  0.32768000E-03
Starting time-step t0=  0.18939923     dt=  0.32768000E-03
Starting time-step t0=  0.18972691     dt=  0.32768000E-03
Starting time-step t0=  0.19005459     dt=  0.32768000E-03
Starting time-step t0=  0.19038227     dt=  0.32768000E-03
Starting time-step t0=  0.19070995     dt=  0.32768000E-03
Starting time-step t0=  0.19103763     dt=  0.32768000E-03
Starting time-step t0=  0.19136531     dt=  0.32768000E-03
Starting time-step t0=  0.19169299     dt=  0.32768000E-03
Starting time-step t0=  0.19202067     dt=  0.65536000E-03
Starting time-step t0=  0.19267603     dt=  0.65536000E-03
Starting time-step t0=  0.19333139     dt=  0.65536000E-03
Starting time-step t0=  0.19398675     dt=  0.65536000E-03
Starting time-step t0=  0.19464211     dt=  0.65536000E-03
Starting time-step t0=  0.19529747     dt=  0.65536000E-03
Starting time-step t0=  0.19595283     dt=  0.13107200E-02
Starting time-step t0=  0.19726355     dt=  0.13107200E-02
```

```
Starting time-step t0=  0.19857427     dt=  0.13107200E-02
Starting time-step t0=  0.19988499     dt=  0.13107200E-02
Starting time-step t0=  0.20119571     dt=  0.13107200E-02
Starting time-step t0=  0.20250643     dt=  0.26214400E-02
Starting time-step t0=  0.20512787     dt=  0.26214400E-02
Starting time-step t0=  0.20774931     dt=  0.52428800E-02
Starting time-step t0=  0.21299219     dt=  0.52428800E-02
Starting time-step t0=  0.21823507     dt=  0.52428800E-02
Starting time-step t0=  0.22347795     dt=  0.10485760E-01
Starting time-step t0=  0.23396371     dt=  0.10485760E-01
Starting time-step t0=  0.24444947     dt=  0.10485760E-01
Starting time-step t0=  0.25493523     dt=  0.10485760E-01
Starting time-step t0=  0.26542099     dt=  0.10485760E-01
Starting time-step t0=  0.27590675     dt=  0.20971520E-01
Starting time-step t0=  0.29687827     dt=  0.20971520E-01
Starting time-step t0=  0.31784979     dt=  0.20971520E-01
Starting time-step t0=  0.33882131     dt=  0.20971520E-01
Starting time-step t0=  0.35979283     dt=  0.20971520E-01
Starting time-step t0=  0.38076435     dt=  0.20971520E-01
Starting time-step t0=  0.40173587     dt=  0.20971520E-01
Starting time-step t0=  0.42270739     dt=  0.20971520E-01
Starting time-step t0=  0.44367891     dt=  0.20971520E-01
Starting time-step t0=  0.46465043     dt=  0.20971520E-01
Starting time-step t0=  0.48562195     dt=  0.20971520E-01
Starting time-step t0=  0.50659347     dt=  0.41943040E-01


output ignored...


... output resumed

 DELETING TIME-RECORD FOR TIME    26647.717
 DELETING TIME-RECORD FOR TIME    26690.666
 DELETING TIME-RECORD FOR TIME    26733.616
 DELETING TIME-RECORD FOR TIME    26776.566
 DELETING TIME-RECORD FOR TIME    26830.253
 DELETING TIME-RECORD FOR TIME    26873.203
 DELETING TIME-RECORD FOR TIME    26916.152
 DELETING TIME-RECORD FOR TIME    26959.102
 DELETING TIME-RECORD FOR TIME    27002.052
 DELETING TIME-RECORD FOR TIME    27045.001
 DELETING TIME-RECORD FOR TIME    27087.951
 DELETING TIME-RECORD FOR TIME    27130.901
 DELETING TIME-RECORD FOR TIME    27184.588
 DELETING TIME-RECORD FOR TIME    27227.537
 DELETING TIME-RECORD FOR TIME    27270.487
 DELETING TIME-RECORD FOR TIME    27313.437
 DELETING TIME-RECORD FOR TIME    27356.386
 DELETING TIME-RECORD FOR TIME    27399.336
 DELETING TIME-RECORD FOR TIME    27442.286
 DELETING TIME-RECORD FOR TIME    27485.235
 DELETING TIME-RECORD FOR TIME    27528.185
 DELETING TIME-RECORD FOR TIME    27571.135
 DELETING TIME-RECORD FOR TIME    27614.084
 DELETING TIME-RECORD FOR TIME    27667.772
 DELETING TIME-RECORD FOR TIME    27721.459
 DELETING TIME-RECORD FOR TIME    27764.408
 DELETING TIME-RECORD FOR TIME    27807.358
 DELETING TIME-RECORD FOR TIME    27850.308
 DELETING TIME-RECORD FOR TIME    27893.257
 DELETING TIME-RECORD FOR TIME    27957.682
 DELETING TIME-RECORD FOR TIME    28000.632
 DELETING TIME-RECORD FOR TIME    28043.581
 DELETING TIME-RECORD FOR TIME    28086.531
 DELETING TIME-RECORD FOR TIME    28129.481
 DELETING TIME-RECORD FOR TIME    28172.430
 DELETING TIME-RECORD FOR TIME    28215.380
 DELETING TIME-RECORD FOR TIME    28258.330
 DELETING TIME-RECORD FOR TIME    28301.279
 DELETING TIME-RECORD FOR TIME    28344.229
 DELETING TIME-RECORD FOR TIME    28387.179
 DELETING TIME-RECORD FOR TIME    28430.128
 DELETING TIME-RECORD FOR TIME    28473.078
 DELETING TIME-RECORD FOR TIME    28516.028
 DELETING TIME-RECORD FOR TIME    28558.977
 DELETING TIME-RECORD FOR TIME    28601.927
 DELETING TIME-RECORD FOR TIME    28644.877
 DELETING TIME-RECORD FOR TIME    28687.826
 DELETING TIME-RECORD FOR TIME    28730.776
 DELETING TIME-RECORD FOR TIME    28773.726
 DELETING TIME-RECORD FOR TIME    28848.888
 DELETING TIME-RECORD FOR TIME    28891.837
 DELETING TIME-RECORD FOR TIME    28945.524
 DELETING TIME-RECORD FOR TIME    28988.474
 DELETING TIME-RECORD FOR TIME    29052.899
 DELETING TIME-RECORD FOR TIME    29095.848
 DELETING TIME-RECORD FOR TIME    29138.798
 DELETING TIME-RECORD FOR TIME    29181.748
 DELETING TIME-RECORD FOR TIME    29224.697
 DELETING TIME-RECORD FOR TIME    29267.647
 DELETING TIME-RECORD FOR TIME    29310.597
 DELETING TIME-RECORD FOR TIME    29353.546
 DELETING TIME-RECORD FOR TIME    29396.496
 DELETING TIME-RECORD FOR TIME    29439.446
 DELETING TIME-RECORD FOR TIME    29482.395
 DELETING TIME-RECORD FOR TIME    29536.082
 DELETING TIME-RECORD FOR TIME    29579.032
 DELETING TIME-RECORD FOR TIME    29621.982
 DELETING TIME-RECORD FOR TIME    29664.931
 DELETING TIME-RECORD FOR TIME    29707.881
 DELETING TIME-RECORD FOR TIME    29750.831
 DELETING TIME-RECORD FOR TIME    29793.780
 DELETING TIME-RECORD FOR TIME    29836.730
 DELETING TIME-RECORD FOR TIME    29879.680
 DELETING TIME-RECORD FOR TIME    29922.629
 DELETING TIME-RECORD FOR TIME    29965.579
 DELETING TIME-RECORD FOR TIME    30008.529
 DELETING TIME-RECORD FOR TIME    30051.478
 DELETING TIME-RECORD FOR TIME    30094.428
 DELETING TIME-RECORD FOR TIME    30137.378
 DELETING TIME-RECORD FOR TIME    30180.327
 DELETING TIME-RECORD FOR TIME    30223.277
 DELETING TIME-RECORD FOR TIME    30266.227
 DELETING TIME-RECORD FOR TIME    30309.176
```

```
 DELETING TIME-RECORD FOR TIME    30352.126
 DELETING TIME-RECORD FOR TIME    30395.076
 DELETING TIME-RECORD FOR TIME    30438.025
 DELETING TIME-RECORD FOR TIME    30491.713
 DELETING TIME-RECORD FOR TIME    30534.662
 DELETING TIME-RECORD FOR TIME    30599.087
 DELETING TIME-RECORD FOR TIME    30642.036
 DELETING TIME-RECORD FOR TIME    30706.461
 DELETING TIME-RECORD FOR TIME    30749.411
 DELETING TIME-RECORD FOR TIME    30813.835
 DELETING TIME-RECORD FOR TIME    30856.785
 DELETING TIME-RECORD FOR TIME    30899.734
 DELETING TIME-RECORD FOR TIME    30942.684
 DELETING TIME-RECORD FOR TIME    30985.634
 DELETING TIME-RECORD FOR TIME    31028.583
 DELETING TIME-RECORD FOR TIME    31082.271
 DELETING TIME-RECORD FOR TIME    31125.220
 DELETING TIME-RECORD FOR TIME    31178.907
 DELETING TIME-RECORD FOR TIME    31221.857
 DELETING TIME-RECORD FOR TIME    31264.807
 DELETING TIME-RECORD FOR TIME    31307.756
 DELETING TIME-RECORD FOR TIME    31350.706
 DELETING TIME-RECORD FOR TIME    31393.656
 DELETING TIME-RECORD FOR TIME    31436.605
 DELETING TIME-RECORD FOR TIME    31479.555
 DELETING TIME-RECORD FOR TIME    31522.505
 DELETING TIME-RECORD FOR TIME    31565.454
 DELETING TIME-RECORD FOR TIME    31608.404
 DELETING TIME-RECORD FOR TIME    31651.354
 DELETING TIME-RECORD FOR TIME    31715.778
 DELETING TIME-RECORD FOR TIME    31758.728
 DELETING TIME-RECORD FOR TIME    31801.678
 DELETING TIME-RECORD FOR TIME    31844.627
 DELETING TIME-RECORD FOR TIME    31887.577
 DELETING TIME-RECORD FOR TIME    31930.527
 DELETING TIME-RECORD FOR TIME    31973.476
 DELETING TIME-RECORD FOR TIME    32016.426
 DELETING TIME-RECORD FOR TIME    32059.376
 DELETING TIME-RECORD FOR TIME    32102.325
 DELETING TIME-RECORD FOR TIME    32145.275
 DELETING TIME-RECORD FOR TIME    32188.225
 DELETING TIME-RECORD FOR TIME    32231.174
 DELETING TIME-RECORD FOR TIME    32274.124
 DELETING TIME-RECORD FOR TIME    32317.074

 KEEPING TIME-RECORD FOR TIME    32360.023
 AND FOR TIME                    32400.000
 WORKSPACE RECLAIMED
 ------------------------------------------------
 INTERPOLATION SCHEME USED THIS FRACTION OF
 THE ALLOCATED MEMORY:   0.826163511075365
 EFFICIENCY FACTOR:    34.6137950051209
 MEMORY FRACTION USAGE PER BRANCH:
   1.00000000000000
  0.700029997000300
  0.722404310871618
 ------------------------------------------------
 DEALLOCATING
 ------------------------------------------------

 TIMESTEP AT     32400.0000     SELECTED

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

**exb7-plot**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exb7\plot.DCM"
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  3.24000E+04
 *** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
 *** ENTERING C1NB1_S AS A DIFFUSION NONE PHASE
DIC> read exb7
 OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1: @@
POST-1: @@ PLOT THE INTERFACE POSITION AS A FUNCTION OF TIME
POST-1: @@
POST-1: s-d-a x time
  INFO: Time is set as independent variable
POST-1: s-d-a y po-o-in aus upp
POST-1:
POST-1: plot
   2019.11.11.17.20.25
   UPPER INTERFACE OF REGION "AUS#1"
   CELL #1
```

```
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ APPEND DATA FROM A CORRESPONDING SIMULATION
POST-1: @@ WITHOUT NIOBIUM
POST-1: @@
POST-1:
POST-1: app y fec.exp 0
DATASET NUMBER(s): /-1/: 1
POST-1:
POST-1: plot
   2019.11.11.17.20.30
   UPPER INTERFACE OF REGION "AUS#1"
   CELL #1
```

```
POST-1:
```

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

# Cell Calculations

# Example exc1

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

This example simulates what happens to a ferrite plate that has inherited the carbon content of its parent austenite. The ferrite plate formed is embedded in an austenite matrix. This setup corresponds to a proposed mechanism for formation of Widmannstätten ferrite or for the ferrite phase of the bainite structure. It is assumed that the phase boundary between ferrite and austenite is immobile, this is achieved in the simulation by putting the ferrite and the austenite in two different cells. See also M. Hillert, L. Höglund and J. Ågren: Acta Metall. Mater. 41 (1993), pp.1951-1957.

**exc1-setup**

```
SYS:About

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

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 21012) 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: Mon Nov 11 11:13:13 2019


SYS:SYS:MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exc1\setup.DCM"
SYS: ?@@
 NO SUCH COMMAND, USE HELP
SYS: @@ Cell calculation.
SYS: @@ Carbon cannon in ferrite/austenite: Fe-C system, 2-cell calculation
SYS: @@ This example simulates what happens to a ferrite plate that has
SYS: @@ inherited the carbon content of its parent austenite. The ferrite
SYS: @@ plate formed is embedded in an austenite matrix. This setup
SYS: @@ corresponds to a proposed mechanism for formation of Widmannstätten
SYS: @@ ferrite or for the ferrite phase of the bainite structure. It is
SYS: @@ assumed that the phase boundary between ferrite and austenite is
SYS: @@ immobile, this is achieved in the simulation by putting the ferrite
SYS: @@ and the austenite in two different cells. See also M. Hillert,
SYS: @@ L. Höglund and J. Ågren: Acta Metall. Mater. 41 (1993), pp.1951-1957.
SYS: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exc1_setup.DCM
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASE
SYS: @@
SYS: go da
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v10.0

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10:
TDB_TCFE10: @@
TDB_TCFE10: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA
TDB_TCFE10: @@
TDB_TCFE10: sw fedemo
 Current database: Iron Demo Database v2.1

 VA                      /-  DEFINED
TDB_FEDEMO: def-sys fe c
 FE                      C  DEFINED
TDB_FEDEMO: rej ph * all
 GAS:G                   LIQUID:L                BCC_A2
 CBCC_A12                CEMENTITE               CUB_A13
 DIAMOND_FCC_A4          FCC_A1                  GRAPHITE
 HCP_A3                  KSI_CARBIDE             LAVES_PHASE_C14
 M23C6                   M5C2                    M7C3
   REJECTED
TDB_FEDEMO: res ph fcc,bcc
 FCC_A1                  BCC_A2  RESTORED
TDB_FEDEMO: get
17:21:48,452 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'P. Franke, Estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
  'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
 -OK-
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE DATA
TDB_FEDEMO: @@
TDB_FEDEMO: app mfedemo
 Current database: Fe-Alloys Mobility demo database v2.0

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

 List of references for assessed data

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

```
 -OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR
APP: @@
APP: go d-m
 NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 673; * N
DIC>
DIC> @@
DIC> @@ IN THE FIRST CELL
DIC> @@
DIC> @@ ENTER REGION aus CONTAINING AUSTENITE
DIC> @@ ENTER A GEOMETRICAL GRID INTO THAT REGION
DIC> @@ ENTER THE INITIAL COMPOSITION INTO THE AUSTENITE
DIC> @@
DIC> enter-region aus
DIC> enter-grid aus  0.2e-6 AUTO
DIC> enter-phase act aus  matrix fcc_a1#1
DIC>
DIC> enter-composition
REGION NAME : /AUS/: aus
PHASE NAME: /FCC_A1/: fcc_a1#1
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: c
TYPE /LINEAR/: lin 0.4 0.4
DIC>
DIC> @@
DIC> @@ IN THE SECOND CELL
DIC> @@
DIC> create-new-cell
CELL DISTRIBUTION FACTOR /1/: 1
 CREATING NEW CELL, NUMBER:  2
 CELL   2 SELECTED
DIC-2>
DIC-2> @@
DIC-2> @@ ENTER REGION fer CONTAINING FERRITE
DIC-2> @@ ENTER A GEOMETRICAL GRID INTO THAT REGION
DIC-2> @@ ENTER THE INITIAL COMPOSITION INTO THE FERRITE
DIC-2> @@
DIC-2> enter-region fer
DIC-2>
DIC-2>
DIC-2>
DIC-2> enter-grid fer  0.2e-6 AUTO
DIC-2> enter-phase act fer  matrix bcc_a2#1
DIC-2>
DIC-2> enter-composition
REGION NAME : /FER/: fer
PHASE NAME: /BCC_A2/: bcc_a2#1
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: c
TYPE /LINEAR/: lin 0.4 0.4
DIC-2>
DIC-2> @@
DIC-2> @@ SET THE SIMULATION TIME AND OTHER SIMULATION PARAMETERS
DIC-2> @@
DIC-2> set-simulation-time
END TIME FOR INTEGRATION /.1/: 0.5
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /.05/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC-2>
DIC-2>
DIC-2>
DIC-2> @@
DIC-2> @@ USE IMPLICIT (1) TIME INTEGRATION
DIC-2> @@
DIC-2> set-simulation-cond
NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /AUTO/:
VARY POTENTIALS OR ACTIVITIES OR LNAC : /POTENTIAL/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/:
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -> 1): /AUTO/: 1.0
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/:
DIC-2> @@
DIC-2> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC-2> @@
DIC-2> save exc1 Y
DIC-2>
DIC-2> set-inter
 --OK---
DIC-2>
```

**exc1-run**

```
DIC-2>About
 NO SUCH COMMAND, USE HELP
DIC-2>DIC-2>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exc1\run.DCM"
DIC-2>
DIC-2>
DIC-2> @@ exc1_run.DCM
DIC-2>
DIC-2> @@
DIC-2> @@ READ THE WORKSPACE AND START THE SIMULATION
DIC-2> @@
DIC-2> go d-m
 TIME STEP AT TIME  0.00000E+00
DIC-2> read exc1
 OK
DIC> sim
 Region: AUS
 single geometric dense at  0.20000E-06
 0.89105       93
 Region: FER
 single geometric dense at  0.20000E-06
 0.96940       72
 U-FRACTION IN SYSTEM:  C = .018673311178274  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
 U-FRACTION IN SYSTEM:  C = .018673311178274  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
 2.570491440876813E-002        2.570457646506868E-002        1.632468387161422E-002        1.481595181147797E-003        4.374341029229313E-
005        2.088304805792750E-007        2.465148218584509E-011        1.324759527745615E-017       TIME =  0.10000000E-06 DT =  0.10000000E-
06 SUM OF SQUARES =  0.13247595E-16
 U-FRACTION IN SYSTEM:  C = .018673311178092  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    1 seconds
 1.721271285522151E-002        1.721309826251351E-002        1.320114680021241E-003        1.780264097991380E-004        4.883616087255494E-
006        2.701426707050831E-008        4.894446465547997E-012        5.060995279251280E-018       TIME =  0.30000000E-06 DT =  0.20000000E-
06 SUM OF SQUARES =  0.50609953E-17
 U-FRACTION IN SYSTEM:  C = .018673311178317  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    1 seconds
 1.723030673037752E-002        1.722973038976220E-002        6.546665119261100E-004        1.540163260513691E-005        9.847912539076782E-
009        1.575452809079496E-013        1.596074202974413E-021       TIME =  0.70000000E-06 DT =  0.40000000E-
06 SUM OF SQUARES =  0.15960742E-20
 U-FRACTION IN SYSTEM:  C = .0186733111783162  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    1 seconds
 2.046536420972576E-003        2.046359859032310E-003        1.093844167326580E-005        4.894917999854999E-008        1.003356970861476E-
012        9.304052991034567E-020       TIME =  0.15000000E-05 DT =  0.80000000E-06 SUM OF SQUARES =  0.93040530E-19
 U-FRACTION IN SYSTEM:  C = .0186733111783284  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    1 seconds
 1.307886964749804E-003        1.307786277163472E-003        8.937182331940690E-006        4.994501074466576E-008        1.605936733334024E-
012        2.925322267681477E-019       TIME =  0.31000000E-05 DT =  0.16000000E-05 SUM OF SQUARES =  0.29253223E-18
 U-FRACTION IN SYSTEM:  C = .0186733111783717  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    0 seconds
 5.482172962185780E-004        5.481699846889124E-004        2.979476091125616E-006        1.354118170477956E-008        2.862903109487713E-
013        2.781361026406541E-020       TIME =  0.63000000E-05 DT =  0.32000000E-05 SUM OF SQUARES =  0.27813610E-19
 U-FRACTION IN SYSTEM:  C = .0186733111783983  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    1 seconds
 2.615717394236799E-002        2.615484476818431E-002        1.336512797281331E-004        5.745045533795560E-007        1.084420984134679E-
011        8.890857792295333E-019       TIME =  0.12700000E-04 DT =  0.64000000E-05 SUM OF SQUARES =  0.88908578E-18
 U-FRACTION IN SYSTEM:  C = .0186733111784285  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    1 seconds
 1.276911017790104E-002        1.276795521546028E-002        6.327036920657389E-005        2.645587374098647E-007        4.737843389821877E-
012        3.570098158612493E-019       TIME =  0.25500000E-04 DT =  0.12800000E-04 SUM OF SQUARES =  0.35700982E-18
 U-FRACTION IN SYSTEM:  C = .0186733111784668  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    0 seconds
 6.319101225972783E-003        6.318525707098414E-003        3.090594166554510E-005        1.275882426541279E-007        2.220821096285124E-
012        1.611614757865490E-019       TIME =  0.51100000E-04 DT =  0.25600000E-04 SUM OF SQUARES =  0.16116148E-18

output ignored...


... output resumed

  CPU time used in timestep                    1 seconds
 1.041680261143076E-005        1.044882763261123E-005        2.673597065080428E-011        6.868679433048460E-
017       TIME =  0.19801409     DT =  0.25429002E-01 SUM OF SQUARES =  0.68686794E-16
 U-FRACTION IN SYSTEM:  C = .0186734961934051  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    1 seconds
 2.750911886589348E-005        2.755302229563082E-005        1.960434722242743E-010        2.118600338709717E-015        5.696655952023327E-
025       TIME =  0.22607048     DT =  0.28056387E-01 SUM OF SQUARES =  0.56966560E-24
 U-FRACTION IN SYSTEM:  C = .0186734961934057  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    1 seconds
 5.476254513395052E-005        5.481399792891838E-005        9.963303739260068E-010        3.091360744603560E-014        1.731549815396808E-
023       TIME =  0.25814941     DT =  0.32078937E-01 SUM OF SQUARES =  0.17315498E-22
 U-FRACTION IN SYSTEM:  C = .0186734961934112  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    1 seconds
 1.037340039688431E-004        1.037913251895321E-004        5.850779319532745E-009        4.333907124400719E-013        1.594527547820133E-
021       TIME =  0.29683922     DT =  0.38689804E-01 SUM OF SQUARES =  0.15945275E-20
 U-FRACTION IN SYSTEM:  C = .0186734961934885  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    1 seconds
 1.750218760480062E-004        1.750799684420316E-004        2.677202769832648E-008        4.755174235095780E-012        1.226189495726562E-
019       TIME =  0.34683922     DT =  0.50000000E-01 SUM OF SQUARES =  0.12261895E-18
 U-FRACTION IN SYSTEM:  C = .0186734961943641  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    1 seconds
 1.655026934222391E-005        1.656587674489186E-005        2.353957912844140E-010        5.747764109154486E-015        9.024788137313696E-
025       TIME =  0.39683922     DT =  0.50000000E-01 SUM OF SQUARES =  0.90247881E-24
 U-FRACTION IN SYSTEM:  C = .0186734961943671  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    1 seconds
 2.721459415892611E-006        2.715794026356017E-006        1.265886507236482E-011        3.006406580786960E-
017       TIME =  0.44683922     DT =  0.50000000E-01 SUM OF SQUARES =  0.30064066E-16
 U-FRACTION IN SYSTEM:  C = .0186734961806587  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
```

```
  CPU time used in timestep                    1 seconds
 2.924257074237546E-005        2.922561803913454E-005        1.420221440177828E-009        5.383685951277357E-014        1.025746498363554E-
022       TIME =  0.49683922     DT =  0.50000000E-01 SUM OF SQUARES =  0.10257465E-21
 U-FRACTION IN SYSTEM:  C = .0186734961806328  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
  CPU time used in timestep                    1 seconds
 1.311639930673761E-002        1.311509713979497E-002        1.933623277214304E-005        2.528817595237144E-008        6.842251204622528E-
014        1.014480225960340E-022       TIME =  0.50000000     DT =  0.31607821E-02 SUM OF SQUARES =  0.10144802E-21
 U-FRACTION IN SYSTEM:  C = .0186734961806345  FE = 1
 TOTAL SIZE OF SYSTEM:  4E-07 [m]
 MUST SAVE WORKSPACE ON FILE
 WORKSPACE SAVED ON FILE
 RECLAIMING WORKSPACE
 DELETING TIME-RECORD FOR TIME    0.0000000
 DELETING TIME-RECORD FOR TIME   0.10000000E-06
 DELETING TIME-RECORD FOR TIME   0.30000000E-06
 DELETING TIME-RECORD FOR TIME   0.70000000E-06
 DELETING TIME-RECORD FOR TIME   0.15000000E-05
 DELETING TIME-RECORD FOR TIME   0.31000000E-05
 DELETING TIME-RECORD FOR TIME   0.63000000E-05
 DELETING TIME-RECORD FOR TIME   0.12700000E-04
 DELETING TIME-RECORD FOR TIME   0.25500000E-04
 DELETING TIME-RECORD FOR TIME   0.51100000E-04
 DELETING TIME-RECORD FOR TIME   0.10230000E-03
 DELETING TIME-RECORD FOR TIME   0.20470000E-03
 DELETING TIME-RECORD FOR TIME   0.40950000E-03
 DELETING TIME-RECORD FOR TIME   0.81910000E-03
 DELETING TIME-RECORD FOR TIME   0.16383000E-02
 DELETING TIME-RECORD FOR TIME   0.32767000E-02
 DELETING TIME-RECORD FOR TIME   0.65535000E-02
 DELETING TIME-RECORD FOR TIME   0.13107100E-01
 DELETING TIME-RECORD FOR TIME   0.26214300E-01
 DELETING TIME-RECORD FOR TIME   0.45184716E-01
 DELETING TIME-RECORD FOR TIME   0.64717392E-01
 DELETING TIME-RECORD FOR TIME   0.84711978E-01
 DELETING TIME-RECORD FOR TIME   0.10530467
 DELETING TIME-RECORD FOR TIME   0.12664930
 DELETING TIME-RECORD FOR TIME   0.14896624
 DELETING TIME-RECORD FOR TIME   0.17258509
 DELETING TIME-RECORD FOR TIME   0.19801409
 DELETING TIME-RECORD FOR TIME   0.22607048
 DELETING TIME-RECORD FOR TIME   0.25814941
 DELETING TIME-RECORD FOR TIME   0.29683922
 DELETING TIME-RECORD FOR TIME   0.34683922
 DELETING TIME-RECORD FOR TIME   0.39683922
 DELETING TIME-RECORD FOR TIME   0.44683922

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

 TIMESTEP AT    0.500000000     SELECTED

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

**exc1-plot**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exc1\plot.DCM"
DIC>
DIC>
DIC> @@ exc1_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE c1
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  5.00000E-01
DIC> read exc1
 OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1: @@
POST-1: @@ FIRST PLOT CARBON CONCENTRATION PROFILES IN FERRITE (CELL-2)
POST-1: @@ THEN SET THE DISTANCE AS X-AXIS (NOT THAT DISTANCE IS SET INDEPENDENT
POST-1: @@ VARIABLE AUTOMATICALLY) AND W-FRACTION CARBON AS Y-AXIS
POST-1: @@ REMEMBER THAT THE PLOT CONDITION ALSO MUST BE SET.
POST-1: @@
POST-1: select-cell
Number /NEXT/: 2
 CELL   2 SELECTED
POST-2:
POST-2: @@
POST-2: @@ NOTICE THAT THE PROMPT INCLUDES THE CURRENT CELL NUMBER
POST-2: @@
POST-2: s-d-a x dist glo
  INFO: Distance is set as independent variable
POST-2: s-d-a y w(c)
POST-2: s-p-c time .0001 .001 .01 .03 .1 .5
POST-2:
POST-2: @@
POST-2: @@ SET THE TITLE ON THE PLOTS
POST-2: @@
POST-2: set-title Figure c1.1
POST-2: plot
```

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

Figure c1.2

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

Figure c1.3

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

Figure c1.4

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

Figure c1.5

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

Figure c1.6

2019.11.11.17.24.29
UPPER INTERFACE OF REGION "LAST"
CELL #1

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

# Example exc2

## Cementite dissolution in an Fe-Cr-C alloy: Three particle sizes and three different cells

This example calculates the dissolution of cementite particles in an austenite matrix. This is the same as exc1 except that there are three particle sizes. Altogether six particles are considered using three different cells. This is to be able to represent some size distribution among the cementite particles. See also Z.-K. Liu, L. Höglund, B. Jönsson and J. Ågren: Metall.Trans.A, v. 22A (1991), pp. 1745-1752.

**exc2-setup**

```
SYS:About

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

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 21012) 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: Mon Nov 11 11:13:13 2019


SYS:SYS:MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exc2\setup.DCM"
SYS: ?@@
 NO SUCH COMMAND, USE HELP
SYS: @@ Cell calculation.
SYS: @@ Cementite dissolution in an Fe-Cr-C alloy: Three particle sizes and
SYS: @@ three different cells
SYS: @@ This example calculates the dissolution of cementite particles
SYS: @@ in an austenite matrix. This example is the same as exc1 but
SYS: @@ instead there are three particle sizes. A total of six
SYS: @@ particles are considered using three different cells. This is to
SYS: @@ represent some size distribution among the cementite particles.
SYS: @@ See also Z.-K. Liu, L. Höglund, B. Jönsson and J. Ågren:
SYS: @@ Metall.Trans.A, v. 22A (1991), pp. 1745-1752.
SYS: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exc2_setup.DCM
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASE
SYS: @@
SYS: go da
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v10.0

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10:
TDB_TCFE10: @@
TDB_TCFE10: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA
TDB_TCFE10: @@
TDB_TCFE10: switch fedemo
 Current database: Iron Demo Database v2.1

 VA                      /-  DEFINED
TDB_FEDEMO: def-sys fe cr c
 FE                      CR                      C
   DEFINED
TDB_FEDEMO: rej ph * all
 GAS:G                   LIQUID:L                BCC_A2
 CBCC_A12                CEMENTITE               CHI_A12
 CUB_A13                 DIAMOND_FCC_A4          FCC_A1
 GRAPHITE                HCP_A3                  KSI_CARBIDE
 LAVES_PHASE_C14         M23C6                   M3C2
 M5C2                    M7C3                    SIGMA
   REJECTED
TDB_FEDEMO: res ph fcc cementite
 FCC_A1                  CEMENTITE  RESTORED
TDB_FEDEMO: get
17:25:47,997 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 Creating a new composition set FCC_A1#2
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'B.-J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
  'P. Villars and L.D. Calvert (1985). Pearson`s handbook of
      crystallographic data for intermetallic phases. Metals park, Ohio.
      American Society for Metals; Molar volumes'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'B. Hallstedt, D. Djurovic, J. von Appen, R. Dronskowski, A. Dick, F.
      Koermann, T. Hickel, J. Neugebauer, CALPHAD, 34, 129 -33(2010); Fe-C'
  'A.V. Khvan, B. Hallstedt, C. Broeckmann, CALPHAD, 46, 24 -33(2014); Cr-Fe
      -C'
  'J. Bratberg, Z. Metallkd., 96 (2005) 335-344; Fe-Cr-Mo-C'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, 2016; FCC Fe-Cr-C and C-Cr-Ni'
  'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
  'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270
      (1986); CR-FE'
 -OK-
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE MOBILITY DATA
TDB_FEDEMO: @@
TDB_FEDEMO: app mobfe4
 Current database: Steels/Fe-Alloys Mobility  v4.0

 VA  DEFINED
 B2_BCC  REJECTED
APP: def-sys fe cr c
 FE                      CR                      C
   DEFINED
APP: rej ph * all
 BCC_A2                  CEMENTITE               FCC_A1
 FE4N_LP1                HCP_A3                  LIQUID:L
   REJECTED
APP: res ph fcc cementite
```

```
 FCC_A1                  CEMENTITE  RESTORED
APP: get
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'This parameter has not been assessed'
  'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'
  'B. Jonsson: Z. Metallkunde 85(1994)502-509; C diffusion in fcc Cr-Fe-Ni'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Fe diffusion fcc Cr-Fe'
  'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
      -Ni'
  'This parameter has been estimated'
 -OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR
APP: @@
APP: go d-m
 NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@  ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob t 0 1183; * n
DIC>
DIC> @@-----------------------------------------------------------------------
DIC> @@ CELL NUMBER ONE
DIC> @@-----------------------------------------------------------------------
DIC>
DIC> @@
DIC> @@ ENTER REGIONS carb AND aus
DIC> @@
DIC> enter-region carb
DIC> enter-region aus
ATTACH TO REGION NAMED /CARB/:
ATTACHED TO THE RIGHT OF CARB /YES/:
DIC> @@
DIC> @@ ENTER GEOMTRICAL GRIDS INTO THE REGIONS
DIC> @@
DIC>
DIC> @@
DIC> @@ THE SIZE OF THE CEMENTITE PARTICLES ARE KNOWN AS WE ASSUME
DIC> @@ IT HAS BEEN MEASURED.
DIC> @@
DIC> enter-grid
REGION NAME : /CARB/: carb
WIDTH OF REGION /1/: 0.700000e-6
TYPE /LINEAR/: AUTO
DIC>
DIC> @@
DIC> @@ THE SIZE OF THE FCC REGION CAN BE CALCULATED FROM A MASS BALANCE
DIC> @@ AFTER ESTIMATING THE INITIAL COMPOSITIONS IN THE TWO PHASES.
DIC> @@
DIC> enter-grid
REGION NAME : /AUS/: aus
WIDTH OF REGION /1/: 7.1832993E-7
TYPE /LINEAR/: AUTO
DIC>
DIC> @@
DIC> @@ ENTER PHASES INTO REGIONS
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /CARB/: carb
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: cementite
DIC>
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /AUS/: aus
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC> @@
DIC> @@ ENTER INITIAL VALUES FOR THE COMPOSITIONS IN THE PHASES
DIC> @@
DIC> enter-composition carb  cementite w-f
PROFILE FOR /CR/: cr lin 0.12423326 0.12423326
DIC>
DIC> enter-composition aus  fcc#1 fe w-f
PROFILE FOR /C/: cr lin 4.6615447E-3 4.6615447E-3
PROFILE FOR /CR/: c lin 1.5135207E-4 1.5135207E-4
DIC>
DIC> @@-----------------------------------------------------------------
DIC> @@ CELL NUMBER TWO
DIC> @@-----------------------------------------------------------------
DIC> create-new-cell
CELL DISTRIBUTION FACTOR /1/: 2
 CREATING NEW CELL, NUMBER:  2
 CELL   2 SELECTED
DIC-2>
DIC-2> @@
DIC-2> @@ ENTER REGIONS carb AND aus
DIC-2> @@
DIC-2> enter-region carb
DIC-2> enter-region aus
ATTACH TO REGION NAMED /CARB/:
ATTACHED TO THE RIGHT OF CARB /YES/:
DIC-2> @@
DIC-2> @@ ENTER GEOMTRICAL GRIDS INTO THE REGIONS
DIC-2> @@
DIC-2> enter-grid carb  0.300000e-6 AUTO
DIC-2> enter-grid aus  3.0785568E-7 AUTO
DIC-2>
DIC-2> @@
DIC-2> @@ ENTER PHASES INTO THE REGIONS
```

```
DIC-2> @@
DIC-2> enter-phase act carb  matrix   cementite
DIC-2> enter-phase act aus   matrix   fcc#1
DIC-2>
DIC-2> @@
DIC-2> @@ ENTER INITIAL VALUES FOR THE COMPOSITIONS IN THE PHASES
DIC-2> @@
DIC-2> enter-composition carb  cementite w-f
PROFILE FOR /CR/: cr lin 0.12423326 0.12423326
DIC-2>
DIC-2> enter-composition aus  fcc#1 fe w-f
PROFILE FOR /C/: cr lin 4.6615447E-3 4.6615447E-3
PROFILE FOR /CR/: c lin 1.5135207E-4 1.5135207E-4
DIC-2>
DIC-2> @@-------------------------------------------------------------
DIC-2> @@ CELL NUMBER THREE
DIC-2> @@-------------------------------------------------------------
DIC-2> create-new-cell
CELL DISTRIBUTION FACTOR /1/: 3
 CREATING NEW CELL, NUMBER:  3
 CELL   3 SELECTED
DIC-3>
DIC-3> @@
DIC-3> @@ ENTER REGIONS carb AND aus
DIC-3> @@
DIC-3> enter-region carb
DIC-3> enter-region aus
ATTACH TO REGION NAMED /CARB/:
ATTACHED TO THE RIGHT OF CARB /YES/:
DIC-3> @@
DIC-3> @@ ENTER GEOMTRICAL GRIDS INTO THE REGIONS
DIC-3> @@
DIC-3> enter-grid carb  0.525500e-6 AUTO
DIC-3> enter-grid aus   5.3926054E-7 AUTO
DIC-3>
DIC-3> @@
DIC-3> @@ ENTER PHASES INTO REGIONS
DIC-3> @@
DIC-3> enter-phase act carb  matrix   cementite
DIC-3> enter-phase act aus   matrix   fcc#1
DIC-3>
DIC-3> @@
DIC-3> @@ ENTER INITIAL VALUES FOR THE COMPOSITIONS IN THE PHASES
DIC-3> @@
DIC-3> enter-composition carb  cementite w-f
PROFILE FOR /CR/: cr lin 0.12423326 0.12423326
DIC-3>
DIC-3> enter-composition aus  fcc#1 fe w-f
PROFILE FOR /C/: cr lin 4.6615447E-3 4.6615447E-3
PROFILE FOR /CR/: c lin 1.5135207E-4 1.5135207E-4
DIC-3>
DIC-3> @@-------------------------------------------------------------
DIC-3> @@ GLOBAL CONDITIONS
DIC-3> @@-------------------------------------------------------------
DIC-3>
DIC-3> @@
DIC-3> @@ SET TO A SPHERICAL GEOMETRY
DIC-3> @@
DIC-3> enter-geo 2
DIC-3>
DIC-3> @s-n-l
's-n-l' is not recognized as an internal or external command,
operable program or batch file.
DIC-3> @
DIC-3> @
DIC-3> @
DIC-3> @
DIC-3> @
DIC-3> @
DIC-3> @
DIC-3> @1E-3
'1E-3' is not recognized as an internal or external command,
operable program or batch file.
DIC-3>
DIC-3>
DIC-3>
DIC-3>
DIC-3> @@
DIC-3> @@ SET THE SIMULATION TIME
DIC-3> @@
DIC-3> set-simulation-time
END TIME FOR INTEGRATION /.1/: 10000
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /1000/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC-3>
DIC-3> @@
DIC-3> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC-3> @@
DIC-3> save exc2 Y
DIC-3>
DIC-3>
DIC-3> set-inter
 --OK---
DIC-3>
```

**exc2-run**

```
DIC-3>About
 NO SUCH COMMAND, USE HELP
DIC-3>DIC-3>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exc2\run.DCM"
DIC-3>
DIC-3>
DIC-3> @@ exc2_run.DCM
DIC-3>
DIC-3> @@
DIC-3> @@ READ THE SET UP FROM FILE AND START THE SIMULATION
DIC-3> @@
DIC-3>
DIC-3> go d-m
 TIME STEP AT TIME  0.00000E+00
DIC-3> read exc2
 OK
DIC> sim yes
 Region: CARB
 single geometric dense at  0.70000E-06
 0.84611       96
 Region: AUS
 double geometric
 dense at outer boundaries, coarse at  0.35916E-06
lower part   1.0486       22
upper part  0.95367       22
 Region: CARB
 single geometric dense at  0.30000E-06
 0.86023       95
 Region: AUS
 double geometric
 dense at outer boundaries, coarse at  0.15393E-06
lower part   1.0067       22
upper part  0.99334       22
 Region: CARB
 single geometric dense at  0.52550E-06
 0.85084       96
 Region: AUS
 double geometric
 dense at outer boundaries, coarse at  0.26963E-06
lower part   1.0222       22
upper part  0.97828       22
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
  Trying old scheme                     4
 GENERATING STARTING VALUES FOR CELL #  1 INTERFACE #  2
 DETERMINING INITIAL EQUILIBRIUM VALUES
CALCULATING STARTING VALUES:       9   EQUILIBRIUM CALCULATIONS               DONE     6 OUT OF     9
89434.0516915
  Trying old scheme                     4
 GENERATING STARTING VALUES FOR CELL #  2 INTERFACE #  2
 DETERMINING INITIAL EQUILIBRIUM VALUES
CALCULATING STARTING VALUES:       9   EQUILIBRIUM CALCULATIONS               DONE     6 OUT OF     9
89434.0516915
  Trying old scheme                     4
 GENERATING STARTING VALUES FOR CELL #  3 INTERFACE #  2
 DETERMINING INITIAL EQUILIBRIUM VALUES
CALCULATING STARTING VALUES:       9   EQUILIBRIUM CALCULATIONS               DONE     6 OUT OF     9
89434.0516915
 U-FRACTION IN SYSTEM:  C = .0406910187346776  CR = .0214382352304608
                        FE = .978561764900046
 TOTAL SIZE OF SYSTEM:  2.90023192349E-17 [m^3]
 U-FRACTION IN SYSTEM:  C = .0406910187346776  CR = .0214382352304608
                        FE = .978561764900046
 TOTAL SIZE OF SYSTEM:  2.90023192349E-17 [m^3]
 0.549881621022649        0.549917064641369        0.549938978099245        0.549921828506974        0.549881463442409        0.549881396770029
002        3.584789101680866E-004        4.707896221871246E-005        1.368538550959717E-006        9.616968063377877E-
006        1.052143983520011E-006        9.010518128198978E-007        8.267746918807358E-007        8.321573841494096E-
007        8.024773010817041E-007        8.036126148686606E-007        7.984608479803817E-007        8.050009080165928E-
007        8.000667876626791E-007        7.984620140545656E-007        7.984782243616622E-007        8.003049929162915E-
007        8.048504050496507E-007        8.013658009098507E-007        7.869048260246039E-007        7.845298608498707E-
007        7.828052493024786E-007        7.795100507689236E-007        7.765420050120344E-007        7.772966895063071E-
007        7.719168100379878E-007        7.729228850378937E-007        7.669031199672529E-007        7.600329286330465E-
007        7.604611933733878E-007        7.600341336989379E-007        7.600503467469419E-007        7.525562576937503E-
007        7.561970193875436E-007        7.540768031134355E-007        7.401555176736862E-007        7.236762720997345E-
007        7.065875829803369E-007        6.785553054611386E-007        6.488671997966662E-007        6.495030271536015E-
007        5.991860187958240E-007        6.000961675353341E-007        5.458302363606085E-007        4.547576392268531E-
007        4.549588564707842E-007        4.547588529061567E-007        4.547750655223542E-007        3.591727438123953E-007

output ignored...



... output resumed

 5.628509259841596E-003        5.628509399139996E-003        5.628509343454668E-003        5.628468751585207E-003        5.628448316187180E-
003        5.628254072092422E-003        5.627629852871229E-003        7.748771066930463E-005        1.407254181427063E-
007        1.720443672727406E-011        4.649786473393236E-015        6.527354000807869E-013        1.361108924042734E-
018       TIME =   7809.6324     DT =   1000.0000     SUM OF SQUARES =  0.13611089E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.11244123E-10 AND  -0.11244123E-10
 POSITION OF INTERFACE CARB / AUS IS   0.41755419E-06
 CELL # 3 VELOCITY AT INTERFACE # 2 IS  -0.12050042E-10 AND  -0.12050042E-10
 POSITION OF INTERFACE CARB / AUS IS   0.24049745E-06
 U-FRACTION IN SYSTEM:  C = .040772595405699  CR = .0215875355468258
                        FE = .978412464583681
 TOTAL SIZE OF SYSTEM:  2.90023192349E-17 [m^3]
  2  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUS

  CPU time used in timestep                    10 seconds
 7.941701039324697E-003        7.941701126769979E-003        7.941701060557927E-003        7.941658579581104E-003        7.941639242379886E-
003        7.941390480464624E-003        7.940628284081996E-003        1.065108524862658E-004        1.618279707790824E-
007        1.993483299416804E-010        4.477064663329279E-014        1.580694811059657E-
018       TIME =   8809.6324     DT =   1000.0000     SUM OF SQUARES =  0.15806948E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.10001876E-10 AND  -0.10001876E-10
 POSITION OF INTERFACE CARB / AUS IS   0.40755231E-06
 CELL # 3 VELOCITY AT INTERFACE # 2 IS  -0.11458739E-10 AND  -0.11458739E-10
 POSITION OF INTERFACE CARB / AUS IS   0.22903871E-06
 U-FRACTION IN SYSTEM:  C = .0407726442653418  CR = .0215873358357055
                        FE = .978412664294802
 TOTAL SIZE OF SYSTEM:  2.90023192349E-17 [m^3]
  CPU time used in timestep                     8 seconds
 1.006818298867124E-002        1.006818304919153E-002        1.006818298106522E-002        1.006814407189043E-002        1.006812857697089E-
002        1.006782788156710E-002        1.006694549542607E-002        1.098508794538804E-004        2.065115440968229E-
007        1.646655274575798E-010        3.815484542468326E-014        1.157702795133675E-
017       TIME =   9809.6324     DT =   1000.0000     SUM OF SQUARES =  0.11577028E-16
```

```
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.90210530E-11 AND  -0.90210530E-11
 POSITION OF INTERFACE CARB / AUS IS   0.39853126E-06
 CELL # 3 VELOCITY AT INTERFACE # 2 IS  -0.11228059E-10 AND  -0.11228059E-10
 POSITION OF INTERFACE CARB / AUS IS   0.21781065E-06
 U-FRACTION IN SYSTEM:  C = .0407726768466095  CR = .0215871924594974
                        FE = .97841280767101
 TOTAL SIZE OF SYSTEM:  2.90023192349E-17 [m^3]
  CPU time used in timestep                    9 seconds
 1.779100376879661E-003        1.779100490333793E-003        1.779100607835709E-003        1.779038350126645E-003        1.779013631509601E-
003        1.779024277428822E-003        1.778985153656587E-003        4.689459193220084E-004        1.294028282392458E-
005        1.327331740159535E-008        2.034632823119645E-012        9.711531430938267E-
017       TIME =   10000.000     DT =   190.36758     SUM OF SQUARES =  0.97115314E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.74899059E-11 AND  -0.74899059E-11
 POSITION OF INTERFACE CARB / AUS IS   0.39710543E-06
 CELL # 3 VELOCITY AT INTERFACE # 2 IS  -0.86394786E-11 AND  -0.86394786E-11
 POSITION OF INTERFACE CARB / AUS IS   0.21616598E-06
 U-FRACTION IN SYSTEM:  C = .0407726973861893  CR = .0215871595332583
                        FE = .978412840597249
 TOTAL SIZE OF SYSTEM:  2.90023192349E-17 [m^3]
 MUST SAVE WORKSPACE ON FILE
 WORKSPACE SAVED ON FILE
 RECLAIMING WORKSPACE
 DELETING TIME-RECORD FOR TIME    3160.9166
 DELETING TIME-RECORD FOR TIME    3467.4552
 DELETING TIME-RECORD FOR TIME    3467.4552
 DELETING TIME-RECORD FOR TIME    3467.4552
 DELETING TIME-RECORD FOR TIME    3467.4552
 DELETING TIME-RECORD FOR TIME    3467.4553
 DELETING TIME-RECORD FOR TIME    3467.4555
 DELETING TIME-RECORD FOR TIME    3467.4558
 DELETING TIME-RECORD FOR TIME    3467.4564
 DELETING TIME-RECORD FOR TIME    3467.4577
 DELETING TIME-RECORD FOR TIME    3467.4603
 DELETING TIME-RECORD FOR TIME    3467.4654
 DELETING TIME-RECORD FOR TIME    3467.4756
 DELETING TIME-RECORD FOR TIME    3467.4961
 DELETING TIME-RECORD FOR TIME    3467.5371
 DELETING TIME-RECORD FOR TIME    3467.6190
 DELETING TIME-RECORD FOR TIME    3467.7828
 DELETING TIME-RECORD FOR TIME    3468.1105
 DELETING TIME-RECORD FOR TIME    3468.7659
 DELETING TIME-RECORD FOR TIME    3470.0766
 DELETING TIME-RECORD FOR TIME    3472.6980
 DELETING TIME-RECORD FOR TIME    3477.9409
 DELETING TIME-RECORD FOR TIME    3488.4267
 DELETING TIME-RECORD FOR TIME    3509.3982
 DELETING TIME-RECORD FOR TIME    3551.3412
 DELETING TIME-RECORD FOR TIME    3635.2273
 DELETING TIME-RECORD FOR TIME    3802.9995
 DELETING TIME-RECORD FOR TIME    4138.5438
 DELETING TIME-RECORD FOR TIME    4809.6324
 DELETING TIME-RECORD FOR TIME    5809.6324
 DELETING TIME-RECORD FOR TIME    6809.6324
 DELETING TIME-RECORD FOR TIME    7809.6324
 DELETING TIME-RECORD FOR TIME    8809.6324

 KEEPING TIME-RECORD FOR TIME    9809.6324
 AND FOR TIME                    10000.000
 WORKSPACE RECLAIMED

 TIMESTEP AT     10000.0000     SELECTED

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

**exc2-plot**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exc2\plot.DCM"
DIC>
DIC>
DIC> @@ exc2_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE c2
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  1.00000E+04
DIC> read exc2
 OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1: @@
POST-1: @@ PLOT THE CHROMIUM CONCENTRATION PROFILES IN THE SAME WAY AS IN exb2
POST-1: @@ BUT NOW FOR EACH PARTICLE. LET US LOOK AT THE PROFILES AFTER 1000s.
POST-1: @@
POST-1:
POST-1: @@
POST-1: @@ FIRST CELL
POST-1: @@
POST-1: enter-symb
Function or table /FUNCTION/: func
NAME: rdist
FUNCTION: gd-poi(carb,u);
POST-1:
POST-1: s-d-a x rdist
POST-1:
POST-1: s-d-a y uf(cr)
POST-1:
POST-1: s-i-v
VARIABLE /TIME/: dist
DISTANCE : /GLOBAL/: glo
POST-1:
POST-1: s-p-c time 1000
POST-1:
POST-1: @@
POST-1: @@ SET THE TITLE ON THE PLOT
POST-1: @@
POST-1: set-title Figure C2.1
POST-1: plot
```

Figure C2.1

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

Figure C2.2

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

Figure C2.3

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

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

Figure C2.4

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

Figure C2.5

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

Figure C2.6

2019.11.11.18.38.53
UPPER INTERFACE OF REGION "CARB#3"
CELL #3

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

Figure C2.7

2019.11.11.18.39.01
CELL #3

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

Figure C2.8

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

Figure C2.9

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

Figure C2.10

2019.11.11.18.39.37
CELL #3

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

# Diffusion in Dispersed Systems

# Example exd1a

## Carburization of a Ni-25% Cr alloy: Dispersed system model

This example is about carburization of a Ni-25Cr alloy. In this case the M3C2 and M7C3 carbides are entered as spheroid phases in a FCC matrix. In this example the DISPERSED SYSTEM MODEL is used. This case is from A. Engström, L. Höglund and J. Ågren: Metall.Trans.A v. 25A (1994), pp. 1127-1134.

**exd1a-setup**

```
SYS:About

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

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 21012) 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: Mon Nov 11 11:13:13 2019


SYS:SYS:MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exd1a\setup.DCM"
SYS: @@
SYS: @@ Diffusion in dispersed systems.
SYS: @@ Carburization of Ni-25%Cr alloy: Dispersed system model
SYS: @@ This example is about carburization of a Ni-25Cr alloy.
SYS: @@ In this case the M3C2 and M7C3 carbides are entered as
SYS: @@ spheroid phases in a FCC matrix. This simulation can be run
SYS: @@ with either the DISPERSED SYSTEM MODEL or the HOMOGENIZATION MODEL.
SYS: @@ In this example the DISPERSED SYSTEM MODEL is used, which requires
SYS: @@ that the default HOMOGENIZATION MODEL is disabled.
SYS: @@ With the DISPERSED SYSTEM MODEL the command
SYS: @@ ENTER_LABYRINTH_FUNCTION is used to take into account the
SYS: @@ impeding effect of dispersed phases on long-range diffusion.
SYS: @@ For the HOMOGENIZATION MODEL the command
SYS: @@ ENTER_HOMOGENIZATION_FUNCTION should be used.
SYS: @@ This case is from A. Engström, L. Höglund and J. Ågren:
SYS: @@ Metall.Trans.A v. 25A (1994), pp. 1127-1134.
SYS: ---------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exd1_setup.DCM
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASE
SYS: @@
SYS: go da
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v10.0

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10:
TDB_TCFE10: @@
TDB_TCFE10: @@ USE THE SSOL DATABASE FOR THERMODYNAMIC DATA
TDB_TCFE10: @@
TDB_TCFE10: sw fedemo
 Current database: Iron Demo Database v2.1

 VA                      /-  DEFINED
TDB_FEDEMO: def-sys ni cr c
 NI                      CR                      C
   DEFINED
TDB_FEDEMO: rej ph * all
 GAS:G                   LIQUID:L                BCC_A2
 CBCC_A12                CEMENTITE               CHI_A12
 CUB_A13                 DIAMOND_FCC_A4          FCC_A1
 GRAPHITE                HCP_A3                  KSI_CARBIDE
 LAVES_PHASE_C14         M23C6                   M3C2
 M7C3                    SIGMA  REJECTED
TDB_FEDEMO: res ph fcc,m7c3,m3c2,grap
 FCC_A1                  M7C3                    M3C2
 GRAPHITE  RESTORED
TDB_FEDEMO: get
18:41:00,442 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 Creating a new composition set FCC_A1#2
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'J. Bratberg, Z. Metallkd., 96 (2005) 335-344; Fe-Cr-Mo-C'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'B.-J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
  'A. Gabriel, C. Chatillon, and I. Ansara, published in High Temp. Sci.
      (Parameters listed in CALPHAD, 11 (1987) 203-218); C-NI'
  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, 2016; FCC Fe-Cr-C and C-Cr-Ni'
  'NPL, Unpublished work (1989); C-Cr-Ni'
  'A. Dinsdale and T. Chart, MTDS NPL, Unpublished work (1986); CR -NI'
  'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121 -127; Molar
      volumes'
  'P. Villars and L.D. Calvert (1985). Pearson`s handbook of
      crystallographic data for intermetallic phases. Metals park, Ohio.
      American Society for Metals; Molar volumes'
  'A. Fernandez Guillermet and G. Grimvall,J. Phys. Chem. Solids, 1992, 53,
      105-125; Molar volumes'
 -OK-
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE MOBILITY DATA
TDB_FEDEMO: @@
TDB_FEDEMO: app mfedemo
 Current database: Fe-Alloys Mobility demo database v2.0

 VA  DEFINED
APP: def-sys ni c cr
 NI                      C                       CR
   DEFINED
APP: rej ph * all
```

```
 BCC_A2                  FCC_A1  REJECTED
APP: res ph fcc,m7c3,m3c2,grap
 *** ERROR M7C3 INPUT IGNORED
 *** ERROR M3C2 INPUT IGNORED
 *** ERROR GRAP INPUT IGNORED
 FCC_A1  RESTORED
APP: get
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 Creating a new composition set FCC_A1#3
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'This parameter has not been assessed'
  'B. Jonsson: Z. Metallkunde 85(1994)502-509; C diffusion in fcc Cr-Fe-Ni'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Fe diffusion fcc Cr-Fe'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Ni diffusion fcc Cr-Ni'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Ni self-diffusion'
 -OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR
APP: @@
APP: go d-m
 NO TIME STEP DEFINED
 *** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
 *** ENTERING M3C2 AS A DIFFUSION NONE PHASE
 *** ENTERING M7C3 AS A DIFFUSION NONE PHASE
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 1123; * N
DIC>
DIC> @@
DIC> @@ SET THE REFERENCE STATE FOR CARBON
DIC> @@
DIC> set-reference-state
Component: C
Reference state: grap
Temperature /*/: *
Pressure /100000/: 101325
DIC>
DIC> @@
DIC> @@ ENTER THE REGION aus
DIC> @@
DIC> enter-region aus
DIC>
DIC> @@
DIC> @@ ENTER A GEOMETRICAL GRID INTO THE REGION
DIC> @@
DIC> enter-grid aus 3e-3 geo 100 1.02
DIC>
DIC> @@
DIC> @@ ENTER A MATRIX PHASE IN THE REGION
DIC> @@
DIC> enter-phase act aus matrix fcc_a1#1
DIC>
DIC> @@
DIC> @@ ENTER THE START COMPOSITION FOR THE MATRIX PHASE
DIC> @@
DIC> enter-composition
REGION NAME : /AUS/: aus
PHASE NAME: /FCC_A1#1/: fcc#1
DEPENDENT COMPONENT ? /NI/: ni
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: cr
TYPE /LINEAR/: lin 25 25
PROFILE FOR /CR/: c
TYPE /LINEAR/: lin 1e-4 1e-4
DIC>
DIC> @@
DIC> @@ ENTER SPHEROIDAL PHASES IN THE REGION
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /AUS/: aus
PHASE TYPE /MATRIX/: sph
PHASE NAME: /NONE/: m7c3
 INFO: EQUILIBRIUM COMPOSITION AND FRACTION OF SPHEROID PHASES USED AS DEFAULT
DIC>
DIC> @@
DIC> @@ ENTER A STOICHOMETRIC SPHEROIDAL PHASE IN THE REGION
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /AUS/: aus
PHASE TYPE /MATRIX/: sph
PHASE NAME: /NONE/: m3c2
 INFO: EQUILIBRIUM COMPOSITION AND FRACTION OF SPHEROID PHASES USED AS DEFAULT
DIC>
DIC>
DIC> @@
DIC> @@ ENTER A START COMPOSITION FOR THE SPHEROIDAL PHASES
DIC> @@
DIC> enter-composition
REGION NAME : /AUS/: aus
PHASE NAME: /FCC_A1#1/: m7c3
USE EQUILIBRIUM VALUE /Y/: Y
DIC> enter-composition
REGION NAME : /AUS/: aus
PHASE NAME: /FCC_A1#1/: m3c2
USE EQUILIBRIUM VALUE /Y/: Y
DIC>
DIC> @@
DIC> @@ SET THE BOUNDARY CONDITION
DIC> @@
DIC> set-cond
```

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

**exd1a-run**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exd1a\run.DCM"
DIC>
DIC>
DIC> @@ exd1_run.DCM
DIC>
DIC> @@
DIC> @@ READ THE SETUP FILE AND START THE SIMULATION
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  0.00000E+00
 *** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
 *** ENTERING M3C2 AS A DIFFUSION NONE PHASE
 *** ENTERING M7C3 AS A DIFFUSION NONE PHASE
DIC> read exd1
 OK
DIC> sim
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
 U-FRACTION IN SYSTEM:  C = 4.73399450059566E-06  CR = .273386452547573
                        NI = .726613547452427
 TOTAL SIZE OF SYSTEM:  .003 [m]
  WARNING:M7C3 HAS NO VOLUME FRACTION, CREATING ONE
  WARNING:M3C2 HAS NO VOLUME FRACTION, CREATING ONE
 U-FRACTION IN SYSTEM:  C = 4.73399450059566E-06  CR = .273386452547573
                        NI = .726613547452427
 TOTAL SIZE OF SYSTEM:  .003 [m]
 TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = 8.32233829951645E-05  CR = .273386452547572
                        NI = .726613547452428
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                     0 seconds
 TIME =  0.10010000E-03 DT =  0.10000000E-03 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = 1.14491977930615E-04  CR = .273386452547544
                        NI = .726613547452456
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                     1 seconds
 TIME =  0.40010010     DT =  0.40000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = 1.34397531949353E-04  CR = .273386452541228
                        NI = .726613547458772
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                     0 seconds
 TIME =   61.226617     DT =   60.826517     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = 1.73234190866323E-04  CR = .273386451404806
                        NI = .726613548595194
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                     0 seconds
 TIME =   136.73132     DT =   75.504702     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = 2.1519536134614E-04  CR = .273386450378639
                        NI = .726613549621361
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                     0 seconds
 TIME =   246.77986     DT =   110.04854     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = 2.65132773423412E-04  CR = .273386449367934
                        NI = .726613550632066
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                     1 seconds
 TIME =   417.73078     DT =   170.95092     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = 3.2670351971475E-04  CR = .273386448427441
                        NI = .726613551572559
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                     0 seconds
 TIME =   700.87762     DT =   283.14684     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = 4.03852183677256E-04  CR = .273386447458974
                        NI = .726613552541025
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                     0 seconds
 TIME =   1196.7621     DT =   495.88443     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = 5.03958315340994E-04  CR = .273386446322885
                        NI = .726613553677115
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                     0 seconds
 TIME =   2136.4660     DT =   939.70399     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = 6.43012086810234E-04  CR = .273386444988436
                        NI = .726613555011564
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                     0 seconds
 TIME =   3936.4660     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = 8.38519749163083E-04  CR = .273386443511134
                        NI = .726613556488866
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                     1 seconds
 TIME =   5736.4660     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00101736970332151  CR = .273386442681224
                        NI = .726613557318776
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                     0 seconds
 TIME =   7536.4660     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00118296902880158  CR = .273386442066142
                        NI = .726613557933858
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                     0 seconds
 TIME =   9336.4660     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00133879540957736  CR = .273386441011293
                        NI = .726613558988707
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                     0 seconds
 TIME =   11136.466     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00148538430057559  CR = .273386439279029
                        NI = .726613560720971
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                     1 seconds
 TIME =   12936.466     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00162329996141555  CR = .273386436825667
                        NI = .726613563174333
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                     0 seconds
 TIME =   14736.466     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00175666371078122  CR = .273386434544898
                        NI = .726613565455102
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                     0 seconds
```

```
 TIME =   16509.560     DT =   1773.0939     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00188419698676039  CR = .273386432317815
                        NI = .726613567682185
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   18202.529     DT =   1692.9692     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00200374370728574  CR = .273386430131715
                        NI = .726613569868284
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1 seconds
 TIME =   19871.496     DT =   1668.9668     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00212043403493915  CR = .273386427985688
                        NI = .726613572014311
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   21585.287     DT =   1713.7913     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00223651041851038  CR = .273386426227075
                        NI = .726613573772925
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   23385.287     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00235302551823152  CR = .273386424970864


output ignored...



... output resumed

  CPU time used in timestep                    0 seconds
 TIME =   3563985.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0314537983526267  CR = .273386325210631
                        NI = .726613674789369
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3565785.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0314617329030149  CR = .273386325190174
                        NI = .726613674809826
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1 seconds
 TIME =   3567585.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0314696650642582  CR = .2733863251695
                        NI = .7266136748305
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3569385.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0314775948480468  CR = .273386325148608
                        NI = .726613674851392
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3571185.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0314855222664732  CR = .273386325127498
                        NI = .726613674872502
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3572985.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0314934473320117  CR = .273386325106171
                        NI = .726613674893829
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3574785.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0315013700574985  CR = .273386325084627
                        NI = .726613674915373
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1 seconds
 TIME =   3576585.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0315092904561121  CR = .273386325062864
                        NI = .726613674937136
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3578385.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0315172085413539  CR = .273386325040883
                        NI = .726613674959117
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3580185.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0315251243270301  CR = .273386325018683
                        NI = .726613674981317
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1 seconds
 TIME =   3581985.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0315330378272334  CR = .273386324996265
                        NI = .726613675003735
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3583785.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0315409490563253  CR = .273386324973629
                        NI = .726613675026371
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3585585.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0315488580289196  CR = .273386324950774
                        NI = .726613675049226
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3587385.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0315567647598653  CR = .273386324927699
                        NI = .726613675072301
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3589185.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .031564669264231  CR = .273386324904406
                        NI = .726613675095595
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1 seconds
 TIME =   3590985.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0315725715572893  CR = .273386324880892
                        NI = .726613675119107
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3592785.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0315804716545019  CR = .27338632485716
                        NI = .726613675142841
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
```

```
 TIME =   3594585.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0315883695715048  CR = .273386324833207
                        NI = .726613675166793
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3596385.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .031596265324095  CR = .273386324809034
                        NI = .726613675190966
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    1 seconds
 TIME =   3598185.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0316041589282161  CR = .273386324784642
                        NI = .726613675215358
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3599985.3     DT =   1800.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0316120503999463  CR = .273386324760028
                        NI = .726613675239972
 TOTAL SIZE OF SYSTEM:  .003 [m]
  CPU time used in timestep                    0 seconds
 TIME =   3600000.0     DT =   14.712794     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0316121157454989  CR = .273386324759817
                        NI = .726613675240183
 TOTAL SIZE OF SYSTEM:  .003 [m]
 MUST SAVE WORKSPACE ON FILE
 WORKSPACE SAVED ON FILE
 RECLAIMING WORKSPACE
 DELETING TIME-RECORD FOR TIME    0.0000000
 DELETING TIME-RECORD FOR TIME   0.10000000E-06
 DELETING TIME-RECORD FOR TIME   0.10010000E-03
 DELETING TIME-RECORD FOR TIME    163785.29
 DELETING TIME-RECORD FOR TIME    341985.29
 DELETING TIME-RECORD FOR TIME    520185.29
 DELETING TIME-RECORD FOR TIME    698385.29
 DELETING TIME-RECORD FOR TIME    876585.29
 DELETING TIME-RECORD FOR TIME    1054785.3
 DELETING TIME-RECORD FOR TIME    1232985.3
 DELETING TIME-RECORD FOR TIME    1411185.3
 DELETING TIME-RECORD FOR TIME    1589385.3
 DELETING TIME-RECORD FOR TIME    1767585.3
 DELETING TIME-RECORD FOR TIME    1945785.3
 DELETING TIME-RECORD FOR TIME    2123985.3
 DELETING TIME-RECORD FOR TIME    2302185.3
 DELETING TIME-RECORD FOR TIME    2480385.3
 DELETING TIME-RECORD FOR TIME    2658585.3
 DELETING TIME-RECORD FOR TIME    2836785.3
 DELETING TIME-RECORD FOR TIME    3014985.3
 DELETING TIME-RECORD FOR TIME    3193185.3
 DELETING TIME-RECORD FOR TIME    3371385.3
 DELETING TIME-RECORD FOR TIME    3549585.3
 DELETING TIME-RECORD FOR TIME    3596385.3
 DELETING TIME-RECORD FOR TIME    3598185.3

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

 TIMESTEP AT     3600000.00     SELECTED

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

**exd1a-plot**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exd1a\plot.DCM"
DIC>
DIC>
DIC> @@ exd1_plot.DCM
DIC>
DIC> @@
DIC> @@ FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE exd1
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  3.60000E+06
 *** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
 *** ENTERING M3C2 AS A DIFFUSION NONE PHASE
 *** ENTERING M7C3 AS A DIFFUSION NONE PHASE
DIC> read exd1
 OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1: @@
POST-1: @@ LOT THE TOTAL CARBON CONCENTRATION PROFILE
POST-1: @@
POST-1: s-d-a y w-p c
POST-1: s-d-a x distance global
  INFO: Distance is set as independent variable
POST-1: s-s-s x n 0 2e-3
POST-1: s-p-c time 3600000
POST-1:
POST-1: app y exd1.exp
PROLOGUE NUMBER: /0/: 1
DATASET NUMBER(s): /-1/: 1
POST-1:
POST-1: @@
POST-1: @@ SET THE TITLE ON THE PLOT
POST-1: @@
POST-1: set-tit d1.1
POST-1:
POST-1: plot
```

```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: @@
POST-1: @@ NOW PLOT THE AMOUNT OF CARBIDES FORMED
POST-1: @@
POST-1: s-d-a y npm(*)
POST-1: s-s-s y n 0 0.4
POST-1: app n
POST-1:
POST-1: set-tit d1.2
POST-1: plot
```

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

# Example exd1b

## Carburization of a Ni-25% Cr alloy: Homogenization model

This example is about carburization of a Ni-25Cr alloy. In this case the M3C2 and M7C3 carbides are entered as spheroid phases in a FCC matrix. It is similar to exd1a except the default HOMOGENIZATION MODEL is used and then ENTER_HOMOGENIZATION_FUNCTION should be used instead of ENTER_LABYRINTH_FUNCTION. This case is from A. Engström, L. Höglund and J. Ågren: Metall.Trans. A, v.25A (1994), pp. 1127-1134.

**exd1b-setup**

```
SYS:About

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

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 21012) 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: Mon Nov 11 11:13:13 2019


SYS:SYS:MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exd1b\setup.DCM"
SYS: ?@@
 NO SUCH COMMAND, USE HELP
SYS: @@ Diffusion in dispersed systems.
SYS: @@ Carburization of Ni-25%Cr alloy: Homogenization model
SYS: @@ This example is about carburization of a Ni-25Cr alloy.
SYS: @@ In this case the M3C2 and M7C3 carbides are entered as
SYS: @@ spheroid phases in a FCC matrix. This case is from
SYS: @@ A. Engström, L. Höglund and J. Ågren: Metall.Trans. A,
SYS: @@ v.25A (1994), pp. 1127-1134.
SYS: @@ This simulation can be run with the DISPERSED SYSTEM MODEL or
SYS: @@ HOMOGENIZATION MODEL. The default HOMOGENIZATION MODEL is used
SYS: @@ and then ENTER_HOMOGENIZATION_FUNCTION should be used instead of
SYS: @@ ENTER_LABYRINTH_FUNCTION.
SYS: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exd1b_setup.DCM
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASE
SYS: @@
SYS:
SYS: @@ This example modifies the database interactively, which is not
SYS: @@ yet supported by GES6. Therefore, we enforce the use of GES5.
SYS: set-ges-version 5
SYS:
SYS: go da
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v10.0

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10:
TDB_TCFE10: @@
TDB_TCFE10: @@ USE THE SSOL DATABASE FOR THERMODYNAMIC DATA
TDB_TCFE10: @@
TDB_TCFE10: sw fedemo
 Current database: Iron Demo Database v2.1

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

 List of references for assessed data

  'J. Bratberg, Z. Metallkd., 96 (2005) 335-344; Fe-Cr-Mo-C'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'B.-J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
  'A. Gabriel, C. Chatillon, and I. Ansara, published in High Temp. Sci.
      (Parameters listed in CALPHAD, 11 (1987) 203-218); C-NI'
  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, 2016; FCC Fe-Cr-C and C-Cr-Ni'
  'NPL, Unpublished work (1989); C-Cr-Ni'
  'A. Dinsdale and T. Chart, MTDS NPL, Unpublished work (1986); CR -NI'
  'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121 -127; Molar
      volumes'
  'P. Villars and L.D. Calvert (1985). Pearson`s handbook of
      crystallographic data for intermetallic phases. Metals park, Ohio.
      American Society for Metals; Molar volumes'
  'A. Fernandez Guillermet and G. Grimvall,J. Phys. Chem. Solids, 1992, 53,
      105-125; Molar volumes'
 -OK-
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE MOBILITY DATA
TDB_FEDEMO: @@
TDB_FEDEMO: app mfedemo
 Current database: Fe-Alloys Mobility demo database v2.0

 VA  DEFINED
APP: def-sys ni c cr
 NI                      C                       CR
   DEFINED
```

```
APP: rej ph * all
 BCC_A2                    FCC_A1  REJECTED
APP: res ph fcc,m7c3,m3c2,grap
 *** ERROR M7C3 INPUT IGNORED
 *** ERROR M3C2 INPUT IGNORED
 *** ERROR GRAP INPUT IGNORED
 FCC_A1  RESTORED
APP: get
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 Creating a new composition set FCC_A1#3
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'This parameter has not been assessed'
  'B. Jonsson: Z. Metallkunde 85(1994)502-509; C diffusion in fcc Cr-Fe-Ni'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Fe diffusion fcc Cr-Fe'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Cr and Ni diffusion fcc Cr-Ni'
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Ni self-diffusion'
 -OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR
APP: @@
APP: go d-m
 NO TIME STEP DEFINED
 *** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
 *** ENTERING M3C2 AS A DIFFUSION NONE PHASE
 *** ENTERING M7C3 AS A DIFFUSION NONE PHASE
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 1123; * N
DIC>
DIC> @@
DIC> @@ SET THE REFERENCE STATE FOR CARBON
DIC> @@
DIC> set-reference-state
Component: C
Reference state: grap
Temperature /*/: *
Pressure /100000/: 101325
DIC>
DIC> @@
DIC> @@ ENTER THE REGION aus
DIC> @@
DIC> enter-region aus
DIC>
DIC> @@
DIC> @@ ENTER A GEOMETRICAL GRID INTO THE REGION
DIC> @@
DIC> enter-grid aus 3e-3 geo 100 1.02
DIC>
DIC> @@
DIC> @@ ENTER A MATRIX PHASE IN THE REGION
DIC> @@
DIC> enter-phase act aus matrix fcc_a1#1
DIC>
DIC> @@
DIC> @@ ENTER THE START COMPOSITION FOR THE MATRIX PHASE
DIC> @@
DIC> enter-composition
REGION NAME : /AUS/: aus
PHASE NAME: /FCC_A1#1/: fcc#1
DEPENDENT COMPONENT ? /NI/: ni
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: cr
TYPE /LINEAR/: lin 25 25
PROFILE FOR /CR/: c
TYPE /LINEAR/: lin 1e-4 1e-4
DIC>
DIC> @@
DIC> @@ ENTER SPHEROIDAL PHASES IN THE REGION
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /AUS/: aus
PHASE TYPE /MATRIX/: sph
PHASE NAME: /NONE/: m7c3
 INFO: EQUILIBRIUM COMPOSITION AND FRACTION OF SPHEROID PHASES USED AS DEFAULT
DIC>
DIC> @@
DIC> @@ ENTER A STOICHOMETRIC SPHEROIDAL PHASE IN THE REGION
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /AUS/: aus
PHASE TYPE /MATRIX/: sph
PHASE NAME: /NONE/: m3c2
 INFO: EQUILIBRIUM COMPOSITION AND FRACTION OF SPHEROID PHASES USED AS DEFAULT
DIC>
DIC>
DIC> @@
DIC> @@ ENTER A START COMPOSITION FOR THE SPHEROIDAL PHASES
DIC> @@
DIC> enter-composition
REGION NAME : /AUS/: aus
PHASE NAME: /FCC_A1#1/: m7c3
USE EQUILIBRIUM VALUE /Y/: Y
DIC> enter-composition
REGION NAME : /AUS/: aus
PHASE NAME: /FCC_A1#1/: m3c2
USE EQUILIBRIUM VALUE /Y/: Y
DIC>
DIC> @@
DIC> @@ SET THE BOUNDARY CONDITION
DIC> @@
```

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

**exd1b-run**

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

```
Starting time-step t0=   50.174361     dt=   1.6777216
Starting time-step t0=   51.852083     dt=   1.6777216
Starting time-step t0=   53.529805     dt=   1.6777216
Starting time-step t0=   55.207526     dt=   1.6777216
Starting time-step t0=   56.885248     dt=   1.6777216
Starting time-step t0=   58.562969     dt=   1.6777216
Starting time-step t0=   60.240691     dt=   1.6777216
Starting time-step t0=   61.918413     dt=   1.6777216
Starting time-step t0=   63.596134     dt=   1.6777216
Starting time-step t0=   65.273856     dt=   1.6777216
Starting time-step t0=   66.951577     dt=   1.6777216
Starting time-step t0=   68.629299     dt=   1.6777216
Starting time-step t0=   70.307021     dt=   1.6777216
Starting time-step t0=   71.984742     dt=   1.6777216
Starting time-step t0=   73.662464     dt=   1.6777216
Starting time-step t0=   75.340185     dt=   1.6777216
Starting time-step t0=   77.017907     dt=   3.3554432
Starting time-step t0=   80.373350     dt=   3.3554432
Starting time-step t0=   83.728793     dt=   3.3554432
Starting time-step t0=   87.084237     dt=   3.3554432
Starting time-step t0=   90.439680     dt=   3.3554432
Starting time-step t0=   93.795123     dt=   3.3554432


output ignored...



... output resumed

 DELETING TIME-RECORD FOR TIME    2328955.9
 DELETING TIME-RECORD FOR TIME    2335827.9
 DELETING TIME-RECORD FOR TIME    2342699.8
 DELETING TIME-RECORD FOR TIME    2349571.8
 DELETING TIME-RECORD FOR TIME    2356443.7
 DELETING TIME-RECORD FOR TIME    2363315.7
 DELETING TIME-RECORD FOR TIME    2370187.6
 DELETING TIME-RECORD FOR TIME    2377059.6
 DELETING TIME-RECORD FOR TIME    2383931.5
 DELETING TIME-RECORD FOR TIME    2390803.5
 DELETING TIME-RECORD FOR TIME    2397675.4
 DELETING TIME-RECORD FOR TIME    2404547.3
 DELETING TIME-RECORD FOR TIME    2411419.3
 DELETING TIME-RECORD FOR TIME    2418291.2
 DELETING TIME-RECORD FOR TIME    2425163.2
 DELETING TIME-RECORD FOR TIME    2432035.1
 DELETING TIME-RECORD FOR TIME    2438907.1
 DELETING TIME-RECORD FOR TIME    2445779.0
 DELETING TIME-RECORD FOR TIME    2452651.0
 DELETING TIME-RECORD FOR TIME    2459522.9
 DELETING TIME-RECORD FOR TIME    2466394.9
 DELETING TIME-RECORD FOR TIME    2473266.8
 DELETING TIME-RECORD FOR TIME    2480138.8
 DELETING TIME-RECORD FOR TIME    2487010.7
 DELETING TIME-RECORD FOR TIME    2493882.7
 DELETING TIME-RECORD FOR TIME    2500754.6
 DELETING TIME-RECORD FOR TIME    2507626.6
 DELETING TIME-RECORD FOR TIME    2514498.5
 DELETING TIME-RECORD FOR TIME    2521370.5
 DELETING TIME-RECORD FOR TIME    2528242.4
 DELETING TIME-RECORD FOR TIME    2535114.4
 DELETING TIME-RECORD FOR TIME    2541986.3
 DELETING TIME-RECORD FOR TIME    2548858.3
 DELETING TIME-RECORD FOR TIME    2555730.2
 DELETING TIME-RECORD FOR TIME    2562602.1
 DELETING TIME-RECORD FOR TIME    2569474.1
 DELETING TIME-RECORD FOR TIME    2576346.0
 DELETING TIME-RECORD FOR TIME    2583218.0
 DELETING TIME-RECORD FOR TIME    2593525.9
 DELETING TIME-RECORD FOR TIME    2600397.9
 DELETING TIME-RECORD FOR TIME    2607269.8
 DELETING TIME-RECORD FOR TIME    2614141.8
 DELETING TIME-RECORD FOR TIME    2621013.7
 DELETING TIME-RECORD FOR TIME    2627885.6
 DELETING TIME-RECORD FOR TIME    2634757.6
 DELETING TIME-RECORD FOR TIME    2641629.5
 DELETING TIME-RECORD FOR TIME    2648501.5
 DELETING TIME-RECORD FOR TIME    2655373.4
 DELETING TIME-RECORD FOR TIME    2662245.4
 DELETING TIME-RECORD FOR TIME    2669117.3
 DELETING TIME-RECORD FOR TIME    2675989.3
 DELETING TIME-RECORD FOR TIME    2682861.2
 DELETING TIME-RECORD FOR TIME    2689733.2
 DELETING TIME-RECORD FOR TIME    2696605.1
 DELETING TIME-RECORD FOR TIME    2703477.1
 DELETING TIME-RECORD FOR TIME    2710349.0
 DELETING TIME-RECORD FOR TIME    2717221.0
 DELETING TIME-RECORD FOR TIME    2724092.9
 DELETING TIME-RECORD FOR TIME    2730964.9
 DELETING TIME-RECORD FOR TIME    2737836.8
 DELETING TIME-RECORD FOR TIME    2744708.8
 DELETING TIME-RECORD FOR TIME    2758452.7
 DELETING TIME-RECORD FOR TIME    2772196.6
 DELETING TIME-RECORD FOR TIME    2785940.4
 DELETING TIME-RECORD FOR TIME    2799684.3
 DELETING TIME-RECORD FOR TIME    2813428.2
 DELETING TIME-RECORD FOR TIME    2827172.1
 DELETING TIME-RECORD FOR TIME    2840916.0
 DELETING TIME-RECORD FOR TIME    2854659.9
 DELETING TIME-RECORD FOR TIME    2868403.8
 DELETING TIME-RECORD FOR TIME    2875275.8
 DELETING TIME-RECORD FOR TIME    2882147.7
 DELETING TIME-RECORD FOR TIME    2895891.6
 DELETING TIME-RECORD FOR TIME    2909635.5
 DELETING TIME-RECORD FOR TIME    2923379.4
 DELETING TIME-RECORD FOR TIME    2937123.3
 DELETING TIME-RECORD FOR TIME    2950867.2
 DELETING TIME-RECORD FOR TIME    2964611.1
 DELETING TIME-RECORD FOR TIME    2978355.0
 DELETING TIME-RECORD FOR TIME    2992098.9
 DELETING TIME-RECORD FOR TIME    3005842.8
 DELETING TIME-RECORD FOR TIME    3019586.7
 DELETING TIME-RECORD FOR TIME    3033330.6
 DELETING TIME-RECORD FOR TIME    3047074.5
 DELETING TIME-RECORD FOR TIME    3060818.4
 DELETING TIME-RECORD FOR TIME    3074562.2
```

```
 DELETING TIME-RECORD FOR TIME    3088306.1
 DELETING TIME-RECORD FOR TIME    3102050.0
 DELETING TIME-RECORD FOR TIME    3115793.9
 DELETING TIME-RECORD FOR TIME    3129537.8
 DELETING TIME-RECORD FOR TIME    3143281.7
 DELETING TIME-RECORD FOR TIME    3157025.6
 DELETING TIME-RECORD FOR TIME    3170769.5
 DELETING TIME-RECORD FOR TIME    3184513.4
 DELETING TIME-RECORD FOR TIME    3198257.3
 DELETING TIME-RECORD FOR TIME    3212001.2
 DELETING TIME-RECORD FOR TIME    3225745.1
 DELETING TIME-RECORD FOR TIME    3232617.0
 DELETING TIME-RECORD FOR TIME    3239489.0
 DELETING TIME-RECORD FOR TIME    3246360.9
 DELETING TIME-RECORD FOR TIME    3253232.9
 DELETING TIME-RECORD FOR TIME    3260104.8
 DELETING TIME-RECORD FOR TIME    3266976.8
 DELETING TIME-RECORD FOR TIME    3273848.7
 DELETING TIME-RECORD FOR TIME    3280720.7
 DELETING TIME-RECORD FOR TIME    3287592.6
 DELETING TIME-RECORD FOR TIME    3294464.6
 DELETING TIME-RECORD FOR TIME    3301336.5
 DELETING TIME-RECORD FOR TIME    3308208.5
 DELETING TIME-RECORD FOR TIME    3315080.4
 DELETING TIME-RECORD FOR TIME    3321952.4
 DELETING TIME-RECORD FOR TIME    3328824.3
 DELETING TIME-RECORD FOR TIME    3335696.3
 DELETING TIME-RECORD FOR TIME    3349440.2
 DELETING TIME-RECORD FOR TIME    3363184.1
 DELETING TIME-RECORD FOR TIME    3376927.9
 DELETING TIME-RECORD FOR TIME    3390671.8
 DELETING TIME-RECORD FOR TIME    3404415.7
 DELETING TIME-RECORD FOR TIME    3418159.6
 DELETING TIME-RECORD FOR TIME    3431903.5
 DELETING TIME-RECORD FOR TIME    3445647.4
 DELETING TIME-RECORD FOR TIME    3459391.3
 DELETING TIME-RECORD FOR TIME    3473135.2
 DELETING TIME-RECORD FOR TIME    3486879.1
 DELETING TIME-RECORD FOR TIME    3500623.0
 DELETING TIME-RECORD FOR TIME    3514366.9
 DELETING TIME-RECORD FOR TIME    3528110.8
 DELETING TIME-RECORD FOR TIME    3541854.7
 DELETING TIME-RECORD FOR TIME    3555598.6
 DELETING TIME-RECORD FOR TIME    3562470.5
 DELETING TIME-RECORD FOR TIME    3572778.5

 KEEPING TIME-RECORD FOR TIME    3586522.3
 AND FOR TIME                    3600000.0
 WORKSPACE RECLAIMED
 ------------------------------------------------
 INTERPOLATION SCHEME USED THIS FRACTION OF
 THE ALLOCATED MEMORY:   0.416857341400993
 EFFICIENCY FACTOR:    65.4571748263559
 ------------------------------------------------
 DEALLOCATING
 ------------------------------------------------

 TIMESTEP AT     3600000.00     SELECTED

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

**exd1b-plot**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exd1b\plot.DCM"
DIC>
DIC>
DIC> @@ exd1_plot.DCM
DIC>
DIC> @@
DIC> @@ FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE exd1b
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  3.60000E+06
 *** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
 *** ENTERING M3C2 AS A DIFFUSION NONE PHASE
 *** ENTERING M7C3 AS A DIFFUSION NONE PHASE
DIC> read exd1
 OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1: @@
POST-1: @@ PLOT THE TOTAL CARBON CONCENTRATION PROFILE
POST-1: @@
POST-1: s-d-a y w-p c
POST-1: s-d-a x distance global
  INFO: Distance is set as independent variable
POST-1: s-s-s x n 0 2e-3
POST-1: s-p-c time 3600000
POST-1:
POST-1: app y exd1.exp
PROLOGUE NUMBER: /0/: 1
DATASET NUMBER(s): /-1/: 1
POST-1:
POST-1: @@
POST-1: @@ SET A TITLE ON THE PLOT
POST-1: @@
POST-1: set-tit d1.1
POST-1:
POST-1: plot
```

```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: @@
POST-1: @@ PLOT THE AMOUNT OF CARBIDES FORMED
POST-1: @@
POST-1: s-d-a y npm(*)
POST-1: s-s-s y n 0 0.4
POST-1: app n
POST-1:
POST-1: set-tit d1.2
POST-1: plot
```

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

# Example exd2a

## Diffusion couple of Fe-Ni-Cr alloys: Step-profile

This example calculates the interdiffusion in a diffusion couple between a two-phase (FCC+BCC) and a single-phase (FCC) Fe-Ni-Cr alloy. Initially it uses a step profile. This simulation can be run with either the DISPERSED SYSTEM MODEL or the HOMOGENIZATION MODEL. In this example the DISPERSED SYSTEM MODEL is used.

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

**exd2a-setup**

```
SYS:About

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

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 21012) 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: Mon Nov 11 11:13:13 2019


SYS:SYS:MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exd2a\setup.DCM"
SYS: @@
SYS: @@ Diffusion in dispersed systems.
SYS: @@ Diffusion couple of Fe-Cr-Ni alloys: Dispersed system model
SYS: @@ This example calculates the interdiffusion in a diffusion
SYS: @@ couple between a two-phase (FCC+BCC) and a single-phase (FCC)
SYS: @@ Fe-Ni-Cr alloy. This case is from A. Engström: Scand. J. Met., v. 24,
SYS: @@ 1995, pp.12-20. This simulation can be run with either the DISPERSED
SYS: @@ SYSTEM MODEL or the HOMOGENIZATION MODEL.
SYS: @@ In this example the DISPERSED SYSTEM MODEL is used, which requires
SYS: @@ that the default HOMOGENIZATION MODEL is disabled.
SYS: @@ With the DISPERSED SYSTEM MODEL the command
SYS: @@ ENTER_LABYRINTH_FUNCTION is used to take into account the
SYS: @@ impeding effect of dispersed phases on long-range diffusion.
SYS: @@ For the HOMOGENIZATION MODEL the command
SYS: @@ ENTER_HOMOGENIZATION_FUNCTION should be used.
SYS: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exd2_setup.DCM
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASE
SYS: @@
SYS: go da
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v10.0

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10: sw fedemo
 Current database: Iron Demo Database v2.1

 VA                      /-  DEFINED
TDB_FEDEMO: def-sys fe ni cr
 FE                      NI                      CR
   DEFINED
TDB_FEDEMO: rej ph * all
 LIQUID:L                BCC_A2                  CBCC_A12
 CHI_A12                 CUB_A13                 FCC_A1
 HCP_A3                  LAVES_PHASE_C14         SIGMA
   REJECTED
TDB_FEDEMO: res ph fcc,bcc
 FCC_A1                  BCC_A2  RESTORED
TDB_FEDEMO: get
18:59:25,805 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

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

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

 List of references for assessed data

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

```
  'B. Jonsson: Scand. J. Metall. 24(1995)21-27; Ni self-diffusion'
  'B. Jonsson: ISIJ International, 35(1995)1415-1421; Cr, Fe and Ni
      diffusion bcc Cr-Fe-Ni'
  'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
      in bcc Fe'
 -OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR
APP: @@
APP: go d-m
 NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 1473; * N
DIC>
DIC> @@
DIC> @@ ENTER THE REGION fer
DIC> @@
DIC> enter-region fer
DIC>
DIC>
DIC> @@
DIC> @@ ENTER A DOUBLE GEOMETRICAL GRID INTO THE REGION
DIC> @@ THIS GIVES A SHORT DISTANCE BETWEEN THE GRIDPOINTS
DIC> @@ IN THE MIDDLE OF THE REGION WHERE THE INITIAL INTERFACE IS
DIC> @@
DIC> enter-grid fer
WIDTH OF REGION /1/: 4e-3
TYPE /LINEAR/: double
NUMBER OF POINTS /50/: 200
VALUE OF R IN THE GEOMETRICAL SERIE FOR LOWER PART OF REGION: 0.97
VALUE OF R IN THE GEOMETRICAL SERIE FOR UPPER PART OF REGION: 1.03093
DIC>
DIC> @@
DIC> @@ ENTER A MATRIX PHASE IN THE REGION
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act fer matrix fcc
DIC>
DIC> @@
DIC> @@ ENTER THE START COMPOSITION FOR THE MATRIX PHASE FROM FILES
DIC> @@
DIC> enter-composition
REGION NAME : /FER/: fer
PHASE NAME: /FCC_A1/: fcc
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /CR/: cr
TYPE /LINEAR/: read d2cr.dat
PROFILE FOR /NI/: ni
TYPE /LINEAR/: read d2ni.dat
DIC>
DIC> @@
DIC> @@ ENTER FERRITE AS THE SPHEROIDAL PHASE IN THE REGION.
DIC> @@ SINCE THE FRACTION OF FERRITE IS SMALL, AND THESE APPEAR
DIC> @@ AS ISOLATED PARTICLES, FERRITE IS ENTERED AS A SPHEROIDAL PHASE
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /FER/: fer
PHASE TYPE /MATRIX/: sph
PHASE NAME: /NONE/: bcc
 INFO: EQUILIBRIUM COMPOSITION AND FRACTION OF SPHEROID PHASES USED AS DEFAULT
DIC>
DIC> @@
DIC> @@ ENTER A COMPOSITION FOR THE SPHEROIDAL PHASE
DIC> @@ USE THE EQUILIBRIUM VALUE
DIC> @@
DIC> enter-composition
REGION NAME : /FER/: fer
PHASE NAME: /FCC_A1/: bcc
USE EQUILIBRIUM VALUE /Y/: y
DIC>
DIC>
DIC> @@
DIC> @@ ENTER A LABYRINTH FACTOR
DIC> @@ IN THIS CASE THE LOW DIFFUSIVITY PHASE IS THE MATRIX AND THE
DIC> @@ "EFFECTIVE" DIFFUSIVITY IN THE AUSTENITE+FERRITE TWO-PHASE
DIC> @@ REGION IS EXPECTED TO BE HIGHER THAN THE DIFFUSIVITY IN THE
DIC> @@ AUSTENITE.
DIC> enter-lab
REGION NAME : fer
f(T,P,VOLFR,X)= 1+3*(1-volfr)/volfr;
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME AND OTHER SIMULATION PARAMETERS
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 720000
AUTOMATIC TIMESTEP CONTROL /YES/: YES
MAX TIMESTEP DURING INTEGRATION /72000/: 5000
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC> set-simulation-condition
NS01A PRINT CONTROL : /0/:
FLUX CORRECTION FACTOR : /1/:
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/:
CHECK INTERFACE POSITION /AUTO/:
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/:
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/:
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/: 99
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -> 1): /AUTO/:
MAX TIMESTEP CHANGE PER TIMESTEP : /2/:
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/:
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/:
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/:
```

```
DIC> @@ BY DEFAULT THE "HOMOGENIZATION MODEL" IS USED WHEN MULTIPLE PHASES
DIC> @@ ARE ENTERED IN A SINGLE REGION. THE HOMOGENIZATION MODEL NEEDS TO BE
DIC> @@ DISABLED FOR THIS EXAMPLE.
DIC> ho n
 HOMOGENIZATION DISABLED
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC>
DIC> save exd2 y
DIC>
DIC> set-inter
 --OK---
DIC>
```

**exd2a-run**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exd2a\run.DCM"
DIC>
DIC>
DIC> @@ exd2_run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING THE SIMULATION OF EXAMPLE D2
DIC> @@
DIC>
DIC> @@
DIC> @@ READ THE SETUP FROM FILE AND START THE SIMULATION
DIC> @@
DIC>
DIC> go d-m
 TIME STEP AT TIME  0.00000E+00
DIC> read exd2
 OK
DIC> sim
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
 U-FRACTION IN SYSTEM:  CR = .297842647391913  FE = .517227320517284
                        NI = .184930032090802
 TOTAL SIZE OF SYSTEM:  .004 [m]
  WARNING:BCC_A2 HAS NO VOLUME FRACTION, CREATING ONE
 U-FRACTION IN SYSTEM:  CR = .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 = .297842648005431  FE = .517227319061159
                        NI = .18493003293341
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                     0 seconds
 TIME =  0.40010010     DT =  0.40000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297842676377595  FE = .517227251840507
                        NI = .184930071781899
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                     1 seconds
 TIME =   281.72200     DT =   281.32190     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297847760270075  FE = .517216317308819
                        NI = .184935922421106
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                     0 seconds
 TIME =   844.36579     DT =   562.64380     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297849615184743  FE = .517212946633452
                        NI = .184937438181805
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                     1 seconds
 TIME =   1969.6534     DT =   1125.2876     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297850550731974  FE = .517211426818697
                        NI = .184938022449329
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                     0 seconds
 TIME =   4220.2286     DT =   2250.5752     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .29785111900064  FE = .517210569323811
                        NI = .184938311675549
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                     0 seconds
 TIME =   8721.3789     DT =   4501.1504     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297851494954335  FE = .517210020163942
                        NI = .184938484881724
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                     1 seconds
 TIME =   13721.379     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .29785173211369  FE = .517209740277052
                        NI = .184938527609258
 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 = .297851883453509  FE = .517209584045533
                        NI = .184938532500959
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                     1 seconds
 TIME =   23721.379     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297851977657555  FE = .517209483265973
                        NI = .184938539076472
 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 = .297852029985827  FE = .51720941242619
                        NI = .184938557587983
 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 = .297852049766011  FE = .517209361691076
                        NI = .184938588542913
 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 = .297852045015469  FE = .517209326359909
                        NI = .184938628624623
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                     0 seconds
 TIME =   43721.379     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852052300693  FE = .517209299378173
                        NI = .184938648321135
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                     1 seconds
 TIME =   48721.379     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852064900642  FE = .517209276184262
                        NI = .184938658915096
 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 = .297852069935261  FE = .517209260646724
                        NI = .184938669418015
 TOTAL SIZE OF SYSTEM:  .004 [m]
```

```
 CPU time used in timestep                    0 seconds
TIME =   58721.379     DT =   5000.0000     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  CR = .297852077632326  FE = .517209244116553
                       NI = .184938678251121
TOTAL SIZE OF SYSTEM:  .004 [m]
 CPU time used in timestep                    0 seconds
TIME =   63721.379     DT =   5000.0000     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  CR = .29785208730734  FE = .517209229697543
                       NI = .184938682995118
TOTAL SIZE OF SYSTEM:  .004 [m]
 CPU time used in timestep                    1 seconds
TIME =   68721.379     DT =   5000.0000     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  CR = .297852092166834  FE = .517209219702969
                       NI = .184938688130196
TOTAL SIZE OF SYSTEM:  .004 [m]
 CPU time used in timestep                    0 seconds
TIME =   73721.379     DT =   5000.0000     SUM OF SQUARES =   0.0000000


output ignored...



... output resumed

U-FRACTION IN SYSTEM:  CR = .297852035243632  FE = .517209097316278
                       NI = .184938867440089
TOTAL SIZE OF SYSTEM:  .004 [m]
 CPU time used in timestep                    0 seconds
TIME =   608721.38     DT =   5000.0000     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  CR = .297852040343916  FE = .517209095828342
                       NI = .184938863827742
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 = .29785204675656  FE = .517209094403528
                       NI = .184938858839911
TOTAL SIZE OF SYSTEM:  .004 [m]
 CPU time used in timestep                    0 seconds
TIME =   618721.38     DT =   5000.0000     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  CR = .297852053277544  FE = .517209093263191
                       NI = .184938853459265
TOTAL SIZE OF SYSTEM:  .004 [m]
 CPU time used in timestep                    0 seconds
TIME =   623721.38     DT =   5000.0000     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  CR = .297852059288762  FE = .517209092514196
                       NI = .184938848197042
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 = .297852064436493  FE = .51720909221795
                       NI = .184938843345556
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 = .297852068500943  FE = .517209092415532
                       NI = .184938839083525
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 = .297852071392546  FE = .517209093083931
                       NI = .184938835523522
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 = .297852073681692  FE = .517209091807034
                       NI = .184938834511274
TOTAL SIZE OF SYSTEM:  .004 [m]
 CPU time used in timestep                    1 seconds
TIME =   648721.38     DT =   5000.0000     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  CR = .297852074518779  FE = .517209091190447
                       NI = .184938834290774
TOTAL SIZE OF SYSTEM:  .004 [m]
 CPU time used in timestep                    0 seconds
TIME =   653721.38     DT =   5000.0000     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  CR = .297852073880057  FE = .517209091158175
                       NI = .184938834961769
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 = .297852071737293  FE = .517209091673231
                       NI = .184938836589476
TOTAL SIZE OF SYSTEM:  .004 [m]
 CPU time used in timestep                    1 seconds
TIME =   663721.38     DT =   5000.0000     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  CR = .297852068061707  FE = .517209092719061
                       NI = .184938839219232
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 = .297852062825046  FE = .517209094290038
                       NI = .184938842884916
TOTAL SIZE OF SYSTEM:  .004 [m]
 CPU time used in timestep                    0 seconds
TIME =   673721.38     DT =   5000.0000     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  CR = .297852056000142  FE = .517209096387321
                       NI = .184938847612537
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 = .297852047560718  FE = .517209099016377
                       NI = .184938853422905
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 = .297852037481158  FE = .517209102185646
                       NI = .184938860333196
TOTAL SIZE OF SYSTEM:  .004 [m]
 CPU time used in timestep                    1 seconds
TIME =   688721.38     DT =   5000.0000     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  CR = .297852031720917  FE = .517209104528003
                       NI = .184938863751081
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 = .297852035107029  FE = .517209102778463
```

```
                        NI = .184938862114509
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0 seconds
 TIME =   698721.38     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .29785204126568  FE = .517209100862438
                        NI = .184938857871882
 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 = .297852048239013  FE = .517209099115003
                        NI = .184938852645985
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    1 seconds
 TIME =   708721.38     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852055131708  FE = .517209097666819
                        NI = .184938847201473
 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 = .297852061470738  FE = .517209096580473
                        NI = .184938841948789
 TOTAL SIZE OF SYSTEM:  .004 [m]
  CPU time used in timestep                    0 seconds
 TIME =   718721.38     DT =   5000.0000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  CR = .297852066979958  FE = .51720909589139
                        NI = .184938837128652
 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 = .297852071767318  FE = .517209095429356
                        NI = .184938832803326
 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>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exd2a\plot.DCM"
DIC>
DIC>
DIC> @@ exd2_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE D2
DIC> @@
DIC> @@ ENTER THE DICTRA MODULE AND SPECIFY THE STORE-RESULT FILE
DIC> @@
DIC>
DIC> go d-m
 TIME STEP AT TIME  7.20000E+05
DIC> read  exd2
 OK
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA POST PROCESSOR
DIC> @@
DIC> post
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:
POST-1: @@
POST-1: @@ LET US SEE HOW THE FRACTION OF FERRITE HAS CHANGED
POST-1: @@ AS A RESULT OF THE DIFFUSION
POST-1: @@
POST-1: s-d-a y npm(bcc)
POST-1: s-d-a x distance global
  INFO: Distance is set as independent variable
POST-1: s-p-c time 0 720000
POST-1: set-tit Figure D2.1
POST-1: plot
```

Figure D2.1

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

Figure D2.2

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

Figure D2.3

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

Figure D2.4

```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1: @@
POST-1: @@ LET US PLOT THE DIFFUSION PATH FOR THE COUPLE.
POST-1: @@ WE APPEND THE TERNARY PHASE-DIAGRAM CALCULATED IN THERMO-CALC
POST-1: @@ AND THE EXPERIMENTAL DATA
POST-1: @@
POST-1: s-d-a x w-p cr
POST-1: s-d-a y w-p ni
POST-1: s-i-v dis gl
POST-1: s-p-c time last
POST-1:
POST-1: app y exd2.exp
PROLOGUE NUMBER: /1/: 1
DATASET NUMBER(s): /-1/: 6 7 8
POST-1:
POST-1: s-s-s x n 10 50
POST-1: s-s-s y n 5 35
POST-1:
POST-1: set-tit Figure D2.5
POST-1: plot
```

Figure D2.5

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

# Example exd2b

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

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

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

**exd2b-setup**

```
SYS:About

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

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 21012) 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: Mon Nov 11 11:13:13 2019


SYS:SYS:MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exd2b\setup.DCM"
SYS: ?@@
 NO SUCH COMMAND, USE HELP
SYS: @@ Diffusion in dispersed systems.
SYS: @@ Diffusion couple of Fe-Cr-Ni alloys: Homogenization model
SYS: @@ This example calculates the interdiffusion in a diffusion
SYS: @@ couple between a two-phase (FCC+BCC) and a single-phase (FCC)
SYS: @@ Fe-Ni-Cr alloy. This case is from A. Engström: Scand. J. Met.,
SYS: @@ v. 24, 1995, pp.12-20. This simulation can be run with either
SYS: @@ the DISPERSED SYSTEM MODEL or the HOMOGENIZATION MODEL.
SYS: @@ Here the default HOMOGENIZATION MODEL is used and then
SYS: @@ ENTER_HOMOGENIZATION_FUNCTION should be used instead of
SYS: @@ ENTER_LABYRINTH_FUNCTION.
SYS: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASE
SYS: @@
SYS: go da
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v10.0

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10: sw fedemo
 Current database: Iron Demo Database v2.1

 VA                      /-  DEFINED
TDB_FEDEMO: def-sys fe ni cr
 FE                      NI                      CR
   DEFINED
TDB_FEDEMO: rej ph * all
 LIQUID:L                BCC_A2                  CBCC_A12
 CHI_A12                 CUB_A13                 FCC_A1
 HCP_A3                  LAVES_PHASE_C14         SIGMA
   REJECTED
TDB_FEDEMO: res ph fcc,bcc
 FCC_A1                  BCC_A2  RESTORED
TDB_FEDEMO: get
19:03:22,840 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

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

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

 List of references for assessed data

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

```
 -OK-
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR
APP: @@
APP: go d-m
 NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 1473; * N
DIC>
DIC> @@
DIC> @@ ENTER THE REGION fer
DIC> @@
DIC> enter-region fer
DIC>
DIC>
DIC> @@
DIC> @@ ENTER A DOUBLE-GEOMETRICAL GRID INTO THE REGION
DIC> @@ THIS GIVES A SHORT DISTANCE BETWEEN THE GRIDPOINTS
DIC> @@ IN THE MIDDLE OF THE REGION WHERE THE INITIAL INTERFACE IS
DIC> @@
DIC> enter-grid fer
WIDTH OF REGION /1/: 4e-3
TYPE /LINEAR/: double
NUMBER OF POINTS /50/: 200
VALUE OF R IN THE GEOMETRICAL SERIE FOR LOWER PART OF REGION: 0.97
VALUE OF R IN THE GEOMETRICAL SERIE FOR UPPER PART OF REGION: 1.03093
DIC>
DIC> @@
DIC> @@ ENTER A MATRIX PHASE IN THE REGION
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act fer matrix fcc
DIC>
DIC> @@
DIC> @@ ENTER THE START COMPOSITION FOR THE MATRIX PHASE FROM FILES
DIC> @@
DIC> enter-composition
REGION NAME : /FER/: fer
PHASE NAME: /FCC_A1/: fcc
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /CR/: cr
TYPE /LINEAR/: read d2cr.dat
PROFILE FOR /NI/: ni
TYPE /LINEAR/: read d2ni.dat
DIC>
DIC> @@
DIC> @@ ENTER FERRITE AS THE SPHEROIDAL PHASE IN THE REGION
DIC> @@ SINCE THE FRACTION OF FERRITE IS SMALL, AND THESE APPEAR
DIC> @@ AS ISOLATED PARTICLES, FERRITE IS ENTERED AS A SPHEROIDAL PHASE
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /FER/: fer
PHASE TYPE /MATRIX/: sph
PHASE NAME: /NONE/: bcc
 INFO: EQUILIBRIUM COMPOSITION AND FRACTION OF SPHEROID PHASES USED AS DEFAULT
DIC>
DIC> @@
DIC> @@ ENTER THE COMPOSITION FOR THE SPHEROIDAL PHASE
DIC> @@ USE THE EQUILIBRIUM VALUE
DIC> @@
DIC> enter-composition
REGION NAME : /FER/: fer
PHASE NAME: /FCC_A1/: bcc
USE EQUILIBRIUM VALUE /Y/: y
DIC>
DIC> @@ SELECT A HOMOGENIZATION FUNCTION
DIC> @@ IN THIS CASE THE LOWER HASHIN-SHTRIKMAN BOUND
DIC> en-ho 1
 SELECTED FUNCTION IS HASHIN-SHTRIKMAN BOUND: GENERAL LOWER
DIC>
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME AND OTHER SIMULATION PARAMETERS
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 720000
AUTOMATIC TIMESTEP CONTROL /YES/: YES
MAX TIMESTEP DURING INTEGRATION /72000/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC> set-simulation-condition
NS01A PRINT CONTROL : /0/: 0
FLUX CORRECTION FACTOR : /1/: 1
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/: 2
CHECK INTERFACE POSITION /AUTO/: n
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/: act
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/: y
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/: 99
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -> 1): /AUTO/: 1
MAX TIMESTEP CHANGE PER TIMESTEP : /2/: 2
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/: n
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/: y
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/: n
DIC>
DIC>
DIC> @@
DIC> @@ SAVE THE SETUP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC>
DIC> save exd2 y
DIC>
DIC> set-inter
 --OK---
```

DIC>

**exd2b-run**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exd2b\run.DCM"
DIC>
DIC>
DIC> @@ exd2_run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING THE SIMULATION OF EXAMPLE D2
DIC> @@
DIC>
DIC> @@
DIC> @@ READ THE SETUP FROM FILE AND START THE SIMULATION
DIC> @@
DIC>
DIC> go d-m
 TIME STEP AT TIME  0.00000E+00
DIC> read exd2
 OK
DIC> sim
 STARTING SIMULATION USING HOMOGENIZATION MODEL
 ----------------------------------------------
  WARNING:BCC_A2 HAS NO VOLUME FRACTION, CREATING ONE
Starting time-step t0=   0.0000000     dt=  0.10000000E-06
Starting time-step t0=  0.10000000E-06 dt=  0.20000000E-06
Starting time-step t0=  0.30000000E-06 dt=  0.40000000E-06
Starting time-step t0=  0.70000000E-06 dt=  0.80000000E-06
Starting time-step t0=  0.15000000E-05 dt=  0.16000000E-05
Starting time-step t0=  0.31000000E-05 dt=  0.32000000E-05
Starting time-step t0=  0.63000000E-05 dt=  0.64000000E-05
Starting time-step t0=  0.12700000E-04 dt=  0.12800000E-04
Starting time-step t0=  0.25500000E-04 dt=  0.25600000E-04
Starting time-step t0=  0.51100000E-04 dt=  0.51200000E-04
Starting time-step t0=  0.10230000E-03 dt=  0.10240000E-03
Starting time-step t0=  0.20470000E-03 dt=  0.20480000E-03
Starting time-step t0=  0.40950000E-03 dt=  0.40960000E-03
Starting time-step t0=  0.81910000E-03 dt=  0.81920000E-03
Starting time-step t0=  0.16383000E-02 dt=  0.16384000E-02
Starting time-step t0=  0.32767000E-02 dt=  0.32768000E-02
Starting time-step t0=  0.65535000E-02 dt=  0.65536000E-02
Starting time-step t0=  0.13107100E-01 dt=  0.13107200E-01
Starting time-step t0=  0.26214300E-01 dt=  0.26214400E-01
Starting time-step t0=  0.52428700E-01 dt=  0.52428800E-01
Starting time-step t0=  0.10485750     dt=  0.10485760
Starting time-step t0=  0.20971510     dt=  0.20971520
Starting time-step t0=  0.41943030     dt=  0.41943040
Starting time-step t0=  0.83886070     dt=  0.83886080
Starting time-step t0=   1.6777215     dt=   1.6777216
Starting time-step t0=   3.3554431     dt=   3.3554432
Starting time-step t0=   6.7108863     dt=   6.7108864
Starting time-step t0=   13.421773     dt=   13.421773
Starting time-step t0=   26.843545     dt=   26.843546
Starting time-step t0=   53.687091     dt=   26.843546
Starting time-step t0=   80.530637     dt=   26.843546
Starting time-step t0=   107.37418     dt=   26.843546
Starting time-step t0=   134.21773     dt=   26.843546
Starting time-step t0=   161.06127     dt=   26.843546
Starting time-step t0=   187.90482     dt=   26.843546
Starting time-step t0=   214.74836     dt=   53.687091
Starting time-step t0=   268.43546     dt=   53.687091
Starting time-step t0=   322.12255     dt=   53.687091
Starting time-step t0=   375.80964     dt=   53.687091
Starting time-step t0=   429.49673     dt=   53.687091
Starting time-step t0=   483.18382     dt=   53.687091
Starting time-step t0=   536.87091     dt=   53.687091
Starting time-step t0=   590.55800     dt=   107.37418
Starting time-step t0=   697.93219     dt=   107.37418
Starting time-step t0=   805.30637     dt=   107.37418
Starting time-step t0=   912.68055     dt=   107.37418
Starting time-step t0=   1020.0547     dt=   107.37418
Starting time-step t0=   1127.4289     dt=   214.74836
Starting time-step t0=   1342.1773     dt=   214.74836
Starting time-step t0=   1556.9256     dt=   214.74836
Starting time-step t0=   1771.6740     dt=   214.74836
Starting time-step t0=   1986.4224     dt=   214.74836
Starting time-step t0=   2201.1707     dt=   214.74836
Starting time-step t0=   2415.9191     dt=   214.74836
Starting time-step t0=   2630.6675     dt=   429.49673
Starting time-step t0=   3060.1642     dt=   429.49673
Starting time-step t0=   3489.6609     dt=   429.49673
Starting time-step t0=   3919.1577     dt=   429.49673
Starting time-step t0=   4348.6544     dt=   429.49673
Starting time-step t0=   4778.1511     dt=   429.49673
Starting time-step t0=   5207.6478     dt=   429.49673
Starting time-step t0=   5637.1446     dt=   858.99346
Starting time-step t0=   6496.1380     dt=   858.99346
Starting time-step t0=   7355.1315     dt=   858.99346
Starting time-step t0=   8214.1250     dt=   858.99346
Starting time-step t0=   9073.1184     dt=   858.99346
Starting time-step t0=   9932.1119     dt=   858.99346
Starting time-step t0=   10791.105     dt=   858.99346
Starting time-step t0=   11650.099     dt=   1717.9869
Starting time-step t0=   13368.086     dt=   1717.9869
Starting time-step t0=   15086.073     dt=   1717.9869
Starting time-step t0=   16804.060     dt=   1717.9869
Starting time-step t0=   18522.046     dt=   1717.9869
Starting time-step t0=   20240.033     dt=   1717.9869
Starting time-step t0=   21958.020     dt=   3435.9738
Starting time-step t0=   25393.994     dt=   3435.9738
Starting time-step t0=   28829.968     dt=   3435.9738
Starting time-step t0=   30547.955     dt=   3435.9738
Starting time-step t0=   33983.929     dt=   3435.9738
Starting time-step t0=   37419.903     dt=   3435.9738
Starting time-step t0=   40855.876     dt=   3435.9738
Starting time-step t0=   44291.850     dt=   6871.9477
Starting time-step t0=   51163.798     dt=   6871.9477
Starting time-step t0=   58035.746     dt=   6871.9477
Starting time-step t0=   64907.693     dt=   6871.9477
Starting time-step t0=   71779.641     dt=   6871.9477
Starting time-step t0=   78651.589     dt=   6871.9477
Starting time-step t0=   85523.536     dt=   6871.9477
Starting time-step t0=   88959.510     dt=   6871.9477
```

```
Starting time-step t0=   95831.458     dt=   13743.895
Starting time-step t0=   109575.35     dt=   13743.895
Starting time-step t0=   116447.30     dt=   13743.895
Starting time-step t0=   130191.20     dt=   13743.895
Starting time-step t0=   143935.09     dt=   13743.895
Starting time-step t0=   147371.07     dt=   6871.9477
Starting time-step t0=   150807.04     dt=   3435.9738
Starting time-step t0=   154243.01     dt=   6871.9477
Starting time-step t0=   161114.96     dt=   13743.895
Starting time-step t0=   174858.86     dt=   13743.895
Starting time-step t0=   188602.75     dt=   27487.791
Starting time-step t0=   216090.54     dt=   27487.791
Starting time-step t0=   229834.44     dt=   13743.895
Starting time-step t0=   243578.33     dt=   27487.791
Starting time-step t0=   271066.12     dt=   27487.791
Starting time-step t0=   277938.07     dt=   13743.895
Starting time-step t0=   291681.97     dt=   27487.791
Starting time-step t0=   319169.76     dt=   27487.791
Starting time-step t0=   346657.55     dt=   27487.791
Starting time-step t0=   374145.34     dt=   27487.791
Starting time-step t0=   387889.23     dt=   27487.791
Starting time-step t0=   394761.18     dt=   13743.895
Starting time-step t0=   408505.08     dt=   13743.895
Starting time-step t0=   422248.97     dt=   27487.791
Starting time-step t0=   449736.76     dt=   27487.791
Starting time-step t0=   463480.66     dt=   27487.791
Starting time-step t0=   470352.61     dt=   6871.9477
Starting time-step t0=   477224.55     dt=   13743.895
Starting time-step t0=   490968.45     dt=   27487.791
Starting time-step t0=   518456.24     dt=   27487.791
Starting time-step t0=   532200.14     dt=   27487.791
Starting time-step t0=   545944.03     dt=   27487.791
Starting time-step t0=   573431.82     dt=   27487.791
Starting time-step t0=   600919.61     dt=   54975.581
Starting time-step t0=   628407.40     dt=   27487.791
Starting time-step t0=   642151.30     dt=   13743.895
Starting time-step t0=   655895.19     dt=   27487.791
Starting time-step t0=   683382.98     dt=   36617.016
 MUST SAVE WORKSPACE ON FILE
 WORKSPACE SAVED ON FILE
 RECLAIMING WORKSPACE
 DELETING TIME-RECORD FOR TIME    0.0000000
 DELETING TIME-RECORD FOR TIME   0.10000000E-06
 DELETING TIME-RECORD FOR TIME    805.30637
 DELETING TIME-RECORD FOR TIME    1556.9256
 DELETING TIME-RECORD FOR TIME    2415.9191
 DELETING TIME-RECORD FOR TIME    3489.6609
 DELETING TIME-RECORD FOR TIME    4348.6544
 DELETING TIME-RECORD FOR TIME    5207.6478
 DELETING TIME-RECORD FOR TIME    6496.1380
 DELETING TIME-RECORD FOR TIME    7355.1315
 DELETING TIME-RECORD FOR TIME    8214.1250
 DELETING TIME-RECORD FOR TIME    9073.1184
 DELETING TIME-RECORD FOR TIME    9932.1119
 DELETING TIME-RECORD FOR TIME    10791.105
 DELETING TIME-RECORD FOR TIME    11650.099
 DELETING TIME-RECORD FOR TIME    13368.086
 DELETING TIME-RECORD FOR TIME    15086.073
 DELETING TIME-RECORD FOR TIME    16804.060
 DELETING TIME-RECORD FOR TIME    18522.046
 DELETING TIME-RECORD FOR TIME    20240.033
 DELETING TIME-RECORD FOR TIME    21958.020
 DELETING TIME-RECORD FOR TIME    25393.994
 DELETING TIME-RECORD FOR TIME    28829.968
 DELETING TIME-RECORD FOR TIME    30547.955
 DELETING TIME-RECORD FOR TIME    33983.929
 DELETING TIME-RECORD FOR TIME    37419.903
 DELETING TIME-RECORD FOR TIME    40855.876
 DELETING TIME-RECORD FOR TIME    44291.850
 DELETING TIME-RECORD FOR TIME    51163.798
 DELETING TIME-RECORD FOR TIME    58035.746
 DELETING TIME-RECORD FOR TIME    64907.693
 DELETING TIME-RECORD FOR TIME    71779.641
 DELETING TIME-RECORD FOR TIME    78651.589
 DELETING TIME-RECORD FOR TIME    85523.536
 DELETING TIME-RECORD FOR TIME    88959.510
 DELETING TIME-RECORD FOR TIME    95831.458
 DELETING TIME-RECORD FOR TIME    109575.35
 DELETING TIME-RECORD FOR TIME    116447.30
 DELETING TIME-RECORD FOR TIME    130191.20
 DELETING TIME-RECORD FOR TIME    143935.09
 DELETING TIME-RECORD FOR TIME    147371.07
 DELETING TIME-RECORD FOR TIME    150807.04
 DELETING TIME-RECORD FOR TIME    154243.01
 DELETING TIME-RECORD FOR TIME    161114.96
 DELETING TIME-RECORD FOR TIME    174858.86
 DELETING TIME-RECORD FOR TIME    188602.75
 DELETING TIME-RECORD FOR TIME    216090.54
 DELETING TIME-RECORD FOR TIME    229834.44
 DELETING TIME-RECORD FOR TIME    243578.33
 DELETING TIME-RECORD FOR TIME    271066.12
 DELETING TIME-RECORD FOR TIME    277938.07
 DELETING TIME-RECORD FOR TIME    291681.97
 DELETING TIME-RECORD FOR TIME    319169.76
 DELETING TIME-RECORD FOR TIME    346657.55
 DELETING TIME-RECORD FOR TIME    374145.34
 DELETING TIME-RECORD FOR TIME    387889.23
 DELETING TIME-RECORD FOR TIME    394761.18
 DELETING TIME-RECORD FOR TIME    408505.08
 DELETING TIME-RECORD FOR TIME    422248.97
 DELETING TIME-RECORD FOR TIME    449736.76
 DELETING TIME-RECORD FOR TIME    463480.66
 DELETING TIME-RECORD FOR TIME    470352.61
 DELETING TIME-RECORD FOR TIME    477224.55
 DELETING TIME-RECORD FOR TIME    490968.45
 DELETING TIME-RECORD FOR TIME    518456.24
 DELETING TIME-RECORD FOR TIME    532200.14
 DELETING TIME-RECORD FOR TIME    545944.03
 DELETING TIME-RECORD FOR TIME    573431.82
 DELETING TIME-RECORD FOR TIME    600919.61
 DELETING TIME-RECORD FOR TIME    628407.40
 DELETING TIME-RECORD FOR TIME    642151.30
 DELETING TIME-RECORD FOR TIME    655895.19

 KEEPING TIME-RECORD FOR TIME    683382.98
 AND FOR TIME                    720000.00
```

```
 WORKSPACE RECLAIMED
 ------------------------------------------------
 INTERPOLATION SCHEME USED THIS FRACTION OF
 THE ALLOCATED MEMORY:   0.308576207705314
 EFFICIENCY FACTOR:    36.6887815225077
 ------------------------------------------------
 DEALLOCATING
 ------------------------------------------------

 TIMESTEP AT     720000.000     SELECTED

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

**exd2b-plot**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exd2b\plot.DCM"
DIC>
DIC>
DIC> @@ exd2_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE D2
DIC> @@
DIC> @@ ENTER THE DICTRA MODULE AND SPECIFY THE STORE-RESULT FILE
DIC> @@
DIC>
DIC> go d-m
 TIME STEP AT TIME  7.20000E+05
DIC> read  exd2
 OK
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA POST PROCESSOR
DIC> @@
DIC> post
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:
POST-1: @@
POST-1: @@ LET US FIRST SEE HOW THE FRACTION OF FERRITE  HAS CHANGED
POST-1: @@ AS A RESULT OF THE DIFFUSION
POST-1: @@
POST-1: s-d-a y npm(bcc)
POST-1: s-d-a x distance global
  INFO: Distance is set as independent variable
POST-1: s-p-c time 0 720000
POST-1: set-tit Figure D2.1
POST-1: plot
```

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

Figure D2.2

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

Figure D2.3

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

Figure D2.4

```
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1: @@
POST-1: @@ LET US PLOT THE DIFFUSION PATH FOR THE COUPLE
POST-1: @@ WE APPEND THE TERNARY PHASE-DIAGRAM CALCULATED IN THERMO-CALC
POST-1: @@ AND THE EXPERIMENTAL DATA
POST-1: @@
POST-1: s-d-a x w-p cr
POST-1: s-d-a y w-p ni
POST-1: s-i-v dis gl
POST-1: s-p-c time last
POST-1:
POST-1: app y exd2.exp
PROLOGUE NUMBER: /1/: 1
DATASET NUMBER(s): /-1/: 6 7 8
POST-1:
POST-1: s-s-s x n 10 50
POST-1: s-s-s y n 5 35
POST-1:
POST-1: set-tit Figure D2.5
POST-1: plot
```

Figure D2.5

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

# Example exd3

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

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

**exd3-setup**

```
SYS:About

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

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 21012) 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: Mon Nov 11 11:13:13 2019


SYS:SYS:MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exd3\setup.DCM.test"
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  v10.0

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10: sw fedemo
 Current database: Iron Demo Database v2.1

 VA                      /-  DEFINED
TDB_FEDEMO: def-sys fe cr ni
 FE                      CR                      NI
   DEFINED
TDB_FEDEMO: rej-ph *
 LIQUID:L                BCC_A2                  CBCC_A12
 CHI_A12                 CUB_A13                 FCC_A1
 HCP_A3                  LAVES_PHASE_C14         SIGMA
   REJECTED
TDB_FEDEMO: rest-ph bcc,fcc
 BCC_A2                  FCC_A1  RESTORED
TDB_FEDEMO: get
19:07:07,134 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270
      (1986); CR-FE'
  'B.-J. Lee, CALPHAD, 17 (1993) 251-268; revision of Fe-Cr and Fe -Ni liquid'
  'B.-J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
  'A. Dinsdale and T. Chart, MTDS NPL, Unpublished work (1986); CR -NI'
  'A. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); FE-NI'
 -OK-
TDB_FEDEMO:
TDB_FEDEMO: 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
 INFO: EQUILIBRIUM COMPOSITION AND FRACTION OF SPHEROID PHASES USED AS DEFAULT
DIC>
DIC> ent-comp
REGION NAME : /FECRNI/: fecrni
PHASE NAME: /FCC_A1/: fcc#1
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: m-f
PROFILE FOR /CR/: cr
TYPE /LINEAR/: read cr.dat
PROFILE FOR /NI/: ni
TYPE /LINEAR/: read ni.dat
DIC>
DIC> ent-comp
REGION NAME : /FECRNI/: fecrni
PHASE NAME: /FCC_A1/: bcc
USE EQUILIBRIUM VALUE /Y/: y
DIC>
DIC> se-si-ti
END TIME FOR INTEGRATION /.1/: 3.6e5
AUTOMATIC TIMESTEP CONTROL /YES/: yes
MAX TIMESTEP DURING INTEGRATION /36000/: 3.6e4
INITIAL TIMESTEP : /1E-07/: 1
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/: 1e-7
DIC>
DIC> @@ SIMULATIONS ARE FASTER WHEN THE RESULTS ARE NOT SAVED
DIC> @@ FOR EVERY TIME STEP
DIC> s-s-c
NS01A PRINT CONTROL : /0/: 0
FLUX CORRECTION FACTOR : /1/: 1
NUMBER OF DELTA TIMESTEPS IN CALLING MULDIF: /2/: 2
CHECK INTERFACE POSITION /AUTO/: n
VARY POTENTIALS OR ACTIVITIES OR LNAC : /ACTIVITIES/: act
ALLOW AUTOMATIC SWITCHING OF VARYING ELEMENT : /YES/: y
SAVE WORKSPACE ON FILE (YES,NO,0-999) /YES/: 99
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs (AUTO, 0 -> 0.5 -> 1): /AUTO/: .5
MAX TIMESTEP CHANGE PER TIMESTEP : /2/: 2
USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION /AUTO/: n
ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF /YES/: y
CALCULATE RESIDUAL FOR DEPENDENT COMPONENT /NO/:
DIC>
DIC> @@ There are a several options available for the homogenization
DIC> @@ model. There is also an interpolation scheme that may reduce
DIC> @@ simulation times. However, for this example, the default settings
DIC> @@ are kept and the interpolation scheme is turned off.
DIC> @@
DIC> homogen yes yes
 INFO: HOMOGENIZATION MODEL ENABLED
DIC>
DIC> @@ There are a large number of homogenization functions
DIC> @@ available. These determine how the average kinetics
DIC> @@ of the multiphase mixture is evaluated. For this example
DIC> @@ the General lower Hashin-Shtrikman bound is a good choice.
DIC> en-ho
ENTER HOMOGENIZATION FUNCTION # /5/: 1
 SELECTED FUNCTION IS HASHIN-SHTRIKMAN BOUND: GENERAL LOWER
DIC>
DIC>
DIC>
DIC> save exd3 Y
DIC>
DIC>
DIC> set-inter
 --OK---
DIC>
```

**exd3-run**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exd3\run.DCM.test"
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
 ----------------------------------------------
  WARNING:BCC_A2 HAS NO VOLUME FRACTION, CREATING ONE
Starting time-step t0=   0.0000000     dt=   1.0000000
Starting time-step t0=   1.0000000     dt=   2.0000000
Starting time-step t0=   3.0000000     dt=   4.0000000
Starting time-step t0=   7.0000000     dt=   8.0000000
Starting time-step t0=   15.000000     dt=   16.000000
Starting time-step t0=   31.000000     dt=   32.000000
Starting time-step t0=   63.000000     dt=   64.000000
Starting time-step t0=   127.00000     dt=   128.00000
Starting time-step t0=   255.00000     dt=   256.00000
Starting time-step t0=   511.00000     dt=   256.00000
Starting time-step t0=   767.00000     dt=   256.00000
Starting time-step t0=   1023.0000     dt=   512.00000
Starting time-step t0=   1535.0000     dt=   512.00000
Starting time-step t0=   2047.0000     dt=   1024.0000
Starting time-step t0=   3071.0000     dt=   1024.0000
Starting time-step t0=   4095.0000     dt=   2048.0000
Starting time-step t0=   6143.0000     dt=   2048.0000
Starting time-step t0=   8191.0000     dt=   2048.0000
Starting time-step t0=   10239.000     dt=   2048.0000
Starting time-step t0=   12287.000     dt=   4096.0000
Starting time-step t0=   16383.000     dt=   8192.0000
Starting time-step t0=   24575.000     dt=   8192.0000
Starting time-step t0=   32767.000     dt=   8192.0000
Starting time-step t0=   40959.000     dt=   8192.0000
Starting time-step t0=   49151.000     dt=   16384.000
Starting time-step t0=   65535.000     dt=   16384.000
Starting time-step t0=   81919.000     dt=   16384.000
Starting time-step t0=   98303.000     dt=   16384.000
Starting time-step t0=   114687.00     dt=   16384.000
Starting time-step t0=   131071.00     dt=   16384.000
Starting time-step t0=   147455.00     dt=   16384.000
Starting time-step t0=   163839.00     dt=   16384.000
Starting time-step t0=   180223.00     dt=   16384.000
Starting time-step t0=   196607.00     dt=   16384.000
Starting time-step t0=   212991.00     dt=   16384.000
Starting time-step t0=   229375.00     dt=   16384.000
Starting time-step t0=   245759.00     dt=   16384.000
Starting time-step t0=   262143.00     dt=   16384.000
Starting time-step t0=   278527.00     dt=   16384.000
Starting time-step t0=   294911.00     dt=   16384.000
Starting time-step t0=   311295.00     dt=   16384.000
Starting time-step t0=   327679.00     dt=   16384.000
Starting time-step t0=   344063.00     dt=   15937.000
 MUST SAVE WORKSPACE ON FILE
 WORKSPACE SAVED ON FILE
 RECLAIMING WORKSPACE
 DELETING TIME-RECORD FOR TIME    0.0000000
 DELETING TIME-RECORD FOR TIME    1.0000000
 DELETING TIME-RECORD FOR TIME    511.00000
 DELETING TIME-RECORD FOR TIME    1023.0000
 DELETING TIME-RECORD FOR TIME    1535.0000
 DELETING TIME-RECORD FOR TIME    2047.0000
 DELETING TIME-RECORD FOR TIME    3071.0000
 DELETING TIME-RECORD FOR TIME    4095.0000
 DELETING TIME-RECORD FOR TIME    6143.0000
 DELETING TIME-RECORD FOR TIME    8191.0000
 DELETING TIME-RECORD FOR TIME    10239.000
 DELETING TIME-RECORD FOR TIME    12287.000
 DELETING TIME-RECORD FOR TIME    16383.000
 DELETING TIME-RECORD FOR TIME    24575.000
 DELETING TIME-RECORD FOR TIME    32767.000
 DELETING TIME-RECORD FOR TIME    40959.000
 DELETING TIME-RECORD FOR TIME    49151.000
 DELETING TIME-RECORD FOR TIME    65535.000
 DELETING TIME-RECORD FOR TIME    81919.000
 DELETING TIME-RECORD FOR TIME    98303.000
 DELETING TIME-RECORD FOR TIME    114687.00
 DELETING TIME-RECORD FOR TIME    131071.00
 DELETING TIME-RECORD FOR TIME    147455.00
 DELETING TIME-RECORD FOR TIME    163839.00
 DELETING TIME-RECORD FOR TIME    180223.00
 DELETING TIME-RECORD FOR TIME    196607.00
 DELETING TIME-RECORD FOR TIME    212991.00
 DELETING TIME-RECORD FOR TIME    229375.00
 DELETING TIME-RECORD FOR TIME    245759.00
 DELETING TIME-RECORD FOR TIME    262143.00
 DELETING TIME-RECORD FOR TIME    278527.00
 DELETING TIME-RECORD FOR TIME    294911.00
 DELETING TIME-RECORD FOR TIME    311295.00
 DELETING TIME-RECORD FOR TIME    327679.00

 KEEPING TIME-RECORD FOR TIME    344063.00
 AND FOR TIME                    360000.00
 WORKSPACE RECLAIMED
 ----------------------------------------------
 INTERPOLATION SCHEME USED THIS FRACTION OF
 THE ALLOCATED MEMORY:   0.200698233364327
 EFFICIENCY FACTOR:    7.09082167832168
 ----------------------------------------------
 DEALLOCATING
 ----------------------------------------------
```

```
 TIMESTEP AT     360000.000     SELECTED

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

**exd3-plot**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exd3\plot.DCM.test"
DIC>
DIC>
DIC> @@ exd3_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE d3
DIC> @@
DIC> @@ ENTER THE DICTRA MODULE AND SPECIFY THE STORE-RESULT FILE
DIC> @@
DIC>
DIC> go d-m
 TIME STEP AT TIME  3.60000E+05
DIC> read  exd3
 OK
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA POST PROCESSOR
DIC> @@
DIC> post
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:
POST-1: @@
POST-1: @@ First study the composition profiles of Cr and Ni
POST-1: @@
POST-1: s-d-a x distance global
  INFO: Distance is set as independent variable
POST-1: s-d-a y w-p Cr
POST-1: s-p-c time 0 360000
POST-1: set-tit Figure D3.1
POST-1:
POST-1: app yes k5k7cr.exp 0; 1
POST-1:
POST-1: s-s-s x n 1e-3 2e-3
POST-1:
POST-1: s-s-s y n 20 45
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 3
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

Figure D3.1

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

Figure D3.2

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

Figure D3.3

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

Figure D3.4

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

# Cooperative Growth

# Example exe1

## Growth of pearlite in an Fe-Mn-C alloy

This is an example of pearlite growth in an Fe-0.50wt%C - 0.91wt%Mn steel.

**exe1-setup**

```
SYS:About

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

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 21012) 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: Mon Nov 11 11:13:13 2019


SYS:SYS:MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exe1\setup.DCM.test"
SYS: ?@@
 NO SUCH COMMAND, USE HELP
SYS: @@ Cooperative growth.
SYS: @@ Growth of pearlite in an Fe-Mn-C alloy
SYS: @@ An example of pearlite growth in an Fe-0.50wt%C-0.91wt%Mn steel.
SYS: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exe1_setup.DCM
SYS:
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASE
SYS: @@
SYS: go da
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v10.0

 VA                       /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10: sw FEDEMO
 Current database: Iron Demo Database v2.1

 VA                       /-  DEFINED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ DEFINE THE SYSTEM
TDB_FEDEMO: @@
TDB_FEDEMO: def-sys fe c mn
 FE                       C                        MN
   DEFINED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ KEEP ONLY THE AUSTENITE, FERRITE AND CEMENTITE PHASES
TDB_FEDEMO: @@
TDB_FEDEMO: rej-ph /all
 GAS:G                    LIQUID:L                 BCC_A2
 CBCC_A12                 CEMENTITE                CUB_A13
 DIAMOND_FCC_A4           FCC_A1                   GRAPHITE
 HCP_A3                   KSI_CARBIDE              LAVES_PHASE_C14
 M23C6                    M5C2                     M7C3
   REJECTED
TDB_FEDEMO: rest-ph fcc,bcc,cem
 FCC_A1                   BCC_A2                   CEMENTITE
   RESTORED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ GET THE THERMODYNAMIC DATA
TDB_FEDEMO: @@
TDB_FEDEMO: get
19:10:36,265 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'P. Franke, Estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
  'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'W. Huang, Metall. Trans. A, 21A (1990) 2115-2123; TRITA-MAC 411 (Rev
      1989); C-FE-MN'
  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, CALPHAD,
      submitted, 2011; Fe-Mn-C'
  'W. Huang, CALPHAD, 13 (1989) 243-252; TRITA-MAC 388 (rev 1989); FE-MN'
  'B. Hallstedt, D. Djurovic, J. von Appen, R. Dronskowski, A. Dick, F.
      Koermann, T. Hickel, J. Neugebauer, CALPHAD, 34, 129 -33(2010); Fe-C'
  'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, CALPHAD, 34, 279
      -85(2010); Mn-C'
  'P. Villars and L.D. Calvert (1985). Pearson`s handbook of
      crystallographic data for intermetallic phases. Metals park, Ohio.
      American Society for Metals; Molar volumes'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
 -OK-
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ APPEND THE KINETIC DATA FROM THE MOBILITY DATABASE
TDB_FEDEMO: @@
TDB_FEDEMO: append mobfe4
 Current database: Steels/Fe-Alloys Mobility  v4.0

 VA  DEFINED
 B2_BCC  REJECTED
APP: def-sys fe c mn
 FE                       C                        MN
   DEFINED
APP: rej-ph /all
 BCC_A2                   CEMENTITE                FCC_A1
 FE4N_LP1                 HCP_A3                   LIQUID:L
```

```
   REJECTED
APP: rest-ph bcc,fcc,cem
 BCC_A2                  FCC_A1                  CEMENTITE
   RESTORED
APP: get
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'This parameter has not been assessed'
  'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'
  'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
      -Ni'
  'Y. Liu, L. Zhang, et al. CALPHAD 33(2009)614-23; Fe-Mn-C (fcc)'
  'B. Jonsson: Z. Metallkunde 85(1994)498-501; C and N diffusion in bcc Cr
      -Fe-Ni'
  'B. Jonsson: Z. Metallkunde 83(1992)349-355; Cr, Co, Fe and Ni diffusion
      in bcc Fe'
  'S. Deng, et al., CALPHAD, 56 (2017) 230-240.'
  'Assessed from data presented in Landholt-Bornstein, Vol. 26, ed. H.
      Mehrer, springer (1990); Impurity diff of Mn in bcc Fe.'
 -OK-
APP:
APP: @@
APP: @@ ALL THE THERMODYNAMIC AND KINETIC DATA HAVE BEEN RETRIEVED.
APP: @@ GO TO THE DICTRA MONITOR TO SET UP YOUR PROBLEM.
APP: @@
APP: go d-m
 NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ SET THE CONDITION FOR TEMPERATURE
DIC> @@
DIC> set-cond glob t 0 900-time*10; * n
DIC>
DIC> @@
DIC> @@ ENTER A REGION
DIC> @@
DIC> enter-reg pearlite
DIC>
DIC> @@
DIC> @@ ENTER A SMALL INITIAL SIZE OF THE GRID IN THE 'PEARLITE' REGION
DIC> @@
DIC> enter-grid pearlite 5e-10 lin 5
DIC>
DIC> @@
DIC> @@ ENTER INTO THE 'PEARLITE' REGION THE PHASES 'BCC' AND 'CEM' AND SPECIFY
DIC> @@ THAT ARE PRESENT IN THE FORM OF A 'LAMELLAR AGGREGATE. SET THE STATUS
DIC> @@ TO 'ACTIVE'. SEVERAL PROMPTS FOLLOW ABOUT THE VALUES OF THE PARAMETERS
DIC> @@ IN THE PEARLITE GROWTH MODEL, FOR EXAMPLE AS SURFACE TENSION, OPTIMUM
DIC> @@ GROWTH RATE FACTOR, AND BOUNDARY DIFFUSION COEFFICIENTS.
DIC> @@
DIC> @@ CARBON(C) IS TREATED IN A SPECIAL WAY. IF 'AUTOMATIC' IS ENTERED
DIC> @@ THE DIFFUSION OF C IS CALCULATED ACCORDING TO AN EQUATION FOR
DIC> @@ MIXED BOUNDARY AND VOLUME DIFFUSION. YOU CAN CHOOSE BETWEEN
DIC> @@ MANUAL OR AUTOMATIC START VALUES FOR ALL VARIABLES EXCEPT THE GROWTH
DIC> @@ RATE. IN THIS EXAMPLE WE WILL TRY 1E-6
DIC> @@
DIC> @@ FOR MORE INFORMATION ABOUT THE PEARLITE GROWTH MODEL SEE
DIC> @@ B. JÖNSSON: TRITA-MAC-0478, 1992 (ROYAL INSTITUTE OF TECHNOLOGY)
DIC> @@ STOCKHOLM, SWEDEN, 1992.
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /PEARLITE/: pearlite
PHASE TYPE /MATRIX/: lam
      Eutectiod reaction is "GAMMA" ==> "ALPHA" + "BETA"
 Enter name of "ALPHA" phase /BCC_A2/: bcc_a2
 Enter name of "BETA" phase /CEMENTITE/: cementite
 Enter name of "GAMMA" phase /FCC_A1/: fcc_a1
 Enter "ALPHA"/"BETA" surface tension
LOW TIME LIMIT /0/: 0
 Surface tension(T,P,TIME)= 1;
HIGH TIME LIMIT /*/: 1000
ANY MORE RANGES /N/: N
 Enter "ALPHA"/"GAMMA" surface tension
LOW TIME LIMIT /0/: 0
 Surface tension(T,P,TIME)= 1;
HIGH TIME LIMIT /*/: 1000
ANY MORE RANGES /N/: N
 Enter "BETA"/"GAMMA" surface tension
LOW TIME LIMIT /0/: 0
 Surface tension(T,P,TIME)= 1;
HIGH TIME LIMIT /*/: 1000
ANY MORE RANGES /N/: N
 Optimum growth condition factor /2/: 2
 Name of dependent element /FE/: fe
 INPUT OF DIFFUSION DATA
   Growth model (VOLUME/BOUNDARY/KIRKALDY) for element C /BOUNDARY/: boundary
     DF(C) = /value/AUTOMATIC/MIXED/: auto
   Growth model (VOLUME/BOUNDARY/KIRKALDY) for element MN /BOUNDARY/: boundary
     DF(MN) = /value/MIXED/: 5.4e-14
     DQ(MN): 155000
 Automatic start values for the S0 determination /Y/: Y
 Growth rate V: 1E-6
 Automatic start values on other variables /Y/: Y
DIC>
DIC> @@
DIC> @@ INITIATE THE COMPOSITION RECORDS FOR THE 'PEARLITE'
DIC> @@
DIC> enter-composition
REGION NAME : /PEARLITE/: pearlite
DIC>
DIC> @@
DIC> @@ NOW CONTINUE BY DEFINING A MATRIX PHASE INTO WHICH THE PEARLITE
DIC> @@ WILL GROW. START BY ENTERING A REGION NAME, 'AUSTENITE'
DIC> @@
```

```
DIC> enter-region austenite
ATTACH TO REGION NAMED /PEARLITE/:
ATTACHED TO THE RIGHT OF PEARLITE /YES/:
DIC> @@
DIC> @@ SPECIFY WHAT PHASE 'FCC' WILL BE PRESENT IN THE 'AUSTENITE' REGION
DIC> @@ AND WHAT TYPE OF PHASE 'MATRIX' IT IS AND ITS INITIAL STATE 'ACTIVE'
DIC> @@
DIC> enter-phase act austenite matrix fcc
DIC>
DIC> @@
DIC> @@ WE ALSO NEED TO HAVE A SPATIAL GRID IN THE 'AUSTENITE' REGION.
DIC> @@ CHOSE SIZE '4E-5' GRIDTYPE 'GEOMETRICAL', '30' GRIDPOINTS AND '1.5'
DIC> @@ AS VALUES FOR THE GEOMETRICAL FACTOR OF THE GRID.
DIC> @@
DIC> enter-grid austenite 4e-5 geo 30 1.5
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL CONCENTRATION PROFILES IN THE 'FCC' PHASE OF THE
DIC> @@ 'AUSTENITE' REGION. CONCENTRATIONS MUST BE GIVEN IN Y-FRACTIONS.
DIC> @@
DIC> enter-composition
REGION NAME : /AUSTENITE/: austenite
PHASE NAME: /FCC_A1/: fcc
DEPENDENT COMPONENT ? /MN/: fe
COMPOSITION TYPE /MOLE_FRACTION/: site-fraction
 PROFILE FOR MN
TYPE /LINEAR/: lin 9.29232973E-3 9.29232973E-3
 PROFILE FOR C
TYPE /LINEAR/: lin 2.3384332E-2 2.3384332E-2
DIC>
DIC> @@
DIC> @@ THE MATRIX PHASE IS NOW COMPLETE.
DIC> @@
DIC>
DIC> @@
DIC> @@ SPECIFY A SPHERICAL '2' GEOMETRY
DIC> @@
DIC> enter-geo 2
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 5
AUTOMATIC TIMESTEP CONTROL /YES/: YES
MAX TIMESTEP DURING INTEGRATION /.5/: 0.1
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exe1 Y
DIC>
DIC> set-inter
 --OK---
DIC>
```

**exe1-run**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exe1\run.DCM.test"
DIC>
DIC>
DIC> @@ exe1_run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING EXAMPLE e1
DIC> @@
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA MONITOR
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  0.00000E+00
DIC>
DIC> @@
DIC> @@ READ SETUP FROM FILE
DIC> @@
DIC> read exe1
 OK
DIC>
DIC> @@
DIC> @@ START THE SIMULATION
DIC> @@
DIC> simulate
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
  Trying old scheme                     4
 U-FRACTION IN SYSTEM:  C = .0233843320030518  FE = .990707670399293
                        MN = .0092923297312127
 TOTAL SIZE OF SYSTEM:  2.68092626329E-13 [m^3]
 U-FRACTION IN SYSTEM:  C = .0233843320030518  FE = .990707670399293
                        MN = .0092923297312127
 TOTAL SIZE OF SYSTEM:  2.68092626329E-13 [m^3]
  17  GRIDPOINT(S) ADDED   TO   CELL #1   REGION: AUSTENITE
 TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =   0.0000000
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.77961766E-05 AND   0.77961766E-05
 POSITION OF INTERFACE PEARLITE / AUSTENITE IS   0.50077962E-09
 U-FRACTION IN SYSTEM:  C = .0233843320030518  FE = .990707670399294
                        MN = .00929232973121272
 TOTAL SIZE OF SYSTEM:  2.68092626329E-13 [m^3]
  10  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUSTENITE

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

```
                        MN = .00929232973121266
 TOTAL SIZE OF SYSTEM:  2.68092626329E-13 [m^3]
  CPU time used in timestep                    0 seconds
  1 GRIDPOINT(S) REMOVED FROM CELL#  1 REGION #  1
 TIME =  0.35283788     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.86617616E-05 AND   0.86617616E-05
 POSITION OF INTERFACE PEARLITE / AUSTENITE IS   0.29374476E-05
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399294
                        MN = .00929232973121271
 TOTAL SIZE OF SYSTEM:  2.68092626329E-13 [m^3]
  CPU time used in timestep                    1 seconds


output ignored...



... output resumed

 WORKSPACE RECLAIMED
  INFO: CELL   1 REGION AUSTENITE   DELETED
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399328
                        MN = .00929232973117857
 TOTAL SIZE OF SYSTEM:  2.68126144219E-13 [m^3]
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399328
                        MN = .00929232973117857
 TOTAL SIZE OF SYSTEM:  2.68126144219E-13 [m^3]
 TIME =   3.2743323     DT =  0.10000000E-04 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399328
                        MN = .00929232973117857
 TOTAL SIZE OF SYSTEM:  2.68126144219E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   3.2843323     DT =  0.10000000E-01 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399328
                        MN = .00929232973117857
 TOTAL SIZE OF SYSTEM:  2.68126144219E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   3.3843323     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399328
                        MN = .00929232973117857
 TOTAL SIZE OF SYSTEM:  2.68126144219E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   3.4843323     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399328
                        MN = .00929232973117857
 TOTAL SIZE OF SYSTEM:  2.68126144219E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   3.5843323     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399328
                        MN = .00929232973117857
 TOTAL SIZE OF SYSTEM:  2.68126144219E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   3.6843323     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399328
                        MN = .00929232973117857
 TOTAL SIZE OF SYSTEM:  2.68126144219E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   3.7843323     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399328
                        MN = .00929232973117857
 TOTAL SIZE OF SYSTEM:  2.68126144219E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   3.8843323     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399328
                        MN = .00929232973117857
 TOTAL SIZE OF SYSTEM:  2.68126144219E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   3.9843323     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399328
                        MN = .00929232973117857
 TOTAL SIZE OF SYSTEM:  2.68126144219E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   4.0843323     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399328
                        MN = .00929232973117857
 TOTAL SIZE OF SYSTEM:  2.68126144219E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   4.1843323     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399328
                        MN = .00929232973117857
 TOTAL SIZE OF SYSTEM:  2.68126144219E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   4.2843323     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399328
                        MN = .00929232973117857
 TOTAL SIZE OF SYSTEM:  2.68126144219E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   4.3843323     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399328
                        MN = .00929232973117857
 TOTAL SIZE OF SYSTEM:  2.68126144219E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   4.4843323     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399328
                        MN = .00929232973117857
 TOTAL SIZE OF SYSTEM:  2.68126144219E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   4.5843323     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399328
                        MN = .00929232973117857
 TOTAL SIZE OF SYSTEM:  2.68126144219E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   4.6843323     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399328
                        MN = .00929232973117857
 TOTAL SIZE OF SYSTEM:  2.68126144219E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   4.7843323     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399328
                        MN = .00929232973117857
 TOTAL SIZE OF SYSTEM:  2.68126144219E-13 [m^3]
  CPU time used in timestep                    0 seconds
 TIME =   4.8843323     DT =  0.10000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399328
                        MN = .00929232973117857
 TOTAL SIZE OF SYSTEM:  2.68126144219E-13 [m^3]
```

```
 CPU time used in timestep                    0 seconds
TIME =   4.9843323     DT =  0.10000000     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399328
                       MN = .00929232973117857
TOTAL SIZE OF SYSTEM:  2.68126144219E-13 [m^3]
 CPU time used in timestep                    0 seconds
TIME =   5.0000000     DT =  0.15667748E-01 SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0233843320030516  FE = .990707670399328
                       MN = .00929232973117857
TOTAL SIZE OF SYSTEM:  2.68126144219E-13 [m^3]
MUST SAVE WORKSPACE ON FILE
WORKSPACE SAVED ON FILE
RECLAIMING WORKSPACE
DELETING TIME-RECORD FOR TIME    3.2528379
DELETING TIME-RECORD FOR TIME    3.2743223
DELETING TIME-RECORD FOR TIME    3.2743323
DELETING TIME-RECORD FOR TIME    3.2843323
DELETING TIME-RECORD FOR TIME    3.3843323
DELETING TIME-RECORD FOR TIME    3.4843323
DELETING TIME-RECORD FOR TIME    3.5843323
DELETING TIME-RECORD FOR TIME    3.6843323
DELETING TIME-RECORD FOR TIME    3.7843323
DELETING TIME-RECORD FOR TIME    3.8843323
DELETING TIME-RECORD FOR TIME    3.9843323
DELETING TIME-RECORD FOR TIME    4.0843323
DELETING TIME-RECORD FOR TIME    4.1843323
DELETING TIME-RECORD FOR TIME    4.2843323
DELETING TIME-RECORD FOR TIME    4.3843323
DELETING TIME-RECORD FOR TIME    4.4843323
DELETING TIME-RECORD FOR TIME    4.5843323
DELETING TIME-RECORD FOR TIME    4.6843323
DELETING TIME-RECORD FOR TIME    4.7843323
DELETING TIME-RECORD FOR TIME    4.8843323

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

TIMESTEP AT     5.00000000     SELECTED

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

**exe1-plot**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exe1\plot.DCM.test"
DIC>
DIC>
DIC> @@ exe1_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE e1
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  5.00000E+00
DIC> read exe1
 OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1: @@
POST-1: @@ PLOT THE TEMPERATURE AS A FUNCTION OF TIME
POST-1: @@
POST-1: s-d-a x time
  INFO: Time is set as independent variable
POST-1: s-d-a y t
POST-1: s-p-c interface first
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 3
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
ORKING ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

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

2019.11.11.19.12.40
CELL #1

```
POST-1:
POST-1:
POST-1:
POST-1:Hit RETURN to continue
POST-1:
POST-1: @@
POST-1: @@ PLOT THE LAMELLAR SPACING AS A FUNCTION OF TIME
POST-1: @@
POST-1: s-d-a
AXIS (X, Y OR Z) : y
VARIABLE : lamellar-sp
IN REGION: /*/: pearlite
POST-1:
POST-1: s-p-c
CONDITION /INTEGRAL/: interface
INTERFACE : pearlite
UPPER OR LOWER INTERFACE OF REGION PEARLITE#1 /LOWER/: upper
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 3
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
ORKING ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

2019.11.11.19.12.40
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:
POST-1: SET_EXP_FILE_FORMAT 3
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
ORKING ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

2019.11.11.19.12.41
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: @@ AND THE C COMPOSITION IN THE FERRITE VS. TEMP
POST-1: @@
POST-1: s-d-a y w(bcc,c)
POST-1:
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 3
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
ORKING ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

2019.11.11.19.12.41
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: @@ FINALLY, LET'S LOOK AT THE VELOCITY OF THE INTERFACE VS. TEMP
POST-1: @@
POST-1: s-d-a y t
POST-1: s-d-a x velocity
INTERFACE : pearlite
UPPER OR LOWER INTERFACE OF REGION PEARLITE#1 /LOWER/: upper
POST-1: set-ax-ty x log
POST-1: s-s-s x n 1e-6 1e-4
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 3
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
ORKING ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

2019.11.11.19.12.42
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: 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.

# Coarsening

Moving phase interface with α and β in local equilibrium.

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

Equilibrium as defined by the average composition in the system.

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

# Example exf1

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

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

**T = 1173K** **$r_p$ = 0.228 μm**

**exf1-setup**

```
SYS:About

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

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 21012) 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: Mon Nov 11 11:13:13 2019


SYS:SYS:MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exf1\setup.DCM.test"
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  v10.0

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10: switch TCFE9
 Current database: Steels/Fe-Alloys  v9.1

 VA                      /-  DEFINED
 L12_FCC                 B2_BCC                  DICTRA_FCC_A1
   REJECTED
TDB_TCFE9: def-sys fe mo c
 FE                      MO                      C
   DEFINED
TDB_TCFE9: rej ph * all
 GAS:G                   LIQUID:L                BCC_A2
 FCC_A1                  HCP_A3                  CBCC_A12
 CUB_A13                 DIAMOND_FCC_A4          GRAPHITE
 CEMENTITE               M23C6                   M7C3
 M6C                     M5C2                    M3C2
 MC_ETA                  MC_SHP                  KSI_CARBIDE
 Z_PHASE                 FE4N_LP1                FECN_CHI
 SIGMA                   MU_PHASE                P_PHASE
 R_PHASE                 CHI_A12                 LAVES_PHASE_C14
 AL5FE4                  M2O3C:I  REJECTED
TDB_TCFE9: res ph fcc m6c
 FCC_A1                  M6C  RESTORED
TDB_TCFE9: get
19:14:03,092 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
  'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
  'J-O. Andersson, CALPHAD, 12 (1988) 1-8; TRITA 0317 (1986); C-MO'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'A. Fernandez Guillermet, CALPHAD, 6 (1982) 127-140; (sigma phase revised
      1986); TRITA-MAC 200 (1982); FE-MO'
  'J-O. Andersson, CALPHAD, 12 (1988) 9-23; TRITA 0321 (1986); C-FE-MO'
  'S. Nagakura, Transactions of the Iron and Steel Institute of Japan, 8
      (1968) 265-294; Molar volumes'
  'I.K. Kupalova, V.I. Pavlova, High Speed Steels: Physical Properties,
      Prop. Data Updat. 2 (1988) 67-78; Molar volumes'
 -OK-
TDB_TCFE9:
TDB_TCFE9: @@
TDB_TCFE9: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE MOBILITY DATA
TDB_TCFE9: @@
TDB_TCFE9: app
 Use one of these databases

 TCFE10  =  Steels/Fe-Alloys  v10.0
 TCFE9   =  Steels/Fe-Alloys  v9.1
 TCFE8   =  Steels/Fe-Alloys  v8.1
 TCFE7   =  Steels/Fe-Alloys  v7.0
 TCFE6   =  Steels/Fe-Alloys  v6.2
 TCFE5   =  Steels/Fe-Alloys  v5.0
 TCFE4   =  Steels/Fe-Alloys  v4.1
 TCFE3   =  Steels/Fe-Alloys  v3.1
 TCFE2   =  Steels/Fe-Alloys  v2.1
 TCFE1   =  Steels/Fe-Alloys  v1.0
 FROST1  =  FROST database v1.2
 FEDAT   =  TCS/TT Steels Database v1.0
 TCNI10  =  Ni-Alloys  v10.0 SNAPSHOT
 TCNI9   =  Ni-Alloys  v9.1
 TCNI8   =  Ni-Alloys  v8.2
 TCNI7   =  Ni-Alloys  v7.2
 TCNI6   =  Ni-Alloys  v6.1
 TCNI5   =  Ni-Alloys  v5.1
 TCNI4   =  Ni-Alloys  v4.0
 TCNI1   =  Ni-Alloys  v1.3
 TCAL6   =  Al-Alloys  v6.0
 TCAL5   =  Al-Alloys  v5.1
 TCAL4   =  Al-Alloys  v4.0
 TCAL3   =  Al-Alloys  v3.0
 TCAL2   =  Al-Alloys  v2.1
```

```
 TCAL1   =  Al-Alloys  v1.2
 TCMG5   =  Mg-Alloys  v5.1
 TCMG4   =  Mg-Alloys  v4.0
 TCMG3   =  Mg-Alloys  v3.0
 TCMG2   =  Mg-Alloys  v2.0
 TCMG1   =  Mg-Alloys  v1.1
 TCTI2   =  Ti-Alloys  v2.1
 TCTI1   =  Ti-Alloys  v1.0
 TCCU3   =  Cu-Alloys  v3.1
 TCCU2   =  Cu-Alloys  v2.0
 TCCU1   =  Cu-Alloys  v1.0
 TCCC1   =  Cemented carbide  v1.0
 TCHEA4  =  High Entropy Alloy  v4.0
 TCHEA3  =  High Entropy Alloy  v3.1
 TCHEA2  =  High Entropy Alloy  v2.1.1
 TCHEA1  =  High Entropy Alloy  v1.0
 SSOL7   =  SGTE Alloy Solutions Database v7.0
 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
 TCOX10  =  Metal Oxide Solutions  v10.0 SNAPSHOT
 TCOX9   =  Metal Oxide Solutions  v9.0
 TCOX8   =  Metal Oxide Solutions  v8.0
 TCOX7   =  Metal Oxide Solutions  v7.0
 TCOX6   =  Metal Oxide Solutions  v6.0
 TCOX5   =  Metal Oxide Solutions  v5.1
 TCOX4   =  Metal Oxide Solutions  v4.1
 ION3    =  Ionic Solutions  v3.0
 ION2    =  Ionic Solutions  v2.6
 ION1    =  Ionic Solutions  v1.5
 NOX2    =  NPL Oxide Solutions Database v2.1
 TCNOBL2 =  Noble Metals Alloys v2.0 SNAPSHOT
 TCNOBL1 =  Noble Metals Alloys v1.0
 TCSLD3  =  Solder Alloys  v3.2
 TCSLD2  =  Solder Alloys  v2.0
 TCSLD1  =  Solder Alloys  v1.1
 TCSI1   =  Ultrapure Silicon  v1.2
 TCMP2   =  Materials Processing  v2.5
 TCES1   =  Combustion/Sintering  v1.1
 TCSC1   =  Super Conductor  v1.0
 TCFC1   =  SOFC Database v1.0
 TCNF2   =  Nuclear Fuels  v2.1b
 NUMT2   =  Nuclear Materials  v2.1
 NUOX4   =  Nuclear Oxides  v4.2
 NUCL15  =  IRSN NUCLEA-15_4
 NUCL10  =  ThermoData NUCLEA Alloys-oxides TDB v10.2
 MEPH15  =  IRSN Mephista-15_1
 MEPH11  =  ThermoData MEPHISTA Nuclear Fuels TDB v11.2
 TCAQ3   =  Aqueous Solution  v3.0
 TCAQ2   =  Aqueous Solution  v2.7
 AQS2    =  TGG Aqueous Solution Database v2.6
 GCE2    =  TGG Geochemical/Environmental TDB v2.3
 FEDEMO  =  Iron Demo Database v2.1
 ALDEMO  =  Aluminum Demo Database v3.0
 NIDEMO  =  Nickel Demo Database v1.1
 CUDEMO  =  Copper Demo Database v1.0
 SLDEMO  =  Solder Demo Database v1.0
 OXDEMO  =  Oxide Demo Database v1.0
 SUBDEMO =  Substance Demo Database v1.0
 PTERN   =  Public Ternary Alloys TDB v1.3
 PAQ2    =  Public Aqueous Soln (SIT) TDB v2.4
 PG35    =  G35 Binary Semi-Conductors TDB v1.2
 PURE5   =  SGTE Unary (Pure Elements) TDB v5.1
 MOB2    =  Alloys Mobility  v2.7
 MOB1    =  Alloys Mobility  v1.3
 MOBFE1  =  Steels/Fe-Alloys Mobility  v1.1
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBFE5  =  Steels/Fe-Alloys Mobility  v5.0
 MOBNI5  =  Ni-Alloys Mobility  v5.1
 MOBNI4  =  Ni-Alloys Mobility  v4.1
 MOBNI3  =  Ni-Alloys Mobility  v3.2
 MOBNI2  =  Ni-Alloys Mobility  v2.4
 MOBNI1  =  Ni-Alloys Mobility  v1.10
 MOBAL5  =  Al-Alloys Mobility  v5.0
 MOBAL4  =  Al-Alloys Mobility  v4.0
 MOBAL3  =  Al-Alloys Mobility  v3.0
 MOBAL2  =  Al-Alloys Mobility  v2.0
 MOBAL1  =  Al-Alloys Mobility  v1.0
 MOBCU1  =  Cu-Alloys Mobility  v1.0
 MOBCU2  =  Cu-Alloys Mobility  v2.0
 MOBCU3  =  Cu-Alloys Mobility  v3.0
 MOBHEA1 =  High Entropy Alloys Mobility  v1.0
 MOBHEA2 =  High Entropy Alloys Mobility  v2.0
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBSLD1 =  Solder-Alloys Mobility  v1.1
 MOBTI3  =  Ti-Alloys Mobility  v3.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v2.0
 MFEDEMO =  Fe-Alloys Mobility demo database v2.0
 MNIDEMO =  Ni-Alloys Mobility demo database v1.0
 MCUDEMO =  Cu-Alloys Mobility demo database v1.0
 USER    =  User defined Database

DATABASE NAME /TCFE9/: mobfe4
 Current database: Steels/Fe-Alloys Mobility  v4.0

 VA  DEFINED
```

```
 B2_BCC  REJECTED
APP: def-sys fe mo c
 FE                      MO                      C
   DEFINED
APP: rej ph * all
 BCC_A2                  CEMENTITE               FCC_A1
 FE4N_LP1                HCP_A3                  LIQUID:L
   REJECTED
APP: res ph fcc m6c
 *** ERROR M6C INPUT IGNORED
 FCC_A1  RESTORED
APP: get
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'This parameter has not been assessed'
  'J. Agren: Scripta Met. 20(1986)1507-1510; C diff in fcc C-Fe'
  'B. Jonsson: Scand. J. Metall. 23(1994)201-208; Fe and Ni diffusion fcc Fe
      -Ni'
  'Y. Liu et al., Calphad 34(2010)253-262; fcc Cu-Fe.'
  'W. Zheng, et al., Metall Mater Trans, 48 (2017) 536-550; Fe-Mn-Mo (fcc
      and bcc)'
 -OK-
APP:
APP:
APP: @@
APP: @@ ENTER THE DICTRA MONITOR
APP: @@
APP: go d-m
 NO TIME STEP DEFINED
 *** ENTERING M6C AS A DIFFUSION NONE PHASE
DIC>
DIC> @@
DIC> @@  ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> s-cond glob t 0 1173; * N
DIC>
DIC> @@
DIC> @@ ENTER REGIONS part AND aus
DIC> @@
DIC> enter-region
REGION NAME : part
DIC> enter-region aus
ATTACH TO REGION NAMED /PART/:
ATTACHED TO THE RIGHT OF PART /YES/:
DIC> @@
DIC> @@ ENTER GEOMTRICAL GRIDS INTO THE REGIONS
DIC> @@
DIC>
DIC> @@
DIC> @@ THE INITIAL SIZE OF THE CARBIDE PARTICLE IS ASSUMED TO BE KNOWN
DIC> @@ (IN THIS CASE THE VALUE IS FROM NISHIZAWA ET. AL.).  THE
DIC> @@ AVERAGE PARTICLE SIZE IS ASSUMED TO BE 0.152E-6 METERS. HOWEVER, THE
DIC> @@ CALCULATIONS ARE PERFORMED ON A MAXIMUM SIZE PARTICLE, WHICH IS ASSUMED
DIC> @@ TO BE 1.5 TIMES THE AVERAGE SIZE. THE SURROUNDING AUSTENITIC MATRIX
DIC> @@ SIZE IS CHOOSEN TO MAINTAIN THE AVERAGE COMPOSITION.
DIC> @@
DIC> enter-grid
REGION NAME : /PART/: part
WIDTH OF REGION /1/: 0.228E-6
TYPE /LINEAR/: AUTO
DIC>
DIC> enter-grid
REGION NAME : /AUS/: aus
WIDTH OF REGION /1/: 4.53147041E-7
TYPE /LINEAR/: AUTO
DIC>
DIC> @@
DIC> @@ ENTER PHASES INTO REGIONS
DIC> @@
DIC> enter-phase active part matrix m6c
DIC>
DIC> enter-phase active aus matrix fcc#1
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITIONS IN THE PHASES
DIC> @@
DIC> enter-composition
REGION NAME : /PART/: part
PHASE NAME: /M6C/: m6c
DEPENDENT COMPONENT ? /MO/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-f
PROFILE FOR /MO/: mo lin 6.20117E-01 6.20117E-01
DIC>
DIC> ent-composition
REGION NAME : /AUS/: aus
PHASE NAME: /FCC_A1/: fcc#1
DEPENDENT COMPONENT ? /MO/: fe
COMPOSITION TYPE /MOLE_FRACTION/: w-f
PROFILE FOR /C/: mo lin 1.82099E-02 1.82099E-02
PROFILE FOR /MO/: c lin 2.83351E-03 2.83351E-03
DIC>
DIC>
DIC> @@
DIC> @@ SET A SPHERICAL GEOMETRY
DIC> @@
DIC> ent-geo 2
DIC>
DIC> @@
DIC> @@ ENTER THE SURFACE TENSION ENERGY CONTRIBUTION AS A FUNCTION OF
DIC> @@ THE INTERFACE POSITION (THE RADIUS OF THE PARTICLE).
DIC> @@ ALSO ENTER THE MOLAR VOLUME OF THE PHASE CORRECTED TO BE THE
DIC> @@ MOLAR VOLUME PER SUBSTITIONAL ATOM.
DIC> @@
DIC> @@ THE SURFACE TENSION IS 0.7, THE MOLAR VOLUME IS 0.71 AND THE
```

```
DIC> @@ TRANSFORMATION TO MOLAR VOLUME PER SUBSTITIONAL ATOM IS 7/6.
DIC> @@
DIC> set-surf 2*0.7*0.71*(7/6)/X;
 ENTERED FUNCTION :2*.7*.71*7/6/X FOR CELL #1
DIC>
DIC>
DIC> @@
DIC> @@ ENABLE THE SIMPLIFIED MODEL FOR THE COARSENING (OSTWALD-RIPENING)
DIC> @@
DIC> coarse  YES
DIC>
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME AND OTHER SIMULATION PARAMETERS
DIC> @@
DIC> set-simulation-time 1E6
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /100000/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exf1 Y
DIC>
DIC> set-inter
 --OK---
DIC>
```

**exf1-run**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exf1\run.DCM.test"
DIC> @@ exf1_run.DCM
DIC>
DIC> @@
DIC> @@ READ THE SETUP FROM FILE AND START THE SIMULATION
DIC> @@
DIC>
DIC> go d-m
 TIME STEP AT TIME  0.00000E+00
 *** ENTERING M6C AS A DIFFUSION NONE PHASE
DIC> read exf1
 OK
DIC> sim
 Region: PART
 single geometric dense at  0.22800E-06
 0.80000       64
 Region: AUS
 single geometric dense at   0.0000
  1.0060       63
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
  Trying old scheme                    4
 GENERATING STARTING VALUES FOR CELL #  1 INTERFACE #  2
 DETERMINING INITIAL EQUILIBRIUM VALUES
CALCULATING STARTING VALUES:        9   EQUILIBRIUM CALCULATIONS               DONE     6 OUT OF     9
 U-FRACTION IN SYSTEM:  C = .0190652843033664  FE = .970761291162784
                        MO = .0292387089677228
 TOTAL SIZE OF SYSTEM:  1.32376603026E-18 [m^3]
 U-FRACTION IN SYSTEM:  C = .0190652843033664  FE = .970761291162784
                        MO = .0292387089677228
 TOTAL SIZE OF SYSTEM:  1.32376603026E-18 [m^3]
 0.610222970497625        0.610391048253360        0.610222911134902        2.564830792704480E-002        2.191933775609301E-
003        1.266865150888817E-004        1.096501654713504E-003        1.278319049399803E-004        4.432656450601522E-
007        1.566395317892607E-009        1.947833765313978E-009        3.659996125120900E-009        1.418022110198698E-
009        1.309139507131020E-009        1.103984934282495E-009        3.800021059935427E-009        7.446660066835144E-
010        2.344008708335420E-010        1.080152259451965E-013        1.867047547869683E-018       TIME =  0.10000000E-06 DT =  0.10000000E-
06 SUM OF SQUARES =  0.18670475E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.50349408E-05 AND  -0.50349408E-05
 POSITION OF INTERFACE PART / AUS IS   0.22799950E-06
 U-FRACTION IN SYSTEM:  C = .0190659317665348  FE = .97075948763499
                        MO = .0292405124955171
 TOTAL SIZE OF SYSTEM:  1.32375726043E-18 [m^3]
  6  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: PART

  CPU time used in timestep                    1 seconds
 5.960103082658641E-005        5.961330244474372E-005        5.959458009984615E-005        3.934421749594752E-007        1.790907374778079E-
012        8.025352262139553E-020       SWITCHING ACTIVITIES FOR INTERFACE #2, CELL #1
 FROM: C  TO: MO
 TIME =  0.25446964E-05 DT =  0.24446964E-05 SUM OF SQUARES =  0.80253523E-19
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.39293667E-08 AND  -0.39293667E-08
 POSITION OF INTERFACE PART / AUS IS   0.22799949E-06
 U-FRACTION IN SYSTEM:  C = .0190664790756638  FE = .970759484159471
                        MO = .029240515971036
 TOTAL SIZE OF SYSTEM:  1.32375709311E-18 [m^3]
  CPU time used in timestep                    0 seconds
 2.515158582734376E-008        2.515761992373896E-008        2.499573885918378E-008        2.005534171990356E-008        1.975331987583105E-
008        1.917061730215090E-008        1.798309030793897E-008        1.798198230198828E-008        1.576453662265046E-
008        1.173116061551727E-008        5.468961674452001E-009        5.475062053761667E-009        2.640250145577584E-
011        1.077667083838249E-019       TIME =  0.74340891E-05 DT =  0.48893927E-05 SUM OF SQUARES =  0.10776671E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.56129636E-09 AND  -0.56129636E-09
 POSITION OF INTERFACE PART / AUS IS   0.22799948E-06
 U-FRACTION IN SYSTEM:  C = .0190671017629171  FE = .970759483986866
                        MO = .0292405161436416
 TOTAL SIZE OF SYSTEM:  1.32375704531E-18 [m^3]
  CPU time used in timestep                    1 seconds
 4.333438086144453E-010        4.334345196764508E-010        4.419215188854006E-010        4.026611772398112E-010        4.018893336315161E-
010        4.003483958744234E-010        3.972574076728677E-010        3.977091043595048E-010        3.911287923829839E-
010        3.789974358120385E-010        3.553242192263789E-010        3.559796397397647E-010        3.102532489719920E-
010        2.292896934307506E-010        1.040111342076072E-010        1.045003395199620E-010        9.690615339079709E-
014        4.712033016180720E-024       TIME =  0.17212874E-04 DT =  0.97787854E-05 SUM OF SQUARES =  0.47120330E-23
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.11440105E-09 AND  -0.11440105E-09
 POSITION OF INTERFACE PART / AUS IS   0.22799948E-06
 U-FRACTION IN SYSTEM:  C = .0190679130516543  FE = .970759484521662
                        MO = .0292405156088451
 TOTAL SIZE OF SYSTEM:  1.32375702582E-18 [m^3]
  CPU time used in timestep                    0 seconds


output ignored...



... output resumed

 2.171297419387849E-011        9.341085573155101E-013        1.185627712128642E-013        1.159839298471633E-
022       TIME =   667998.25     DT =   100000.00     SUM OF SQUARES =  0.11598393E-21
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.22669488E-13 AND   0.22669488E-13
 POSITION OF INTERFACE PART / AUS IS   0.24398484E-06
 U-FRACTION IN SYSTEM:  C = .0195561971881839  FE = .970692497669242
                        MO = .0293075024612658
 TOTAL SIZE OF SYSTEM:  1.62216577705E-18 [m^3]
  29  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: PART
  29  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUS

  CPU time used in timestep                    1 seconds
 8.463228520121981E-012        8.732923055065668E-012        1.106305607473807E-011        1.671261335042640E-012        8.083195081402649E-
013        2.031410415325825E-015        4.526659080965921E-
025       TIME =   767998.25     DT =   100000.00     SUM OF SQUARES =  0.45266591E-24
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.22252996E-13 AND   0.22252996E-13
 POSITION OF INTERFACE PART / AUS IS   0.24621014E-06
 U-FRACTION IN SYSTEM:  C = .0195587075255012  FE = .970694293020119
                        MO = .029305707110388
 TOTAL SIZE OF SYSTEM:  1.66695743697E-18 [m^3]
  16  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: PART
  16  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUS

  CPU time used in timestep                    0 seconds
 4.716189848333446E-012        4.737893961990167E-012        6.250071128404940E-012        2.547264377747085E-012        1.906488212836178E-
012        8.178985716571513E-013        4.536304958318062E-
022       TIME =   867998.25     DT =   100000.00     SUM OF SQUARES =  0.45363050E-21
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.21855116E-13 AND   0.21855116E-13
```

```
 POSITION OF INTERFACE PART / AUS IS   0.24839565E-06
 U-FRACTION IN SYSTEM:  C = .0195611435098945  FE = .97069604845685
                        MO = .0293039516736582
 TOTAL SIZE OF SYSTEM:  1.71174343902E-18 [m^3]
  25  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: PART
  25  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUS

  CPU time used in timestep                     0 seconds
 3.963242876932314E-012        3.789984561463865E-012        4.665295371421832E-012        3.497963842959495E-012        3.136690283117291E-
012        2.396321610548591E-012        1.082065633024848E-012        1.796674171817538E-015        5.649670291045813E-
025       TIME =   967998.25     DT =   100000.00     SUM OF SQUARES =  0.56496703E-24
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.21474553E-13 AND   0.21474553E-13
 POSITION OF INTERFACE PART / AUS IS   0.25054311E-06
 U-FRACTION IN SYSTEM:  C = .0195635100799357  FE = .970697758696432
                        MO = .0293022414340753
 TOTAL SIZE OF SYSTEM:  1.75652397337E-18 [m^3]
  13  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: PART
  13  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: AUS

  CPU time used in timestep                     1 seconds
 3.163580377257607E-010        3.128551222089807E-010        3.018312584807434E-010        3.724165520990264E-011        1.354264929717906E-
011        1.037034966532211E-019       TIME =   1000000.0     DT =   32001.746     SUM OF SQUARES =  0.10370350E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.21247167E-13 AND   0.21247167E-13
 POSITION OF INTERFACE PART / AUS IS   0.25122306E-06
 U-FRACTION IN SYSTEM:  C = .0195660575765356  FE = .970698831747598
                        MO = .0293011683829089
 TOTAL SIZE OF SYSTEM:  1.77086385839E-18 [m^3]
 MUST SAVE WORKSPACE ON FILE
 WORKSPACE SAVED ON FILE
 RECLAIMING WORKSPACE
 DELETING TIME-RECORD FOR TIME    0.0000000
 DELETING TIME-RECORD FOR TIME   0.10000000E-06
 DELETING TIME-RECORD FOR TIME   0.25446964E-05
 DELETING TIME-RECORD FOR TIME   0.74340891E-05
 DELETING TIME-RECORD FOR TIME   0.17212874E-04
 DELETING TIME-RECORD FOR TIME   0.36770445E-04
 DELETING TIME-RECORD FOR TIME   0.75885587E-04
 DELETING TIME-RECORD FOR TIME   0.15411587E-03
 DELETING TIME-RECORD FOR TIME   0.31057644E-03
 DELETING TIME-RECORD FOR TIME   0.62349757E-03
 DELETING TIME-RECORD FOR TIME   0.12493398E-02
 DELETING TIME-RECORD FOR TIME   0.25010244E-02
 DELETING TIME-RECORD FOR TIME   0.50043934E-02
 DELETING TIME-RECORD FOR TIME   0.10011132E-01
 DELETING TIME-RECORD FOR TIME   0.20024608E-01
 DELETING TIME-RECORD FOR TIME   0.40051560E-01
 DELETING TIME-RECORD FOR TIME   0.80105465E-01
 DELETING TIME-RECORD FOR TIME   0.16021328
 DELETING TIME-RECORD FOR TIME   0.32042890
 DELETING TIME-RECORD FOR TIME   0.64086014
 DELETING TIME-RECORD FOR TIME    1.2817226
 DELETING TIME-RECORD FOR TIME    2.5634476
 DELETING TIME-RECORD FOR TIME    5.1268975
 DELETING TIME-RECORD FOR TIME    10.253797
 DELETING TIME-RECORD FOR TIME    20.507597
 DELETING TIME-RECORD FOR TIME    41.015196
 DELETING TIME-RECORD FOR TIME    82.030395
 DELETING TIME-RECORD FOR TIME    164.06079
 DELETING TIME-RECORD FOR TIME    328.12159
 DELETING TIME-RECORD FOR TIME    656.24318
 DELETING TIME-RECORD FOR TIME    1312.4864
 DELETING TIME-RECORD FOR TIME    2624.9727
 DELETING TIME-RECORD FOR TIME    5249.9454
 DELETING TIME-RECORD FOR TIME    10499.891
 DELETING TIME-RECORD FOR TIME    20999.782
 DELETING TIME-RECORD FOR TIME    41999.564
 DELETING TIME-RECORD FOR TIME    83999.127
 DELETING TIME-RECORD FOR TIME    167998.25
 DELETING TIME-RECORD FOR TIME    267998.25
 DELETING TIME-RECORD FOR TIME    367998.25
 DELETING TIME-RECORD FOR TIME    467998.25
 DELETING TIME-RECORD FOR TIME    567998.25
 DELETING TIME-RECORD FOR TIME    667998.25
 DELETING TIME-RECORD FOR TIME    767998.25
 DELETING TIME-RECORD FOR TIME    867998.25

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

 TIMESTEP AT     1000000.00     SELECTED

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

**exf1-plot**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exf1\plot.DCM.test"
DIC> @@ exf1_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE f1
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  1.00000E+06
 *** ENTERING M6C AS A DIFFUSION NONE PHASE
DIC> read exf1
 OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1: @@
POST-1: @@ PLOT THE AVERAGE PARTICLE SIZE (CUBED) AS THIS ASSUMED TO
POST-1: @@ SCALE LINEARLY WITH TIME. THEN A FUNCTION IS ENTERED SO
POST-1: @@ THIS QUANTITY CAN BE ACCESSED. WE ALSO WANT TO PLOT THIS
POST-1: @@ QUANTITY VERSUS TIME (IN HOURS) SO A FUNCTION IS ENTERED.
POST-1: @@
POST-1: enter-symbol func rr3=(poi(part,u)/1.5)**3;
POST-1: enter-symbol func hours=time/3600;
POST-1: s-d-a x hours
POST-1: s-d-a y rr3
POST-1:
POST-1: @@
POST-1: @@ AS WE ARE PLOTTING FUNCTIONS ON BOTH AXES WE MUST EXPLICITLY
POST-1: @@ DEFINE THE INDEPENDENT VARIABLE AND THE PLOT CONDITION
POST-1: @@
POST-1: s-ind time
POST-1: s-p-c inter
INTERFACE : part upper
POST-1:
POST-1:
POST-1: set-axis-text-status x n
AXIS TEXT : Time [h]
POST-1:
POST-1: @@
POST-1: @@ WHEN THIS IS PLOTTED, THIS AXIS TEXT NOTATION WORKS WELL FOR
POST-1: @@ THE AVERAGE RADIUS CUBED. FOR MORE INFORMATION ABOUT HOW TO
POST-1: @@ ADJUST TEXT IN THE POST PROCESSOR USING THE DATAPLOT LANGUAGE,
POST-1: @@ SEARCH THE ONLINE HELP (FROM THE MAIN MENU -> HELP > ONLINE HELP)
POST-1:
POST-1:
POST-1: set-axis-text-status y n
AXIS TEXT : \latex r^3\, [m^3]
POST-1:
POST-1:
POST-1: @@
POST-1: @@ COMPARE WITH EXPERIMENTAL DATA FROM NISHIZAWA ET AL.
POST-1: @@ TRANS. JPN. INST. MET. VOL. 22 1981 PP. 733-742.
POST-1: @@
POST-1:
POST-1: app y exf1
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 1
POST-1:
POST-1: s-s-s y n 0 6e-21
POST-1:
POST-1: @@
POST-1: @@ SET A TITLE ON THE PLOT
POST-1: @@
POST-1: set-title Figure f1.1
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

Figure f1.1

2019.11.11.19.16.30
UPPER INTERFACE OF REGION "PART#1"
CELL #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:
```

**exg1-setup**

```
SYS:About

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

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 21012) 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: Mon Nov 11 11:13:13 2019


SYS:SYS:MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exg1\setup.DCM.test"
SYS: @@
SYS: @@ Kinetic data example.
SYS: @@ Checking mobilities and diffusivities in an Fe-Ni alloy
SYS: @@ This is an example file to check the mobilities and diffusivities
SYS: @@ in an Fe-Ni alloy.
SYS: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exg1_setup.DCM
SYS:
SYS: @@
SYS: @@ START BY GOING TO THE DATABASE MODULE
SYS: @@
SYS: go da
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v10.0

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10:
TDB_TCFE10: @@
TDB_TCFE10: @@ SELECT A DATABASE FOR THERMODYNAMIC DATA
TDB_TCFE10: @@
TDB_TCFE10: sw fedemo
 Current database: Iron Demo Database v2.1

 VA                      /-  DEFINED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ DEFINE THE SYSTEM TO WORK WITH
TDB_FEDEMO: @@
TDB_FEDEMO: def-sys fe ni
 FE                      NI  DEFINED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ EXCLUDE THE THERMODYNAMIC DATA FOR THE PHASES THAT ARE NOT NEEDED
TDB_FEDEMO: @@
TDB_FEDEMO: rej ph * all
 LIQUID:L                BCC_A2                  CBCC_A12
 CUB_A13                 FCC_A1                  HCP_A3
 LAVES_PHASE_C14  REJECTED
TDB_FEDEMO: res ph fcc
 FCC_A1  RESTORED
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ RETRIEVE DATA FROM THE DATABASE FILE
TDB_FEDEMO: @@
TDB_FEDEMO: get
19:17:50,663 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

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

 TCFE10  =  Steels/Fe-Alloys  v10.0
 TCFE9   =  Steels/Fe-Alloys  v9.1
 TCFE8   =  Steels/Fe-Alloys  v8.1
 TCFE7   =  Steels/Fe-Alloys  v7.0
 TCFE6   =  Steels/Fe-Alloys  v6.2
 TCFE5   =  Steels/Fe-Alloys  v5.0
 TCFE4   =  Steels/Fe-Alloys  v4.1
 TCFE3   =  Steels/Fe-Alloys  v3.1
 TCFE2   =  Steels/Fe-Alloys  v2.1
 TCFE1   =  Steels/Fe-Alloys  v1.0
 FROST1  =  FROST database v1.2
 FEDAT   =  TCS/TT Steels Database v1.0
 TCNI10  =  Ni-Alloys  v10.0 SNAPSHOT
 TCNI9   =  Ni-Alloys  v9.1
 TCNI8   =  Ni-Alloys  v8.2
 TCNI7   =  Ni-Alloys  v7.2
 TCNI6   =  Ni-Alloys  v6.1
 TCNI5   =  Ni-Alloys  v5.1
 TCNI4   =  Ni-Alloys  v4.0
 TCNI1   =  Ni-Alloys  v1.3
 TCAL6   =  Al-Alloys  v6.0
 TCAL5   =  Al-Alloys  v5.1
 TCAL4   =  Al-Alloys  v4.0
```

```
 TCAL3   =  Al-Alloys  v3.0
 TCAL2   =  Al-Alloys  v2.1
 TCAL1   =  Al-Alloys  v1.2
 TCMG5   =  Mg-Alloys  v5.1
 TCMG4   =  Mg-Alloys  v4.0
 TCMG3   =  Mg-Alloys  v3.0
 TCMG2   =  Mg-Alloys  v2.0
 TCMG1   =  Mg-Alloys  v1.1
 TCTI2   =  Ti-Alloys  v2.1
 TCTI1   =  Ti-Alloys  v1.0
 TCCU3   =  Cu-Alloys  v3.1
 TCCU2   =  Cu-Alloys  v2.0
 TCCU1   =  Cu-Alloys  v1.0
 TCCC1   =  Cemented carbide  v1.0
 TCHEA4  =  High Entropy Alloy  v4.0
 TCHEA3  =  High Entropy Alloy  v3.1
 TCHEA2  =  High Entropy Alloy  v2.1.1
 TCHEA1  =  High Entropy Alloy  v1.0
 SSOL7   =  SGTE Alloy Solutions Database v7.0
 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
 TCOX10  =  Metal Oxide Solutions  v10.0 SNAPSHOT
 TCOX9   =  Metal Oxide Solutions  v9.0
 TCOX8   =  Metal Oxide Solutions  v8.0
 TCOX7   =  Metal Oxide Solutions  v7.0
 TCOX6   =  Metal Oxide Solutions  v6.0
 TCOX5   =  Metal Oxide Solutions  v5.1
 TCOX4   =  Metal Oxide Solutions  v4.1
 ION3    =  Ionic Solutions  v3.0
 ION2    =  Ionic Solutions  v2.6
 ION1    =  Ionic Solutions  v1.5
 NOX2    =  NPL Oxide Solutions Database v2.1
 TCNOBL2 =  Noble Metals Alloys v2.0 SNAPSHOT
 TCNOBL1 =  Noble Metals Alloys v1.0
 TCSLD3  =  Solder Alloys  v3.2
 TCSLD2  =  Solder Alloys  v2.0
 TCSLD1  =  Solder Alloys  v1.1
 TCSI1   =  Ultrapure Silicon  v1.2
 TCMP2   =  Materials Processing  v2.5
 TCES1   =  Combustion/Sintering  v1.1
 TCSC1   =  Super Conductor  v1.0
 TCFC1   =  SOFC Database v1.0
 TCNF2   =  Nuclear Fuels  v2.1b
 NUMT2   =  Nuclear Materials  v2.1
 NUOX4   =  Nuclear Oxides  v4.2
 NUCL15  =  IRSN NUCLEA-15_4
 NUCL10  =  ThermoData NUCLEA Alloys-oxides TDB v10.2
 MEPH15  =  IRSN Mephista-15_1
 MEPH11  =  ThermoData MEPHISTA Nuclear Fuels TDB v11.2
 TCAQ3   =  Aqueous Solution  v3.0
 TCAQ2   =  Aqueous Solution  v2.7
 AQS2    =  TGG Aqueous Solution Database v2.6
 GCE2    =  TGG Geochemical/Environmental TDB v2.3
 FEDEMO  =  Iron Demo Database v2.1
 ALDEMO  =  Aluminum Demo Database v3.0
 NIDEMO  =  Nickel Demo Database v1.1
 CUDEMO  =  Copper Demo Database v1.0
 SLDEMO  =  Solder Demo Database v1.0
 OXDEMO  =  Oxide Demo Database v1.0
 SUBDEMO =  Substance Demo Database v1.0
 PTERN   =  Public Ternary Alloys TDB v1.3
 PAQ2    =  Public Aqueous Soln (SIT) TDB v2.4
 PG35    =  G35 Binary Semi-Conductors TDB v1.2
 PURE5   =  SGTE Unary (Pure Elements) TDB v5.1
 MOB2    =  Alloys Mobility  v2.7
 MOB1    =  Alloys Mobility  v1.3
 MOBFE1  =  Steels/Fe-Alloys Mobility  v1.1
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBFE5  =  Steels/Fe-Alloys Mobility  v5.0
 MOBNI5  =  Ni-Alloys Mobility  v5.1
 MOBNI4  =  Ni-Alloys Mobility  v4.1
 MOBNI3  =  Ni-Alloys Mobility  v3.2
 MOBNI2  =  Ni-Alloys Mobility  v2.4
 MOBNI1  =  Ni-Alloys Mobility  v1.10
 MOBAL5  =  Al-Alloys Mobility  v5.0
 MOBAL4  =  Al-Alloys Mobility  v4.0
 MOBAL3  =  Al-Alloys Mobility  v3.0
 MOBAL2  =  Al-Alloys Mobility  v2.0
 MOBAL1  =  Al-Alloys Mobility  v1.0
 MOBCU1  =  Cu-Alloys Mobility  v1.0
 MOBCU2  =  Cu-Alloys Mobility  v2.0
 MOBCU3  =  Cu-Alloys Mobility  v3.0
 MOBHEA1 =  High Entropy Alloys Mobility  v1.0
 MOBHEA2 =  High Entropy Alloys Mobility  v2.0
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBSLD1 =  Solder-Alloys Mobility  v1.1
 MOBTI3  =  Ti-Alloys Mobility  v3.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v2.0
 MFEDEMO =  Fe-Alloys Mobility demo database v2.0
 MNIDEMO =  Ni-Alloys Mobility demo database v1.0
 MCUDEMO =  Cu-Alloys Mobility demo database v1.0
 USER    =  User defined Database

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

```
 VA  DEFINED
APP: def-sys fe ni
 FE                    NI  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'
  '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> @@ CHECK THE DIFFUSIVITES
DIC> @@
DIC> check-diffusion-matrix
OUTPUT TO SCREEN OR FILE /SCREEN/:
PHASE NAME : fcc
DEPENDENT COMPONENT ? /NI/: fe
CONCENTRATION OF NI IN U-FRACTION /1/: 0.3
Pressure /100000/: 101325
Temperature /298.15/: 1409
OPTION ( dlpbmx0ez or * ) /D/: dl

  Dkj (reduced n=FE)
  k / j NI
  NI   +3.83335E-15
   L0kj = Uk*Mvak IF (kES) ELSE Uk*Yva*Mvak
  k / j   FE             NI
  FE    +9.0901E-20
  NI                   +9.0901E-20


  Volume =   1.000000000000000E-005

DIC>
DIC>
DIC>@?<Hit_return_to_continue>
DIC>
DIC> @@
DIC> @@ USE STEPPING IN POLY-3 TO CALCULATE THE DIFFUSIVITIES VS. COMPOSITION
DIC> @@
DIC> go p-3
POLY: s-c t=1409,p=101325,n=1,x(ni)=0.3
POLY: c-e
 Using global minimization procedure
Calculated           209 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY:

POLY: s-a-v
Axis number: /1/: 1
Condition /NONE/: x(ni)
Min value /0/: 0
Max value /1/: 1
Increment /.025/: 1e-3
POLY:
POLY: step
Option? /NORMAL/: normal
 No initial equilibrium, using default
 Step will start from axis value   0.300000
...OK

 Phase Region from   0.300000     for:
     FCC_A1
 Global test at  3.08000E-01 .... OK
 Global test at  3.18000E-01 .... OK
 Global test at  3.28000E-01 .... OK
 Global test at  3.38000E-01 .... OK
 Global test at  3.48000E-01 .... OK
 Global test at  3.58000E-01 .... OK
 Global test at  3.68000E-01 .... OK
 Global test at  3.78000E-01 .... OK
 Global test at  3.88000E-01 .... OK
 Global test at  3.98000E-01 .... OK
 Global test at  4.08000E-01 .... OK
 Global test at  4.18000E-01 .... OK
 Global test at  4.28000E-01 .... OK
 Global test at  4.38000E-01 .... OK
 Global test at  4.48000E-01 .... OK
 Global test at  4.58000E-01 .... OK
 Global test at  4.68000E-01 .... OK
 Global test at  4.78000E-01 .... OK
 Global test at  4.88000E-01 .... OK
 Global test at  4.98000E-01 .... OK
 Global test at  5.08000E-01 .... OK
 Global test at  5.18000E-01 .... OK
 Global test at  5.28000E-01 .... OK
 Global test at  5.38000E-01 .... OK
 Global test at  5.48000E-01 .... OK
 Global test at  5.58000E-01 .... OK
 Global test at  5.68000E-01 .... OK
 Global test at  5.78000E-01 .... OK
 Global test at  5.88000E-01 .... OK
 Global test at  5.98000E-01 .... OK
 Global test at  6.08000E-01 .... OK
```

```
 Global test at  6.18000E-01 .... OK
 Global test at  6.28000E-01 .... OK
 Global test at  6.38000E-01 .... OK
 Global test at  6.48000E-01 .... OK
 Global test at  6.58000E-01 .... OK
 Global test at  6.68000E-01 .... OK
 Global test at  6.78000E-01 .... OK
 Global test at  6.88000E-01 .... OK
 Global test at  6.98000E-01 .... OK
 Global test at  7.08000E-01 .... OK
 Global test at  7.18000E-01 .... OK
 Global test at  7.28000E-01 .... OK
 Global test at  7.38000E-01 .... OK
 Global test at  7.48000E-01 .... OK
 Global test at  7.58000E-01 .... OK
 Global test at  7.68000E-01 .... OK
 Global test at  7.78000E-01 .... OK
 Global test at  7.88000E-01 .... OK
 Global test at  7.98000E-01 .... OK
 Global test at  8.08000E-01 .... OK
 Global test at  8.18000E-01 .... OK
 Global test at  8.28000E-01 .... OK
 Global test at  8.38000E-01 .... OK
 Global test at  8.48000E-01 .... OK
 Global test at  8.58000E-01 .... OK
 Global test at  8.68000E-01 .... OK
 Global test at  8.78000E-01 .... OK
 Global test at  8.88000E-01 .... OK
 Global test at  8.98000E-01 .... OK
 Global test at  9.08000E-01 .... OK
 Global test at  9.18000E-01 .... OK
 Global test at  9.28000E-01 .... OK
 Global test at  9.38000E-01 .... OK
 Global test at  9.48000E-01 .... OK
 Global test at  9.58000E-01 .... OK
 Global test at  9.68000E-01 .... OK
 Global test at  9.78000E-01 .... OK
 Global test at  9.88000E-01 .... OK
 Global test at  9.98000E-01 .... OK
 Terminating at    1.00000
 Calculated   703 equilibria

 Phase Region from   0.300000     for:
     FCC_A1
 Global test at  2.92000E-01 .... OK
 Global test at  2.82000E-01 .... OK
 Global test at  2.72000E-01 .... OK
 Global test at  2.62000E-01 .... OK
 Global test at  2.52000E-01 .... OK
 Global test at  2.42000E-01 .... OK
 Global test at  2.32000E-01 .... OK
 Global test at  2.22000E-01 .... OK
 Global test at  2.12000E-01 .... OK
 Global test at  2.02000E-01 .... OK
 Global test at  1.92000E-01 .... OK
 Global test at  1.82000E-01 .... OK
 Global test at  1.72000E-01 .... OK
 Global test at  1.62000E-01 .... OK
 Global test at  1.52000E-01 .... OK
 Global test at  1.42000E-01 .... OK
 Global test at  1.32000E-01 .... OK
 Global test at  1.22000E-01 .... OK
 Global test at  1.12000E-01 .... OK
 Global test at  1.02000E-01 .... OK
 Global test at  9.20000E-02 .... OK
 Global test at  8.20000E-02 .... OK
 Global test at  7.20000E-02 .... OK
 Global test at  6.20000E-02 .... OK
 Global test at  5.20000E-02 .... OK
 Global test at  4.20000E-02 .... OK
 Global test at  3.20000E-02 .... OK
 Global test at  2.20000E-02 .... OK
 Global test at  1.20000E-02 .... OK
 Global test at  2.00000E-03 .... OK
 Terminating at   0.100000E-11
 Calculated   303 equilibria
 *** Buffer saved on file: C:\Users\vagrant\AppData\Local\Temp\RESULT_002.POLY3
POLY:
POLY: @@
POLY: @@ ENTER THE POST PROCESSOR AND PLOT THE RESULT
POLY: @@
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2
POST:
POST:
POST:
POST: @@
POST: @@ PLOT THE MOBILITY OF Ni VS. X(Ni)
POST: @@
POST: s-d-a y m(fcc,ni)
POST: s-d-a x m-f ni
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
```

2019.11.11.19.17.55
MFEDEMO: FE, NI
T=1409, P=1.01325E5, N=1.

```
POST:
POST:
POST:
POST:@?<Hit_return_to_continue>
POST:
POST: @@
POST: @@ THEN PLOT THE DIFFUSIVITY OF Ni VS. X(Ni)
POST: @@
POST: s-d-a y dc(fcc,ni,ni,fe)
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
```

2019.11.11.19.17.56
MFEDEMO: 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:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
```

2019.11.11.19.17.56
MFEDEMO: 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**

```
SYS:About

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

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 21012) 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: Mon Nov 11 11:13:13 2019


SYS:SYS:MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exg2\setup.DCM.test"
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: @@
SYS: @@ EXPLICITLY SELECTING GES VERSION 5 BECAUSE PARAMETER OPTIMIZATION
SYS: @@ IS NOT SUPPORTED IN GES VERSION 6
SYS: @@
SYS: set-ges-version 5
SYS:
SYS: @@
SYS: @@ RETRIEVE THERMODYNAMIC DATA FROM A USER-DEFINED DATABASE
SYS: @@
SYS: go data
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v10.0

 VA                       /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10: sw us tdata.TDB
 Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

 VA  DEFINED
TDB_USER: def-sys al ni
 AL                       NI  DEFINED
TDB_USER: rej ph *
 LIQUID                   B2_BCC                   BCC_A2
 FCC_A1                   GAMMA_PRIME  REJECTED
TDB_USER: rest ph fcc_a1
 FCC_A1  RESTORED
TDB_USER: get
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....
 -OK-
TDB_USER:
TDB_USER: @@
TDB_USER: @@ APPEND THE KINETIC DATA FROM THE MOBILITY DATABASE IN ORDER TO
TDB_USER: @@ HAVE SOME DUMMY PARAMETERS.
TDB_USER: @@
TDB_USER: app mob2
 Current database: Alloys Mobility  v2.7

 VA  DEFINED
 GAS:G  REJECTED
APP: def-sys al ni
 AL                       NI  DEFINED
APP: rej ph *
 BCC_A2                   FCC_A1                   M4N
 HCP_A3                   LIQUID:L  REJECTED
APP: res ph fcc_a1
 FCC_A1  RESTORED
APP: get
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 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:About
 NO SUCH COMMAND, USE HELP
PARROT:PARROT:MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exg2\run.DCM.test"
PARROT: @@ exg2_run.DCM
PARROT:
PARROT: @@-----------------------------------------------------------------
PARROT: @@ FILE FOR DOING THE OPTIMIZATION IN PARROT
PARROT: @@-----------------------------------------------------------------
PARROT:
PARROT: @@
PARROT: @@ GO TO PARROT AND READ THE SETUP
PARROT: @@
PARROT: go dic_parrot
 PARROT  VERSION 5.3d RUNNING ON PC/WINDOWS NT
PARROT: set-store-file opt
PARROT:
PARROT:
PARROT: @@
PARROT: @@ COMPILE THE EXPERIMENTAL DATA IN exp.DOP INTO STRUCTURED BINARY DATA.
PARROT: @@
PARROT: compile-experiments exp
OUTPUT TO SCREEN OR FILE /SCREEN/:
INITIATE STORE FILE: /Y/:

 $-------------------------------------------------------------------
 $ DOP-FILE CONTAINING EXPERIMENTAL INFORMATION USED DURING THE
 $ OTIMIZATION IN PARROT (COMPARE WITH POP-FILE USED WHEN EVALUATING
 $ THERMODYNAMIC DATA). THE EXPERIMENTAL DATA HERE STEAM FROM A STUDY BY
 $ YAMAMOTO ET AL. TRANS. JPN. INST. MET. VOL. 21,NO. 9 (1980), P. 601.
 $
 $ CONSULT THE THERMO-CALC USER'S GUIDE TO LEARN MORE ABOUT SYNTAXES
 $ FOR OPTIMIZATION OF THERMODYNAMIC DATA.
 $-------------------------------------------------------------------

 ENTER CONST P0=101325

 TABLE_HEAD 10
 CREATE_NEW 0010,1
 C-S PH FCC=ENT 1
 S-C T=1573,N=1,P=P0
 S-C X(AL)=.01055
 EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.6:.1
 CREATE_NEW 0011,1
 C-S PH FCC=ENT 1
 S-C T=1573,N=1,P=P0
 S-C X(AL)=.02032
 EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.56:.1
 CREATE_NEW 0012,1
 C-S PH FCC=ENT 1
 S-C T=1573,N=1,P=P0
 S-C X(AL)=.02957
 EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.65:.1
 CREATE_NEW 0013,1
 C-S PH FCC=ENT 1
 S-C T=1573,N=1,P=P0
 S-C X(AL)=.03884
 EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.52:.1
 CREATE_NEW 0014,1
 C-S PH FCC=ENT 1
 S-C T=1573,N=1,P=P0
 S-C X(AL)=.03884
 EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.52:.1
 CREATE_NEW 0015,1
 C-S PH FCC=ENT 1
 S-C T=1573,N=1,P=P0
 S-C X(AL)=.04927
 EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.48:.1
 CREATE_NEW 0016,1
 C-S PH FCC=ENT 1
 S-C T=1573,N=1,P=P0
 S-C X(AL)=.06062
 EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.43:.1
 CREATE_NEW 0017,1
 C-S PH FCC=ENT 1
 S-C T=1573,N=1,P=P0
 S-C X(AL)=.07029
 EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.41:.1
 CREATE_NEW 0018,1
 C-S PH FCC=ENT 1
 S-C T=1573,N=1,P=P0
 S-C X(AL)=.08113
 EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.37:.1
 CREATE_NEW 0019,1
 C-S PH FCC=ENT 1
 S-C T=1573,N=1,P=P0
 S-C X(AL)=.09166
 EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.32:.1
 CREATE_NEW 0020,1
 C-S PH FCC=ENT 1
 S-C T=1573,N=1,P=P0
 S-C X(AL)=.09945
 EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.28:.1
 CREATE_NEW 0021,1
 C-S PH FCC=ENT 1
 S-C T=1573,N=1,P=P0
 S-C X(AL)=.1099
 EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.24:.1
 CREATE_NEW 0022,1
 C-S PH FCC=ENT 1
 S-C T=1573,N=1,P=P0
 S-C X(AL)=.1207
 EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.2:.1
 CREATE_NEW 0023,1
 C-S PH FCC=ENT 1
 S-C T=1573,N=1,P=P0
 S-C X(AL)=.129
 EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.18:.1
 CREATE_NEW 0024,1
 C-S PH FCC=ENT 1
 S-C T=1573,N=1,P=P0
 S-C X(AL)=.1392
 EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.16:.1
```

```
 CREATE_NEW 0025,1
 C-S PH FCC=ENT 1
 S-C T=1573,N=1,P=P0
 S-C X(AL)=.1503
 EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.1:.1
 CREATE_NEW 0026,1
 C-S PH FCC=ENT 1
 S-C T=1573,N=1,P=P0
 S-C X(AL)=.1589
 EXPERIMENT LOGDC(FCC_A1,AL,AL,NI)=-12.08:.1
 CREATE_NEW 0027,1
 C-S PH FCC=ENT 1
 S-C T=1573,N=1,P=P0


output ignored...



... output resumed

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

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


 Sorry, LIST-DATA disabled for this database

 ======  BLOCK NUMBER  1

 DEFINED CONSTANTS
    P0=101325
10 LOGDC(F...,AL,NI)=-12.6       -12.56      0.10      4.3827E-02  0.4383
11 LOGDC(F...,AL,NI)=-12.56      -12.55      0.10      1.2341E-02  0.1234
12 LOGDC(F...,AL,NI)=-12.65      -12.53      0.10      0.1167       1.167
13 LOGDC(F...,AL,NI)=-12.52      -12.51      0.10      5.8843E-03  5.8843E-02
14 LOGDC(F...,AL,NI)=-12.52      -12.51      0.10      5.8843E-03  5.8843E-02
15 LOGDC(F...,AL,NI)=-12.48      -12.49      0.10     -8.4123E-03 -8.4123E-02
16 LOGDC(F...,AL,NI)=-12.43      -12.46      0.10     -2.6851E-02 -0.2685
17 LOGDC(F...,AL,NI)=-12.41      -12.43      0.10     -1.7821E-02 -0.1782
18 LOGDC(F...,AL,NI)=-12.37      -12.39      0.10     -2.3493E-02 -0.2349
19 LOGDC(F...,AL,NI)=-12.32      -12.36      0.10     -3.8626E-02 -0.3863
20 LOGDC(F...,AL,NI)=-12.28      -12.33      0.10     -5.1933E-02 -0.5193
21 LOGDC(F...,AL,NI)=-12.24      -12.29      0.10     -5.4919E-02 -0.5492
22 LOGDC(F...,AL,NI)=-12.2       -12.26      0.10     -5.5128E-02 -0.5513
23 LOGDC(F...,AL,NI)=-12.18      -12.22      0.10     -4.3400E-02 -0.4340
24 LOGDC(F...,AL,NI)=-12.16      -12.18      0.10     -2.2927E-02 -0.2293
25 LOGDC(F...,AL,NI)=-12.1       -12.14      0.10     -3.6888E-02 -0.3689
26 LOGDC(F...,AL,NI)=-12.08      -12.10      0.10     -1.9703E-02 -0.1970
27 LOGDC(F...,AL,NI)=-12.02      -12.04      0.10     -2.2272E-02 -0.2227
28 LOGDC(F...,AL,NI)=-11.98      -11.99      0.10     -9.0917E-03 -9.0917E-02
29 LOGDC(F...,AL,NI)=-11.94      -11.95      0.10     -9.1618E-03 -9.1618E-02
30 LOGDC(F...,AL,NI)=-13         -12.86      0.10      0.1360       1.360
31 LOGDC(F...,AL,NI)=-12.96      -12.85      0.10      0.1059       1.059
32 LOGDC(F...,AL,NI)=-12.92      -12.84      0.10      8.4799E-02  0.8480
33 LOGDC(F...,AL,NI)=-12.9       -12.82      0.10      8.2549E-02  0.8255
34 LOGDC(F...,AL,NI)=-12.77      -12.79      0.10     -1.5173E-02 -0.1517
35 LOGDC(F...,AL,NI)=-12.74      -12.75      0.10     -1.1192E-02 -0.1119
36 LOGDC(F...,AL,NI)=-12.82      -12.72      0.10      9.5223E-02  0.9522
37 LOGDC(F...,AL,NI)=-12.82      -12.72      0.10      9.5223E-02  0.9522
38 LOGDC(F...,AL,NI)=-12.69      -12.68      0.10      5.7856E-03  5.7856E-02
39 LOGDC(F...,AL,NI)=-12.65      -12.65      0.10      2.6229E-03  2.6229E-02
40 LOGDC(F...,AL,NI)=-12.64      -12.62      0.10      1.9222E-02  0.1922
41 LOGDC(F...,AL,NI)=-12.61      -12.58      0.10      2.8492E-02  0.2849
42 LOGDC(F...,AL,NI)=-12.55      -12.54      0.10      9.2091E-03  9.2091E-02
43 LOGDC(F...,AL,NI)=-12.53      -12.51      0.10      2.1034E-02  0.2103
44 LOGDC(F...,AL,NI)=-12.47      -12.47      0.10      2.0402E-03  2.0402E-02
45 LOGDC(F...,AL,NI)=-12.41      -12.42      0.10     -1.0621E-02 -0.1062
46 LOGDC(F...,AL,NI)=-12.38      -12.38      0.10     -1.6323E-04 -1.6323E-03
47 LOGDC(F...,AL,NI)=-12.36      -12.32      0.10      3.6256E-02  0.3626
48 LOGDC(F...,AL,NI)=-12.36      -12.32      0.10      3.6256E-02  0.3626
49 LOGDC(F...,AL,NI)=-12.3       -12.27      0.10      3.0494E-02  0.3049
50 LOGDC(F...,AL,NI)=-13.23      -13.19      0.10      3.8416E-02  0.3842
51 LOGDC(F...,AL,NI)=-13.23      -13.19      0.10      3.8416E-02  0.3842
52 LOGDC(F...,AL,NI)=-13.19      -13.18      0.10      1.3209E-02  0.1321
53 LOGDC(F...,AL,NI)=-13.15      -13.16      0.10     -5.5530E-03 -5.5530E-02
54 LOGDC(F...,AL,NI)=-13.12      -13.13      0.10     -1.4736E-02 -0.1474
55 LOGDC(F...,AL,NI)=-13.09      -13.10      0.10     -1.2913E-02 -0.1291
56 LOGDC(F...,AL,NI)=-13.06      -13.07      0.10     -6.9397E-03 -6.9397E-02
57 LOGDC(F...,AL,NI)=-13.02      -13.04      0.10     -1.5971E-02 -0.1597
58 LOGDC(F...,AL,NI)=-12.99      -13.00      0.10     -1.0672E-02 -0.1067
59 LOGDC(F...,AL,NI)=-12.96      -12.96      0.10      8.0069E-04  8.0069E-03
60 LOGDC(F...,AL,NI)=-12.91      -12.93      0.10     -2.0470E-02 -0.2047
61 LOGDC(F...,AL,NI)=-12.88      -12.89      0.10     -7.3947E-03 -7.3947E-02
62 LOGDC(F...,AL,NI)=-12.86      -12.85      0.10      1.4312E-02  0.1431
63 LOGDC(F...,AL,NI)=-12.86      -12.85      0.10      1.4312E-02  0.1431
64 LOGDC(F...,AL,NI)=-12.83      -12.81      0.10      1.7076E-02  0.1708
65 LOGDC(F...,AL,NI)=-12.8       -12.77      0.10      2.9558E-02  0.2956
66 LOGDC(F...,AL,NI)=-12.75      -12.72      0.10      2.5293E-02  0.2529
67 LOGDC(F...,AL,NI)=-12.71      -12.68      0.10      2.6861E-02  0.2686
68 LOGDC(F...,AL,NI)=-12.67      -12.63      0.10      4.4033E-02  0.4403
70 LOGDC(F...,AL,NI)=-13.5       -13.54      0.10     -4.2456E-02 -0.4246
71 LOGDC(F...,AL,NI)=-13.47      -13.53      0.10     -5.5160E-02 -0.5516
72 LOGDC(F...,AL,NI)=-13.45      -13.50      0.10     -5.0384E-02 -0.5038
73 LOGDC(F...,AL,NI)=-13.42      -13.48      0.10     -5.6139E-02 -0.5614
74 LOGDC(F...,AL,NI)=-13.39      -13.44      0.10     -5.3034E-02 -0.5303
75 LOGDC(F...,AL,NI)=-13.36      -13.40      0.10     -4.3865E-02 -0.4386
76 LOGDC(F...,AL,NI)=-13.34      -13.37      0.10     -3.0943E-02 -0.3094
77 LOGDC(F...,AL,NI)=-13.31      -13.33      0.10     -2.0539E-02 -0.2054
78 LOGDC(F...,AL,NI)=-13.24      -13.29      0.10     -5.0311E-02 -0.5031
79 LOGDC(F...,AL,NI)=-13.22      -13.26      0.10     -4.1318E-02 -0.4132
80 LOGDC(F...,AL,NI)=-13.19      -13.22      0.10     -2.6230E-02 -0.2623
81 LOGDC(F...,AL,NI)=-13.13      -13.17      0.10     -4.3098E-02 -0.4310
82 LOGDC(F...,AL,NI)=-13.12      -13.14      0.10     -1.9773E-02 -0.1977
```

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


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

**exg2-plot**

```
PARROT:About
 NO SUCH COMMAND, USE HELP
PARROT:PARROT:MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exg2\plot.DCM.test"
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: s-c n=1,p=101325,t=1573
POLY: s-c x(al)=.1
POLY: c-e,,,,
 Using global minimization procedure
Calculated           209 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY: add,,
POLY:

POLY: s-a-v 1 x(al) 0.0001 .20 0.001,,,,
POLY: step
Option? /NORMAL/:
 Step will start from axis value   0.100000
...OK

 Phase Region from   0.100000     for:
     FCC_A1
 Global test at  1.08000E-01 .... OK
 Global test at  1.18000E-01 .... OK
 Global test at  1.28000E-01 .... OK
 Global test at  1.38000E-01 .... OK
 Global test at  1.48000E-01 .... OK
 Global test at  1.58000E-01 .... OK
 Global test at  1.68000E-01 .... OK
 Global test at  1.78000E-01 .... OK
 Global test at  1.88000E-01 .... OK
 Global test at  1.98000E-01 .... OK
 Terminating at   0.200000
 Calculated   103 equilibria

 Phase Region from   0.100000     for:
     FCC_A1
 Global test at  9.20000E-02 .... OK
 Global test at  8.20000E-02 .... OK
 Global test at  7.20000E-02 .... OK
 Global test at  6.20000E-02 .... OK
 Global test at  5.20000E-02 .... OK
 Global test at  4.20000E-02 .... OK
 Global test at  3.20000E-02 .... OK
 Global test at  2.20000E-02 .... OK
 Global test at  1.20000E-02 .... OK
 Global test at  2.00000E-03 .... OK
 Terminating at   0.100000E-03
 Calculated   103 equilibria
 *** Buffer saved on file: C:\Users\vagrant\AppData\Local\Temp\RESULT_002.POLY3
POLY: @@
POLY: @@ REPEATE THE PROCEDURE FOR SOME OTHER TEMPERATURES
POLY: @@
POLY: s-c t=1523,x(al)=.1
POLY: c-e,,,,,,,
 Using global minimization procedure
Calculated           209 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY: s-a-v 1 x(al) 0.0001 .20 0.001,,,,
POLY: step
Option? /NORMAL/:
 Step will start from axis value   0.100000
...OK

 Phase Region from   0.100000     for:
     FCC_A1
 Global test at  1.08000E-01 .... OK
 Global test at  1.18000E-01 .... OK
 Global test at  1.28000E-01 .... OK
 Global test at  1.38000E-01 .... OK
 Global test at  1.48000E-01 .... OK
 Global test at  1.58000E-01 .... OK
 Global test at  1.68000E-01 .... OK
 Global test at  1.78000E-01 .... OK
 Global test at  1.88000E-01 .... OK
 Global test at  1.98000E-01 .... OK
 Terminating at   0.200000
 Calculated   103 equilibria

 Phase Region from   0.100000     for:
     FCC_A1
 Global test at  9.20000E-02 .... OK
 Global test at  8.20000E-02 .... OK
 Global test at  7.20000E-02 .... OK
 Global test at  6.20000E-02 .... OK
 Global test at  5.20000E-02 .... OK
 Global test at  4.20000E-02 .... OK
 Global test at  3.20000E-02 .... OK
 Global test at  2.20000E-02 .... OK
 Global test at  1.20000E-02 .... OK
 Global test at  2.00000E-03 .... OK
```

```
 Terminating at   0.100000E-03
 Calculated   103 equilibria
 *** Buffer saved on file: C:\Users\vagrant\AppData\Local\Temp\RESULT_002.POLY3
POLY: s-c t=1473,x(al)=.1
POLY: c-e,,,,,,,
 Using global minimization procedure
Calculated           209 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY: s-a-v 1 x(al) 0.0001 .20 0.001,,,,
POLY: step
Option? /NORMAL/:
 Step will start from axis value   0.100000
...OK

 Phase Region from   0.100000     for:
     FCC_A1
 Global test at  1.08000E-01 .... OK
 Global test at  1.18000E-01 .... OK
 Global test at  1.28000E-01 .... OK
 Global test at  1.38000E-01 .... OK
 Global test at  1.48000E-01 .... OK
 Global test at  1.58000E-01 .... OK
 Global test at  1.68000E-01 .... OK
 Global test at  1.78000E-01 .... OK
 Global test at  1.88000E-01 .... OK
 Global test at  1.98000E-01 .... OK
 Terminating at   0.200000
 Calculated   103 equilibria

 Phase Region from   0.100000     for:
     FCC_A1
 Global test at  9.20000E-02 .... OK
 Global test at  8.20000E-02 .... OK
 Global test at  7.20000E-02 .... OK
 Global test at  6.20000E-02 .... OK
 Global test at  5.20000E-02 .... OK
 Global test at  4.20000E-02 .... OK
 Global test at  3.20000E-02 .... OK
 Global test at  2.20000E-02 .... OK
 Global test at  1.20000E-02 .... OK
 Global test at  2.00000E-03 .... OK
 Terminating at   0.100000E-03
 Calculated   103 equilibria
 *** Buffer saved on file: C:\Users\vagrant\AppData\Local\Temp\RESULT_002.POLY3
POLY: s-c t=1423,x(al)=.1
POLY: c-e,,,,,,,
 Using global minimization procedure
Calculated           209 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY: s-a-v 1 x(al) 0.0001 .20 0.001,,,,
POLY: step
Option? /NORMAL/:
 Step will start from axis value   0.100000
...OK

 Phase Region from   0.100000     for:
     FCC_A1
 Global test at  1.08000E-01 .... OK
 Global test at  1.18000E-01 .... OK
 Global test at  1.28000E-01 .... OK
 Global test at  1.38000E-01 .... OK
 Global test at  1.48000E-01 .... OK
 Global test at  1.58000E-01 .... OK
 Global test at  1.68000E-01 .... OK
 Global test at  1.78000E-01 .... OK
 Global test at  1.88000E-01 .... OK
 Global test at  1.98000E-01 .... OK
 Terminating at   0.200000
 Calculated   103 equilibria

 Phase Region from   0.100000     for:
     FCC_A1
 Global test at  9.20000E-02 .... OK
 Global test at  8.20000E-02 .... OK
 Global test at  7.20000E-02 .... OK
 Global test at  6.20000E-02 .... OK
 Global test at  5.20000E-02 .... OK
 Global test at  4.20000E-02 .... OK
 Global test at  3.20000E-02 .... OK
 Global test at  2.20000E-02 .... OK
 Global test at  1.20000E-02 .... OK
 Global test at  2.00000E-03 .... OK
 Terminating at   0.100000E-03
 Calculated   103 equilibria
 *** Buffer saved on file: C:\Users\vagrant\AppData\Local\Temp\RESULT_002.POLY3
POLY: s-c t=1373,x(al)=.1
POLY: c-e,,,,,,,
 Using global minimization procedure
Calculated           209 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY: s-a-v 1 x(al) 0.0001 .20 0.001,,,,
POLY: step
Option? /NORMAL/:
 Step will start from axis value   0.100000
...OK

 Phase Region from   0.100000     for:
     FCC_A1
 Global test at  1.08000E-01 .... OK
 Global test at  1.18000E-01 .... OK
 Global test at  1.28000E-01 .... OK
 Global test at  1.38000E-01 .... OK
 Global test at  1.48000E-01 .... OK
 Global test at  1.58000E-01 .... OK
 Global test at  1.68000E-01 .... OK
 Global test at  1.78000E-01 .... OK
 Global test at  1.88000E-01 .... OK
 Global test at  1.98000E-01 .... OK
 Terminating at   0.200000
 Calculated   103 equilibria

 Phase Region from   0.100000     for:
```

```
     FCC_A1
 Global test at  9.20000E-02 .... OK
 Global test at  8.20000E-02 .... OK
 Global test at  7.20000E-02 .... OK
 Global test at  6.20000E-02 .... OK
 Global test at  5.20000E-02 .... OK
 Global test at  4.20000E-02 .... OK
 Global test at  3.20000E-02 .... OK
 Global test at  2.20000E-02 .... OK
 Global test at  1.20000E-02 .... OK
 Global test at  2.00000E-03 .... OK
 Terminating at   0.100000E-03
 Calculated   103 equilibria
 *** Buffer saved on file: C:\Users\vagrant\AppData\Local\Temp\RESULT_002.POLY3
POLY: s-c t=1323,x(al)=.1
POLY: c-e,,,,,,,
 Using global minimization procedure
Calculated           209 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY: s-a-v 1 x(al) 0.0001 .20 0.001,,,,
POLY: step
Option? /NORMAL/:
 Step will start from axis value   0.100000
...OK

 Phase Region from   0.100000     for:
     FCC_A1
 Global test at  1.08000E-01 .... OK
 Global test at  1.18000E-01 .... OK
 Global test at  1.28000E-01 .... OK
 Global test at  1.38000E-01 .... OK
 Global test at  1.48000E-01 .... OK
 Global test at  1.58000E-01 .... OK
 Global test at  1.68000E-01 .... OK
 Global test at  1.78000E-01 .... OK
 Global test at  1.88000E-01 .... OK
 Global test at  1.98000E-01 .... OK
 Terminating at   0.200000
 Calculated   103 equilibria

 Phase Region from   0.100000     for:
     FCC_A1
 Global test at  9.20000E-02 .... OK
 Global test at  8.20000E-02 .... OK
 Global test at  7.20000E-02 .... OK
 Global test at  6.20000E-02 .... OK
 Global test at  5.20000E-02 .... OK
 Global test at  4.20000E-02 .... OK
 Global test at  3.20000E-02 .... OK
 Global test at  2.20000E-02 .... OK
 Global test at  1.20000E-02 .... OK
 Global test at  2.00000E-03 .... OK
 Terminating at   0.100000E-03
 Calculated   103 equilibria
 *** Buffer saved on file: C:\Users\vagrant\AppData\Local\Temp\RESULT_002.POLY3
POLY: s-c t=1273,x(al)=.1
POLY: c-e,,,,,,,
 Using global minimization procedure
Calculated           209 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY: s-a-v 1 x(al) 0.0001 .20 0.001,,,,
POLY: step
Option? /NORMAL/:
 Step will start from axis value   0.100000
...OK

 Phase Region from   0.100000     for:
     FCC_A1
 Global test at  1.08000E-01 .... OK
 Global test at  1.18000E-01 .... OK
 Global test at  1.28000E-01 .... OK
 Global test at  1.38000E-01 .... OK
 Global test at  1.48000E-01 .... OK
 Global test at  1.58000E-01 .... OK
 Global test at  1.68000E-01 .... OK
 Global test at  1.78000E-01 .... OK
 Global test at  1.88000E-01 .... OK
 Global test at  1.98000E-01 .... OK
 Terminating at   0.200000
 Calculated   103 equilibria

 Phase Region from   0.100000     for:
     FCC_A1
 Global test at  9.20000E-02 .... OK
 Global test at  8.20000E-02 .... OK
 Global test at  7.20000E-02 .... OK
 Global test at  6.20000E-02 .... OK
 Global test at  5.20000E-02 .... OK
 Global test at  4.20000E-02 .... OK
 Global test at  3.20000E-02 .... OK
 Global test at  2.20000E-02 .... OK
 Global test at  1.20000E-02 .... OK
 Global test at  2.00000E-03 .... OK
 Terminating at   0.100000E-03
 Calculated   103 equilibria
 *** Buffer saved on file: C:\Users\vagrant\AppData\Local\Temp\RESULT_002.POLY3
POLY: @@
POLY: @@ ENTER THE POST MODULE, PLOT THE DIFFUSIVITY ON THE Y-AXIS
POLY: @@ AND MOLE-FRACTION Al ON THE X-AXIS.
POLY: @@
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2
POST:
POST: s-d-a x m-f al
POST: s-d-a y logdc(fcc,al,al,ni)
POST:
POST: app y yama.exp
PROLOGUE NUMBER: /0/: 1
DATASET NUMBER(s): /-1/: 1 2 3 4 5 6 7
POST:
POST:
POST: s-t-m-s y
```

```
 COMMAND NOT SUPPORTED IN THIS PLOT DRIVER
POST: s-s-s y n -15 -11.7
POST: s-t-m-s y
 COMMAND NOT SUPPORTED IN THIS PLOT DRIVER
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
```

2019.11.11.19.21.13
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**

```
SYS:About

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

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 21012) 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: Mon Nov 11 11:13:13 2019


SYS:SYS:MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exh1\setup.DCM.test"
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  v10.0

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10:
TDB_TCFE10: @@
TDB_TCFE10: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE THE DATA
TDB_TCFE10: @@
TDB_TCFE10: sw FEDEMO
 Current database: Iron Demo Database v2.1

 VA                      /-  DEFINED
TDB_FEDEMO: def-sys fe c
 FE                      C  DEFINED
TDB_FEDEMO: rej ph * all
 GAS:G                   LIQUID:L                BCC_A2
 CBCC_A12                CEMENTITE               CUB_A13
 DIAMOND_FCC_A4          FCC_A1                  GRAPHITE
 HCP_A3                  KSI_CARBIDE             LAVES_PHASE_C14
 M23C6                   M5C2                    M7C3
   REJECTED
TDB_FEDEMO: res ph bcc fcc
 BCC_A2                  FCC_A1  RESTORED
TDB_FEDEMO: get
19:22:31,764 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'P. Franke, Estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
  'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
 -OK-
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ SWITCH TO A MOBILITY DATABASE TO RETRIEVE MOBILITY DATA
TDB_FEDEMO: @@
TDB_FEDEMO: app mfedemo
 Current database: Fe-Alloys Mobility demo database v2.0

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

 List of references for assessed data

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

```
DIC> @@ ENTER THE GLOBAL CONDITION T
DIC> @@
DIC> set-cond glob T 0 1000; * N
DIC>
DIC> @@
DIC> @@ START BY ENTERING THE REGIONS ferrite AND austenite WHERE
DIC> @@ THE BCC AND FCC PHASES ARE PUT, RESPECTIVELY. THE FERRITE REGION IS
DIC> @@ ASSUMED INITIALLY TO BE VERY THIN, 1E-9 METERS.
DIC> @@
DIC> enter-region
REGION NAME : ferrite
DIC>
DIC> enter-region
REGION NAME : austenite
ATTACH TO REGION NAMED /FERRITE/:
ATTACHED TO THE RIGHT OF FERRITE /YES/:
DIC>
DIC> @@
DIC> @@ ENTER GRIDS INTO THE REGIONS
DIC> @@
DIC> enter-grid
REGION NAME : /FERRITE/: ferrite
WIDTH OF REGION /1/: 1e-9
TYPE /LINEAR/: AUTO
DIC>
DIC> enter-grid austenite
WIDTH OF REGION /1/: 0.999e-6
TYPE /LINEAR/: AUTO
DIC>
DIC> @@
DIC> @@ ENTER THE active PHASES INTO THE REGIONS
DIC> @@
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /FERRITE/: ferrite
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: bcc
DIC>
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: active
REGION NAME : /AUSTENITE/: austenite
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: fcc#1
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITION INTO BCC
DIC> @@
DIC> enter-composition
REGION NAME : /FERRITE/: ferrite
PHASE NAME: /BCC_A2/: bcc
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: C
TYPE /LINEAR/: linear
VALUE OF FIRST POINT : 0.019091893
VALUE OF LAST POINT : /1.9091893E-2/: 0.019091893
DIC>
DIC> @@
DIC> @@ ENTER THE INITIAL COMPOSITION INTO FCC
DIC> @@
DIC> enter-composition
REGION NAME : /AUSTENITE/: austenite
PHASE NAME: /FCC_A1/: fcc#1
COMPOSITION TYPE /MOLE_FRACTION/: w-p
PROFILE FOR /C/: C
TYPE /LINEAR/: linear
VALUE OF FIRST POINT : 0.0191
VALUE OF LAST POINT : /1.91E-2/: 0.0191
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exh1 y
DIC>
DIC> set-inter
 --OK---
DIC>
```

**exh1-run**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exh1\run.DCM.test"
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
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
  Trying old scheme                     3
 U-FRACTION IN SYSTEM:  C = 8.8825328568563E-04  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-06 [m]
 U-FRACTION IN SYSTEM:  C = 8.8825328568563E-04  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-06 [m]
 2.137709938543949E-004        2.137625593783627E-004         13.8289494082011        2.120998911035789E-004        2.112667987438772E-
004        2.108508673179424E-004        2.106430552934355E-004        2.104353457279473E-004        2.101948159848891E-
004        2.097141691265310E-004        2.087545259209826E-004        2.068418415541200E-004        2.030428809977812E-
004        1.955505925945084E-004        1.809885466255661E-004        1.535545780378763E-004        1.054471342636204E-
004        3.627422031933180E-005         13.8289493973143        3.615700659637290E-005        3.609847086651284E-
005        3.606922078447431E-005        3.605460018916993E-005        3.603998255771458E-005        3.602477866736845E-
005        3.599438050954132E-005        3.593362268572064E-005        3.581226100506191E-005        3.557015351193050E-
005        3.508840199823097E-005        3.413475286112764E-005        3.226687014812406E-005        2.868876696680698E-
005        2.216320958311595E-005        1.163469073143171E-005         7.48347184238138        1.161266681061649E-
005        1.160166267452470E-005        1.159616256257289E-005        1.159341299561144E-005        1.159066375466364E-
005        1.158790566549404E-005        1.158239047172325E-005        1.157136402252789E-005        1.154932687740117E-
005        1.150531560030047E-005        1.141754509870998E-005        1.124301230593695E-005        1.089797956220244E-
005        1.022404544182420E-005        1.490118163906617E-002        1.019021768213511E-005        1.017332482286429E-
005        1.016488364835814E-005        1.016066437488455E-005        1.015644597727906E-005        1.015204956612225E-
005        1.014325959902083E-005        1.012569108573464E-005        1.009059974271581E-005        1.002059979098280E-
005        9.881330824735401E-006        4.762707176426177E-006        4.438313282537391E-003        2.058831396523542E-
006        2.181365075882774E-007        6.215862814898044E-009        1.005966772581293E-011        2.807707694406453E-
008        1.740878115116929E-015        2.916483858551415E-008        3.123161389050897E-019       TIME =  0.10000000E-06 DT =  0.10000000E-
06 SUM OF SQUARES =  0.31231614E-18
 CELL # 1 VELOCITY AT INTERFACE # 2 IS    4.9961063     AND    4.9961063
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.50061063E-06


output ignored...



... output resumed

TIME =  0.24974221E-02 DT =  0.18903327E-05 SUM OF SQUARES =  0.87228773E-22
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.83033508E-03 AND   0.83033508E-03
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.93676957E-06
 U-FRACTION IN SYSTEM:  C = 8.98900765940845E-04  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-06 [m]
  CPU time used in timestep                    1 seconds
 7.855333440683324E-008        7.845460238641636E-008        2.895741339936800E-010        1.377394760819383E-012        3.299231770250781E-
017       TIME =  0.24986191E-02 DT =  0.11969968E-05 SUM OF SQUARES =  0.32992318E-16
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.95215868E-03 AND   0.95215868E-03
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.93790930E-06
 U-FRACTION IN SYSTEM:  C = 8.989534719341E-04  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-06 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: FERRITE

  CPU time used in timestep                    1 seconds
 1.224785681270332E-007        1.223256121098784E-007        2.395879096322191E-010        6.518559811356232E-013        4.308838477575707E-
018       TIME =  0.24993550E-02 DT =  0.73586305E-06 SUM OF SQUARES =  0.43088385E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.10897996E-02 AND   0.10897996E-02
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.93871124E-06
 U-FRACTION IN SYSTEM:  C = 8.98994461883804E-04  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-06 [m]
  CPU time used in timestep                    0 seconds
 3.060408066093171E-007        3.057361975974857E-007        3.253001848907352E-010        5.404633214996537E-013        1.316152270107155E-
018       TIME =  0.24997404E-02 DT =  0.38538384E-06 SUM OF SQUARES =  0.13161523E-17
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.12900929E-02 AND   0.12900929E-02
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.93920842E-06
 U-FRACTION IN SYSTEM:  C = 8.990521408474E-04  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-06 [m]
  1  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: FERRITE

  CPU time used in timestep                    0 seconds
 3.534169346408812E-007        3.530044344472758E-007        1.634714103406208E-010        8.223319780560527E-014        2.121725976031438E-
020       TIME =  0.24999375E-02 DT =  0.19709686E-06 SUM OF SQUARES =  0.21217260E-19
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.14857381E-02 AND   0.14857381E-02
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.93950126E-06
 U-FRACTION IN SYSTEM:  C = 8.99110504480419E-04  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-06 [m]
  CPU time used in timestep                    1 seconds
 1.382373355427484E-006        1.381370849163780E-006        1.794175805973575E-010        9.492163681654640E-015        3.810061969864780E-
022       TIME =  0.25000000E-02 DT =  0.62514865E-07 SUM OF SQUARES =  0.38100620E-21
```

```
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.18529423E-02 AND   0.18529423E-02
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.93961709E-06
 U-FRACTION IN SYSTEM:  C = 8.99171784693228E-04  FE = 1
 TOTAL SIZE OF SYSTEM:  1E-06 [m]
 MUST SAVE WORKSPACE ON FILE
 WORKSPACE SAVED ON FILE
 RECLAIMING WORKSPACE
 DELETING TIME-RECORD FOR TIME    0.0000000
 DELETING TIME-RECORD FOR TIME   0.10000000E-06
 DELETING TIME-RECORD FOR TIME   0.30000000E-06
 DELETING TIME-RECORD FOR TIME   0.70000000E-06
 DELETING TIME-RECORD FOR TIME   0.15000000E-05
 DELETING TIME-RECORD FOR TIME   0.28565341E-05
 DELETING TIME-RECORD FOR TIME   0.52015356E-05
 DELETING TIME-RECORD FOR TIME   0.98915386E-05
 DELETING TIME-RECORD FOR TIME   0.19271545E-04
 DELETING TIME-RECORD FOR TIME   0.33687181E-04
 DELETING TIME-RECORD FOR TIME   0.53417477E-04
 DELETING TIME-RECORD FOR TIME   0.78654361E-04
 DELETING TIME-RECORD FOR TIME   0.10952899E-03
 DELETING TIME-RECORD FOR TIME   0.14613094E-03
 DELETING TIME-RECORD FOR TIME   0.18853082E-03
 DELETING TIME-RECORD FOR TIME   0.23679896E-03
 DELETING TIME-RECORD FOR TIME   0.29104871E-03
 DELETING TIME-RECORD FOR TIME   0.35145426E-03
 DELETING TIME-RECORD FOR TIME   0.41823583E-03
 DELETING TIME-RECORD FOR TIME   0.48723339E-03
 DELETING TIME-RECORD FOR TIME   0.55628740E-03
 DELETING TIME-RECORD FOR TIME   0.62546249E-03
 DELETING TIME-RECORD FOR TIME   0.69481220E-03
 DELETING TIME-RECORD FOR TIME   0.76438013E-03
 DELETING TIME-RECORD FOR TIME   0.83419603E-03
 DELETING TIME-RECORD FOR TIME   0.90425851E-03
 DELETING TIME-RECORD FOR TIME   0.97473728E-03
 DELETING TIME-RECORD FOR TIME   0.10456577E-02
 DELETING TIME-RECORD FOR TIME   0.11169997E-02
 DELETING TIME-RECORD FOR TIME   0.11887868E-02
 DELETING TIME-RECORD FOR TIME   0.12609692E-02
 DELETING TIME-RECORD FOR TIME   0.13331752E-02
 DELETING TIME-RECORD FOR TIME   0.14056137E-02
 DELETING TIME-RECORD FOR TIME   0.14782827E-02
 DELETING TIME-RECORD FOR TIME   0.15511176E-02
 DELETING TIME-RECORD FOR TIME   0.16239995E-02
 DELETING TIME-RECORD FOR TIME   0.16973710E-02
 DELETING TIME-RECORD FOR TIME   0.17714237E-02
 DELETING TIME-RECORD FOR TIME   0.18459454E-02
 DELETING TIME-RECORD FOR TIME   0.19208360E-02
 DELETING TIME-RECORD FOR TIME   0.19960899E-02
 DELETING TIME-RECORD FOR TIME   0.20715733E-02
 DELETING TIME-RECORD FOR TIME   0.21477959E-02
 DELETING TIME-RECORD FOR TIME   0.22245451E-02
 DELETING TIME-RECORD FOR TIME   0.23020845E-02
 DELETING TIME-RECORD FOR TIME   0.23637496E-02
 DELETING TIME-RECORD FOR TIME   0.24066139E-02
 DELETING TIME-RECORD FOR TIME   0.24364991E-02
 DELETING TIME-RECORD FOR TIME   0.24572378E-02
 DELETING TIME-RECORD FOR TIME   0.24715984E-02
 DELETING TIME-RECORD FOR TIME   0.24814555E-02
 DELETING TIME-RECORD FOR TIME   0.24881136E-02
 DELETING TIME-RECORD FOR TIME   0.24925865E-02
 DELETING TIME-RECORD FOR TIME   0.24955318E-02
 DELETING TIME-RECORD FOR TIME   0.24974221E-02
 DELETING TIME-RECORD FOR TIME   0.24986191E-02
 DELETING TIME-RECORD FOR TIME   0.24993550E-02
 DELETING TIME-RECORD FOR TIME   0.24997404E-02

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

 TIMESTEP AT    0.250000000E-02 SELECTED

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

**exh1-plot**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exh1\plot.DCM.test"
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  2.50000E-03
DIC>
DIC> read exh1
 OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1: @@
POST-1: @@ SET THE DATA APPENDED FROM THE "EXP" FILE TO BE READ
POST-1: @@
POST-1: set-col for for red
 COMMAND NOT SUPPORTED IN THIS PLOT DRIVER
POST-1:
POST-1: @@
POST-1: @@ COMPARE THE POSITION OF THE INTERFACE AS A FUNCTION OF TIME
POST-1: @@
POST-1: s-d-a x time
  INFO: Time is set as independent variable
POST-1: s-d-a y posi aus low
POST-1:
POST-1: @@
POST-1: @@ APPEND THE SIMULATION (WITHOUT THE ENERGY CONTRIBUTION) FROM FILE
POST-1: @@
POST-1: app y noadd.exp 1; 1
POST-1:
POST-1: @@
POST-1: @@ SET A TITLE ON THE PLOT
POST-1: @@
POST-1: set-title Figure h1
POST-1:
POST-1: @@
POST-1: @@ PLOT THE RESULTS
POST-1: @@
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
ORKING ...          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

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

# Example exh2

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

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

**exh2-setup**

```
SYS:About

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

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 21012) 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: Mon Nov 11 11:13:13 2019


SYS:SYS:MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exh2\setup.DCM.test"
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  v10.0

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10:
TDB_TCFE10: @@
TDB_TCFE10: @@ SELECT A DATABASE FOR THERMODYNAMIC DATA
TDB_TCFE10: @@
TDB_TCFE10: sw fedemo
 Current database: Iron Demo Database v2.1

 VA                      /-  DEFINED
TDB_FEDEMO: def-sys fe ni c
 FE                      NI                      C
   DEFINED
TDB_FEDEMO: rej ph * all
 GAS:G                   LIQUID:L                BCC_A2
 CBCC_A12                CEMENTITE               CUB_A13
 DIAMOND_FCC_A4          FCC_A1                  GRAPHITE
 HCP_A3                  KSI_CARBIDE             LAVES_PHASE_C14
 M23C6                   M5C2                    M7C3
   REJECTED
TDB_FEDEMO: res ph bcc fcc
 BCC_A2                  FCC_A1  RESTORED
TDB_FEDEMO: get
19:26:41,807 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'P. Franke, Estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
  'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'A. Gabriel, C. Chatillon, and I. Ansara, published in High Temp. Sci.
      (Parameters listed in CALPHAD, 11 (1987) 203-218); C-NI'
  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'A. Gabriel, P. Gustafson, and I. Ansara, CALPHAD, 11 (1987) 203 -218;
      TRITA-MAC 285 (1986); C-FE-NI'
  'A. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); FE-NI'
  'B.-J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
 -OK-
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ 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>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exh2\run.DCM.test"
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ FILE TO RUN EXAMPLE exh2
DIC> @@
DIC>
DIC> @@
DIC> @@ READ THE SETUP FROM FILE
DIC> @@
DIC>
DIC> go d-m
 TIME STEP AT TIME  0.00000E+00
DIC>
DIC> read exh2
 OK
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME
DIC> @@
DIC> set-sim-time 50,,,,,,,,,
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ ENABLE THE PARA-EQUILIBRIUM MODEL
DIC> @@
DIC> para
ENABLE PARAEQ : /NO/: YES
U-FRACTION OF COMPONENT FE /AUTO/: AUTO
U-FRACTION OF COMPONENT NI /AUTO/: AUTO
DIC>
DIC> @@
DIC> @@ START THE SIMULATION
DIC> @@
DIC> sim
 Region: FERRITE
 single geometric dense at  0.10000E-08
 0.99997       24
 Region: AUSTENITE
 single geometric dense at   0.0000
  1.1602       98
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
  Trying old scheme                      4
 GENERATING STARTING VALUES FOR CELL #  1 INTERFACE #  2
 DETERMINING INITIAL EQUILIBRIUM VALUES
CALCULATING STARTING VALUES:       9   EQUILIBRIUM CALCULATIONS                DONE     6 OUT OF     9
 U-FRACTION IN SYSTEM:  C = .00412262676333  FE = .980742621143594
                        NI = .0192573788564064
 TOTAL SIZE OF SYSTEM:  5.0001E-05 [m]
 U-FRACTION IN SYSTEM:  C = .00412262676333  FE = .980742621143594
                        NI = .0192573788564064
 TOTAL SIZE OF SYSTEM:  5.0001E-05 [m]
  13403.6958745515         13403.6958745544         13396.6824657623         181.652816596437         1.24966115125195         3.83383224797661
003        1.422760370068196E-005        4.522016552102631E-007        2.881115035337984E-014       TIME =  0.10000000E-06 DT =  0.10000000E-
06 SUM OF SQUARES =  0.28811150E-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 = .00412273714809208  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
  13162.2365643736         13162.2365643871         13155.2460353445         172.785445511666         1.16154682475210         4.14452150354471
003        1.903424222643867E-003        2.796485935687478E-006        4.535465492522392E-007        1.548523230771471E-
009        7.179388844618737E-013       TIME =  0.20000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =  0.71793888E-12
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.28504281E-02 AND   0.28504281E-02
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.32995912E-08
 U-FRACTION IN SYSTEM:  C = .00412273399769255  FE = .980742621143594
                        NI = .0192573788564064
 TOTAL SIZE OF SYSTEM:  5.0001E-05 [m]
  CPU time used in timestep                    2 seconds
  12924.7969674934         12924.7969674966         12917.8299122818         164.371510588806         1.07976167312770         5.304375861029674
002

output ignored...



... output resumed

 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.12884768E-04
 U-FRACTION IN SYSTEM:  C = .00412855131241517  FE = .980742621143593
                        NI = .0192573788564065
 TOTAL SIZE OF SYSTEM:  5.0001E-05 [m]
  12  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: FERRITE

  CPU time used in timestep                    2 seconds
  6134.60951334372         6134.60951334461         6128.88995332177         24.2689894207182         6.413323263101194E-
002        8.380049164198499E-004        3.990461784559268E-006        5.061503059272618E-011        1.608627864064461E-
003        1.355253114191093E-020       TIME =   41.718584     DT =   3.7168197     SUM OF SQUARES =  0.13552531E-19
 CELL # 1 VELOCITY AT INTERFACE # 2 IS   0.19118081E-06 AND   0.19118081E-06
 POSITION OF INTERFACE FERRITE / AUSTENITE IS   0.13595352E-04
 U-FRACTION IN SYSTEM:  C = .00412892447598192  FE = .980742621143593
                        NI = .0192573788564065
 TOTAL SIZE OF SYSTEM:  5.0001E-05 [m]
  14  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: FERRITE

  CPU time used in timestep                    2 seconds
  6019.29790049771         6019.29790049740         6013.61359254602         23.1752711370790         5.988603172030072E-
002        6.191105985224194E-004        3.230252623246713E-006        5.179386172606324E-011        1.618147715945773E-
003        1.529953697989539E-020       TIME =   45.525738     DT =   3.8071537     SUM OF SQUARES =  0.15299537E-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 = .00412927023802926  FE = .980742621143593
                        NI = .0192573788564066
 TOTAL SIZE OF SYSTEM:  5.0001E-05 [m]
```

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

  CPU time used in timestep                    3 seconds
  5906.07319970474         5906.07319970558         5900.42420052966         22.1323479634626        5.592492743369468E-
002        1.888925052028504E-003        1.151756742879570E-006        1.342517986229353E-010        1.162543001321810E-
003        2.376456812917080E-019       TIME =   49.001916     DT =   3.4761784     SUM OF SQUARES =  0.23764568E-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 = .00412980312100919  FE = .980742621143593
                        NI = .0192573788564066
 TOTAL SIZE OF SYSTEM:  5.0001E-05 [m]
  12  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: FERRITE

  CPU time used in timestep                    2 seconds
  5794.90030702302         5794.90030702527         5789.28666554224         21.1377744510757        5.223026173575411E-
002        1.429845858158202E-002        3.466078141492284E-005        1.478441968367781E-007        1.640219092461051E-
003        7.208303413817830E-018       TIME =   50.000000     DT =  0.99808402     SUM OF SQUARES =  0.72083034E-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 = .00413094813368856  FE = .980742621143593
                        NI = .0192573788564066
 TOTAL SIZE OF SYSTEM:  5.0001E-05 [m]
 MUST SAVE WORKSPACE ON FILE
 WORKSPACE SAVED ON FILE
 RECLAIMING WORKSPACE
 DELETING TIME-RECORD FOR TIME    0.0000000
 DELETING TIME-RECORD FOR TIME   0.10000000E-06
 DELETING TIME-RECORD FOR TIME   0.20000000E-06
 DELETING TIME-RECORD FOR TIME   0.35656740E-06
 DELETING TIME-RECORD FOR TIME   0.63794974E-06
 DELETING TIME-RECORD FOR TIME   0.11506591E-05
 DELETING TIME-RECORD FOR TIME   0.21687314E-05
 DELETING TIME-RECORD FOR TIME   0.42048761E-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>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exh2\plot.DCM.test"
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  5.00000E+01
DIC>
DIC> read exh2
 OK
DIC>
DIC> @@
DIC> @@ GO TO THE POST PROCESSOR
DIC> @@
DIC> post
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1:
POST-1: @@
POST-1: @@ WE WANT TO PLOT THE POSITION OF THE INTERFACE AS A FUNCTION OF TIME
POST-1: @@ I.E. THE FERRITE HALF-THICKNESS
POST-1: @@
POST-1: s-d-a x time
  INFO: Time is set as independent variable
POST-1: s-d-a y posi aus low
POST-1:
POST-1: @@
POST-1: @@ APPEND THE EXPERIMENTAL INFORMATION
POST-1: @@
POST-1: app y exh2.exp 1; 1
POST-1:
POST-1: @@
POST-1: @@ SET A TITLE ON THE PLOT
POST-1: @@
POST-1: set-title Figure h2
POST-1:
POST-1: @@
POST-1: @@ RENAME THE AXIS LABELS
POST-1: @@
POST-1: set-axis-text-status
AXIS (X, Y OR Z) : x
AUTOMATIC AXIS TEXT  (Y OR N) /N/: NO
AXIS TEXT : Time [s]
POST-1:
POST-1: set-axis-text-status
AXIS (X, Y OR Z) : y
AUTOMATIC AXIS TEXT  (Y OR N) /N/: NO
AXIS TEXT : Ferrite half-thickness
POST-1:
POST-1: @@
POST-1: @@ PLOT THE RESULTS
POST-1: @@
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

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

# Example exh3

## Diffusion induced by a temperature gradient (thermomigration)

This calculation shows how a temperature gradient induces diffusion.

$$J_C = -\frac{u_C}{V_s} y_{Va} M_{CVa} \left( \frac{\partial \mu_C}{\partial x} + \frac{Q_C^*}{T} \frac{\partial T}{\partial x} \right)$$

**exh3-setup**

```
SYS:About

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

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 21012) 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: Mon Nov 11 11:13:13 2019


SYS:SYS:MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exh3\setup.DCM.test"
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  v10.0

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10: sw fedemo
 Current database: Iron Demo Database v2.1

 VA                      /-  DEFINED
TDB_FEDEMO: def-sys fe ni c
 FE                      NI                      C
   DEFINED
TDB_FEDEMO: rej ph * all
 GAS:G                   LIQUID:L                BCC_A2
 CBCC_A12                CEMENTITE               CUB_A13
 DIAMOND_FCC_A4          FCC_A1                  GRAPHITE
 HCP_A3                  KSI_CARBIDE             LAVES_PHASE_C14
 M23C6                   M5C2                    M7C3
   REJECTED
TDB_FEDEMO: res ph fcc graph
 FCC_A1                  GRAPHITE  RESTORED
TDB_FEDEMO: get
19:31:33,479 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'B.-J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
  'A. Gabriel, C. Chatillon, and I. Ansara, published in High Temp. Sci.
      (Parameters listed in CALPHAD, 11 (1987) 203-218); C-NI'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'A. Gabriel, P. Gustafson, and I. Ansara, CALPHAD, 11 (1987) 203 -218;
      TRITA-MAC 285 (1986); C-FE-NI'
  'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
  'A. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); FE-NI'
  'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121 -127; Molar
      volumes'
 -OK-
TDB_FEDEMO: 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>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exh3\run.DCM.test"
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
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
 U-FRACTION IN SYSTEM:  C = .00662305741857945  FE = .68534915460493
                        NI = .31465084539507
 TOTAL SIZE OF SYSTEM:  .025 [m]
 U-FRACTION IN SYSTEM:  C = .00662305741857945  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 = .00662305741857945  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 = .00662305741857945  FE = .68534915460493
                        NI = .31465084539507
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                     0 seconds
 TIME =  0.40010010     DT =  0.40000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741857945  FE = .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 = .00662305741857939  FE = .68534915460493
                        NI = .31465084539507
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                     1 seconds
 TIME =   75752.427     DT =   74152.027     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741850891  FE = .68534915460493
                        NI = .31465084539507
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                     0 seconds
 TIME =   224056.48     DT =   148304.05     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741822246  FE = .68534915460493
                        NI = .31465084539507
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                     1 seconds
 TIME =   520664.59     DT =   296608.11     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741822199  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 = .00662305741822179  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 = .00662305741819816  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 = .00662305741817878  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 = .00662305741819076  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 = .00662305741819606  FE = .68534915460493
                        NI = .31465084539507
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                     1 seconds
 TIME =   12348045.     DT =   2268061.6     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741820038  FE = .68534915460493
                        NI = .31465084539507
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                     0 seconds
 TIME =   14506749.     DT =   2158703.9     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0066230574182025  FE = .68534915460493
                        NI = .31465084539507
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                     1 seconds
 TIME =   16599481.     DT =   2092732.2     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741820529  FE = .68534915460493
                        NI = .31465084539507
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                     0 seconds
 TIME =   18648923.     DT =   2049441.3     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741790997  FE = .68534915460493
                        NI = .31465084539507
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                     1 seconds
 TIME =   20668354.     DT =   2019431.3     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741737892  FE = .68534915460493
                        NI = .31465084539507
 TOTAL SIZE OF SYSTEM:  .025 [m]
  CPU time used in timestep                     0 seconds
 TIME =   22666114.     DT =   1997759.7     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .00662305741692793  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 = .00662305741653927  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 = .00662305741620168  FE = .68534915460493
                       NI = .31465084539507
TOTAL SIZE OF SYSTEM:  .025 [m]
 CPU time used in timestep                    1 seconds
TIME =   28576276.     DT =   1959399.6     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00662305741590666  FE = .68534915460493
                       NI = .31465084539507
TOTAL SIZE OF SYSTEM:  .025 [m]
 CPU time used in timestep                    0 seconds
TIME =   30527808.     DT =   1951532.4     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00662305741564812  FE = .68534915460493
                       NI = .31465084539507
TOTAL SIZE OF SYSTEM:  .025 [m]
 CPU time used in timestep                    1 seconds
TIME =   32472884.     DT =   1945075.6     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00662305741542068  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 = .00662305741522134  FE = .68534915460493
                       NI = .31465084539507
TOTAL SIZE OF SYSTEM:  .025 [m]
 CPU time used in timestep                    0 seconds
TIME =   36347704.     DT =   1935131.5     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00662305741504439  FE = .68534915460493
                       NI = .31465084539507
TOTAL SIZE OF SYSTEM:  .025 [m]
 CPU time used in timestep                    1 seconds
TIME =   38278937.     DT =   1931233.7     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00662305741488771  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 = .0066230574147487  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 = .0066230574146271  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 = .00662305741451714  FE = .68534915460493
                       NI = .31465084539507
TOTAL SIZE OF SYSTEM:  .025 [m]
 CPU time used in timestep                    1 seconds
TIME =   45974292.     DT =   1920148.0     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00662305741442006  FE = .68534915460493
                       NI = .31465084539507
TOTAL SIZE OF SYSTEM:  .025 [m]
 CPU time used in timestep                    0 seconds
TIME =   47614300.     DT =   1640007.6     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00662305741434941  FE = .68534915460493
                       NI = .31465084539507
TOTAL SIZE OF SYSTEM:  .025 [m]
 CPU time used in timestep                    0 seconds
TIME =   48910464.     DT =   1296163.5     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .0066230574143039  FE = .68534915460493
                       NI = .31465084539507
TOTAL SIZE OF SYSTEM:  .025 [m]
 CPU time used in timestep                    1 seconds
TIME =   49749384.     DT =   838920.23     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00662305741428246  FE = .68534915460493
                       NI = .31465084539507
TOTAL SIZE OF SYSTEM:  .025 [m]
 CPU time used in timestep                    0 seconds
TIME =   50000000.     DT =   250616.21     SUM OF SQUARES =   0.0000000
U-FRACTION IN SYSTEM:  C = .00662305741428195  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>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exh3\plot.DCM.test"
DIC> go d-m
 TIME STEP AT TIME  5.00000E+07
 *** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
DIC>
DIC>
DIC> read exh3
 OK
DIC>
DIC> post
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1: s-d-a x dist glob
  INFO: Distance is set as independent variable
POST-1: s-d-a y w-p c
POST-1: s-p-c time 367200 5E7
POST-1: s-s-s y n 0.1 0.18
POST-1: s-s-s y y
POST-1: app y exh3.exp 0; 1 3;
POST-1: s-p-o n y y n y n n,,,,,,,,
POST-1:
POST-1: set-ax-text-st x
AUTOMATIC AXIS TEXT  (Y OR N) /N/: n
AXIS TEXT : Distance [m]
POST-1:
POST-1: set-ax-text-st y
AUTOMATIC AXIS TEXT  (Y OR N) /N/: n
AXIS TEXT : Mass percent C
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

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

# Diffusion in Complex Phases

# Example exi1

## Diffusion in system with B2 ordering

Diffusion in including effects from chemical ordering. In this example folder, there is also a datafile `AlFeNi-data.TDB`, which contains both a thermodynamic and kinetic description for the ordered and disordered bcc.

**exi1-setup**

```
SYS:About

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

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 21012) 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: Mon Nov 11 11:13:13 2019


SYS:SYS:MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exi1\setup.DCM.test"
SYS: @@
SYS: @@ Diffusion in complex phases.
SYS: @@ Diffusion in a system with B2 ordering
SYS: @@ This example shows diffusion in a system with B2 ordering.
SYS: @@ The datafile AlFeNi-data.TDB contains both a thermodynamic
SYS: @@ and kinetic description for the ordered and disordered BCC.
SYS: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exi1_setup.DCM
SYS:
SYS:
SYS: go da
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v10.0

 VA                       /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10: sw user AlFeNi-data.TDB
 Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

 VA  DEFINED
19:35:05,429 INFO  USER_1151090780_7, number of lines read: 608
19:35:06,213 INFO  Parsing of USER_1151090780_7 completed in 906 ms
TDB_USER: def-sys fe al ni
 FE                       AL                       NI
   DEFINED
TDB_USER: rej ph *
 B2_BCC                   BCC_DIS                  B2_ORD
   REJECTED
TDB_USER: res ph bcc_dis b2_ord
 BCC_DIS                  B2_ORD  RESTORED
TDB_USER: get
19:35:06,428 INFO  *** Invoking Gibbs Energy System v6 ***
19:35:07,457 INFO  Preparing system for use: USER_1151090780_7
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....
 INFO: Forcing option USE_POLY3 for complex phase B2_ORD
 -OK-
TDB_USER: go -m
 NO TIME STEP DEFINED
DIC> set-cond glob T 0 1277; * N
DIC>
DIC> enter-region beta
DIC>
DIC> enter-grid beta
WIDTH OF REGION /1/: 2e-3
TYPE /LINEAR/: double
NUMBER OF POINTS /50/: 50
VALUE OF R IN THE GEOMETRICAL SERIE FOR LOWER PART OF REGION: 0.85
VALUE OF R IN THE GEOMETRICAL SERIE FOR UPPER PART OF REGION: 1.1765
DIC>
DIC> enter-phase
ACTIVE OR INACTIVE PHASE /ACTIVE/: act
REGION NAME : /BETA/: beta
PHASE TYPE /MATRIX/: matrix
PHASE NAME: /NONE/: b2_ord
DIC>
DIC> enter-composition
REGION NAME : /BETA/: beta
PHASE NAME: /B2_ORD/: b2_ord
DEPENDENT COMPONENT ? /NI/: fe
COMPOSITION TYPE /MOLE_FRACTION/: mole-fraction
PROFILE FOR /AL/: ni
TYPE /LINEAR/: function
Function F(X)= 0.28-0.277*erf((x-1e-3)/3e-6);
PROFILE FOR /NI/: al
TYPE /LINEAR/: function
Function F(X)= 0.4295-0.0105*erf((x-1e-3)/3e-6);
19:35:09,119 INFO  Preparing phase for use: B2_ORD
19:35:09,627 INFO  Preparing phase for use: BCC_DIS
DIC>
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 345600
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /34560/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC> s-a-s-v
AUTOMATIC STARTING VALUES FOR PHASE COMPOSITIONS /YES/: no
START VALUES FOR PHASES IN REGION BETA
PHASE: B2_ORD
MAJOR CONSTITUENTS IN PHASE B2_ORD: NI;AL
DIC>
DIC>
DIC>
DIC>
DIC>
DIC> save exi1 yes
DIC>
```

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

**exi1-run**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exi1\run.DCM.test"
DIC>
DIC>
DIC> @@ exi1_run.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR RUNNING EXAMPLE i1
DIC> @@
DIC>
DIC> @@
DIC> @@ ENTER THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  0.00000E+00
DIC> read exi1
 OK
DIC>
DIC> @@
DIC> @@ START THE SIMULATION
DIC> @@
DIC> sim
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
 INFO: FORCED STARTING VALUES TURNED ON
 U-FRACTION IN SYSTEM:  AL = .429499345639258  FE = .290517917020317
                        NI = .279982737340425
 TOTAL SIZE OF SYSTEM:  .002 [m]
 U-FRACTION IN SYSTEM:  AL = .429499345639258  FE = .290517917020317
                        NI = .279982737340425
 TOTAL SIZE OF SYSTEM:  .002 [m]
  6  GRIDPOINT(S) ADDED   TO   CELL #1   REGION: BETA
 TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  AL = .429499345639258  FE = .290517917020317
                        NI = .279982737340425
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                     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                     1 seconds
 TIME =  0.40010010     DT =  0.40000000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  AL = .429499345639258  FE = .290517917020317
                        NI = .279982737340425
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                     0 seconds
 TIME =   513.08856     DT =   512.68846     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  AL = .429499345639248  FE = .290517917020327
                        NI = .279982737340426
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                     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 = .290517917020345
                        NI = .279982737340424
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                     2 seconds
 TIME =   7690.7270     DT =   4101.5077     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  AL = .429499345639227  FE = .290517917020346
                        NI = .279982737340427
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                     1 seconds
 TIME =   15893.742     DT =   8203.0154     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  AL = .429499345639233  FE = .290517917020342
                        NI = .279982737340425
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                     1 seconds
 TIME =   32299.773     DT =   16406.031     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  AL = .42949934563921  FE = .290517917020363
                        NI = .279982737340427
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                     2 seconds
 TIME =   65111.835     DT =   32812.062     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  AL = .429499345639174  FE = .290517917020383
                        NI = .279982737340444
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                     2 seconds
 TIME =   99671.835     DT =   34560.000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  AL = .429499345639088  FE = .290517917020497
                        NI = .279982737340415
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                     1 seconds
 TIME =   134231.83     DT =   34560.000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  AL = .429499345639131  FE = .290517917020483
                        NI = .279982737340385
 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                     1 seconds
 TIME =   203351.83     DT =   34560.000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  AL = .429499345639156  FE = .290517917020456
                        NI = .279982737340387
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                     2 seconds
 TIME =   237911.83     DT =   34560.000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  AL = .429499345639151  FE = .290517917020442
                        NI = .279982737340408
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                     1 seconds
 TIME =   272471.83     DT =   34560.000     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  AL = .429499345639151  FE = .290517917020426
                        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 = .429499345639159  FE = .290517917020413
                        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 = .429499345639172  FE = .290517917020402
                        NI = .279982737340425
 TOTAL SIZE OF SYSTEM:  .002 [m]
  CPU time used in timestep                    1 seconds
 TIME =   345600.00     DT =   4008.1652     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  AL = .429499345639173  FE = .290517917020402
                        NI = .279982737340426
 TOTAL SIZE OF SYSTEM:  .002 [m]
 MUST SAVE WORKSPACE ON FILE
 WORKSPACE SAVED ON FILE
 RECLAIMING WORKSPACE
 DELETING TIME-RECORD FOR TIME    0.0000000
 DELETING TIME-RECORD FOR TIME   0.10000000E-06
 DELETING TIME-RECORD FOR TIME   0.10010000E-03
 DELETING TIME-RECORD FOR TIME   0.40010010
 DELETING TIME-RECORD FOR TIME    513.08856
 DELETING TIME-RECORD FOR TIME    1538.4655
 DELETING TIME-RECORD FOR TIME    3589.2193
 DELETING TIME-RECORD FOR TIME    7690.7270
 DELETING TIME-RECORD FOR TIME    15893.742
 DELETING TIME-RECORD FOR TIME    32299.773
 DELETING TIME-RECORD FOR TIME    65111.835
 DELETING TIME-RECORD FOR TIME    99671.835
 DELETING TIME-RECORD FOR TIME    134231.83
 DELETING TIME-RECORD FOR TIME    168791.83
 DELETING TIME-RECORD FOR TIME    203351.83
 DELETING TIME-RECORD FOR TIME    237911.83
 DELETING TIME-RECORD FOR TIME    272471.83
 DELETING TIME-RECORD FOR TIME    307031.83

 KEEPING TIME-RECORD FOR TIME    341591.83
 AND FOR TIME                    345600.00
 WORKSPACE RECLAIMED

 TIMESTEP AT     345600.000     SELECTED

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

**exi1-plot**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exi1\plot.DCM.test"
DIC>
DIC> @@ exi1_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE i1
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  3.45600E+05
DIC> read exi1
 OK
DIC>
DIC> @@
DIC> @@ ENTER THE POST PROCESSOR
DIC> @@
DIC> post
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1: s-d-a x dist glob
  INFO: Distance is set as independent variable
POST-1:
POST-1: s-d-a y m-f al
POST-1:
POST-1: s-p-c time last
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

```
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: ent tab prof
Variable(s) x(al) x(ni)
POST-1:
POST-1: ent fun rdist
FUNCTION: 1e6*(gd-10e-4)
&
POST-1: s-d-a y prof
COLUMN NUMBER /*/: 1 2
POST-1:
POST-1: s-d-a x rdist
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

2019.11.11.19.37.30
Time = 345600
CELL #1

```
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: app y exi1.exp
PROLOGUE NUMBER: /0/: 1
DATASET NUMBER(s): /-1/: 1
POST-1:
POST-1: s-s-s x n -300 300
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

2019.11.11.19.37.31
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**

```
SYS:About

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

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 21012) 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: Mon Nov 11 11:13:13 2019


SYS:SYS:MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exi2\setup.DCM.test"
SYS: @@
SYS: @@ Diffusion in complex phases.
SYS: @@ Diffusion of carbon in cementite
SYS: @@ This example demonstrates the use of the model for calculation of
SYS: @@ diffusion through a stoichiometric phase. The flux of a component in
SYS: @@ the stoichiometric phase is assumed to be proportional to the
SYS: @@ difference in chemical potential at each side of the stoichiometric
SYS: @@ phase multiplied with the mobility for the component in the phase. The
SYS: @@ mobility is assessed from experimental information and is basically
SYS: @@ the tracer diffusivity for the component.
SYS: @@
SYS: @@ This calculation is compared with experimental data where a sample of
SYS: @@ pure iron has been exposed to a gas atmosphere with a certain carbon
SYS: @@ activity. The weight gain is then measured as a function of time.
SYS: @@ The experimental data is obtained from Ozturk B., Fearing V. L.,
SYS: @@ Ruth A. Jr. and Simkovich G., Met. Trans A, vol 13A (1982), pp. 1871-1873.
SYS: ---------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM THE DATABASES
SYS: @@
SYS: go da
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v10.0

 VA                       /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10:
TDB_TCFE10: @@
TDB_TCFE10: @@ USE A THERMODYNAMIC DATABASE TO RETRIEVE DATA
TDB_TCFE10: @@
TDB_TCFE10: switch FEDEMO
 Current database: Iron Demo Database v2.1

 VA                       /-  DEFINED
TDB_FEDEMO: def-sys fe c
 FE                       C  DEFINED
TDB_FEDEMO: rej ph * all
 GAS:G                    LIQUID:L                 BCC_A2
 CBCC_A12                 CEMENTITE                CUB_A13
 DIAMOND_FCC_A4           FCC_A1                   GRAPHITE
 HCP_A3                   KSI_CARBIDE              LAVES_PHASE_C14
 M23C6                    M5C2                     M7C3
   REJECTED
TDB_FEDEMO: res ph bcc fcc cementite grap
 BCC_A2                   FCC_A1                   CEMENTITE
 GRAPHITE  RESTORED
TDB_FEDEMO: get
19:38:49,784 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'P. Franke, Estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
  'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'B. Hallstedt, D. Djurovic, J. von Appen, R. Dronskowski, A. Dick, F.
      Koermann, T. Hickel, J. Neugebauer, CALPHAD, 34, 129 -33(2010); Fe-C'
  'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
  'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121 -127; Molar
      volumes'
 -OK-
TDB_FEDEMO:
TDB_FEDEMO: @@
TDB_FEDEMO: @@ 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
19:38:51,190 INFO  USER_876738828_7, number of lines read: 51
19:38:51,441 INFO  Parsing of USER_876738828_7 completed in 291 ms
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
 *** ERROR FCC INPUT IGNORED
 BCC_A2                   CEMENTITE  RESTORED
TDB_APP: get
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....
```

```
 -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
19:38:51,791 INFO  Preparing system for use: USER_876738828_7
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
19:38:53,091 INFO  Preparing phase for use: BCC_A2
DIC>
DIC> set-cond bound upp
CONDITION TYPE /CLOSED_SYSTEM/: mix
Dependent substitutional element:FE
Dependent interstitial element:VA
LOW TIME LIMIT /0/: 0
ACR(C)(TIME)= 9;
HIGH TIME LIMIT /*/: *
ANY MORE RANGES /N/: N
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ SIMULATE FOR 150 MINUTES
DIC> @@
DIC> set-simulation-time
END TIME FOR INTEGRATION /.1/: 9000
AUTOMATIC TIMESTEP CONTROL /YES/:
MAX TIMESTEP DURING INTEGRATION /900/:
INITIAL TIMESTEP : /1E-07/:
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exi2 Y
DIC>
DIC> set-inter
 --OK---
DIC>
```

**exi2-run**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exi2\run.DCM.test"
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
 DEGREE OF IMPLICITY SET TO TRAPEZOIDAL RULE
  Trying old scheme                     3
 U-FRACTION IN SYSTEM:  C = 4.6598005784384E-05  FE = 1
 TOTAL SIZE OF SYSTEM:  3.300001E-06 [m]
 U-FRACTION IN SYSTEM:  C = 4.6598005784384E-05  FE = 1
 TOTAL SIZE OF SYSTEM:  3.300001E-06 [m]
19:39:49,134 INFO  Preparing phase for use: CEMENTITE
 0.111094107740055        0.111116327660160        1.168933545268372E-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                    1 seconds
 1.985503622653896E-006        1.986016682715921E-006        8.569006692077880E-023       TIME =  0.25999666E-05 DT =  0.24999666E-
05 SUM OF SQUARES =  0.85690067E-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
 9.632817666939915E-007        9.640732404382838E-007        1.188386949892457E-025       TIME =  0.75998999E-05 DT =  0.49999333E-
05 SUM OF SQUARES =  0.11883869E-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
 5.520598281728859E-007        5.525040595679611E-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
 3.294904029785889E-007        3.297431202262135E-007        1.295444436331959E-026       TIME =  0.37599500E-04 DT =  0.19999733E-
04 SUM OF SQUARES =  0.12954444E-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
 1.842051604944532E-007        1.843420424822769E-007        2.883351411658548E-025       TIME =  0.77598966E-04 DT =  0.39999466E-
04 SUM OF SQUARES =  0.28833514E-24
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.34957854E-07 AND  -0.34957854E-07
 POSITION OF INTERFACE FER / CARB IS   0.32999961E-05
 U-FRACTION IN SYSTEM:  C = 4.69308608646657E-05  FE = 1
 TOTAL SIZE OF SYSTEM:  3.300001E-06 [m]
  14  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: CARB

  CPU time used in timestep                    0 seconds
 9.778279834954463E-008        9.785422397002213E-008        4.603903155444994E-026       TIME =  0.15759790E-03 DT =  0.79998933E-
04 SUM OF SQUARES =  0.46039032E-25
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.24876846E-07 AND  -0.24876846E-07
 POSITION OF INTERFACE FER / CARB IS   0.32999941E-05
 U-FRACTION IN SYSTEM:  C = 4.7107484088289E-05  FE = 1
 TOTAL SIZE OF SYSTEM:  3.300001E-06 [m]
  49  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: CARB

  CPU time used in timestep                    0 seconds
 5.038045607965860E-006        5.041694023499918E-006

output ignored...



... output resumed

TIME =   3142.1594     DT =   900.00000     SUM OF SQUARES =  0.30310202E-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 = .00283057618776225  FE = 1
 TOTAL SIZE OF SYSTEM:  3.300001E-06 [m]
  55  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: CARB

  CPU time used in timestep                    0 seconds
 3.512901236418004E-008        3.518395504613353E-008        9.193038624674948E-
```

```
029       TIME =   4042.1594     DT =   900.00000     SUM OF SQUARES =  0.91930386E-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 = .00317904137490811  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
 1.337273691002185E-008        1.340171249711458E-008        1.442674507444166E-
026       TIME =   4942.1594     DT =   900.00000     SUM OF SQUARES =  0.14426745E-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 = .00348899893656278  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
 6.238597393560772E-009        6.256204153621230E-009        6.091408152458267E-
030       TIME =   5842.1594     DT =   900.00000     SUM OF SQUARES =  0.60914082E-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 = .0037712160470436  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
 3.280281446382724E-009        3.291907995858972E-009        1.340043917426806E-
030       TIME =   6742.1594     DT =   900.00000     SUM OF SQUARES =  0.13400439E-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 = .00403216870914771  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
 1.864873577148230E-007        1.872981046499102E-007        1.766718431636158E-
029       TIME =   7642.1594     DT =   900.00000     SUM OF SQUARES =  0.17667184E-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 = .00427612481768571  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
 1.118941666112022E-007        1.124814013565127E-007        5.965760595733902E-
030       TIME =   8542.1594     DT =   900.00000     SUM OF SQUARES =  0.59657606E-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 = .00450607892012243  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
 6.975845441408309E-008        7.019562007454278E-008        8.604937630166184E-
030       TIME =   9000.0000     DT =   457.84063     SUM OF SQUARES =  0.86049376E-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 = .00461705531635636  FE = 1
 TOTAL SIZE OF SYSTEM:  3.300001E-06 [m]
 MUST SAVE WORKSPACE ON FILE
 WORKSPACE SAVED ON FILE
 RECLAIMING WORKSPACE
 DELETING TIME-RECORD FOR TIME    0.0000000
 DELETING TIME-RECORD FOR TIME   0.10000000E-06
 DELETING TIME-RECORD FOR TIME   0.25999666E-05
 DELETING TIME-RECORD FOR TIME   0.75998999E-05
 DELETING TIME-RECORD FOR TIME   0.17599767E-04
 DELETING TIME-RECORD FOR TIME   0.37599500E-04
 DELETING TIME-RECORD FOR TIME   0.77598966E-04
 DELETING TIME-RECORD FOR TIME   0.15759790E-03
 DELETING TIME-RECORD FOR TIME   0.31759576E-03
 DELETING TIME-RECORD FOR TIME   0.63759149E-03
 DELETING TIME-RECORD FOR TIME   0.12775830E-02
 DELETING TIME-RECORD FOR TIME   0.25575659E-02
 DELETING TIME-RECORD FOR TIME   0.51175317E-02
 DELETING TIME-RECORD FOR TIME   0.10237463E-01
 DELETING TIME-RECORD FOR TIME   0.20477327E-01
 DELETING TIME-RECORD FOR TIME   0.40957054E-01
 DELETING TIME-RECORD FOR TIME   0.81916507E-01
 DELETING TIME-RECORD FOR TIME   0.16383541
 DELETING TIME-RECORD FOR TIME   0.32767323
 DELETING TIME-RECORD FOR TIME   0.65534886
 DELETING TIME-RECORD FOR TIME    1.3107001
 DELETING TIME-RECORD FOR TIME    2.6214026
 DELETING TIME-RECORD FOR TIME    5.2428076
 DELETING TIME-RECORD FOR TIME    10.485618
 DELETING TIME-RECORD FOR TIME    20.971238
 DELETING TIME-RECORD FOR TIME    41.942478
 DELETING TIME-RECORD FOR TIME    83.884958
 DELETING TIME-RECORD FOR TIME    167.76992
 DELETING TIME-RECORD FOR TIME    335.53984
 DELETING TIME-RECORD FOR TIME    671.07968
 DELETING TIME-RECORD FOR TIME    1342.1594
 DELETING TIME-RECORD FOR TIME    2242.1594
 DELETING TIME-RECORD FOR TIME    3142.1594
 DELETING TIME-RECORD FOR TIME    4042.1594
 DELETING TIME-RECORD FOR TIME    4942.1594
 DELETING TIME-RECORD FOR TIME    5842.1594
 DELETING TIME-RECORD FOR TIME    6742.1594
 DELETING TIME-RECORD FOR TIME    7642.1594

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

 TIMESTEP AT     9000.00000     SELECTED

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

**exi2-plot**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exi2\plot.DCM.test"
DIC>
DIC> @@ exi2_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE i2
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  9.00000E+03
 *** ENTERING FCC_A1 AS A DIFFUSION NONE PHASE
 *** ENTERING GRAPHITE AS A DIFFUSION NONE PHASE
DIC>
DIC>
DIC> read exi2 Y
 OK
DIC>
DIC>
DIC> @@
DIC> @@ PLOT THE SIZE OF THE CEMENTITE LAYER AS A FUNCTION OF TIME
DIC> @@
DIC> post
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1: ent-symb func csize
FUNCTION: 1e6*(poi(car,u)-poi(car,l));
POST-1:
POST-1: ent-symb func minutes
FUNCTION: time/60;
POST-1:
POST-1: s-d-a x minutes
POST-1: s-d-a y csize
POST-1:
POST-1: s-p-c inter first
POST-1:
POST-1: s-a-t-s x n Time [min]
POST-1: s-a-t-s y n Distance [?m]
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
           OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

```
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1:
POST-1: @@
POST-1: @@ ASSUME A CERTAIN TIME FOR NUCLEATION OF THE CEMENTITE LAYER
POST-1: @@
POST-1: ent-symb func cortim
FUNCTION: (time+1400)/60;
POST-1:
POST-1: @@
POST-1: @@ PLOT THE WEIGHT GAIN AS A FUNCTION OF TIME
POST-1: @@
POST-1: ent-symb func cwei
FUNCTION: 1e12*((poi(car,u)-poi(car,l)-1E-12)*12.01/2.33E-5*1e-4)**2;
POST-1:
POST-1:
POST-1: s-d-a x cortim
POST-1: s-d-a y cwei
POST-1:
POST-1: @@
POST-1: @@ COMPARE WITH EXPERIMENTAL DATA
POST-1: @@
POST-1: app y exi2.exp 0; 1
POST-1:
POST-1:
```

```
POST-1: s-a-t-s x n Time [min]
POST-1: s-a-t-s y n \latex \Delta m^2/A^2\, [g^2/cm^4\times 10^{12}]
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

2019.11.11.19.40.52
"FIRST" INTERFACE OF SYSTEM
CELL #1

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

# Example exi3a

## Diffusion in iron oxide (FeO)

This example shows the oxidation of an iron sample and the consequent growth of an oxide layer using the grain boundary diffusion contribution model.

**exi3a-setup**

```
SYS:About

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

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 21012) 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: Mon Nov 11 11:13:13 2019


SYS:SYS:MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exi3a\setup.DCM.test"
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  v10.0

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10:
TDB_TCFE10: @@
TDB_TCFE10: @@ SELECT A USER DATABASE FOR READING THE THERMODYNAMIC DATA
TDB_TCFE10: @@
TDB_TCFE10: sw user FeO.TDB
 Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

 VA                      /-  DEFINED
19:42:10,943 INFO  USER_467798867_7, number of lines read: 217
19:42:11,626 INFO  Parsing of USER_467798867_7 completed in 795 ms
TDB_USER: def-sys fe o
 FE                      O  DEFINED
TDB_USER: rej sp *
 /-                      VA                      FE
 O                       FE+2                    FE+3
 FE+4                    FE2O3                   FEO
 FEO3/2                  O-2                     O2
   REJECTED
TDB_USER: res sp fe fe+2 fe+3 o o2 o-2 va
 FE                      FE+2                    FE+3
 O                       O2                      O-2
 VA  RESTORED
TDB_USER: rej ph * all
 GAS:G                   BCC_A2                  SPINEL:I
   REJECTED
TDB_USER: res ph bcc spinel gas
 BCC_A2                  SPINEL:I                GAS:G
   RESTORED
TDB_USER:
TDB_USER: get
19:42:11,756 INFO  *** Invoking Gibbs Energy System v6 ***
19:42:12,892 INFO  Preparing system for use: USER_467798867_7
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317 -425'
  'M. Kowalski and P.J. Spencer, Calphad, 19 (1995), 229-243; Cr-O, Fe-O and
      Ni-O'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
      Molar volumes'
  'B. Sundman, J. Phase Equil., 12 (1991), 127-140; Fe-O'
 -OK-
TDB_USER:
TDB_USER: @@
TDB_USER: @@ SWITCH TO A USER-DEFINED MOBILITY DATABASE TO RETRIEVE MOBILITY DATA
TDB_USER: @@
TDB_USER: app user FeOmob.TDB
 Current database: User defined Database
         test database

 VA                      /-                      O
   DEFINED
19:42:14,098 INFO  USER_1724833957_7, number of lines read: 129
19:42:14,176 INFO  Parsing of USER_1724833957_7 completed in 79 ms
TDB_APP: def-sys fe o
 FE  DEFINED
TDB_APP: rej sp *
 /-                      VA                      FE
 O                       FE+2                    FE+3
 FE2O3                   FEO                     FEO3/2
 O-2                     O2  REJECTED
TDB_APP: res sp fe fe+2 fe+3 o o2 o-2 va
 FE                      FE+2                    FE+3
 O                       O2                      O-2
 VA  RESTORED
TDB_APP: rej ph * all
 SPINEL:I                GAS:G                   BCC_A2
   REJECTED
TDB_APP: res ph bcc spinel gas
 BCC_A2                  SPINEL:I                GAS:G
```

```
   RESTORED
TDB_APP:
TDB_APP: get
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 *** ERROR  2018 IN DESHPH: DIFFUSION DATA NOT POSSIBLE FOR GAS PHASE
 *** ERROR  2018 IN DESHPH: DIFFUSION DATA NOT POSSIBLE FOR GAS PHASE
 FUNCTIONS ....
 -OK-
TDB_APP:
TDB_APP:
TDB_APP: @@
TDB_APP: @@ ENTER THE DICTRA MONITOR
TDB_APP: @@
TDB_APP: go d-m
 NO TIME STEP DEFINED
19:42:14,620 INFO  Preparing system for use: USER_1724833957_7
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
19:42:14,961 INFO  Preparing phase for use: BCC_A2
19:42:15,299 INFO  Preparing phase for use: BCC_A2
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
19:42:16,214 INFO  Preparing phase for use: SPINEL
19:42:16,640 INFO  Preparing phase for use: SPINEL
DIC>
DIC>
DIC> @@
DIC> @@ ENTER A BOUNDARY CONDITION "GAS" ON THE UPPER (RIGHT-MOST) INTERFACE
DIC> @@ OF THE OXIDE. THIS ALLOWS THE SYSTEM TO EXPAND AND THE OXIDE LAYER
DIC> @@ TO GROW EXTERNALY. FOR THIS EXAMPLE AN OXYGEN ACTIVITY IS SPECIFIED
DIC> @@ THAT IS LOW ENOUGH NOT TO FORM CORUNDUM (FE2O3). WE ALSO SPECIFY
DIC> @@ THAT THERE IS NO FLUX OF Fe ACROSS THIS INTERFACE, I.E. NO Fe
DIC> @@ IS ALLOWED TO ENTER OR LEAVE THE SYSTEM.
DIC> @@
DIC> set-cond boundary upper gas
TYPE OF CONDITION FOR COMPONENT FE /ZERO_FLUX/: zero-flux
TYPE OF CONDITION FOR COMPONENT O /ZERO_FLUX/: act
LOW TIME LIMIT /0/: 0 4.5e-4; * N
DIC>
DIC>
DIC> @@
DIC> @@ ENTER START VALUES FOR THE INITIAL INTERFACE VELOCITIES
DIC> @@
DIC> s-a-s-v -1e-5 1e-5 yes
 STARTING VALUES WILL BE TAKEN FROM PROFILES
DIC>
DIC>
DIC> @@
DIC> @@ SIMULATE FOR 24 HOURS
DIC> @@
DIC> s-s-time 86400,,,,
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
DIC>
```

```
DIC> @@
DIC> @@ SPECIFY THAT POTENTIALS AND NOT ACTIVITIES ARE VARIED AT THE PHASE
DIC> @@ INTERFACE. ALSO USE A FULLY IMPLICIT SCHEME FOR TIME INTEGRATION.
DIC> @@
DIC> s-s-c 0 1 1 YES POT YES YES 1 2,,,,,,,,,,
 RELEASING OLD STARTING VALUES
DIC>
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exi3.DIC Y
DIC>
DIC> set-inter
 --OK---
DIC>
```

**exi3a-run**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exi3a\run.DCM.test"
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
 0.87701       95
 Region: SP
 double geometric
 dense at outer boundaries, coarse at  0.50000E-10
lower part   1.2500        9
upper part  0.80000        9
  Trying old scheme                    3
 U-FRACTION IN SYSTEM:  FE = 0.99999999500542  O = 2.10000395011622E-08
 TOTAL SIZE OF SYSTEM:  .0049999901 [m]
 U-FRACTION IN SYSTEM:  FE = 0.99999999500542  O = 2.10000395011622E-08
 TOTAL SIZE OF SYSTEM:  .0049999901 [m]
 0.347387301620383        0.347386528700296        0.347386701355531        4.618089871971189E-002        3.060231557192546E-
023       TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =  0.30602316E-22
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.39646054E-03 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49999900E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.66982674E-03 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.49999901E-02
 U-FRACTION IN SYSTEM:  FE = 0.99999998954903  O = 3.44025119032269E-08
 TOTAL SIZE OF SYSTEM:  .00499999012734 [m]
  9  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: FER

  CPU time used in timestep                    2 seconds
 1.507552605918995E-005        1.507739146395544E-005        1.507822847215681E-005        2.226308396844897E-007        1.088156531149413E-
031       TIME =  0.30000000E-06 DT =  0.20000000E-06 SUM OF SQUARES =  0.10881565E-30
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.14849229E-03 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49999899E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.20393047E-03 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.49999901E-02
 U-FRACTION IN SYSTEM:  FE = 0.99999998713864  O = 4.25594164341045E-08
 TOTAL SIZE OF SYSTEM:  .00499999013842 [m]
  CPU time used in timestep                    1 seconds
 1.398975102000987E-008        1.397926495102674E-008        1.395940586866040E-008        3.137487097492559E-011        2.576683617002454E-
034       TIME =  0.70000000E-06 DT =  0.40000000E-06 SUM OF SQUARES =  0.25766836E-33
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.14913262E-03 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49999899E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.21655229E-03 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.49999902E-02
 U-FRACTION IN SYSTEM:  FE = 0.99999998167656  O = 5.98849352760284E-08
 TOTAL SIZE OF SYSTEM:  .00499999016539 [m]
  CPU time used in timestep                    0 seconds
 5.609742547861760E-007        5.611284846522786E-007        5.611264634808881E-007        2.444637653827850E-010        5.154425178920648E-
034       TIME =  0.15000000E-05 DT =  0.80000000E-06 SUM OF SQUARES =  0.51544252E-33
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.93393028E-04 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49999898E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.13339356E-03 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.49999902E-02
 U-FRACTION IN SYSTEM:  FE = 0.99999997507588  O = 8.12308039073763E-08
 TOTAL SIZE OF SYSTEM:  .00499999019739 [m]
  23  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    1 seconds
 8.108701238937232E-006        8.112502967110108E-006        8.112138099507566E-006        1.121067578901924E-008        8.358084568809888E-
032       TIME =  0.31000000E-05 DT =  0.16000000E-05 SUM OF SQUARES =  0.83580846E-31
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.70760985E-04 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49999897E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.10183290E-03 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.49999902E-02
 U-FRACTION IN SYSTEM:  FE = 0.99999996490465  O = 1.13822384430487E-07
 TOTAL SIZE OF SYSTEM:  .00499999024711 [m]
  35  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    0 seconds
 8.100481734332299E-006        8.103302413472336E-006        8.103162850392707E-006        7.195354231104727E-009        1.751400066340988E-
031       TIME =  0.63000000E-05 DT =  0.32000000E-05 SUM OF SQUARES =  0.17514001E-30
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.49011444E-04 AND    0.0000000


output ignored...



... output resumed

 POSITION OF INTERFACE FER / SP IS   0.49497263E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.85406534E-09 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.50216007E-02
 U-FRACTION IN SYSTEM:  FE = .995601423066384  O = .0143132204530917
 TOTAL SIZE OF SYSTEM:  .005021600735 [m]
  23  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    0 seconds
 2.789556771490803E-007        2.794057583737726E-007        2.793655766546490E-007        3.800585458161961E-010        3.226308815040883E-
032       TIME =   56943.895     DT =   8640.0000     SUM OF SQUARES =  0.32263088E-31
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.54743813E-09 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49449965E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.78319309E-09 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.50236377E-02
```

```
 U-FRACTION IN SYSTEM:  FE = .995194725257643  O = .015654406467856
 TOTAL SIZE OF SYSTEM:  .00502363765793 [m]
  8  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    0 seconds
 1.595105700144953E-007        1.598217866198838E-007        1.597953811113808E-007        2.020602967915836E-010        2.692164182027236E-
032       TIME =   65583.895     DT =   8640.0000     SUM OF SQUARES =  0.26921642E-31
 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 = .994817249745992  O = .0168979971924709
 TOTAL SIZE OF SYSTEM:  .0050255321232 [m]
  7  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    1 seconds
 9.568367503403812E-008        9.590684468208239E-008        9.588874686948297E-008        1.147888045917204E-010        2.727146893907707E-
033       TIME =   74223.895     DT =   8640.0000     SUM OF SQUARES =  0.27271469E-32
 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 = .994463754813102  O = .0180617615442109
 TOTAL SIZE OF SYSTEM:  .00502730918328 [m]
  10  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    0 seconds
 5.962030955772009E-008        5.978502095949167E-008        5.977212454512204E-008        6.869420004186038E-011        1.745374012100932E-
033       TIME =   82863.895     DT =   8640.0000     SUM OF SQUARES =  0.17453740E-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 = .994130359456919  O = .0191587681410784
 TOTAL SIZE OF SYSTEM:  .00502898750134 [m]
  8  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    0 seconds
 9.162180981273464E-009        9.108164939659235E-009        9.224421751578580E-009        1.011580317017117E-011        1.083335593717820E-
034       TIME =   86400.000     DT =   3536.1047     SUM OF SQUARES =  0.10833356E-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 = .994008758985556  O = .0195911680902176
 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>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exi3a\plot.DCM.test"
DIC>
DIC> @@ exi3_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE i3
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  8.64000E+04
DIC> read exi3
 OK
DIC>
DIC> @@
DIC> @@ ENTER THE POST PROCESSOR
DIC> @@
DIC> post
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1: @@
POST-1: @@ PLOT THE THICKNESS OF THE OXIDE LAYER GROWING AT THE SURFACE.
POST-1: @@ FOR THIS WE NEED TO ENTER A FUNCTION ACCORDING TO THE FOLLOWING.
POST-1: ent func oxideth
FUNCTION: poi(sp,upper)-poi(sp,lower)
&
POST-1: @@
POST-1: @@ PUT THIS FUNCTION ON THE Y-AXIS
POST-1: @@
POST-1: s-d-a y oxideth
POST-1:
POST-1: @@
POST-1: @@ AND PLOT THE OXIDE THICKNESS VERSUS TIME
POST-1: @@
POST-1: s-d-a x time
  INFO: Time is set as independent variable
POST-1:
POST-1: @@
POST-1: @@ SINCE WE ARE PLOTTING A FUNCTION, SPECIFY A PLOT CONDITION
POST-1: @@
POST-1: s-p-c interface sp upper
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

```
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1:
POST-1: @@
POST-1: @@ NOW PLOT THE MOBILITY IN A SPINEL FOR Fe+2 ON THE SECOND SUBLATTICE
POST-1: @@
POST-1: s-d-a y logm(sp,fe+2#2)
POST-1:
POST-1: @@
POST-1: @@ LIMIT THE PLOT TO THE SPINEL PHASE
POST-1: @@
POST-1: s-d-a x dis local sp
  INFO: Distance is set as independent variable
POST-1:
POST-1: s-p-c time 86400
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

2019.11.11.19.44.28
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:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

2019.11.11.19.44.29
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:
POST-1: SET_EXP_FILE_FORMAT 5
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
POST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

2019.11.11.19.44.31
Time = 86400
CELL #1

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

# Example i3b

## Diffusion in iron oxide (FeO) with grain boundary contribution

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

**exi3b-setup**

```
SYS:About

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

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 21012) 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: Mon Nov 11 11:13:13 2019


SYS:SYS:MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exi3b\setup.DCM.test"
SYS: @@
SYS: @@ Diffusion in complex phases.
SYS: @@ Diffusion in iron oxide (FeO) with a grain boundary contribution
SYS: @@ This example shows the oxidation of an iron sample and consequent
SYS: @@ growth of an oxide layer using the grain boundary diffusion
SYS: @@ contribution model.
SYS: ------------------------------------------------------------------
 NO SUCH COMMAND, USE HELP
SYS:
SYS: @@ exi3_setup.DCM
SYS:
SYS: @@
SYS: @@ START BY GOING TO THE DATABASE MODULE
SYS: @@
SYS: go da
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v10.0

 VA                       /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10:
TDB_TCFE10: @@
TDB_TCFE10: @@ SELECT A USER DATABASE TO READ THE THERMODYNAMIC DATA
TDB_TCFE10: @@
TDB_TCFE10: sw user FeO.TDB
 Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

 VA                       /-  DEFINED
19:45:49,811 INFO  USER_2019713966_7, number of lines read: 217
19:45:50,375 INFO  Parsing of USER_2019713966_7 completed in 683 ms
TDB_USER: def-sys fe o
 FE                       O  DEFINED
TDB_USER: rej sp *
 /-                       VA                       FE
 O                        FE+2                     FE+3
 FE+4                     FE2O3                    FEO
 FEO3/2                   O-2                      O2
   REJECTED
TDB_USER: res sp fe fe+2 fe+3 o o2 o-2 va
 FE                       FE+2                     FE+3
 O                        O2                       O-2
 VA  RESTORED
TDB_USER: rej ph * all
 GAS:G                    BCC_A2                   SPINEL:I
   REJECTED
TDB_USER: res ph bcc spinel gas
 BCC_A2                   SPINEL:I                 GAS:G
   RESTORED
TDB_USER:
TDB_USER: get
19:45:50,703 INFO  *** Invoking Gibbs Energy System v6 ***
19:45:51,785 INFO  Preparing system for use: USER_2019713966_7
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317 -425'
  'M. Kowalski and P.J. Spencer, Calphad, 19 (1995), 229-243; Cr-O, Fe-O and
      Ni-O'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
      Molar volumes'
  'B. Sundman, J. Phase Equil., 12 (1991), 127-140; Fe-O'
 -OK-
TDB_USER:
TDB_USER: @@
TDB_USER: @@ SWITCH TO A USER-DEFINED MOBILITY DATABASE TO RETRIEVE MOBILITY DATA
TDB_USER: @@
TDB_USER: app user FeOmob.TDB
 Current database: User defined Database
         test database

 VA                       /-                       O
   DEFINED
19:45:52,986 INFO  USER_1595751238_7, number of lines read: 128
19:45:53,070 INFO  Parsing of USER_1595751238_7 completed in 84 ms
TDB_APP: def-sys fe o
 FE  DEFINED
TDB_APP: rej sp *
 /-                       VA                       FE
 O                        FE+2                     FE+3
 FE2O3                    FEO                      FEO3/2
 O-2                      O2  REJECTED
TDB_APP: res sp fe fe+2 fe+3 o o2 o-2 va
 FE                       FE+2                     FE+3
 O                        O2                       O-2
 VA  RESTORED
TDB_APP: rej ph * all
 SPINEL:I                 GAS:G                    BCC_A2
   REJECTED
TDB_APP: res ph bcc spinel gas
```

```
 BCC_A2                  SPINEL:I                GAS:G
   RESTORED
TDB_APP:
TDB_APP: get
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 *** ERROR  2018 IN DESHPH: DIFFUSION DATA NOT POSSIBLE FOR GAS PHASE
 *** ERROR  2018 IN DESHPH: DIFFUSION DATA NOT POSSIBLE FOR GAS PHASE
 FUNCTIONS ....
 -OK-
TDB_APP:
TDB_APP:
TDB_APP: @@
TDB_APP: @@ ENTER THE DICTRA MONITOR
TDB_APP: @@
TDB_APP: go d-m
 NO TIME STEP DEFINED
19:45:53,290 INFO  Preparing system for use: USER_1595751238_7
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
19:45:53,629 INFO  Preparing phase for use: BCC_A2
19:45:53,826 INFO  Preparing phase for use: BCC_A2
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
19:45:54,750 INFO  Preparing phase for use: SPINEL
19:45:55,230 INFO  Preparing phase for use: SPINEL
DIC>
DIC>
DIC> @@
DIC> @@ ENTER A BOUNDARY CONDITION "GAS" ON THE UPPER (RIGHT-MOST) INTERFACE
DIC> @@ OF THE OXIDE. THIS ALLOWS THE SYSTEM TO EXPAND AND THE OXIDE LAYER
DIC> @@ TO GROW EXTERNALY. FOR THIS EXAMPLE AN OXYGEN ACTIVITY IS SPECIFIED
DIC> @@ THAT IS LOW ENOUGH NOT TO FORM CORUNDUM (FE2O3). ALSO SPECIFY THAT
DIC> @@ THERE IS NO FLUX OF Fe ACROSS THIS INTERFACE, I.E. NO Fe IS
DIC> @@ ALLOWED TO ENTER OR LEAVE THE SYSTEM.
DIC> @@
DIC> set-cond boundary upper gas
TYPE OF CONDITION FOR COMPONENT FE /ZERO_FLUX/: zero-flux
TYPE OF CONDITION FOR COMPONENT O /ZERO_FLUX/: act
LOW TIME LIMIT /0/: 0 4.5e-4; * N
DIC>
DIC>
DIC> @@
DIC> @@ ENTER START VALUES FOR THE INITIAL INTERFACE VELOCITIES
DIC> @@
DIC> s-a-s-v -1e-5 1e-5 yes
 STARTING VALUES WILL BE TAKEN FROM PROFILES
DIC>
DIC>
DIC> @@
DIC> @@ SIMULATE FOR 24 HOURS
DIC> @@
DIC> s-s-time 86400,,,,
SMALLEST ACCEPTABLE TIMESTEP : /1E-07/:
```

```
DIC>
DIC> @@
DIC> @@ SPECIFY THAT POTENTIALS AND NOT ACTIVITIES ARE VARIED AT THE PHASE
DIC> @@ INTERFACE. ALSO USE A FULLY IMPLICIT SCHEME FOR TIME INTEGRATION.
DIC> @@
DIC> s-s-c 0 1 1 YES POT YES YES 1 2,,,,,,,,,
 RELEASING OLD STARTING VALUES
DIC>
DIC>
DIC> @@ ENABLE THE GRAIN BOUNDARY DIFFUSION CONTRIBUTION MODEL
DIC> GB
REGION NAME : /SP/: SP
PHASE NAME: /SPINEL/: SPINEL
Enable model for grainboundary contribution to diffusion /YES/: YES
Grainboundary thickness /5E-10/: 5e-10
Grainsize(T,P,TIME)= 10.0e-6;
Bulkdiffusion activation energy multiplier /.5/: 0.333333
Enable model for dislocation contribution to diffusion /YES/: NO
DIC>
DIC>
DIC>
DIC> @@
DIC> @@ SAVE THE SET UP TO A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exi3b.DIC Y
DIC>
DIC>
DIC>
DIC> set-inter
 --OK---
DIC>
```

**exi3b-run**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exi3b\run.DCM.test"
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
 0.87701       95
 Region: SP
 double geometric
 dense at outer boundaries, coarse at  0.50000E-10
lower part   1.2500        9
upper part  0.80000        9
  Trying old scheme                    3
 U-FRACTION IN SYSTEM:  FE = 0.99999999500542  O = 2.10000395011622E-08
 TOTAL SIZE OF SYSTEM:  .0049999901 [m]
 U-FRACTION IN SYSTEM:  FE = 0.99999999500542  O = 2.10000395011622E-08
 TOTAL SIZE OF SYSTEM:  .0049999901 [m]
 6.141064823797707E-002        6.141034147853782E-002        6.141038569194786E-002        8.444667162402950E-003        1.735854061037513E-
024       TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =  0.17358541E-23
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.16338022E-03 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49999900E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.29859771E-03 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.49999901E-02
 U-FRACTION IN SYSTEM:  FE = 0.99999999230859  O = 2.69779165557198E-08
 TOTAL SIZE OF SYSTEM:  .00499999011352 [m]
  9  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: FER

  CPU time used in timestep                    0 seconds
 8.109431941180634E-006        8.108744539988769E-006        8.108693416853126E-006        3.429194121551169E-007        9.371262898088711E-
031       TIME =  0.30000000E-06 DT =  0.20000000E-06 SUM OF SQUARES =  0.93712629E-30
 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   0.57006113E-03 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.49999902E-02
 U-FRACTION IN SYSTEM:  FE = 0.99999998461782  O = 4.97800757628426E-08
 TOTAL SIZE OF SYSTEM:  .00499999015258 [m]
  CPU time used in timestep                    1 seconds
 8.244220574618579E-006        8.245625310494682E-006        8.245834813729388E-006        5.265217528900878E-009        1.048766655848838E-
032       TIME =  0.70000000E-06 DT =  0.40000000E-06 SUM OF SQUARES =  0.10487667E-31
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.17607363E-03 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49999898E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.24106843E-03 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.49999902E-02
 U-FRACTION IN SYSTEM:  FE = 0.99999997890226  O = 6.90668894023925E-08
 TOTAL SIZE OF SYSTEM:  .00499999017858 [m]
  CPU time used in timestep                    1 seconds
 1.134917486802709E-007        1.135891987656391E-007        1.135503628192808E-007        5.608688598427207E-010        1.002409390432070E-
031       TIME =  0.15000000E-05 DT =  0.80000000E-06 SUM OF SQUARES =  0.10024094E-30
 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   0.20898652E-03 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.49999902E-02
 U-FRACTION IN SYSTEM:  FE = 0.99999996836327  O = 1.02507655166001E-07
 TOTAL SIZE OF SYSTEM:  .00499999023031 [m]
  8  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    1 seconds
 4.495117146315590E-007        4.496453310860320E-007        4.496431989768027E-007        2.514741997590077E-010        3.652354987552913E-
033       TIME =  0.31000000E-05 DT =  0.16000000E-05 SUM OF SQUARES =  0.36523550E-32
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.94208031E-04 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49999896E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.13424764E-03 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.49999903E-02
 U-FRACTION IN SYSTEM:  FE = 0.99999995509026  O = 1.4547197126829E-07
 TOTAL SIZE OF SYSTEM:  .00499999029437 [m]
  32  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    1 seconds
 1.153180115059997E-005        1.153636432478212E-005        1.153593600363959E-005        1.797715626630339E-008        6.738497856201747E-
032       TIME =  0.63000000E-05 DT =  0.32000000E-05 SUM OF SQUARES =  0.67384979E-31
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.67615624E-04 AND    0.0000000


output ignored...



... output resumed

 POSITION OF INTERFACE FER / SP IS   0.49333470E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.11009830E-08 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.50286092E-02
 U-FRACTION IN SYSTEM:  FE = .994180844230443  O = .0189442386383345
 TOTAL SIZE OF SYSTEM:  .00502860924783 [m]
  21  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    1 seconds
 5.273110613037545E-007        5.281039636597586E-007        5.280421006006052E-007        7.076325929812446E-010        2.294564972805105E-
034       TIME =   56943.895     DT =   8640.0000     SUM OF SQUARES =  0.22945650E-33
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.70247281E-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 = .993661317137569  O = .0206594864287854
 TOTAL SIZE OF SYSTEM:  .00503121911323 [m]
  9  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    1 seconds
 2.946692395761351E-007        2.952132480192080E-007        2.951644504133431E-007        3.823716784870093E-010        8.802101698957289E-
035       TIME =   65583.895     DT =   8640.0000     SUM OF SQUARES =  0.88021017E-34
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.64894659E-09 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49216707E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.92920430E-09 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.50336405E-02
 U-FRACTION IN SYSTEM:  FE = .993180429214222  O = .0222444821602594
 TOTAL SIZE OF SYSTEM:  .00503364053991 [m]
  8  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    1 seconds
 1.646050194307750E-007        1.649796223234198E-007        1.649485636756252E-007        1.988147189996472E-010        6.695615822283750E-
034       TIME =   74223.895     DT =   8640.0000     SUM OF SQUARES =  0.66956158E-33
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.60654804E-09 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49164301E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.86919594E-09 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.50359098E-02
 U-FRACTION IN SYSTEM:  FE = .992730593250164  O = .0237257185885361
 TOTAL SIZE OF SYSTEM:  .00503590981773 [m]
  11  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    0 seconds
 1.056447174728819E-007        1.059234014799306E-007        1.059040983328184E-007        1.220607100044091E-010        6.837803618959214E-
033       TIME =   82863.895     DT =   8640.0000     SUM OF SQUARES =  0.68378036E-32
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.57100501E-09 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49114966E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.81838267E-09 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.50380472E-02
 U-FRACTION IN SYSTEM:  FE = .992307543457158  O = .0251191385412454
 TOTAL SIZE OF SYSTEM:  .00503804716073 [m]
  7  GRIDPOINT(S) REMOVED FROM CELL #1   REGION: SP

  CPU time used in timestep                    1 seconds
 1.518630594855703E-008        1.512784240291555E-008        1.530720135745792E-008        1.085163171698853E-011        1.925929944387236E-
034       TIME =   86400.000     DT =   3536.1047     SUM OF SQUARES =  0.19259299E-33
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.56483672E-09 AND    0.0000000
 POSITION OF INTERFACE FER / SP IS   0.49094993E-02
 CELL # 1 VELOCITY AT INTERFACE # 3 IS   0.78548545E-09 AND    0.0000000
 POSITION OF INTERFACE SP / gas interface IS   0.50388274E-02
 U-FRACTION IN SYSTEM:  FE = .992153350504448  O = .0256664800740252
 TOTAL SIZE OF SYSTEM:  .00503882739771 [m]
 MUST SAVE WORKSPACE ON FILE
 WORKSPACE SAVED ON FILE
 RECLAIMING WORKSPACE
 DELETING TIME-RECORD FOR TIME    0.0000000
 DELETING TIME-RECORD FOR TIME   0.10000000E-06
 DELETING TIME-RECORD FOR TIME   0.30000000E-06
 DELETING TIME-RECORD FOR TIME   0.70000000E-06
 DELETING TIME-RECORD FOR TIME   0.15000000E-05
 DELETING TIME-RECORD FOR TIME   0.31000000E-05
 DELETING TIME-RECORD FOR TIME   0.63000000E-05
 DELETING TIME-RECORD FOR TIME   0.12700000E-04
 DELETING TIME-RECORD FOR TIME   0.25500000E-04
 DELETING TIME-RECORD FOR TIME   0.51100000E-04
 DELETING TIME-RECORD FOR TIME   0.10230000E-03
 DELETING TIME-RECORD FOR TIME   0.20470000E-03
 DELETING TIME-RECORD FOR TIME   0.40950000E-03
 DELETING TIME-RECORD FOR TIME   0.81910000E-03
 DELETING TIME-RECORD FOR TIME   0.16383000E-02
 DELETING TIME-RECORD FOR TIME   0.32767000E-02
 DELETING TIME-RECORD FOR TIME   0.65535000E-02
 DELETING TIME-RECORD FOR TIME   0.13107100E-01
 DELETING TIME-RECORD FOR TIME   0.26214300E-01
 DELETING TIME-RECORD FOR TIME   0.52428700E-01
 DELETING TIME-RECORD FOR TIME   0.10485750
 DELETING TIME-RECORD FOR TIME   0.20971510
 DELETING TIME-RECORD FOR TIME   0.41943030
 DELETING TIME-RECORD FOR TIME   0.83886070
 DELETING TIME-RECORD FOR TIME    1.6777215
 DELETING TIME-RECORD FOR TIME    3.3554431
 DELETING TIME-RECORD FOR TIME    6.7108863
 DELETING TIME-RECORD FOR TIME    13.421773
 DELETING TIME-RECORD FOR TIME    26.843545
 DELETING TIME-RECORD FOR TIME    53.687091
 DELETING TIME-RECORD FOR TIME    107.37418
 DELETING TIME-RECORD FOR TIME    214.74836
 DELETING TIME-RECORD FOR TIME    429.49673
 DELETING TIME-RECORD FOR TIME    858.99346
 DELETING TIME-RECORD FOR TIME    1717.9869
 DELETING TIME-RECORD FOR TIME    3435.9738
 DELETING TIME-RECORD FOR TIME    6871.9477
 DELETING TIME-RECORD FOR TIME    13743.895
 DELETING TIME-RECORD FOR TIME    22383.895
 DELETING TIME-RECORD FOR TIME    31023.895
 DELETING TIME-RECORD FOR TIME    39663.895
 DELETING TIME-RECORD FOR TIME    48303.895
 DELETING TIME-RECORD FOR TIME    56943.895
 DELETING TIME-RECORD FOR TIME    65583.895
 DELETING TIME-RECORD FOR TIME    74223.895

 KEEPING TIME-RECORD FOR TIME    82863.895
 AND FOR TIME                    86400.000
 WORKSPACE RECLAIMED

 TIMESTEP AT     86400.0000     SELECTED

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

**exi3b-plot**

```
DIC>About
 NO SUCH COMMAND, USE HELP
DIC>DIC>MACRO "c:\jenkins\workspace\dictra_generate_console_examples\examples\exi3b\plot.DCM.test"
DIC>
DIC> @@ exi3_plot.DCM
DIC>
DIC> @@
DIC> @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE i3
DIC> @@
DIC>
DIC> @@
DIC> @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
DIC> @@
DIC> go d-m
 TIME STEP AT TIME  8.64000E+04
DIC> read exi3b
 OK
DIC>
DIC> @@
DIC> @@ ENTER THE POST PROCESSOR
DIC> @@
DIC> post
  POST PROCESSOR VERSION   1.7
  Implemented by Bjorn Jonsson
POST-1:
POST-1: @@
POST-1: @@ PLOT THE THICKNESS OF THE OXIDE LAYER GROWING AT THE SURFACE.
POST-1: @@ FOR THIS WE NEED TO ENTER A FUNCTION ACCORDING TO THE FOLLOWING.
POST-1: ent func oxideth
FUNCTION: poi(sp,upper)-poi(sp,lower)
&
POST-1: @@
POST-1: @@ PUT THIS FUNCTION ON THE Y-AXIS
POST-1: @@
POST-1: s-d-a y oxideth
POST-1:
POST-1: @@
POST-1: @@ AND PLOT THE OXIDE THICKNESS VERSUS TIME
POST-1: @@
POST-1: s-d-a x time
  INFO: Time is set as independent variable
POST-1:
POST-1: @@
POST-1: @@ SINCE WE ARE PLOTTING A FUNCTION, SPECIFY A PLOT CONDITION
POST-1: @@
POST-1: s-p-c interface sp upper
POST-1:
POST-1: app y exi3a.exp 0; 1;
POST-1:
POST-1:
POST-1: SET_EXP_FILE_FORMAT 4
POST-1: MAKE c:/jenkins/workspace/dictra_generate_console_examples/unite/distribution\macroResult.exp Y
          OST-1: SET_EXP_FILE_FORMAT 10
POST-1:
POST-1: plot
```

2019.11.11.19.48.24
UPPER INTERFACE OF REGION "SP#1"
CELL #1

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

This page was generated 2019-11-11 19:49