Thermo-Calc Software

Thermo-Calc On-line Training

Day 3, *April 11, 2024*

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Schedule

Thermo-Calc Day 3

9:00	About the home assignment.
9:10	Scheil solidification simulation.
9:40	App1: Alloy design, duplex stainless steel.
10:20	Demo of console mode.
10:30	Q & A
10:45	Property Model Calculation.
11:15	Process Metallurgy Module Calculation.
11:35	Resources for help.
11:45	Q & A
12:00	End.

App = Thermo-Calc calculation applied to a real case.

Home Assignment 2

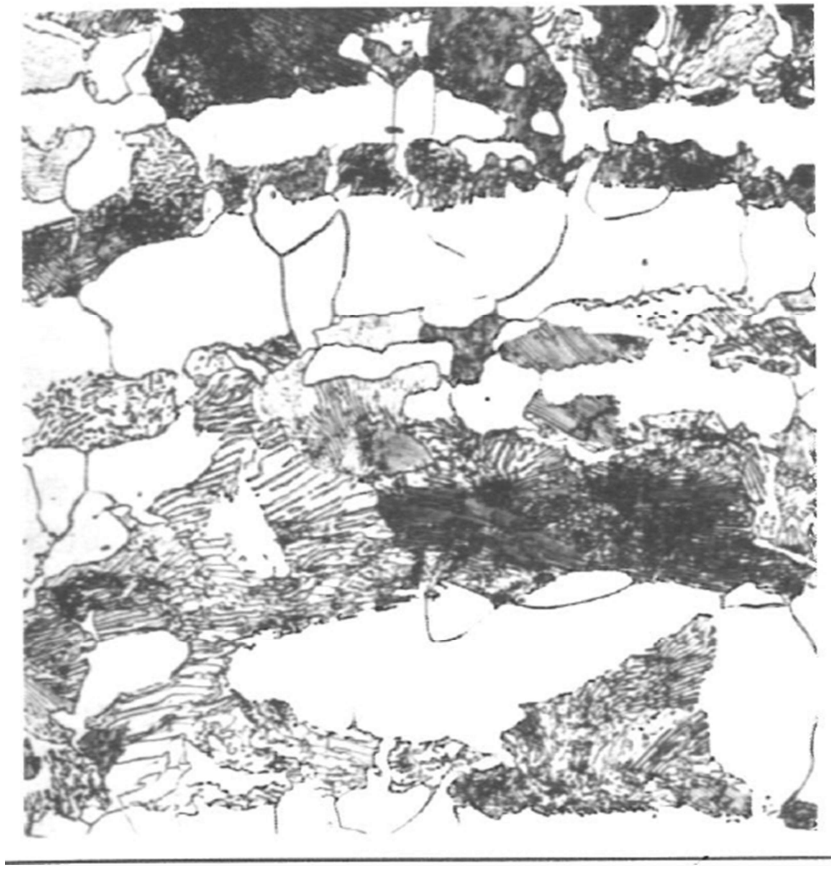
Thermo-Calc Software

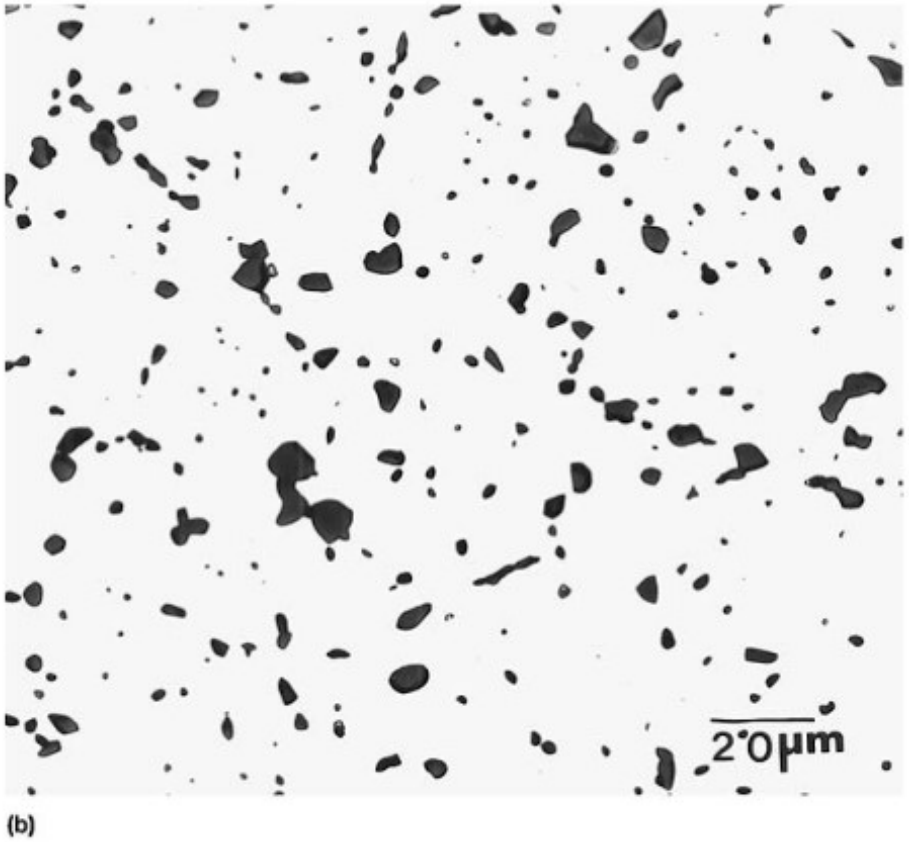
Calculate Equilibrium at 600 ºC for the following steel:

- AISI 1040 with Fe (bal.) – 0.4C - 0.7Mn (wt-%)

Which microstructure aligns with your result?

Is this Graphite or Fe_3C (Cementite)?





From ASM International: Heat Treaters Guide (1995).

Home Assignment 2 - solution

- Which microstructure aligns with your result?
- Is this Graphite or Fe_3C (Cementite)?

Both do! Equilibrium calculations with Thermo-Calc can give volume fraction/composition data but not tell you about the morphology. The steel on the left is air cooled and the steel on the right is spheroidized (= held below A1 in the ferrite + cementite two-phase field for long time to increase ductility).

Both micrographs have the same amount of Cementite (no graphite!), around 6 vol-%. The pearlite lamellae are too small to see in some regions on the left.

Cementite + Bcc is a metastable equilibrium compared to Graphite + Bcc, but it is the equilibrium that will show up in normal circumstances.

Thermo-Calc Software

Scheil Module

Solidification simulations

Thermo-Calc Software

Equilibrium methods (lever-rule)

Solute diffusion is rapid, i.e. complete solute back diffusion → uniform composition in both solids and liquid.

Non equilibrium methods (SCHEIL)

Negligible diffusion in solids, i.e. no solute back diffusion → solids retain same composition through solidification.

Partial equilibrium methods/ Fast diffusing species

Complete interstitial but negligible substitutional solute back diffusion. No diffusion calculation – equilibration of chemical potential for fast diffusing species.

Back diffusion calculated in the Primary Phase

Scheil with a simultaneous diffusion calculation in the primary phase. Requires additional kinetic data and takes dendrite spacing and cooling rate into account.

Scheil with Solute Trapping

Intended for simulation of very fast cooling, e.g. during Additive Manufacturing. Requires assumption about scanning speed and angle.

Moving phase boundary methods (DICTRA)

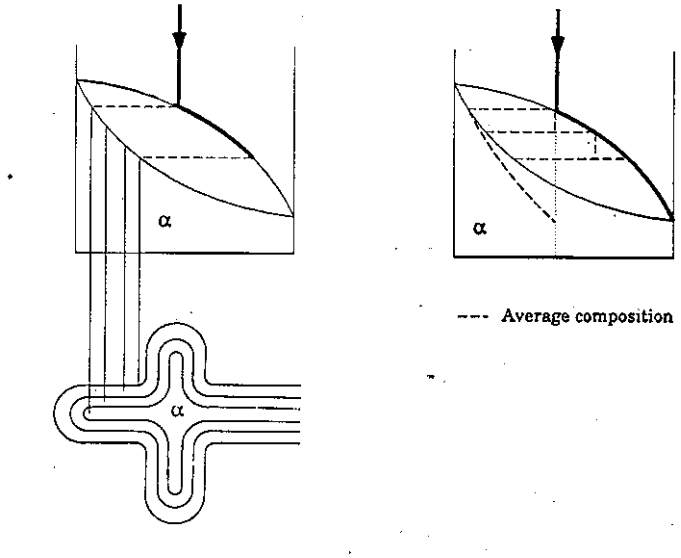
Full integration of thermodynamics and kinetics in all phases. Requires additional kinetic database and takes dendrite spacing and cooling rate into account.

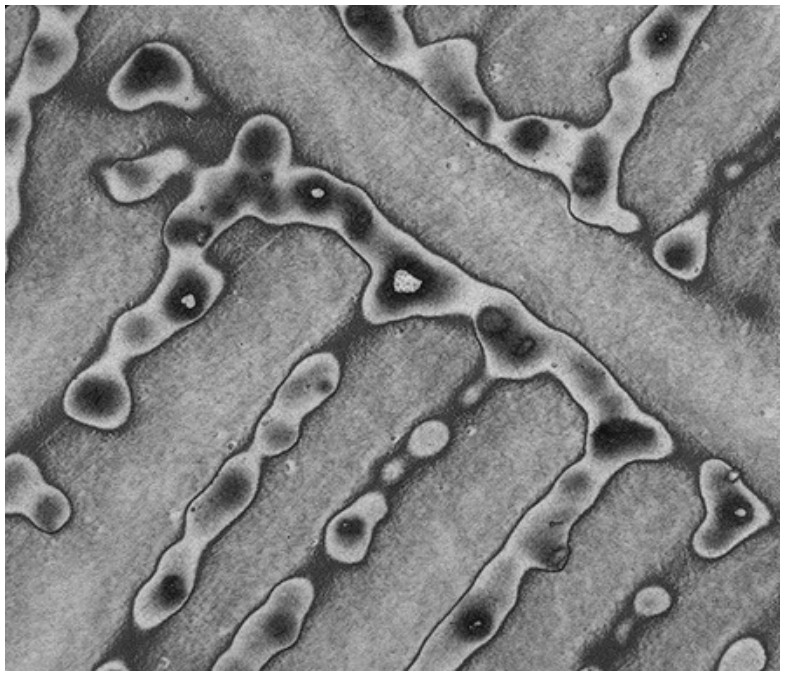
Scheil model

Thermo-Calc Software

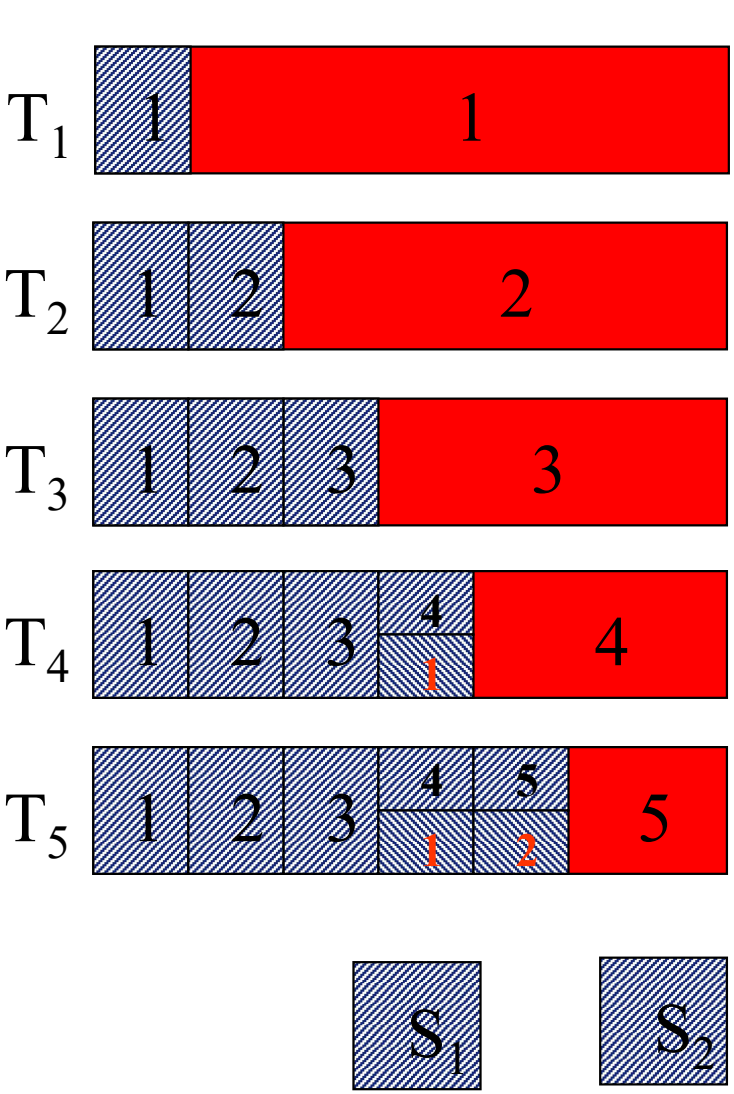
Assumptions in traditional Scheil:

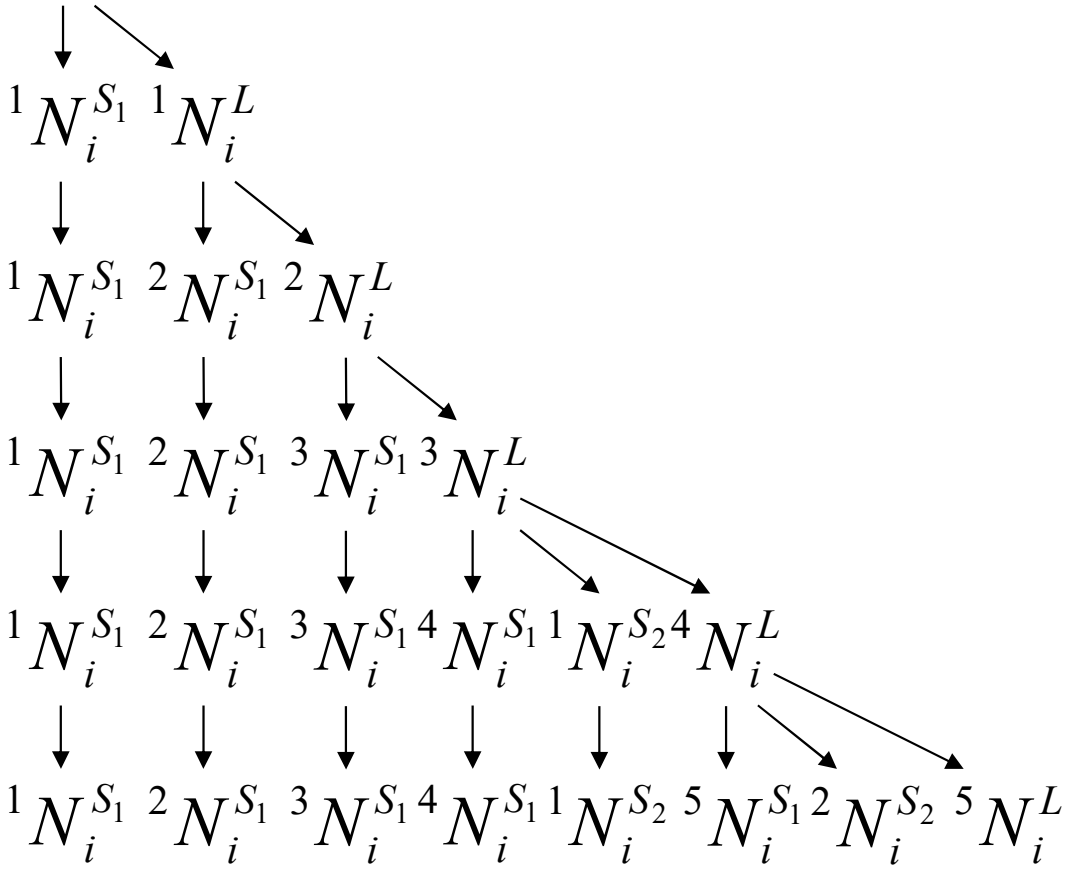
- Fast diffusion in liquid → homogenous liquid
- No diffusion in solid phases → segregations in the solid





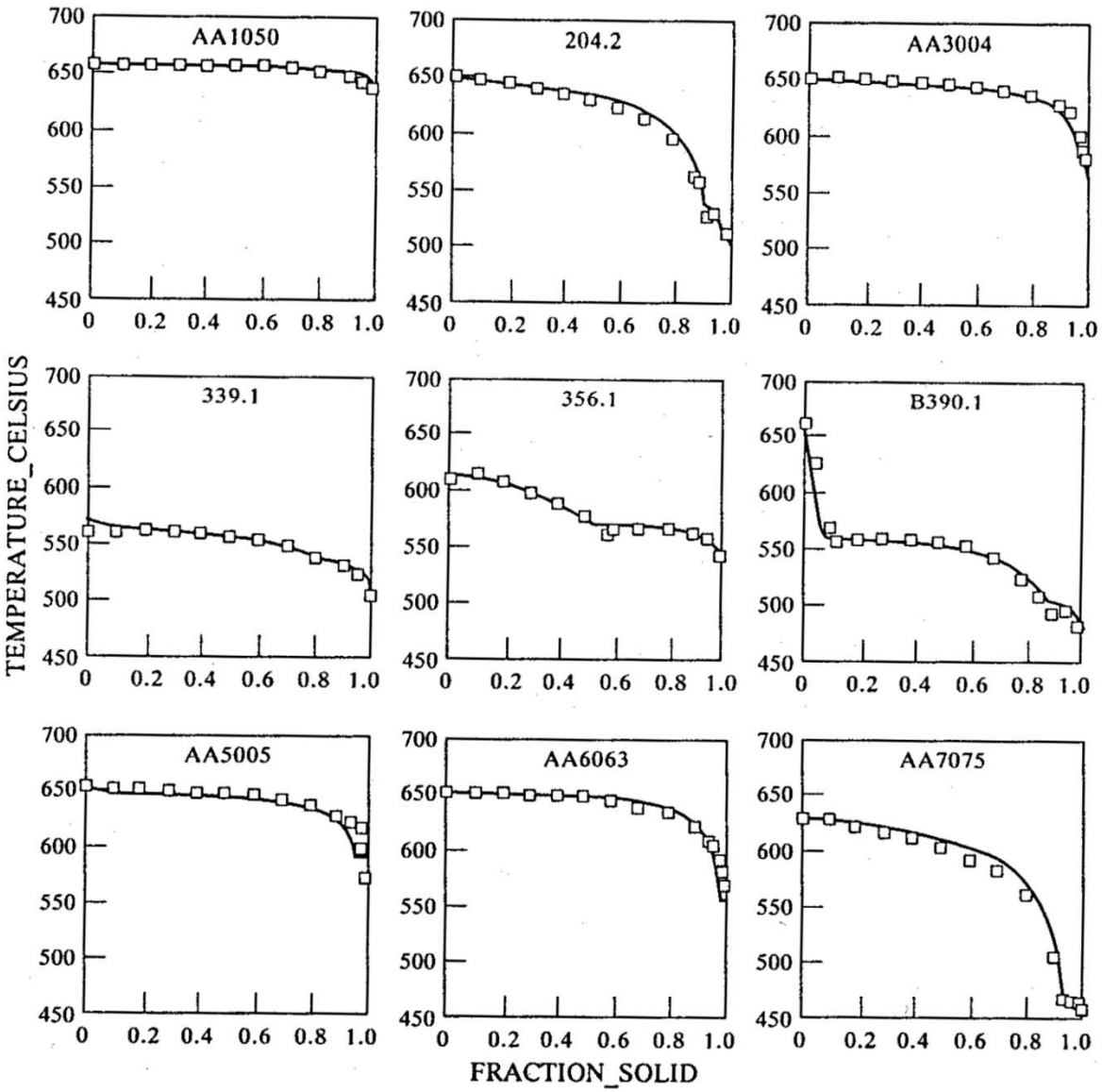
Algorithm in traditional Scheil





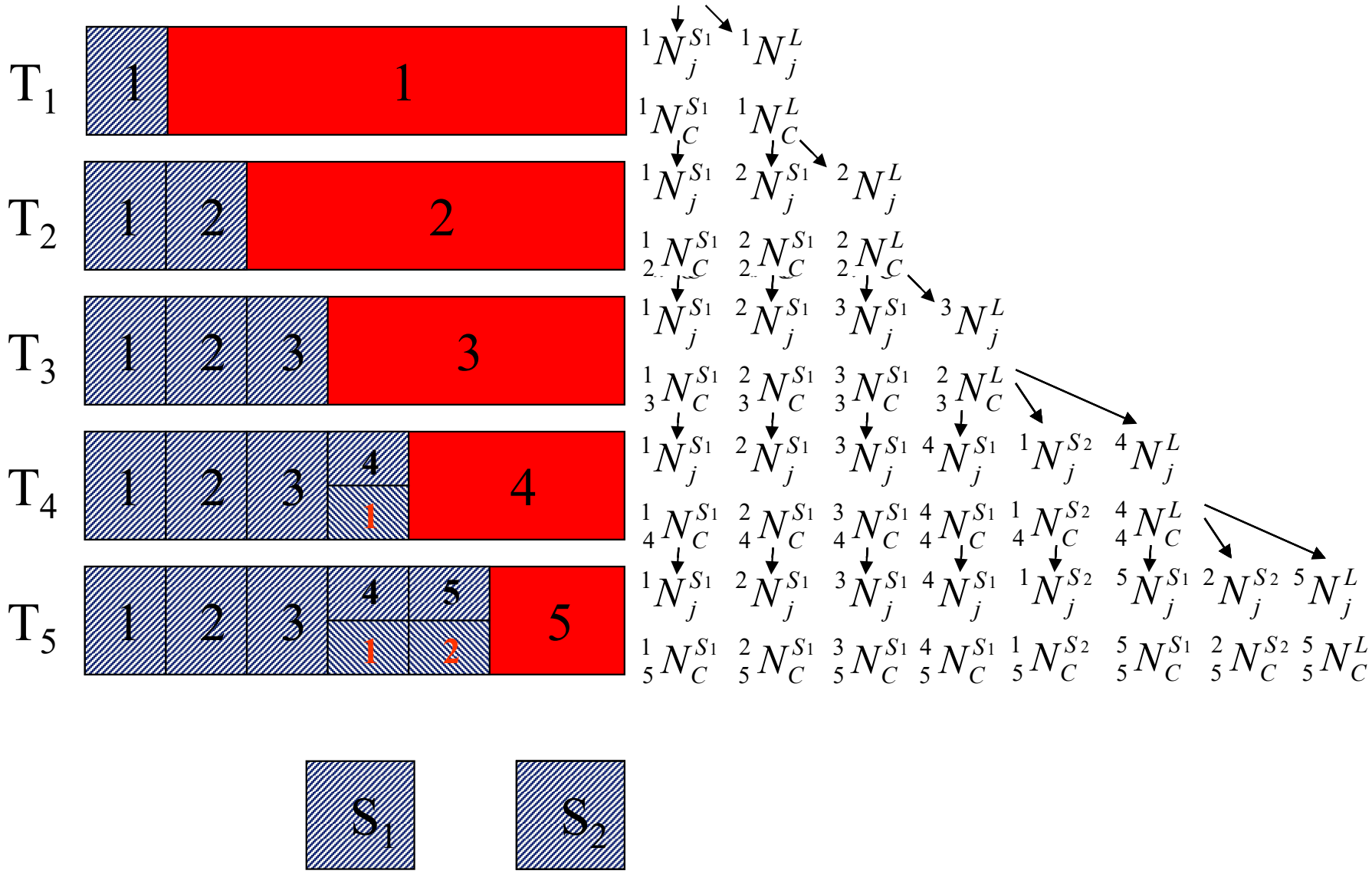
Some Examples

- T vs. fraction solid
- Results from commercial Al-alloys



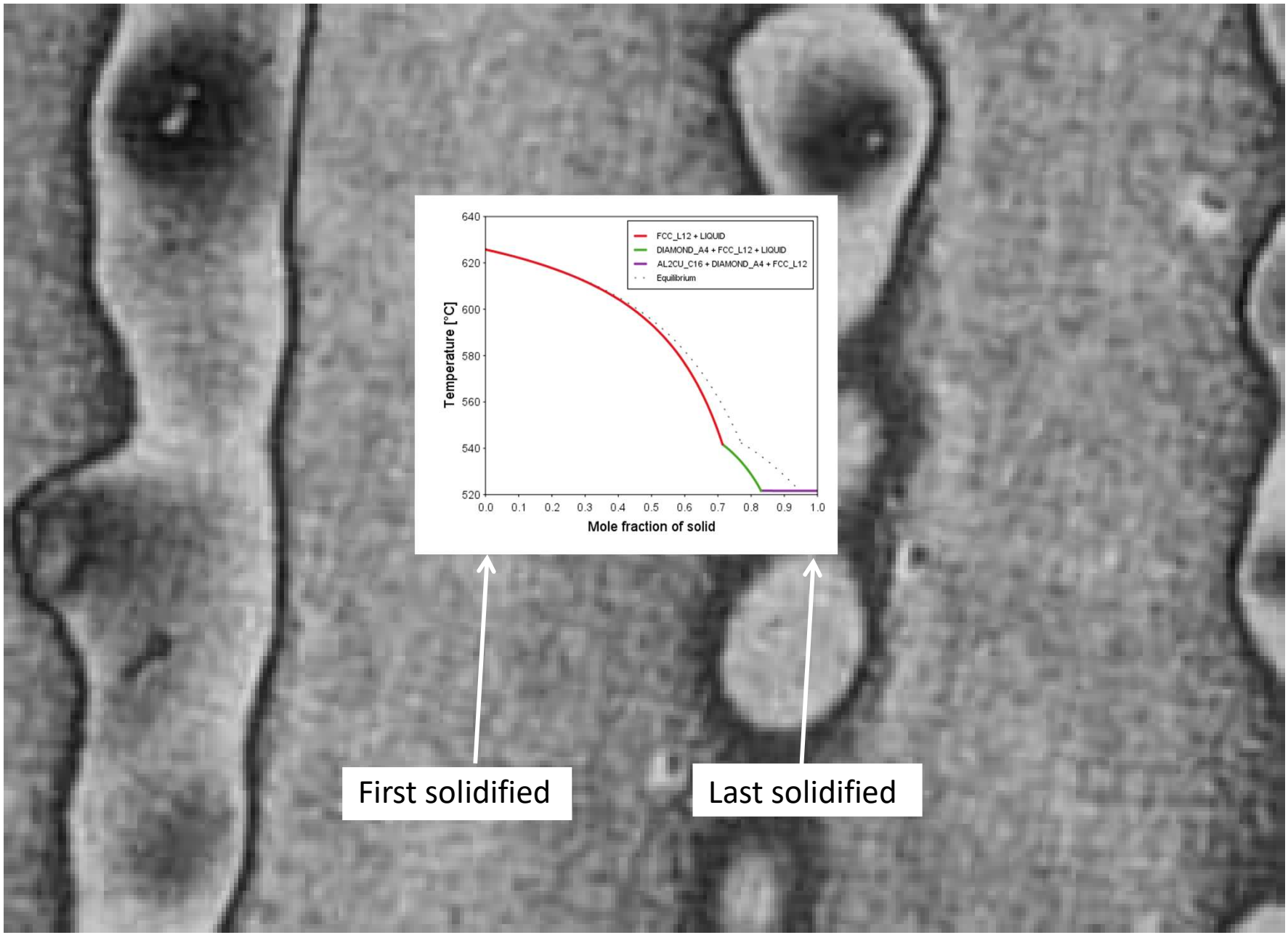
From: Saunders & Miedownik: "Calphad -a comprehensive review"

Algorithm in modified Scheil (partial eq.)



Translating the Scheil to Microstructure

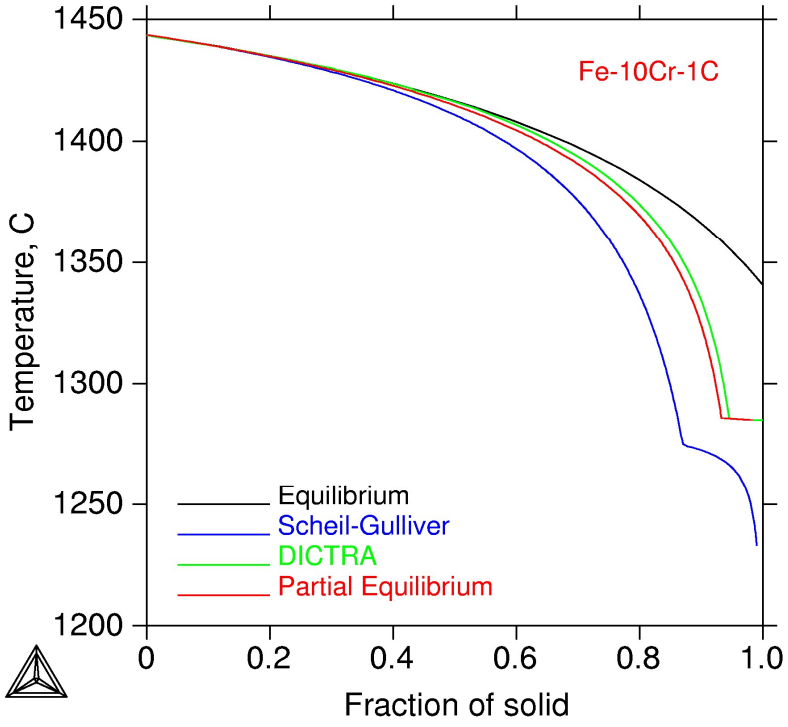
Thermo-Calc Software



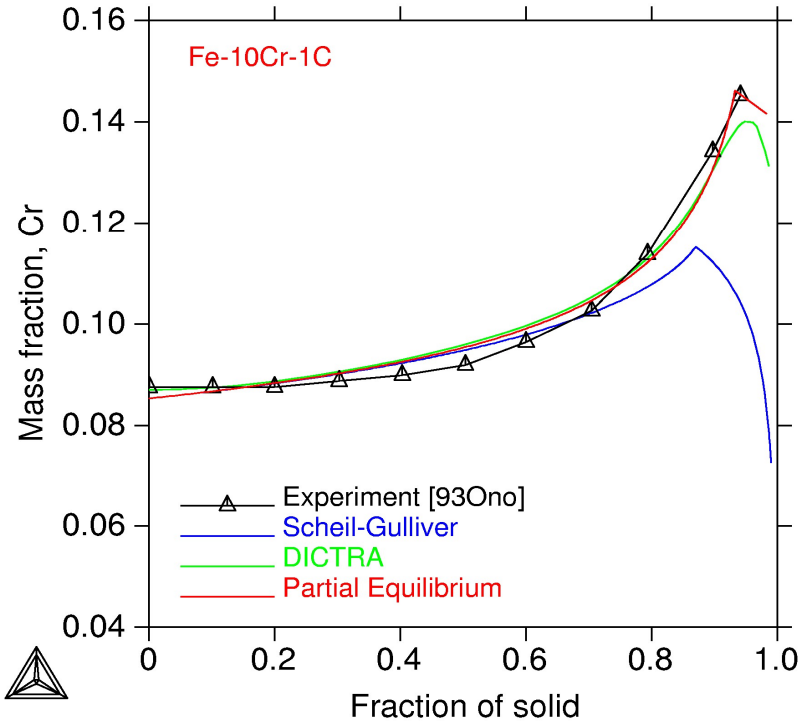
Some results: Fe-10Cr-1C

Comparison of equilibrium, Scheil, and partial eq

Freezing Range



Microsegregation



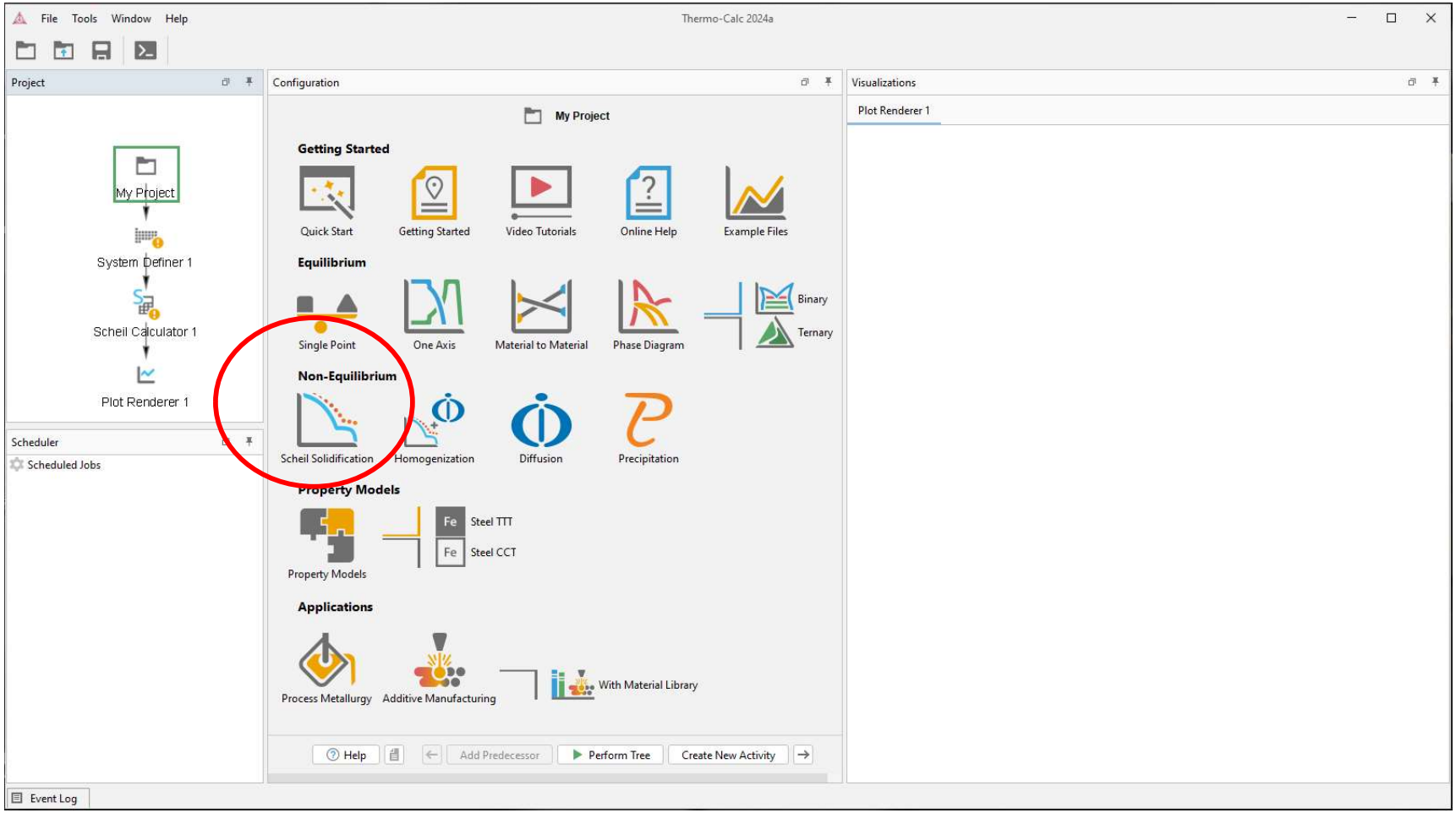
Q. Chen & B. Sundman, Materials Transactions, 43(3)551(2002).

Scheil solidification simulation

Alloy composition:

Fe – 1.00% Mn - 0.40% Mo - 0.10% C - 0.90% Ni - 0.20% Si (wt-%)

- ❑ Plot “mass fraction of solid” vs T and the segregation in the liquid.
- ❑ C as fast diffusing element – or not? Will it make a difference?



Scheil solidification simulation

Thermo-Calc Software

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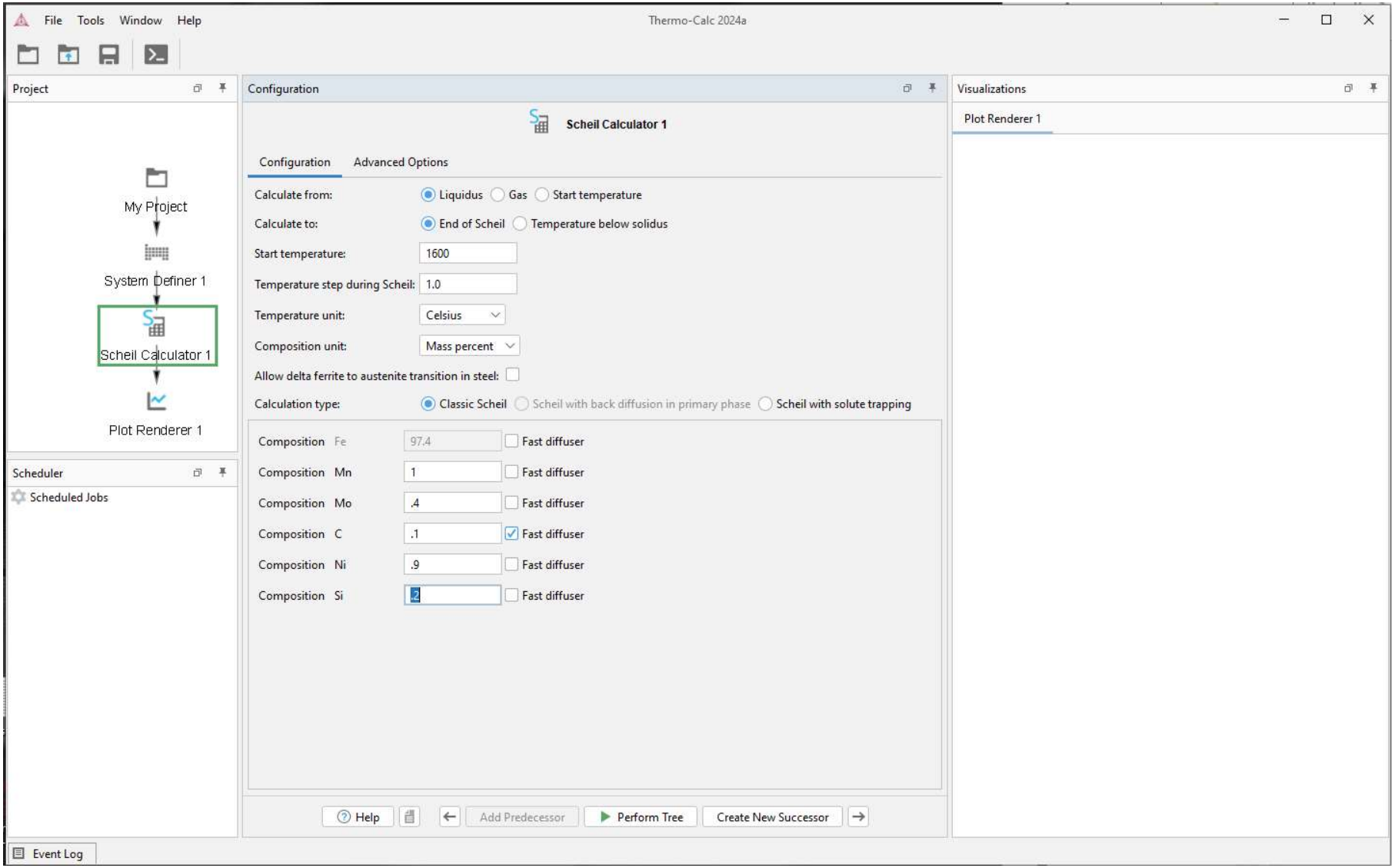
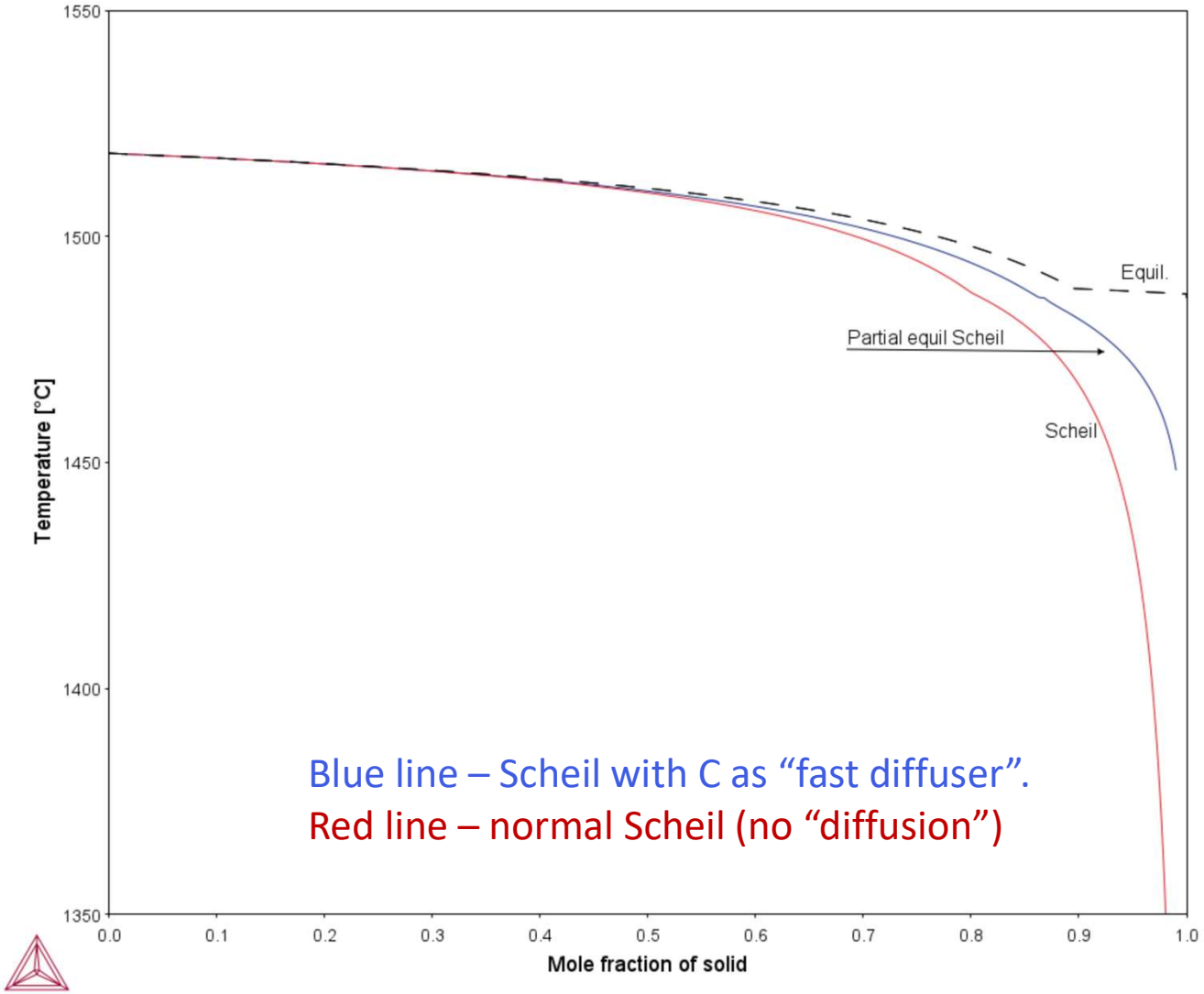


Scheil solidification simulation

Thermo-Calc Software

Alloy composition:

Fe – 1.00% Mn - 0.40% Mo - 0.10% C - 0.90% Ni - 0.20% Si



Applied Example:

Alloy design – duplex stainless steel

Alloy design example: Designing a duplex stainless steel for off-shore use.

- Based on a real example at Sandvik Steel, late 1980's.
- SAF 2507
- Said to be the world's first computer designed steel

Image from https://www.materials.sandvik/en/products/tube-pipe-fittings-and-flanges/

PRE-number for duplex stainless steel

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- PRE (Pitting Resistance Equivalence) is an empirical measure for corrosion resistance in stainless steels.

- PRE can be defined as:

  PRE=w%Cr+3*w%Mo+16*w%N

- For duplex stainless steels, it is desirable to have a high and balanced PRE-numbers in ferrite and austenite.

- Approximate composition (weight-%):

  Fe (bal.) – 25 Cr – 7 Ni – 4 Mo – 0.3 Mn – 0.3 Si – 0.27 N – 0.002 C

Effect of alloy elements on phase stability

Thermo-Calc Software

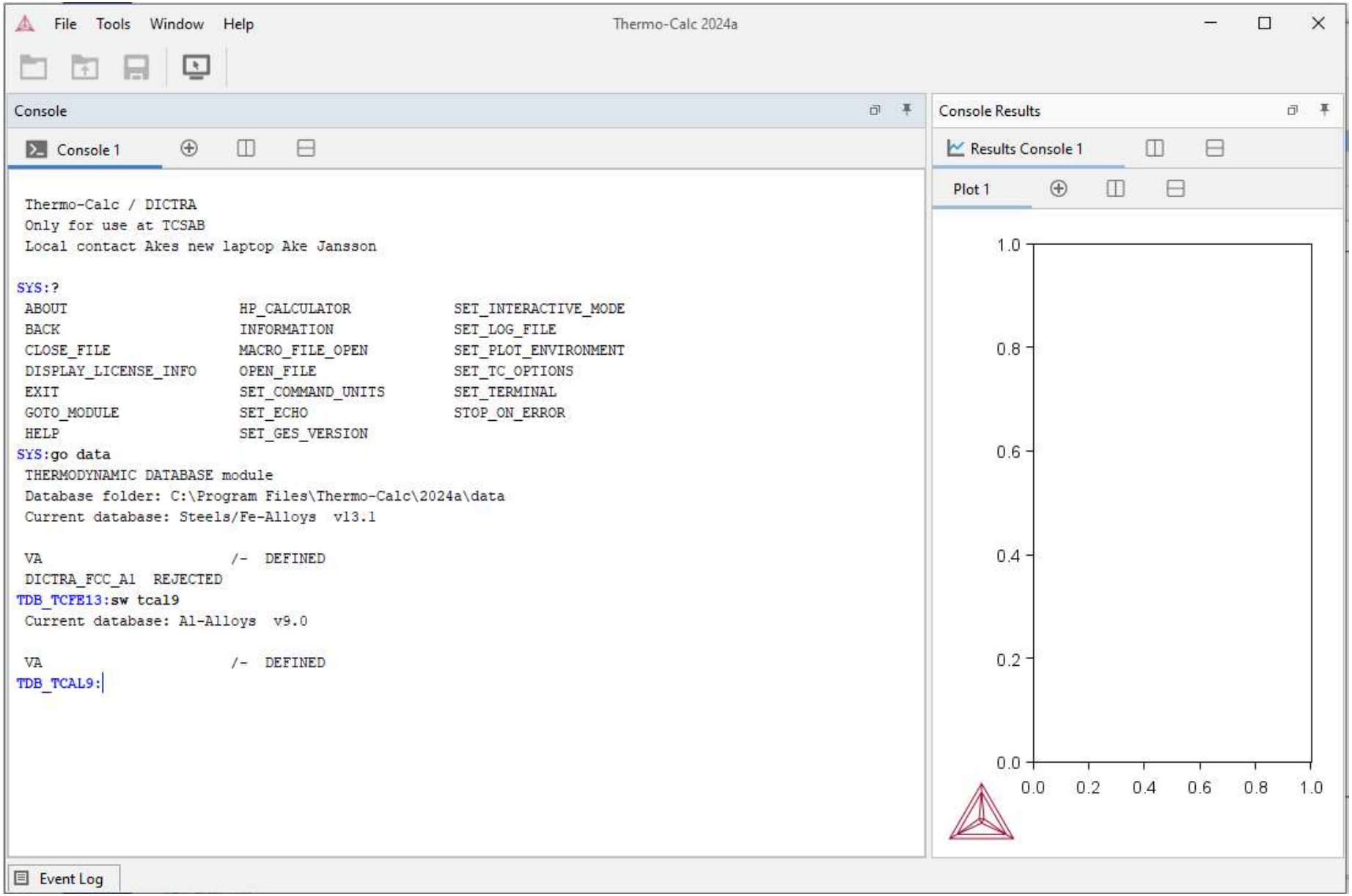
- May be evaluated by entering variables which are derivatives
- The phase of interest with status fixed=0
- No condition for T

- Evaluate $\frac{\partial T}{\partial w(i)}$ by entering user defined variables

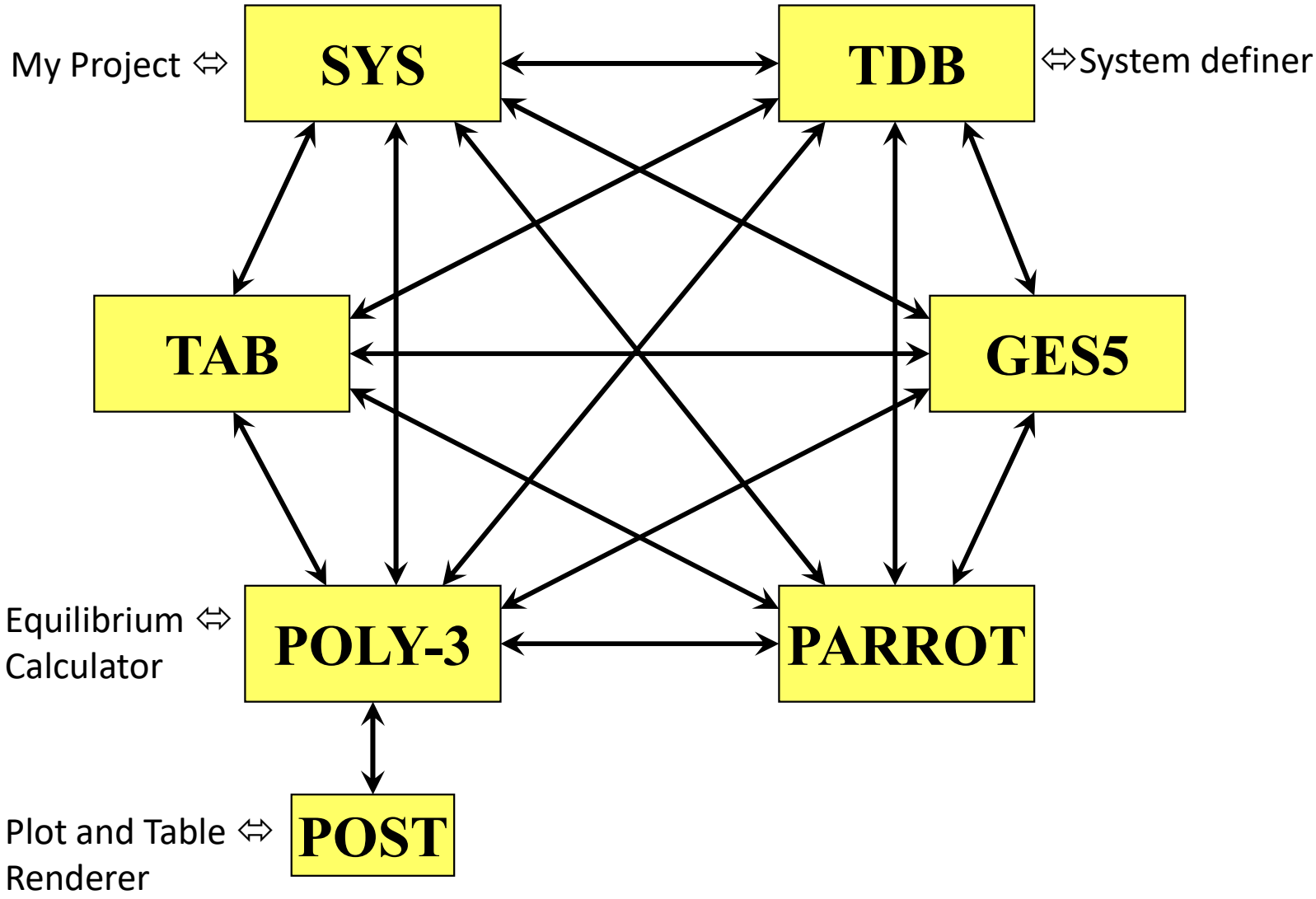
Syntax: T.w(Cr) equals $\frac{\partial T}{\partial w(Cr)}$

Console mode

Using Console Mode



Modules in Thermo-Calc Console mode



Special modules in Console mode

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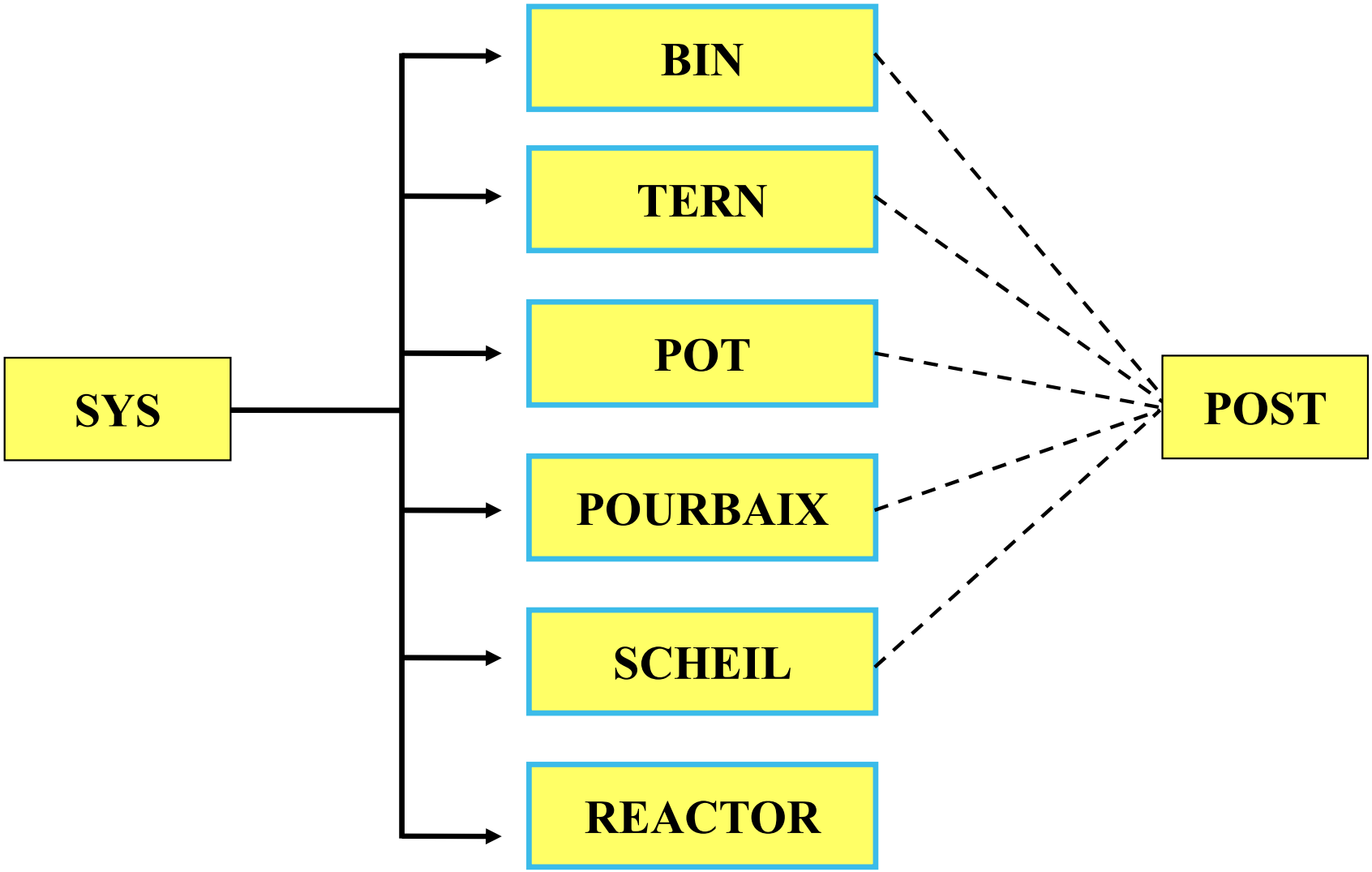
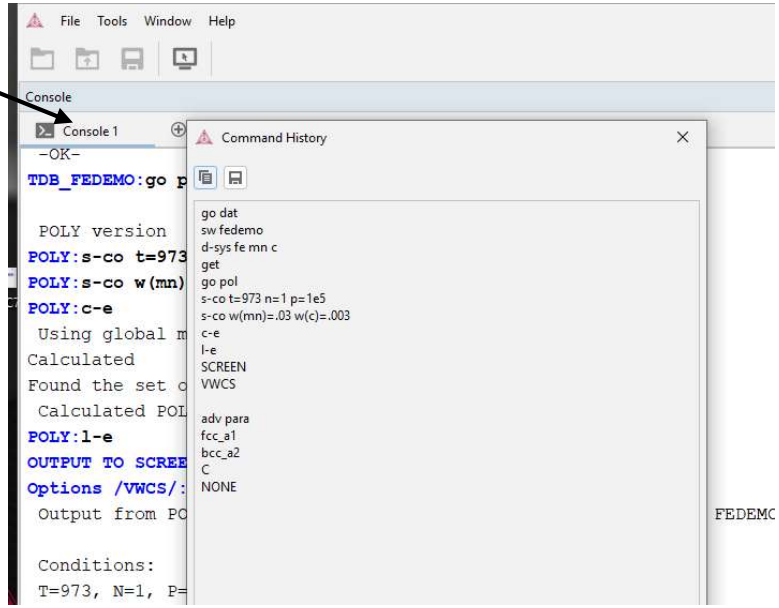
These modules* are very automatic and after entering a few conditions, the calculation will start and end with a plotted diagram.

*) except REACTOR



Console Mode Macros

- Text files with Console mode commands
- Preferred file extension: .TCM
- Can easily be produced from log-files (SET-LOG command) – or by right-clicking ”Console 1” and opening ”Command history”
- Can be rewritten in a text editor.



LOGFILE → MACRO FILE

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

go data
switch tcni12
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 tcni12
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
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step
NORMAL
post
set-diag-ax x t-c
set-diag-ax y vpv(*),,
plot,,

set-interact
```

Thermo-Calc Software

Questions

&

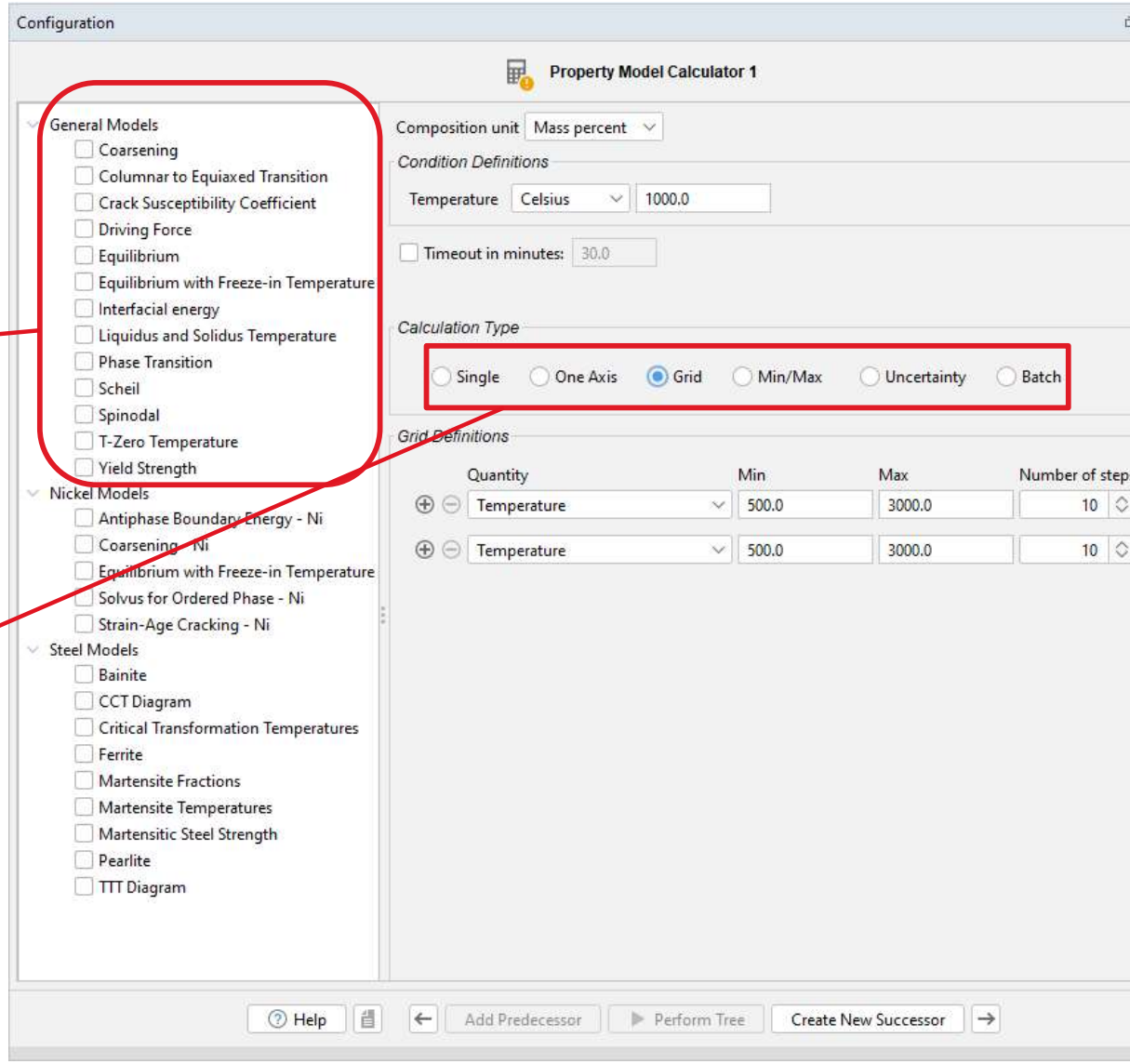
Answers

Thermo-Calc Software

Property Model Calculator

Property model calculator

- Calculation activity which allows users to predict and optimize properties of materials based on models.
- Thirteen general models have been introduced.
- Further models are in development.
- Different calculation types.
- Users can develop their own models based on python script.



Variation of A1 over a composition range

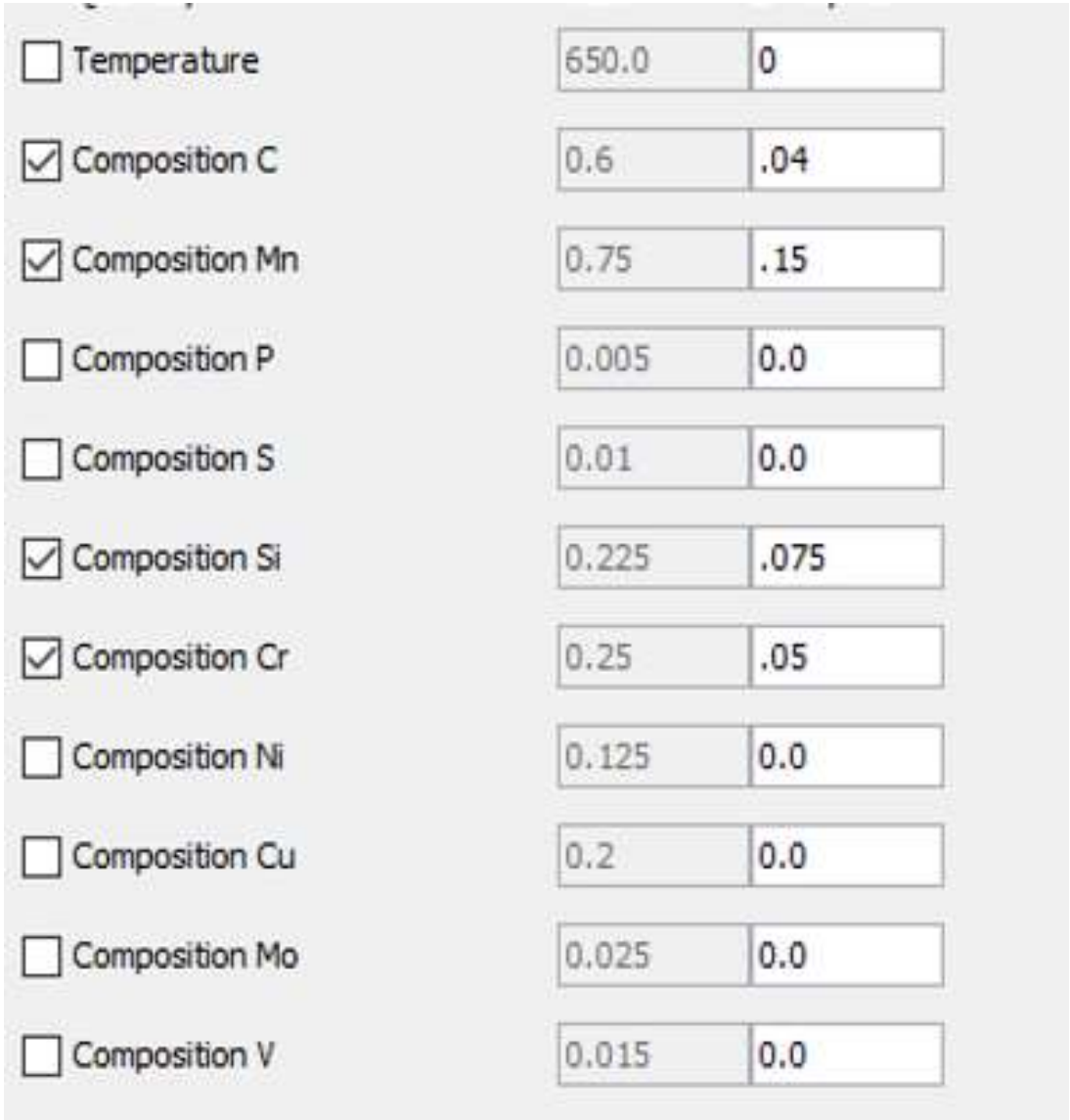
Thermo-Calc Software

Composition of this steel:

Fe (bal.) + (in wt-%)

200 random samples, where
4 elements were varied:
C Mn Si Cr

The other elements were constant at their nominal composition.



Variation of A1 over a composition range - result

Thermo-Calc Software

Configuration

Property Model Calculator 1

Composition V 0.015

Phase transition

Configuration | Description

Matrix phase: BCC_A2

Phase to form: FCC_A1

Condition to vary: Temperature

Search direction: Positive

Calculation Type

Single | One axis | Grid | Min/Max | Uncertainty

Sampling of Data from Gaussian Distributions

Quantity	Mean	Δ Min/Max
Temperature	650.0	0
Composition C	0.6	.04
Composition Mn	0.75	.15
Composition P	0.005	0.0
Composition S	0.01	0.0
Composition Si	0.225	.075
Composition Cr	0.25	.05
Composition Ni	0.125	0.0
Composition Cu	0.2	0.0
Composition Mo	0.025	0.0
Composition V	0.015	0.0

Sampling Parameters

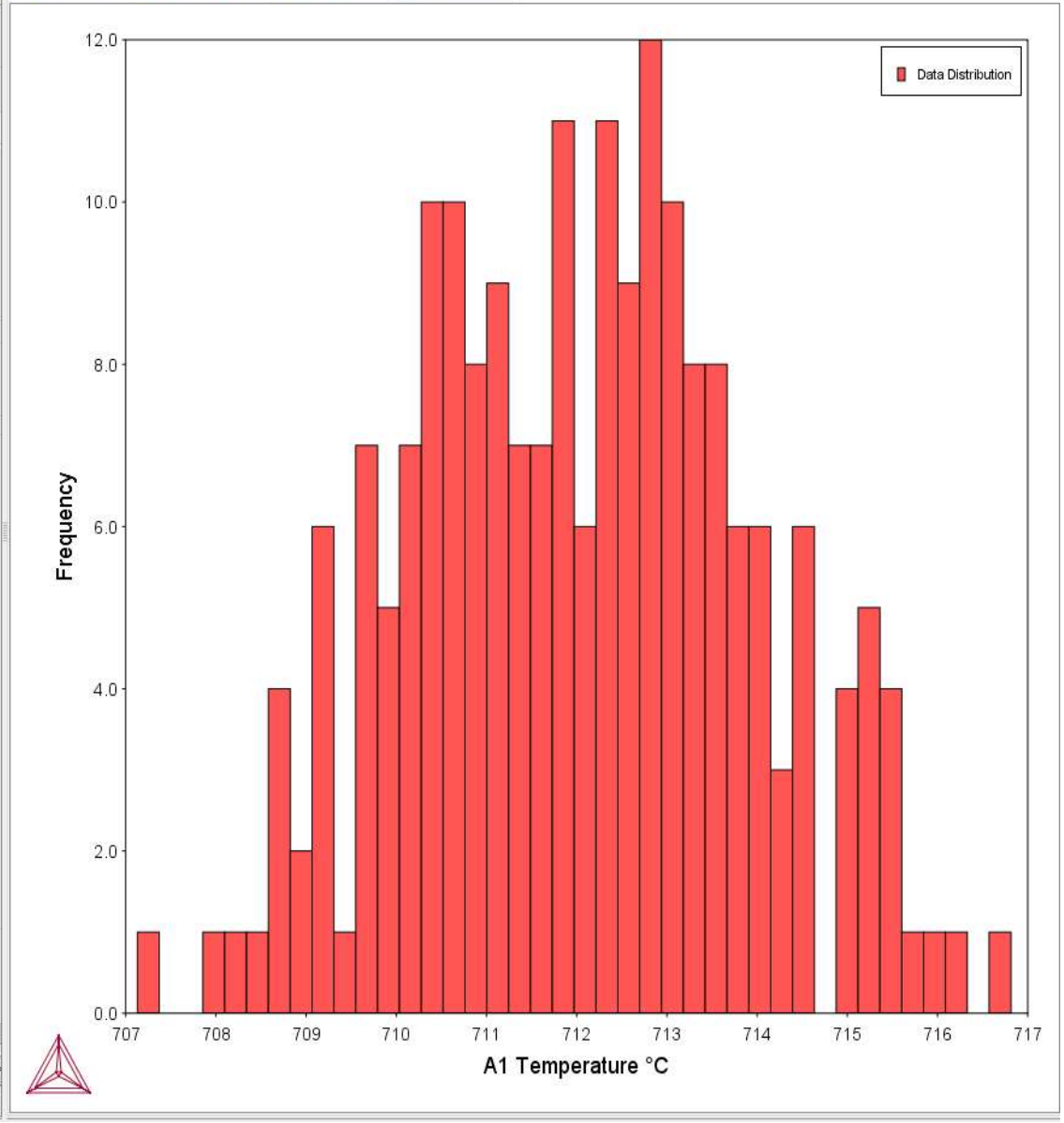
Truncate distribution at 3 standard deviations

Total number of samples 200

Help | < | Add Predecessor | Perform Tree | Create New Successor | >

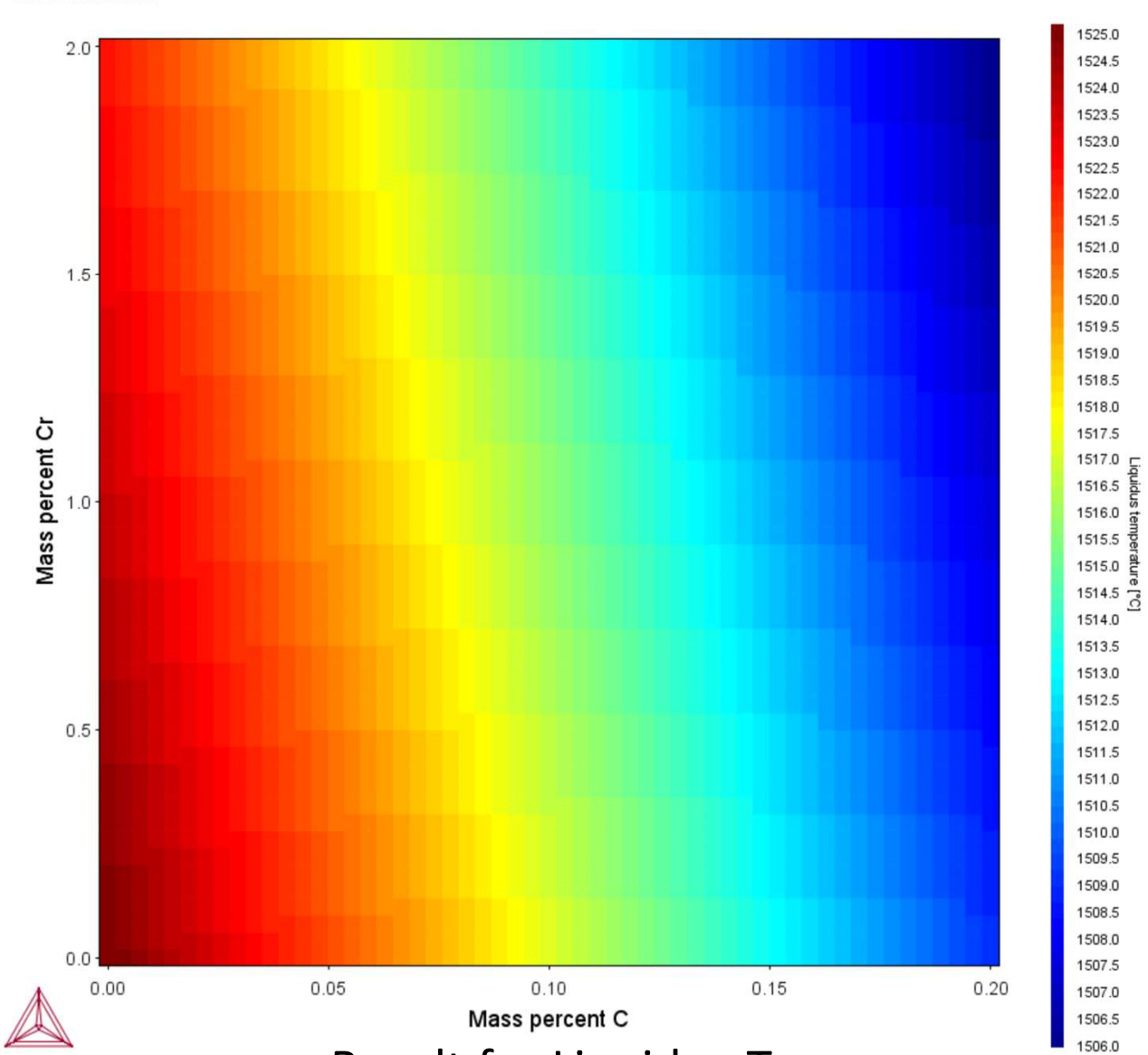
Results

Plot Renderer 1 | Plot Renderer 3 | Plot Renderer 4 | Plot Renderer 5



Property Model Calculator result – Liquidus/(Solidus)

Fe – 1Cr – 1Mn – 0.7Ni – 0.5Si – 0.1C (wt-%)

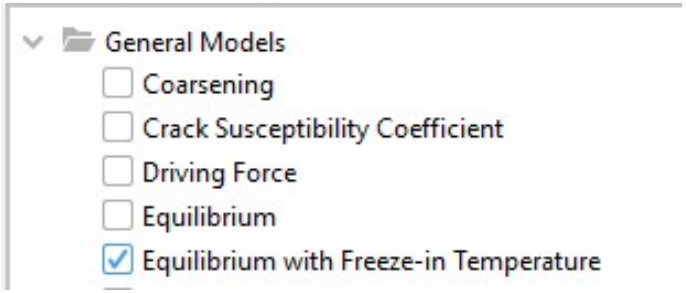


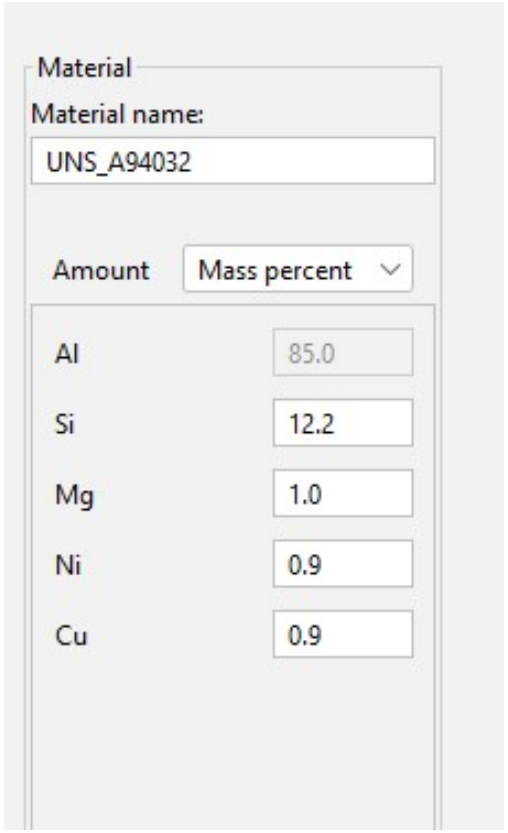
Result for Liquidus-T.

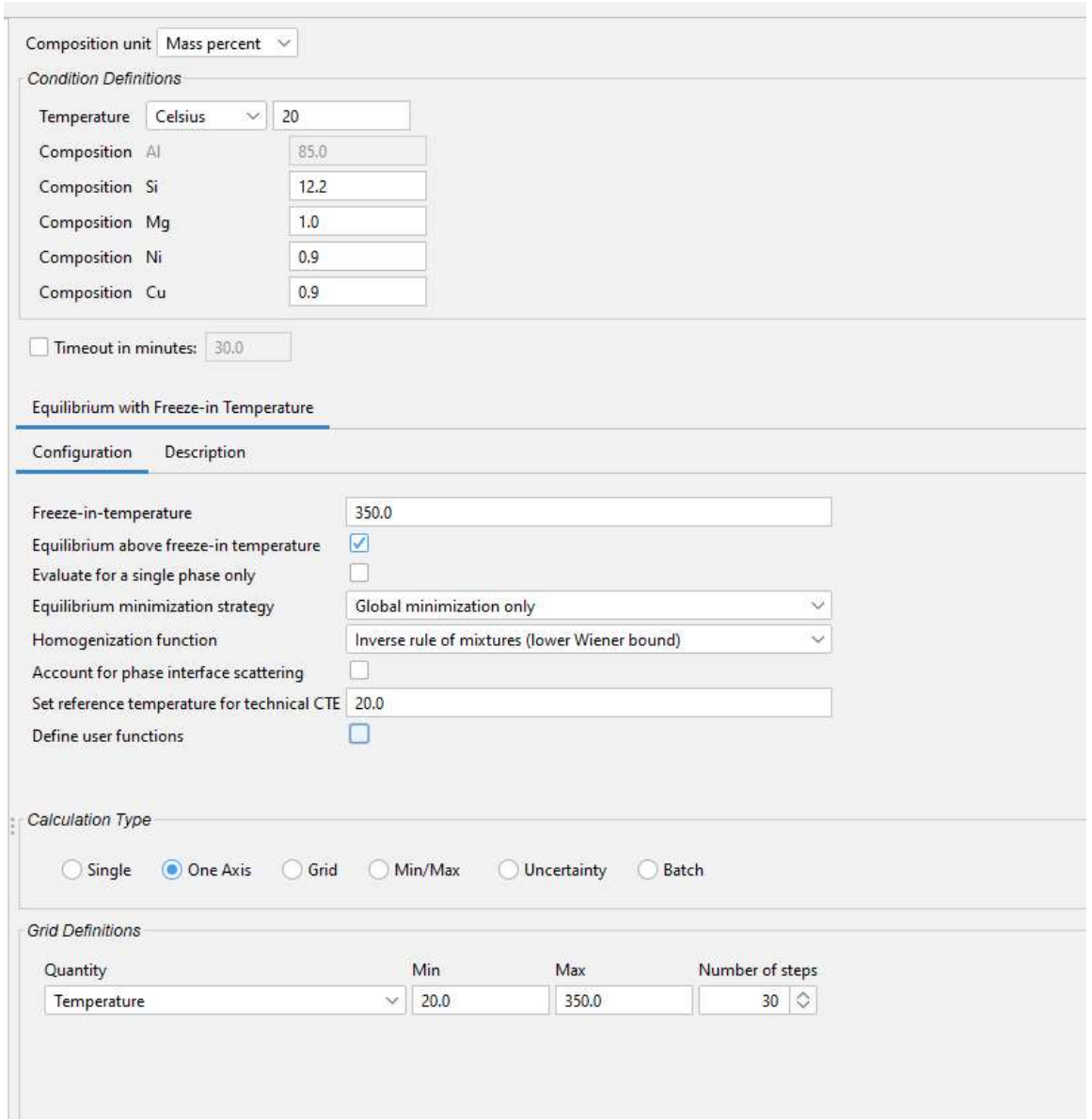
Property Model Calculator:
Electrical resistivity, freeze-in temperature

Step in temperature for Al-alloy AA4032.

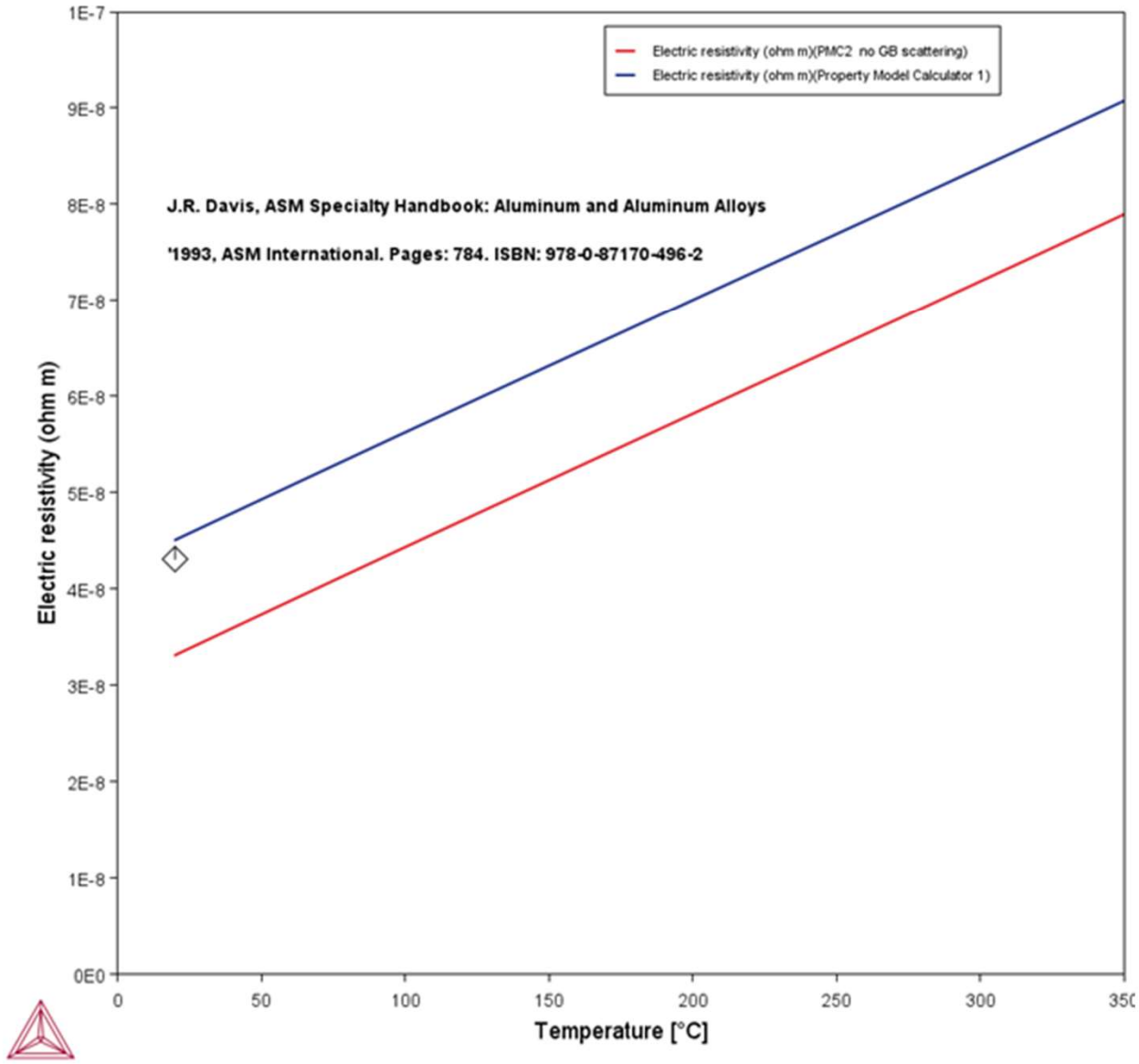
Plot the Electrical resistivity. Heat treatment at 350 C.







Property Model Calculator result – Electrical resistivity, freeze-in

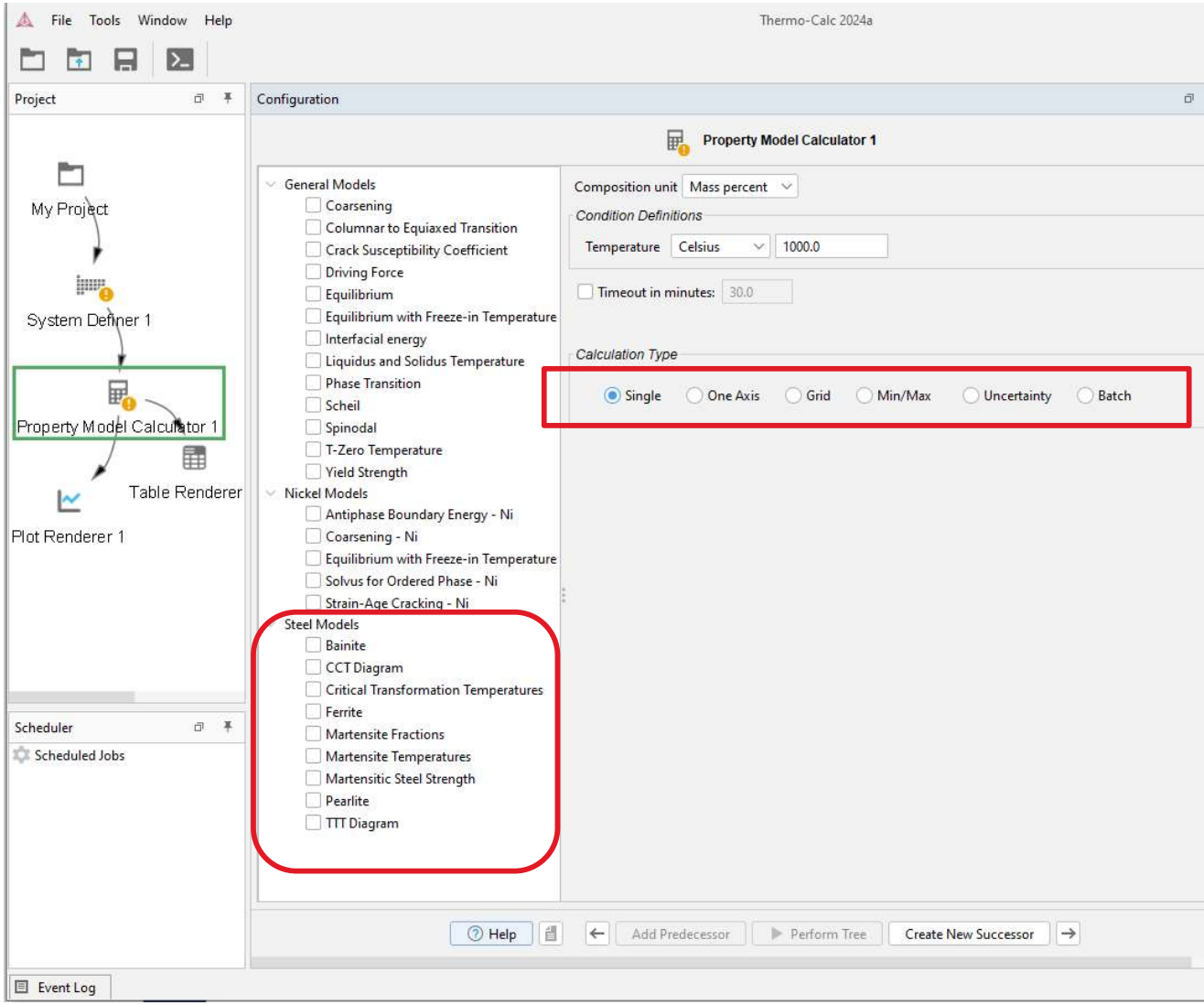


Thermo-Calc Software

Steel Model Library

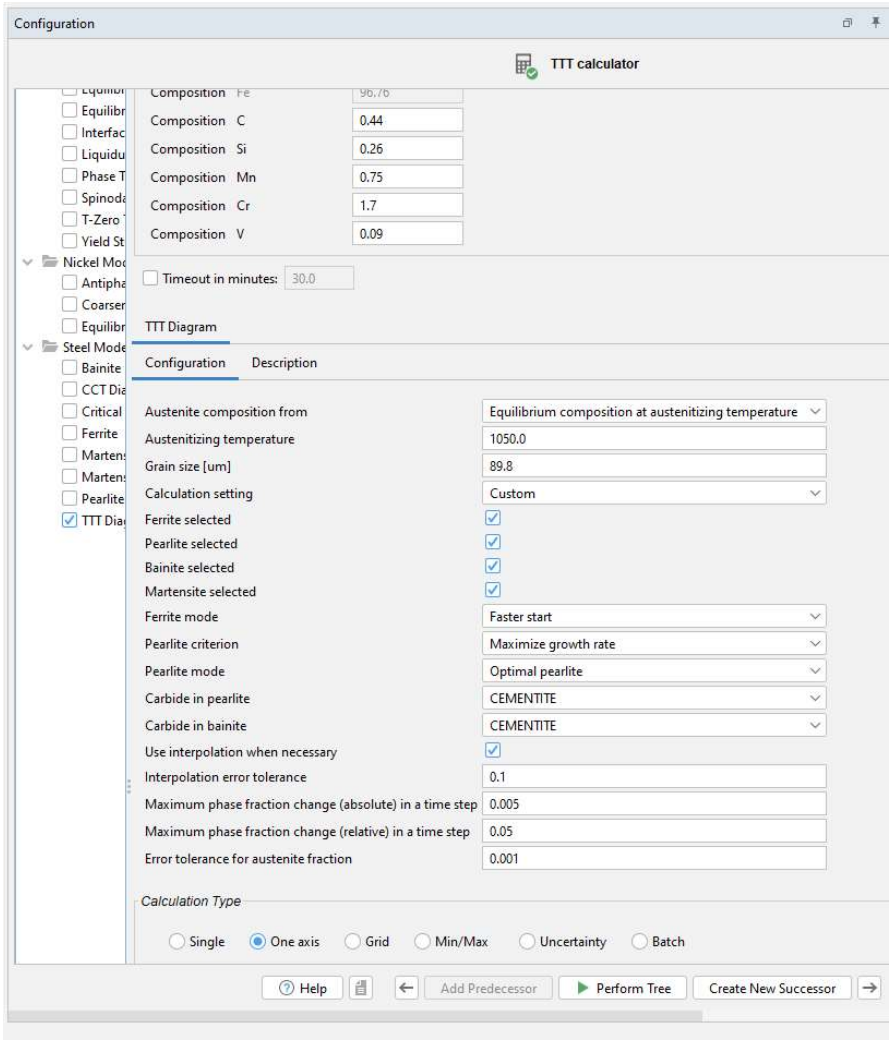
Steel Model Library

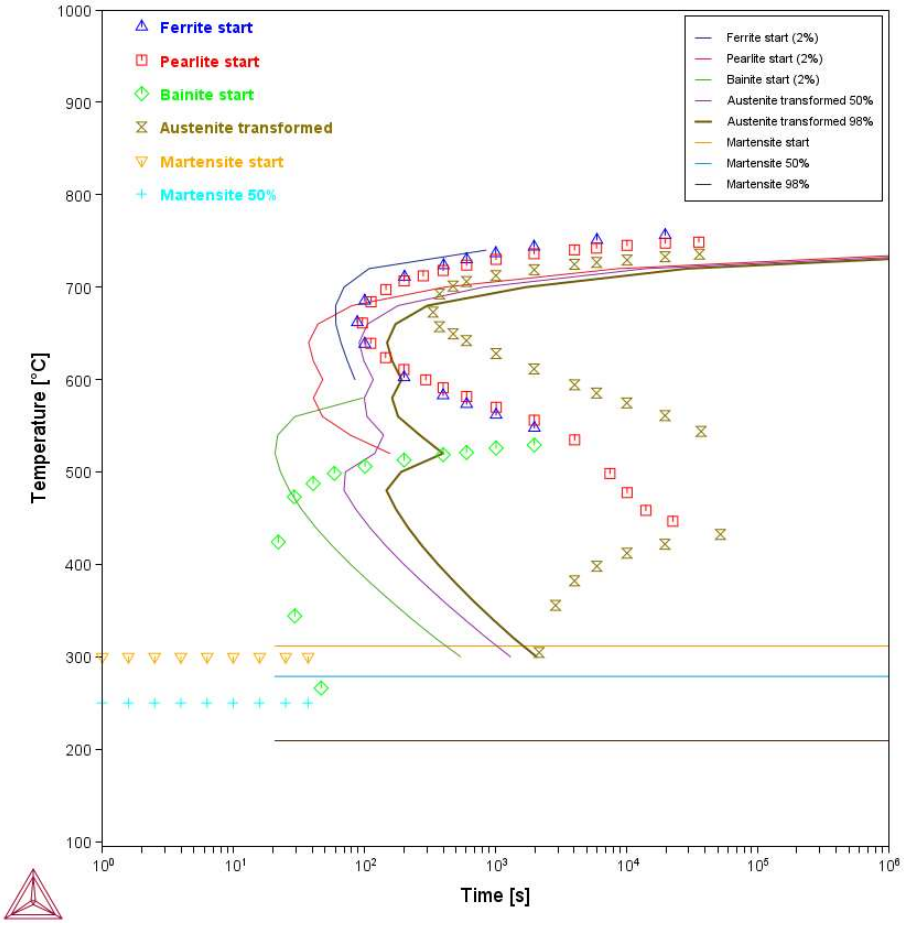
- Advanced models for formation of structures in steel.
- Introduced in 2019, martensite and pearlite models.
- Bainite and TTT-diagram model were added in 2021, CCT new in 2022.
- Other material specific property model libraries will be added in the future. Ni-library was new in 2022.



Steel Model Library

Fe (bal.) – 0.44 C – 1.7 Cr – 0.75 Mn - 0.26 Si – 0.09 V



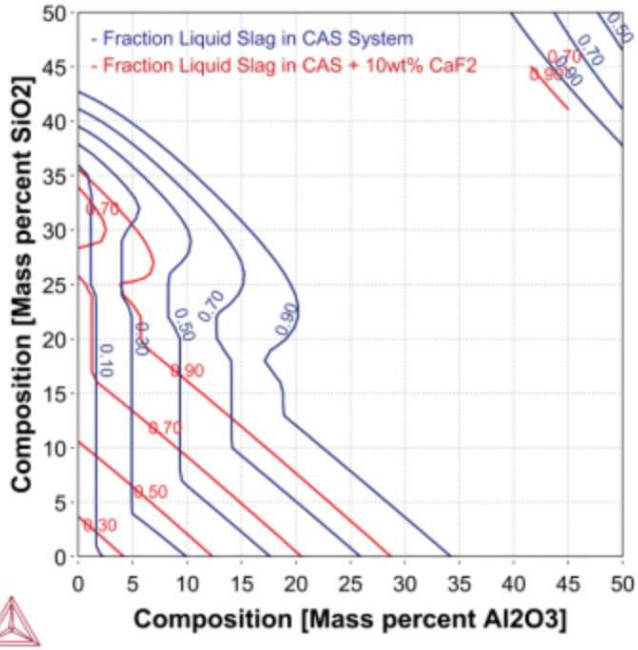


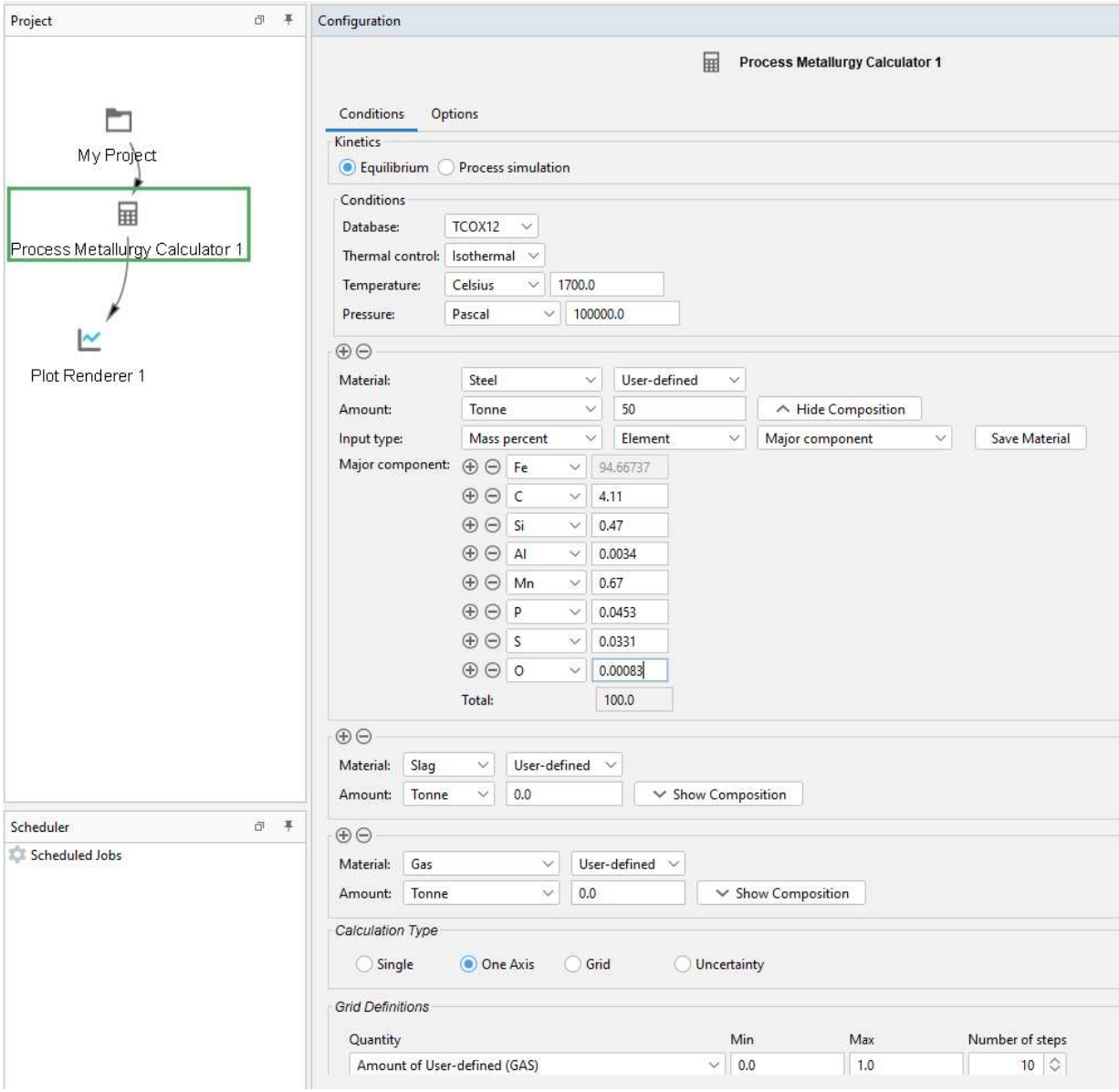
Thermo-Calc Software

Process Metallurgy Module

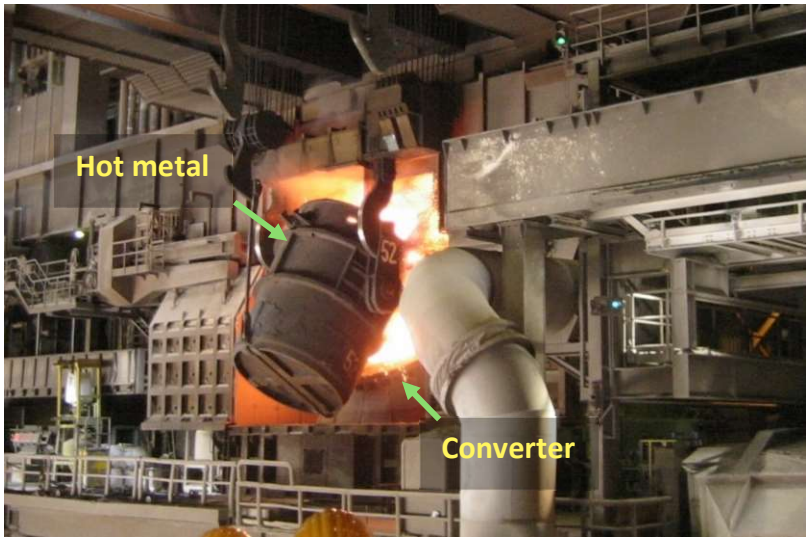
Process Metallurgy Module (PMM)

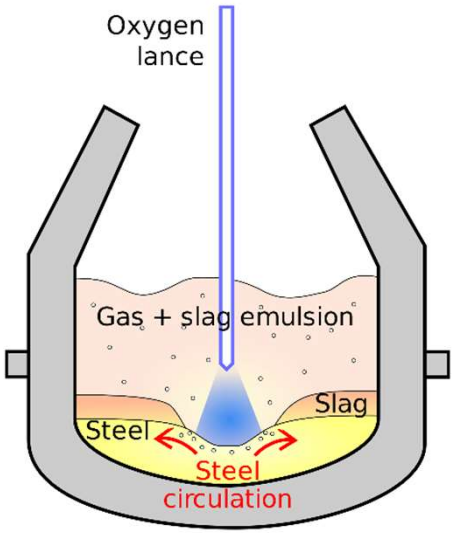
- Module for easy set-up of Steel-Slag-Gas equilibria.
- New in 2019.
- Designed for steel making and steel refining processes, BOF, EAF, LF and more.





PMM Example
Calculation of decarburization (steelmaking)





The hot metal from a blast furnace contains about 4.5 wt% Carbon. This makes it brittle and unsuitable for forging and rolling. The carbon content therefore needs to be reduced. This is termed steel-making and is mostly carried out in a converter (basic oxygen furnace, BOF) by blowing oxygen into the hot metal. The main reaction taking place is

Hot metal + O_2(gas) = Steel + CO (gas)

This reaction is highly exothermic and results in a temperature increase in the converter from ~1450°C to over 1650°C.

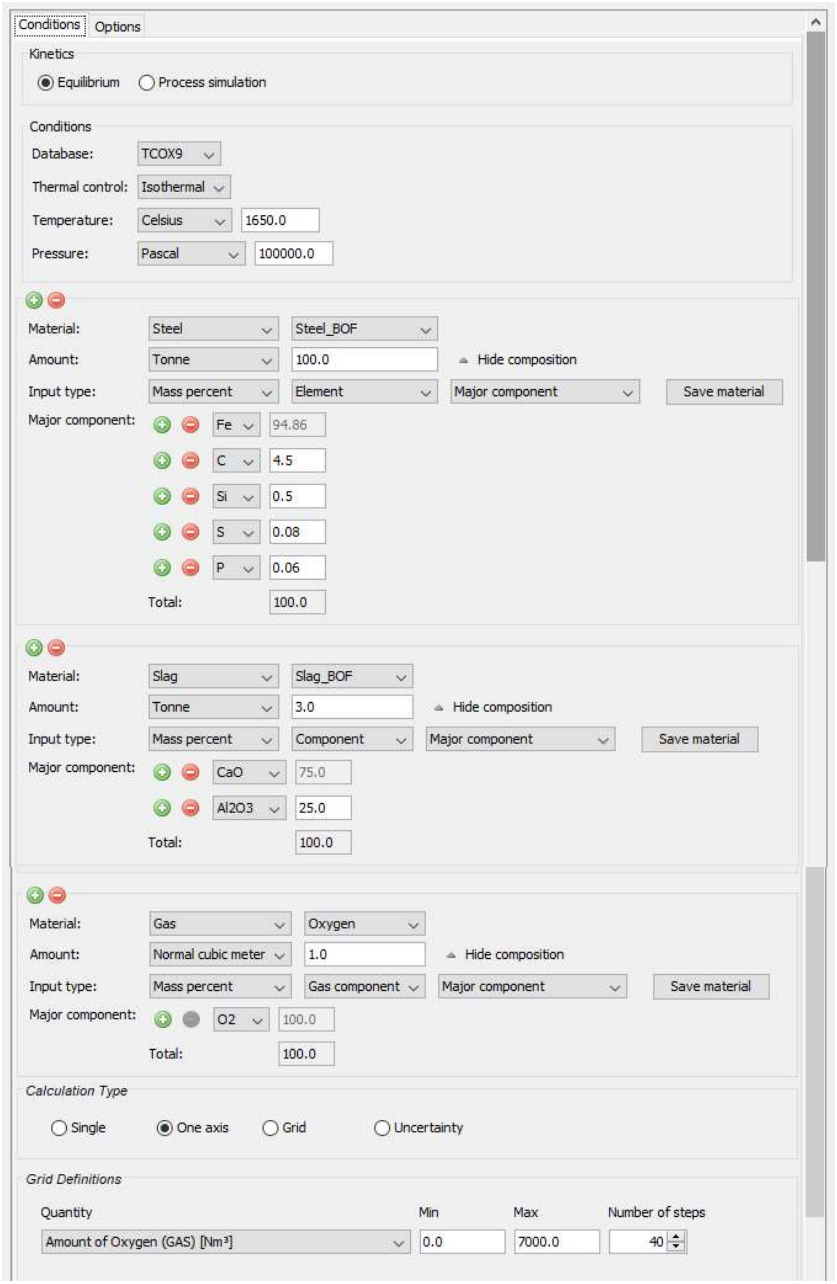
During the blowing process other oxidizing reactions can take place. Some are desirable such as the oxidation of Phosphorous and removal from the hot metal

P (hot metal) + O_2 (gas) → P_2O_5 (slag)

Other oxidation reactions are not desirable, such as the oxidation of the iron itself, that results in a reduced yield of the process:

Fe (hot metal) + O_2 (gas) → FeO_x (slag)

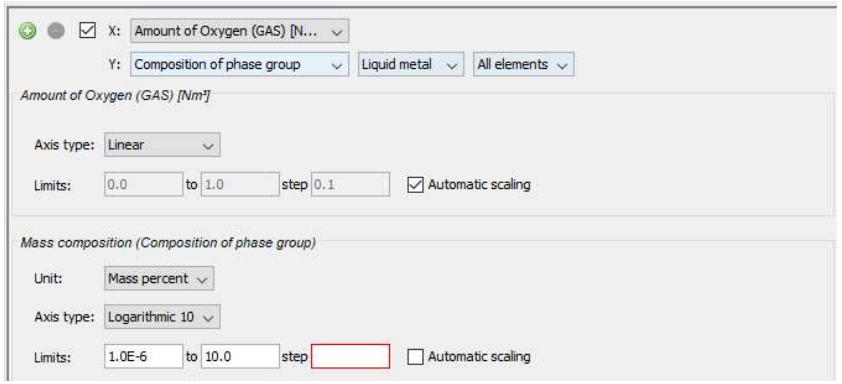
PMM Example 1
Calculation of decarburization EQUILIBRIUM



Setting up equilibrium calculation

This assumes that all the oxygen added to the converter immediately reaches equilibrium with all the hot metal. This is certainly a simplification but important information about the reactions can be obtained.

1) Set-up and run equilibrium calculation as shown
2) Experiment with various plots of the results:



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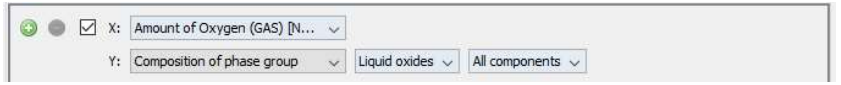

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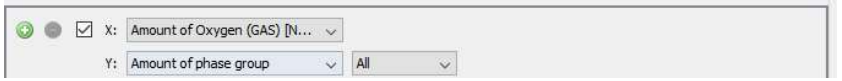
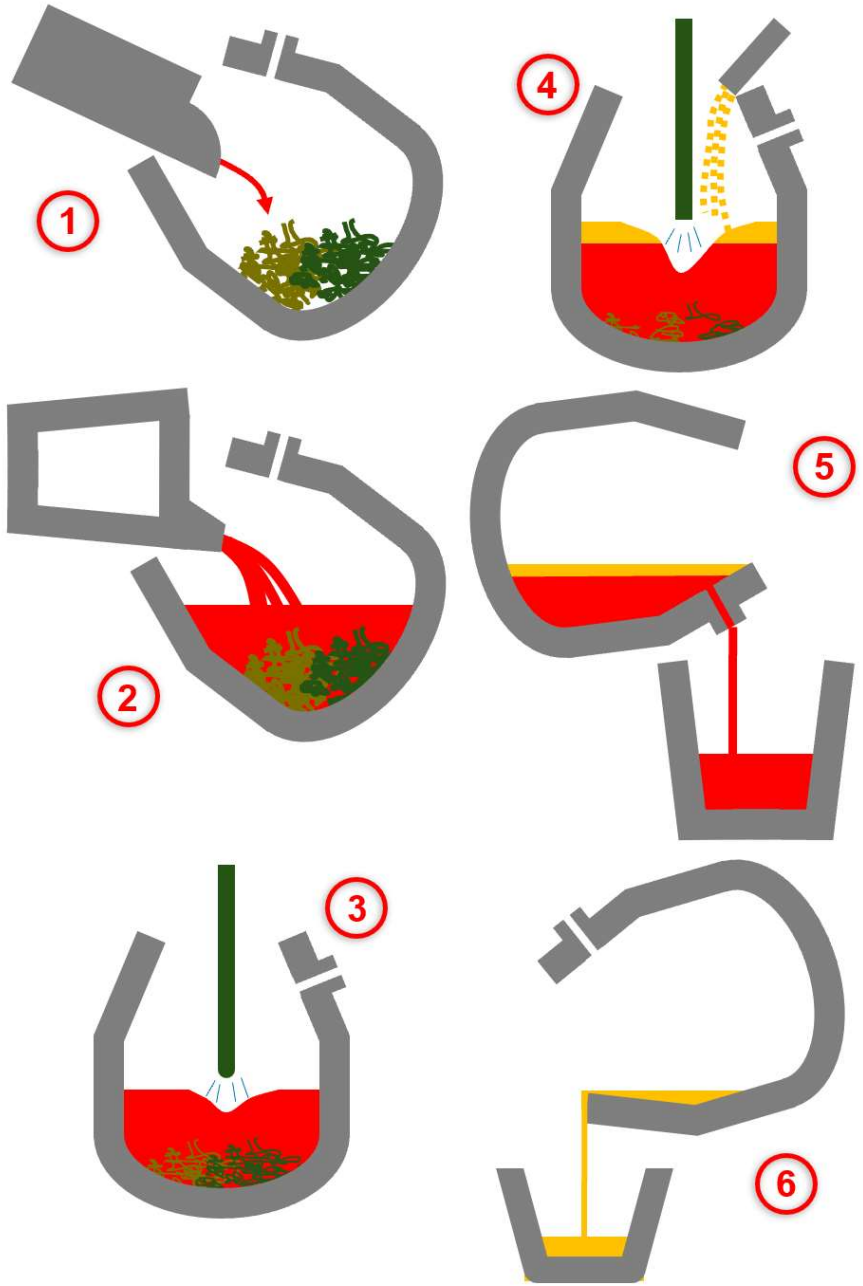


Experiment with different calculations

a) Adiabatic instead of Isothermal. For this the initial temperatures of the steel and slag will have to be set. Put both at 1450°C.

b) Add 0t of slag. Note that this will result in no dephosphorization.

PMM Example 2
Calculation of decarburization PROCESS SIMULATION

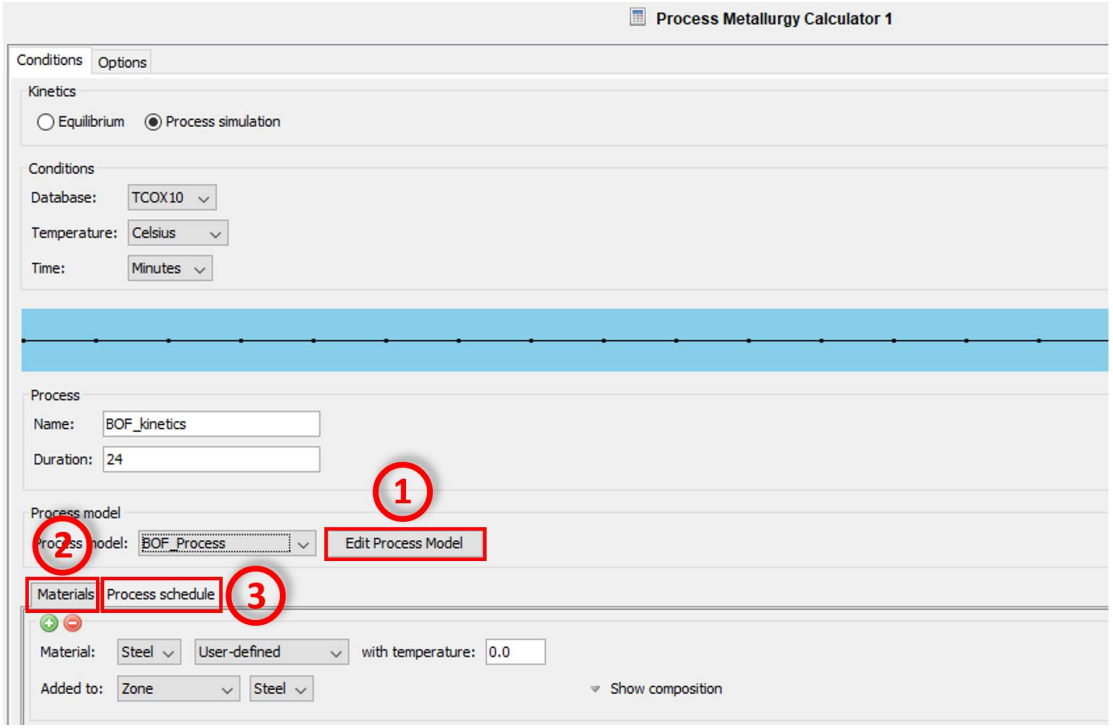


Setting up equilibrium calculation

The aim of a process simulation is to describe the complete process:

1) Initial situation with cold scrap in the converter
2) Hot metal is poured onto the cold scrap
3) Oxygen lance is lowered and blows oxygen into the hot metal, at the same time scrap gradually melts
4) Slag formers are added to the converter
5) Aim is to find the final steel and slag composition and temperature

PMM Example 2
Calculation of decarburization PROCESS SIMULATION



The 3 steps for setting up a process simulation:

1) Define kinetics of steel – slag reactions.
2) Define materials to be used in simulation.
3) Define process schedule

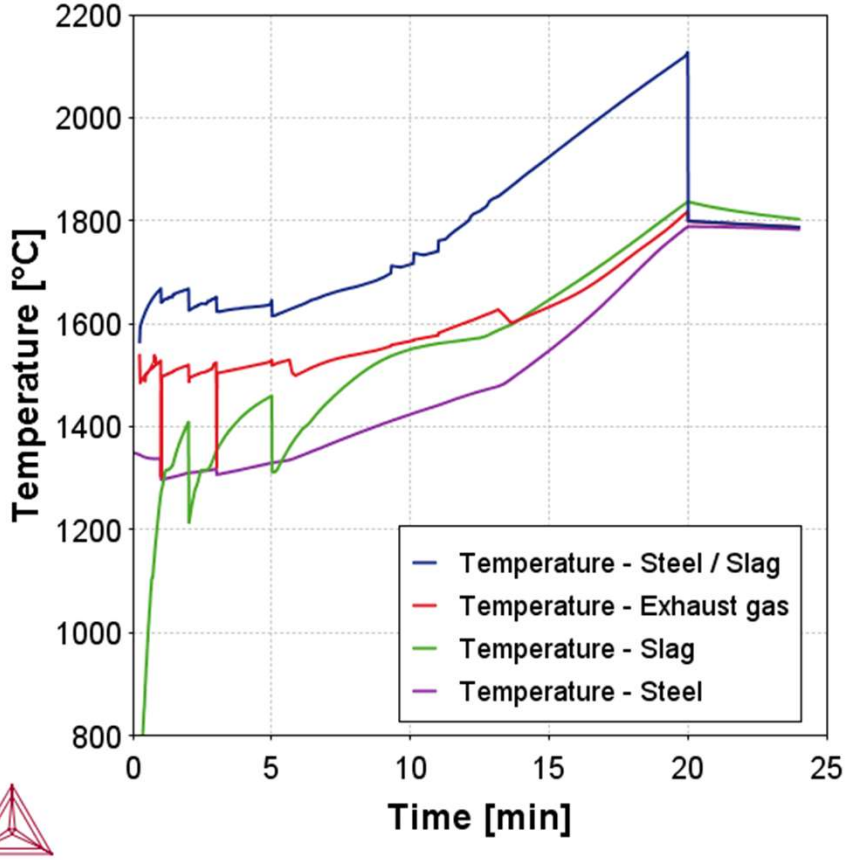
Note: Calculation times for a full process simulation can be 30 min or more

Detailed description of simulations as video tutorials, pdfs and example files can be found under https://www.thermocalc.com/products-services/process-metallurgy-module/

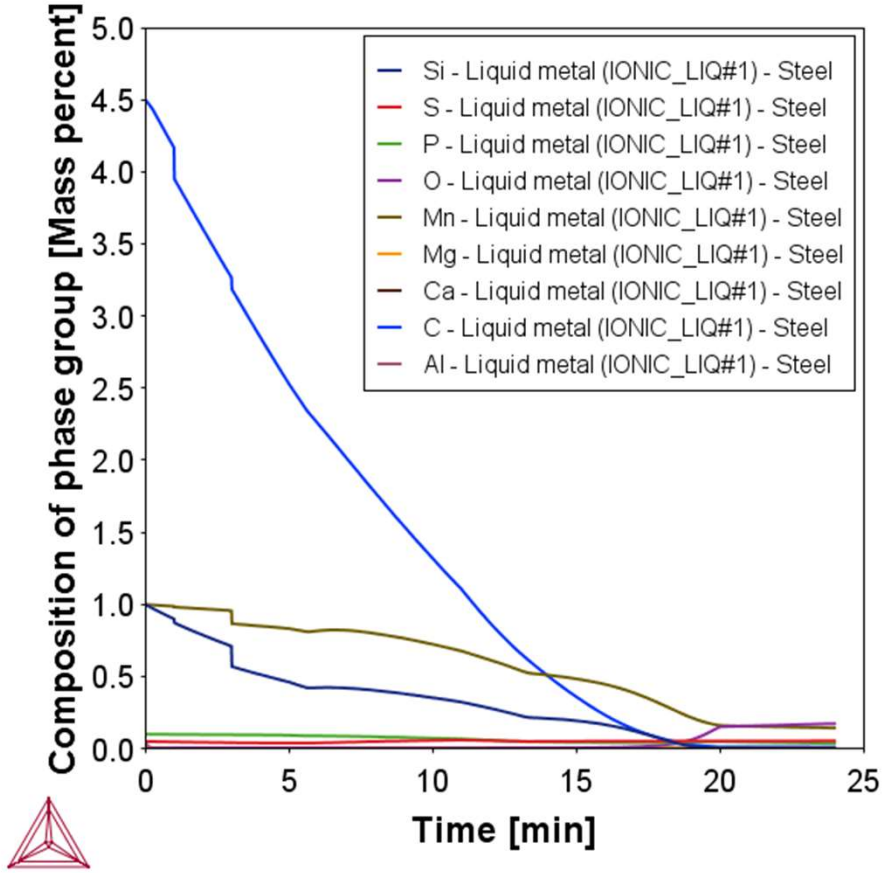
PMM Example 2
Calculation of decarburization PROCESS SIMULATION

Thermo-Calc Software

Some typical results of the simulation



Temperature increase in different zones of the converter during the oxygen blowing process



Reduction in carbon content as the hot metal is transformed into steel

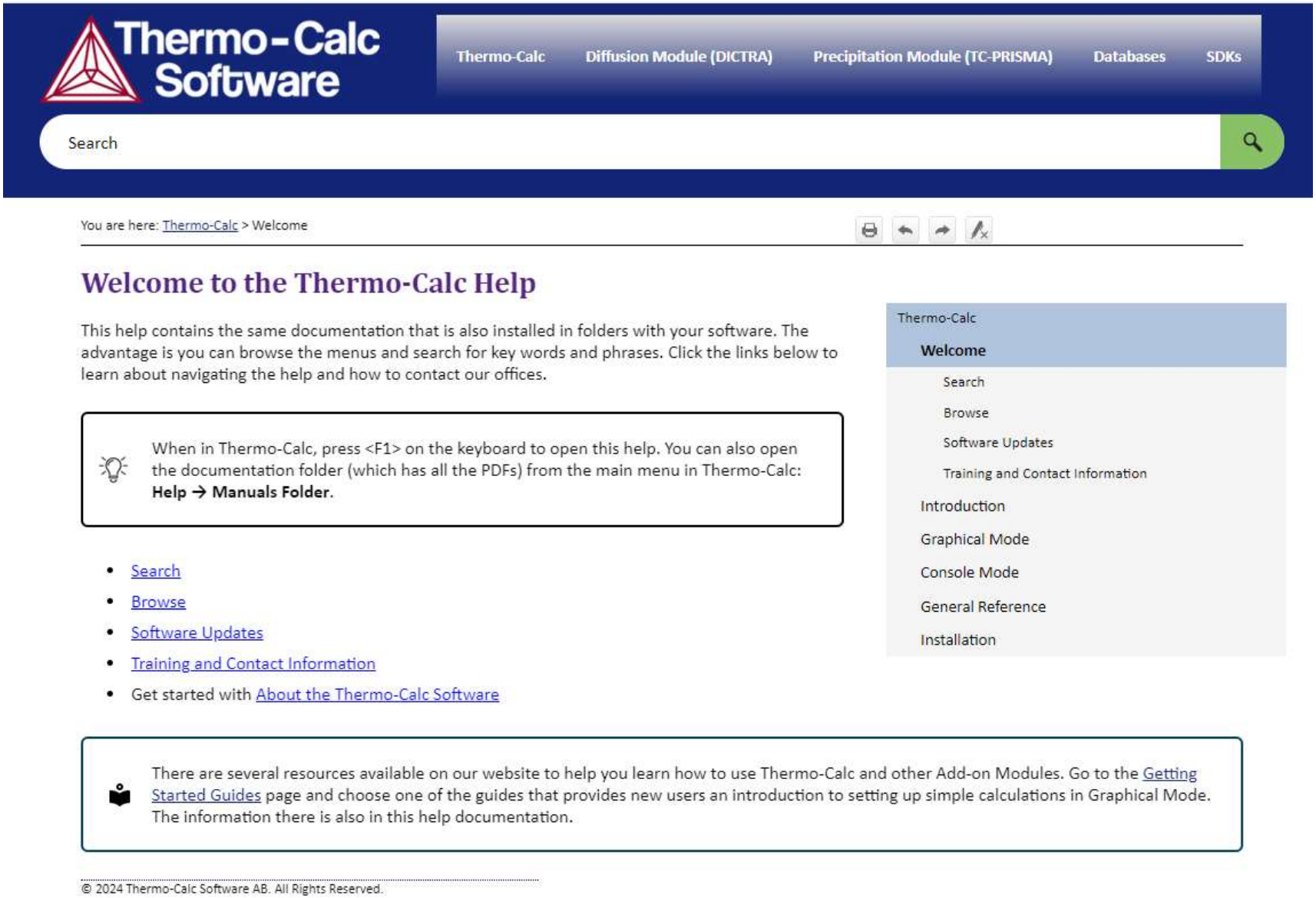
→ Much more and more detailed process information can be obtained...

Detailed description of simulations as video tutorials, pdfs and example files can be found under https://www.thermocalc.com/products-services/process-metallurgy-module/

Resources:
Where to find Help

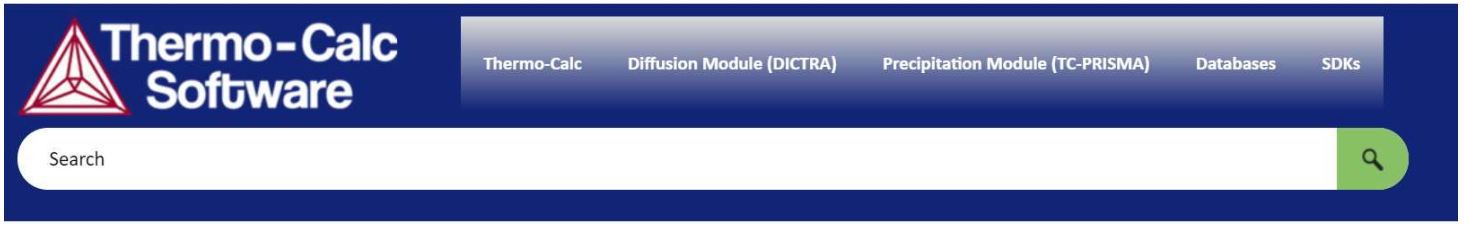
The Online Help

Use the Help menu or press F1.
Help for all software and more.



The Online Help

Below a search for “State variables” and then browsing among the search results.



Intensive Variables

V	Abbrev.	Unit	Descript.	Domain	Suffix
T	T[1]	K	Temperature	System	
P	P	Pa	Pressure	System	
μ	MU(comp)	J/mol	Chemical potential	Component	R
	MU(sp,ph)[2]			Species relative to a solution phase	R
a	AC(comp)	N/A	Activity	Component	R
	AC(sp,ph)[2]			Species relative to a solution phase	R
	LNAC (comp)[3]		ln(Activity)	Component	R
	LNAC (sp,ph) [2]			Species relative to a solution phase	R

[1] When plotting in POST, besides T (Kelvin), you can also use T_C or T_F to plot temperature in °C or °F.

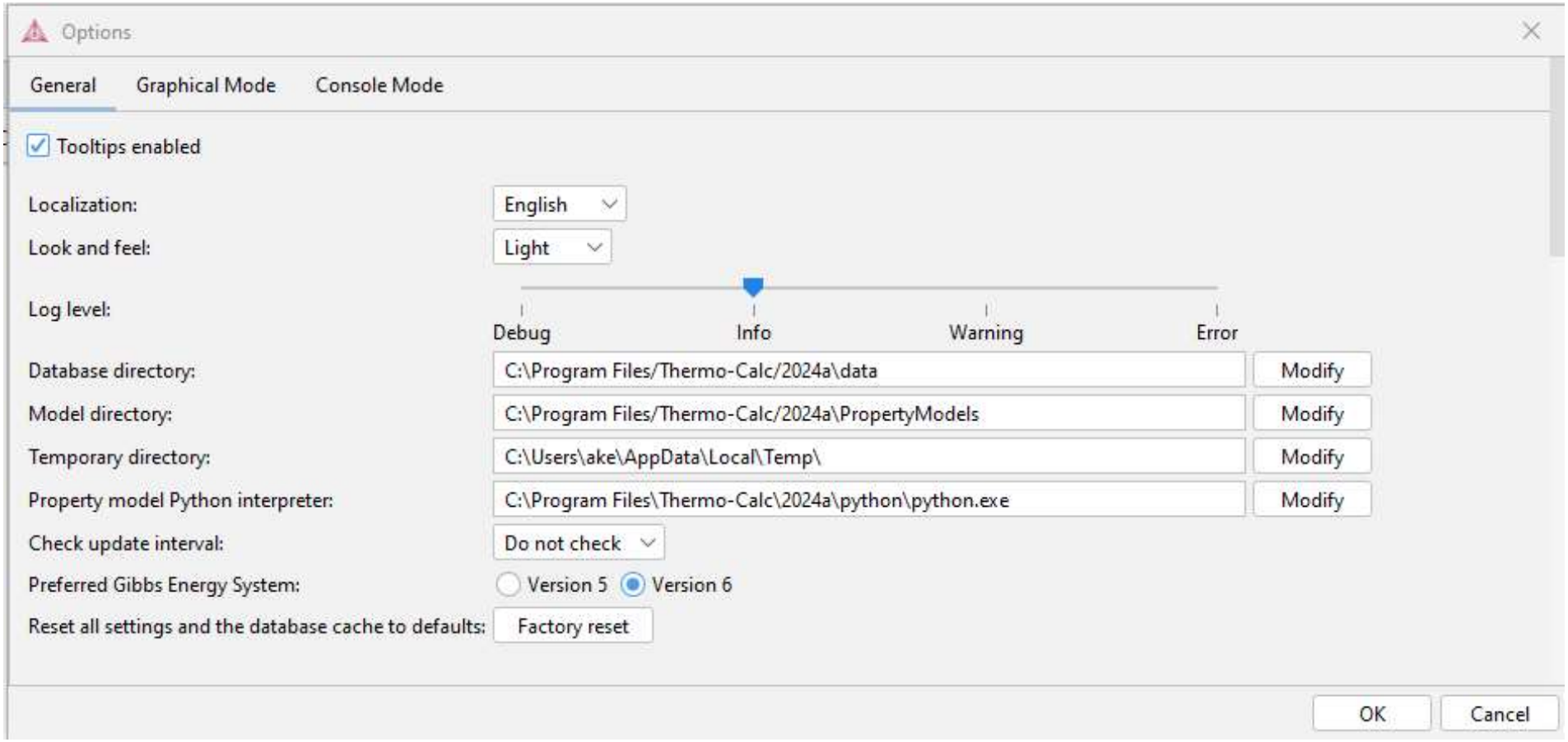
[2] Only for single-substitutional-lattice solution phases such as AQUEOUS solution and GASeous mixture phases and for interacting species on the substitutional sublattice of two-sublattice solution phases (such as the phases BCC_A2 and M6C phases).

[3] In natural logarithm (lnAC=MU/RT)

Settings

Thermo-Calc Software

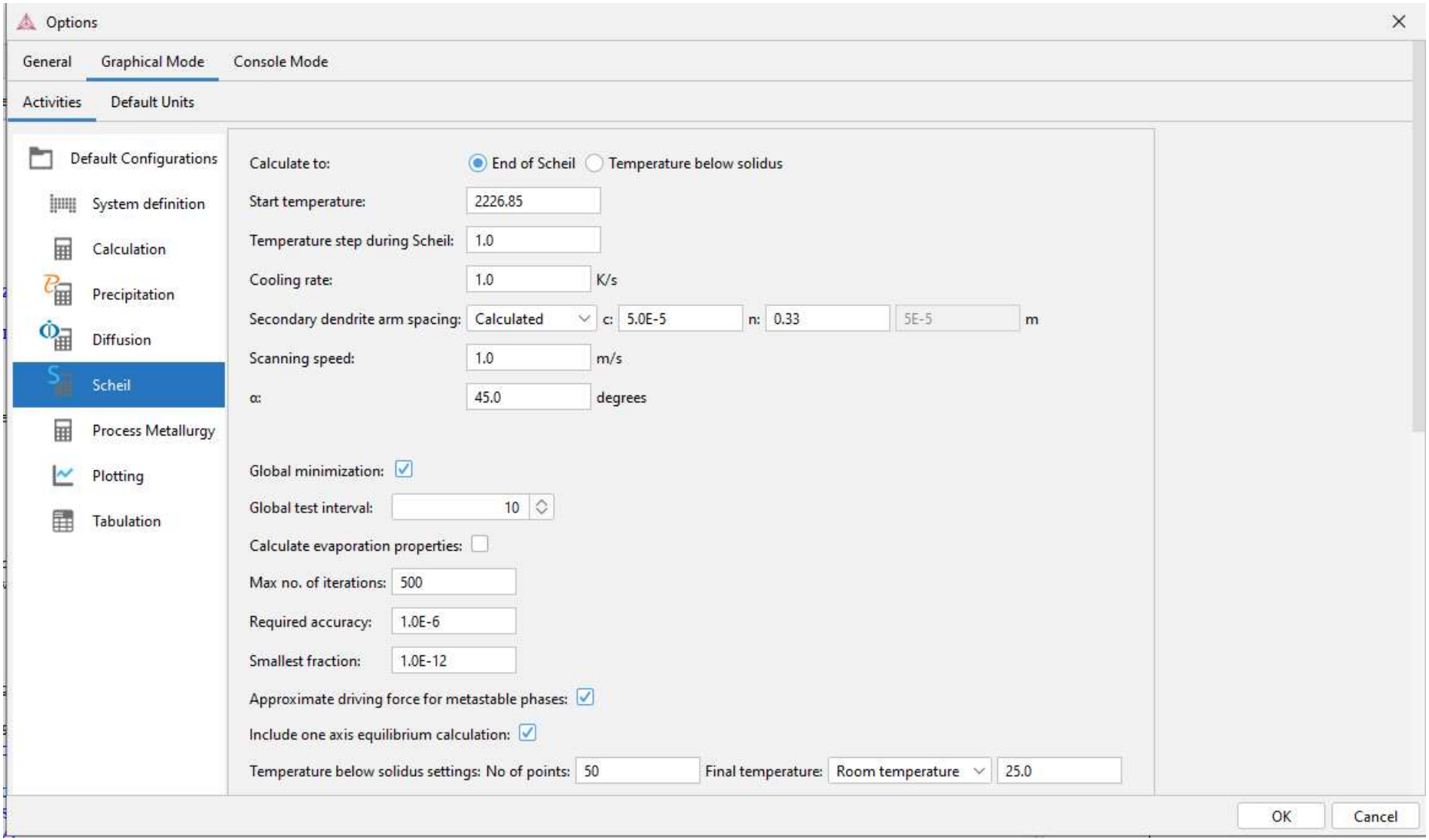
Tools -> Options



Settings

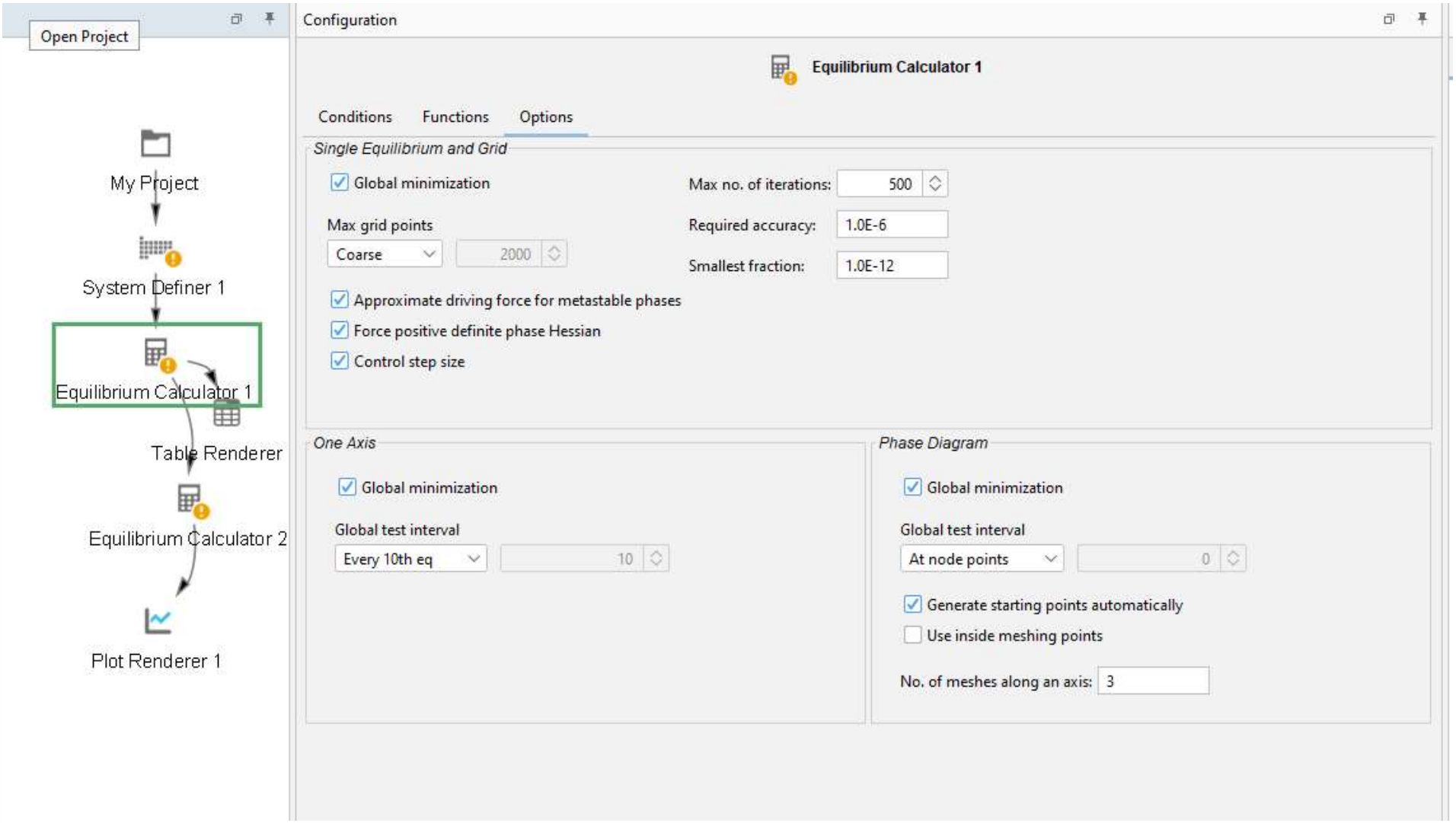
Thermo-Calc Software

Tools -> Options -> Graphical mode



Settings

Same “Options” windows can also be reached from inside each activity.



Thermo-Calc Software

Questions

&

Answers

The End

Please take a few minutes to fill out the anonymous Course Evaluation. Link here:

https://www.surveymonkey.com/r/F3BBQMN

(If you have filled out this survey before 09:00 this morning you will have to do it again.)

The End

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.