Thermo-Calc Software

DICTRA On-line Training

Day 3: 16 October 2025

www.thermocalc.com

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Diffusion Module (DICTRA)

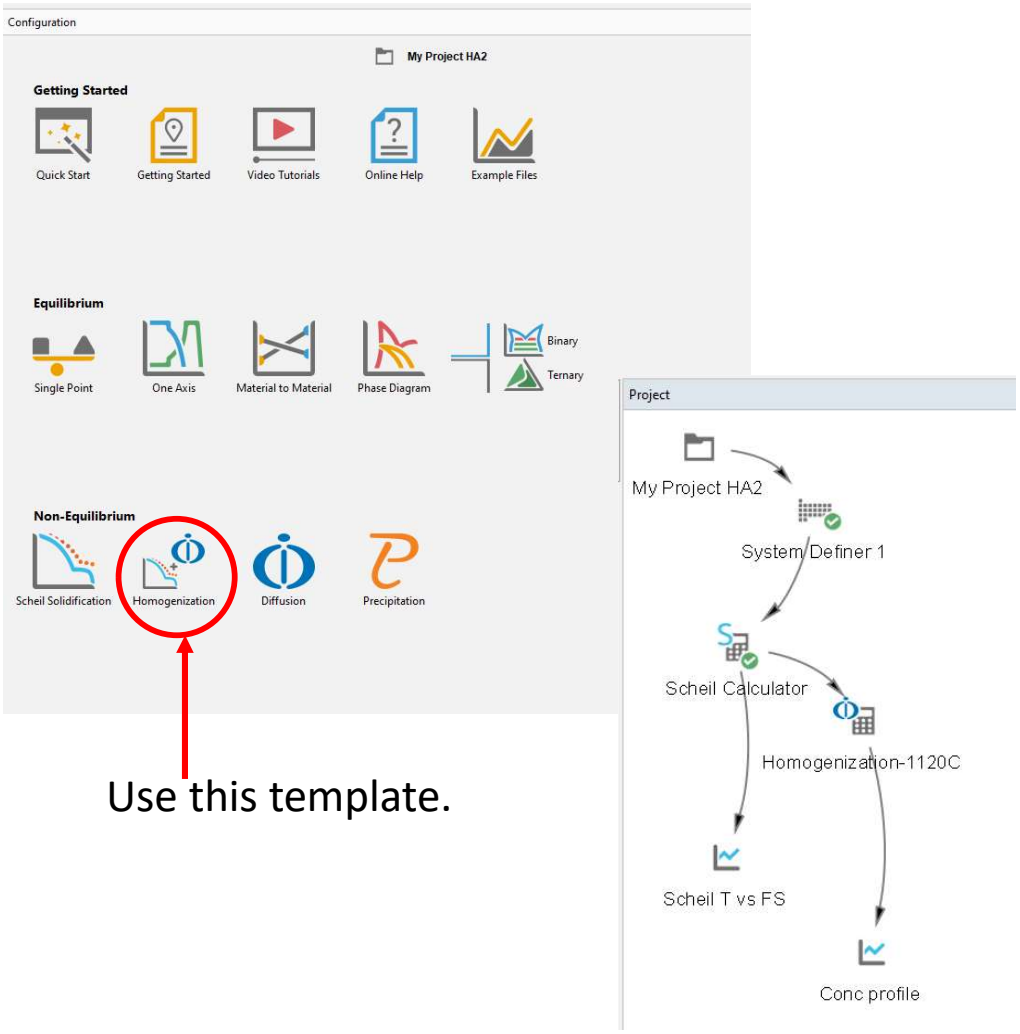
Day 3

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

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-%)



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.

Half the secondary dendrite arm spacing: 200 µm.
Temperature 1120 °C.
Time for homogenisation: 72 hours.

<u>Task: Check how the concentration profiles for Ni and Cr change over time.</u>

Compare with exp. data: Fuchs_1120.exp

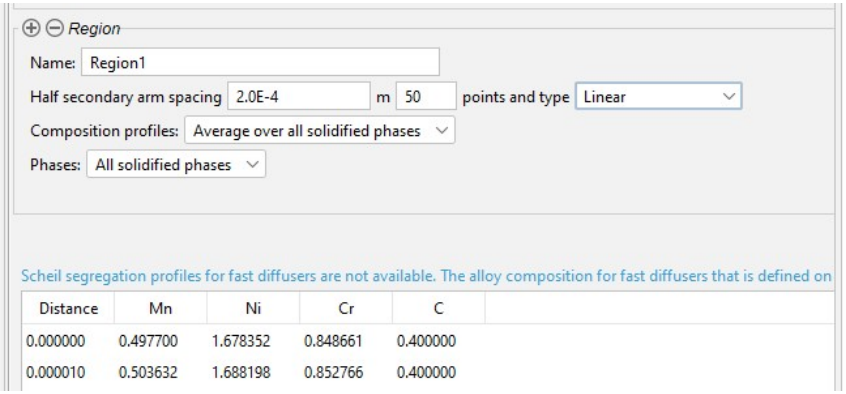
Home assignment 2: Solidification & Homogenisation

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

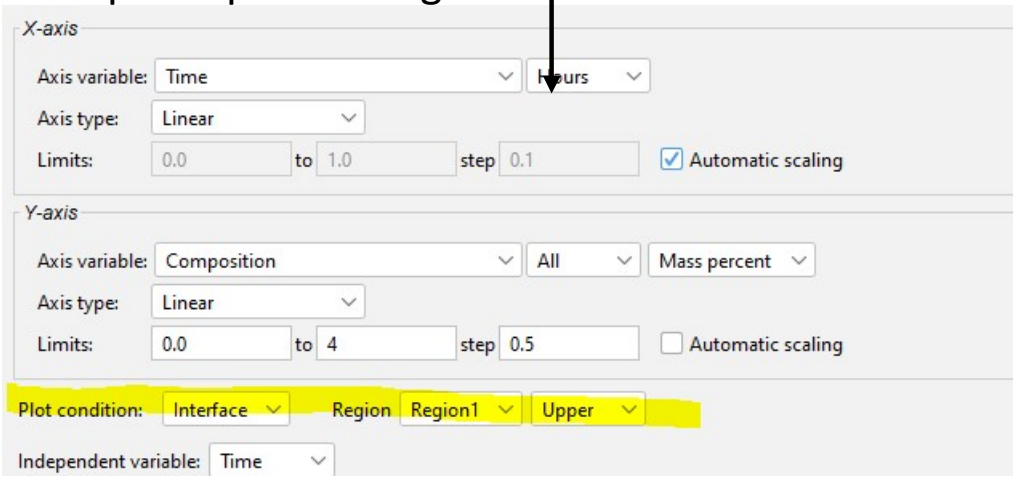
Considerations:
To export the scheil concentration profile to a DICTRA simulation, the Homogenisation template must be used.

Set a Classic Scheil simulation with C as fast diffuser. However, the calculated carbon profile will not be used. The other elements (Cr,Mn,Ni) profiles are used.

In the Diffusion Calculator, use these settings.



Example of plot settings.



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

Home assignment 2: Solidification & Homogenisation

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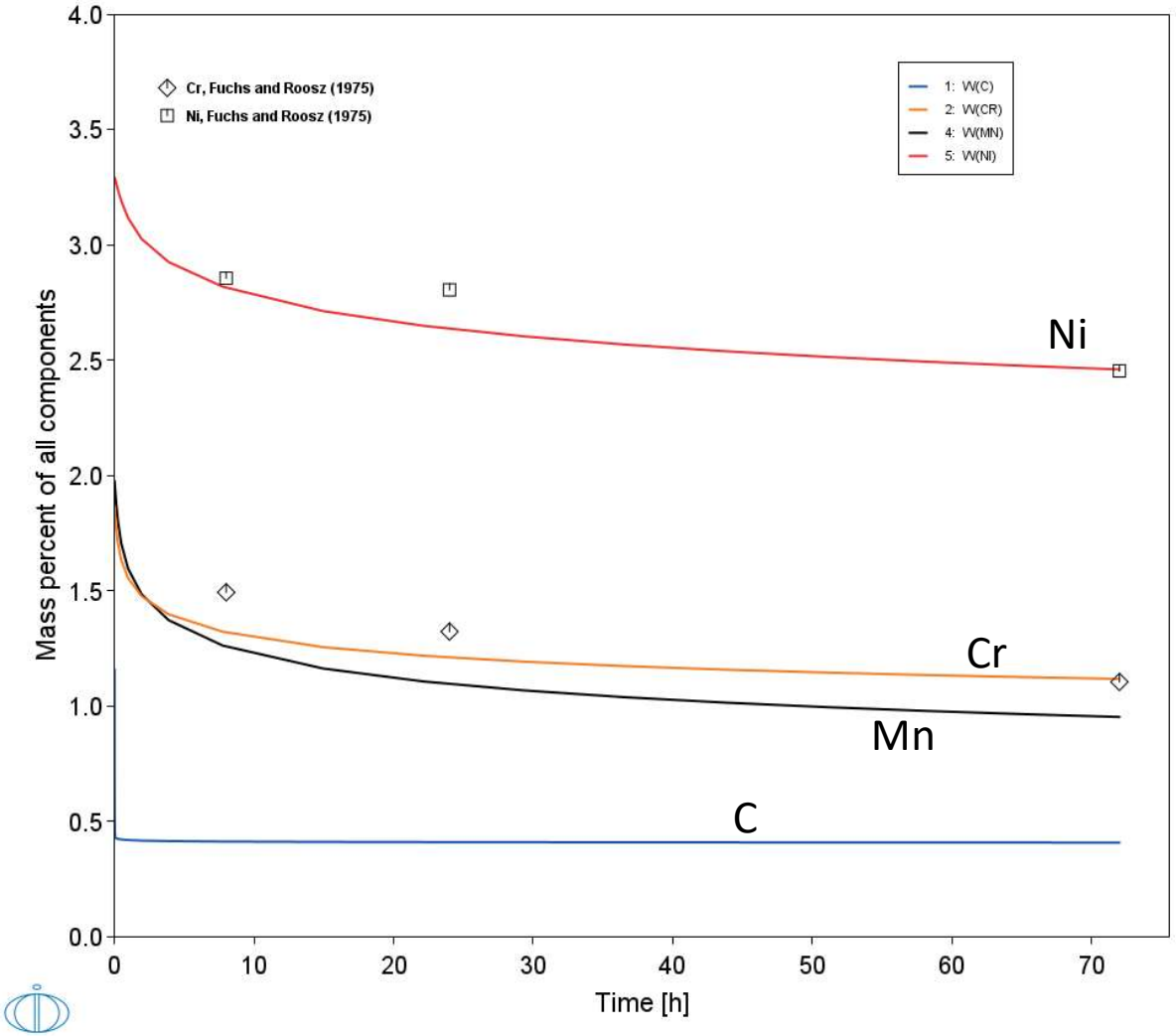
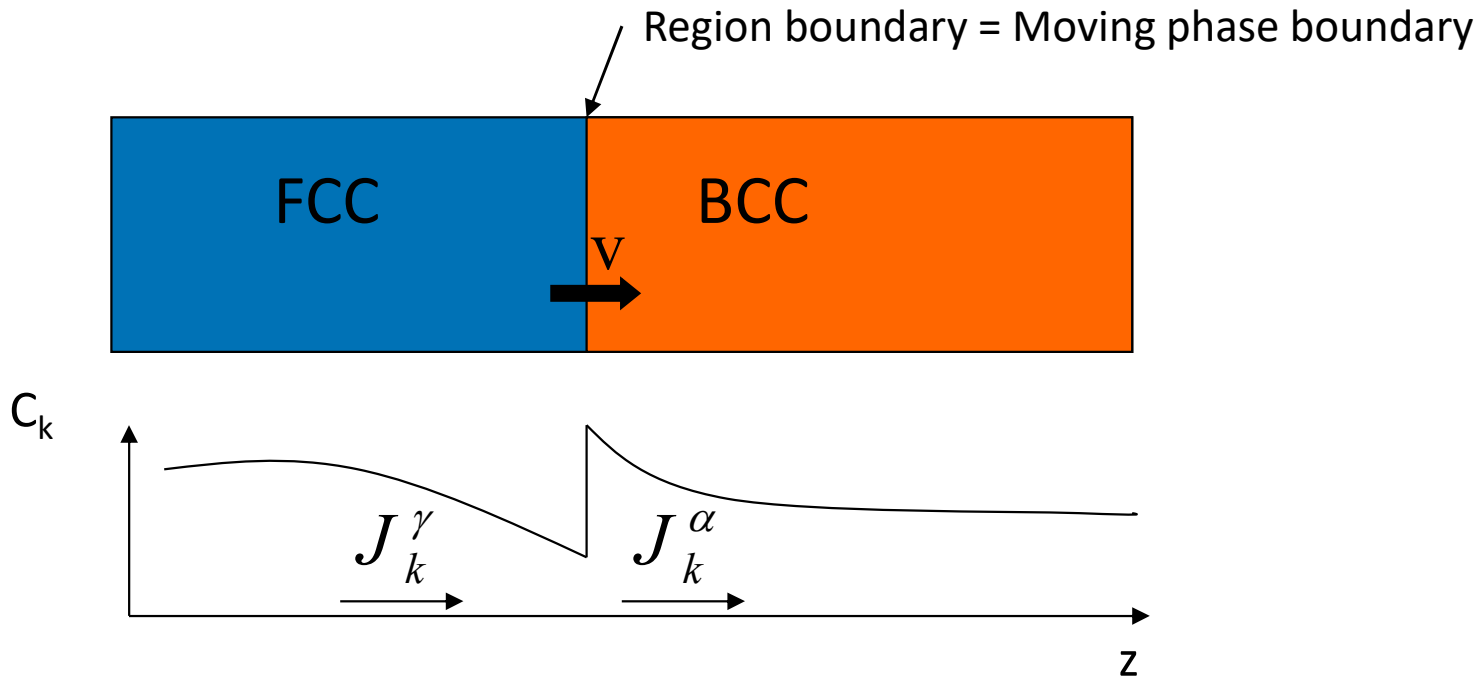
CrNi-steel: Fe(bal.) – 1.9 Ni – 0.95 Cr – 0.65 Mn – 0.4 C (wt-%)



Result.

Moving Phase Boundary – Cementite dissolution

Moving phase boundary simulation



Solve diffusion equation in each phase

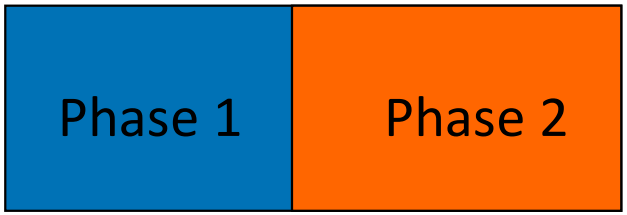
Calculate displacement of phase boundary

Thermo-Calc is used to find tie-lines

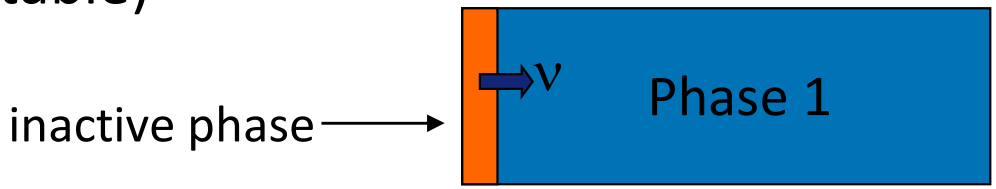
Moving Phase Boundary

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

1) Introducing two or more adjacent regions containing different phases



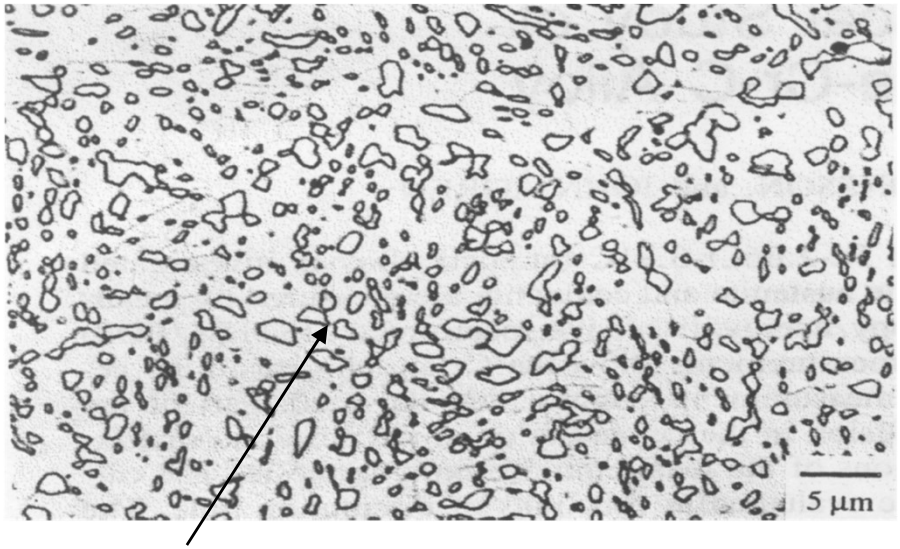
2) Entering an inactive phase (formed when thermodynamically stable)



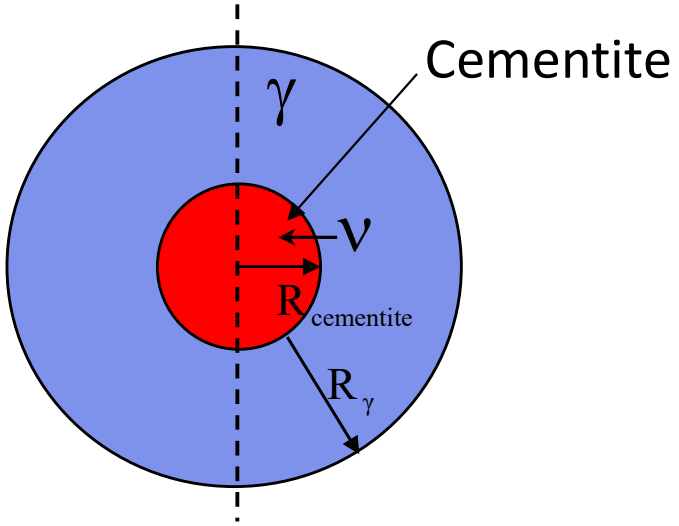
Cementite dissolution in an Fe–Cr-C alloy

Dissolution of cementite at 910°C (1183K)

x(Cr)= 0.0206, x(C)=0.0391, bal. Fe.



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

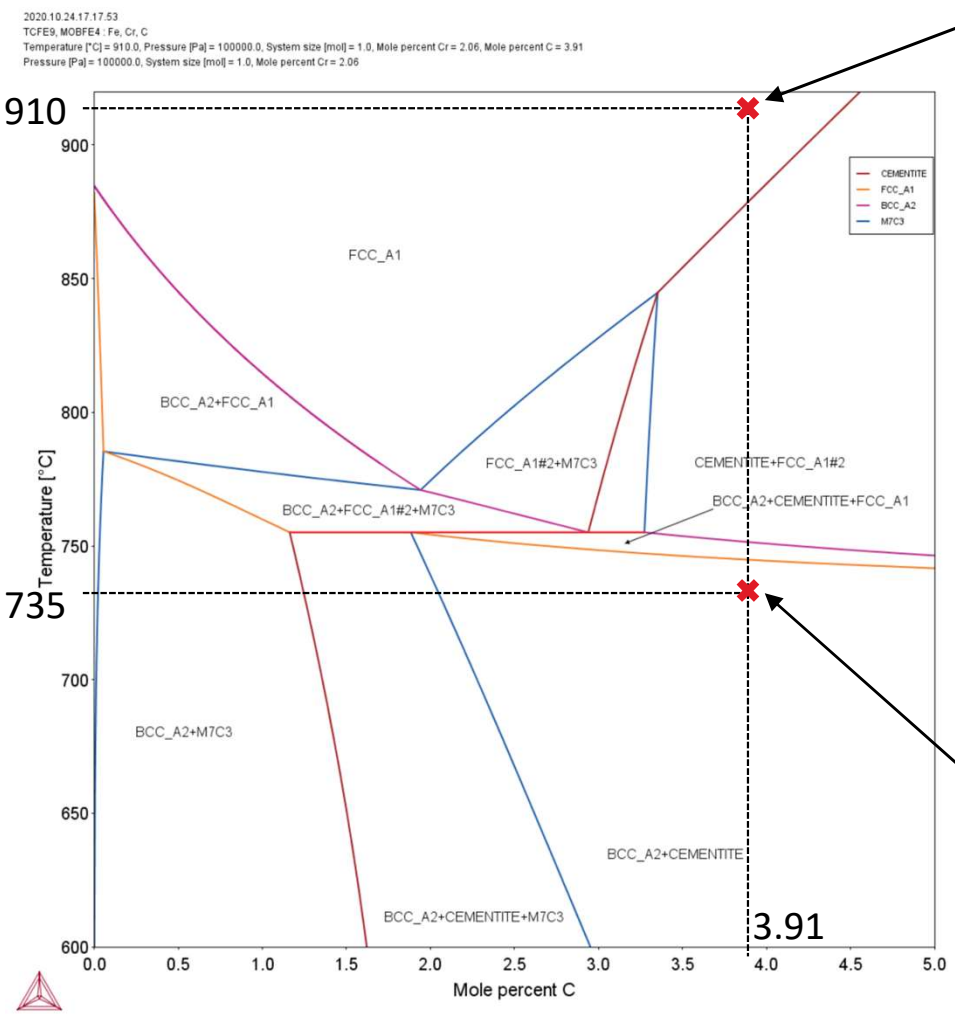


FCC (γ) is the matrix phase during dissolution. BCC is the matrix when the structure is formed.

Liu et al, Metall Trans A 22A(1991)1745

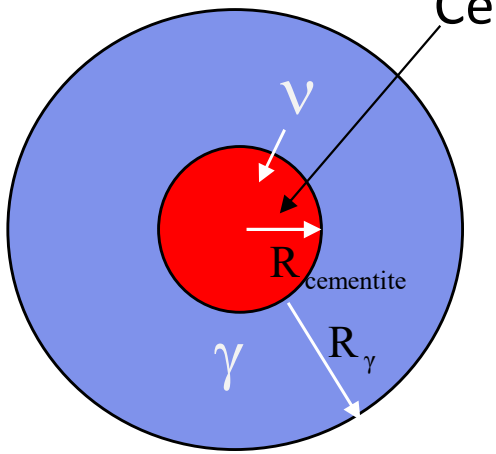
Cementite dissolution in an Fe–Cr-C alloy

910°C x(Cr)= 0.0206, x(C)=0.0391, bal. Fe.



Dissolution

Annealing



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:

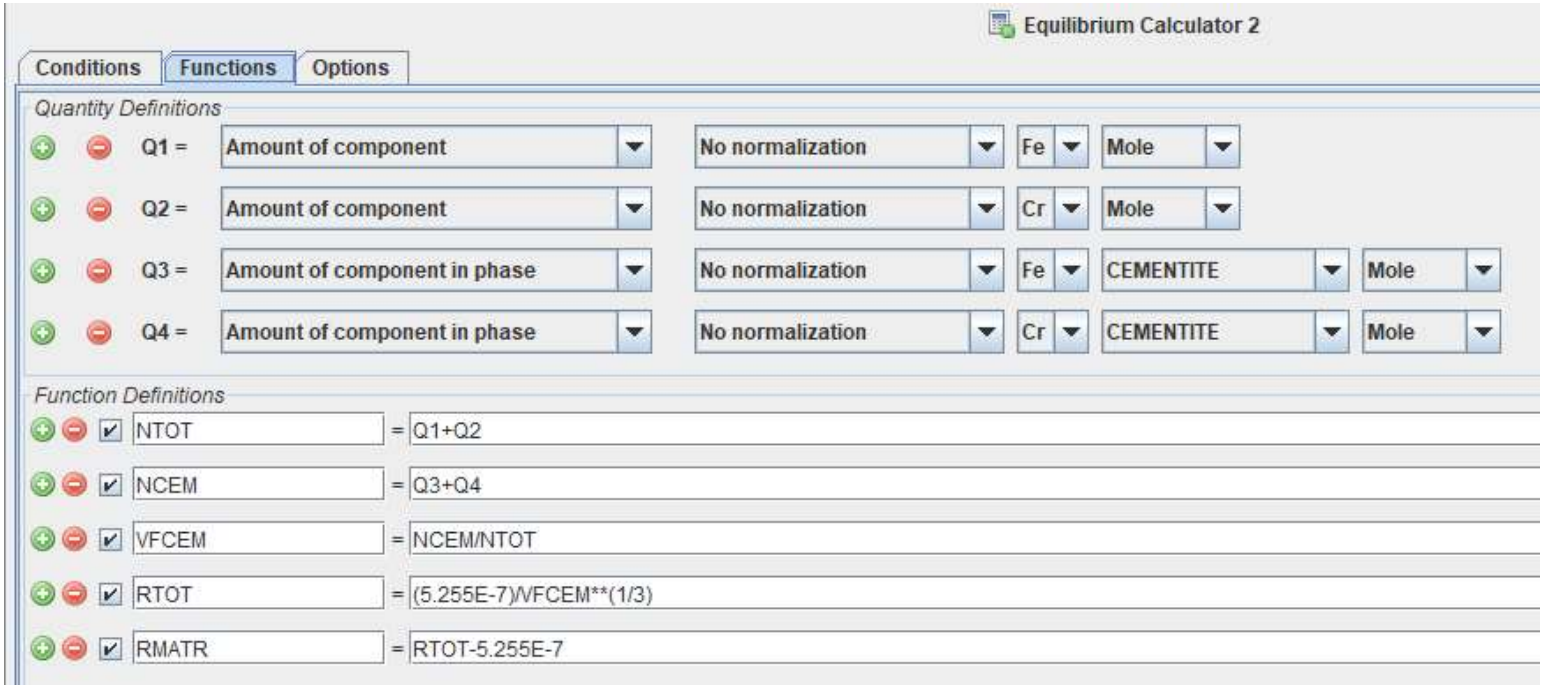
$$\frac{R^3_{\text{cementite}}}{R^3_{\text{tot}}} = \frac{V_{\text{cementite}}}{V_{\text{tot}}} = V^f_{\text{cementite}}$$

$$\Longrightarrow \quad R_\gamma = R_{\text{tot}} - R_{\text{cementite}} = \frac{R_{\text{cementite}}}{\sqrt[3]{V^f_{\text{cementite}}}} - R_{\text{cementite}}$$

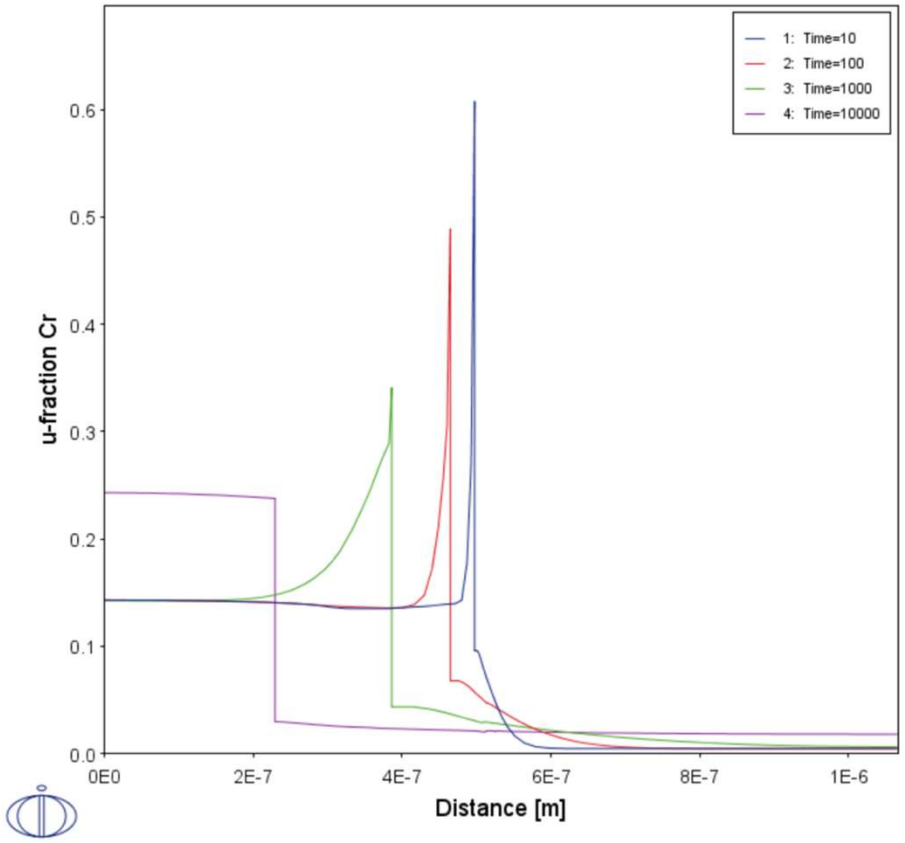
$$\left(V^{\,f}_{\text{cementite}} = \text{n(cem, Cr)} + \text{n(cem, Fe)} \Big/ \text{n(Cr)} + \text{n(Fe)} \right)$$

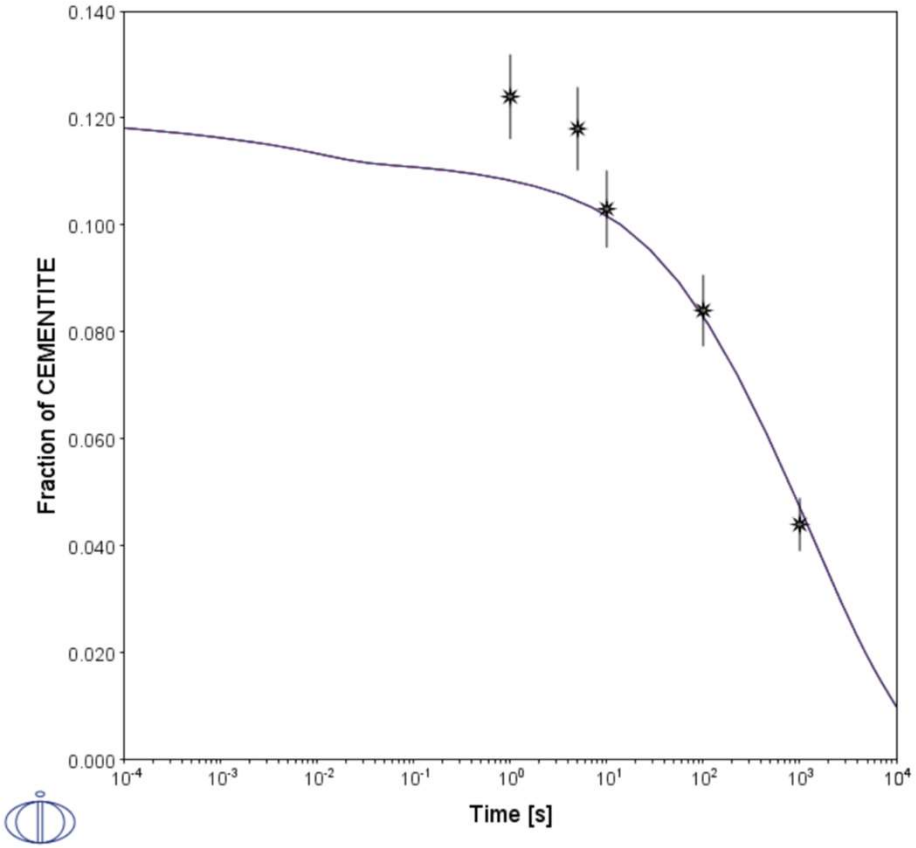
Cementite dissolution in an Fe–Cr-C alloy

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:



Results – cementite dissolution





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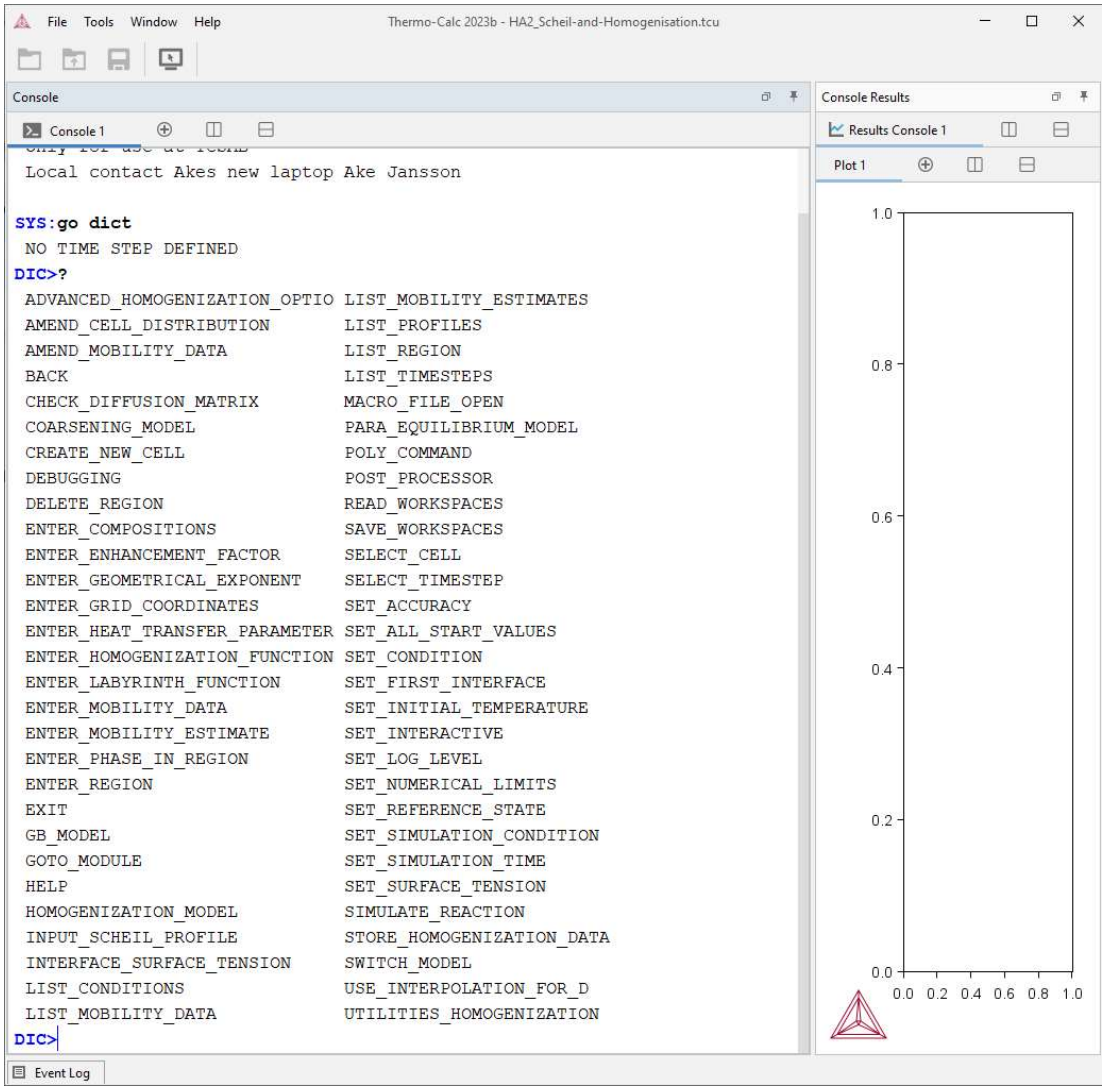
Console Mode

Console mode – DICTRA monitor



Typical calculation scheme - Console

DICTRA Monitor

Define and get thermodynamic and kinetic data	DEF-SYS; GET; APPEND
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 or just copy paste from the Console tab (right-click top))
- Can be rewritten in a text editor, e.g. NotePad

LOG file to Macro file

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```
@@ 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 tcfe14
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.

There is also a macro file for the plotting.

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Q & A

Example – Gradient Sintering of Cemented Carbide

Gradient sintering of cemented carbide

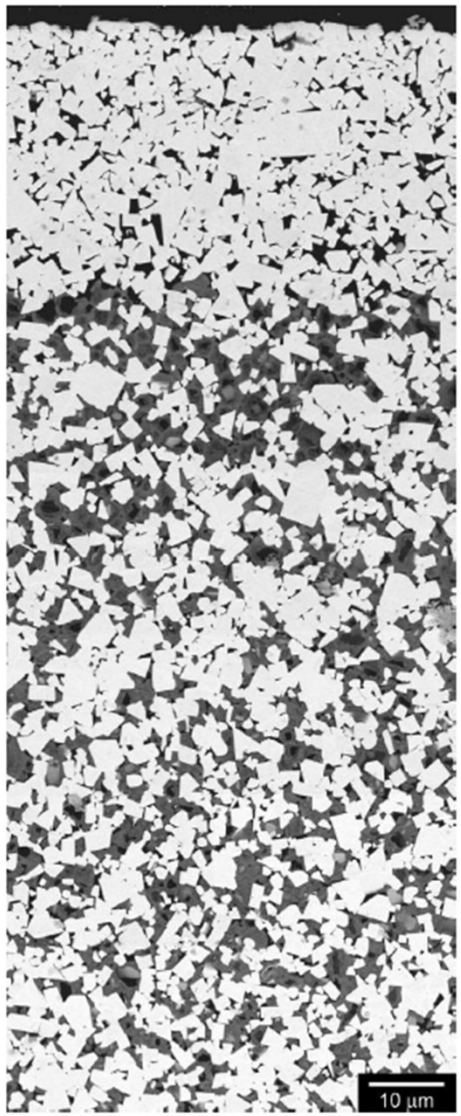
- A process used by the cemented carbide industry to increase surface toughness away from the cutting edge and increase hardness at the edge. The latter effect is due to geometry reasons and not considered further here.

- Cemented carbides are composite materials made up of hard refractory phases (mainly WC + other carbides/carbonitrides) in a minority Co-base matrix phase. Mostly used for cutting tools.

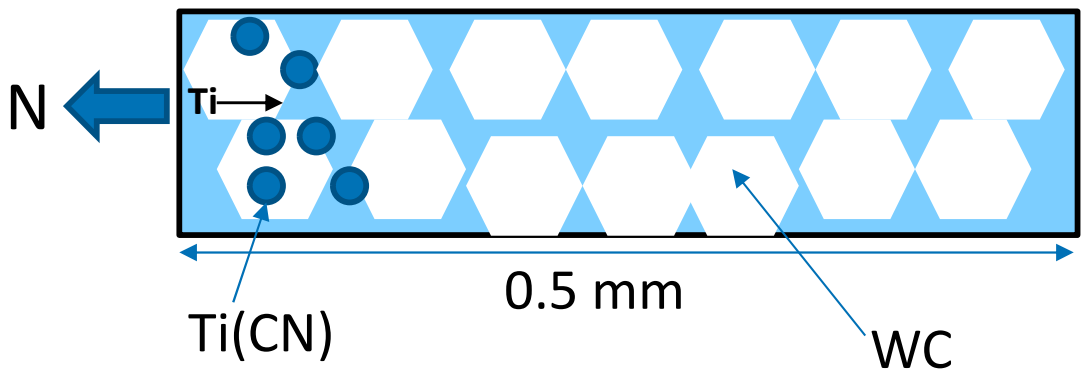
- Gradient sintering typically depend on the high nitrogen affinity of titanium (though other elements are possible).

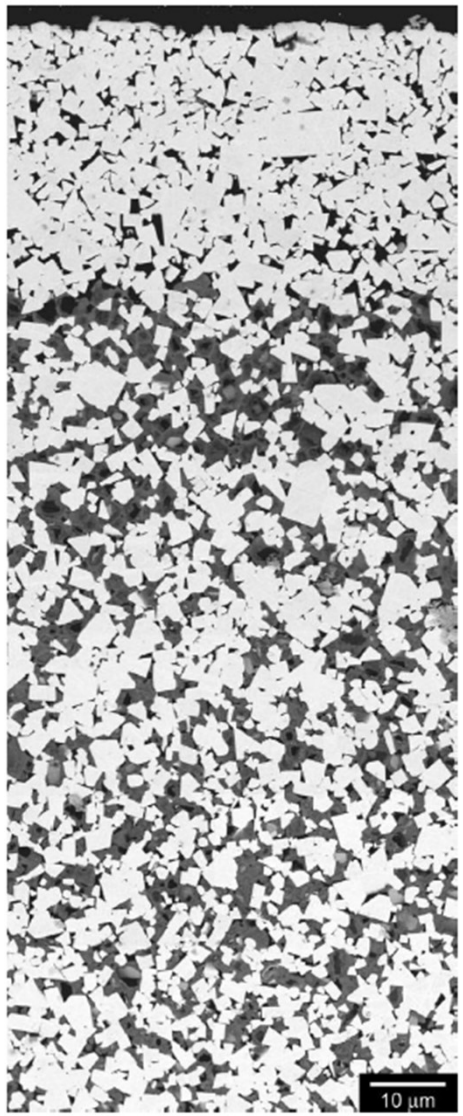
- During vacuum sintering the cemented carbide is de-nitrided resulting in an inward diffusion of titanium and dissolution of the carbonitride phase in a surface zone.

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



Gradient sintering of cemented carbide



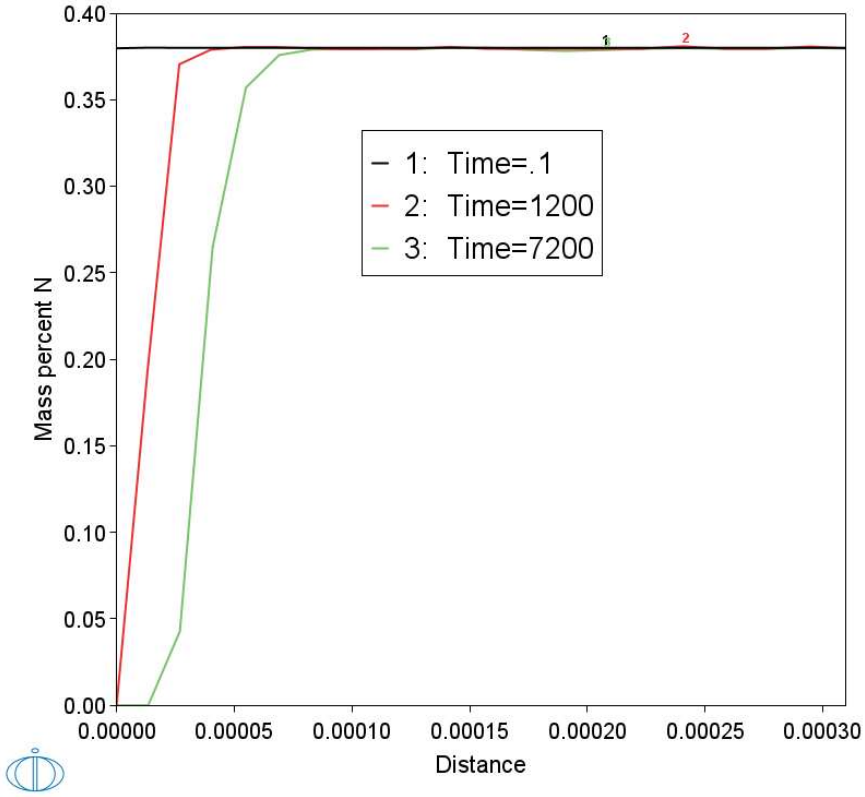


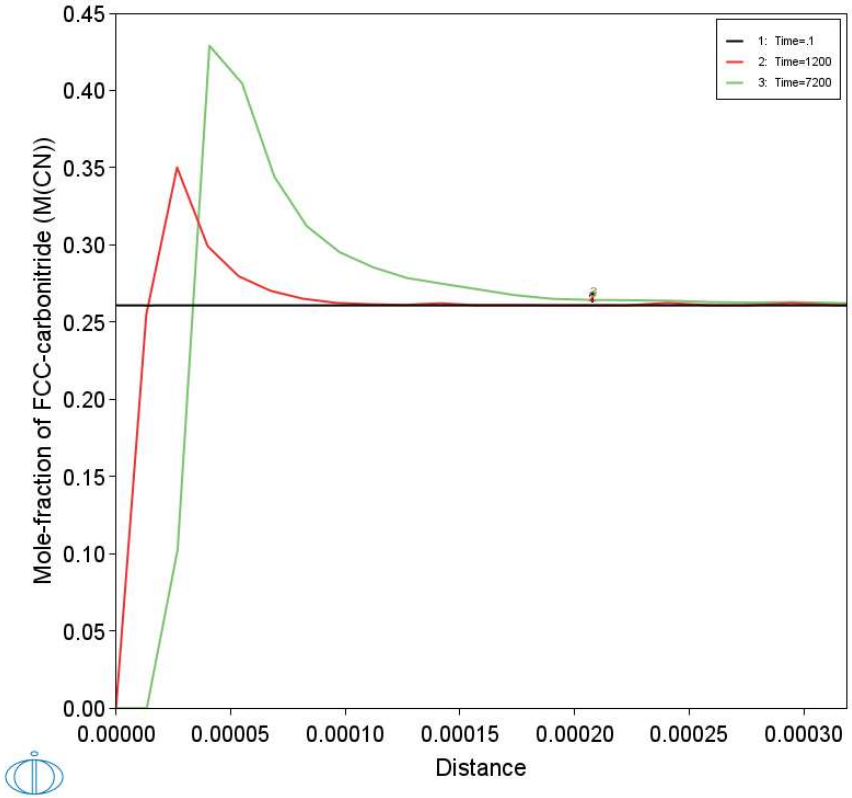
- Use TCFE14 + MOBFE8 - works for these systems.
- Sintering temperature 1450 °C.
- Matrix phase: LIQUID.
- Secondary phases: WC (=MC_SHP), TiCN (FCC_A1#2).
- Alloy composition:

  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 one or two hours.

Gradient sintering of cemented carbide

Results (console mode simulation)





Trouble Shooting

Troubleshooting in DICTRA

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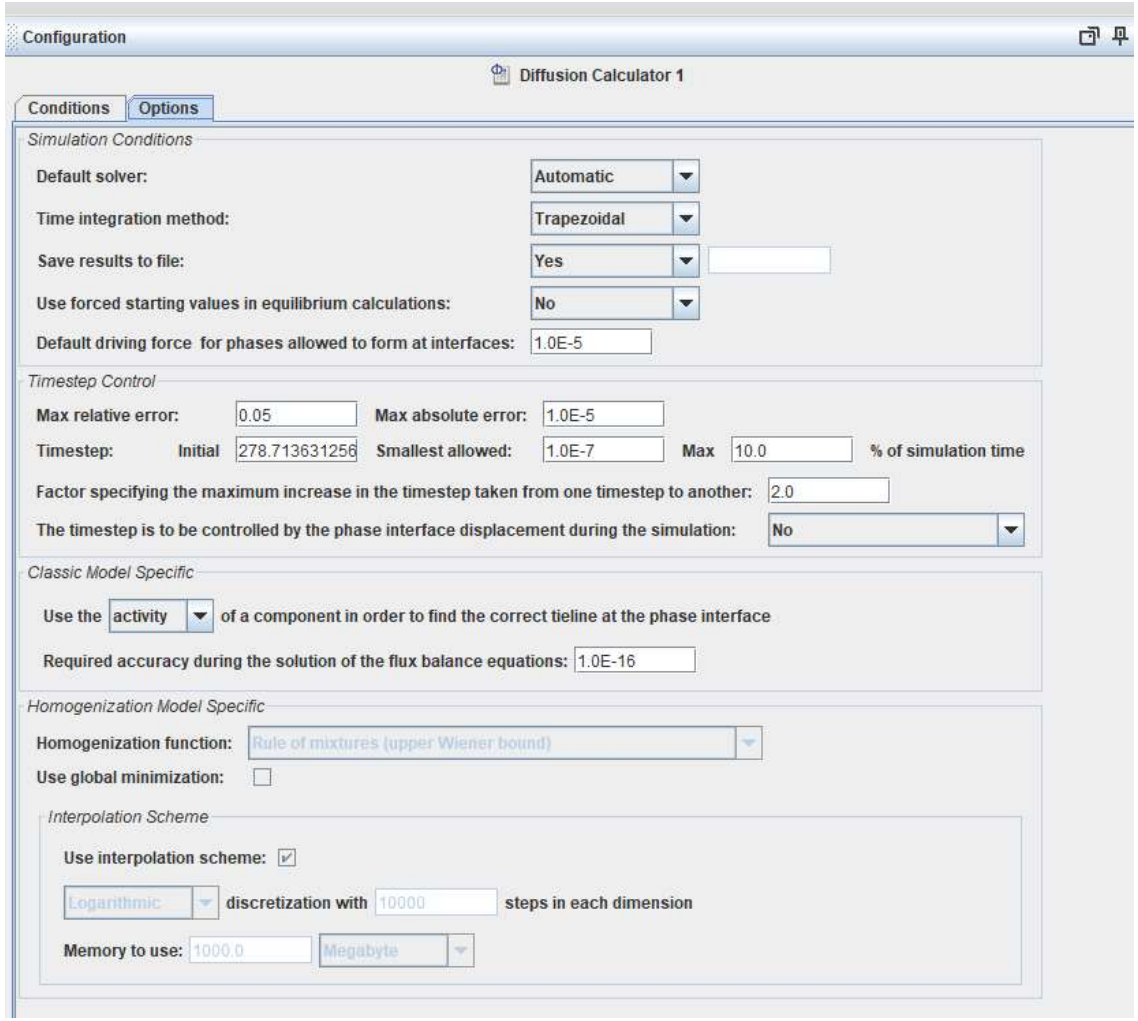
What to do when things go wrong.

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



One-Phase Calculations

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These normally work well.

<u>Some sources of problems can be:</u>

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 compostions and plot the diffusivities (e.g. DC(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 look at this in the included *CALC_NiCrAl-Step.tcu*

One-Phase Calculations

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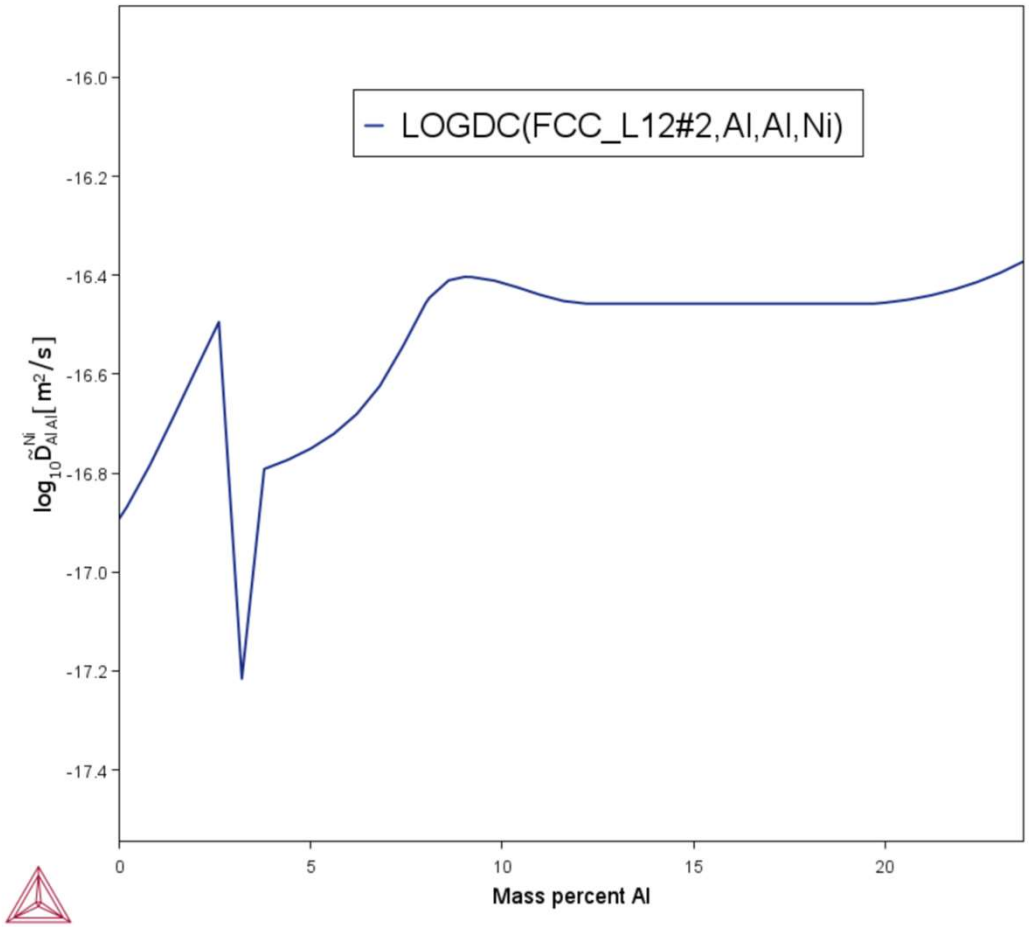
Perform a step calculation in one of the changing compostions and plot the diffusivities (e.g. DC(phase,x,y,z)) as a function of concentration.



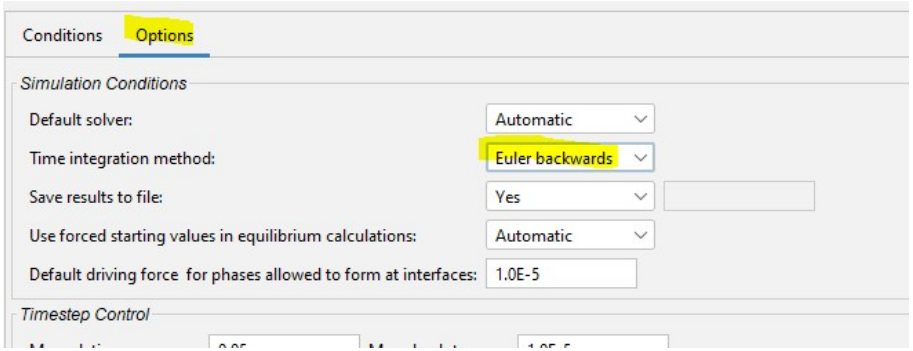
One-Phase Calculations

”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.

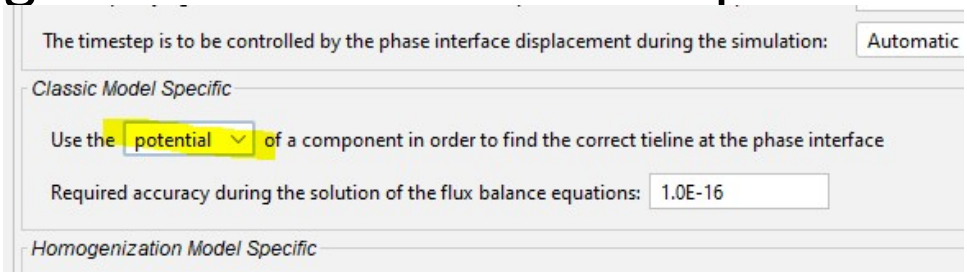
Moving Phase Boundary Simulations

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.

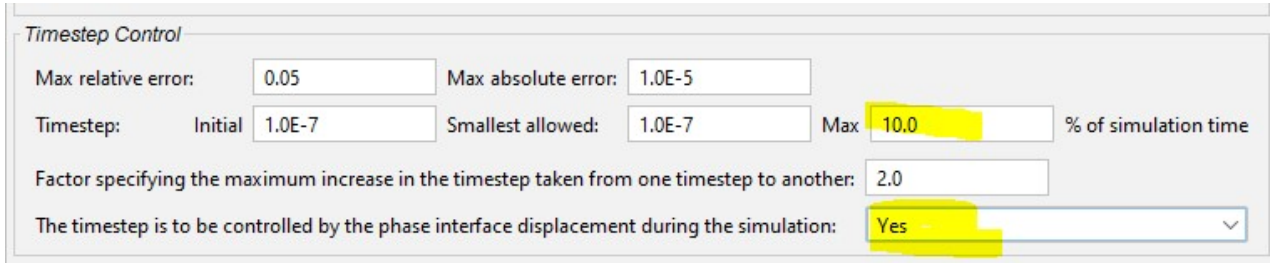
Moving Phase Boundary Simulations

Problems with varying temperatures.

First check that your time-temperature curve is correct.

Limit the maximum timestep in the calculation by:

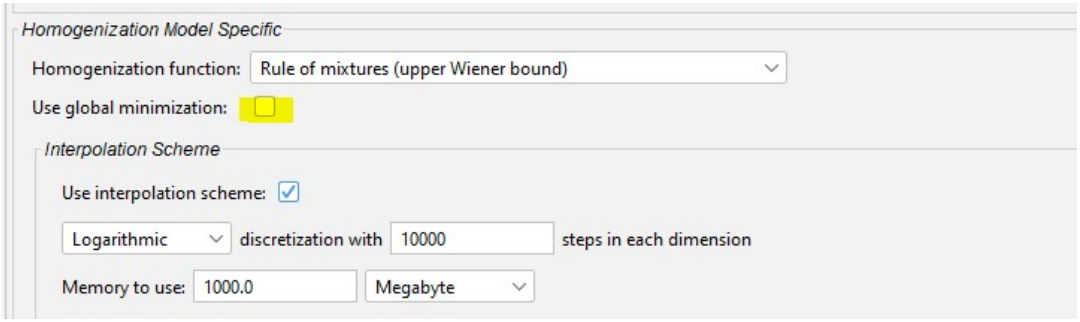
1. Decreasing the max timestep from 10% to a smaller value.
2. Set the time step to be controlled by the movement of the phase interface. This is standard for any solidification simulation.



Homogenization Model

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

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



* e.g. systems with many composition sets of the same phase, and/or ordered/disordered phases.

Changing settings in Graphical mode

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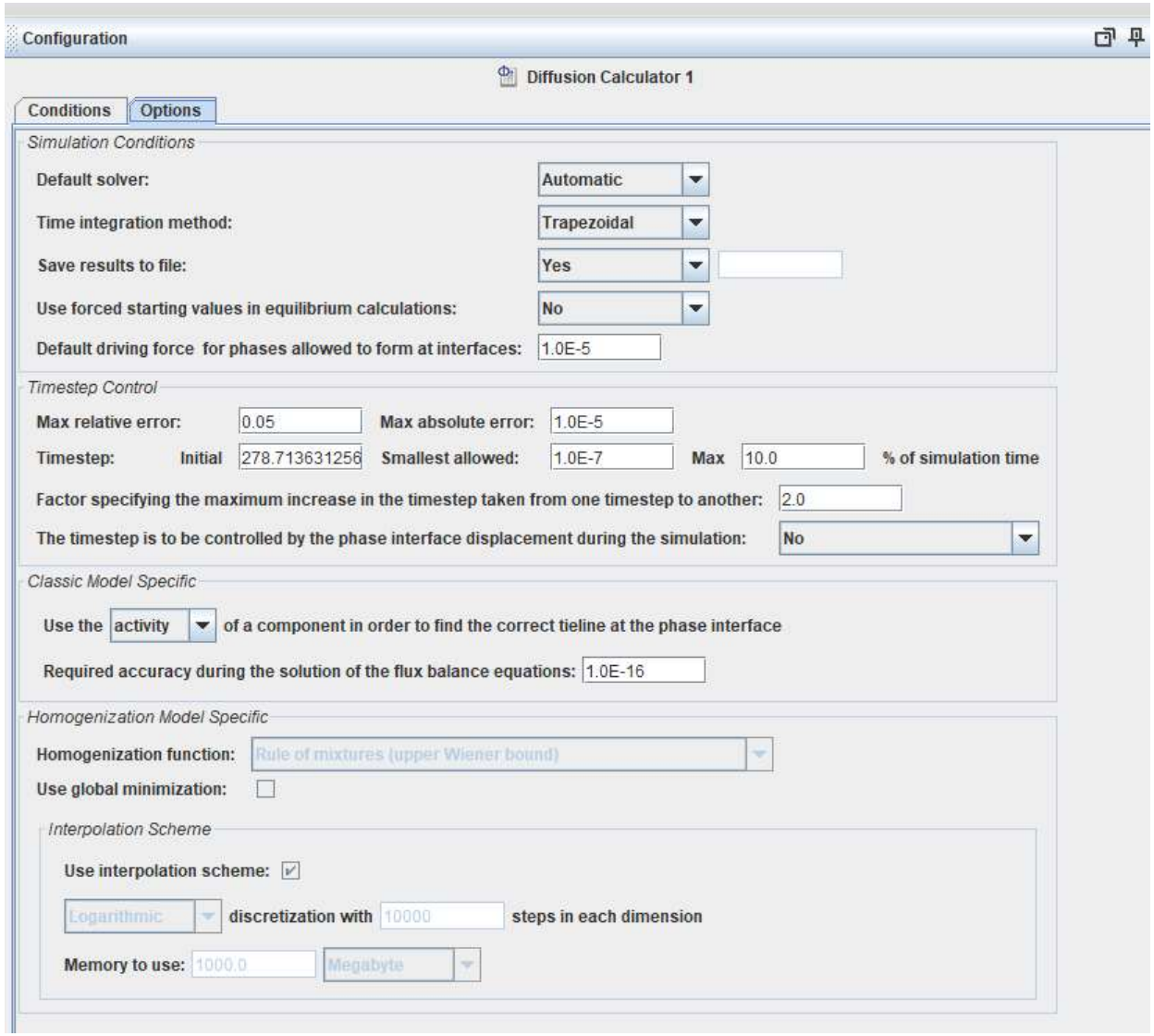


Thermo-Calc Software

Q & A

For those of you who will take part in any of the coming courses:

TC-Prisma 21-22 Oct.

AM 28-29 Oct.

You already have the software and database installation you need. Just keep it.

You will be mailed new license credentials, and new details for Zoom meetings and material.

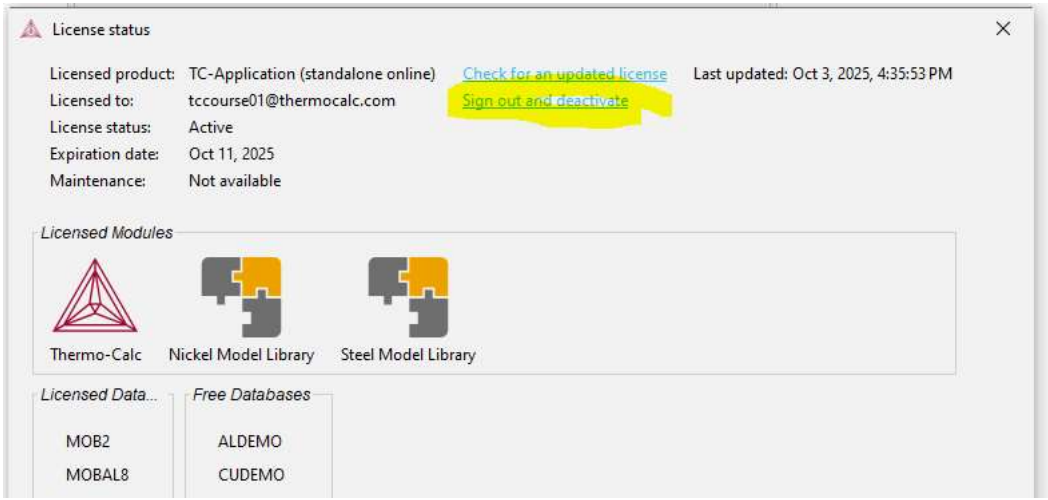
The current course license will be valid on Friday 17 Oct., but not on Saturday.

For those of you who will take part in

TC-Prisma 21 -22 Oct

It will be easiest if you deactivate the current license today or on Friday 10 Oct. You will be sent a new license for TC + TC-PRISMA on Friday.

Help > Show License Info



The End

We will email you a certificate of course completion just after all four online courses are finished (i.e. early November).

For some of you we might not have the correct details for your name and affiliation. Email to

ake@thermocalc.se

if you are uncertain if we have it correct.