Sharp interface model

Comparison between

- Analytical / numerical solutions
- Phase field model
- Sharp interface model

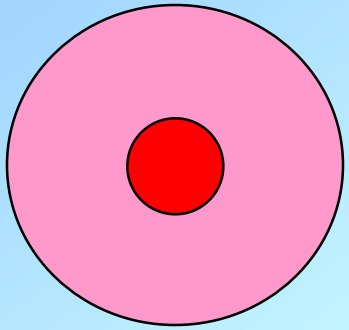
Moving Phase Boundary Calculations

- Used for calculating growth or dissolution of a phase.
- Assumptions:
  - Local equilibrium holds at the phase boundary, i.e. concentrations at the boundary can be calculated from an equilibrium calculation in T-C.
  - Diffusion controls the movement of the phase boundary
- Application examples:
  - ✓Carbide dissolution
  - ✓Solidification
  - ✓Growth of σ–phase in a stainless steel

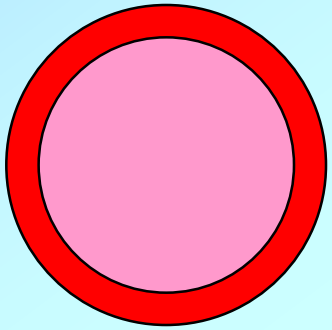
Advantages / Disadvantages ”Analytical” solutions

+ exact solution
- limited to simple problems
  (constant coefficients)

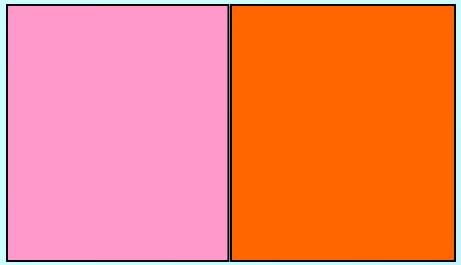
Some different possible geometries



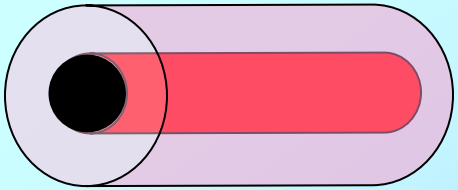
Growth or dissolution of spherical precipitate



Growth of spherical film (Grain-boundrary film)



Planar growth



Growth of cylindrical precipitate

Advantages / Disadvantages Phase field model

+ 2-D / 3-D problems
- complex calculation scheme
- Position of interface not well defined
- Often explicit integration schemes

Advantages / Disadvantages Sharp interface model

+ simple calculation scheme
+ accurate position of phase interface
- 1-D problems

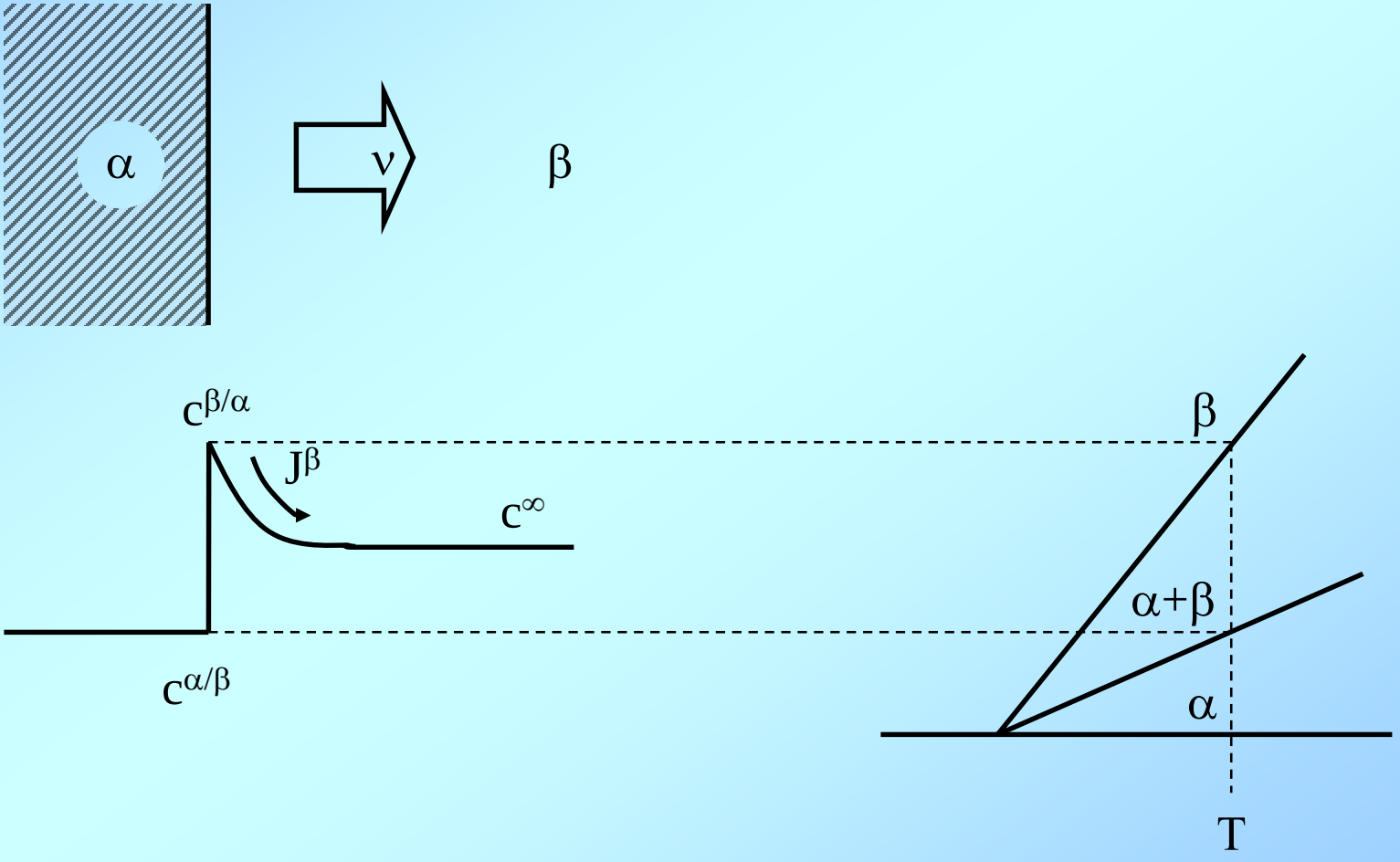
Assumptions – Sharp interface model

- local equilibrium
- profiles as piecewise linear functions
- volume is independent of composition
- volume fixed frame of reference

Calculation scheme - binary case

- determine tieline
- solve PDE
- solve flux balance equation
- update grid

LE Tieline in Binary system



PDE

$$\frac{\partial c_k}{\partial t} = \frac{\partial}{\partial z}\left(D_k \frac{\partial c_k}{\partial z} \right)$$

Solved by FDM / FEM

Flux balance equation

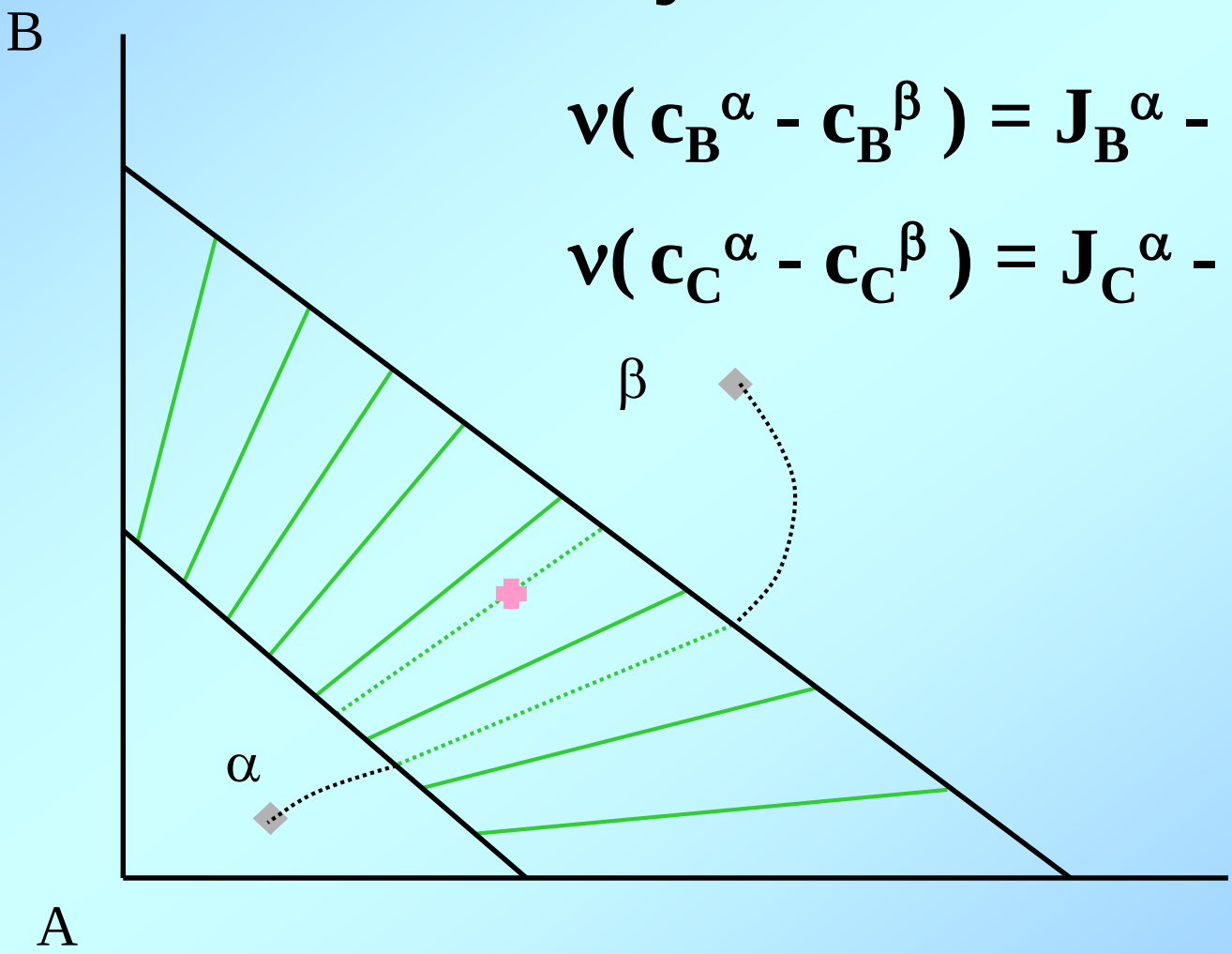
$$\nu^{\alpha} c_k^{\alpha} - \nu^{\beta} c_k^{\beta} = J_k^{\alpha} - J_k^{\beta}$$

$c_k^{\alpha}, c_k^{\beta}$ from LE

$J_k^{\alpha}, J_k^{\beta}$ from PDE (and LE)

$$\Rightarrow \nu^{p}(\nu^{\alpha}, \nu^{\beta})$$

LE Tieline in multicomponent system



$$\nu(c_B^{\alpha} - c_B^{\beta}) = J_B^{\alpha} - J_B^{\beta}$$

$$\nu(c_C^{\alpha} - c_C^{\beta}) = J_C^{\alpha} - J_C^{\beta}$$

Flux balance equation

$$\nu^{\alpha} c_k^{\alpha} - \nu^{\beta} c_k^{\beta} = J_k^{\alpha} - J_k^{\beta} \qquad k=1,2\ldots.n-1$$

$c_k^{\alpha}, c_k^{\beta}$ from LE

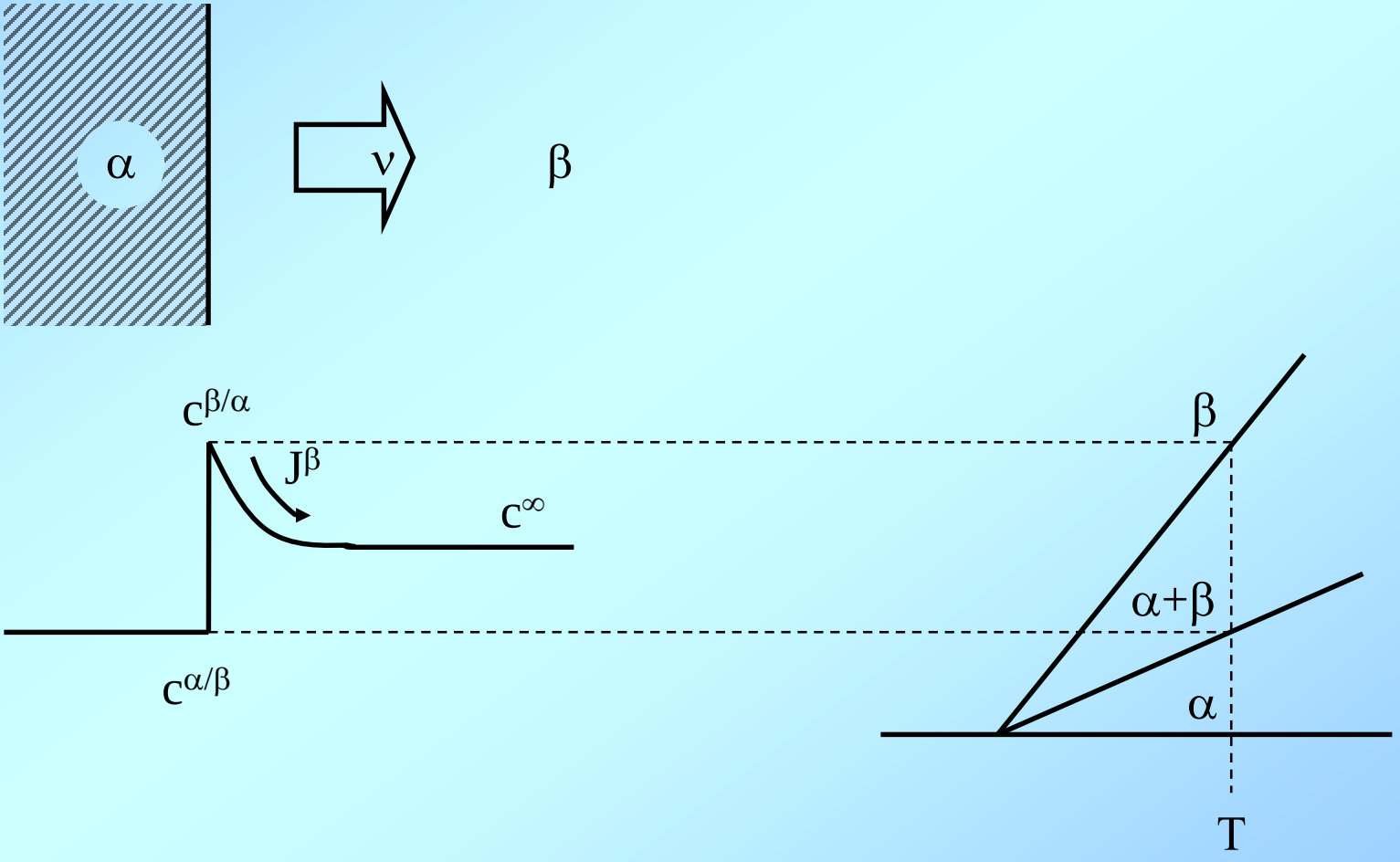
$J_k^{\alpha}, J_k^{\beta}$ from PDE (and LE)

$$\Rightarrow \nu^{p}(\nu^{\alpha}, \nu^{\beta})$$

Flux balance equation cont.

- Simple case, binary system α growing into supersaturated β

Flux balance equation cont.



Flux balance equation cont.

Solving PDE, boundary conditions

α:

left side:	closed system	(Neumann)
right side:	$c^{\alpha/\beta}$ from LE	(Dirichlet)

β:

left side:	$c^{\beta/\alpha}$ from LE	(Dirichlet)
right side:	closed system	(Neumann)

Flux balance equation cont.

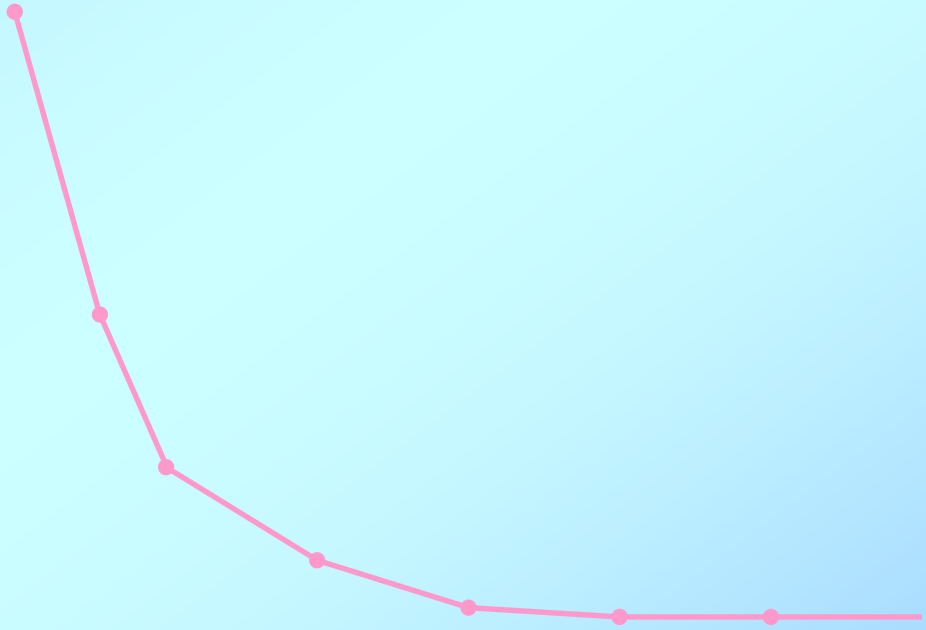
In this case

$J^{\alpha} = 0$ as α grows with equilibrium composition

$J^{\beta} \neq 0$

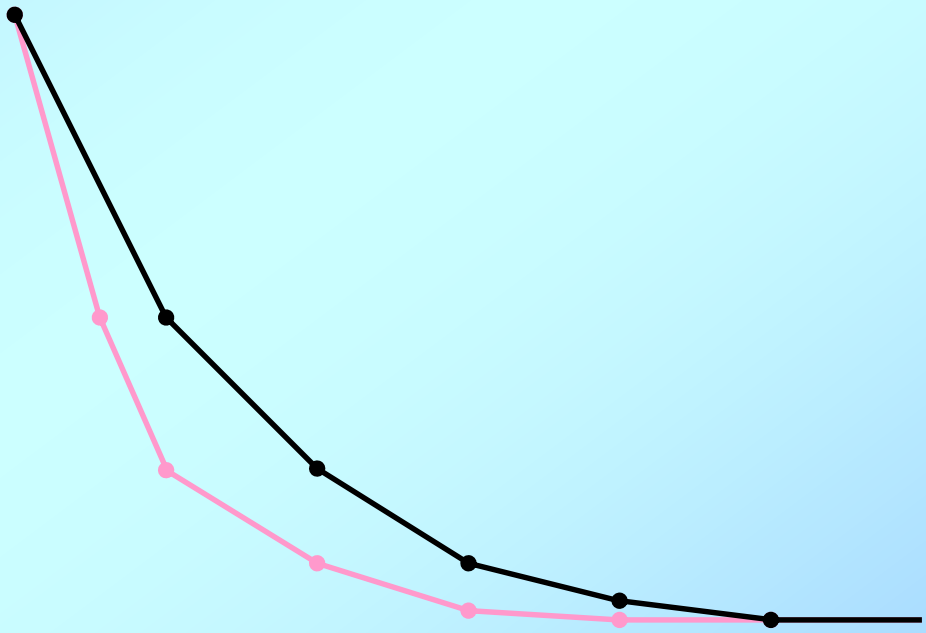
Flux balance equation cont.

$t=t_0$



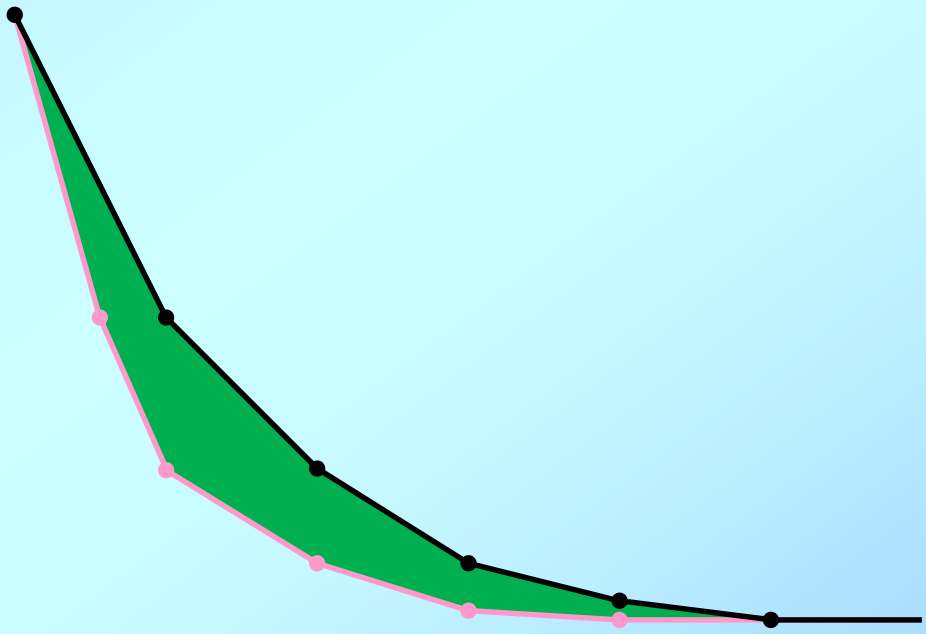
Flux balance equation cont.

$t=t_0+\Delta t$



Flux balance equation cont.

$J^{\beta}\Delta t$



Flux balance equation cont.

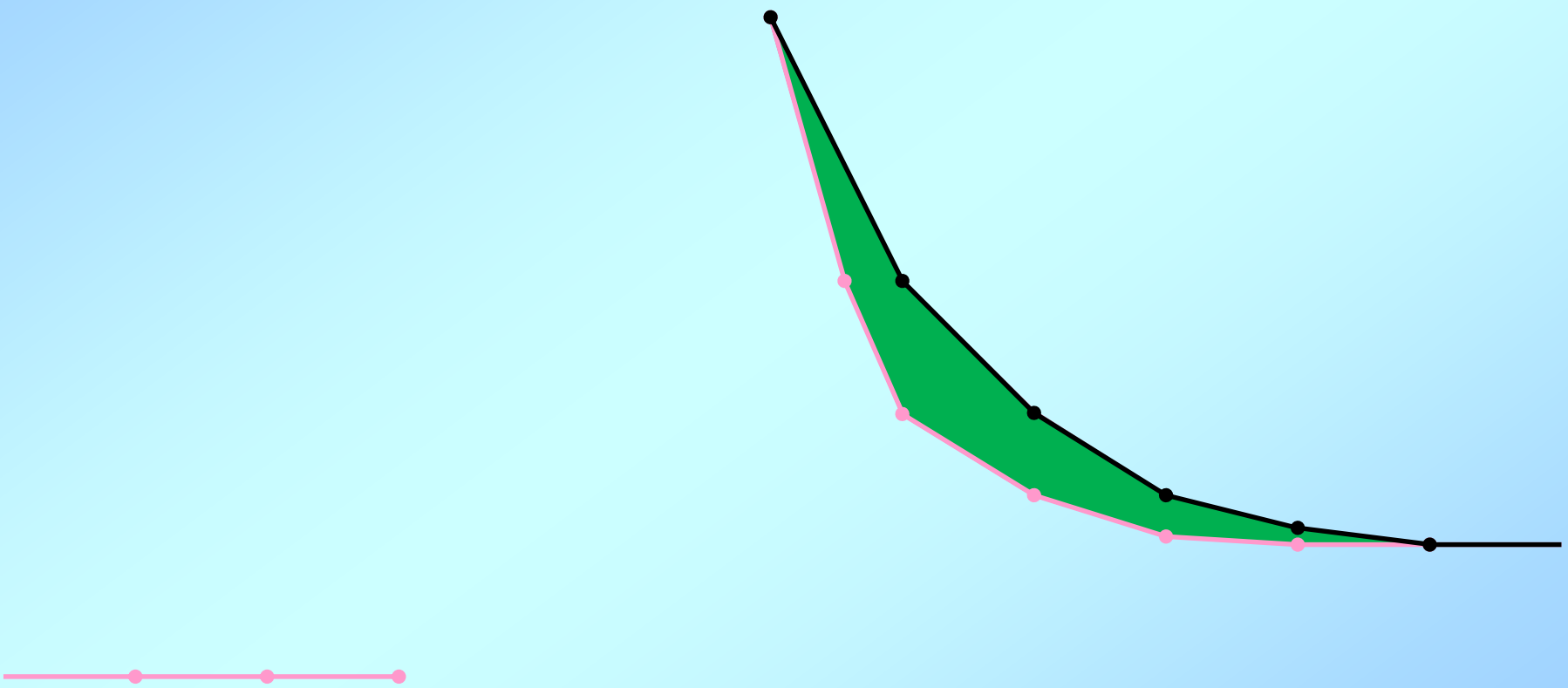
The change in total amount in the β phase must be compensated by the displacement of the interface (assume $v^{\alpha} = v^{\beta}$)

$$v(c^{\alpha} - c^{\beta}) = (J^{\alpha} - J^{\beta})\Delta t$$

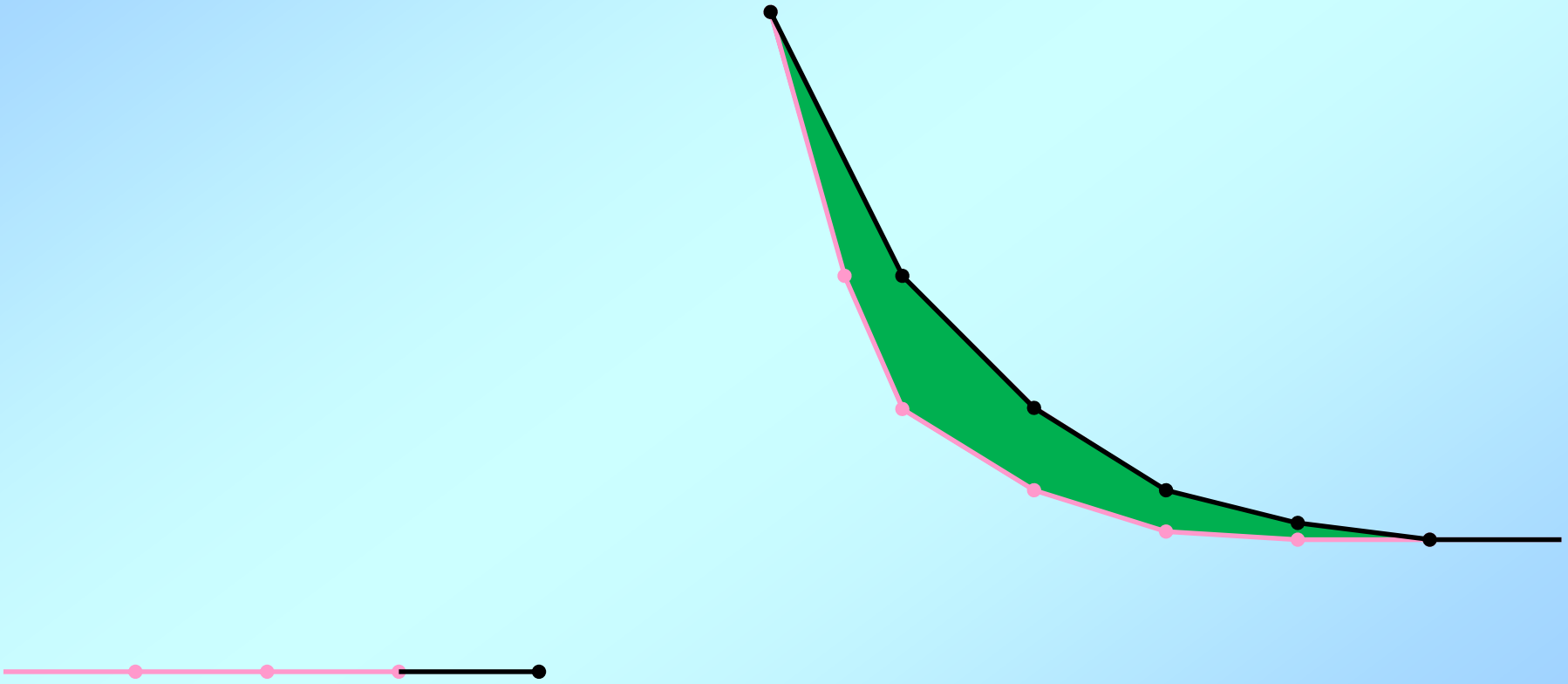
Assuming $J^{\alpha}=0$ then

$$v(c^{\alpha} - c^{\beta}) = -J^{\beta}\Delta t$$

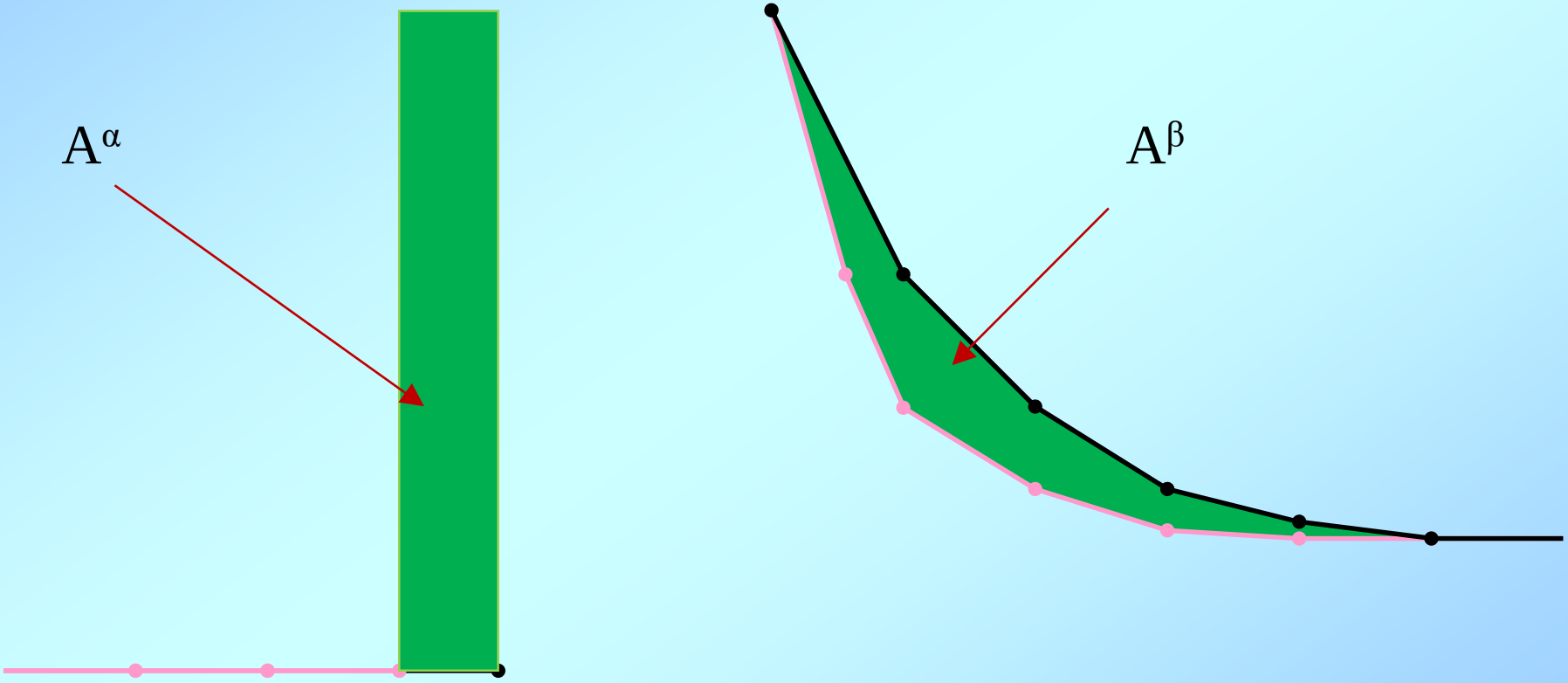
Flux balance equation cont.



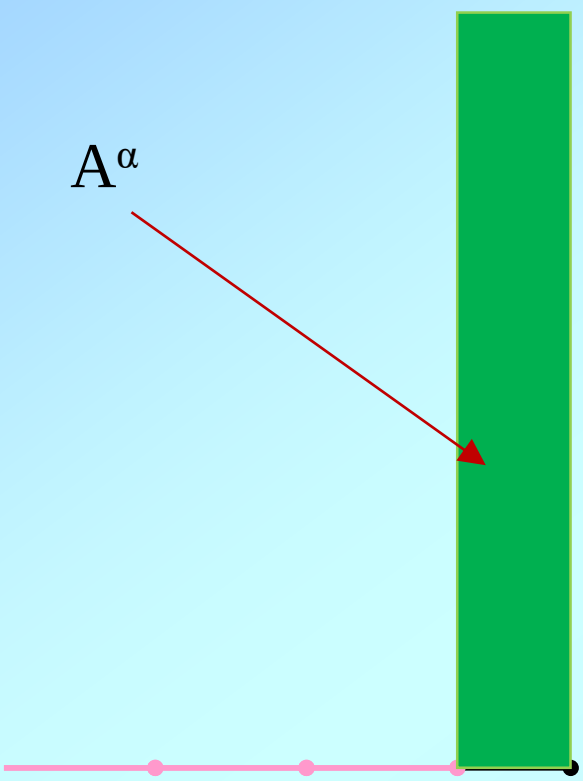
Flux balance equation cont.

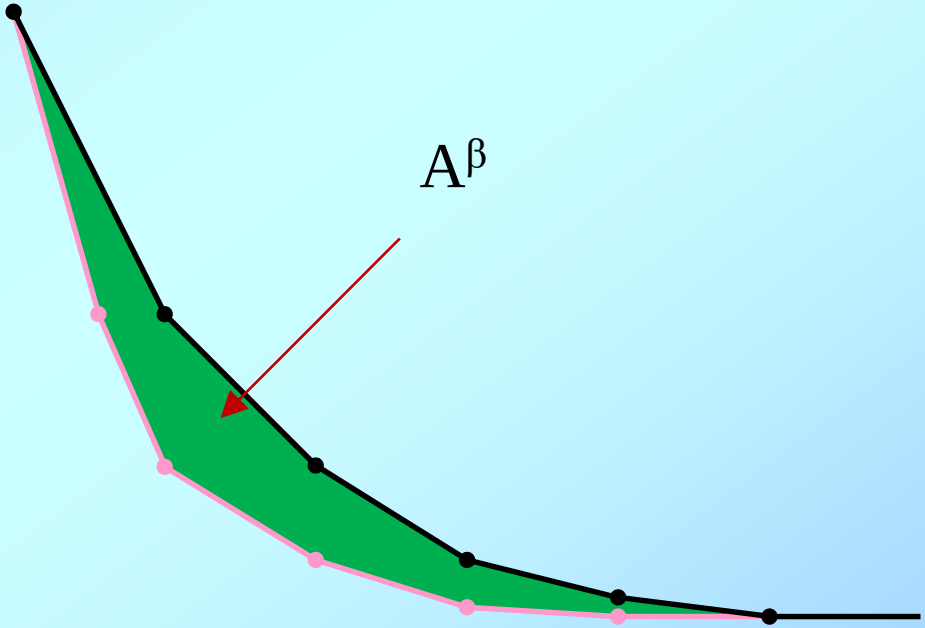


Flux balance equation cont.



Flux balance equation cont.





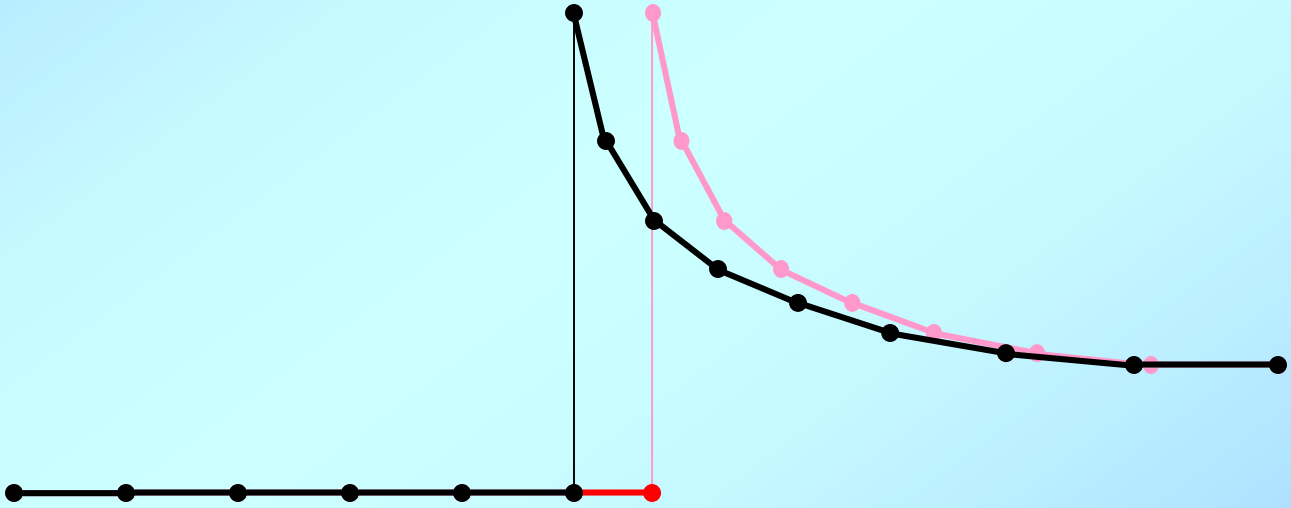
$A^{\alpha}=A^{\beta}$

Grid update

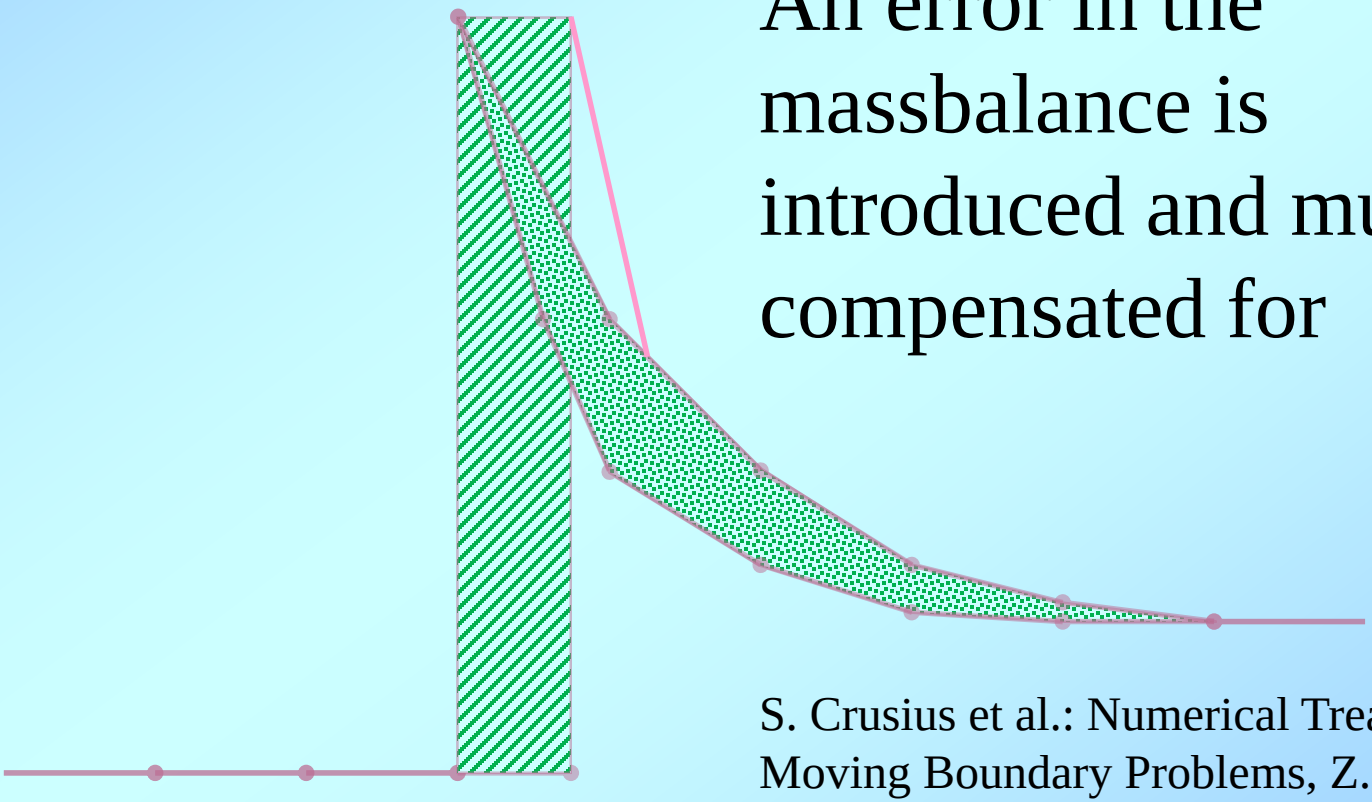
Howto update the grid according to the calculated displacement?

- For growing phase: add one gridpoint
- For shrinking phase: linearly contract the grid

Grid update



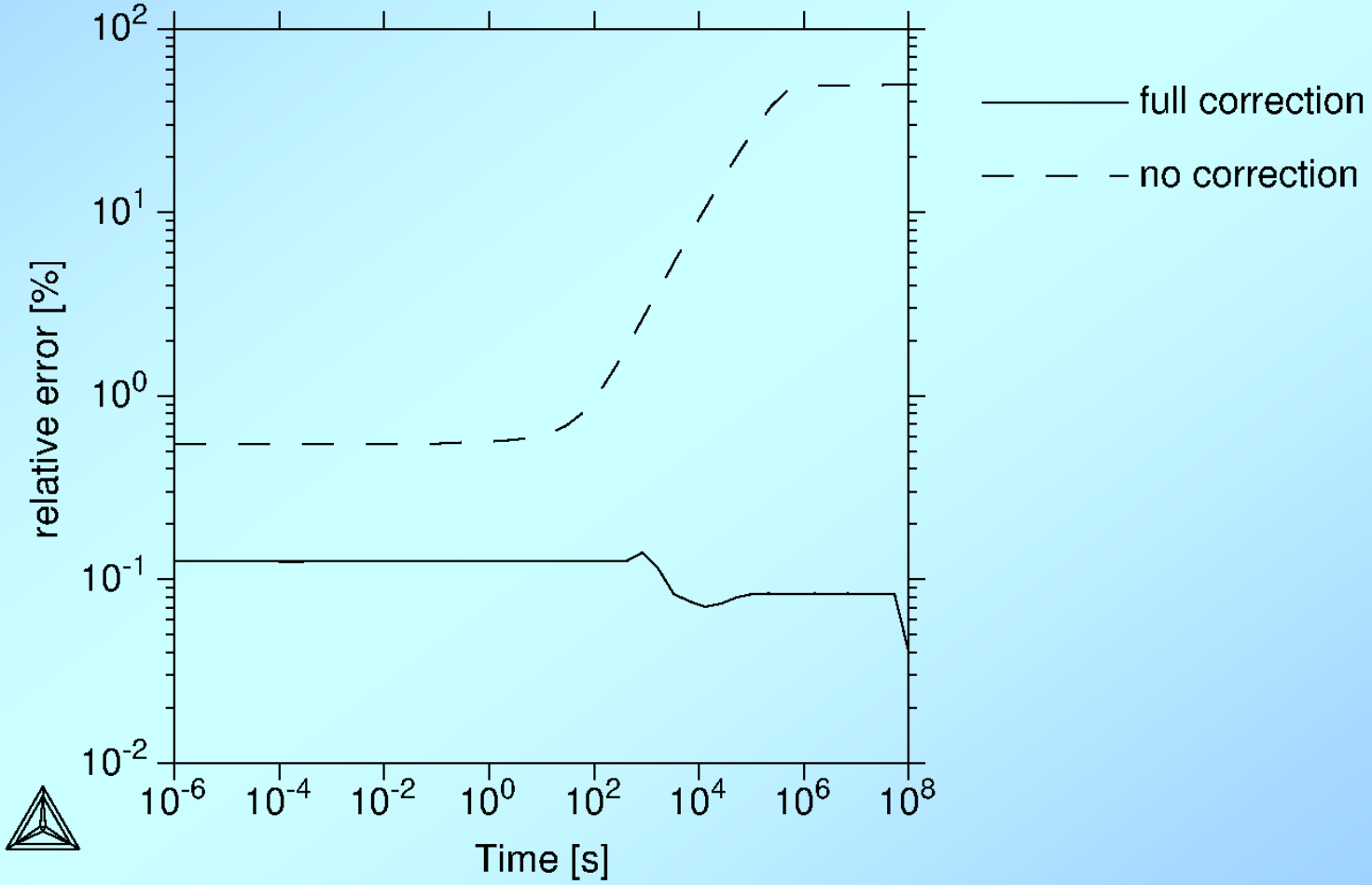
Grid update



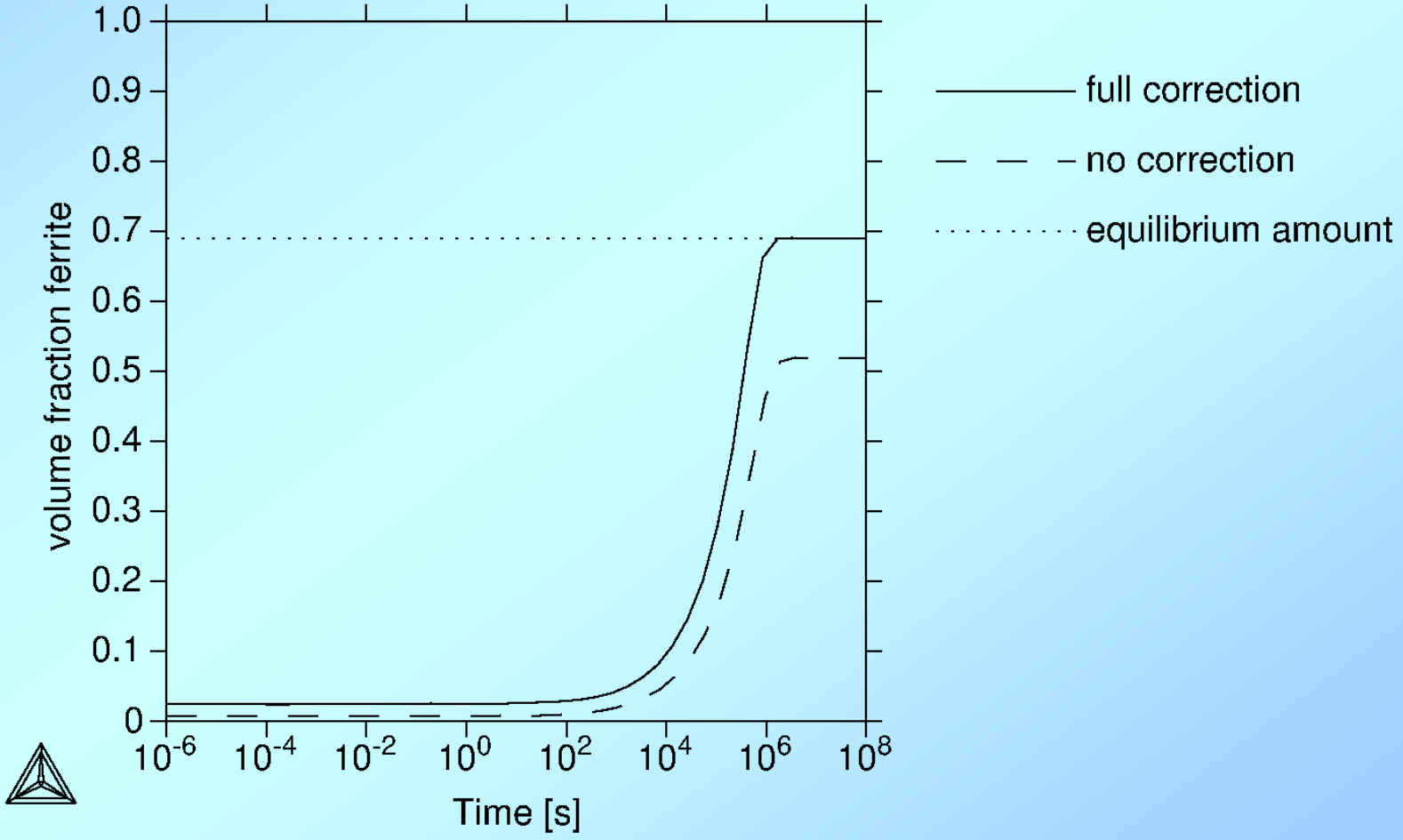
An error in the massbalance is introduced and must be compensated for

S. Crusius et al.: Numerical Treatment of Moving Boundary Problems, Z. Metallkd. 83 (l992) 9

Error in massbalance



Volume fraction ferrite



Frame of reference

- number fixed frame of reference
- lattice fixed frame of reference
- volume fixed frame of reference

Composition variable

- mass fraction
- mole fraction
- site fraction
- u-fraction

u-fraction

mole fraction: $$x_k = \frac{N_k}{\sum_i N_i}$$

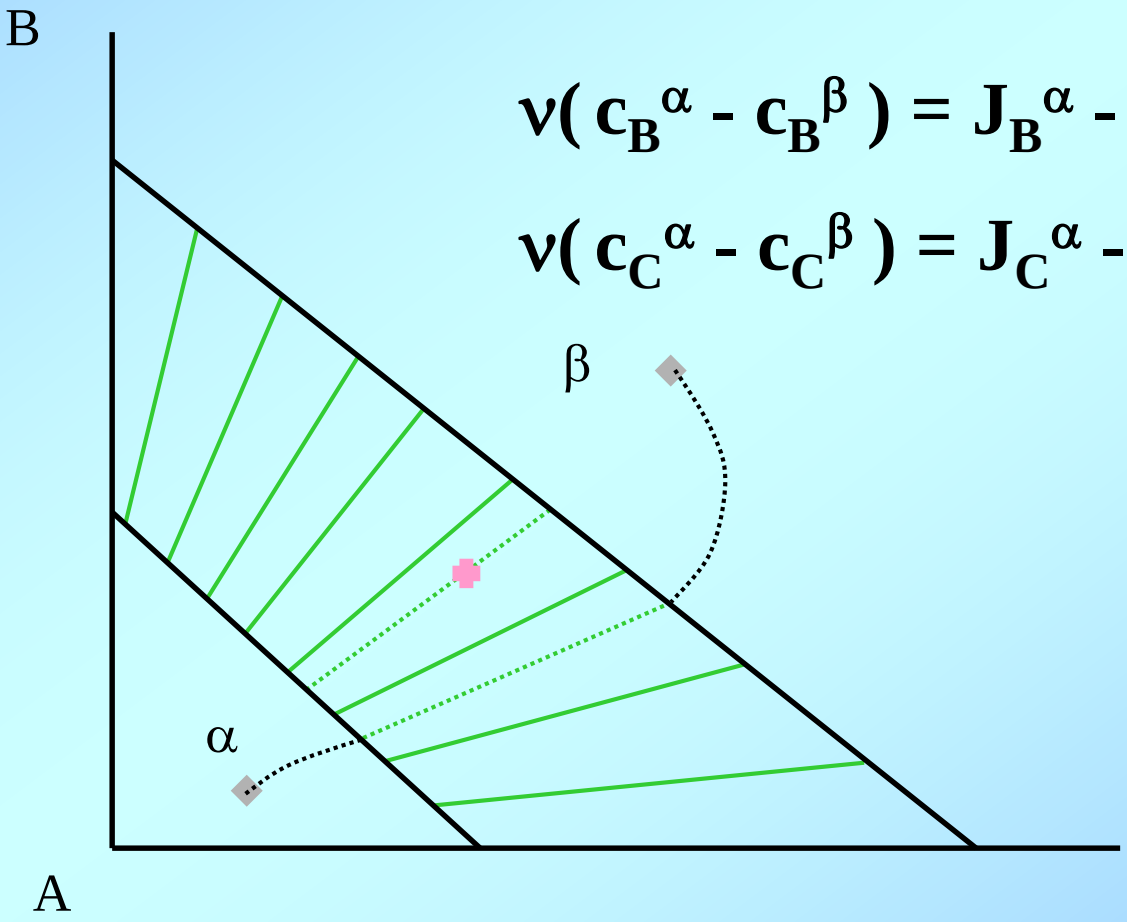
mass fraction: $$w_k = \frac{N_k m_k}{\sum_i N_i m_i}$$

u-fraction: $$u_k = \frac{N_k}{\sum_{i \in s} N_i}$$

Calculation scheme - multicomponent case

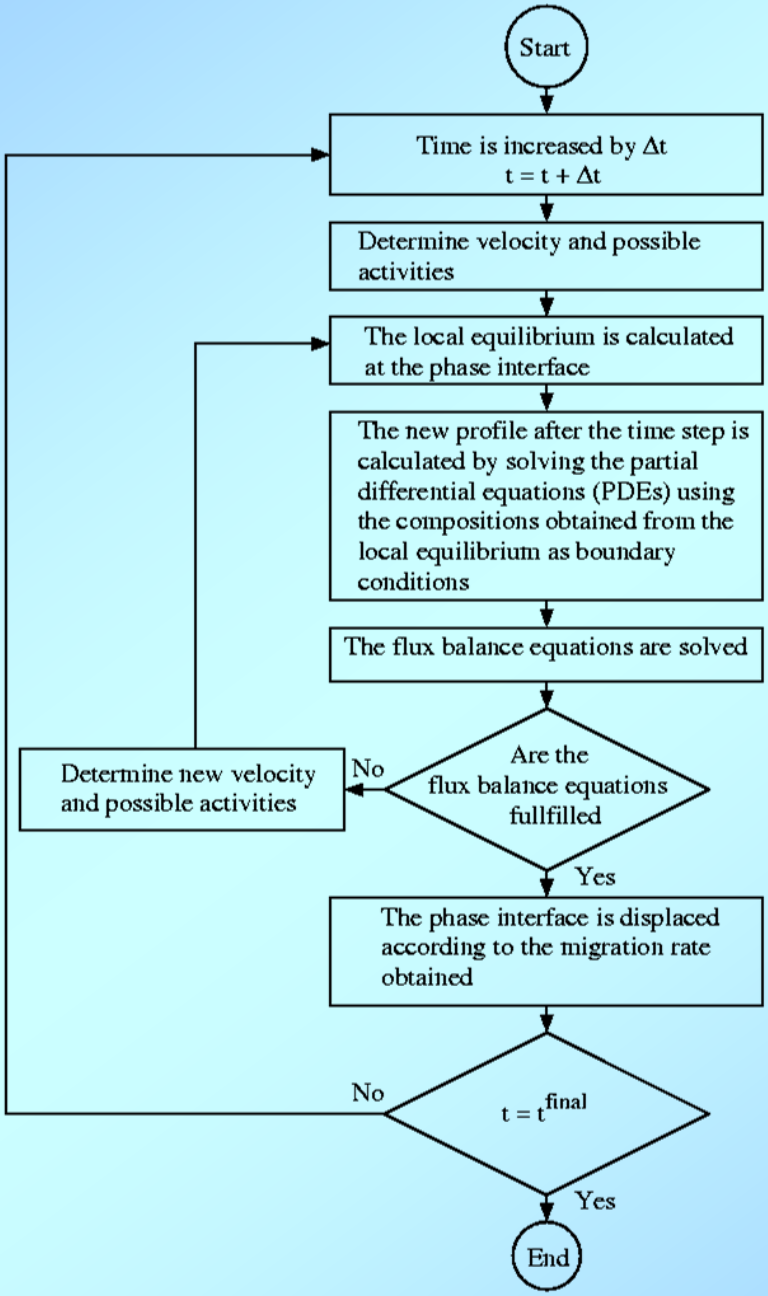
- fix activities/potentials
- determine tieline
- solve PDE
- solve flux balance equations
- guess new activities/potentials until flux balance equations are fulfilled
- update grid

LE in multicomponent systems



$$\nu(c_B^{\alpha} - c_B^{\beta}) = J_B^{\alpha} - J_B^{\beta}$$

$$\nu(c_C^{\alpha} - c_C^{\beta}) = J_C^{\alpha} - J_C^{\beta}$$


Start
Time is increased by Δt
t = t + Δt
Determine velocity and possible activities
The local equilibrium is calculated at the phase interface
The new profile after the time step is calculated by solving the partial differential equations (PDEs) using the compositions obtained from the local equilibrium as boundary conditions
The flux balance equations are solved
Are the flux balance equations fullfilled
No
Determine new velocity and possible activities
Yes
The phase interface is displaced according to the migration rate obtained
t = t final
No
Yes
End

HA 1

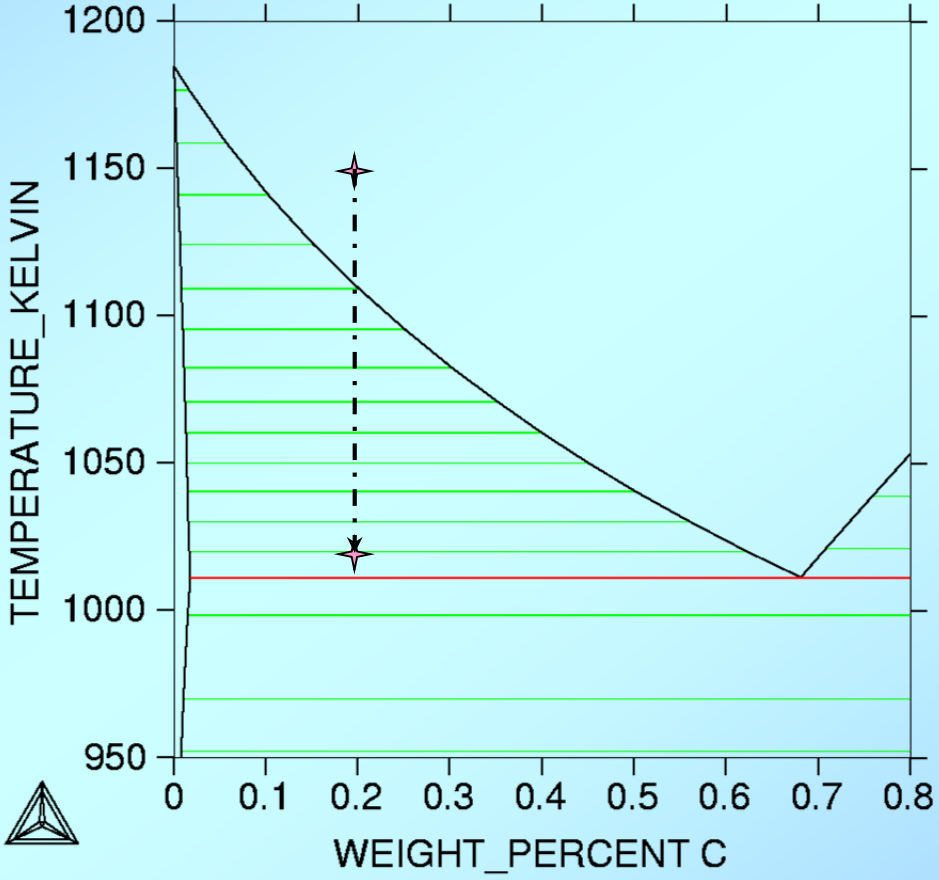
Use MATLAB (or any other appropriate package) to solve the moving boundary problem in a Fe-C alloy with 0.2 mass percent C.

The alloy is cooled from an equilibrium state with single phase FCC down to the two phase BCC/FCC region at 1120 K.

Use $D_c^{FCC} = 2.5 \cdot 10^{-10} \cdot u_c + 5.9 \cdot 10^{-13}$

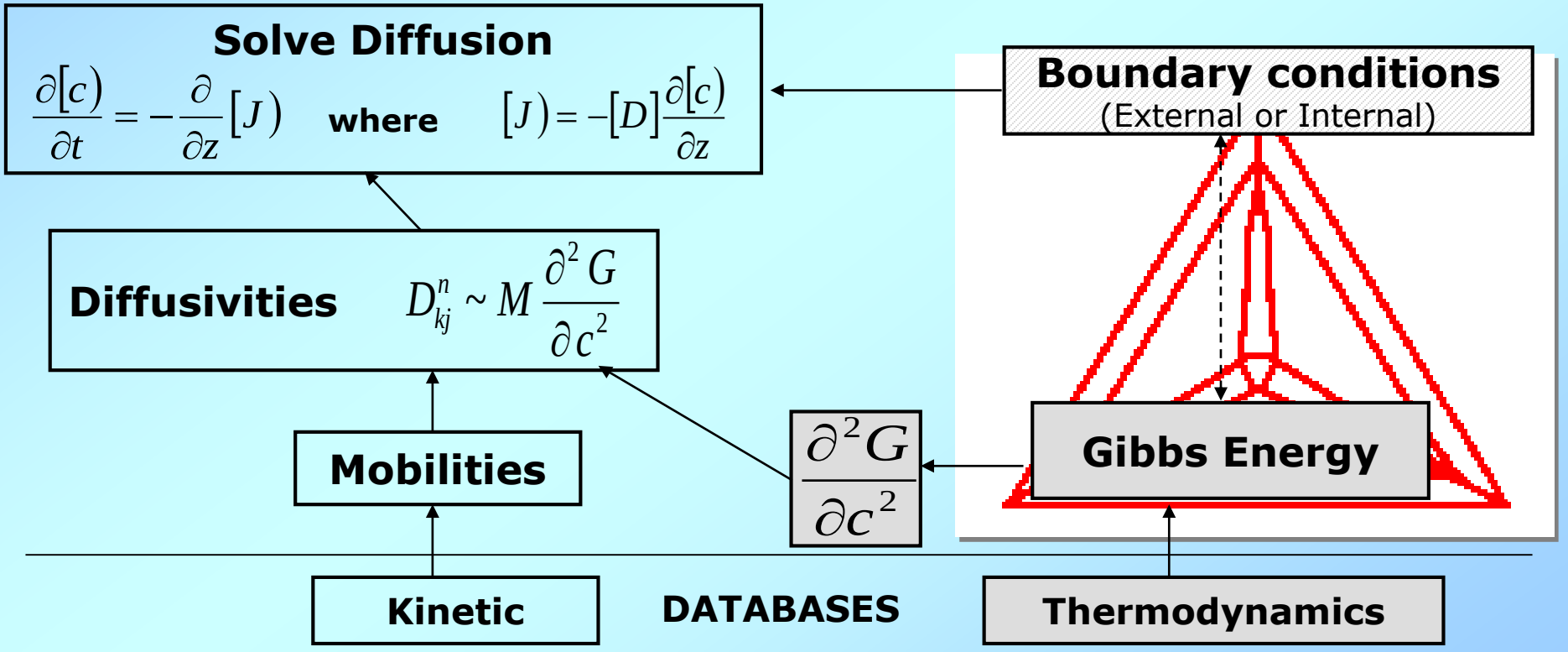
Compare results with the DICTRA software package.

HA1


1200
1150
1100
1050
1000
950
TEMPERATURE_KELVIN
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
WEIGHT_PERCENT C

Basic calculation scheme

A numerical finite difference scheme is used for solving a system of coupled parabolic partial differential equations



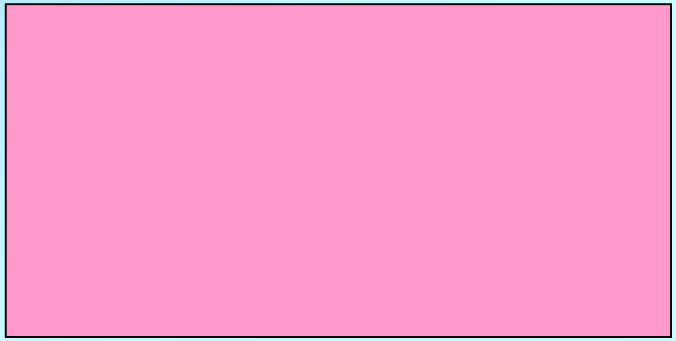
All simulations depend on assessed kinetic and thermodynamic data, which are stored in databases

DICTRA – basic concepts

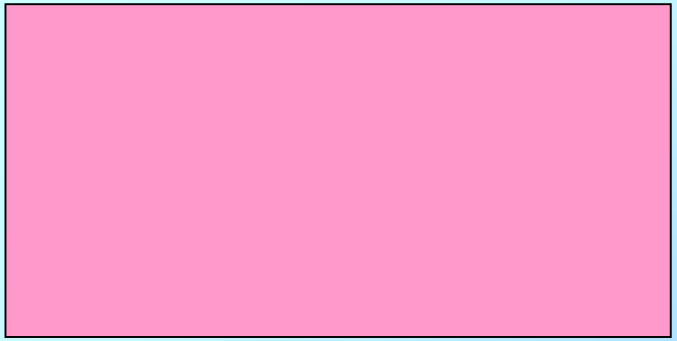
- Regions
- Grid
- Phase
- Composition
- Boundary conditions
- Global conditions

DICTRA – Region

REGION #1

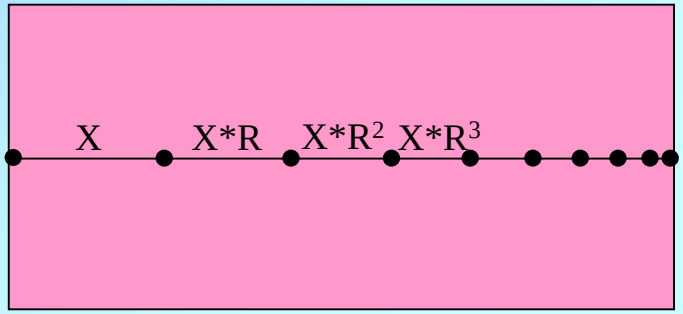


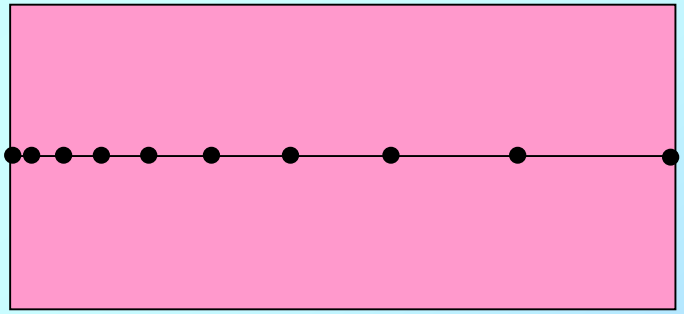
REGION #2



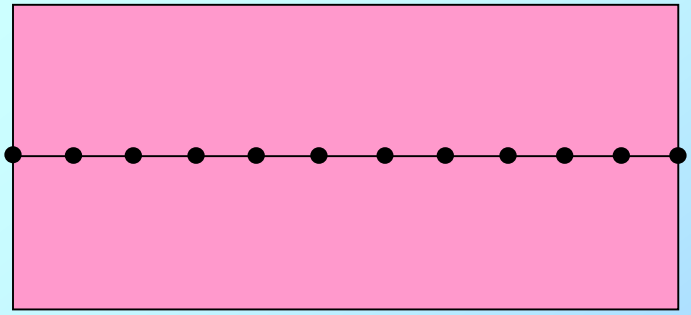
DICTRA - Grids

Geometric grids

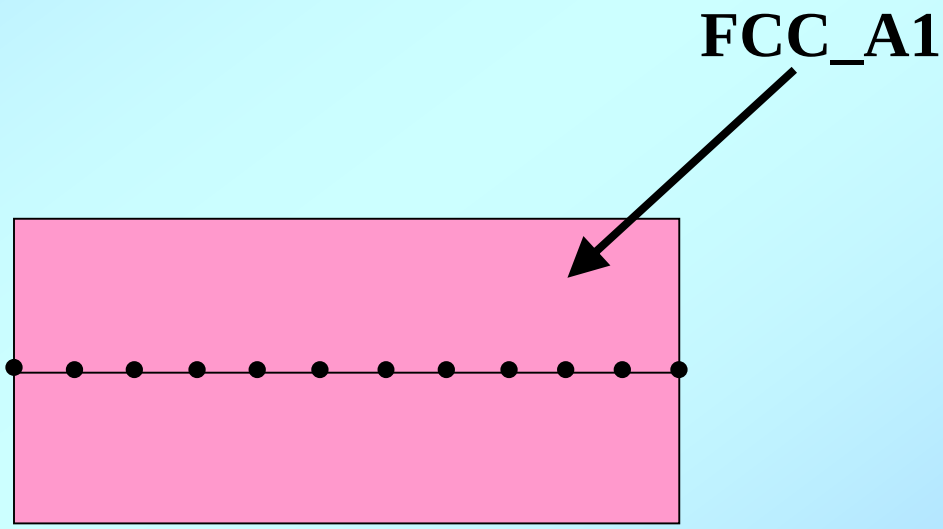




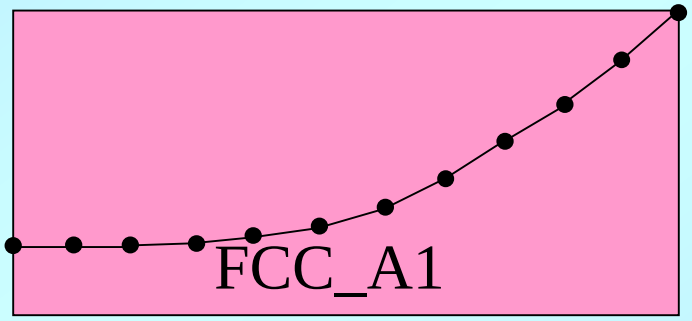
Linear grid



DICTRA - Phases

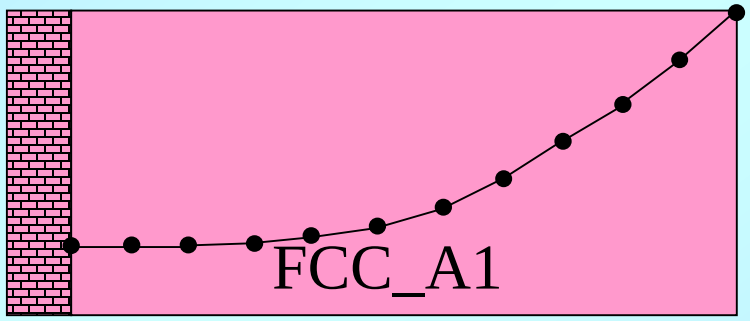


DICTRA - Composition



DICTRA – Boundary conditions

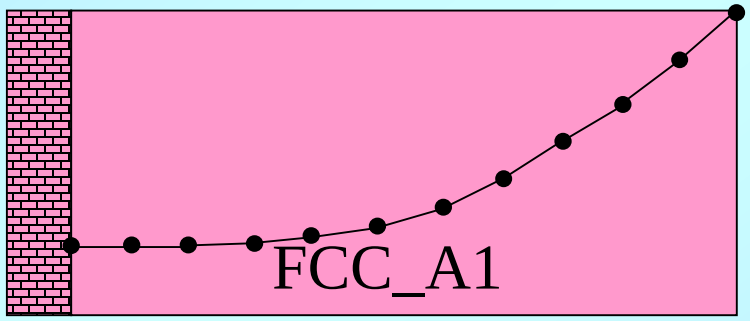
$J_i = 0$



$u_i = C$

DICTRA – Global conditions

$J_i = 0$



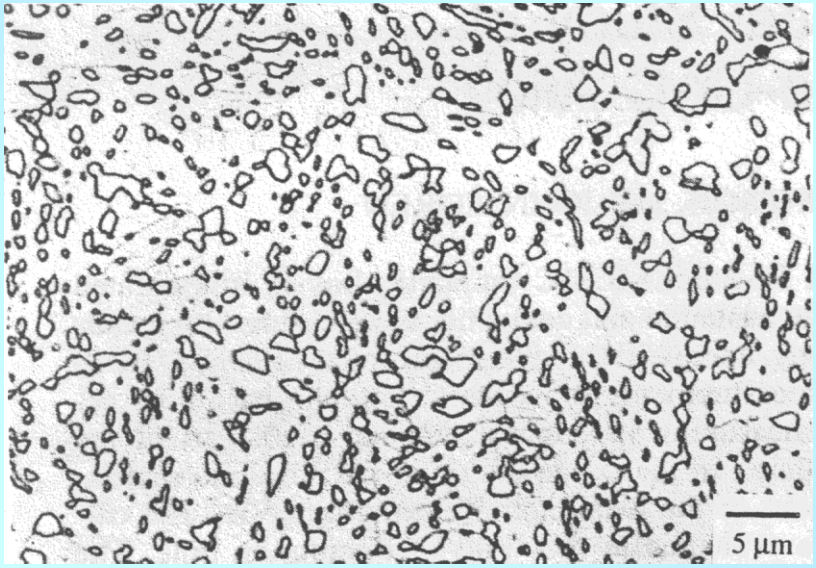
$u_i = C$

T = 1273 K

P = 101325 (1 bar)

Carbide dissolution

- Fe-Cr-C alloy (2.06 at%Cr, 3.91 at%C)
- Soft annealed microstructure (α+cem.)



- Dissolution at 910°C

```
 D I C T R A service version  22 on Linux
 Copyright (1993,1995) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 17-12-02 12:38:55

SYS: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: SGTE solution database with Thermo-Calc extentions
```

```
SYS: @@
SYS: go da
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: SGTE solution database with Thermo-Calc extentions

 VA  DEFINED
 B2_BCC                  L12_FCC                 AL5FE4:
 FE4N                    GAS:G  REJECTED
TDB_SSOL:
TDB_SSOL: @@
TDB_SSOL: @@ USE SSOL DATABASE FOR THERMODYNAMIC DATA
TDB_SSOL: @@
TDB_SSOL: sw ssol
TDB_SSOL: def-sys fe cr c
 FE                      CR                      C
   DEFINED
TDB_SSOL: rej ph * all
 LIQUID:L                FCC_A1                  BCC_A2
 HCP_A3                  DIAMOND_A4              GRAPHITE
 CBCC_A12                CUB_A13                 SIGMA
 CHI_A12                 CEMENTITE               KSI_CARBIDE
 M23C6                   M7C3                    M3C2
 V3C2                    M5C2                    CR3SI
 CRSI2                   FECN_CHI  REJECTED
TDB_SSOL: res ph fcc bcc cem
 FCC_A1                  BCC_A2                  CEMENTITE
   RESTORED
TDB_SSOL: get
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   'J-O Andersson, Calphad Vol 11 (1987) p 271-276, TRITA 0314; C-CR'
   'P. Gustafson, Scan. J. Metall. vol 14, (1985) p 259-267
```

```
      TRITA 0237 (1984); C-FE'
   'Alan Dinsdale, SGTE Data for Pure Elements,
      Calphad Vol 15(1991) p 317-425,
      also in NPL Report DMA(A)195 Rev. August 1990'
   'Byeong-Joo Lee, unpublished revision (1991); C-Cr-Fe-Ni'
   'Alan Dinsdale, SGTE Data for Pure Elements, NPL Report DMA(A)195
      September 1989'
   'J-O Andersson, B. Sundman, CALPHAD Vol 11, (1987), p 83-92
      TRITA 0270 (1986); CR-FE'
   'J-O Andersson, Met. Trans A, Vol 19A, (1988) p 627-636
      TRITA 0207 (1986); C-CR-FE'

 The list of references can be obtained in the Gibbs Energy System also
 by the command LIST_DATA and option R

 -OK-
TDB_SSOL:
TDB_SSOL: @@
TDB_SSOL: @@ ENTER THE POLY-3 MONITOR
TDB_SSOL: @@
TDB_SSOL: go p-3

 POLY version  3.32,  Aug 2001
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: @@ 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
 Automatic start values will be set
  42 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=5.39260539E-7
POLY_3: show w(cem,cr),w(bcc,cr),w(bcc,c)
 W(CEMENTITE,CR)=1.24233467E-1
 W(BCC_A2,CR)=4.66155363E-3
 W(BCC_A2,C)=1.51352072E-4
POLY_3:
POLY_3:
POLY_3:
```

```
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SYS: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: SGTE solution database with Thermo-Calc extentions

 VA  DEFINED
 B2_BCC                  L12_FCC                 AL5FE4:
 FE4N                    GAS:G   REJECTED
TDB_SSOL:
TDB_SSOL: @@
TDB_SSOL: @@ USE SSOL DATABASE FOR THERMODYNAMIC DATA
TDB_SSOL: @@
TDB_SSOL: switch ssol
TDB_SSOL: def-species fe cr c
 FE                      CR                      C
   DEFINED
TDB_SSOL: rej ph * all
 LIQUID:L                FCC_A1                  BCC_A2
```

```
TDB_SSOL: def-species fe cr c
 FE                     CR                     C
   DEFINED
TDB_SSOL: rej ph * all
 LIQUID:L               FCC_A1                 BCC_A2
 HCP_A3                 DIAMOND_A4             GRAPHITE
 CBCC_A12               CUB_A13                SIGMA
 CHI_A12                CEMENTITE              KSI_CARBIDE
 M23C6                  M7C3                   M3C2
 V3C2                   M5C2                   CR3SI
 CRSI2                  FECN_CHI  REJECTED
TDB_SSOL: res ph fcc cementite
 FCC_A1                 CEMENTITE  RESTORED
TDB_SSOL: get
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   'Byeong-Joo Lee, unpublished revision (1991); C-Cr-Fe-Ni'
   'P. Gustafson, Scan. J. Metall. vol 14, (1985) p 259-267
       TRITA 0237 (1984); C-FE'
   'Alan Dinsdale, SGTE Data for Pure Elements, NPL Report DMA(A)195
       September 1989'
   'Alan Dinsdale, SGTE Data for Pure Elements,
       Calphad Vol 15(1991) p 317-425,
       also in NPL Report DMA(A)195 Rev. August 1990'
   'J-O Andersson, B. Sundman, CALPHAD Vol 11, (1987), p 83-92
       TRITA 0270 (1986); CR-FE'

 The list of references can be obtained in the Gibbs Energy System also
 by the command LIST_DATA and option R

 -OK-
TDB_SSOL:
```

```
TDB_SSOL: @@
TDB_SSOL: @@ SWITCH TO MOBILITY DATABASE TO RETRIEVE MOBILITY DATA
TDB_SSOL: @@
TDB_SSOL: app mob2
 Current database: Mobility database, last update 1998-04-08

         Mobility database version 1998-04-08

 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'
```

```
      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'

 The list of references can be obtained in the Gibbs Energy System also
 by the command LIST_DATA and option R

 -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/: 5.39260539E-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 /SITE_FRACTION/: weig-fraction
PROFILE FOR /CR/: cr lin 1.24233467E-1 1.24233467E-1
DIC>
DIC> enter-composition
REGION NAME : /AUS/: aus
PHASE NAME: /FCC_A1#1/: fcc#1
DEPENDENT SUBSTITUTIONAL SPECIES ? (CR,FE) : fe
COMPOSITION TYPE /SITE_FRACTION/: weig-fraction
PROFILE FOR /C/: CR lin 4.66155363E-3 4.66155363E-3
```

```
REGION NAME : /AUS/: aus
PHASE NAME: /FCC_A1#1/: fcc#1
DEPENDENT SUBSTITUTIONAL SPECIES ? (CR,FE) : fe
COMPOSITION TYPE /SITE_FRACTION/: weig-fraction
PROFILE FOR /C/: CR lin 4.66155363E-3 4.66155363E-3
PROFILE FOR /CR/: C  lin 1.51352072E-4 1.51352072E-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  3 seconds
```

```
 D I C T R A service version  22 on Linux
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SYS: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
 GENERATING STARTING VALUES FOR CELL #  1 INTERFACE #  2
 DETERMINING INITIAL EQUILIBRIUM VALUES
 Forcing automatic start values
 Automatic start values will be set
 Forcing automatic start values
 Automatic start values will be set
 Forcing automatic start values
 Automatic start values will be set
 Forcing automatic start values
 Automatic start values will be set
 Forcing automatic start values
 Automatic start values will be set
 Convergence problems, increasing smallest sitefraction from 1.00E-30
 to hardware precision 2.00E-14.  You can restore using SET-NUMERICAL-LIMITS
```

```
Automatic start values will be set
Forcing automatic start values
Automatic start values will be set
Convergence problems, increasing smallest sitefraction from 1.00E-30
to hardware precision 2.00E-14.  You can restore using SET-NUMERICAL-LIMITS
CALCULATING STARTING VALUES:       9   EQUILIBRIUM CALCULATIONS
Forcing automatic start values
Automatic start values will be set
 DONE     6 OUT OF     9
Forcing automatic start values
Automatic start values will be set
Forcing automatic start values
Automatic start values will be set
 DONE     9 OUT OF     9
DETERMINED POTENTIALS  MUR(CR) -89262.4117252

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 = .0406910188227072  CR = .0214382349621405
                       FE = .978561765168366
TOTAL SIZE OF SYSTEM:  5.05643526484E-18 [m^3]
U-FRACTION IN SYSTEM:  C = .0406910188227072  CR = .0214382349621405
                       FE = .978561765168366
TOTAL SIZE OF SYSTEM:  5.05643526484E-18 [m^3]
TIME =  0.10000000E-06 DT =  0.10000000E-06 SUM OF SQUARES =  0.13412399E-18
CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.31449081E-02 AND  -0.31449081E-02
POSITION OF INTERFACE CARB / AUS IS   0.52518551E-06
U-FRACTION IN SYSTEM:  C = .0407188294145162  CR = .0214513918945723
                       FE = .978548608235038
TOTAL SIZE OF SYSTEM:  5.05643526484E-18 [m^3]

TIME =  0.30000000E-06 DT =  0.20000000E-06 SUM OF SQUARES =  0.22235163E-19
CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.30344577E-03 AND  -0.30344577E-03
  :
  :
  :
```

```
  :
CELL # 1 VELOCITY AT INTERFACE # 2 IS  -0.12026667E-10 AND  -0.12026667E-10
POSITION OF INTERFACE CARB / AUS IS   0.20222504E-06
U-FRACTION IN SYSTEM:  C = .0407046660870136  CR = .0213869852397216
                       FE = .978613014890578
TOTAL SIZE OF SYSTEM:  5.05643526484E-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   0.31931434E-02
DELETING TIME-RECORD FOR TIME   0.59299308E-02
DELETING TIME-RECORD FOR TIME   0.10440483E-01
DELETING TIME-RECORD FOR TIME   0.17567552E-01
DELETING TIME-RECORD FOR TIME   0.28913822E-01
DELETING TIME-RECORD FOR TIME   0.48255937E-01
DELETING TIME-RECORD FOR TIME   0.85983057E-01
DELETING TIME-RECORD FOR TIME   0.16143730
DELETING TIME-RECORD FOR TIME   0.31234578
DELETING TIME-RECORD FOR TIME   0.34252747
DELETING TIME-RECORD FOR TIME   0.40289087
DELETING TIME-RECORD FOR TIME   0.52361765
DELETING TIME-RECORD FOR TIME   0.76507122
DELETING TIME-RECORD FOR TIME   0.81336193
DELETING TIME-RECORD FOR TIME   0.90994336
```

```
 DELETING TIME-RECORD FOR TIME    0.40289087
 DELETING TIME-RECORD FOR TIME    0.52361765
 DELETING TIME-RECORD FOR TIME    0.76507122
 DELETING TIME-RECORD FOR TIME    0.81336193
 DELETING TIME-RECORD FOR TIME    0.90994336
 DELETING TIME-RECORD FOR TIME     1.1031062
 DELETING TIME-RECORD FOR TIME     1.4894319
 DELETING TIME-RECORD FOR TIME     1.5666971
 DELETING TIME-RECORD FOR TIME     1.7212274
 DELETING TIME-RECORD FOR TIME     2.0302879
 DELETING TIME-RECORD FOR TIME     2.6484091
 DELETING TIME-RECORD FOR TIME     3.8846513
 DELETING TIME-RECORD FOR TIME     6.3571359
 DELETING TIME-RECORD FOR TIME     11.302105
 DELETING TIME-RECORD FOR TIME     21.192043
 DELETING TIME-RECORD FOR TIME     40.971920
 DELETING TIME-RECORD FOR TIME     80.531672
 DELETING TIME-RECORD FOR TIME     159.65118
 DELETING TIME-RECORD FOR TIME     317.89019
 DELETING TIME-RECORD FOR TIME     634.36821
 DELETING TIME-RECORD FOR TIME     1267.3243
 DELETING TIME-RECORD FOR TIME     2267.3243
 DELETING TIME-RECORD FOR TIME     3267.3243
 DELETING TIME-RECORD FOR TIME     4267.3243
 DELETING TIME-RECORD FOR TIME     5267.3243
 DELETING TIME-RECORD FOR TIME     6267.3243
 DELETING TIME-RECORD FOR TIME     7267.3243
 DELETING TIME-RECORD FOR TIME     8267.3243

 KEEPING TIME-RECORD FOR TIME     9267.3243
 AND FOR TIME                     10000.000
 WORKSPACE RECLAIMED
DIC>
DIC> set-inter
 --OK---
DIC>DIC> CPU time  219 seconds
```

```
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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
```
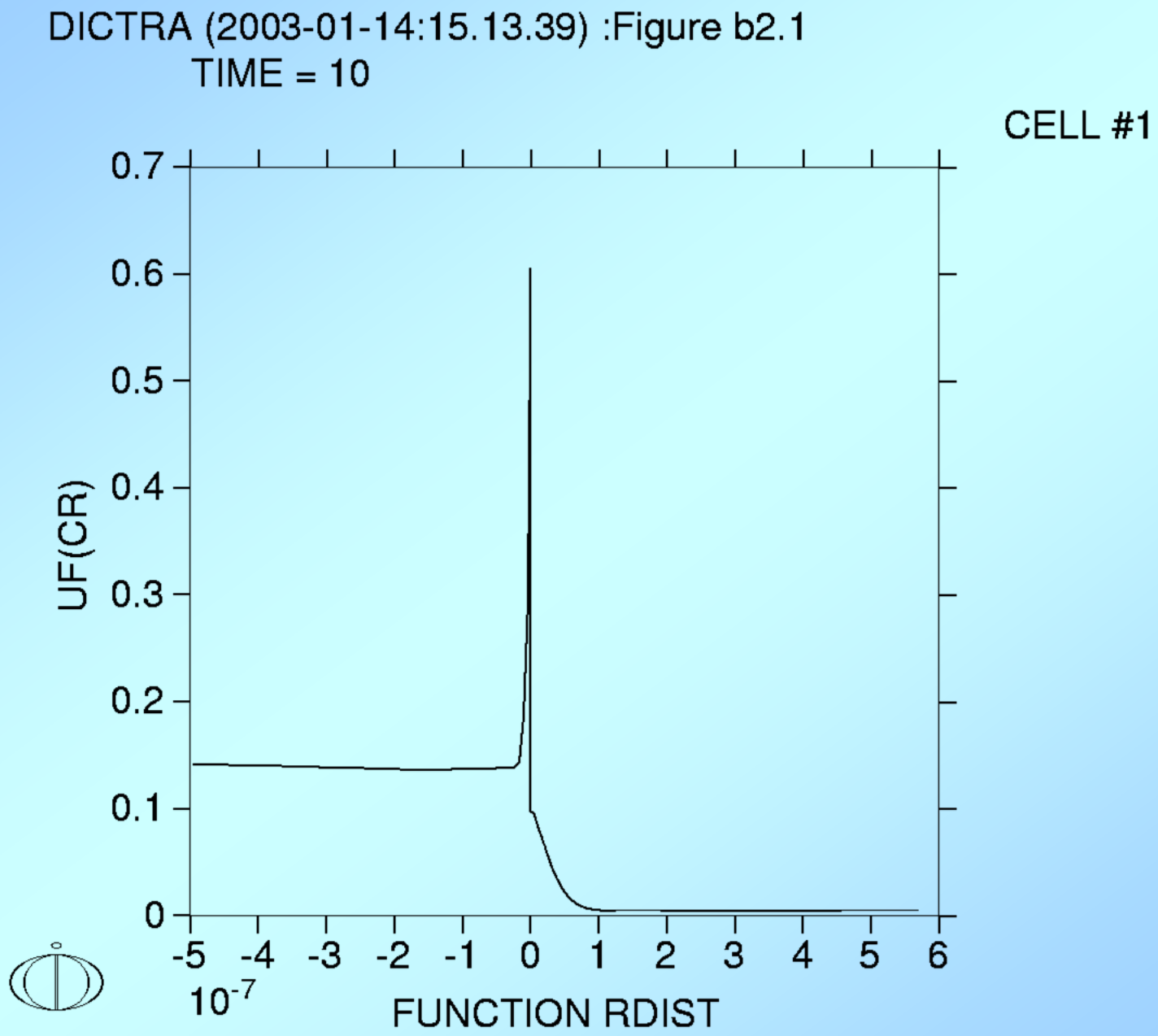
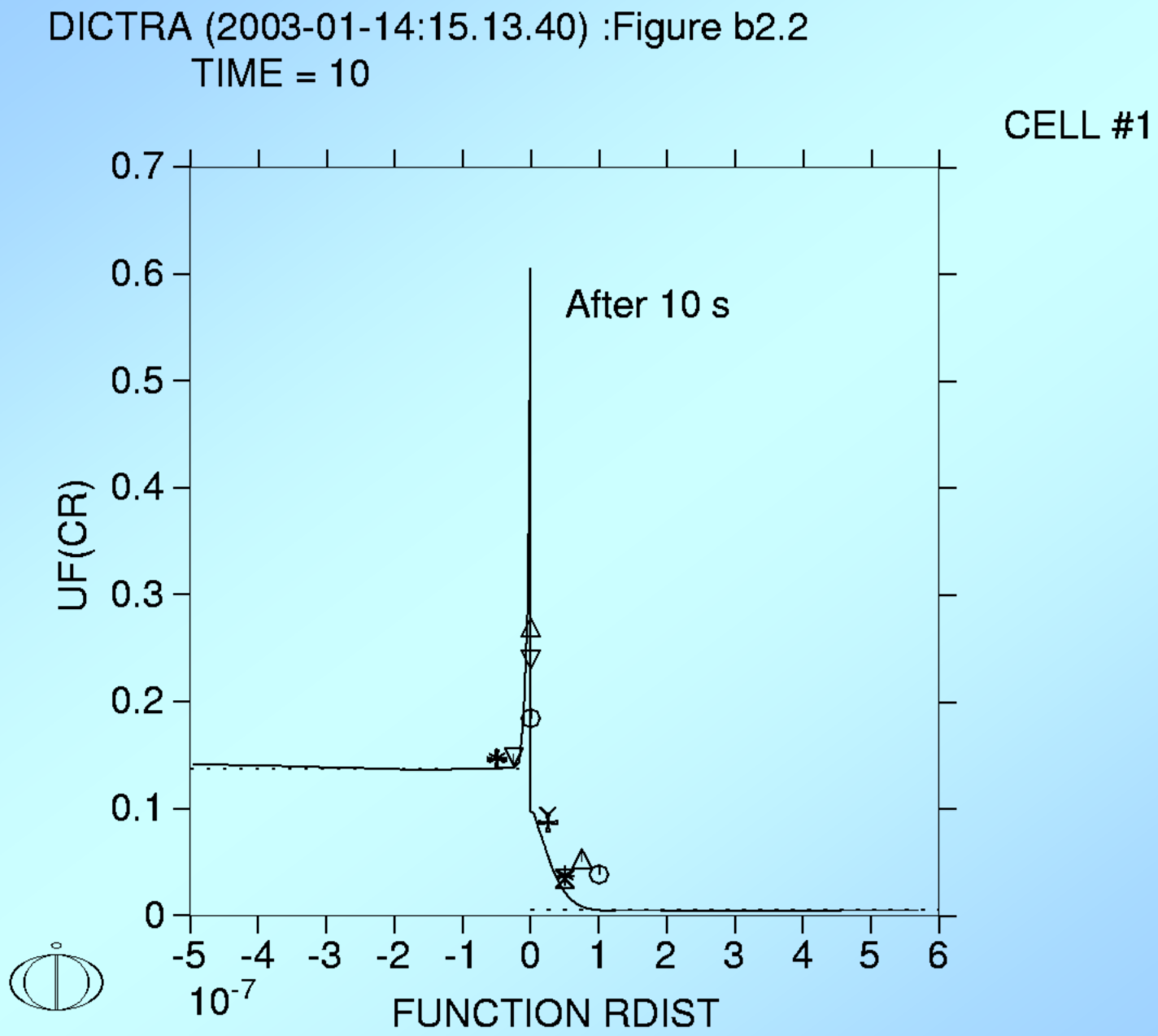
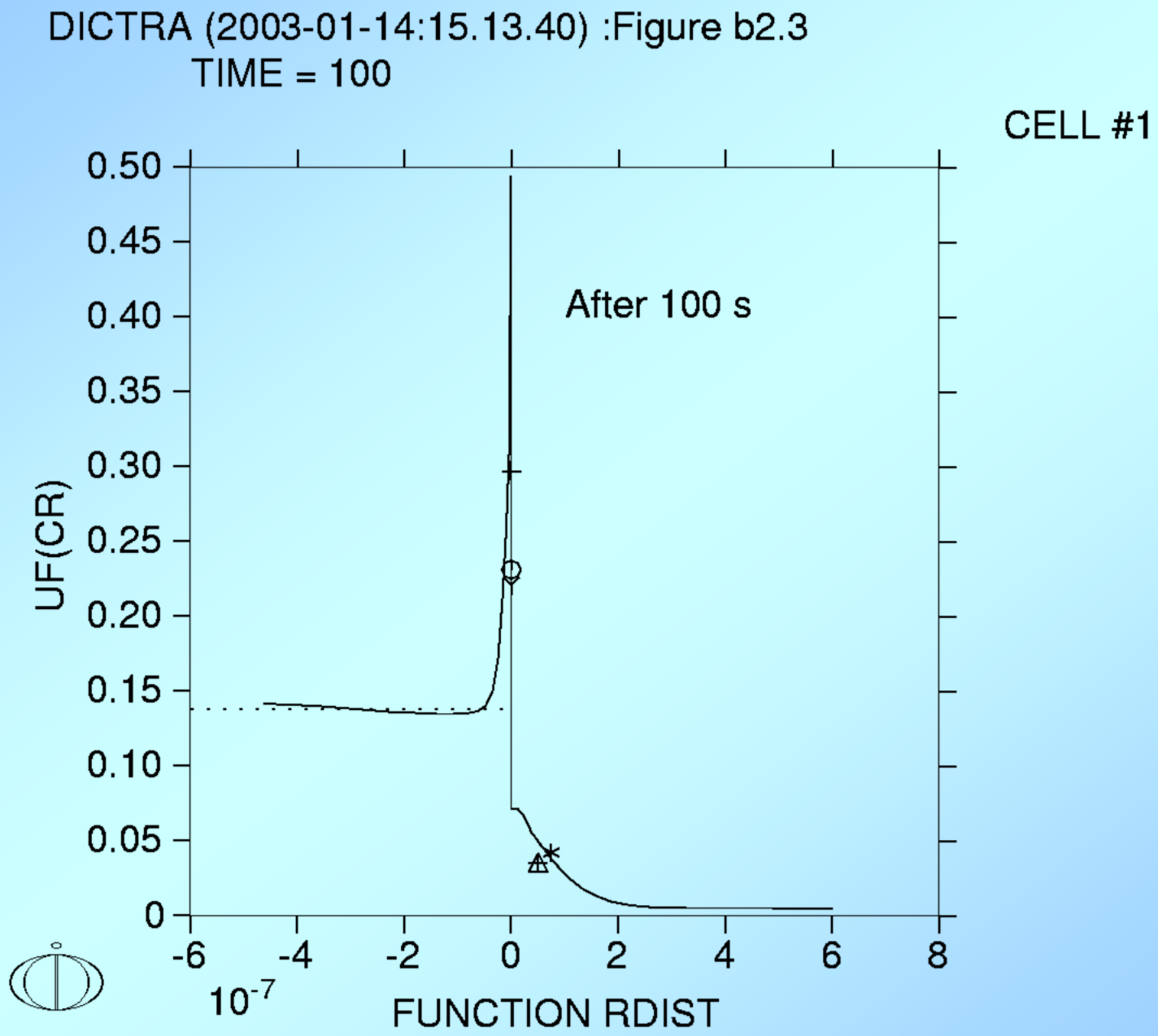

```
POST-1:
POST-1: @@
POST-1: @@ LET US PLOT CHROMIUM CONCENTRATION PROFILES
POST-1: @@ WE THEN SET DISTANCE AS X-AXIS (NOTE THAT DISTANCE IS SET AS
POST-1: @@ INDEPENDENT VARIABLE AUTOMATICALLY) AND U-FRACTION CARBON AS Y-AXIS
POST-1: @@ REMEMBER THAT ONE ALSO HAS TO SET PLOT CONDITION
POST-1: @@
POST-1: @@ 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_>
```


DICTRA (2003-01-14:15.13.39) :Figure b2.1
TIME = 10
CELL #1
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
UF(CR)
-5 -4 -3 -2 -1 0 1 2 3 4 5 6
10-7
FUNCTION RDIST

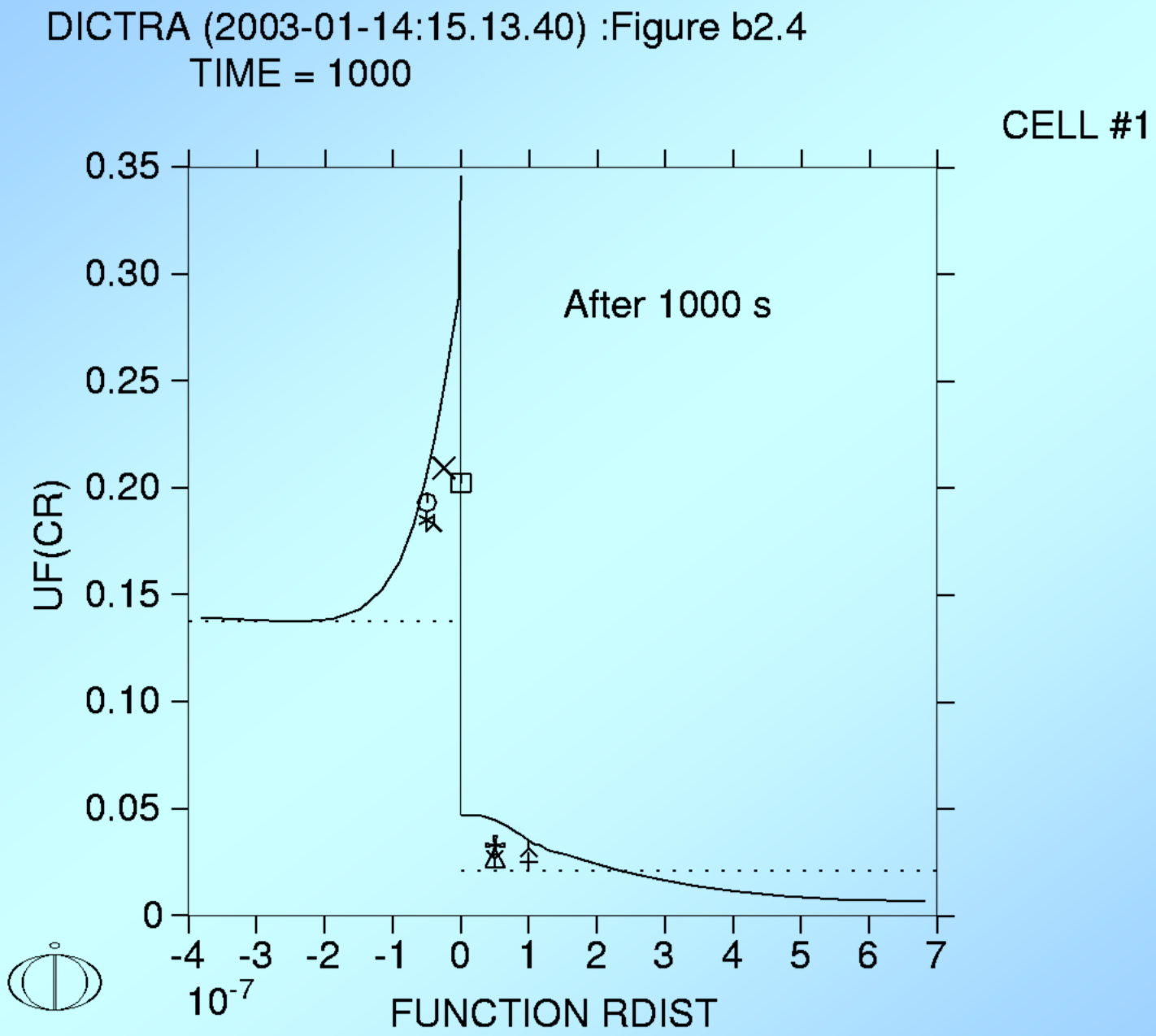
```
POST-1:
POST-1: @@
POST-1: @@ INCLUDE EXPERIMENTAL DATAPOINTS ON THE FIGURE FOR COMPARISION
POST-1: @@
POST-1: @@ FIRST LIST DATASETS
POST-1: @@
POST-1: app y exb2.exp
PROLOGUE NUMBER: /0/:  0
DATASET NUMBER(s): /-1/:  -1
 DATASET 1 CONCENTRATION PROFILE T=10S
 DATASET 2 CONCENTRATION PROFILE T=100S
 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:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: @@
```


DICTRA (2003-01-14:15.13.40) :Figure b2.2
TIME = 10
CELL #1
After 10 s
UF(CR)
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
-5 -4 -3 -2 -1 0 1 2 3 4 5 6
10-7
FUNCTION RDIST

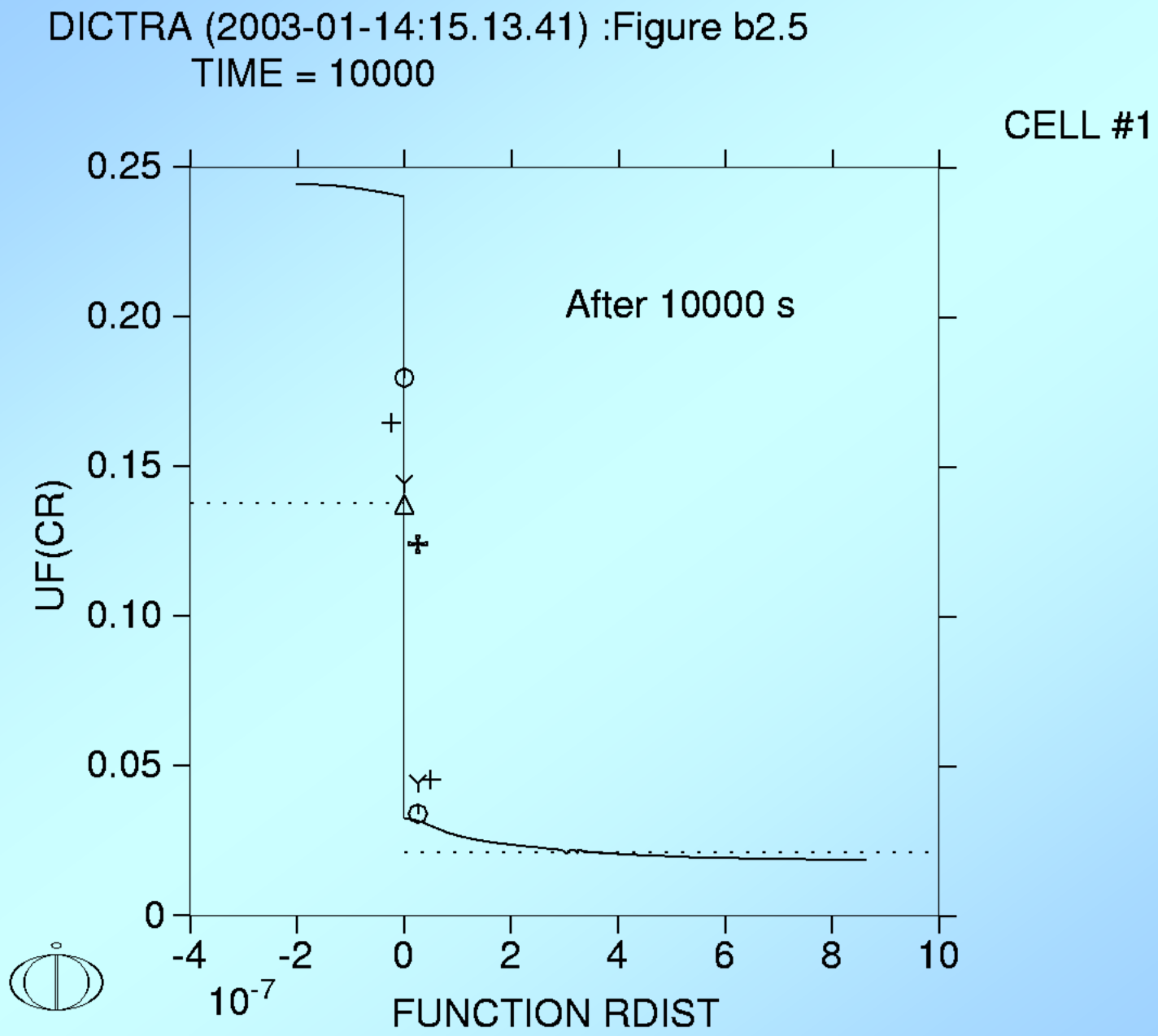
```
POST-1:
POST-1:
POST-1:@?<_hit_return_to_continue_>
POST-1:
POST-1: @@
POST-1: @@ PLOT ALSO FOR 100, 1000 AND 10000S
POST-1: @@
POST-1:
POST-1: s-p-c time 100
POST-1:
POST-1: app y exb2.exp
PROLOGUE NUMBER: /0/:  0
DATASET NUMBER(s): /-1/:  2
POST-1:
POST-1: set-title Figure b2.3
POST-1: plo SCREEN

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


DICTRA (2003-01-14:15.13.40) :Figure b2.3
TIME = 100
CELL #1
After 100 s
UF(CR)
0.50
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0
-6
-4
-2
0
2
4
6
8
10-7
FUNCTION RDIST

```
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:
```

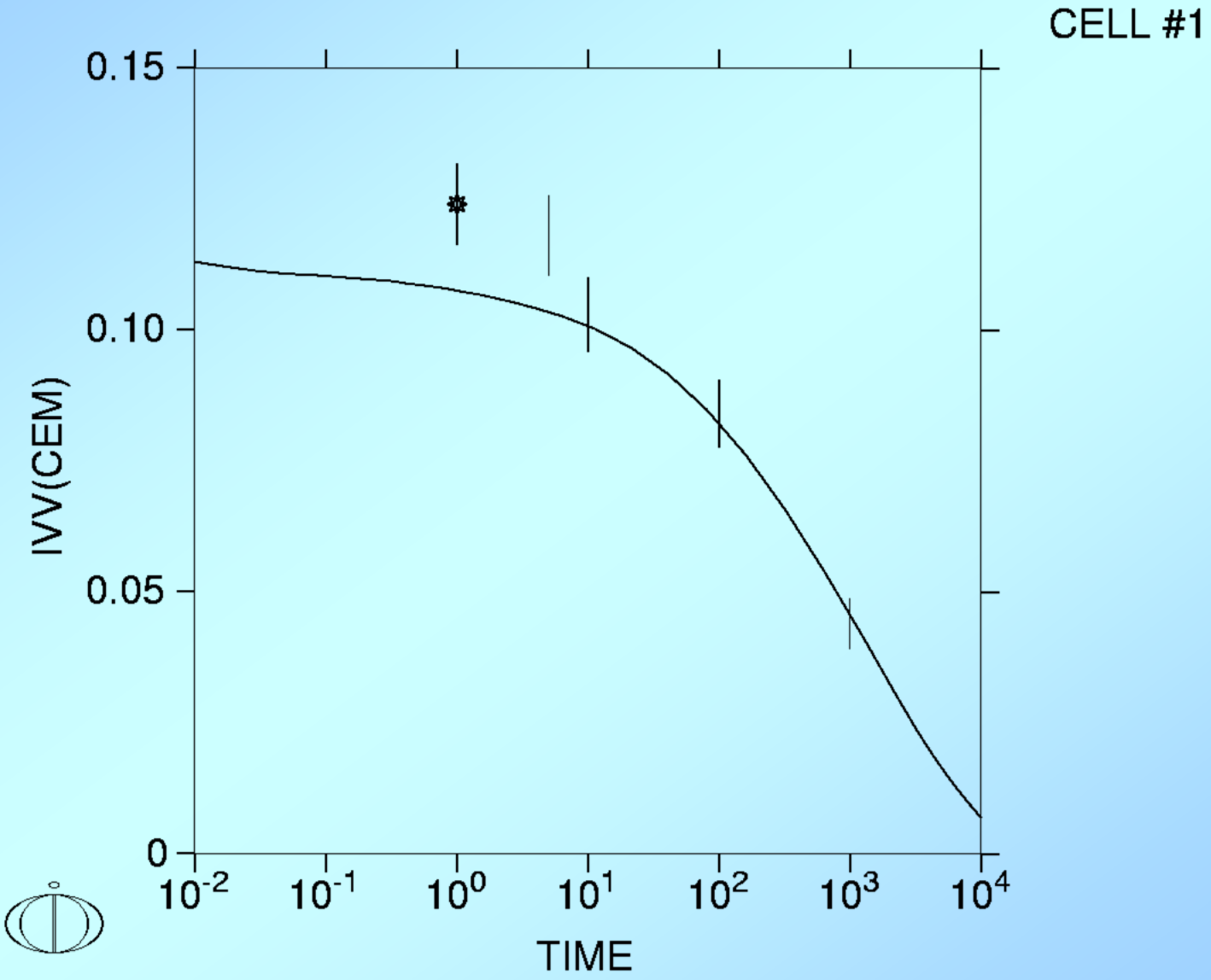

DICTRA (2003-01-14:15.13.40) :Figure b2.4
TIME = 1000
CELL #1
After 1000 s
UF(CR)
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0
-4
-3
-2
-1
0
1
2
3
4
5
6
7
10-7
FUNCTION RDIST

```
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
```

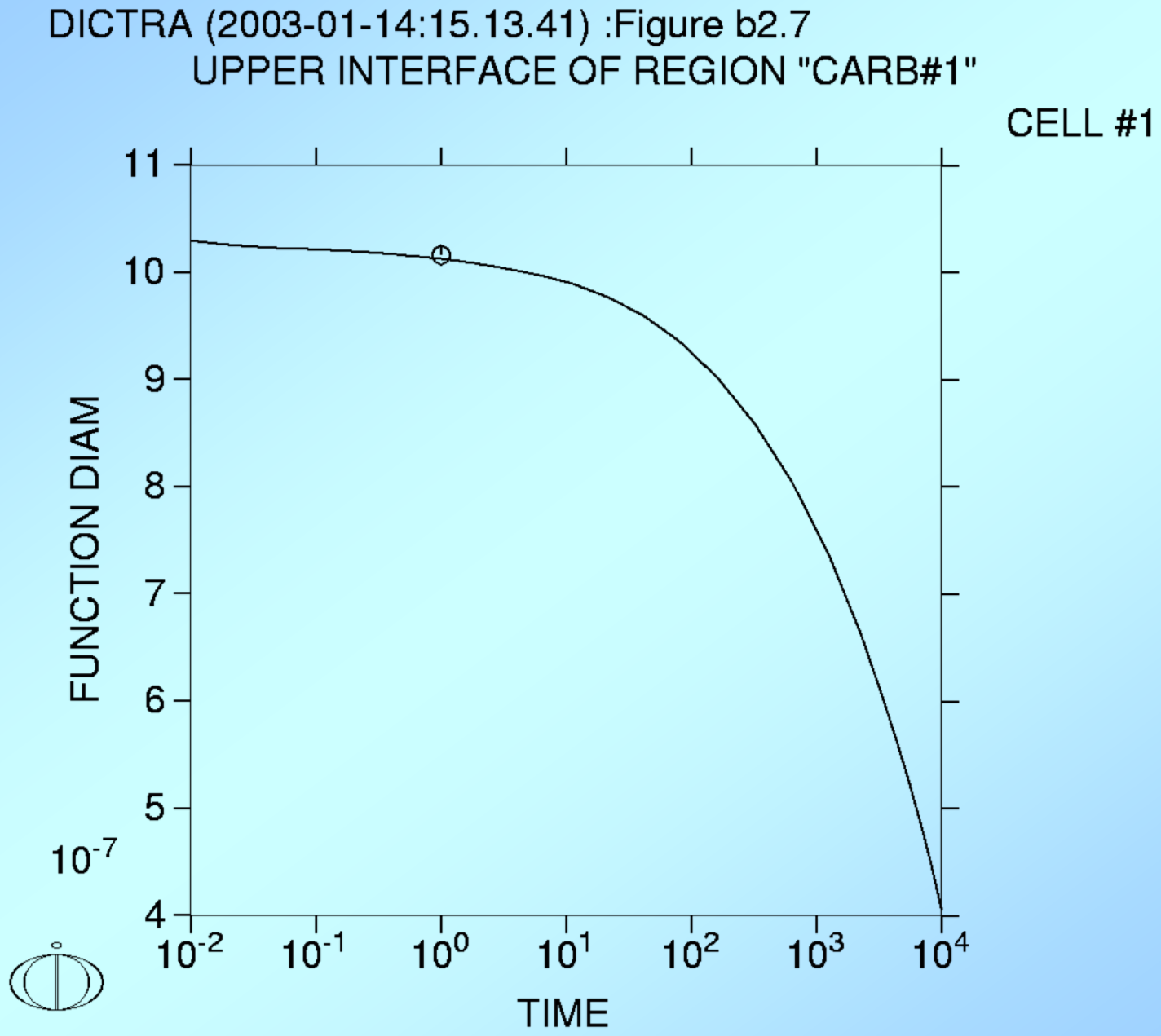

DICTRA (2003-01-14:15.13.41) :Figure b2.5
TIME = 10000
CELL #1
After 10000 s
UF(CR)
0.25
0.20
0.15
0.10
0.05
0
-4
-2
0
2
4
6
8
10
10-7
FUNCTION RDIST

```
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:
```

DICTRA (2003-01-14:15.13.41) :Figure b2.6



```
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  2 seconds
```


DICTRA (2003-01-14:15.13.41) :Figure b2.7
UPPER INTERFACE OF REGION "CARB#1"
CELL #1
FUNCTION DIAM
10^{-7}
11
10
9
8
7
6
5
4
10^{-2}
10^{-1}
10^{0}
10^{1}
10^{2}
10^{3}
10^{4}
TIME