



DICTRA On-line Training

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Day 3: 18 April 2024



www.thermocalc.com

Diffusion Module (DICTRA)

Day 3

9:00	Home assignment 2
9:10	Example – Dissolution of cementite particles (moving phase boundary calculation)
10:10	Console mode and macro files.
10:30	Q&A
10:45	Example – Gradient sintering in Cemented carbide
11:30	Trouble shooting
11:45	Q&A
12:00	End

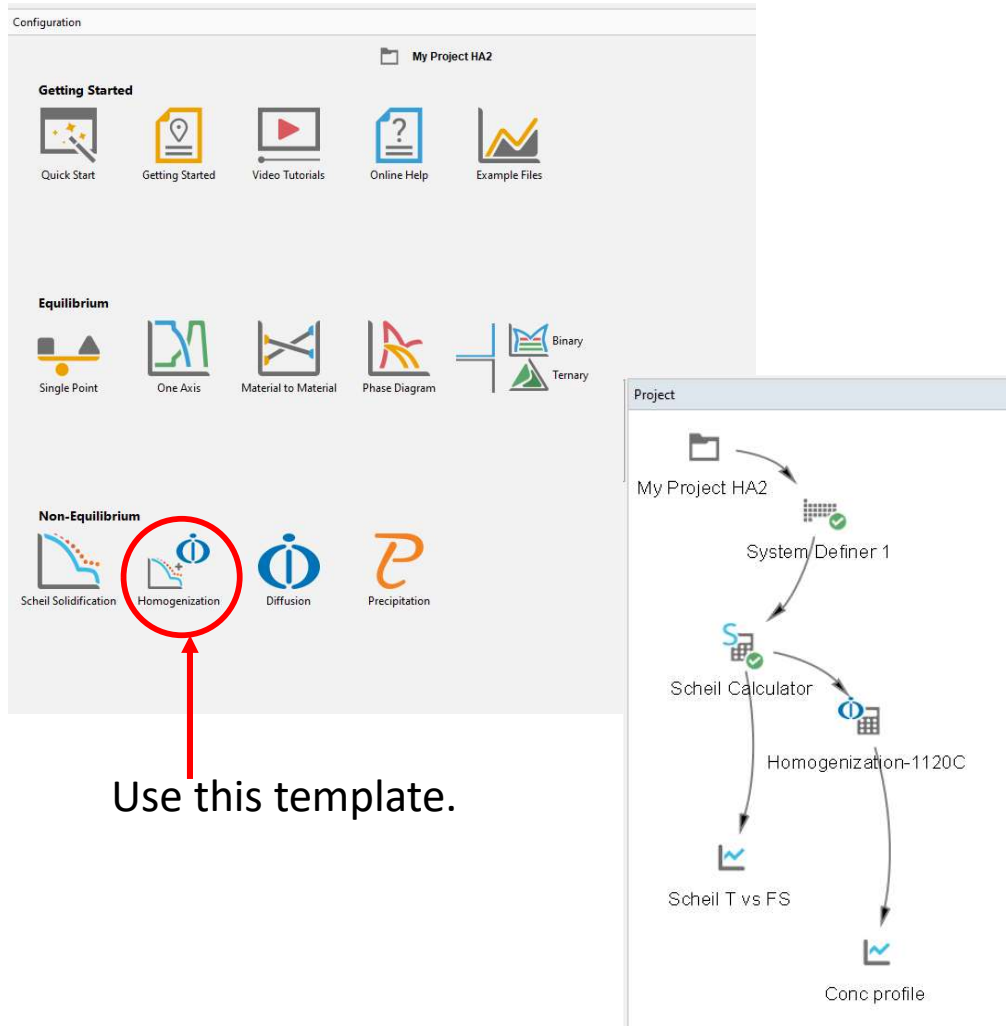
Today's download:

<https://download.thermocalc.com/courses/DICTRA/DICT-Day3/>

Home assignment 2

Home assignment 2: Solidification & Homogenisation

CrNi-steel: Fe(bal.) – 1.9 Ni – 0.95 Cr – 0.65 Mn – 0.4 C (wt-%)



Configuration

My Project HA2

Getting Started

Quick Start Getting Started Video Tutorials Online Help Example Files

Equilibrium

Single Point One Axis Material to Material Phase Diagram Binary Ternary

Non-Equilibrium

Scheil Solidification Homogenization Diffusion Precipitation

Project

My Project HA2

System Definer 1

Scheil Calculator

Homogenization-1120C

Scheil T vs FS

Conc profile

Use this template.

Start with a Classic Scheil simulation, with carbon as a fast diffusing element.

Then use the result of the Scheil as start composition in the homogenisation simulation. Use default settings.

Secondary dendrite arm spacing: 200 μm .
Temperature 1120 $^{\circ}\text{C}$.

Time for homogenisation: 72 hours.

Task: Check how the concentration profiles for Ni and Cr change over time.

Compare with exp. data: Fuchs_1120.exp

Home assignment 2: Solidification & Homogenisation



CrNi-steel: Fe(bal.) – 1.9 Ni – 0.95 Cr – 0.65 Mn – 0.4 C (wt-%)

Considerations:

To export the Scheil concentration profile to a DICTRA simulation, the Homogenisation template must be used.

Set a Classic Scheil simulation with C as fast diffuser. However, the calculated carbon profile will not be used.

In the Diffusion Calculator, use these settings.

And for instance these plot settings.

The screenshot shows the plot settings for the Diffusion Calculator. The X-axis is set to 'Time' in 'Hours' with a 'Linear' axis type and limits from 0.0 to 1.0 with a step of 0.1. The Y-axis is set to 'Composition' in 'All' 'Mass percent' with a 'Linear' axis type and limits from 0.0 to 4 with a step of 0.5. The plot condition is set to 'Interface' for 'Region' 'Region1' 'Upper'. The independent variable is 'Time'.

The screenshot shows the 'Region' settings in the Diffusion Calculator. The Name is 'Region1', Half secondary arm spacing is 2.0E-4 m, 50 points and type is 'Linear'. Composition profiles are set to 'Average over all solidified phases' and Phases are 'All solidified phases'. Below the settings is a table of Scheil segregation profiles for fast diffusers.

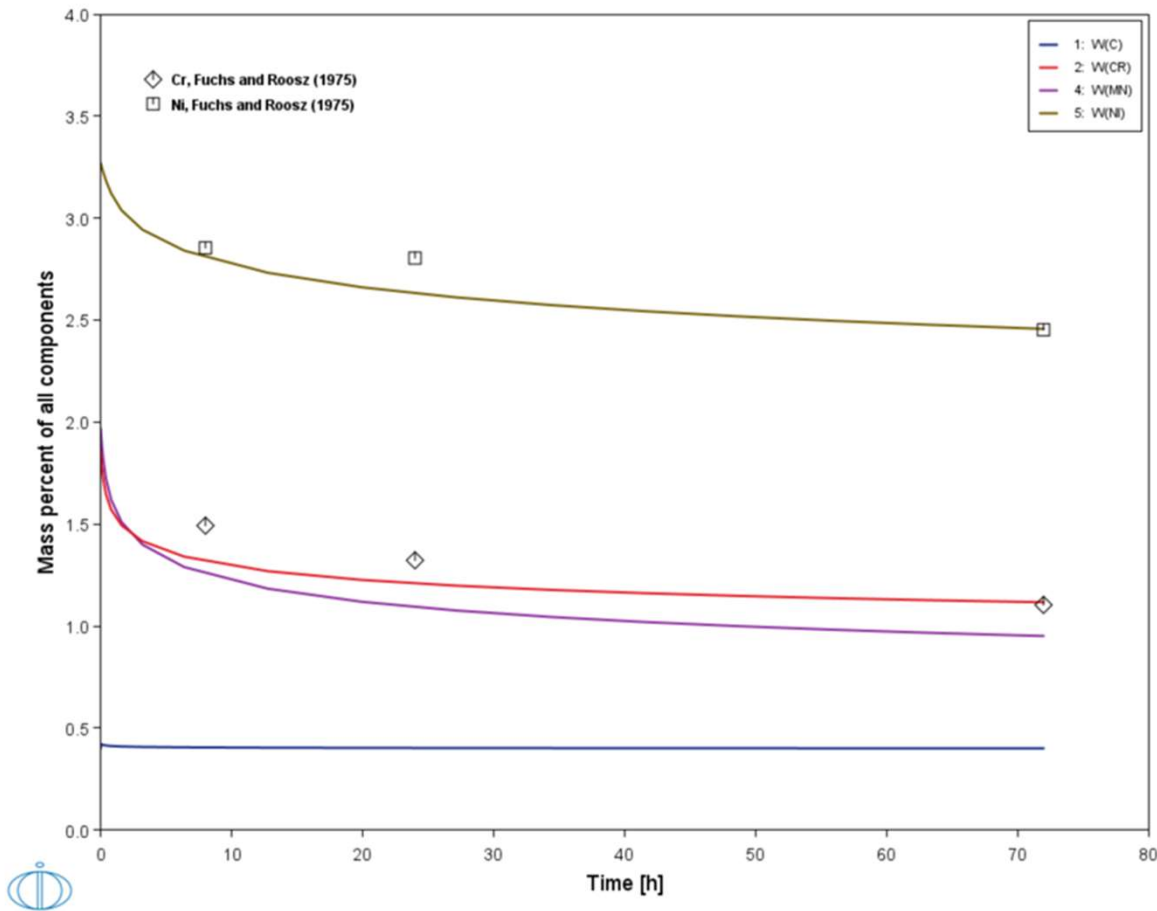
Distance	Mn	Ni	Cr	C
0.000000	0.497700	1.678352	0.848661	0.400000
0.000010	0.503632	1.688198	0.852766	0.400000

There are two TCU files for HA2 included in today's download, one of them with calculated results.

Home assignment 2: Solidification & Homogenisation

CrNi-steel: Fe(bal.) – 1.9 Ni – 0.95 Cr – 0.65 Mn – 0.4 C (wt-%)

2023.10.10.14.37.19
Diffusion Calculator 1:
TCFE13, MOBFE8 : Fe, Mn, Ni, Cr, C
W(Mn) = 0.65, W(Ni) = 1.9, W(Cr) = 0.95, W(C) = 0.4
Mass percent Mn = 0.65, Mass percent Ni = 1.9, Mass percent Cr = 0.95

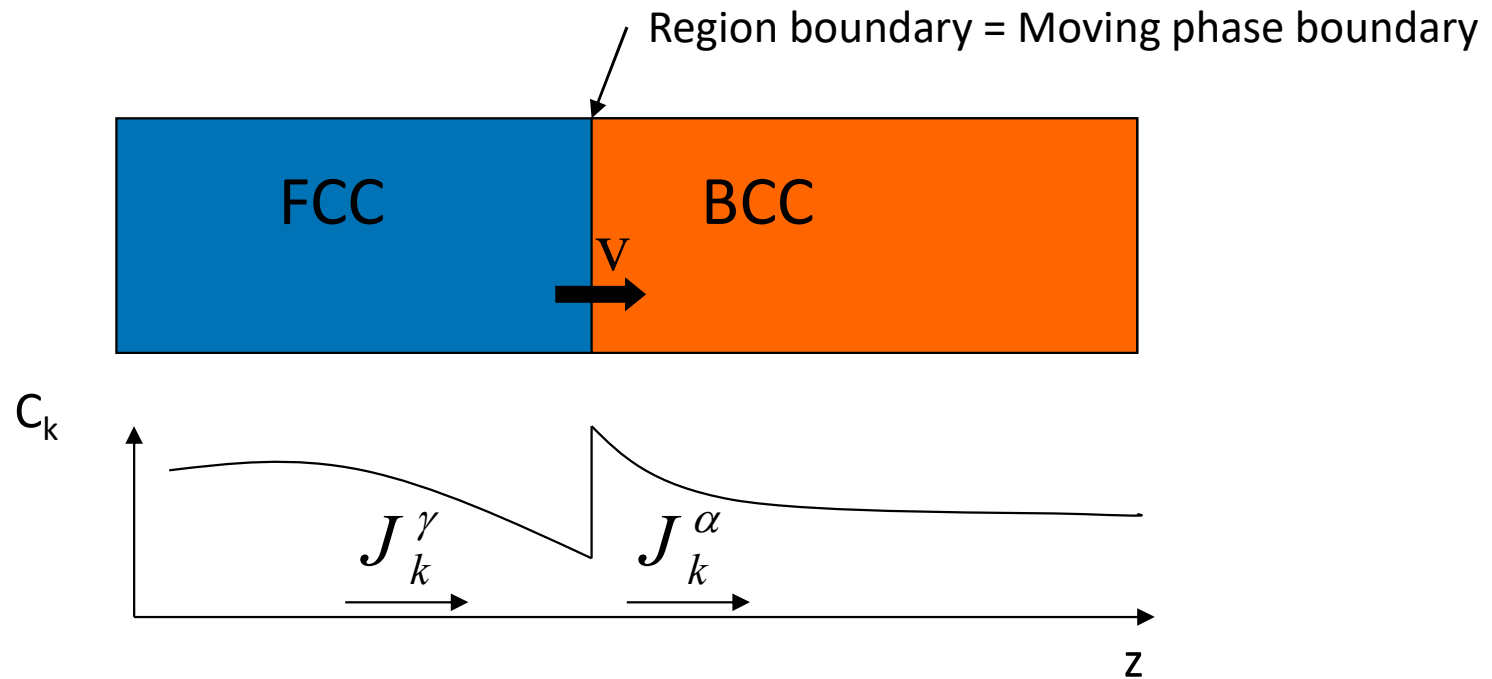


Result.



Moving Phase Boundary – Cementite dissolution

Moving phase boundary simulation



Solve diffusion equation in each phase

Calculate displacement of phase boundary

Thermo-Calc is used to find tie-lines

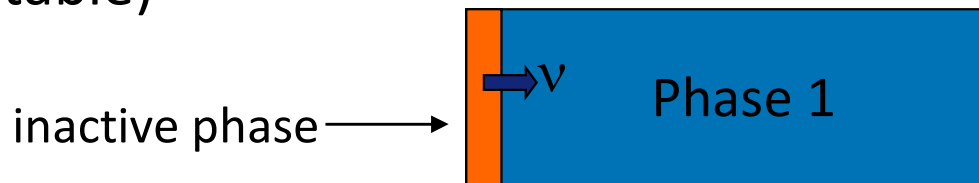
Moving Phase Boundary

- Moving phase boundary simulations may be set up in DICTRA in two different ways:

1) Introducing two or more adjacent regions containing different phases



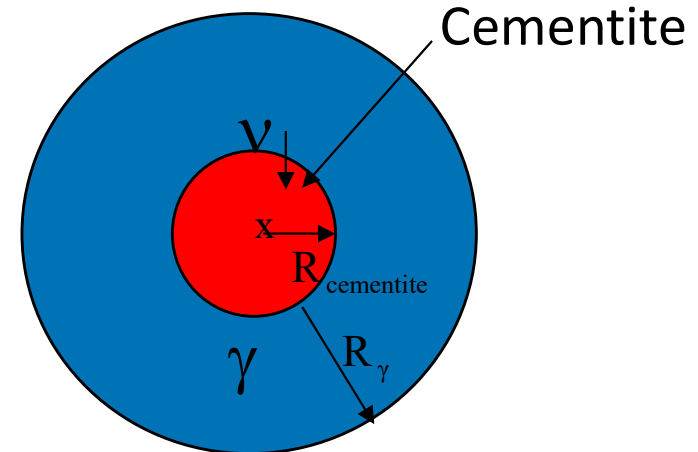
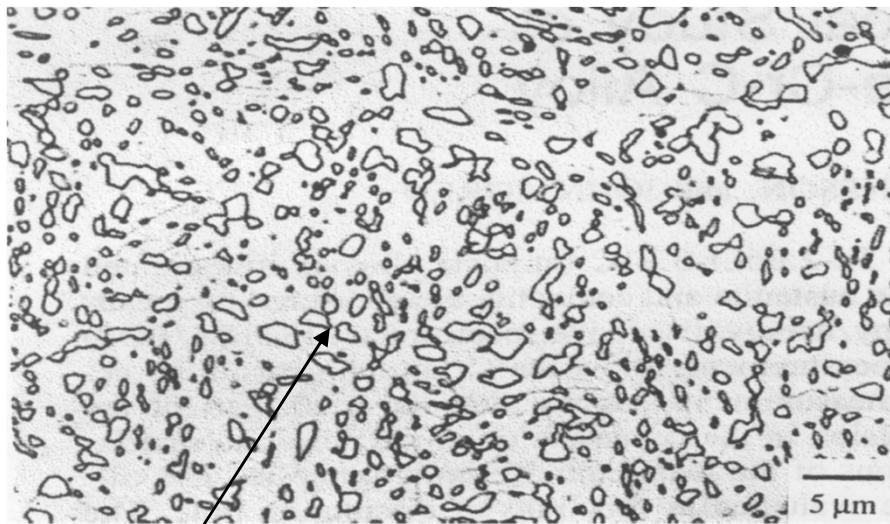
2) Entering an inactive phase (formed when thermodynamically stable)



Cementite dissolution in an Fe–Cr–C alloy

Dissolution of cementite at 910°C (1183K)

$x(\text{Cr})= 0.0206$, $x(\text{C})=0.0391$, bal. Fe.

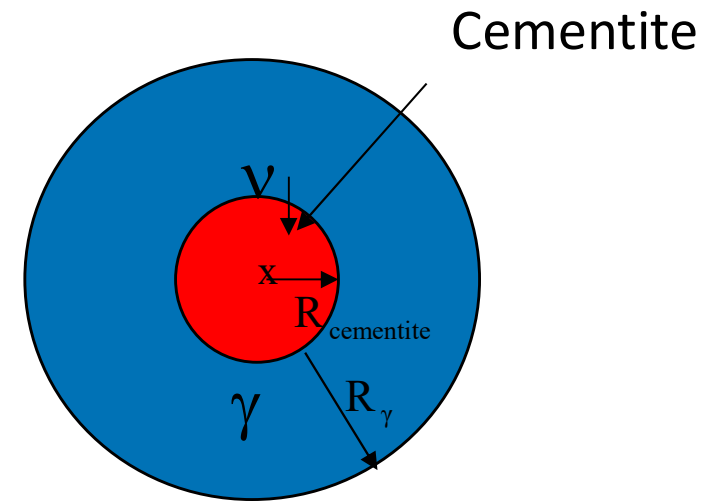
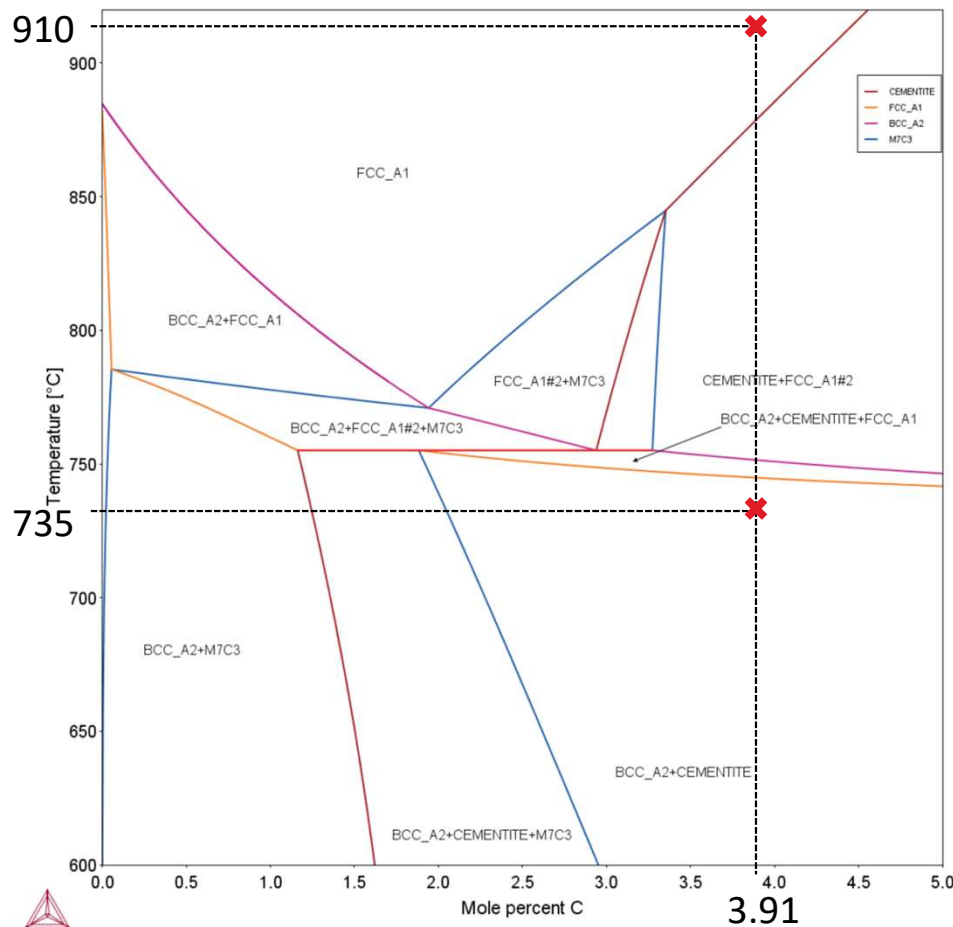


Initial particle radius is estimated to 0.5255 μm. Heat treatment at 735°C.

Cementite dissolution in an Fe–Cr–C alloy

910°C $x(\text{Cr}) = 0.0206$, $x(\text{C}) = 0.0391$, bal. Fe.

2020.10.24.17.17.53
 TCFE9, MOBFE4: Fe, Cr, C
 Temperature [°C] = 910.0, Pressure [Pa] = 100000.0, System size [mol] = 1.0, Mole percent Cr = 2.06, Mole percent C = 3.91
 Pressure [Pa] = 100000.0, System size [mol] = 1.0, Mole percent Cr = 2.06



Phase diagram section at 2.06 mol-% Cr.

Cementite dissolution in an Fe–Cr–C alloy

The volume fraction of cementite and the composition in the cementite, is calculated at the normalizing temperature 735°C (1008 K).

The size of the γ region is calculated from:

$$\frac{R_{\text{cementite}}^3}{R_{\text{tot}}^3} = \frac{V_{\text{cementite}}}{V_{\text{tot}}} = V_{\text{cementite}}^f$$

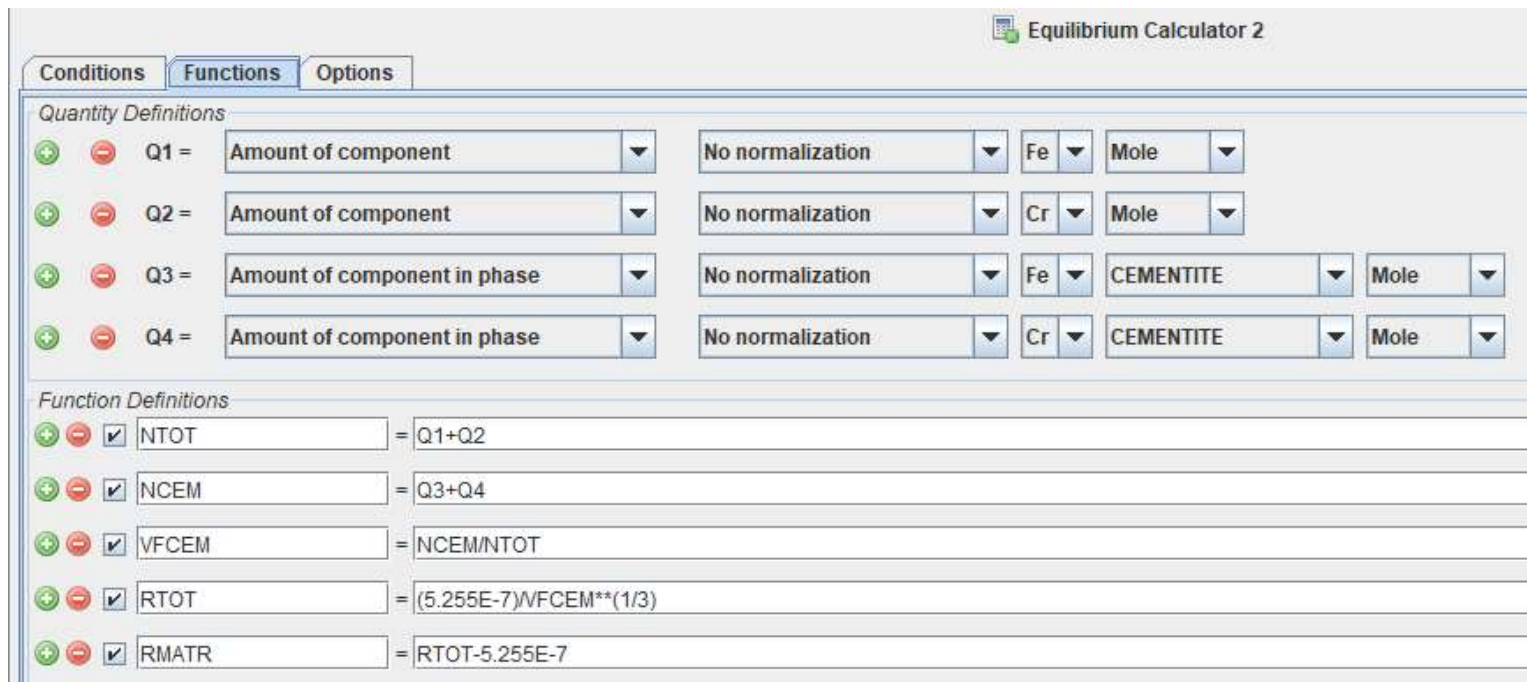
$$\Rightarrow R_{\gamma} = R_{\text{tot}} - R_{\text{cementite}} = \frac{R_{\text{cementite}}}{\sqrt[3]{V_{\text{cementite}}^f}} - R_{\text{cementite}}$$

$$\left(V_{\text{cementite}}^f = \frac{n(\text{cem, Cr}) + n(\text{cem, Fe})}{n(\text{Cr}) + n(\text{Fe})} \right)$$

Cementite dissolution in an Fe–Cr–C alloy

The volume fraction of cementite and the composition in the cementite, is calculated at the normalizing temperature 735°C (1008 K).

Here is how to set it up in the Equilibrium Calculator's Functions page:



The screenshot shows the 'Equilibrium Calculator 2' software interface, specifically the 'Functions' tab. The interface is divided into two main sections: 'Quantity Definitions' and 'Function Definitions'.

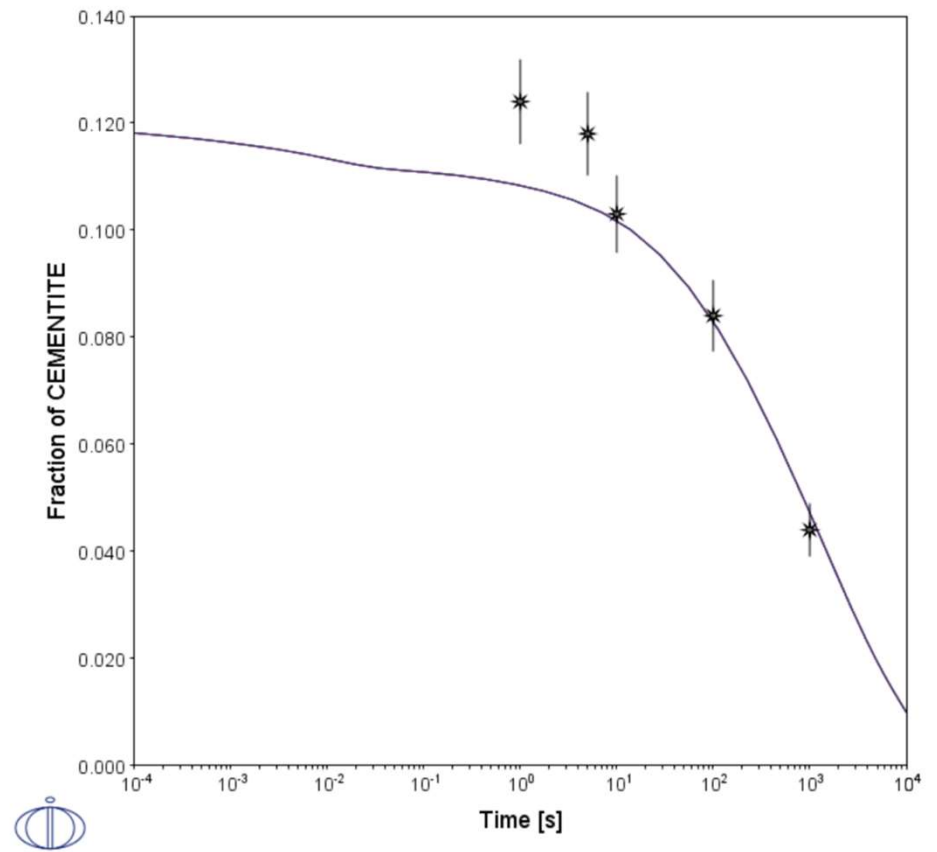
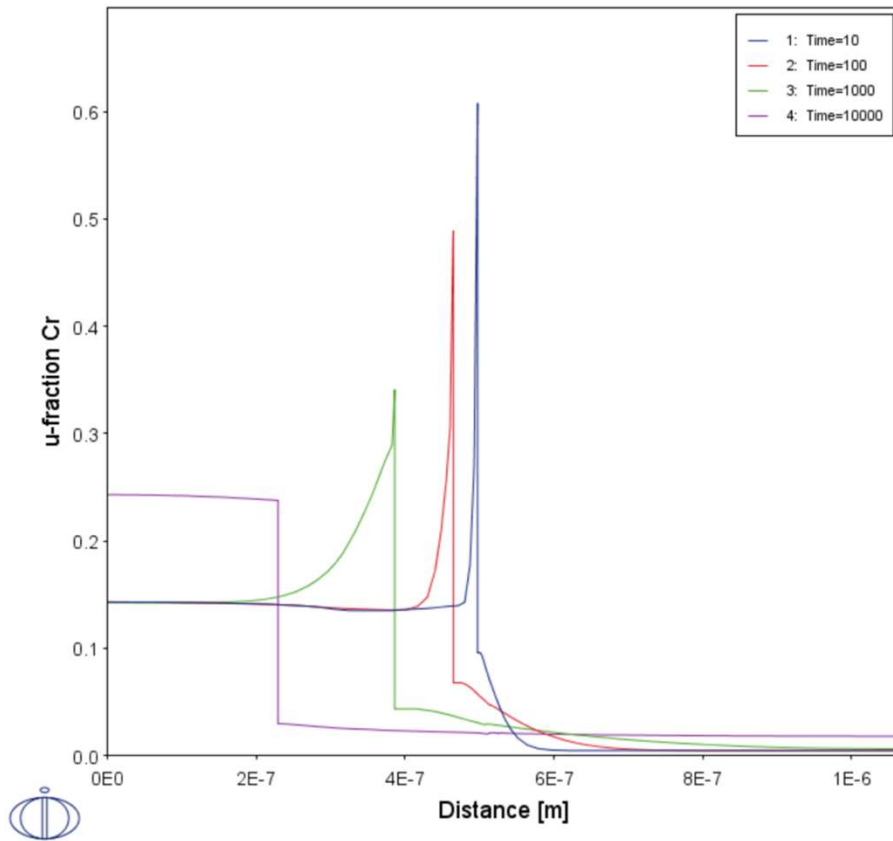
Quantity Definitions:

Quantity	Definition	Normalization	Element	Phase	Unit
Q1	Amount of component	No normalization	Fe		Mole
Q2	Amount of component	No normalization	Cr		Mole
Q3	Amount of component in phase	No normalization	Fe	CEMENTITE	Mole
Q4	Amount of component in phase	No normalization	Cr	CEMENTITE	Mole

Function Definitions:

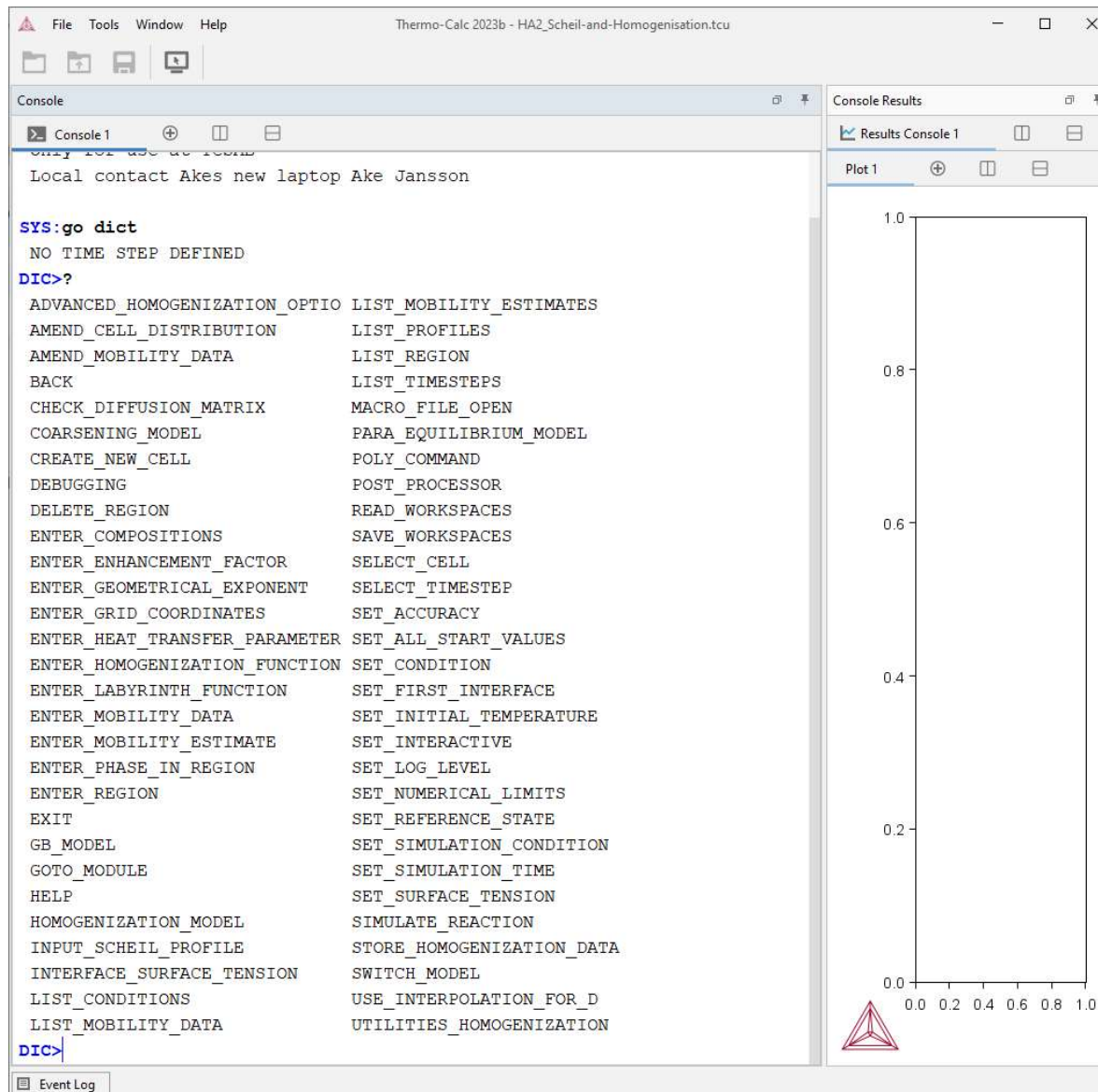
Function	Equation
NTOT	Q1+Q2
NCEM	Q3+Q4
VFCEM	NCEM/NTOT
RTOT	(5.255E-7)/VFCEM**(1/3)
RMATR	RTOT-5.255E-7

Results – cementite dissolution



Console Mode

Console mode – DICTRA monitor



The screenshot displays the Thermo-Calc 2023b interface. The main window title is "Thermo-Calc 2023b - HA2_Scheil-and-Homogenisation.tcu". The interface is divided into several panels:

- Console:** Shows the command prompt with the following text:

```
Local contact Akes new laptop Ake Jansson  
  
SYS:go dict  
NO TIME STEP DEFINED  
DIC>?  
ADVANCED_HOMOGENIZATION_OPTIO LIST_MOBILITY_ESTIMATES  
AMEND_CELL_DISTRIBUTION LIST_PROFILES  
AMEND_MOBILITY_DATA LIST_REGION  
BACK LIST_TIMESTEPS  
CHECK_DIFFUSION_MATRIX MACRO_FILE_OPEN  
COARSENING_MODEL PARA_EQUILIBRIUM_MODEL  
CREATE_NEW_CELL POLY_COMMAND  
DEBUGGING POST_PROCESSOR  
DELETE_REGION READ_WORKSPACES  
ENTER_COMPOSITIONS SAVE_WORKSPACES  
ENTER_ENHANCEMENT_FACTOR SELECT_CELL  
ENTER_GEOMETRICAL_EXPONENT SELECT_TIMESTEP  
ENTER_GRID_COORDINATES SET_ACCURACY  
ENTER_HEAT_TRANSFER_PARAMETER SET_ALL_START_VALUES  
ENTER_HOMOGENIZATION_FUNCTION SET_CONDITION  
ENTER_LABYRINTH_FUNCTION SET_FIRST_INTERFACE  
ENTER_MOBILITY_DATA SET_INITIAL_TEMPERATURE  
ENTER_MOBILITY_ESTIMATE SET_INTERACTIVE  
ENTER_PHASE_IN_REGION SET_LOG_LEVEL  
ENTER_REGION SET_NUMERICAL_LIMITS  
EXIT SET_REFERENCE_STATE  
GB_MODEL SET_SIMULATION_CONDITION  
GOTO_MODULE SET_SIMULATION_TIME  
HELP SET_SURFACE_TENSION  
HOMOGENIZATION_MODEL SIMULATE_REACTION  
INPUT_SCHEIL_PROFILE STORE_HOMOGENIZATION_DATA  
INTERFACE_SURFACE_TENSION SWITCH_MODEL  
LIST_CONDITIONS USE_INTERPOLATION_FOR_D  
LIST_MOBILITY_DATA UTILITIES_HOMOGENIZATION  
DIC>
```
- Console Results:** Contains a plot titled "Plot 1". The plot area is currently empty, with axes ranging from 0.0 to 1.0 on both the x and y axes. A small Thermo-Calc logo is visible in the bottom-left corner of the plot area.
- Event Log:** Located at the bottom of the console panel, it is currently empty.

Typical calculation scheme - Console



	Define and get thermodynamic and kinetic data	DEF-SYS; GET; APPEND
DICTRA Monitor	Set global conditions (usually only T)	SET-COND GLOB T.....
	Enter region(s)	ENT-REG
	Enter grid(s) and size in region(s)	ENT-GRID
	Enter phase(s) in region(s)	ENT-PH
	Enter composition(s) for the phases	ENT-COMP
	Enter geometrical factor (optional)	(ENT-GEO)
	(Set boundary conditions)	(SET-CO BOU
	Set simulation time	SET-SIM-TIME
	Start simulation	SIM
	Move to Plot module (the Post processor)	POST
	Set diagram axes	S-D-A
	Set plot condition (often time or distance)	S-P-C
	Plot diagram	PLOT

Console mode Macro files



- Text files with Console mode commands
- File extension: .TCM or .DCM
- Can easily be produced from log-files (SET-LOG command)
- Can be rewritten in a text editor, e.g. NotePad

LOG file

to

Macro file



```
@@ Log file generated 2020-10-13
@@

go data
switch tcni11
def-elements ni cr co al ti
get-data
go poly
set-cond t=1000 n=1 p=1e5 w(co)=0.20
set-cond w(cr)=0.195 w(al)=0.4E-2 w(ti)=0.021
s-a-v 1 t
773.15 1773.15 10

step
NORMAL
post
set-diag-ax x t-c
set-diag-ax y vpv(*),,
plot,,
exit
```



```
set-echo

go data
switch tcni11
def-elements ni cr co al ti
get-data
go poly
set-cond t=1000 n=1 p=1e5 w(co)=0.20
set-cond w(cr)=0.195 w(al)=0.4E-2 w(ti)=0.021
s-a-v 1 t
773.15 1773.15 10

step
NORMAL
post
set-diag-ax x t-c
set-diag-ax y vpv(*),,
plot,,

set-interact
```

DICTRA Macro file



```
go data
sw tcfe13
def-sys fe cr ni
rej-ph *
rest-ph bcc fcc
get
```

```
app mobfe8
def-sys fe cr ni
rej-ph *
rest-ph bcc fcc
get
```

```
go dict
```

```
set-cond glob T 0 1373.15; * N
```

```
ent-region
fecrni
```

```
ent-grid
fecrni
3e-3
double
60
0.85
1.15
```

```
ent-phase
act
fecrni
matrix
fcc#1
```

```
ent-ph
act
fecrni
sph
bcc
```

```
ent-comp
fecrni
fcc#1
fe
w-p
cr
fun 24.3+15.7*HS(x-0.0015)
ni
fun 6.9+22.5*HS(x-0.0015)
```

```
ent-comp
fecrni
bcc
y
```

```
set-sim-time
3.6e5
yes
3.6e4
1e-7
1e-7
```

```
homogen yes yes
ent-hom 1
```

```
save FECRNI y
```

```
set-inter
```

DICTRA Macro file



The macro file from previous slide is included in the download as *fecrni_hom_setup.DCM*

It is the same Fe-Cr-Ni diffusion couple simulation that we performed yesterday.

Run it by drag-and-drop to an open console window or by simply double-clicking the DCM file.

Q & A

Example – Gradient Sintering of Cemented Carbide

Gradient sintering of cemented carbide

- A process used by the cemented carbide industry to increase surface toughness away from the cutting edge and increase hardness at the edge. The latter effect is due to geometry reasons and not considered further here.
- Cemented carbides are composite materials made up of hard refractory phases (mainly WC + other carbides/carbonitrides) in a minority Co-base matrix phase.
- Gradient sintering typically depend on the high nitrogen affinity of titanium (though other elements are possible).
- During vacuum sintering the cemented carbide is de-nitrided resulting in an inward diffusion of titanium and dissolution of the carbonitride phase in a surface zone.

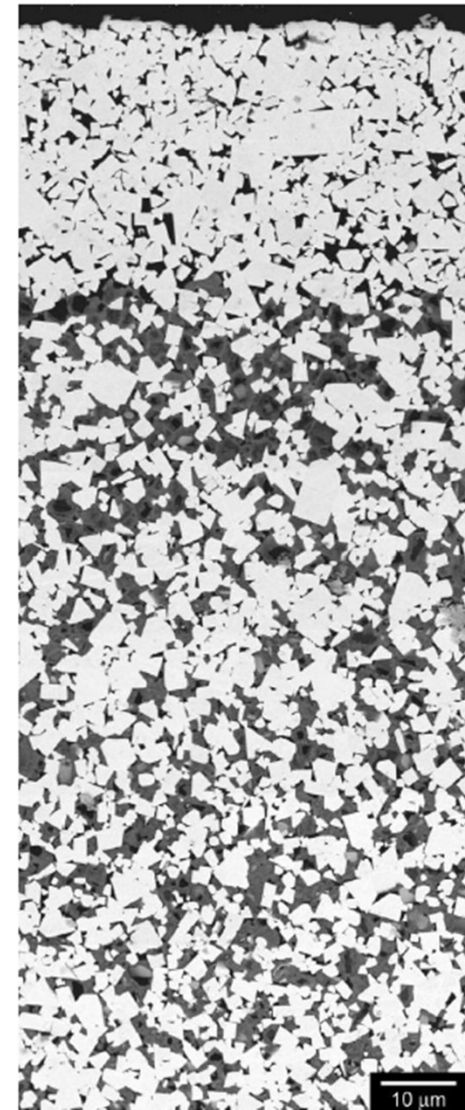
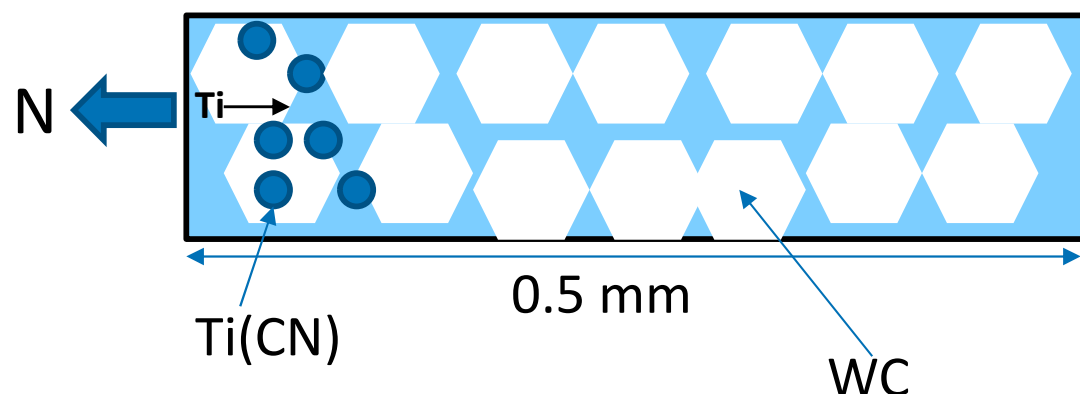
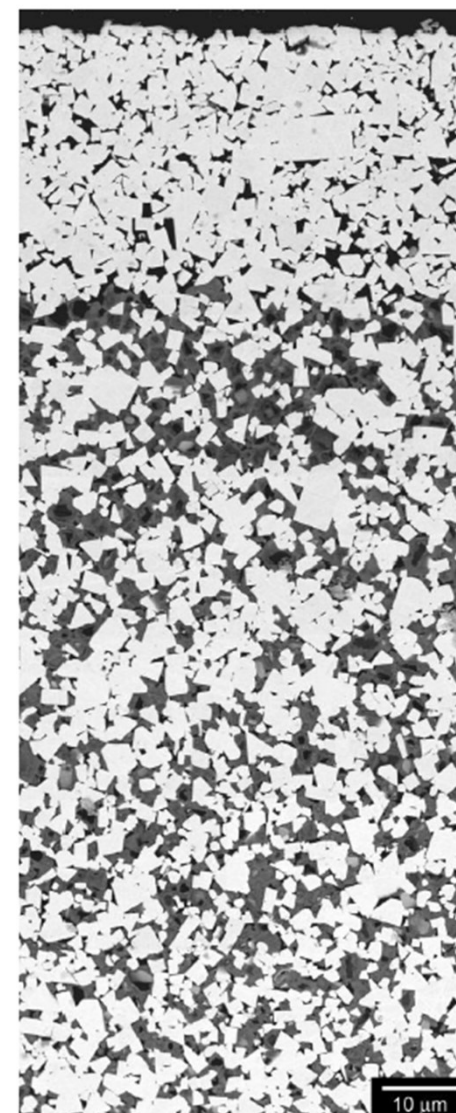


Image from: Ekroth et al. Acta Mater 48(2000)2177

Gradient sintering of cemented carbide

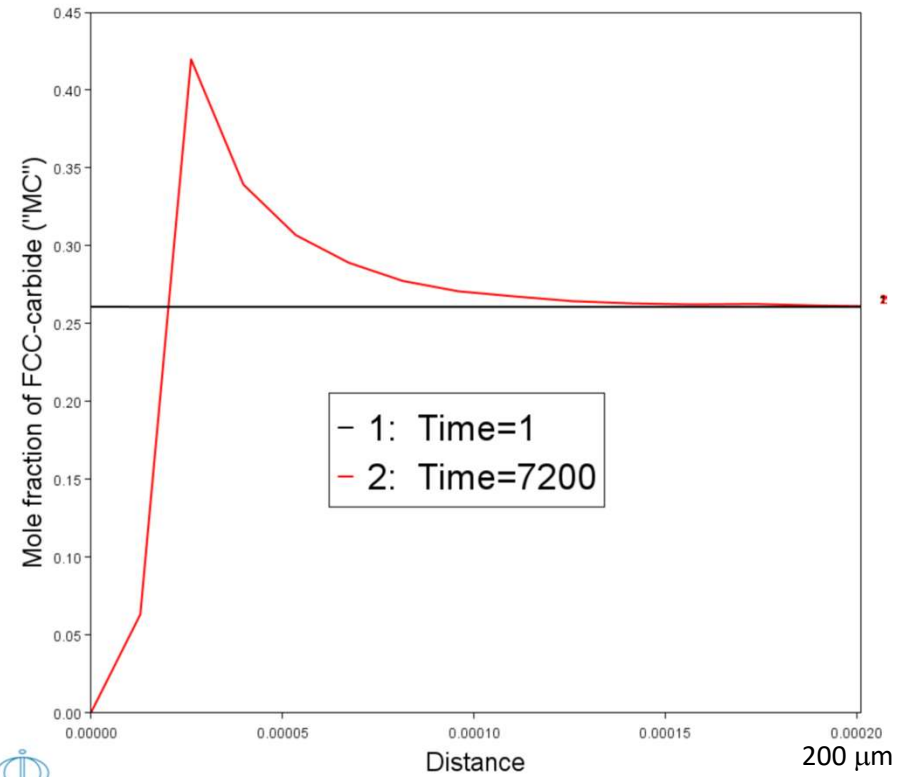
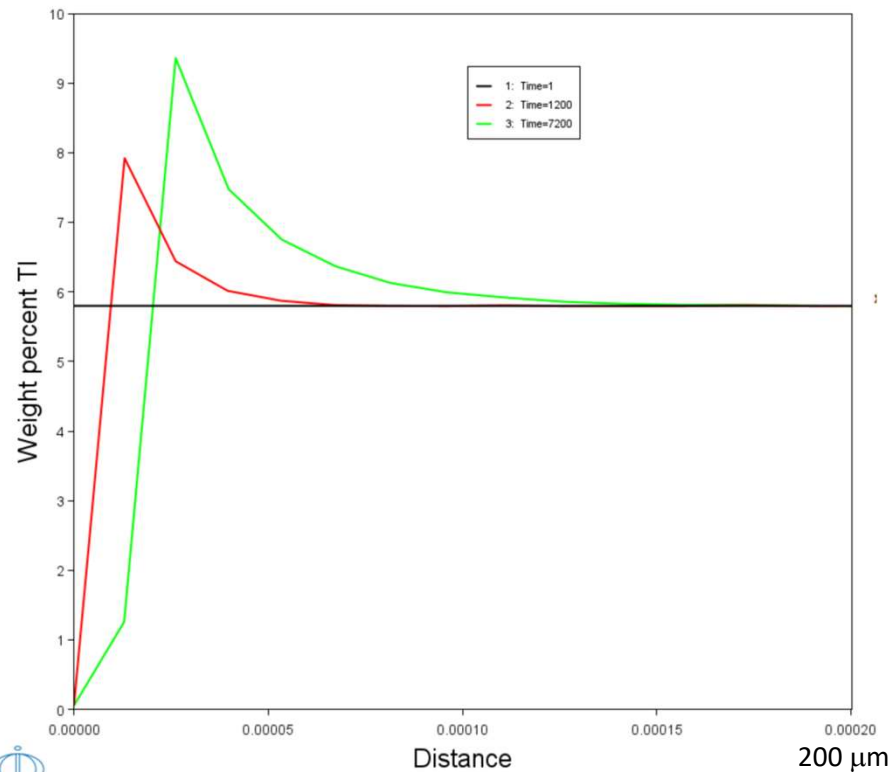


- Use TCFE13, works for these systems.
- Sintering temperature 1450 °C.
- Matrix phase: LIQUID.
- Secondary phases: WC (=MC_SHP), TiCN (FCC_A1#2).
- Alloy composition:
6.85 Co – 5.8 Ti – 6.35 C – 0.38 N – bal. W (wt-%)
- Boundary condition on activity N, $ACR(N)=1e-5$.
- Run simulation for two hours.



Gradient sintering of cemented carbide

Results (console mode simulation)



Trouble Shooting

Troubleshooting in DICTRA

What to do when things go wrong.

1. Check that the settings are what you want.
2. Simplify, e.g. use fewer elements.
3. Note that "ERROR 1234 in DXXYYZ" and similar are not considered errors (but rather information messages) as long as the simulation continues to run.

Options tab – this is where settings are changed in Graphical mode

Configuration

Diffusion Calculator 1

Conditions Options

Simulation Conditions

Default solver: Automatic

Time integration method: Trapezoidal

Save results to file: Yes

Use forced starting values in equilibrium calculations: No

Default driving force for phases allowed to form at interfaces: 1.0E-5

Timestep Control

Max relative error: 0.05 Max absolute error: 1.0E-5

Timestep: Initial 278.713631256 Smallest allowed: 1.0E-7 Max 10.0 % of simulation time

Factor specifying the maximum increase in the timestep taken from one timestep to another: 2.0

The timestep is to be controlled by the phase interface displacement during the simulation: No

Classic Model Specific

Use the activity of a component in order to find the correct tieline at the phase interface

Required accuracy during the solution of the flux balance equations: 1.0E-16

Homogenization Model Specific

Homogenization function: Rule of mixtures (upper Wiener bound)

Use global minimization:

Interpolation Scheme

Use interpolation scheme:

Logarithmic discretization with 10000 steps in each dimension

Memory to use: 1000.0 Megabyte

One-Phase Calculations



These normally work well.

Some sources of problems can be:

Unsuitable grid point spacing (use $1e-7$ to $1e-8$ m at boundary conditions or steep gradients)

Problems with mobility data

”Stiff-problems”, large differences in mobilities of different elements

One-Phase Calculations



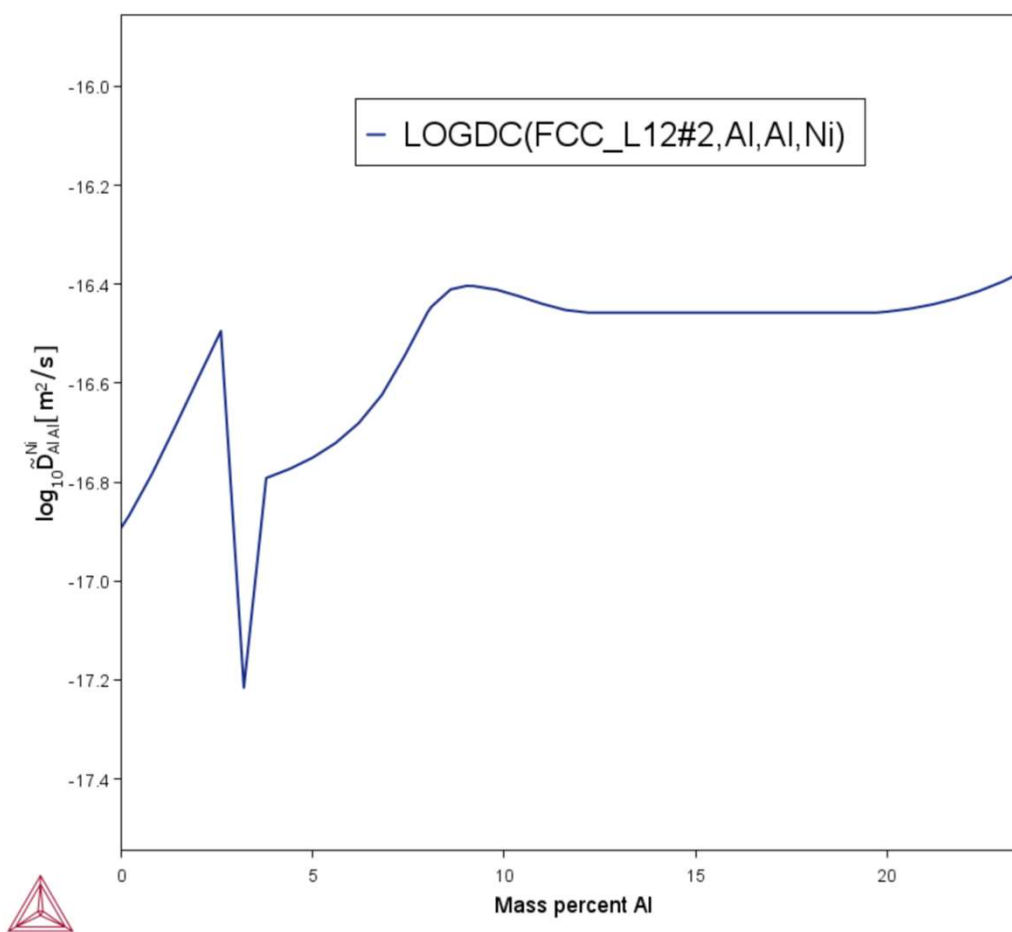
Problems with mobility data:

Perform a step calculation in one of the changing compositions and plot the diffusivities (e.g. $DC(\text{phase}, x, y, z)$) as a function of concentration to check if these vary in an extreme way (i.e. many orders of magnitude).

We can see how using the included *CALC_NiCrAl-Step.tcu*

One-Phase Calculations

Perform a step calculation in one of the changing compositions and plot the diffusivities (e.g. $DC(\text{phase},x,y,z)$) as a function of concentration.



One-Phase Calculations



”Stiff problems”

Show up as fluctuations (wiggles) in the concentration profiles.

Suggestion:

Use implicit time integration of the diffusion equations, i.e.
set the time integration method to Euler Backwards.

In Console mode:

```
SET_SIMULATION_CONDITION ;
```

```
DEGREE OF IMPLICITY WHEN INTEGRATING PDEs = 1
```

Moving Phase Boundary Simulations



The same errors as for one phase simulations may occur, and can be handled in the same way. Additional sources of problems for M-P-B can be:

Problems calculating phase equilibria at the phase interface

Problems when having a varying temperature

Elements with zero solubility in a region or phase.

Moving Phase Boundary Simulations



Problems calculating phase equilibria at the phase interface

Show up as error messages from POLY-3.

Suggestions:

1. Try changing between activities and potentials for specifying the tie-line.

or

2. Try the homogenization model. If the simulation starts and runs nicely you can often switch back to Classic model.

Moving Phase Boundary Simulations



Problems with varying temperatures.

First check that your set temperature curve is correct.

Limit the maximum timestep in the calculation by:

1. Decreasing the max timestep from 10% to a smaller value.
2. Set the time step to be controlled by the movement of the phase interface. This is standard for any solidification simulation.

Homogenization Model



Make sure that the grid point spacing is not too tight; a very dense grid can result in very short time-steps.

For complex systems it may be necessary to use forced starting values in equilibrium calculations or turn on the global minimization

Changing settings in Graphical mode

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1. Link to course evaluation:

<https://www.surveymonkey.com/r/BW87SQY>

2. We will send a certificate of course completion electronically just after all three online courses are finished.

Send your name and affiliation to ake@thermocalc.se if you are uncertain if we have it correctly.

Q & A