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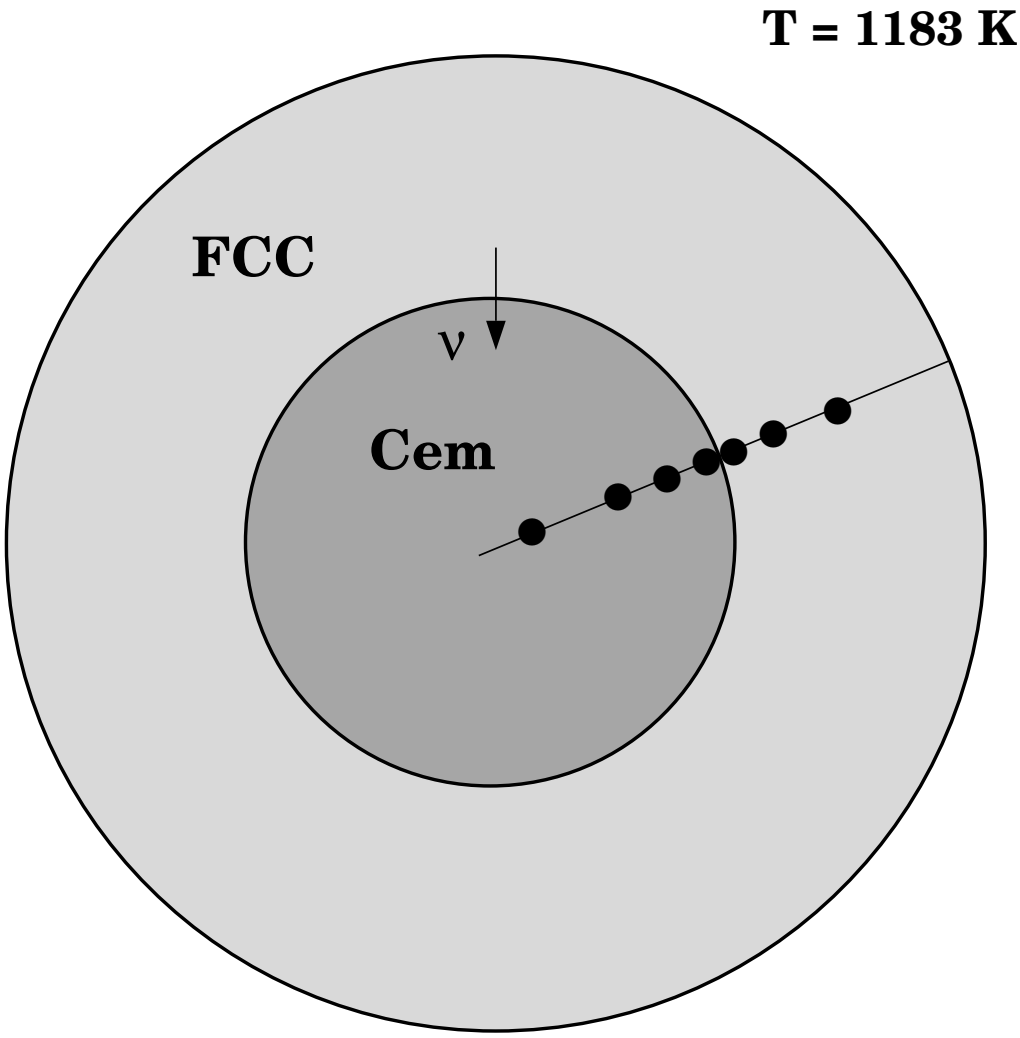
Example b2

Cementite dissolution in an Fe-Cr-C alloy



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```
 D I C T R A service version  25(Build 1315) on Linux
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 Stockholm, Sweden
 Double precision version linked at 21-08-08 10:22:06
 Only for use at MSE
 Local contact Malin Selleby
SYS:ioctl failed: it's not a terminal
SYS:SYS:SYS:
SYS:
SYS: @@
SYS: @@ In order to achieve the correct average composition in the calculation
SYS: @@ it is necessary to take into account the fact that the calculation in
SYS: @@ DICTRA is setup using the volume fraction of the phases. To calculate
SYS: @@ the initiale state at the heattreatment temperature we need first to
SYS: @@ determine the state at the normalizing temperature. To calculate the
SYS: @@ volume 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 system, whereas the interstitial components
SYS: @@ don't.
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 DATABASE
SYS: @@
SYS: go da
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Public Ternary Alloys TDB v1

 VA  DEFINED
TDB_PTERN:
TDB_PTERN: @@
TDB_PTERN: @@ USE SSOL DATABASE FOR THERMODYNAMIC DATA
TDB_PTERN: @@
TDB_PTERN: sw ptern
TDB_PTERN: def-sys fe cr c
 FE                  CR                  C
   DEFINED
TDB_PTERN: rej ph * all
 LIQUID:L            BCC_A2              FCC_A1
 HCP_A3              SIGMA               CEMENTITE
 M3C2                M7C3                M23C6
 V3C2                GRAPHITE  REJECTED
TDB_PTERN: res ph fcc bcc cem
 FCC_A1              BCC_A2              CEMENTITE
   RESTORED
TDB_PTERN: get
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

 -OK-
TDB_PTERN:
TDB_PTERN: @@
TDB_PTERN: @@ ENTER THE POLY-3 MONITOR
TDB_PTERN: @@
```

```
TDB_PTERN: go p-3

 POLY version  3.32,  Dec 2007
POLY_3:
POLY_3: @@
POLY_3: @@  SET THE CONDITIONS AT THE NORMALIZING TEMPERATURE
POLY_3: @@
POLY_3: set-cond T=1008,P=101325,N=1
POLY_3: set-cond X(CR)=0.0206,X(C)=0.0391
POLY_3:
POLY_3:
POLY_3: @@
POLY_3: @@  ENTER FUNCTIONS IN ORDER TO DETERMINE THE VOLUME-FRACTIONS
POLY_3: @@
POLY_3:
POLY_3: @@ Radius of the cementite particle
POLY_3: ent-symb var rcem=0.5255e-6;
POLY_3:
POLY_3: @@ total number of moles of substitutional components
POLY_3: ent-symb func nstot=n(fe)+n(cr);
POLY_3:
POLY_3: @@ number of moles of substitutional components in cementite
POLY_3: ent-symb func nscem=n(cem,fe)+n(cem,cr);
POLY_3:
POLY_3: @@ volume fraction (U-fraction) of cementite
POLY_3: ent-symb func vfcem=nscem/nstot;
POLY_3:
POLY_3: @@ total radius of the system
POLY_3: ent-symb func rtot=rcem/vfcem**(1/3);
POLY_3:
POLY_3: @@ radius of the surrounding austenite matrix
POLY_3: ent-symb func rmat=rtot-rcem;
POLY_3:
POLY_3:
POLY_3: @@
POLY_3: @@  COMPUTE THE EQUILIBRIUM
POLY_3: @@
POLY_3: compute-eq
 Global equilibrium calculation turned off, you can turn it on with
 ADVANCED_OPTIONS GLOBAL_MINIMIZATION Y,,,,,,,,
    36 ITS,  CPU TIME USED   0 SECONDS
POLY_3:
POLY_3:
POLY_3: @@
POLY_3: @@  SHOW THE COMPUTED VALUES THAT ARE TO BE USED IN THE DICTRA CALCULATION
POLY_3: @@
POLY_3: show rmat
 RMAT=5.3926054E-7
POLY_3: show w(cem,cr),w(bcc,cr),w(bcc,c)
 W(CEMENTITE,CR)=0.12423326
 W(BCC_A2,CR)=4.6615447E-3
 W(BCC_A2,C)=1.5135207E-4
POLY_3:
POLY_3:
POLY_3:
POLY_3:
POLY_3: set-inter
POLY_3:POLY_3: CPU time  1 seconds
```

```
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SYS:ioctl failed: it's not a terminal
SYS:SYS:SYS:
SYS:
SYS: @@ exb2_setup.DCM
SYS:
SYS: @@--------------------------------------------------------------------
SYS: @@ SETUP FILE FOR CALCULATING THE DISSOLUTION OF A SPHERICAL CEMENTITE
SYS: @@ PARTICLE IN AN AUSTENITE MATRIX.
SYS: @@
SYS: @@ THIS CASE IS FROM Z.-K. LIU, L. HÖGLUND, B. JÖNSSON AND J. ÅGREN:
SYS: @@ METALL. TRANS. A 22A(1991)1745-1752
SYS: @@--------------------------------------------------------------------
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM DATABASE
SYS: @@
SYS: go da
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Public Ternary Alloys TDB v1

 VA  DEFINED
TDB_PTERN:
TDB_PTERN: @@
TDB_PTERN: @@ USE A PUBLIC DATABASE FOR THERMODYNAMIC DATA
TDB_PTERN: @@
TDB_PTERN: switch ptern
TDB_PTERN: def-species fe cr c
 FE                  CR                  C
   DEFINED
TDB_PTERN: rej ph * all
 LIQUID:L            BCC_A2              FCC_A1
 HCP_A3              SIGMA               CEMENTITE
 M3C2                M7C3                M23C6
 V3C2                GRAPHITE  REJECTED
TDB_PTERN: res ph fcc cementite
 FCC_A1              CEMENTITE  RESTORED
TDB_PTERN: get
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

 -OK-
TDB_PTERN:
TDB_PTERN: @@
TDB_PTERN: @@ SWITCH TO MOBILITY DATABASE TO RETRIEVE MOBILITY DATA
TDB_PTERN: @@
TDB_PTERN: app mob2
 Current database: TCS Alloys Mobility Database v2

 VA  DEFINED
 GAS:G  REJECTED
APP: def-sp fe cr c
 FE                  CR                  C
   DEFINED
APP: rej ph * all
 BCC_A2              CEMENTITE           DIAMOND_A4
 FCC_A1              FE4N                GRAPHITE
 HCP_A3              KSI_CARBIDE         LIQUID:L
 M23C6               M3C2                M5C2
 M7C3                SIGMA  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 diffusion in fcc C-Fe'
   'B. Jönsson: Z. Metallkunde 85(1994)502-509;
      C diffusion in fcc Cr-Fe-Ni'
   'B. Jönsson: Scand. J. Metall. 24(1995)21-27;
      Cr and Fe diffusion fcc Cr-Fe'
   'B. Jönsson: Scand. J. Metall. 23(1994)201-208;
      Fe and Ni diffusion fcc Fe-Ni'
   'BJORN: KOLLA UPP DENNA'
 -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 1183; * n

DIC>
DIC> @@
DIC> @@ ENTER 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 WE TAKE OUR VALUE 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/: 0.525500e-6
TYPE /LINEAR/: geo
NUMBER OF POINTS /50/: 16
VALUE OF R IN THE GEOMETRICAL SERIE : 0.80
DIC>
DIC> @@
DIC> @@ THE SIZE OF THE FCC REGION WE MAY CALCULATE FROM A MASSBALANCE
DIC> @@ AFTER ESTIMATING THE INITIAL COMPOSITIONS IN THE TWO PHASES.
DIC> @@
DIC> enter-grid
REGION NAME : /AUS/: aus
WIDTH OF REGION /1/: 5.3926054E-7
TYPE /LINEAR/: geo
NUMBER OF POINTS /50/: 16
VALUE OF R IN THE GEOMETRICAL SERIE : 1.25
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 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 0.12423326 0.12423326
DIC>
DIC> enter-composition
REGION NAME : /AUS/: aus
PHASE NAME: /FCC_A1/: fcc#1
DEPENDENT COMPONENT ? /FE/: fe
COMPOSITION TYPE /MOLE_FRACTION/: weig-fraction
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> @@ SET SPHERICAL GEOMETRY
DIC> @@
DIC> enter-geo
GEOMETRICAL EXPONENT /0/: 2
DIC>
DIC> @@
DIC> @@ SET THE SIMULATION TIME AND VARIOUS 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 SETUP ON A NEW STORE FILE AND EXIT
DIC> @@
DIC> save exb2 Y
DIC>
DIC> set-inter
 --OK---
DIC>DIC> CPU time  1 seconds
```

```
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SYS:ioctl failed: it's not a terminal
SYS:SYS:SYS:
SYS:
SYS: @@ exb2_run.DCM
SYS:
SYS: @@
SYS: @@ READ THE SETUP FROM FILE AND START THE SIMULATION
SYS: @@
SYS:
SYS: go d-m
 NO TIME STEP DEFINED
DIC> read exb2
 OK
DIC> sim
 Automatic start values will be set
 Old start values kept
 Automatic start values will be set
 Old start values kept
 Automatic start values will be set
  Trying old scheme
 GENERATING STARTING VALUES FOR CELL #  1 INTERFACE #  2
 DETERMINING INITIAL EQUILIBRIUM VALUES
 CALCULATING STARTING VALUES:       9   EQUILIBRIUM CALCULATIONS

 Automatic start values will be set
 Old start values kept
 Automatic start values will be set
 Old start values kept
 Automatic start values will be set
 U-FRACTION IN SYSTEM:  C = .0406910186963101  CR = .0214382352146941
                        FE = .978561764915813
 TOTAL SIZE OF SYSTEM:  5.05643527908E-18 [m^3]
 U-FRACTION IN SYSTEM:  C = .0406910186963101  CR = .0214382352146941
                        FE = .978561764915813
 TOTAL SIZE OF SYSTEM:  5.05643527908E-18 [m^3]
  10  GRIDPOINT(S) ADDED   TO   CELL #1   REGION: CARB
  11  GRIDPOINT(S) ADDED   TO   CELL #1   REGION: AUS
  0.00000000000605
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.31659972E-02 AND  -0.31659972E-02
 POSITION OF INTERFACE CARB / AUS IS   0.52518340E-06
 U-FRACTION IN SYSTEM:  C = .04071882402492  CR = .0214514771061759
                        FE = .978548523024331
 TOTAL SIZE OF SYSTEM:  5.05643527908E-18 [m^3]

  CPU time used in timestep 1 seconds
  2  GRIDPOINT(S) ADDED   TO   CELL #1   REGION: CARB
  1  GRIDPOINT(S) ADDED   TO   CELL #1   REGION: AUS
 TIME 0.20000000E-06 DT =  0.20000000E-06 SUM O
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.27683211E-03 AND  -0.27683211E-03
 POSITION OF INTERFACE CARB / AUS IS   0.52512803E-06
 U-FRACTION IN SYSTEM:  C = .0407211192851271  CR = .0214537406440264
                        FE = .978546259486481
 TOTAL SIZE OF SYSTEM:  5.05643527908E-18 [m^3]

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

  CPU time used in timestep 1 seconds
 TIME 0.60000000E-06 DT =  0.40000000E-06 SUM OF SQUARES =  0.46040234E-20
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.27425480E-03 AND  -0.27425480E-03
 POSITION OF INTERFACE CARB / AUS IS   0.52501833E-06
 U-FRACTION IN SYSTEM:  C = .0407210647298552  CR = .0214581766431546
                        FE = .978541823487352
   :
   :
   :
```

```
  :
 U-FRACTION IN SYSTEM:  C = .040744164178951  CR = .0221316205040515
                        FE = .977868379626456
 TOTAL SIZE OF SYSTEM:  5.05643527908E-18 [m^3]

  CPU time used in timestep 4 seconds
  4.99999999E-10
 CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.11041684E-10 AND  -0.11041684E-10
 POSITION OF INTERFACE CARB / AUS IS   0.21535661E-06
 U-FRACTION IN SYSTEM:  C = .040744153648996  CR = .0221275147313298
                        FE = .977872485399177
 TOTAL SIZE OF SYSTEM:  5.05643527908E-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   0.10230000E-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   0.31944081E-02
 DELETING TIME-RECORD FOR TIME   0.59334799E-02
 DELETING TIME-RECORD FOR TIME   0.10445012E-01
 DELETING TIME-RECORD FOR TIME   0.17559866E-01
 DELETING TIME-RECORD FOR TIME   0.28864666E-01
 DELETING TIME-RECORD FOR TIME   0.48001751E-01
 DELETING TIME-RECORD FOR TIME   0.85070793E-01
 DELETING TIME-RECORD FOR TIME   0.15920888
 DELETING TIME-RECORD FOR TIME   0.30748505
 DELETING TIME-RECORD FOR TIME   0.59608739
 DELETING TIME-RECORD FOR TIME    1.1732921
 DELETING TIME-RECORD FOR TIME    1.2887330
 DELETING TIME-RECORD FOR TIME    1.5196149
 DELETING TIME-RECORD FOR TIME    1.9813787
 DELETING TIME-RECORD FOR TIME    2.9049062
 DELETING TIME-RECORD FOR TIME    4.7519612
 DELETING TIME-RECORD FOR TIME    8.4460713
 DELETING TIME-RECORD FOR TIME    15.834291
 DELETING TIME-RECORD FOR TIME    30.610732
 DELETING TIME-RECORD FOR TIME    60.163612
 DELETING TIME-RECORD FOR TIME    119.26937
 DELETING TIME-RECORD FOR TIME    237.48090
 DELETING TIME-RECORD FOR TIME    473.90394
 DELETING TIME-RECORD FOR TIME    946.75003
 DELETING TIME-RECORD FOR TIME    1892.4422
 DELETING TIME-RECORD FOR TIME    2892.4422
 DELETING TIME-RECORD FOR TIME    3892.4422
 DELETING TIME-RECORD FOR TIME    4892.4422
 DELETING TIME-RECORD FOR TIME    5892.4422
 DELETING TIME-RECORD FOR TIME    6892.4422
 DELETING TIME-RECORD FOR TIME    7892.4422
 DELETING TIME-RECORD FOR TIME    8892.4422

 KEEPING TIME-RECORD FOR TIME    9892.4422
 AND FOR TIME                    10000.000
 WORKSPACE RECLAIMED
DIC>
DIC> set-inter
 --OK---
DIC>DIC> CPU time  307 seconds
```

```
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SYS:ioctl failed: it's not a terminal
SYS:SYS:SYS:



SYS:SYS:
SYS:
SYS: @@ exb2_plot.DCM
SYS:
SYS: @@
SYS: @@ FILE FOR GENERATING GRAPHICAL OUTPUT FOR EXAMPLE b2
SYS: @@
SYS:
SYS: @@
SYS: @@ GO TO THE DICTRA MONITOR AND READ THE STORE RESULT FILE
SYS: @@
SYS: go d-m
 NO TIME STEP DEFINED
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 DISTANCE AS X-AXIS (NOTE THAT DISTANCE IS SET AS
POST-1: @@ INDEPENDENT VARIABLE AUTOMATICALLY) AND U-FRACTION CARBON AS Y-AXIS
POST-1: @@ REMEMBER THAT ONE ALSO HAS TO SET PLOT CONDITION
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 ONE HAS TO GIVE AN OFFSET 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 TITLE ON DIAGRAM
POST-1: @@
POST-1: set-title Figure b2.1
POST-1:
POST-1: plo SCREEN

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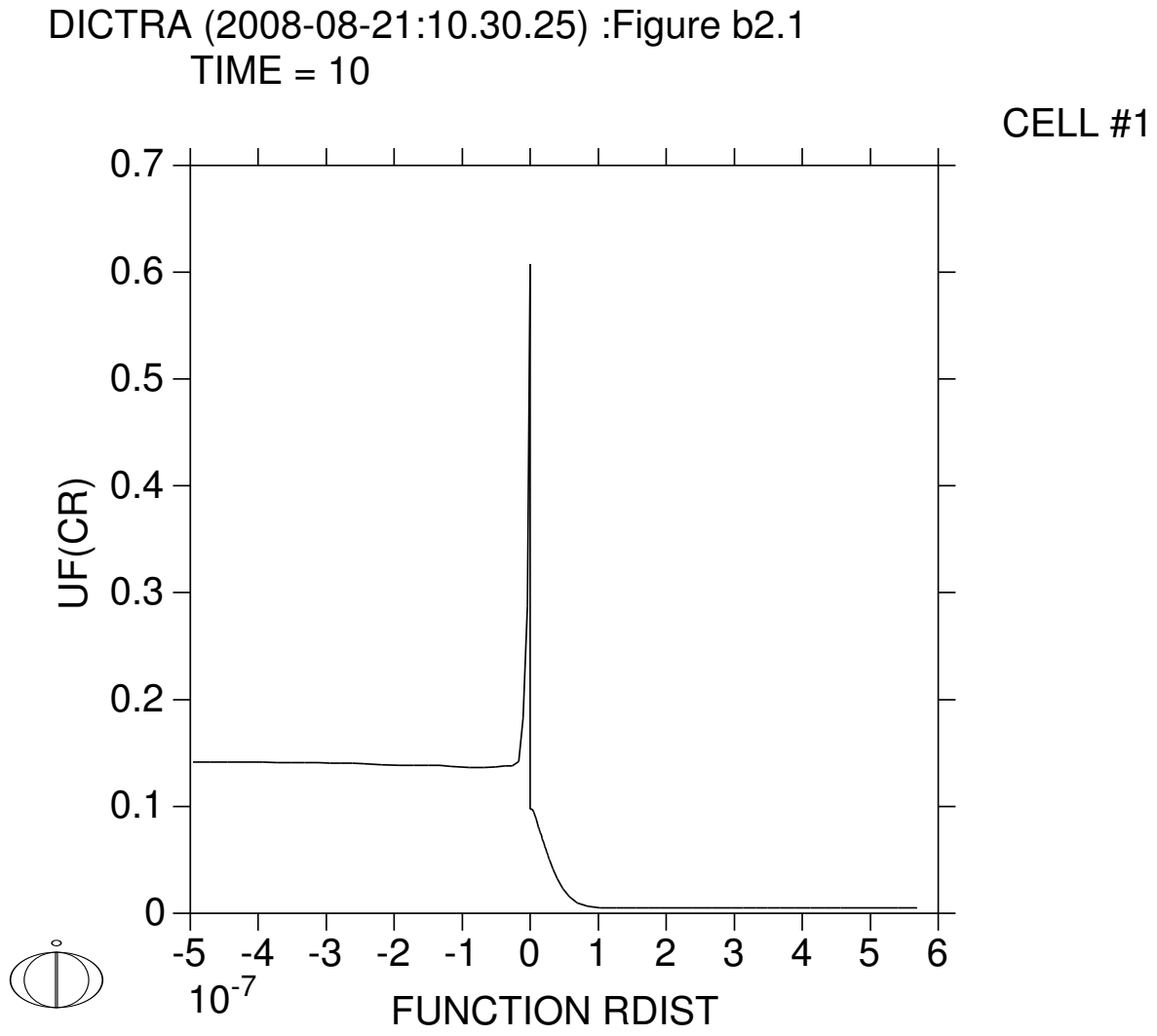

```
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: @@
POST-1: @@ INCLUDE EXPERIMENTAL DATAPOINTS ON THE FIGURE FOR COMPARISION
POST-1: @@
POST-1: @@ FIRST LIST DATASETS
POST-1: @@
POST-1: app y exb2.exp
PROLOGUE NUMBER: /0/:  0
DATASET NUMBER(s): /-1/:  -1
 DATASET 1 CONCENTRATION PROFILE T=10S
 DATASET 2 CONCENTRATION PROFILE T=100S
 DATASET 3 CONCENTRATION PROFILE T=1000S
 DATASET 4 CONCENTRATION PROFILE T=10000S
 DATASET 5 VOLUME FRACTION CEMENTITE VS. TIME
 DATASET 6 MEAN PARTICLE DIAMETER VS. TIME
POST-1:
POST-1: @@
POST-1: @@ SELECT THE PROPER DATASET
POST-1: @@
POST-1: app y exb2.exp
PROLOGUE NUMBER: /0/:  0
DATASET NUMBER(s): /-1/:  1
POST-1:
POST-1: set-title Figure b2.2
POST-1: plo SCREEN
POST-1:
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: @@
POST-1: @@ PLOT ALSO FOR 100, 1000 AND 10000S
POST-1: @@
POST-1:
POST-1: s-p-c time 100
POST-1:
POST-1: app y exb2.exp
PROLOGUE NUMBER: /0/:  0
DATASET NUMBER(s): /-1/:  2
POST-1:
POST-1: set-title Figure b2.3
POST-1: plo SCREEN

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

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

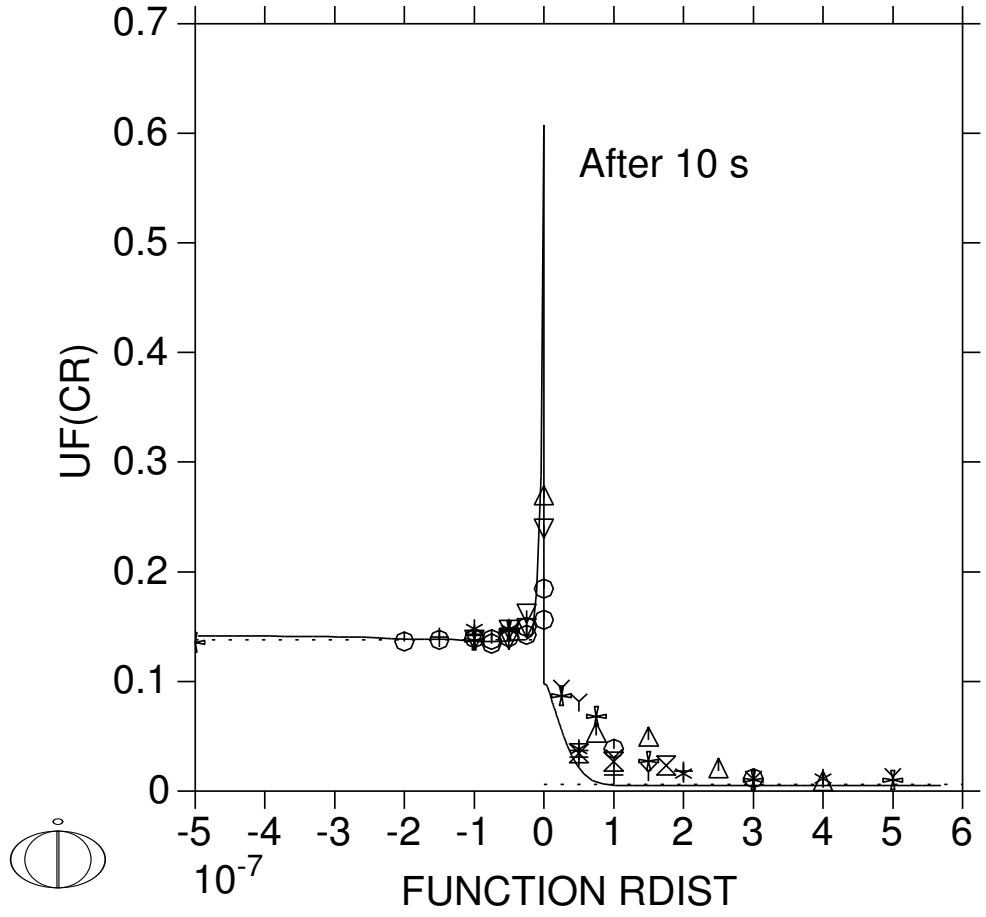
```
POST-1: set-title Figure b2.5
POST-1: plo SCREEN

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

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

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



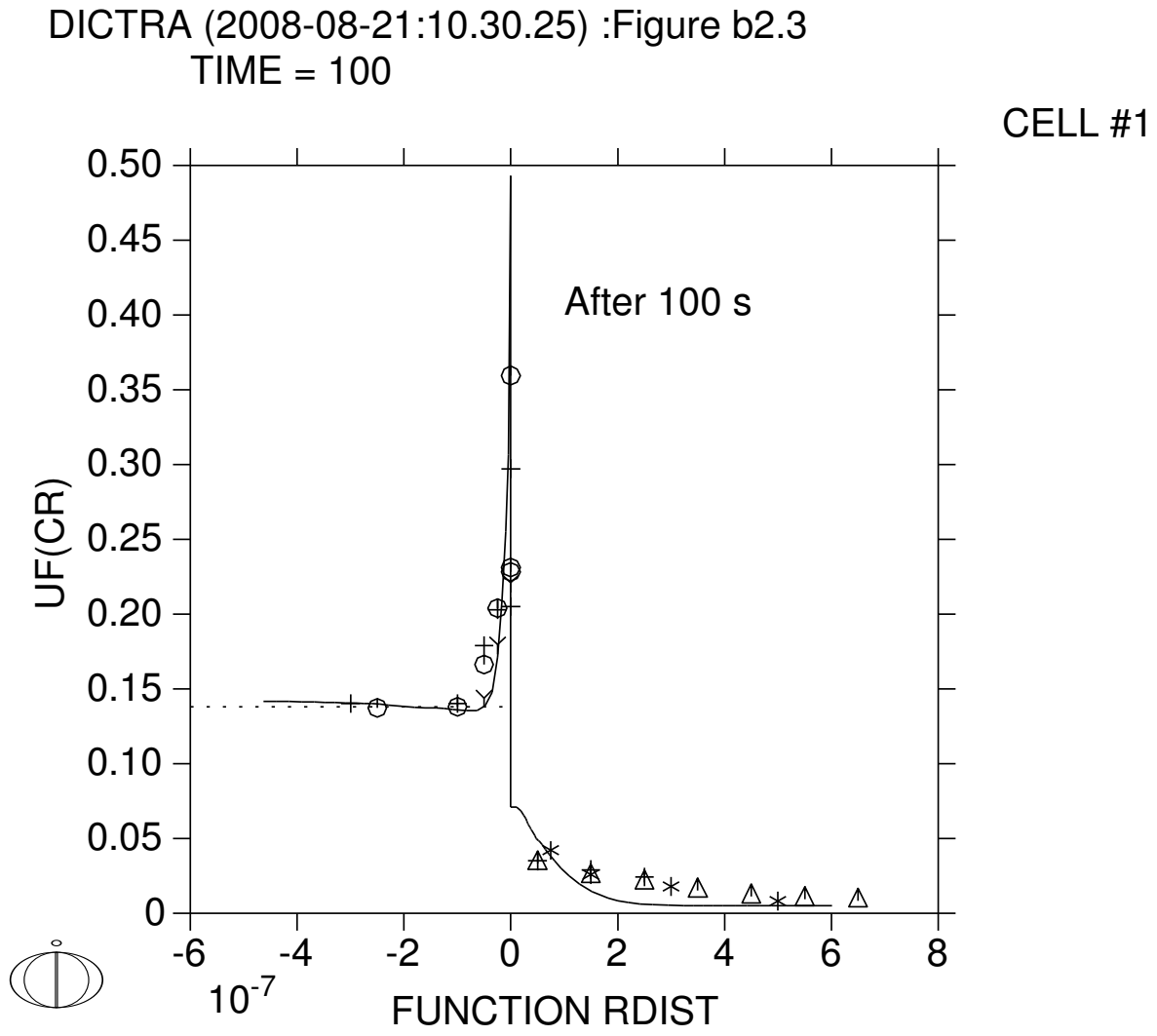
output by user lars on 2008.08.21:10.30

DICTRA (2008-08-21:10.30.25) :Figure b2.2
TIME = 10

CELL #1



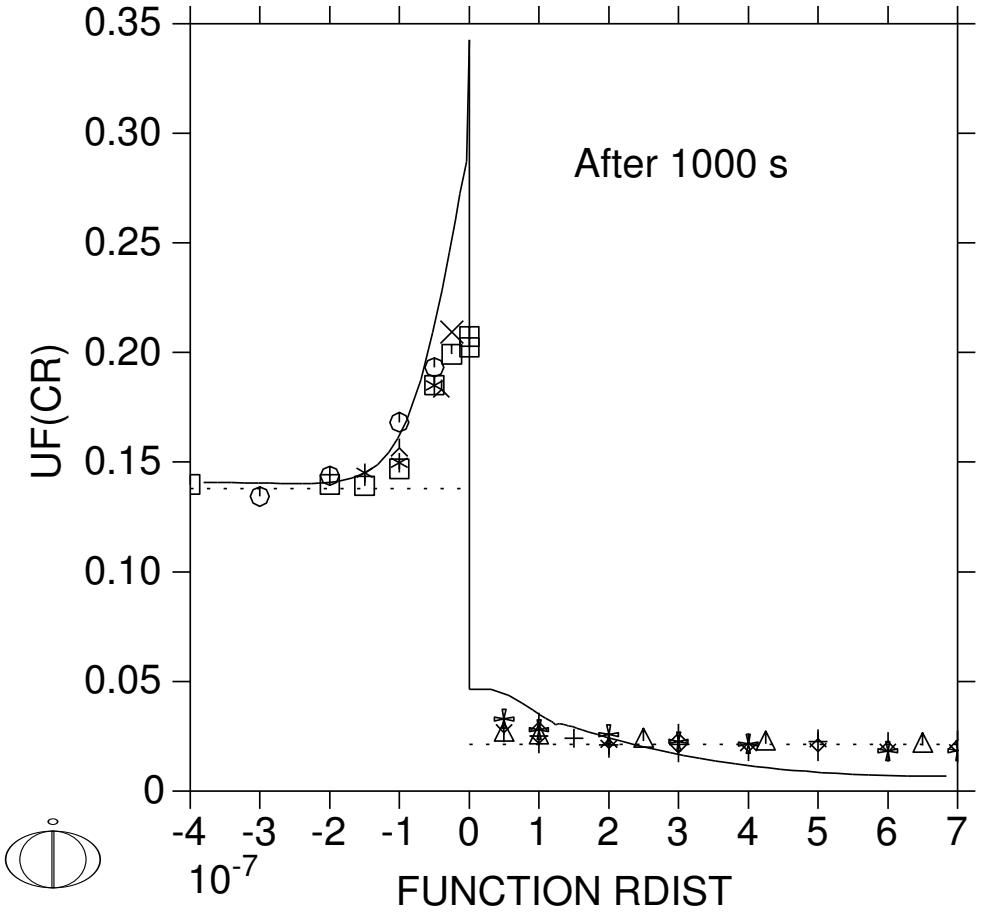
output by user lars on 2008.08.21:10.30



output by user lars on 2008.08.21:10.30

DICTRA (2008-08-21:10.30.25) :Figure b2.4
TIME = 1000

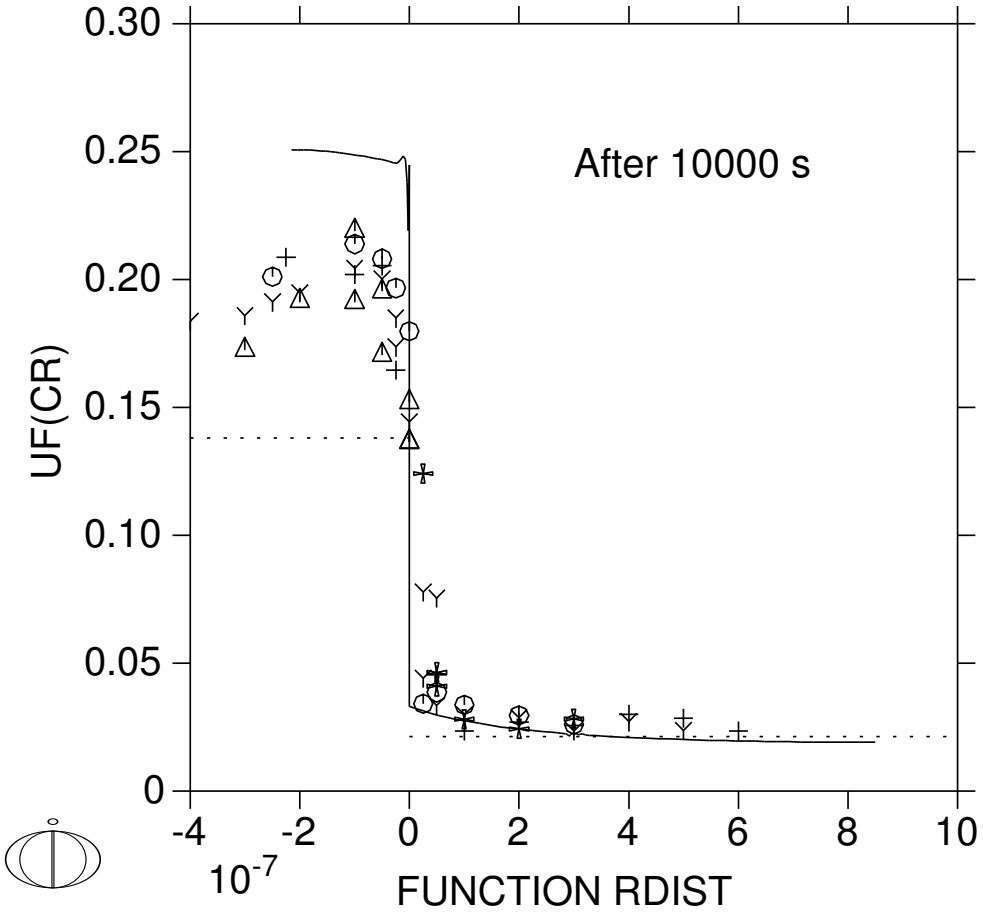
CELL #1



output by user lars on 2008.08.21:10.30

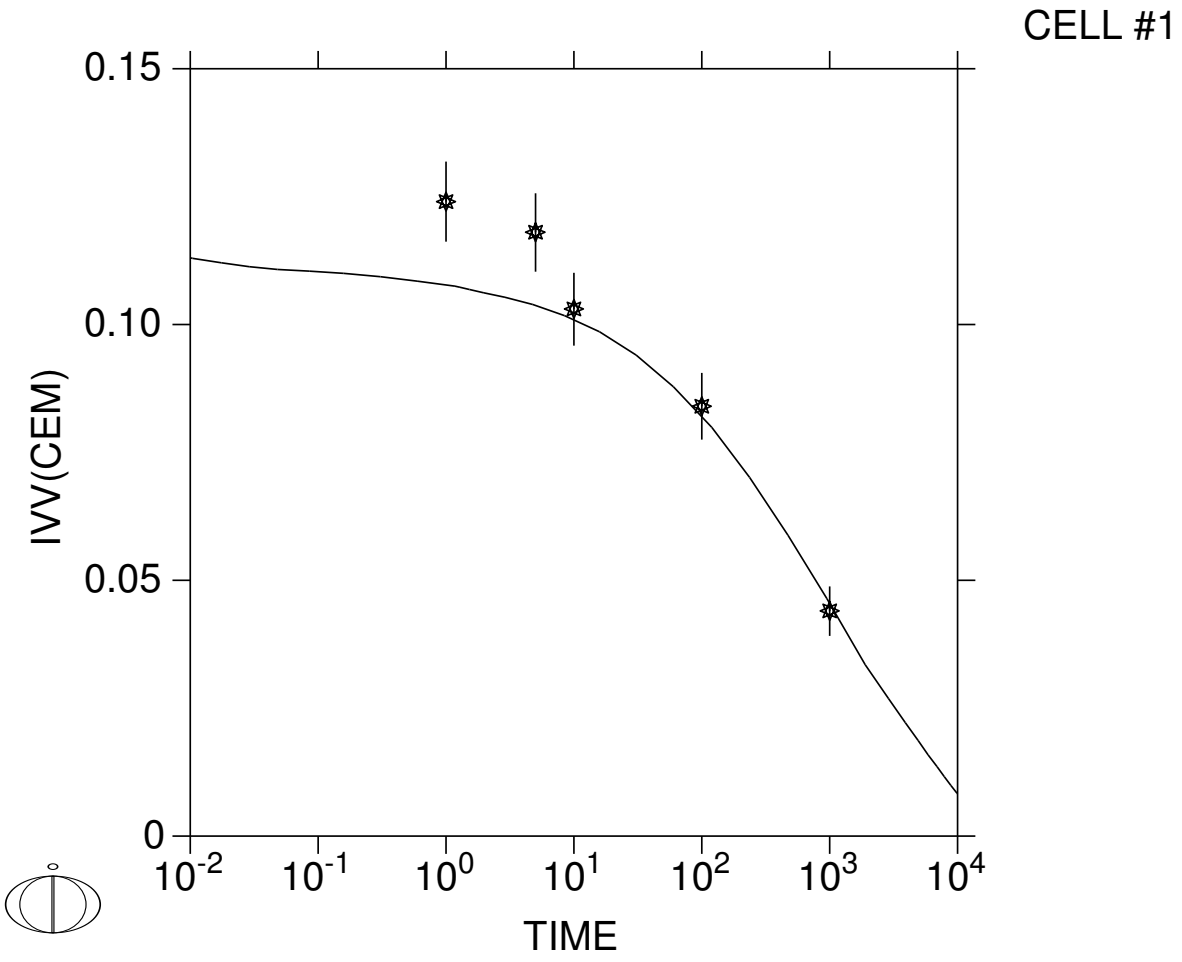
DICTRA (2008-08-21:10.30.26) :Figure b2.5
TIME = 10000

CELL #1



output by user lars on 2008.08.21:10.30

DICTRA (2008-08-21:10.30.26) :Figure b2.6

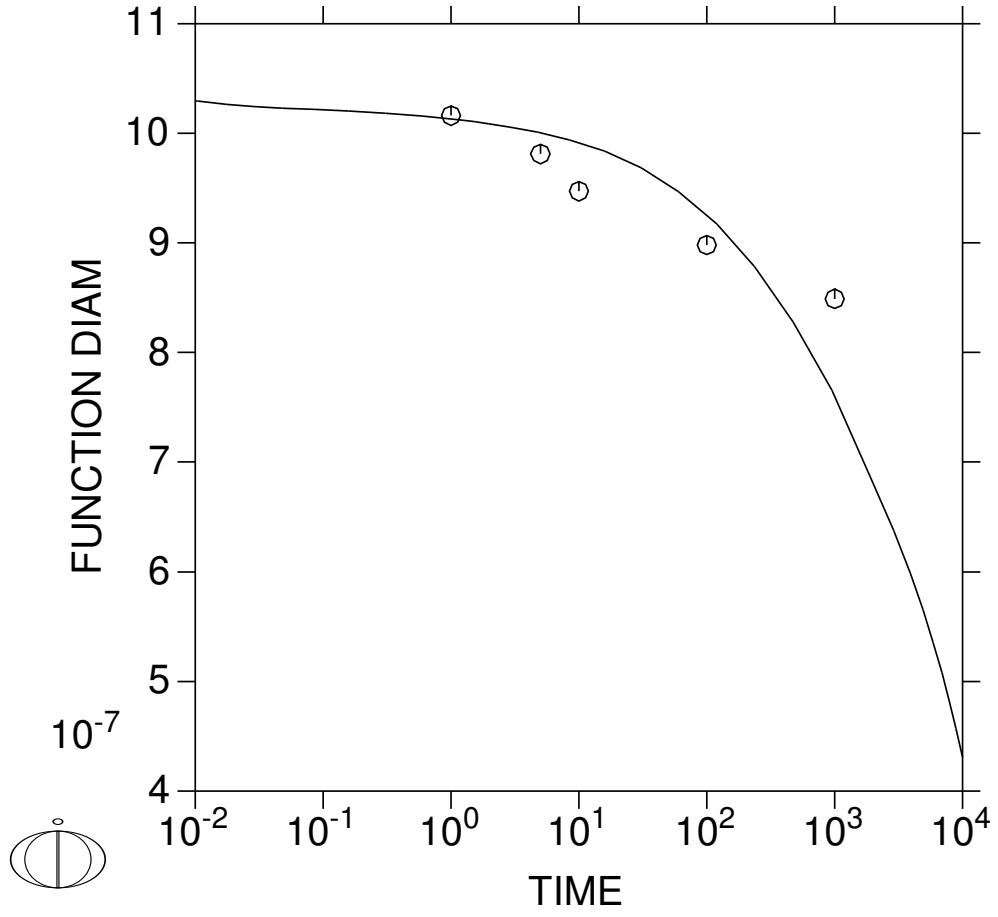


output by user lars on 2008.08.21:10.30

DICTRA (2008-08-21:10.30.26) :Figure b2.7

UPPER INTERFACE OF REGION "CARB#1"

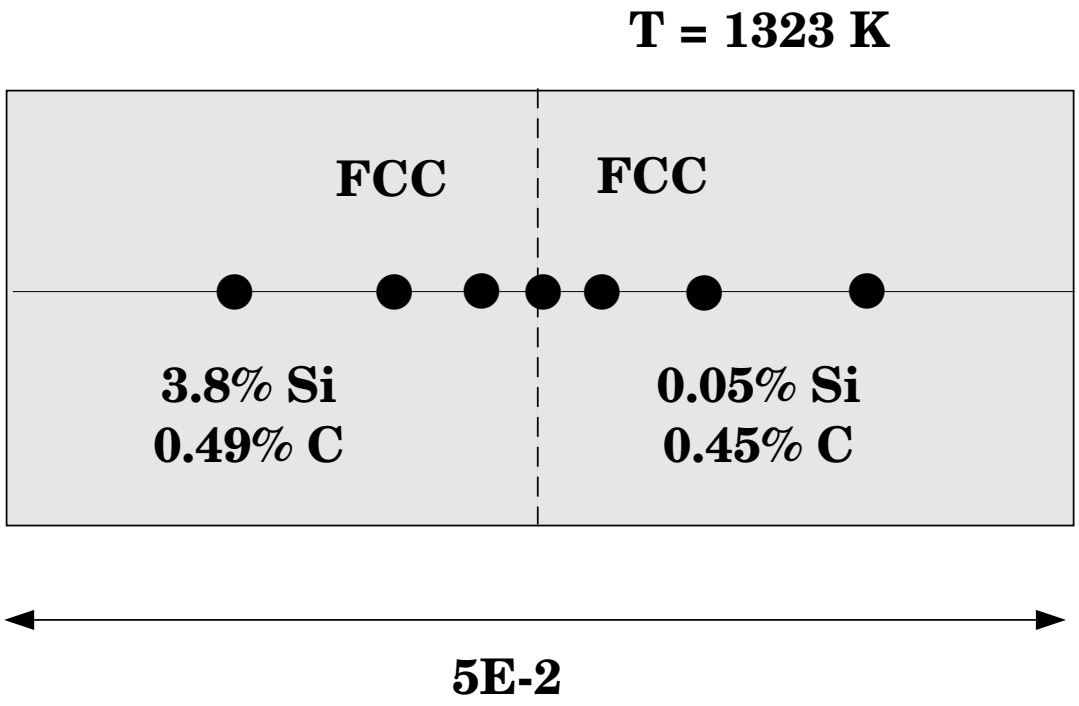
CELL #1



output by user lars on 2008.08.21:10.30

Example a3

Uphill diffusion in an Fe-Si-C alloy



```
 D I C T R A service version  25(Build 1315) on Linux
 Copyright (1993,1995,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 21-08-08 10:22:06
 Only for use at MSE
 Local contact Malin Selleby
SYS:ioctl failed: it's not a terminal
SYS:SYS:SYS:
SYS:
SYS: @@ darken_setup.DCM
SYS:
SYS: @@--------------------------------------------------------------------------------
SYS: @@ SETUP FILE FOR THE SIMULATION OF UPHILL DIFFUSION IN A TERNARY SINGLE PHASE
SYS: @@ AUSTENITE MATRIX DUE TO THE CLASSICAL DARKEN EXPERIMENT PUBLISHED BY
SYS: @@ L.S. DARKEN: TRANS. AIME 180(1949)430-438.
SYS: @@
SYS: @@ IN THIS SETUP 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 1050 C FOR 13 DAYS. AS BOTH PIECES ARE AUSTENITE THEY MUST BE ENTERED
SYS: @@ INTO THE SAME REGION. WE CAN ACCOMPLISH THIS BY GIVING THE COMPOSITIONS
SYS: @@ OF SI AND C IN EACH GRIDPOINT INDIVIDUALLY. FOR CONVENIENCE WE STORE
SYS: @@ THESE DATA ON FILE.
SYS: @@--------------------------------------------------------------------------------
SYS:
SYS: @@
SYS: @@ FROM NOW ON WE STOP USING LOG-FILES AS WE USED IN EXAMPLES a2a and a2b
SYS: @@
SYS:
SYS: @@
SYS: @@ RETRIEVE DATA FROM DATABASE
SYS: @@
SYS: go da
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Public Ternary Alloys TDB v1

 VA  DEFINED
TDB_PTERN:
TDB_PTERN: @@
TDB_PTERN: @@ USE TCFE DATABASE FOR THERMODYNAMIC DATA
TDB_PTERN: @@
TDB_PTERN: sw tcfe6
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA  REJECTED
TDB_TCFE6: def-sys fe si c
 FE                      SI                      C
   DEFINED
TDB_TCFE6: rej ph * all
 LIQUID:L                BCC_A2                  FCC_A1
 HCP_A3                  DIAMOND_FCC_A4          GRAPHITE
 CEMENTITE               M23C6                   M7C3
 M5C2                    KSI_CARBIDE             FE4N_LP1
 FECN_CHI                LAVES_PHASE_C14         M3SI
 CR3SI                   FE2SI                   MSI
 M5SI3                   AL4C3                   FE8SI2C
 SIC  REJECTED
TDB_TCFE6: res ph fcc
 FCC_A1  RESTORED
TDB_TCFE6: get
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

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

```
  'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C
      -FE'
  'J. Lacaze and B. Sundman, Metall. Mater. Trans. A, 22A (1991), 2211-2223;
      Fe-Si and Fe-Si-C'
  'J. Miettinen and B. Hallstedt, Calphad, 22 (1998), 231-256; Fe-Si and Fe
      -Si-C'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
      Molar volumes'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
 -OK-
TDB_TCFE6:
TDB_TCFE6: @@
TDB_TCFE6: @@ SWITCH TO MOBILITY DATABASE TO RETRIEVE MOBILITY DATA
TDB_TCFE6: @@
TDB_TCFE6: app mob2
 Current database: TCS Alloys Mobility Database v2

 VA  DEFINED
 GAS:G  REJECTED
APP: def-sys  fe si c
 FE                    SI                    C
   DEFINED
APP: rej ph * all
 BCC_A2                CEMENTITE             DIAMOND_A4
 FCC_A1                FE4N                  GRAPHITE
 HCP_A3                KSI_CARBIDE           LIQUID:L
 M23C6                 M5C2                  M7C3
   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 diffusion in fcc C-Fe'
   'B. Jönsson: 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 REGION austenite
DIC> @@
DIC> enter-region
REGION NAME : austenite
DIC>
DIC> @@
DIC> @@ ENTER GRID
DIC> @@ N.B. GRIDPOINT DISTANCES ARE SMALLEST AROUND THE MIDDLE
DIC> @@
DIC> enter-grid
REGION NAME : /AUSTENITE/: austenite
WIDTH OF REGION /1/: 50E-3
TYPE /LINEAR/: double
```

```
NUMBER OF POINTS /50/: 50
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 PHASE INTO 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 VARIOUS 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>DIC> CPU time  4 seconds
```

```
 D I C T R A service version  25(Build 1315) on Linux
 Copyright (1993,1995,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 21-08-08 10:22:06
 Only for use at MSE
 Local contact Malin Selleby
SYS:ioctl failed: it's not a terminal
SYS:SYS:SYS:
SYS:
SYS: @@ darken_run.DCM
SYS:
SYS: @@
SYS: @@ ENTER THE DICTRA MONITOR
SYS: @@
SYS: go d-m
 NO TIME STEP DEFINED
DIC>
DIC> @@
DIC> @@ READ SETUP FROM FILE AND START SIMULATION
DIC> @@
DIC> read exa3
 OK
DIC>
DIC> sim
 Automatic start values will be set
 Old start values kept
 Automatic start values will be set
 Automatic start values will be set
 Old start values kept
 Automatic start values will be set
 U-FRACTION IN SYSTEM:  C = .0215326239970656  FE = .963089414810838
                        SI = .0369105851891616
 TOTAL SIZE OF SYSTEM:  .05 [m]
 U-FRACTION IN SYSTEM:  C = .0215326239970656  FE = .963089414810838
                        SI = .0369105851891616
 TOTAL SIZE OF SYSTEM:  .05 [m]
 TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215326239970656  FE = .963089414810838
                        SI = .0369105851891616
 TOTAL SIZE OF SYSTEM:  .05 [m]

  CPU time used in timestep 0 seconds
 TIME =   455.95240     DT =   455.95240     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215326239970656  FE = .963089414810838
                        SI = .0369105851891616
 TOTAL SIZE OF SYSTEM:  .05 [m]

  CPU time used in timestep 0 seconds
 TIME =   1367.8572     DT =   911.90481     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215326239970656  FE = .963089414810838
                        SI = .0369105851891617
 TOTAL SIZE OF SYSTEM:  .05 [m]

  CPU time used in timestep 0 seconds
 TIME =   3191.6668     DT =   1823.8096     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215326239970656  FE = .963089414810838
                        SI = .0369105851891616
 TOTAL SIZE OF SYSTEM:  .05 [m]

  CPU time used in timestep 1 seconds
 TIME =   6839.2860     DT =   3647.6192     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215326239970656  FE = .963089414810838
                        SI = .0369105851891616
 TOTAL SIZE OF SYSTEM:  .05 [m]

  CPU time used in timestep 0 seconds
 TIME =   14134.524     DT =   7295.2384     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215326239970656  FE = .963089414810838
   :
   :
   :
```

```
  :
 U-FRACTION IN SYSTEM:  C = .0215326239970588  FE = .963086148039918
                        SI = .0369138519600817
 TOTAL SIZE OF SYSTEM:  .05 [m]

  CPU time used in timestep 1 seconds
 TIME =  0.79124025E+10 DT =  0.10000000E+10 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215326239970372  FE = .963086148039918
                        SI = .0369138519600824
 TOTAL SIZE OF SYSTEM:  .05 [m]

  CPU time used in timestep 1 seconds
 TIME =  0.89124025E+10 DT =  0.10000000E+10 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215326239970315  FE = .963086148039918
                        SI = .0369138519600827
 TOTAL SIZE OF SYSTEM:  .05 [m]

  CPU time used in timestep 1 seconds
 TIME =  0.99124025E+10 DT =  0.10000000E+10 SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215326239970405  FE = .963086148039917
                        SI = .0369138519600829
 TOTAL SIZE OF SYSTEM:  .05 [m]

  CPU time used in timestep 1 seconds
 TIME =  0.10000000E+11 DT =   87597468.     SUM OF SQUARES =   0.0000000
 U-FRACTION IN SYSTEM:  C = .0215326239970431  FE = .963086148039917
                        SI = .0369138519600827
 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    455.95240
 DELETING TIME-RECORD FOR TIME    1367.8572
 DELETING TIME-RECORD FOR TIME    3191.6668
 DELETING TIME-RECORD FOR TIME    6839.2860
 DELETING TIME-RECORD FOR TIME    14134.524
 DELETING TIME-RECORD FOR TIME    28725.001
 DELETING TIME-RECORD FOR TIME    57905.955
 DELETING TIME-RECORD FOR TIME    116267.86
 DELETING TIME-RECORD FOR TIME    232991.68
 DELETING TIME-RECORD FOR TIME    466439.31
 DELETING TIME-RECORD FOR TIME    933334.57
 DELETING TIME-RECORD FOR TIME    1867125.1
 DELETING TIME-RECORD FOR TIME    3734706.1
 DELETING TIME-RECORD FOR TIME    7469868.2
 DELETING TIME-RECORD FOR TIME    14940192.
 DELETING TIME-RECORD FOR TIME    29880841.
 DELETING TIME-RECORD FOR TIME    59762137.
 DELETING TIME-RECORD FOR TIME   0.11952473E+09
 DELETING TIME-RECORD FOR TIME   0.23904992E+09
 DELETING TIME-RECORD FOR TIME   0.47810029E+09
 DELETING TIME-RECORD FOR TIME   0.95620104E+09
 DELETING TIME-RECORD FOR TIME   0.19124025E+10
 DELETING TIME-RECORD FOR TIME   0.29124025E+10
 DELETING TIME-RECORD FOR TIME   0.39124025E+10
 DELETING TIME-RECORD FOR TIME   0.49124025E+10
 DELETING TIME-RECORD FOR TIME   0.59124025E+10
 DELETING TIME-RECORD FOR TIME   0.69124025E+10
 DELETING TIME-RECORD FOR TIME   0.79124025E+10
 DELETING TIME-RECORD FOR TIME   0.89124025E+10

 KEEPING TIME-RECORD FOR TIME   0.99124025E+10
 AND FOR TIME                   0.10000000E+11
 WORKSPACE RECLAIMED
DIC>
DIC> set-inter
 --OK---
DIC>DIC> CPU time  23 seconds
```

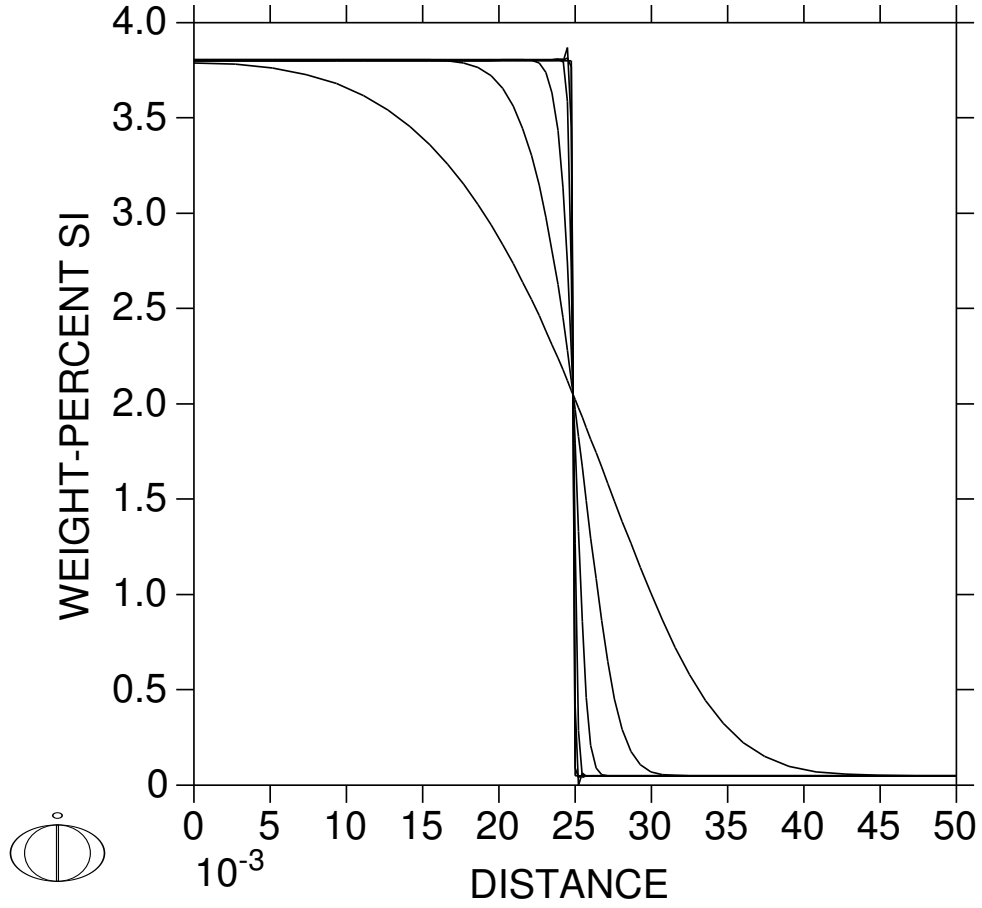
```
 D I C T R A service version  25(Build 1315) on Linux
 Copyright (1993,1995,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 21-08-08 10:22:06
 Only for use at MSE
 Local contact Malin Selleby
SYS:ioctl failed: it's not a terminal
SYS:SYS:SYS:



SYS:SYS:
SYS:
SYS: @@ darken_plot.DCM
SYS:
SYS: @@
SYS: @@ ENTER THE DICTRA MODULE AND SPECIFY THE STORE-RESULT FILE
SYS: @@
SYS: go d-m
 NO TIME STEP DEFINED
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 WE SHALL PLOT THE PROFILES.
POST-1: @@
POST-1: set-diagram-axis x distance global
  INFO: Distance is set as independent variable
POST-1: set-diagram-axis y weight-percent si
POST-1: set-plot-condition time 0 1E5 1123200 1e7 1E8 1E9 1E10
POST-1:
POST-1: @@
POST-1: @@ PLOT THE DIAGRAM
POST-1: @@
POST-1: set-title
TITLE : Figure a3.1
POST-1:
POST-1: plot SCREEN

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 Y-AXIS
POST-1: @@
POST-1: set-diagram-axis y w-p c
POST-1: set-title Figure a3.2
POST-1: plot SCREEN

POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1: @@
POST-1: @@ COMPARE WITH DARKENS EXPERIMENTS
```

```
POST-1: @@
POST-1: append_experimental_data  yes exa3.exp 0; 1
POST-1:
POST-1: set-plot-condition time 1123200
POST-1:
POST-1: s-s-s
AXIS (X, Y OR Z) : y
AUTOMATIC SCALING  (Y OR N) /N/:  n
MIN VALUE : 0.25
MAX VALUE : 0.75
POST-1:
POST-1: set-title Figure a3.3
POST-1: plot SCREEN

POST-1:
POST-1:
POST-1:
POST-1:@?<Hit_return_to_continue>
POST-1: set-inter
 --OK---
POST-1: CPU time  0 seconds
```

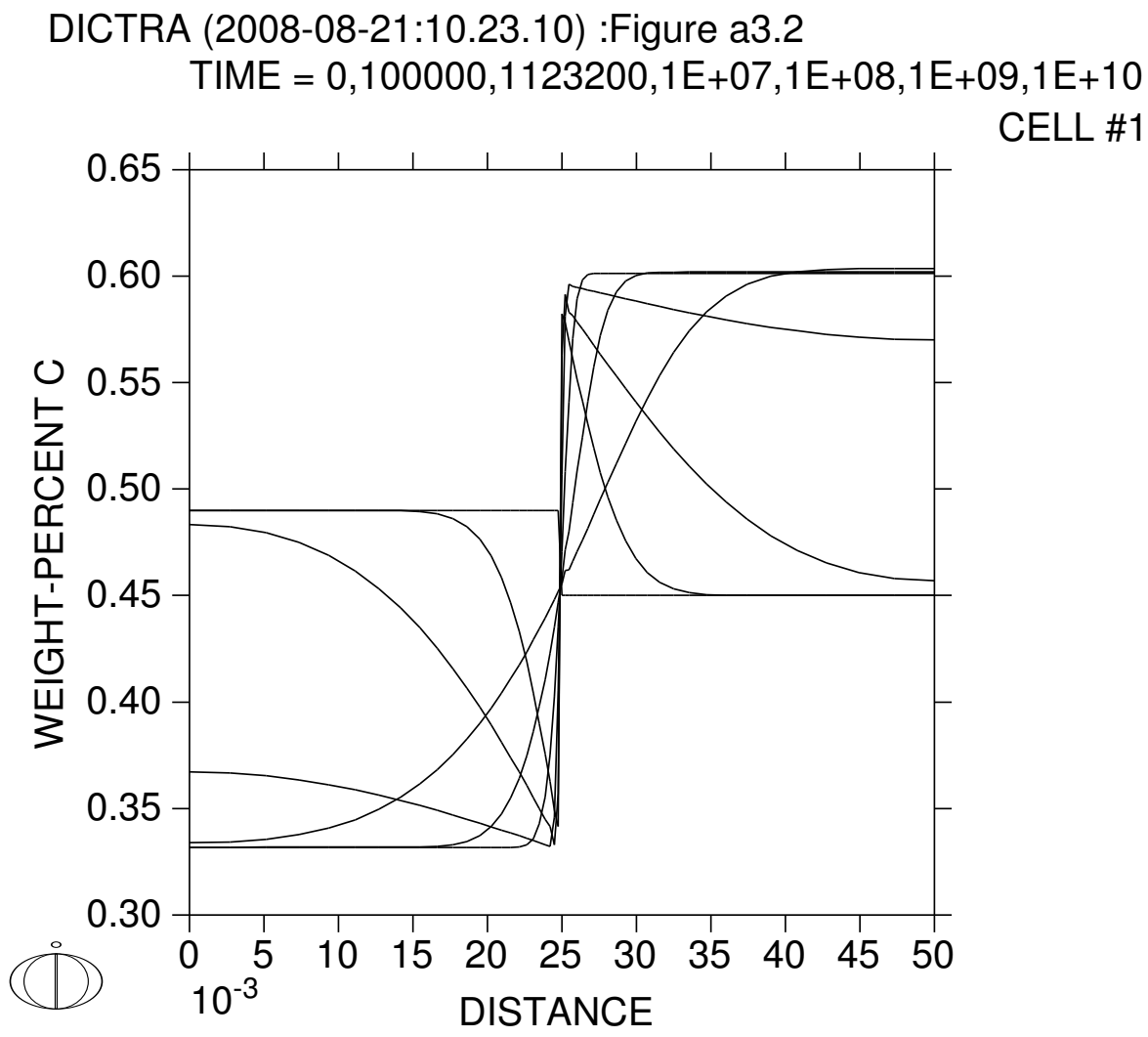
DICTRA (2008-08-21:10.23.10) :Figure a3.1

TIME = 0,100000,1123200,1E+07,1E+08,1E+09,1E+10

CELL #1



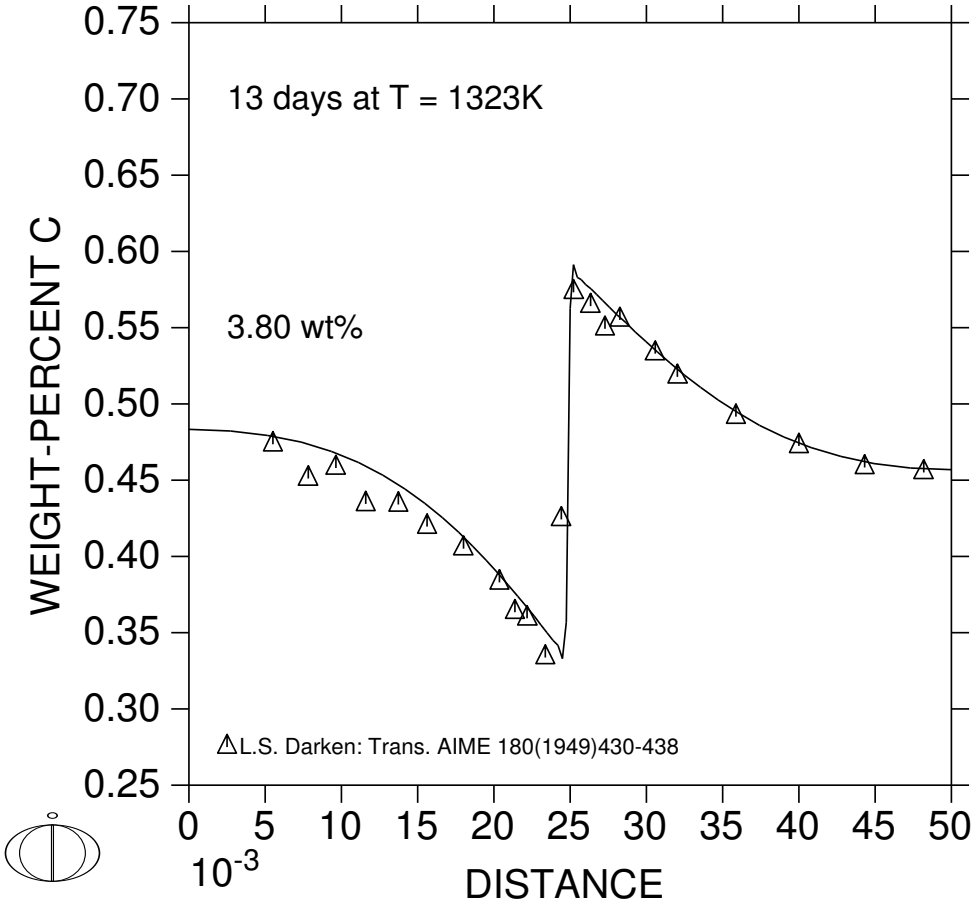
output by user lars on 2008.08.21:10.23



output by user lars on 2008.08.21:10.23

DICTRA (2008-08-21:10.23.10) :Figure a3.3
TIME = 1123200

CELL #1



output by user lars on 2008.08.21:10.23