

Thermo-Calc Software

Thermo-Calc On-line Training

Day 3, October 9, 2025



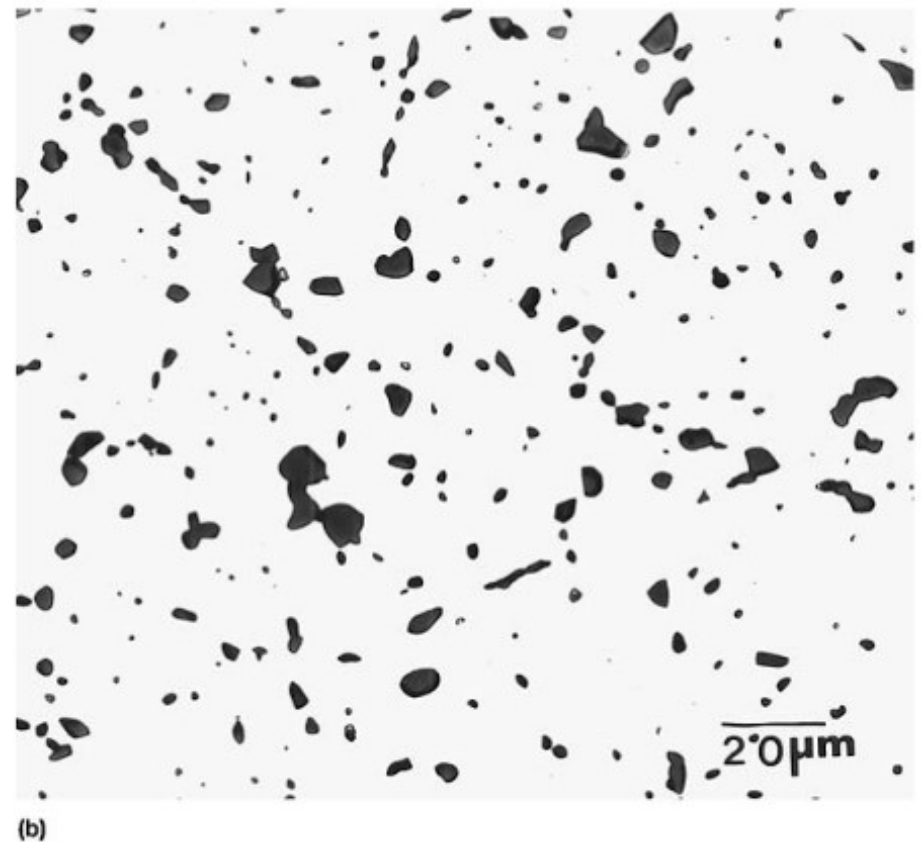
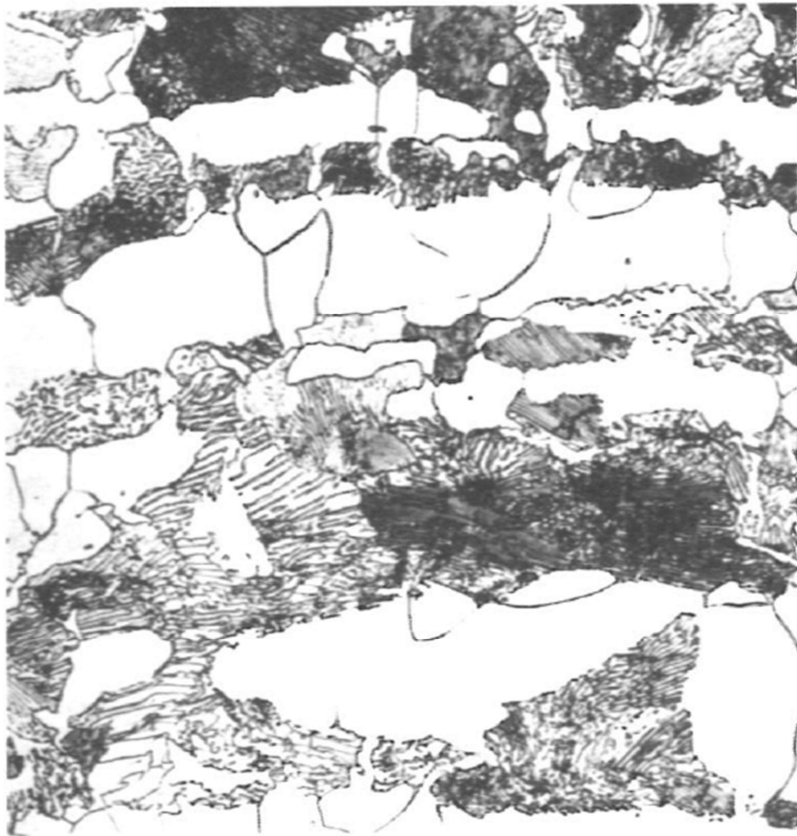
Home Assignment 2

Calculate Equilibrium at 600 °C 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.

Scheil Module

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

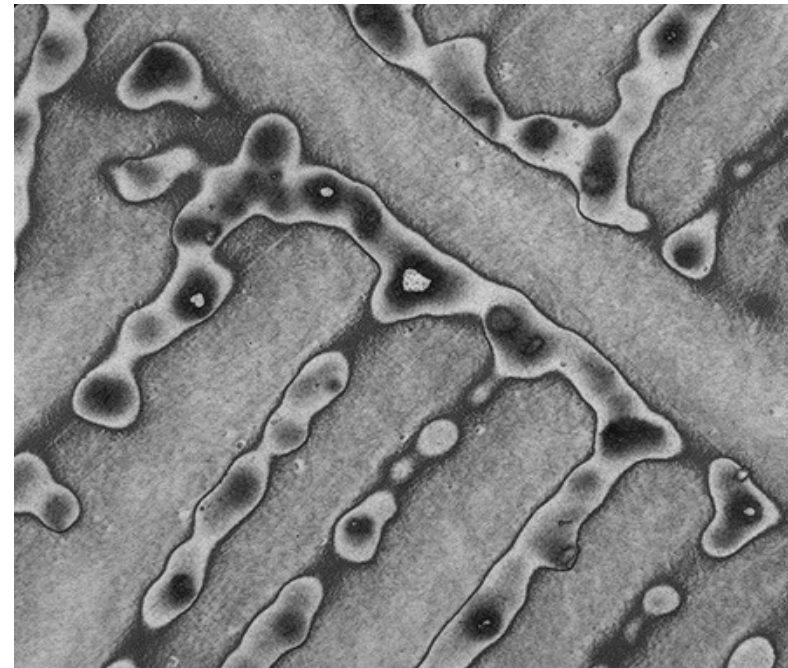
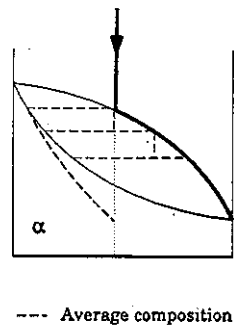
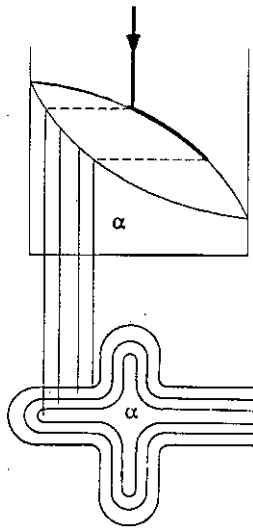
Intended for simulation of very fast cooling, e.g. during Additive Manufacturing. Requires assumption about scanning speed and angle.

Moving phase boundary methods (DICTRA)

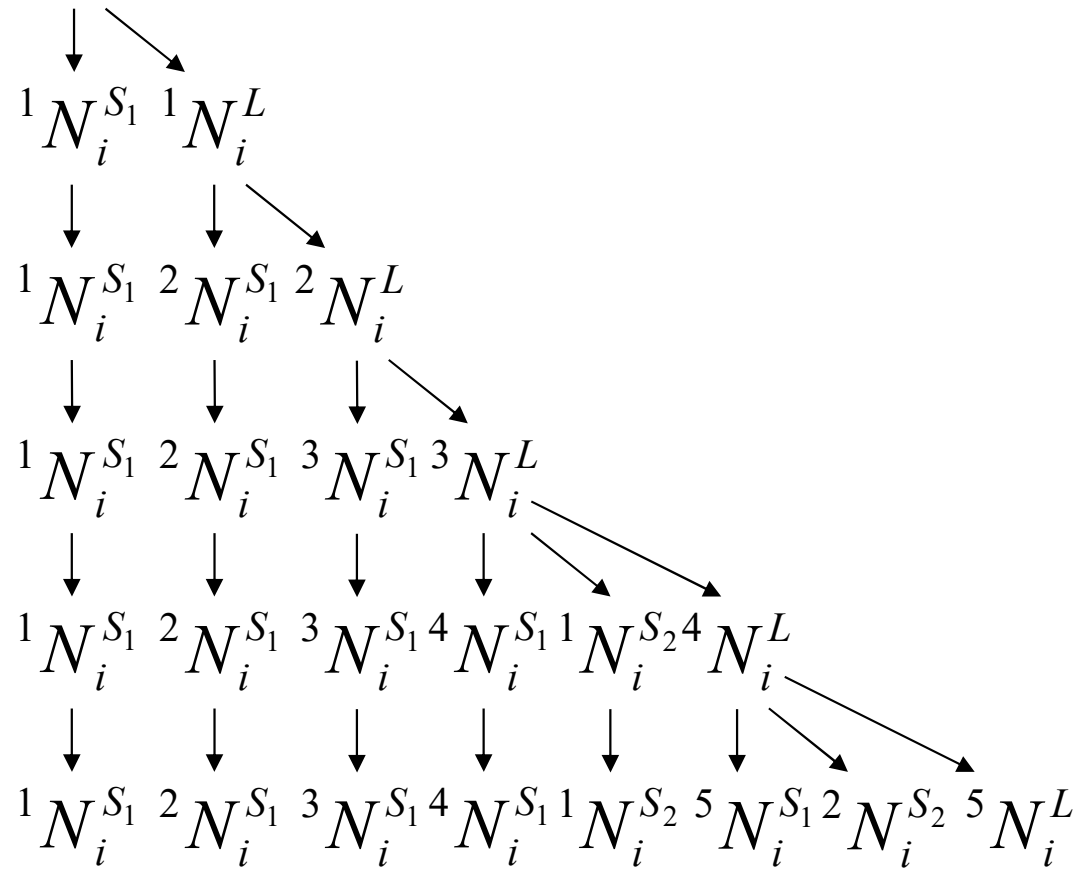
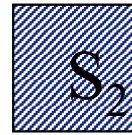
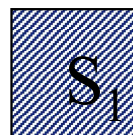
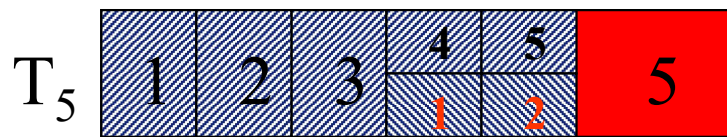
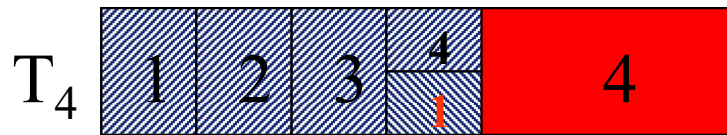
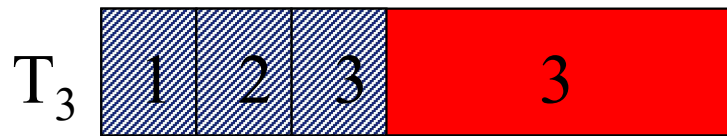
Full integration of thermodynamics and kinetics in all phases. Requires additional kinetic database and takes dendrite spacing and cooling rate into account.

Assumptions in traditional Scheil:

- ❑ Fast diffusion in liquid $\rightarrow$ homogenous liquid
- ❑ No diffusion in solid phases $\rightarrow$ segregations in the solid

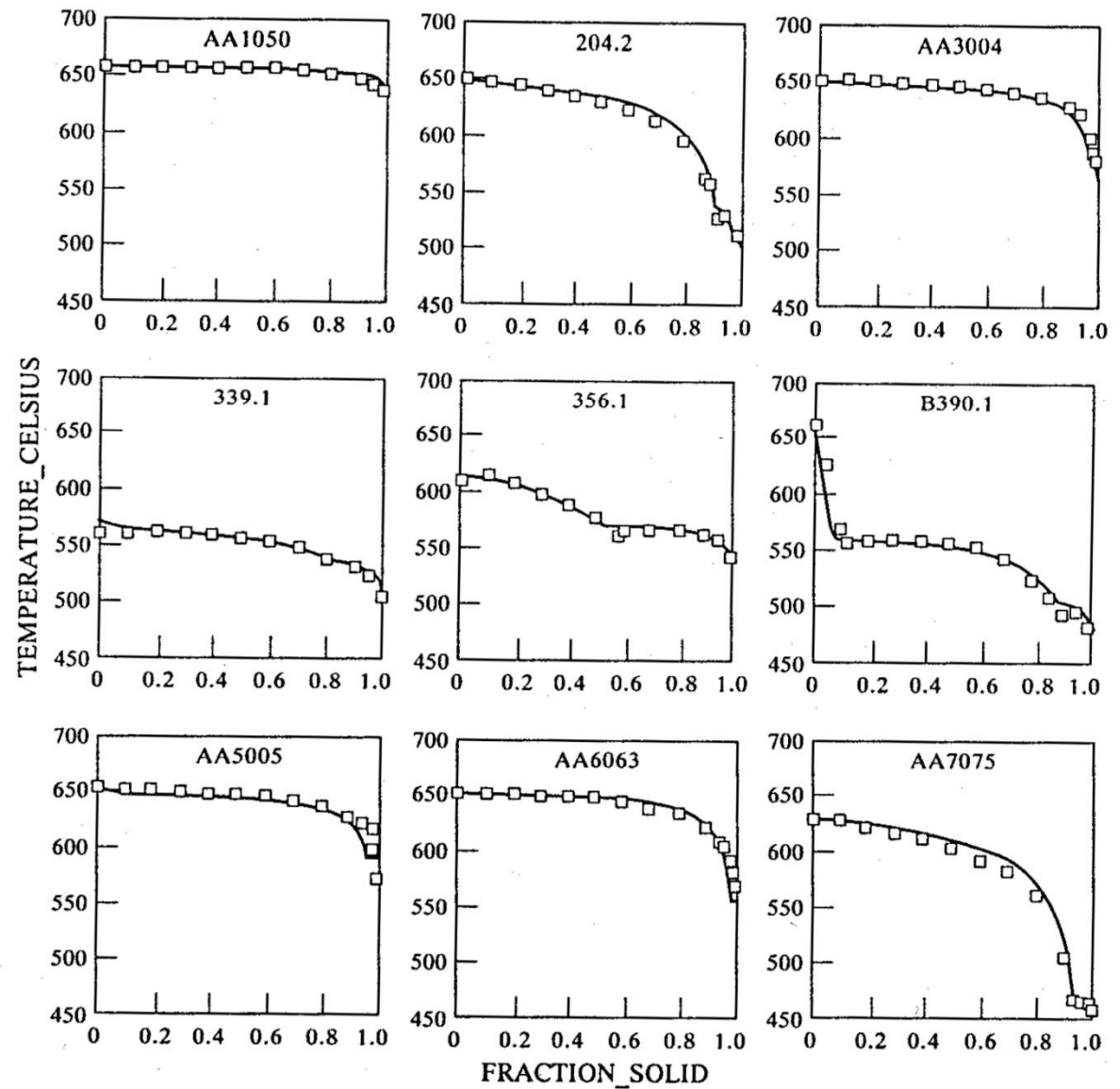


Algorithm in traditional Scheil



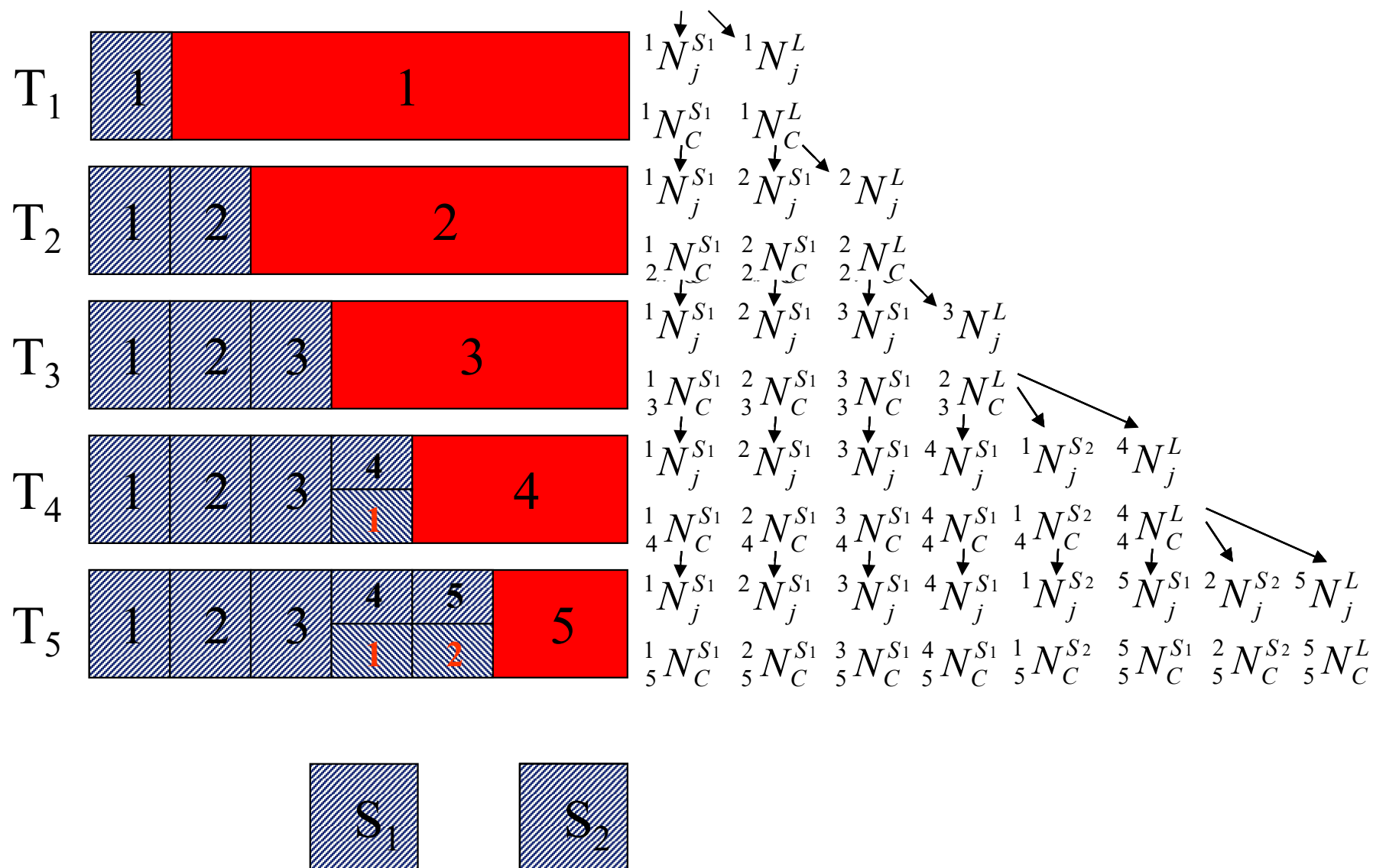
Some Examples

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

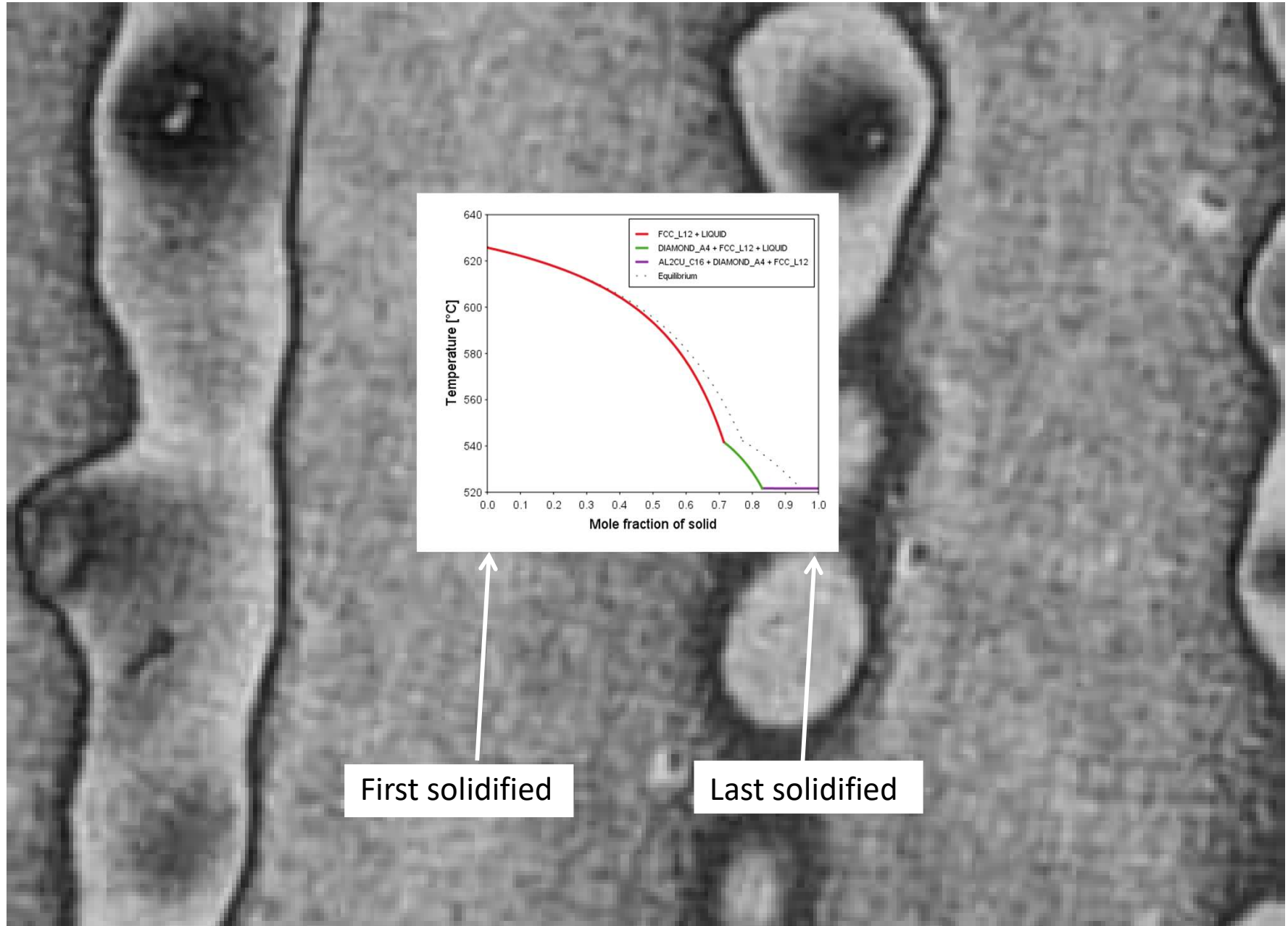


From: Saunders & Miedownik: "Calphad -a comprehensive review"

Algorithm in modified Scheil (partial eq.)



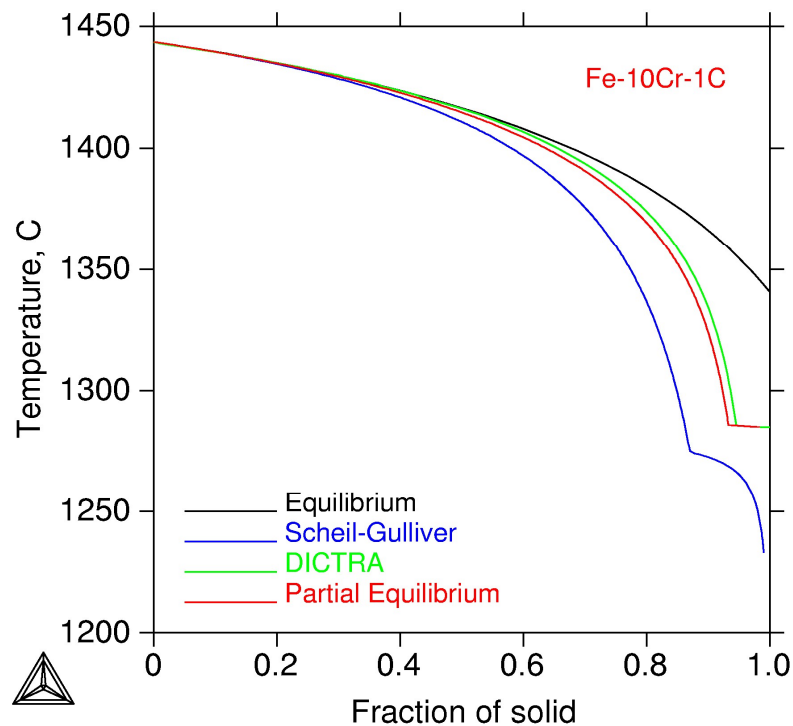
Translating the Scheil to Microstructure



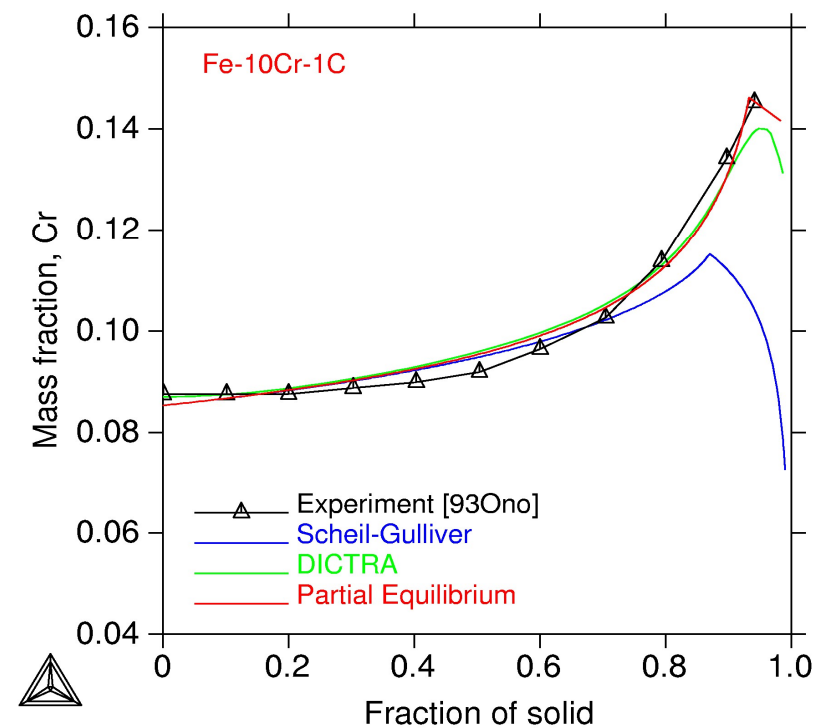
Some results: Fe-10Cr-1C

Comparison of equilibrium, Scheil, and partial eq

Freezing Range



Microsegregation



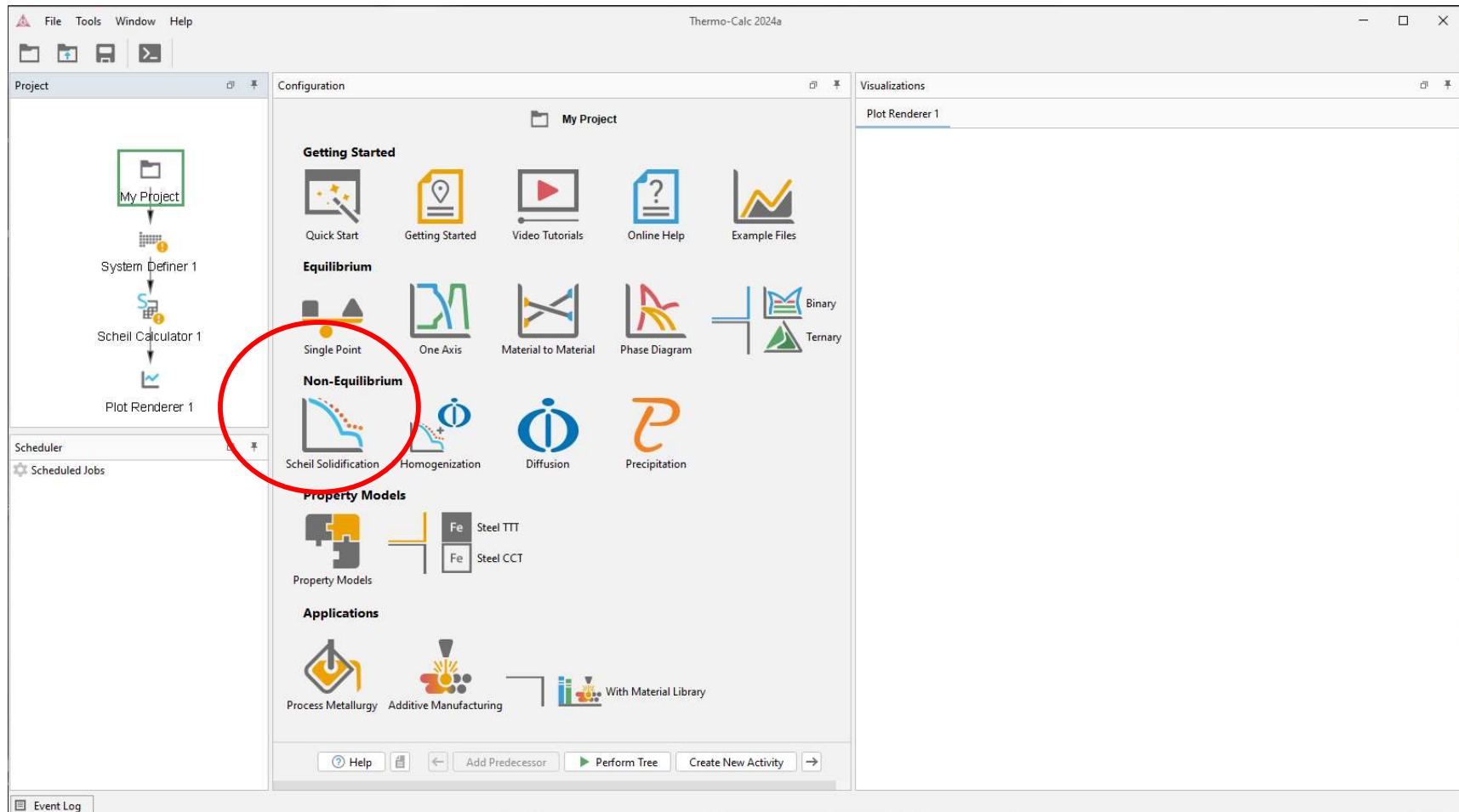
Q. Chen & B. Sundman, Materials Transactions, 43(3)551(2002).

Scheil solidification simulation

Alloy composition:

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

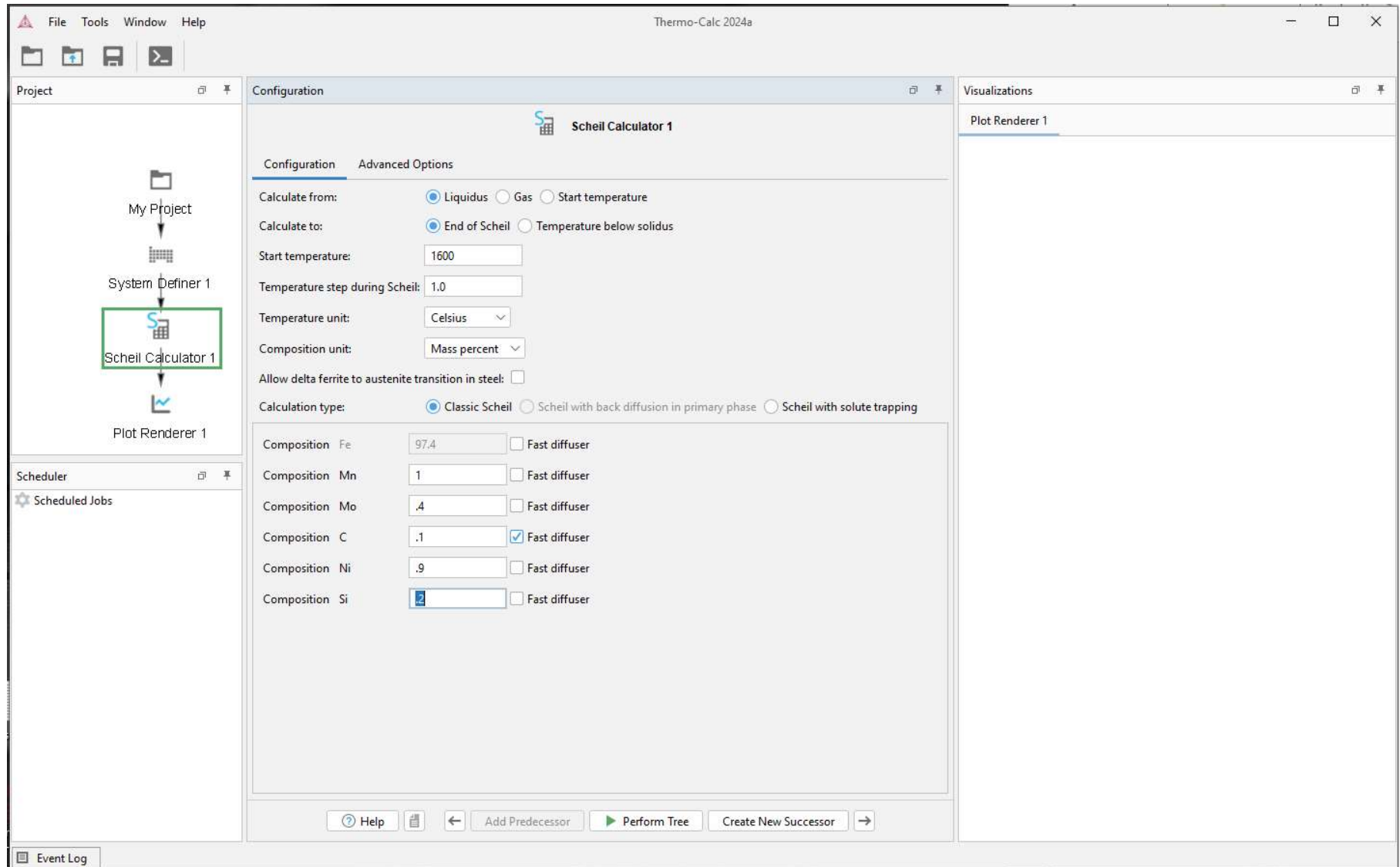
- ☐ Plot “mass fraction of solid” vs T and the segregation in the liquid.
- ☐ C as fast diffusing element – or not? Will it make a difference?



Scheil solidification simulation

Alloy composition:

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



The screenshot displays the Thermo-Calc 2024a software interface. The main window is titled "Thermo-Calc 2024a" and features a menu bar (File, Tools, Window, Help) and a toolbar. The interface is divided into several panes:

- Project Pane:** Shows a hierarchical tree structure with "My Project" at the top, followed by "System Definer 1", "Scheil Calculator 1" (highlighted with a green box), and "Plot Renderer 1".
- Scheduler Pane:** Located at the bottom left, it shows "Scheduled Jobs".
- Configuration Pane:** The central area, titled "Scheil Calculator 1", contains two tabs: "Configuration" and "Advanced Options".
 - Configuration Tab:**
 - Calculate from:** Radio buttons for "Liquidus" (selected), "Gas", and "Start temperature".
 - Calculate to:** Radio buttons for "End of Scheil" (selected) and "Temperature below solidus".
 - Start temperature:** Input field set to "1600".
 - Temperature step during Scheil:** Input field set to "1.0".
 - Temperature unit:** Dropdown menu set to "Celsius".
 - Composition unit:** Dropdown menu set to "Mass percent".
 - Allow delta ferrite to austenite transition in steel:** Unchecked checkbox.
 - Calculation type:** Radio buttons for "Classic Scheil" (selected), "Scheil with back diffusion in primary phase", and "Scheil with solute trapping".
 - Composition Table:**

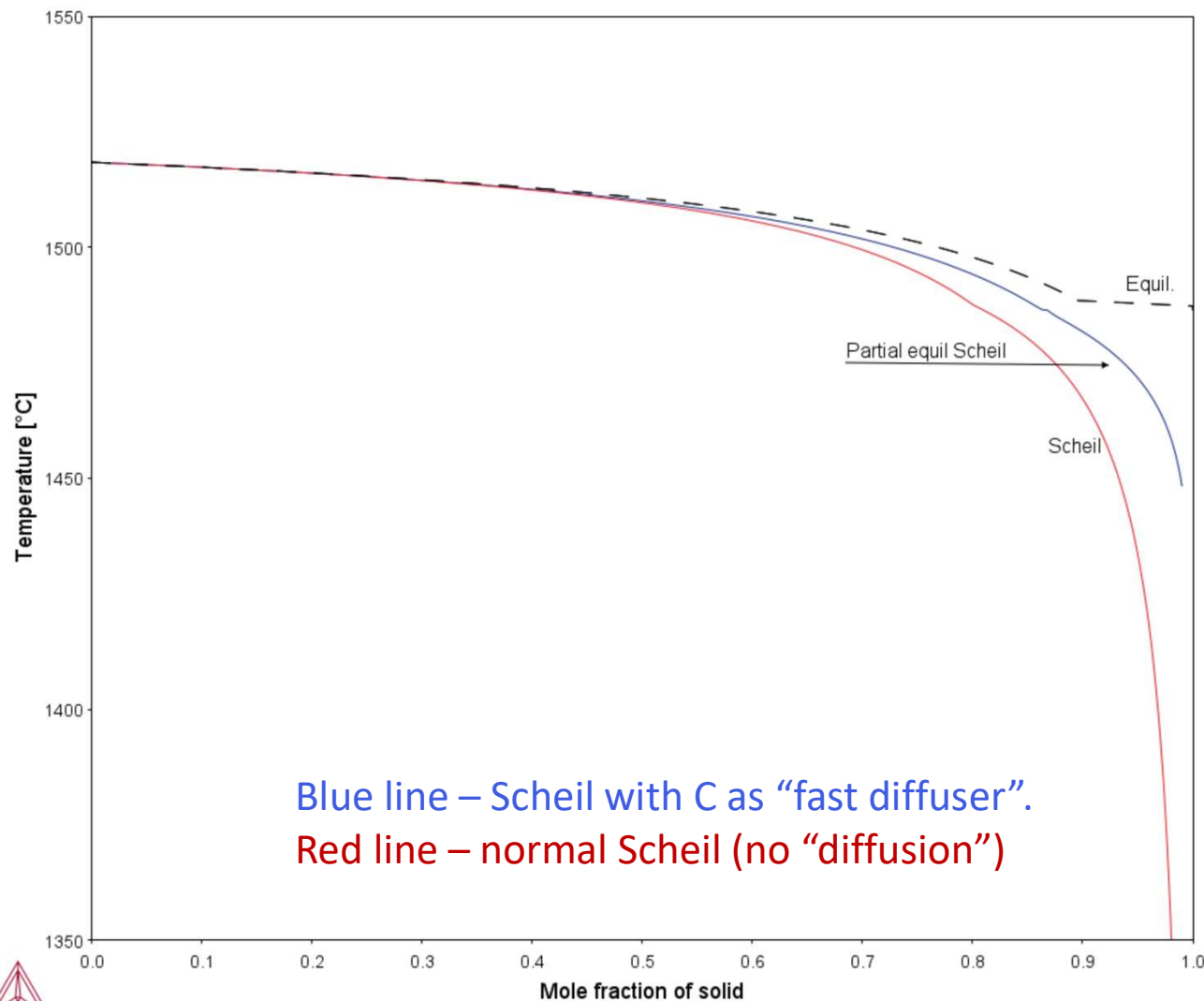
Composition	Value	Fast diffuser
Fe	97.4	☐
Mn	1	☐
Mo	.4	☐
C	.1	☒
Ni	.9	☐
Si	.2	☐
- Visualizations Pane:** Located on the right, it contains a sub-pane titled "Plot Renderer 1".

At the bottom of the Configuration pane, there is a toolbar with buttons: "Help", "Add Predecessor", "Perform Tree", "Create New Successor", and a right arrow.

Scheil solidification simulation

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/>

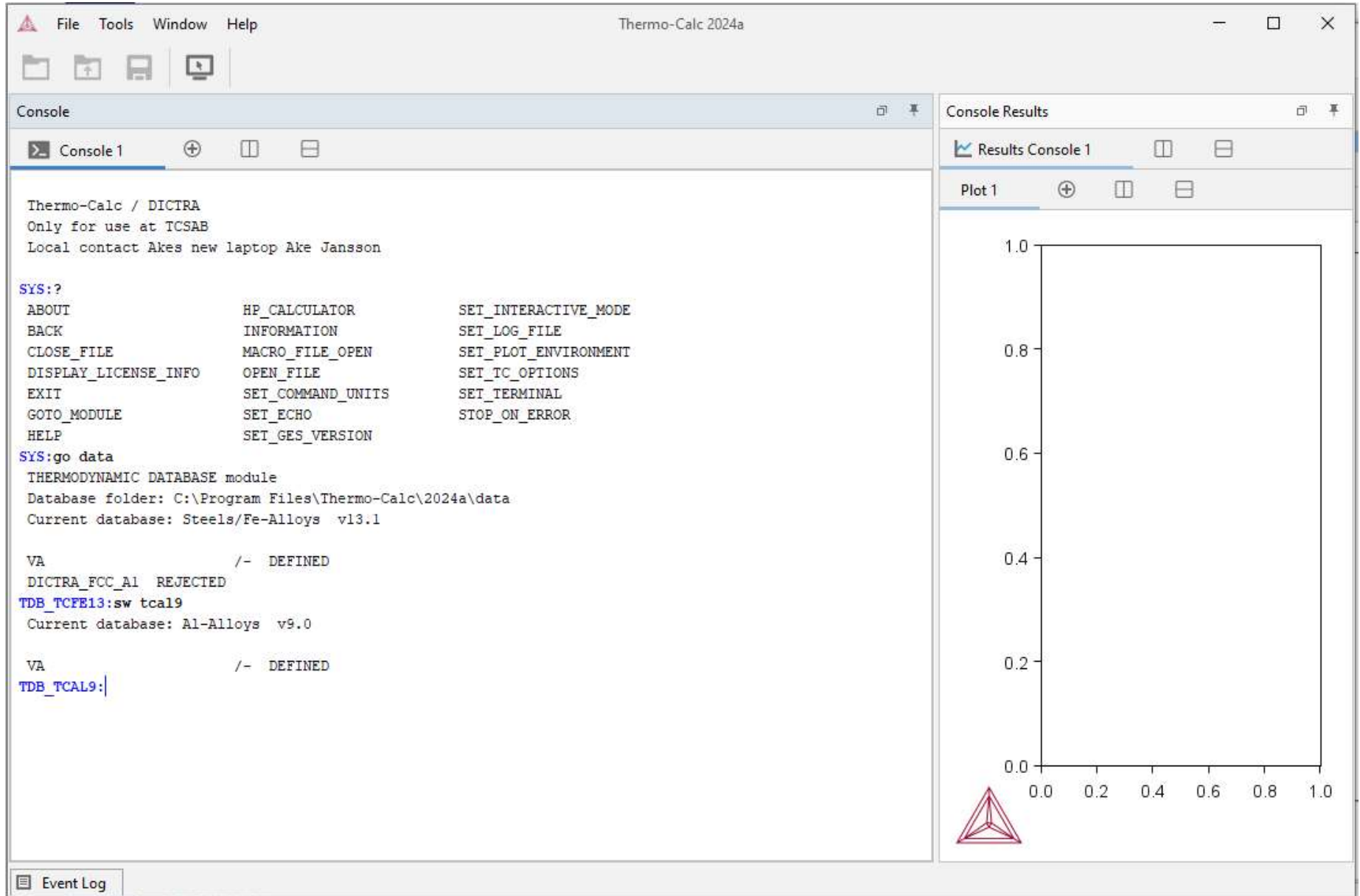
- PRE (Pitting Resistance Equivalence) is an empirical measure for corrosion resistance in stainless steels.
- PRE can be defined as:
$$\text{PRE} = w\% \text{Cr} + 3 * w\% \text{Mo} + 16 * w\% \text{N}$$
- For duplex stainless steels, it is desirable to have a high and balanced PRE-numbers in ferrite 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

- 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



The screenshot displays the Thermo-Calc 2024a software interface. The main window is titled "Thermo-Calc 2024a" and features a menu bar with "File", "Tools", "Window", and "Help". Below the menu bar is a toolbar with icons for file operations and a console window. The console window, titled "Console", shows the following text:

```
Thermo-Calc / DICTRA
Only for use at TCSAB
Local contact Akas new laptop Ake Jansson

SYS:?
ABOUT          HP_CALCULATOR      SET_INTERACTIVE_MODE
BACK            INFORMATION        SET_LOG_FILE
CLOSE_FILE      MACRO_FILE_OPEN    SET_PLOT_ENVIRONMENT
DISPLAY_LICENSE_INFO OPEN_FILE      SET_TC_OPTIONS
EXIT            SET_COMMAND_UNITS  SET_TERMINAL
GOTO_MODULE     SET_ECHO          STOP_ON_ERROR
HELP            SET_GES_VERSION

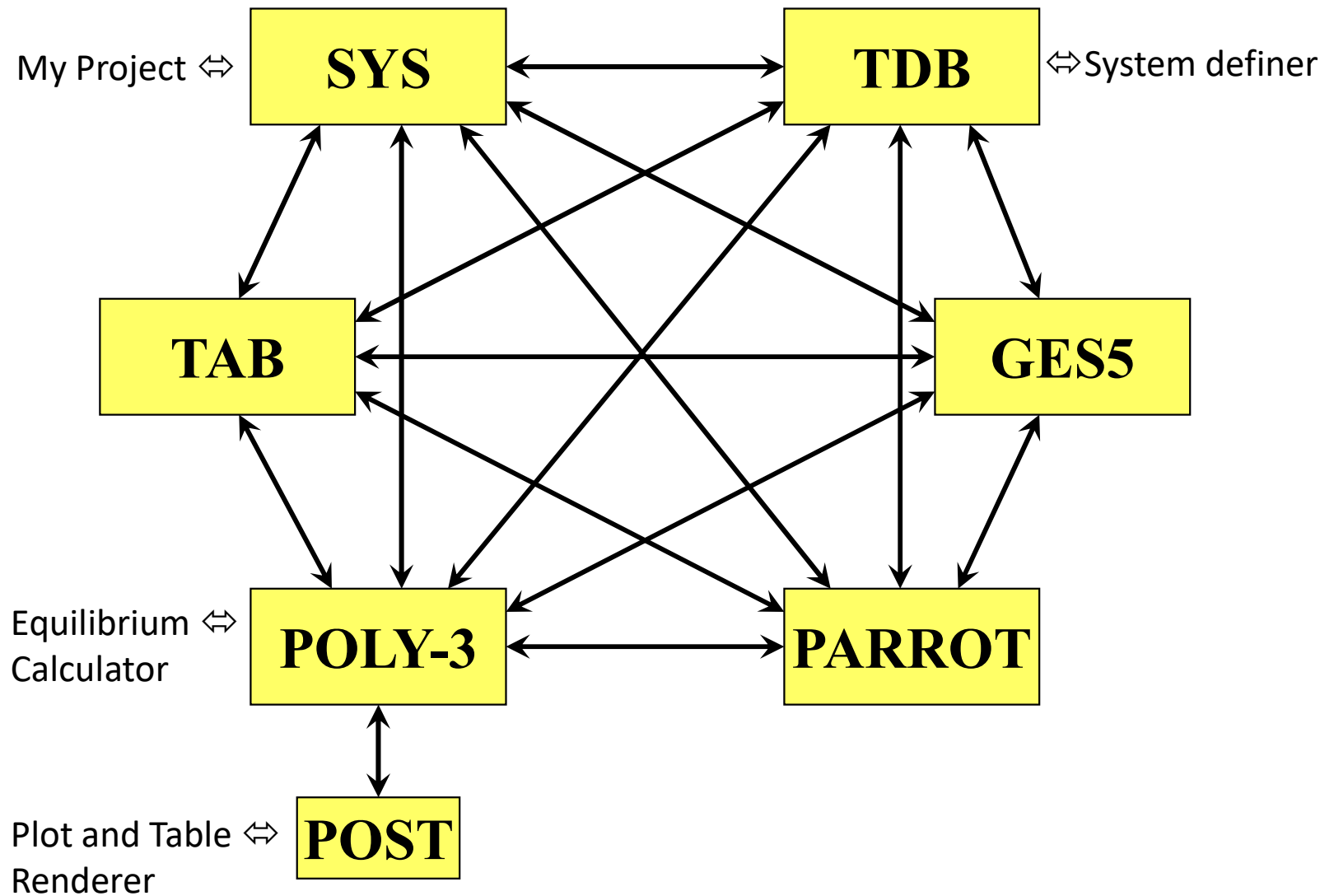
SYS:go data
THERMODYNAMIC DATABASE module
Database folder: C:\Program Files\Thermo-Calc\2024a\data
Current database: Steels/Fe-Alloys v13.1

VA              /- DEFINED
DICTRA_FCC_A1 REJECTED
TDB_TCFE13:sw tcal9
Current database: Al-Alloys v9.0

VA              /- DEFINED
TDB_TCAL9:
```

The right side of the interface shows a "Console Results" panel with a sub-panel titled "Results Console 1". Below this is a "Plot 1" window, which is currently blank. The plot area has axes ranging from 0.0 to 1.0. A small Thermo-Calc logo is visible in the bottom left corner of the plot area.

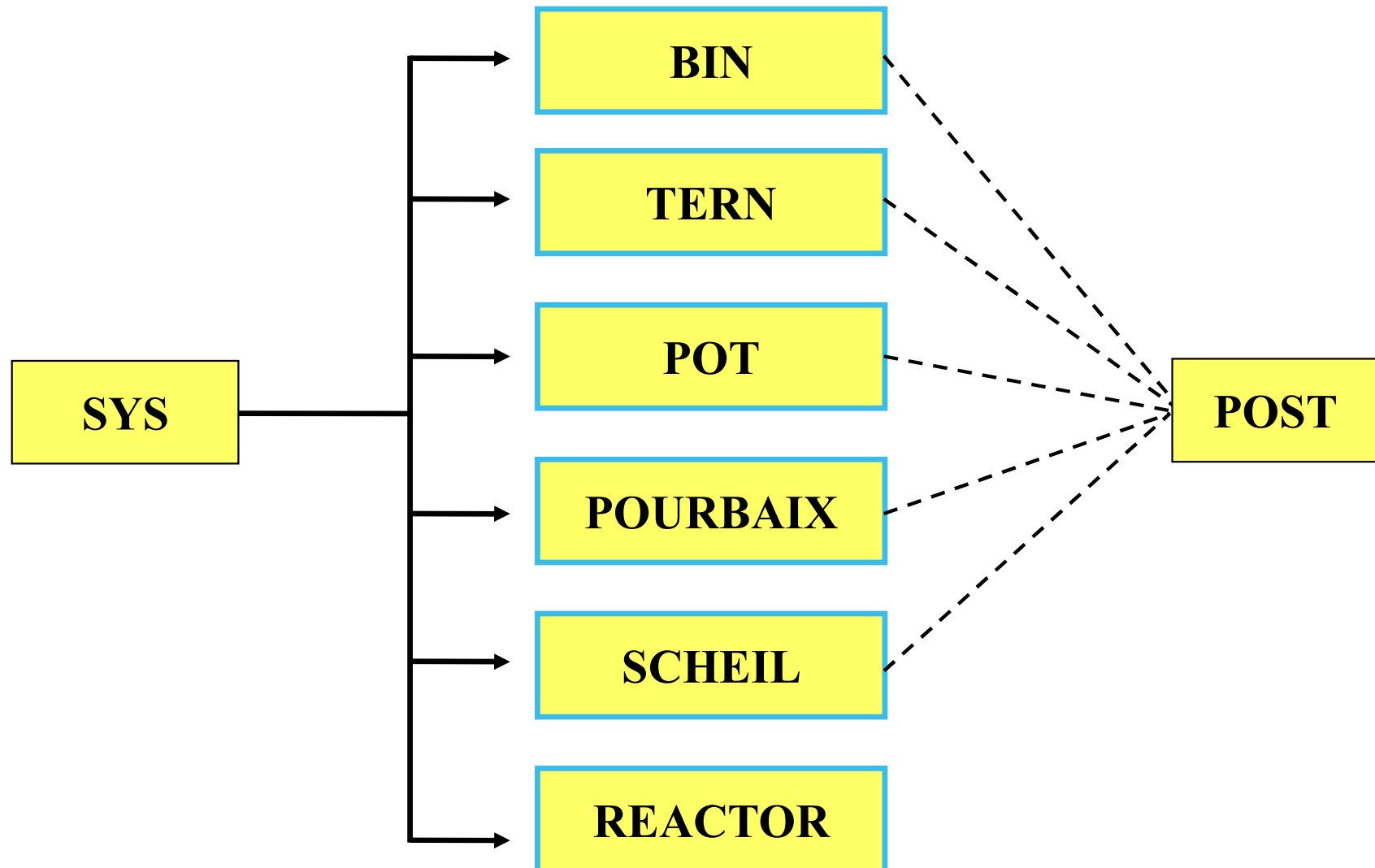
Modules in Thermo-Calc Console mode



Special modules in Console mode

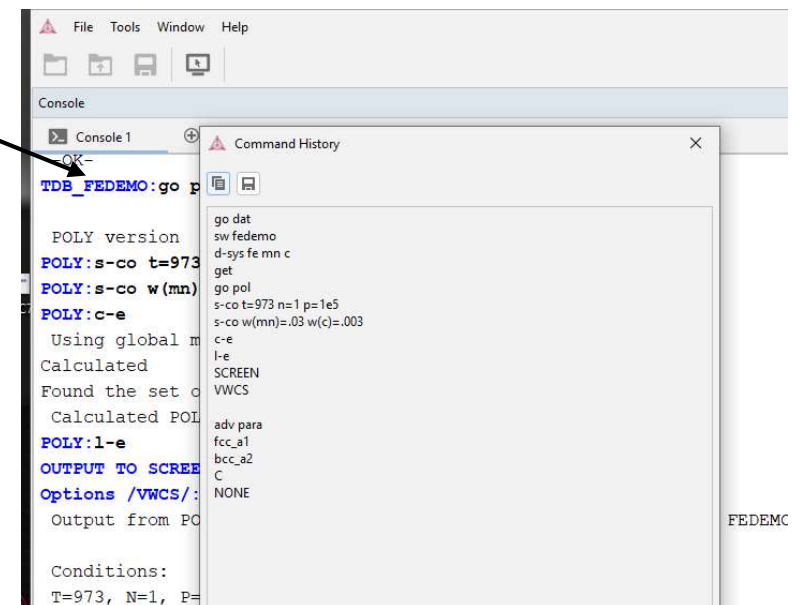
These modules* are very automatic and after entering a few conditions, the calculation will start and end with a plotted diagram.

*) 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

```
@@ 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
773.15 1773.15 10

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

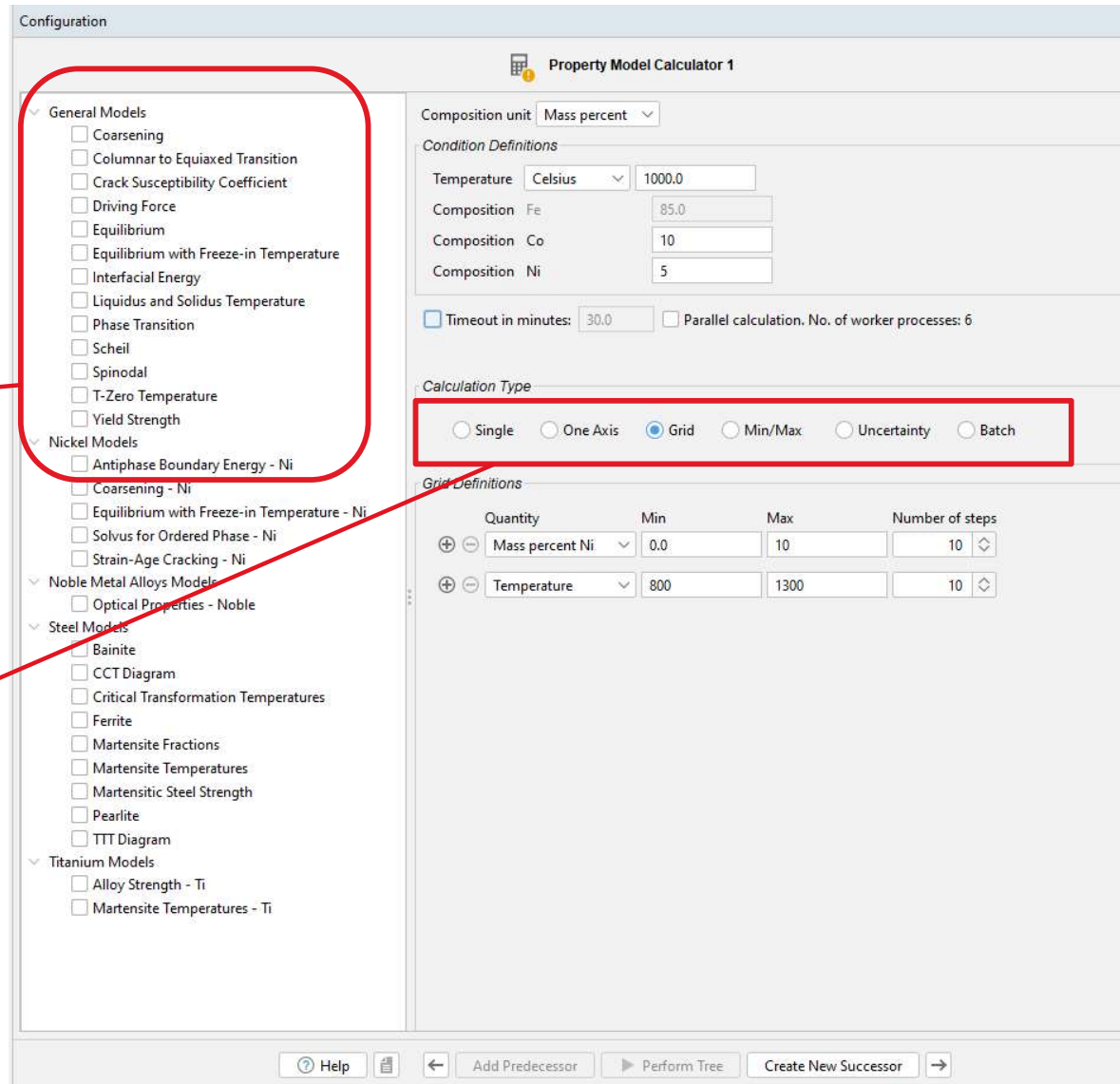
set-interact
```

Questions & Answers

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.



Configuration

Property Model Calculator 1

Composition unit: Mass percent

Condition Definitions

Temperature: Celsius, 1000.0

Composition: Fe 85.0, Co 10, Ni 5

Timeout in minutes: 30.0, Parallel calculation. No. of worker processes: 6

Calculation Type

Single, One Axis, **Grid**, Min/Max, Uncertainty, Batch

Grid Definitions

Quantity	Min	Max	Number of steps
Mass percent Ni	0.0	10	10
Temperature	800	1300	10

Help, Add Predecessor, Perform Tree, Create New Successor

Variation of A1 over a composition range

Phase Transition Property
Model, bcc $\rightarrow$ fcc.

Composition of this steel:
Fe (bal.) + (in wt-%)

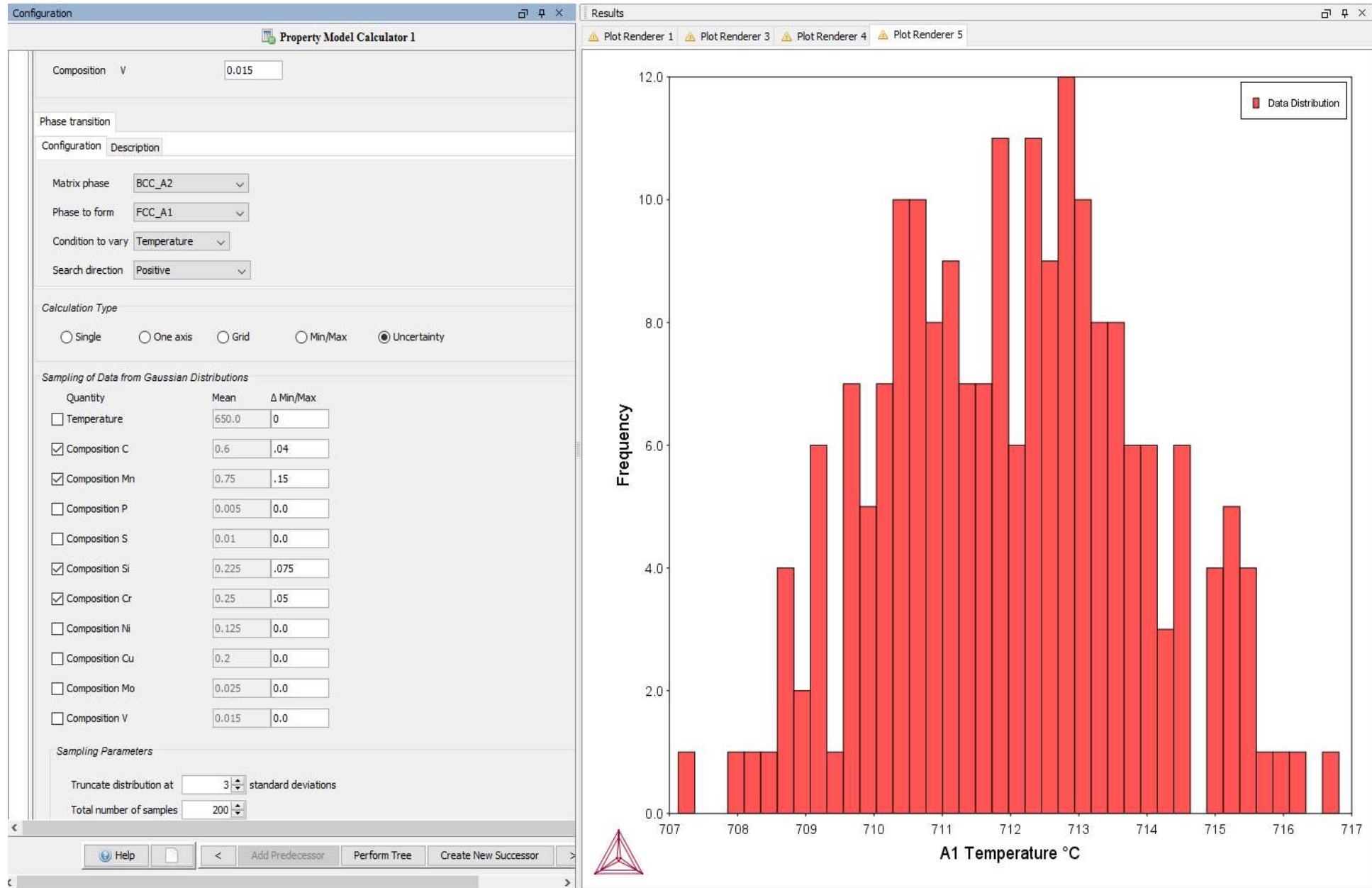
200 random samples, where
4 elements were varied:
C Mn Si Cr

The other elements were
constant at their nominal
composition.

Using the “Uncertainty”
calculation type.

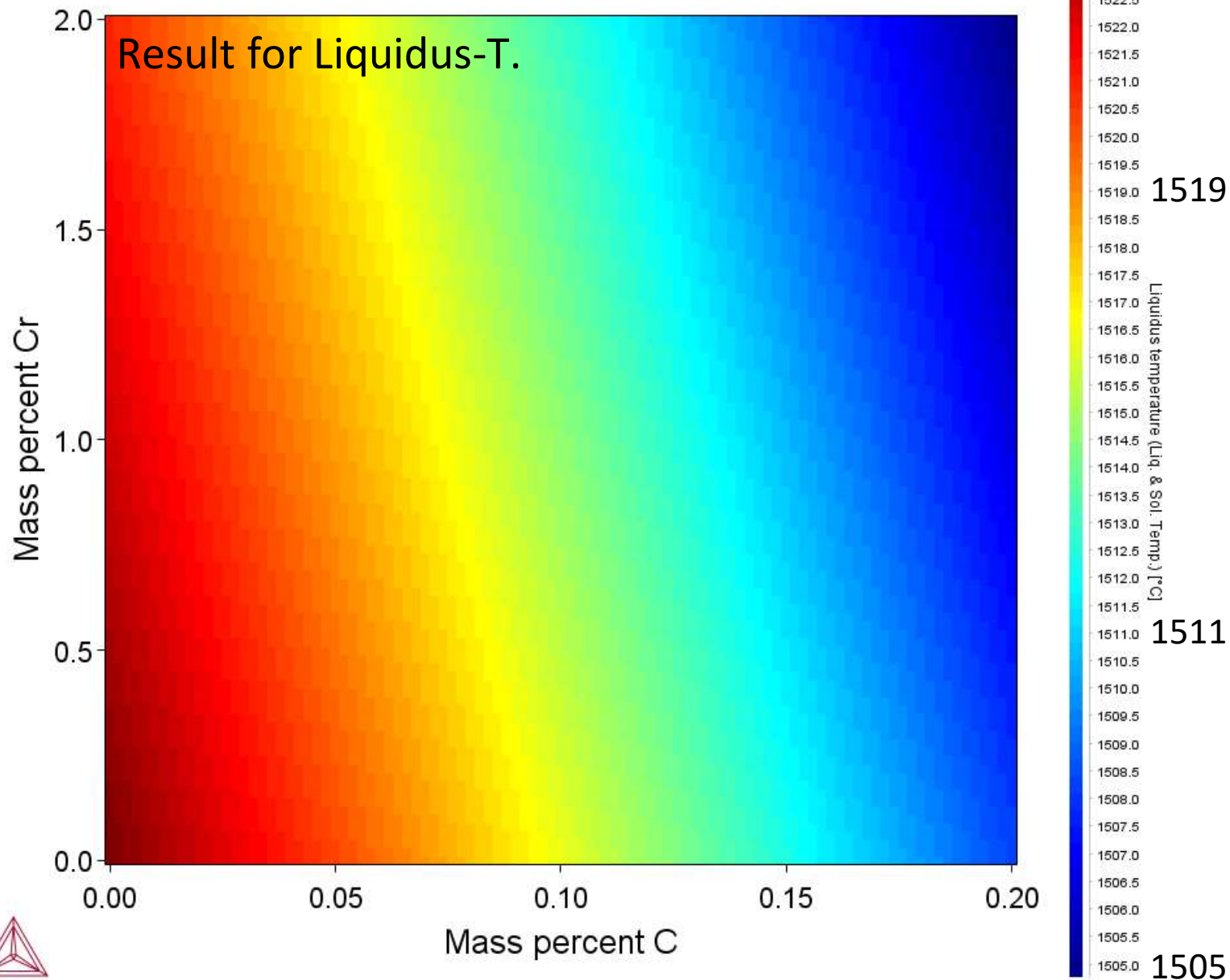
☐ Temperature	650.0	0
☒ Composition C	0.6	.04
☒ Composition Mn	0.75	.15
☐ Composition P	0.005	0.0
☐ Composition S	0.01	0.0
☒ Composition Si	0.225	.075
☒ Composition Cr	0.25	.05
☐ Composition Ni	0.125	0.0
☐ Composition Cu	0.2	0.0
☐ Composition Mo	0.025	0.0
☐ Composition V	0.015	0.0

Variation of A1 over a composition range - result



Property Model Calculator result – Liquidus/(Solidus) – Grid calculation

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



Property Model Calculator:

Electrical resistivity, freeze-in temperature

Step in temperature for Al-alloy AA4032.

Plot the Electrical resistivity. Heat treatment at 350 C.

General Models

☐ Coarsening

☐ Crack Susceptibility Coefficient

☐ Driving Force

☐ Equilibrium

☒ Equilibrium with Freeze-in Temperature

Material

Material name:
UNS_A94032

Amount Mass percent

Al85.0

Si12.2

Mg1.0

Ni0.9

Cu0.9

Composition unitMass percent

Condition Definitions

TemperatureCelsius20

Composition Al85.0

Composition Si12.2

Composition Mg1.0

Composition Ni0.9

Composition Cu0.9

☐ Timeout in minutes: 30.0

Equilibrium with Freeze-in Temperature

ConfigurationDescription

Freeze-in-temperature350.0

Equilibrium above freeze-in temperature☒

Evaluate for a single phase only☐

Equilibrium minimization strategyGlobal minimization only

Homogenization functionInverse rule of mixtures (lower Wiener bound)

Account for phase interface scattering☐

Set reference temperature for technical CTE20.0

Define user functions☐

Calculation Type

☐ Single☒ One Axis☐ Grid☐ Min/Max☐ Uncertainty☐ Batch

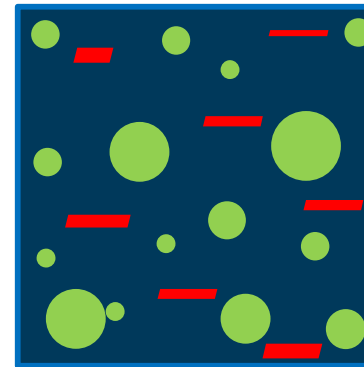
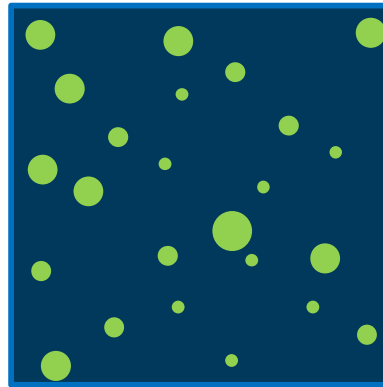
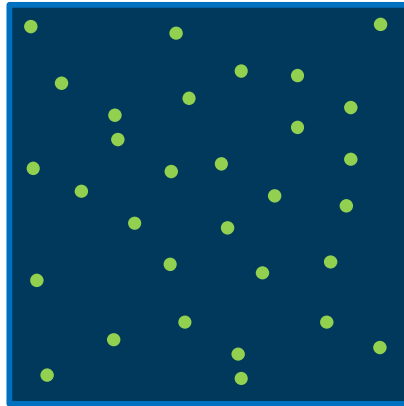
Grid Definitions

QuantityMinMaxNumber of steps

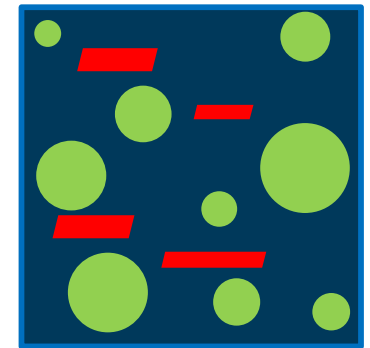
Temperature20.0350.030

Property Model Calculator: Freeze-in temperature

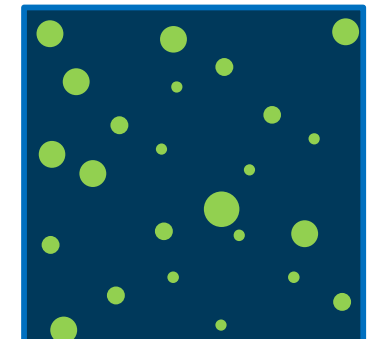
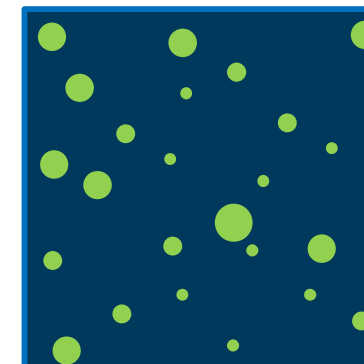
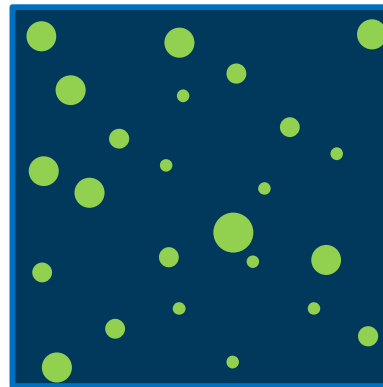
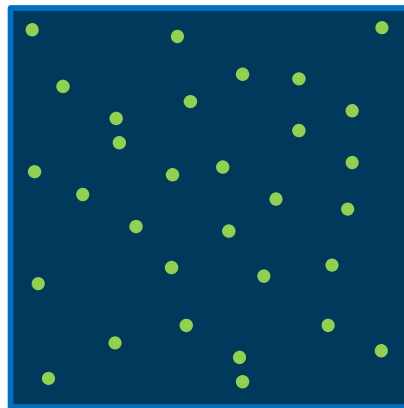
T = high



T = low



Microstructure frozen in



T = high

T = low

- ☒ Equilibrium with Freeze-in Temperature
- ☐ Interfacial Energy
- ☐ Liquidus and Solidus Temperature
- ☐ Phase Transition
- ☐ Scheil
- ☐ Spinodal
- ☐ T-Zero Temperature
- ☐ Yield Strength

Equilibrium with Freeze-in Temperature

Configuration Description

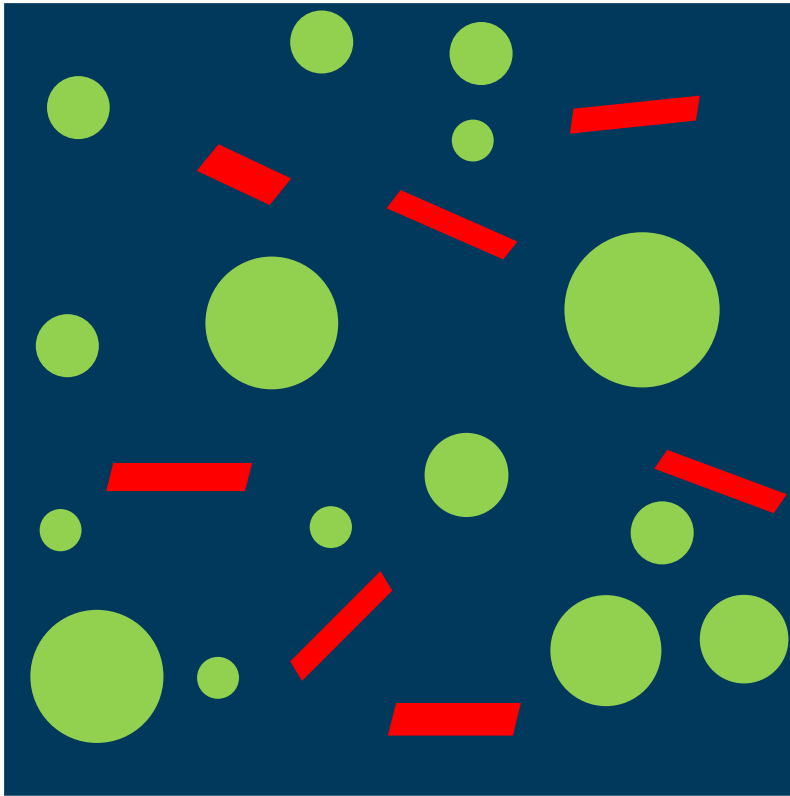
Freeze-in-temperature 350.0

Equilibrium above freeze-in temperature ☒

Evaluate for a single phase only ☐

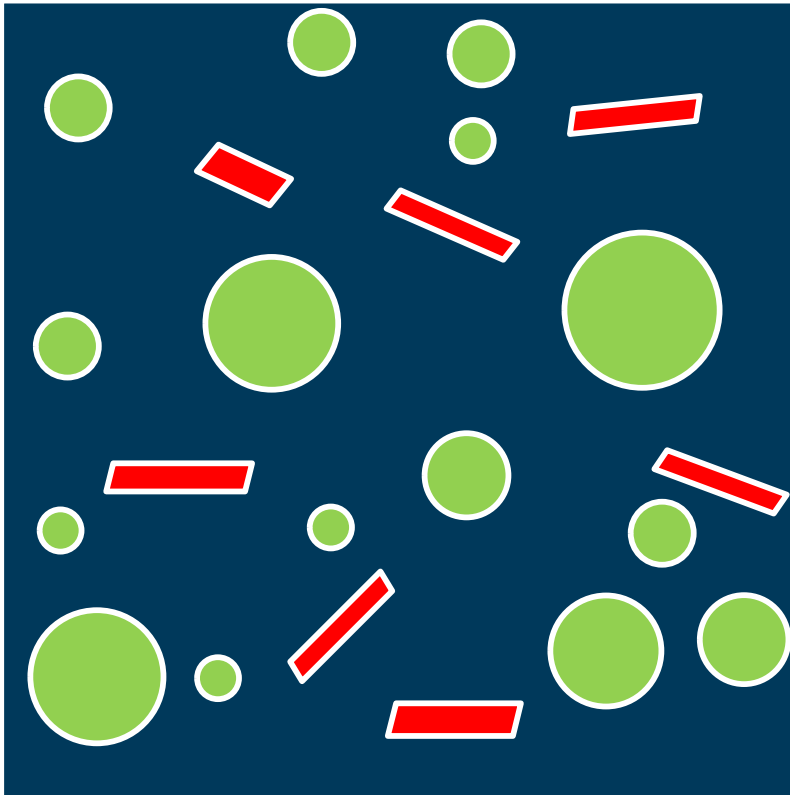
Property Model Calculator: Scattering effects

Phase Interface scattering

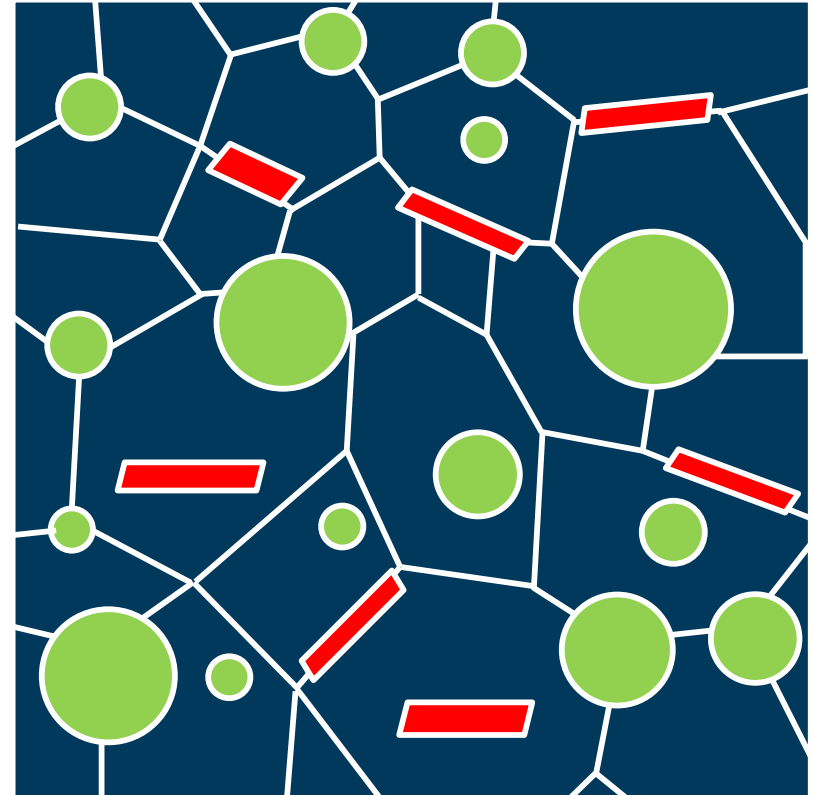


Property Model Calculator: Scattering effects

Phase Interface scattering



Grain boundary scattering:
Not considered!



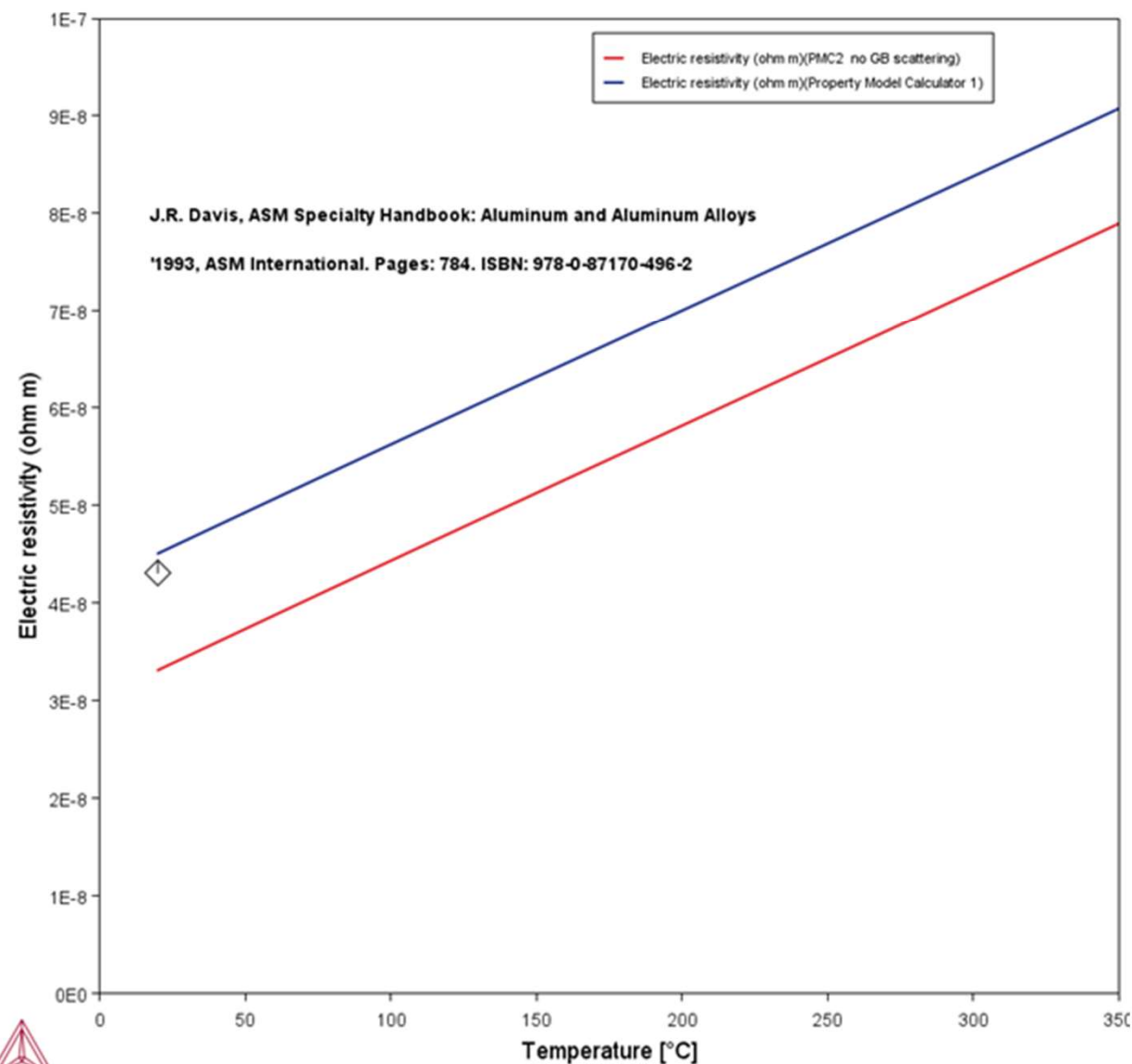
Account for phase interface scattering



Phase interface scattering constant

4.0E-8

Property Model Calculator result – Electrical resistivity, freeze-in



Steel Model Library

Steel Model Library

- ❑ Advanced models for formation of structures in steel.
- ❑ Introduced in 2019 with martensite and pearlite models.
- ❑ Bainite and TTT-diagram model were added in 2021, CCT new in 2022.
- ❑ Other material specific property model libraries have been added. Ni-library was new in 2022, Ti-library in 2024 and Noble Metals-library in 2025.

Configuration

Property Model Calculator 1

Composition unit: Mass percent

Condition Definitions

Temperature: Celsius 1000.0

Composition: Fe 85.0

Composition: Co 10

Composition: Ni 5

Timeout in minutes: 30.0 Parallel calculation, No. of worker processes: 6

Calculation Type

☐ Single ☐ One Axis ☒ Grid ☐ Min/Max ☐ Uncertainty ☐ Batch

Grid Definitions

Quantity	Min	Max	Number of steps
Mass percent Ni	0.0	10	10
Temperature	800	1300	10

General Models

- ☐ Coarsening
- ☐ Columnar to Equiaxed Transition
- ☐ Crack Susceptibility Coefficient
- ☐ Driving Force
- ☐ Equilibrium
- ☐ Equilibrium with Freeze-in Temperature
- ☐ Interfacial Energy
- ☐ Liquidus and Solidus Temperature
- ☐ Phase Transition
- ☐ Scheil
- ☐ Spinodal
- ☐ T-Zero Temperature
- ☐ Yield Strength

Nickel Models

- ☐ Antiphase Boundary Energy - Ni
- ☐ Coarsening - Ni
- ☐ Equilibrium with Freeze-in Temperature - Ni
- ☐ Solvus for Ordered Phase - Ni
- ☐ Strain-Age Cracking - Ni

Noble Metal Alloys Models

- ☐ Optical Properties - Noble

Steel Models

- ☐ Bainite
- ☐ CCT Diagram
- ☐ Critical Transformation Temperature
- ☐ Ferrite
- ☐ Martensite Fractions
- ☐ Martensite Temperatures
- ☐ Martensitic Steel Strength
- ☐ Pearlite
- ☐ TTT Diagram

Titanium Models

- ☐ Alloy Strength - Ti
- ☐ Martensite Temperatures - Ti

Help Add Predecessor Perform Tree Create New Successor

Steel Model Library

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

Configuration

TTT calculator

Composition Fe 96.76
Composition C 0.44
Composition Si 0.26
Composition Mn 0.75
Composition Cr 1.7
Composition V 0.09

Timeout in minutes: 30.0

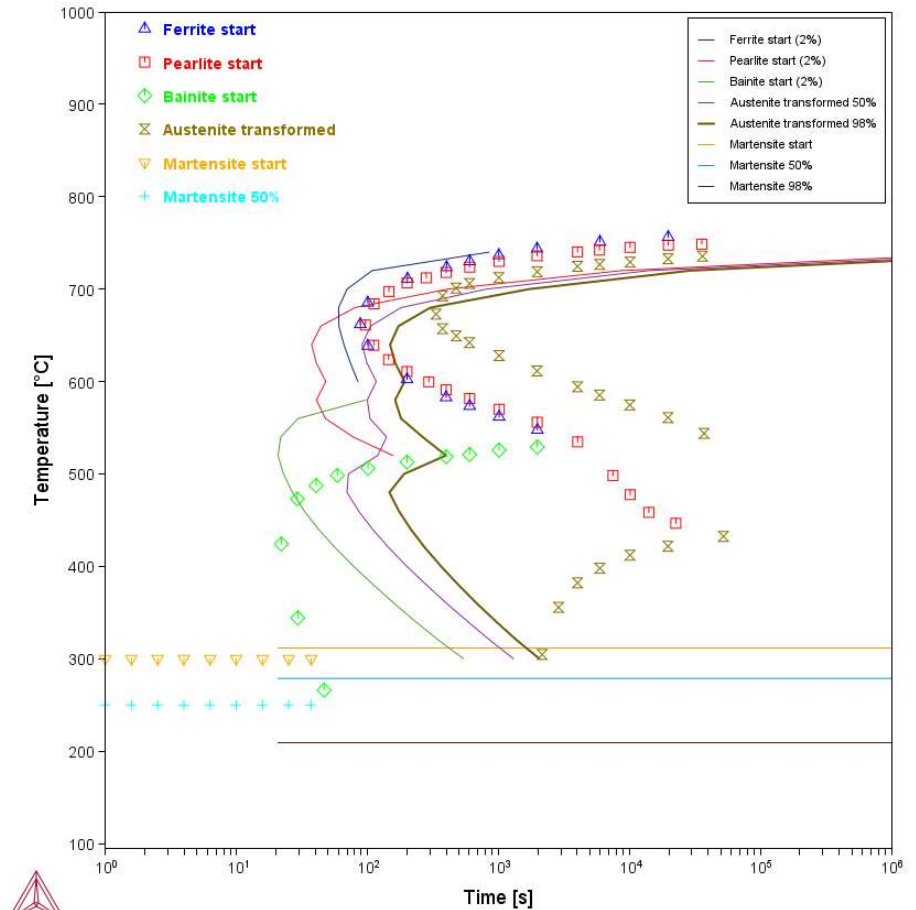
TTT Diagram

Configuration	Description
Austenite composition from	Equilibrium composition at austenitizing temperature
Austenitizing temperature	1050.0
Grain size [um]	89.8
Calculation setting	Custom
Ferrite selected	☒
Pearlite selected	☒
Bainite selected	☒
Martensite selected	☒
Ferrite mode	Faster start
Pearlite criterion	Maximize growth rate
Pearlite mode	Optimal pearlite
Carbide in pearlite	CEMENTITE
Carbide in bainite	CEMENTITE
Use interpolation when necessary	☒
Interpolation error tolerance	0.1
Maximum phase fraction change (absolute) in a time step	0.005
Maximum phase fraction change (relative) in a time step	0.05
Error tolerance for austenite fraction	0.001

Calculation Type

☐ Single ☒ One axis ☐ Grid ☐ Min/Max ☐ Uncertainty ☐ Batch

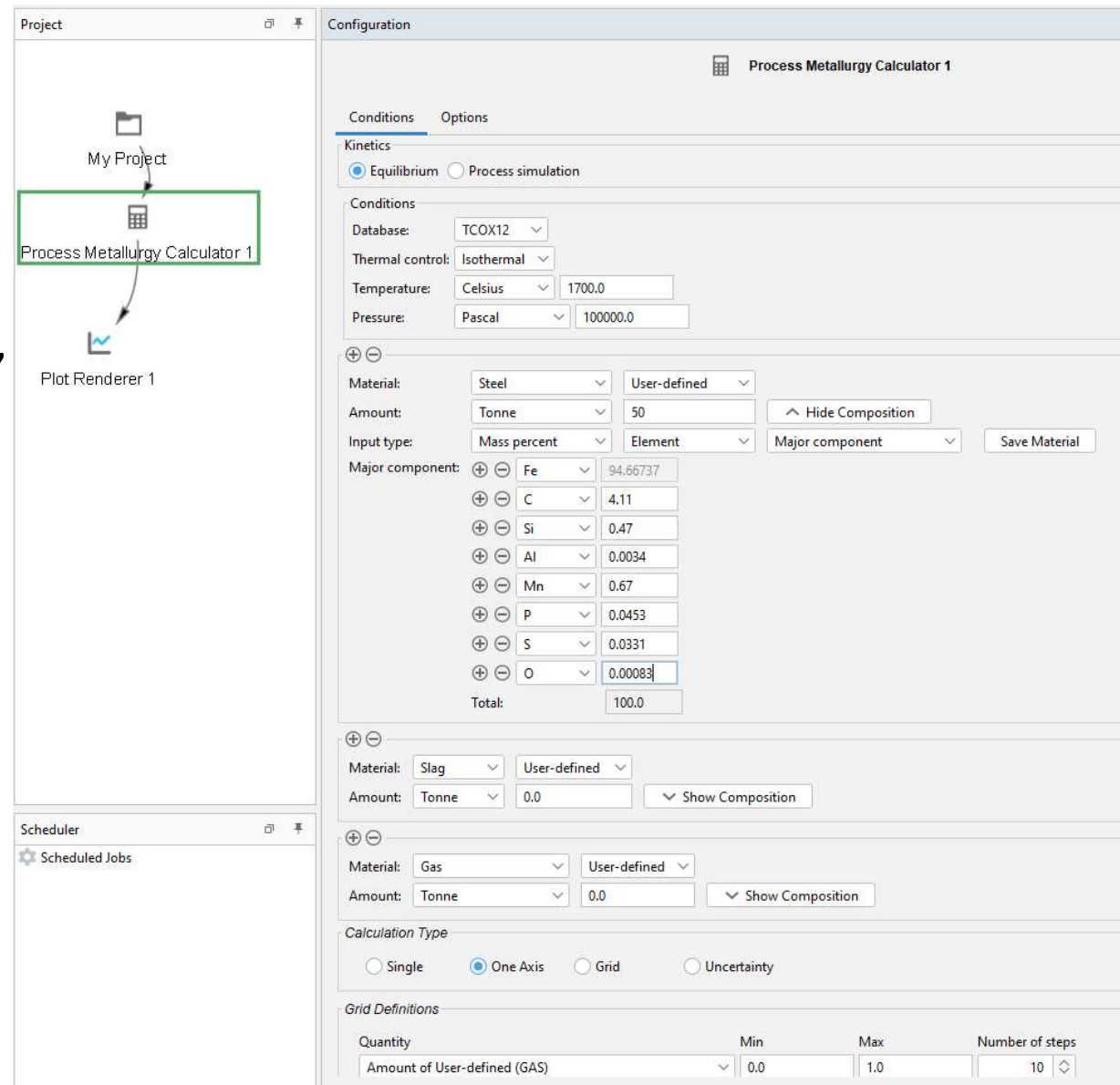
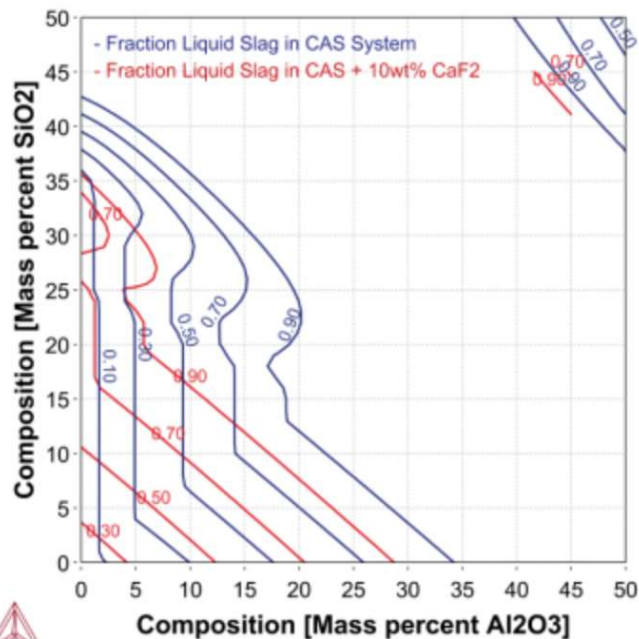
Help Add Predecessor Perform Tree Create New Successor



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.



Project

My Project

Process Metallurgy Calculator 1

Plot Renderer 1

Configuration

Process Metallurgy Calculator 1

Conditions Options

Kinetics

☒ Equilibrium ☐ Process simulation

Conditions

Database: TCOX12

Thermal control: Isothermal

Temperature: Celsius 1700.0

Pressure: Pascal 100000.0

Material: Steel User-defined

Amount: Tonne 50

Input type: Mass percent Element

Major component:

Element	Value
Fe	94.66737
C	4.11
Si	0.47
Al	0.0034
Mn	0.67
P	0.0453
S	0.0331
O	0.00083
Total	100.0

Material: Slag User-defined

Amount: Tonne 0.0

Calculation Type

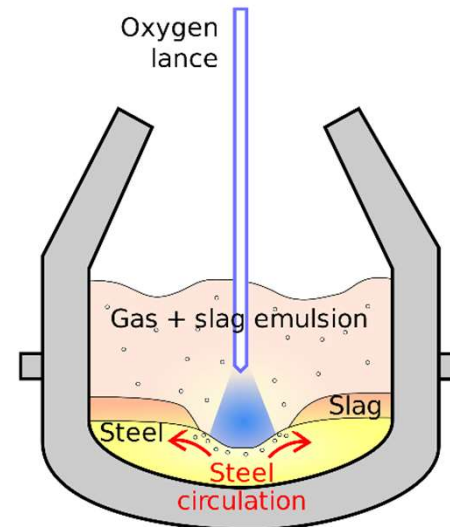
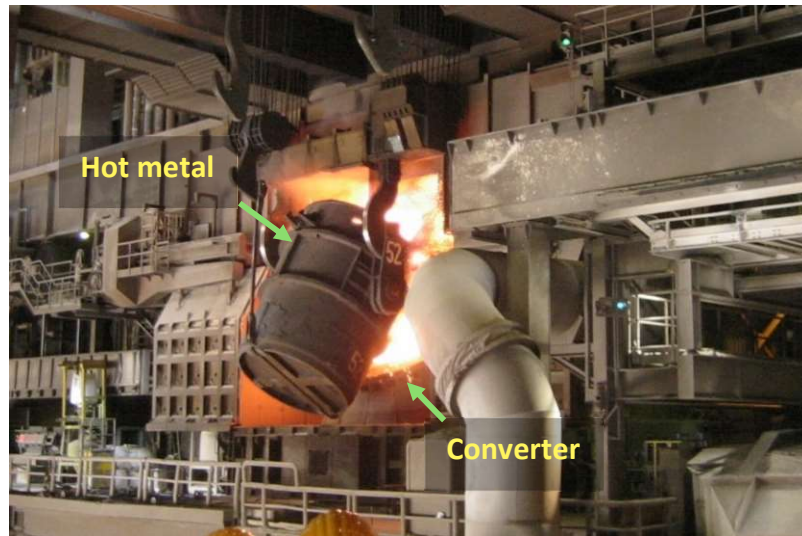
☐ Single ☒ One Axis ☐ Grid ☐ Uncertainty

Grid Definitions

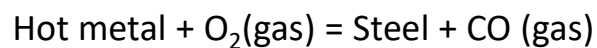
Quantity	Min	Max	Number of steps
Amount of User-defined (GAS)	0.0	1.0	10

PMM Example

Calculation of decarburization (steelmaking)

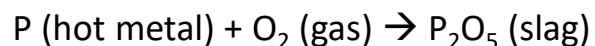


The hot metal from a blast furnace contains about 4.5 wt% Carbon. This makes it brittle and unsuitable for forging and rolling. The carbon content therefore needs to be reduced. This is termed steel-making and is mostly carried out in a converter (basic oxygen furnace, BOF) by blowing oxygen into the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

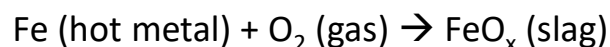


This reaction is highly exothermic and results in a temperature increase in the converter from $\sim 1450^\circ\text{C}$ to over 1650°C .

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



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



PMM Example 1

Calculation of decarburization (EQUILIBRIUM)

Conditions Options

Kinetics

☒ Equilibrium ☐ Process simulation

Conditions

Database: TCOX9

Thermal control: Isothermal

Temperature: Celsius 1650.0

Pressure: Pascal 100000.0

Material: Steel Steel_BOF

Amount: Tonne 100.0 Hide composition

Input type: Mass percent Element Major component Save material

Major component:

+	-	Fe	94.86
+	-	C	4.5
+	-	Si	0.5
+	-	S	0.08
+	-	P	0.06
Total:			100.0

Material: Slag Slag_BOF

Amount: Tonne 3.0 Hide composition

Input type: Mass percent Component Major component Save material

Major component:

+	-	CaO	75.0
+	-	Al2O3	25.0
Total:			100.0

Material: Gas Oxygen

Amount: Normal cubic meter 1.0 Hide composition

Input type: Mass percent Gas component Major component Save material

Major component:

+	-	O2	100.0
Total:			100.0

Calculation Type

☐ Single ☒ One axis ☐ Grid ☐ Uncertainty

Grid Definitions

Quantity	Min	Max	Number of steps
Amount of Oxygen (GAS) [Nm ³]	0.0	7000.0	40

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:

☒ X: Amount of Oxygen (GAS) [Nm³]

Y: Composition of phase group Liquid metal All elements

Amount of Oxygen (GAS) [Nm³]

Axis type: Linear

Limits: 0.0 to 1.0 step 0.1 ☒ Automatic scaling

Mass composition (Composition of phase group)

Unit: Mass percent

Axis type: Logarithmic 10

Limits: 1.0E-6 to 10.0 step ☐ Automatic scaling

or

☒ X: Amount of Oxygen (GAS) [Nm³]

Y: Composition of phase group Liquid oxides All components

or

☒ X: Amount of Oxygen (GAS) [Nm³]

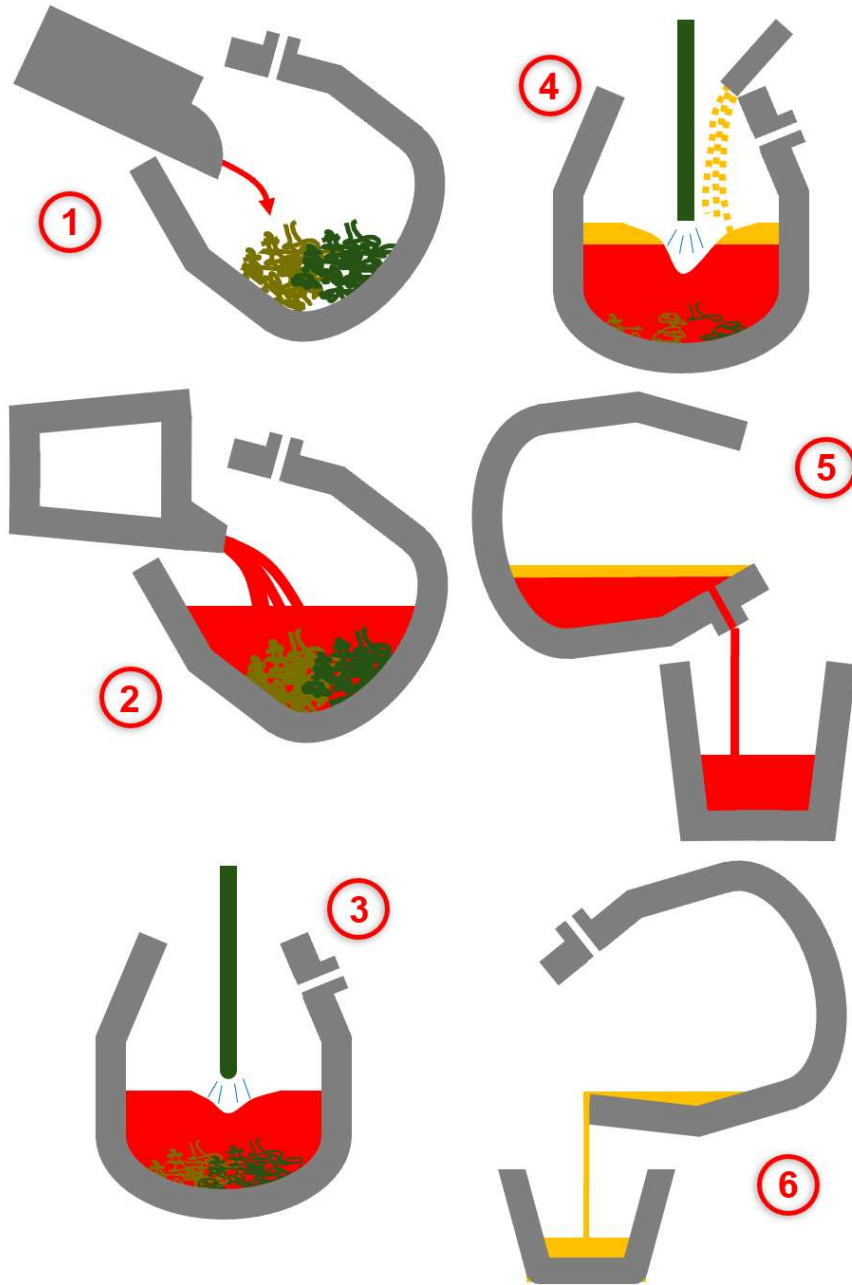
Y: Amount of phase group All

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



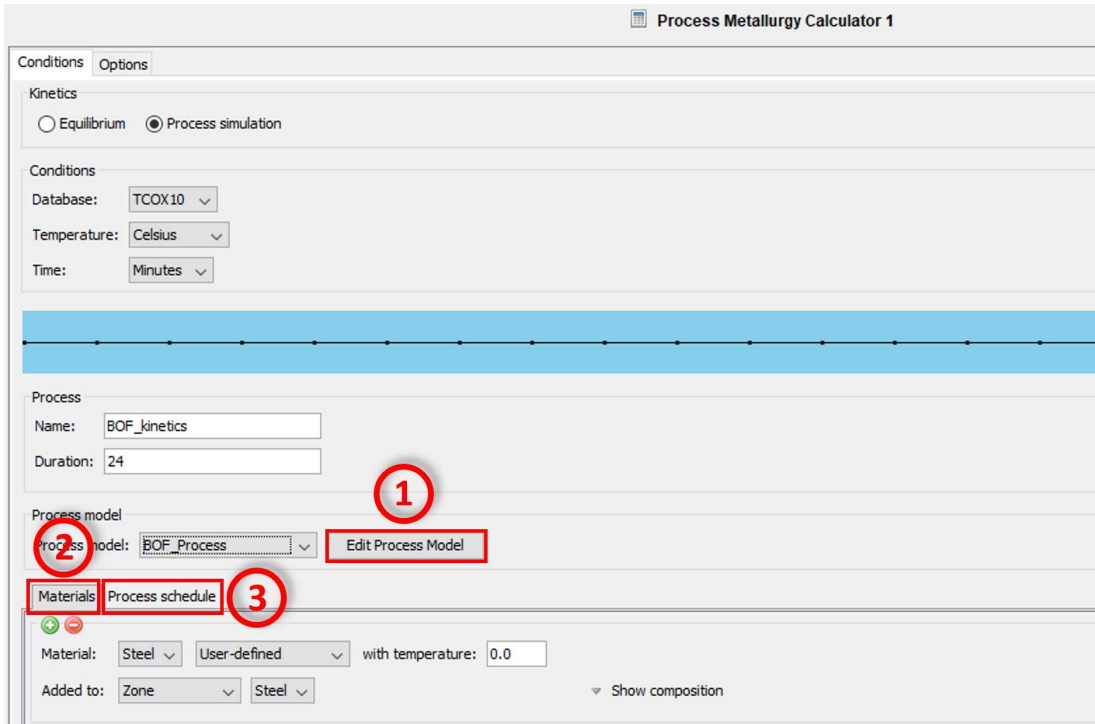
Setting up equilibrium calculation

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



Process Metallurgy Calculator 1

Conditions Options

Kinetics

☐ Equilibrium ☒ Process simulation

Conditions

Database: TCOX10

Temperature: Celsius

Time: Minutes

Process

Name: BOF_kinetics

Duration: 24

Process model

Process model: BOF_Process Edit Process Model

Materials Process schedule

Material: Steel User-defined with temperature: 0.0

Added to: Zone Steel Show composition

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

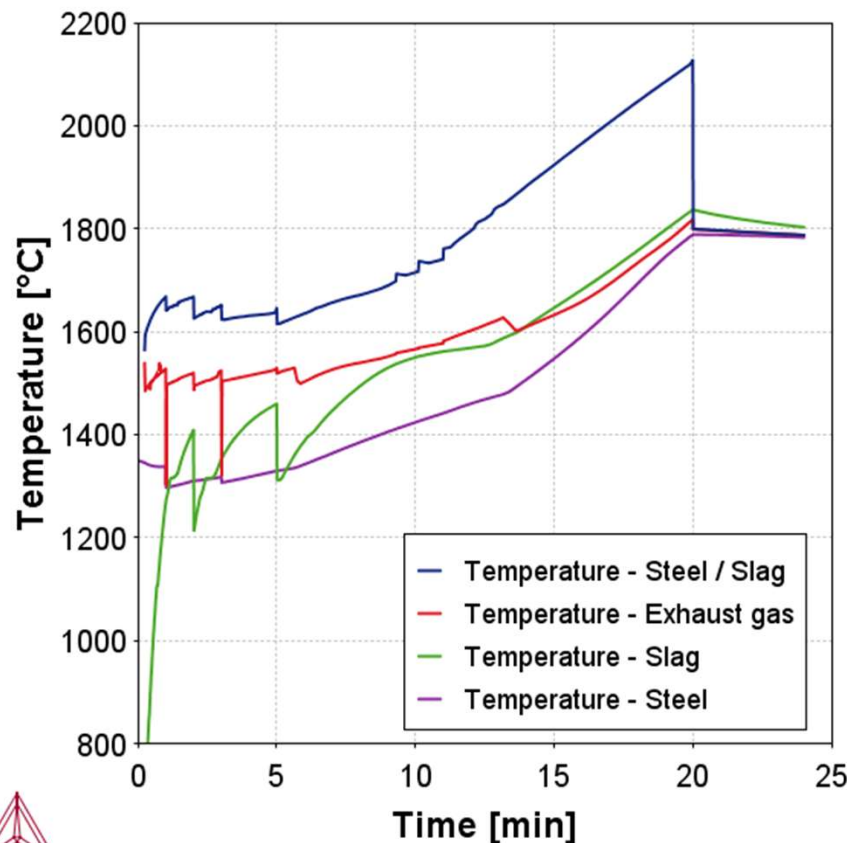
Note: Calculation times for a full process simulation can be 45 minutes or more

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

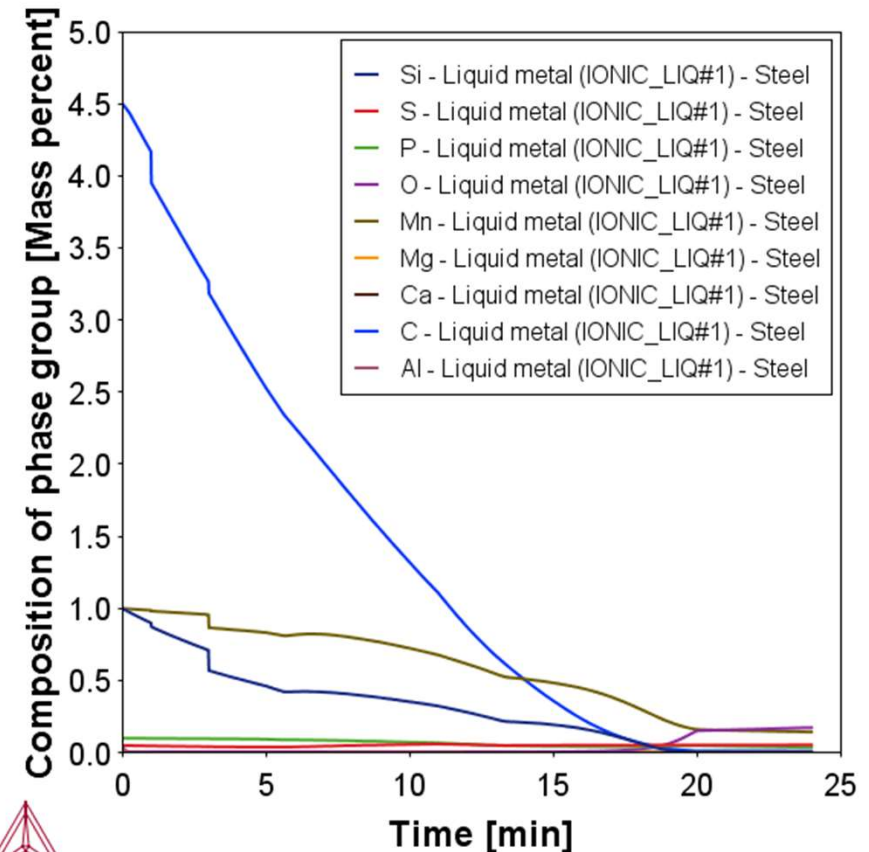
PMM Example 2

Calculation of decarburization PROCESS SIMULATION

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.

Thermo-Calc Software

- Welcome to Thermo-Calc ▾
- Introduction ▾
- Key Concepts and Features ▾
- Calculations in Graphical Mode ▾
- Visualizations in Graphical Mode ▾
- Thermo-Calc Console Mode ▾
- Software Examples All Products ▾
- Databases ▾
- Add-on Modules and Property Model Libraries ▾
- Software Development Kits (SDKs) ▾
- Installation ▾
- General Reference ▾

Get Started



Browse

Get familiar with navigating the help and technical content.



Learn

Discover training and self-paced learning opportunities.



Getting Started Guides on the Web

In addition to the technical content in this help, you can also access resources on our website including guides for Thermo-Calc as well as the Add-on Diffusion Module (DICTRA) and Additive Manufacturing Module.



The Online Help

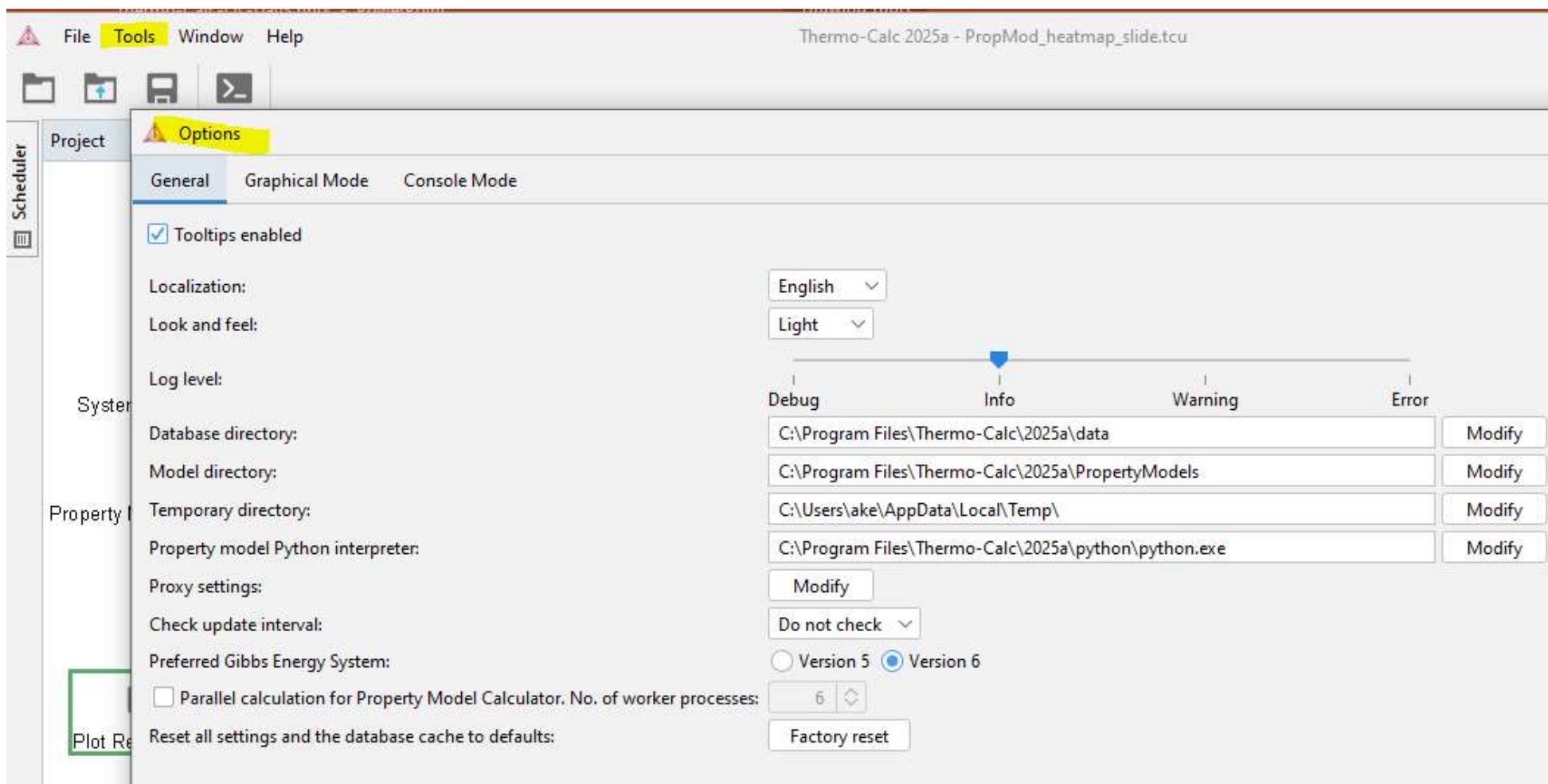
Below a search for “State variables” and then browsing among the search results.

You are here: [General Reference](#) > [Parameters, Functions, and Variables](#) > [Thermodynamic Variables and Units](#) > Intensive Variables

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

Tools -> Options menu



Tools -> Options -> Graphical mode

Options

General Graphical Mode Console Mode

Activities Default Units

Default Configurations

- System definition
- Calculation
- Precipitation
- Diffusion
- Scheil**
- Process Metallurgy
- Plotting
- Tabulation

Calculate to: ☒ End of Scheil ☐ Temperature below solidus

Start temperature: 2226.85

Temperature step during Scheil: 1.0

Cooling rate: 1.0 K/s

Secondary dendrite arm spacing: Calculated c: 5.0E-5 n: 0.33 5E-5 m

Scanning speed: 1.0 m/s

α : 45.0 degrees

Trans-interface diffusivity: Same for all elements Pre-exponential factor: 5.0E-9 m²/s Activation energy: 0.0 J/mol

Maximum velocity for infinite driving force: 2000 m/s

Model: Aziz

Interface driving force: Driving energy

Global minimization: ☒

Global test interval: 10

Max grid points: 2000

Calculate evaporation properties: ☐

Max no. of iterations: 500

Required accuracy: 1.0E-6

Smallest fraction: 1.0E-12

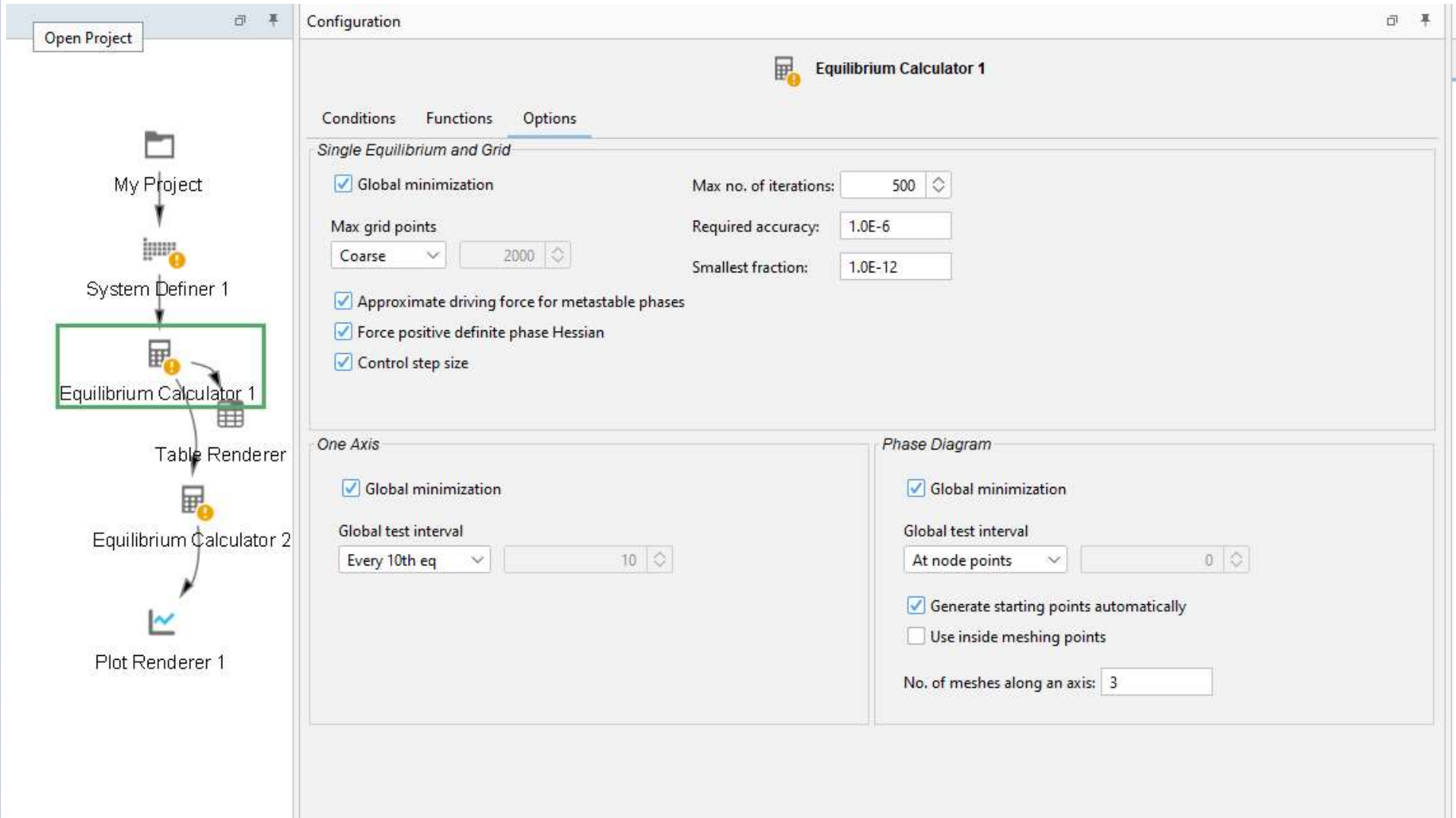
Approximate driving force for metastable phases: ☒

Include one axis equilibrium calculation: ☒

Temperature below solidus settings: No. of points: 50 Final temperature: Room temperature 25.0

Settings

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



The screenshot displays the Thermo-Calc software interface, illustrating the workflow and the configuration settings for the Equilibrium Calculator 1.

Workflow Diagram (Left Panel):

- Open Project
- My Project
- System Definer 1
- Equilibrium Calculator 1** (highlighted with a green box)
- Table Renderer
- Equilibrium Calculator 2
- Plot Renderer 1

Configuration Window (Right Panel):

The Configuration window for **Equilibrium Calculator 1** is shown, with the **Options** tab selected.

Single Equilibrium and Grid:

- ☒ Global minimization
- Max no. of iterations: 500
- Max grid points: Coarse (dropdown), 2000 (spinbox)
- Required accuracy: 1.0E-6
- Smallest fraction: 1.0E-12
- ☒ Approximate driving force for metastable phases
- ☒ Force positive definite phase Hessian
- ☒ Control step size

One Axis:

- ☒ Global minimization
- Global test interval: Every 10th eq (dropdown), 10 (spinbox)

Phase Diagram:

- ☒ Global minimization
- Global test interval: At node points (dropdown), 0 (spinbox)
- ☒ Generate starting points automatically
- ☐ Use inside meshing points
- No. of meshes along an axis: 3

Questions & Answers

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

DICTRA 14 -16 Oct.

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.

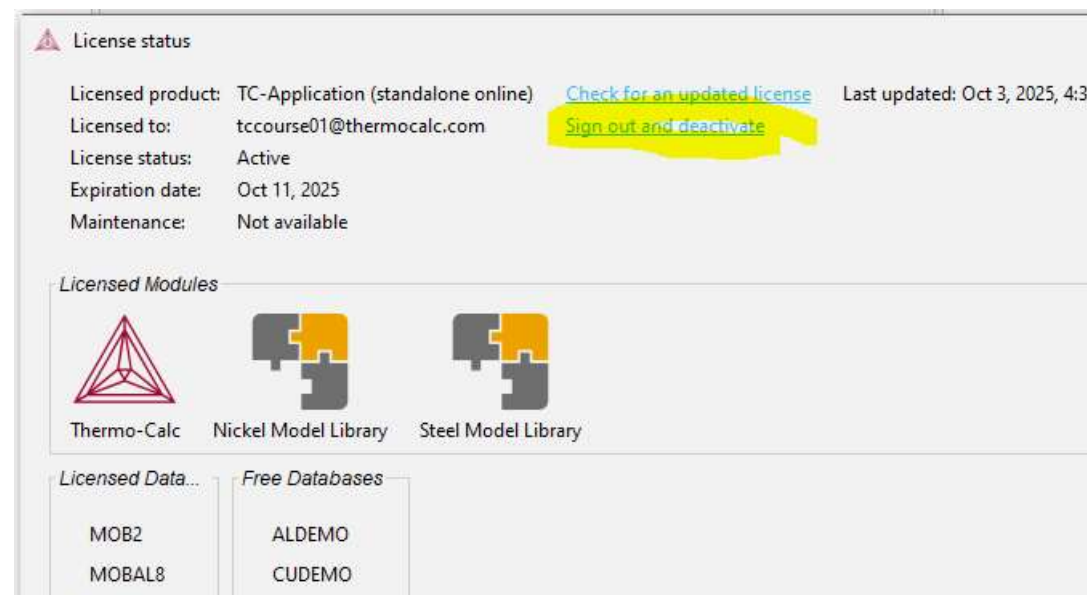
The current course license will be valid on Friday
10 Oct., but not on Saturday.

For those of you who will take part in

DICTRA 14 -16 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 + DICTRA 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 think we might have it wrong.