



Thermo-Calc On-line Training

Day 3, April 11, 2024

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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.

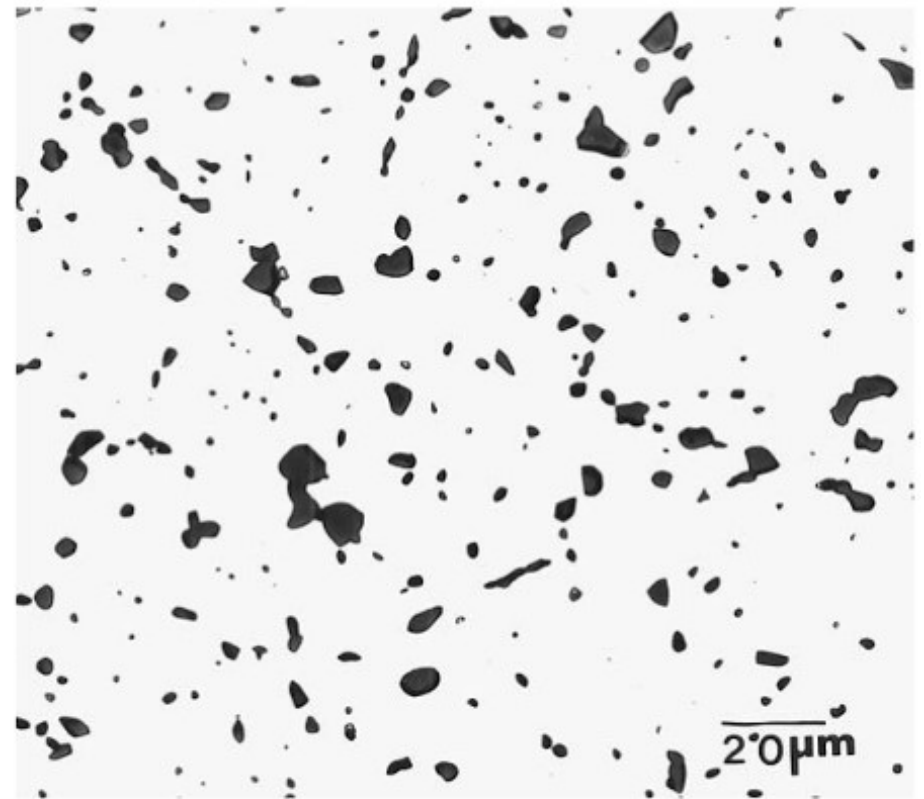
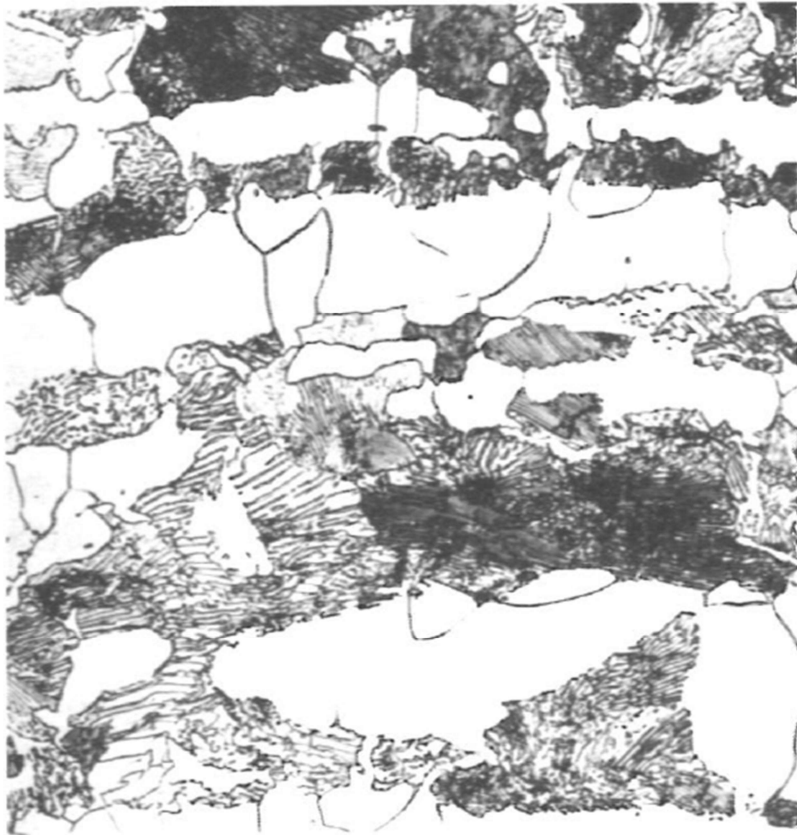
Home Assignment 2

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 Fe₃C (Cementite)?



(b)

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

Solidification simulations

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.

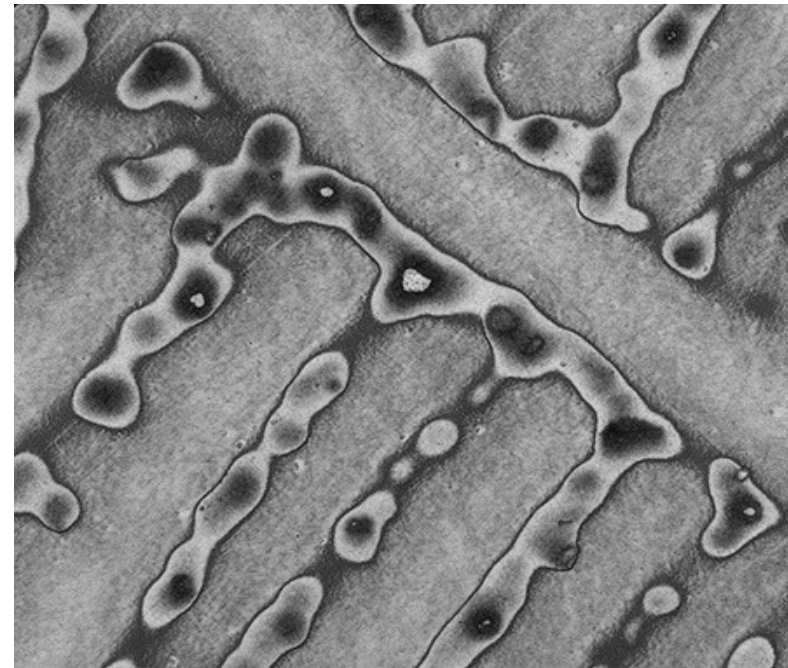
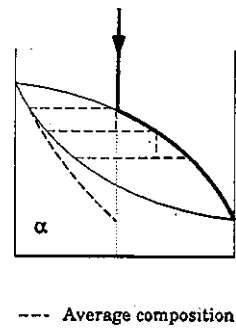
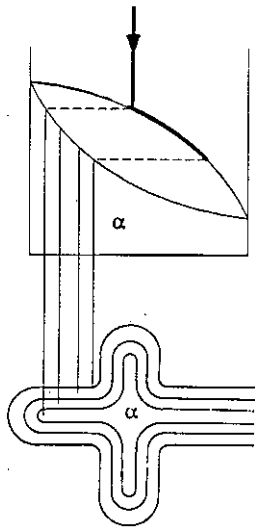
Moving phase boundary methods (DICTRA)

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

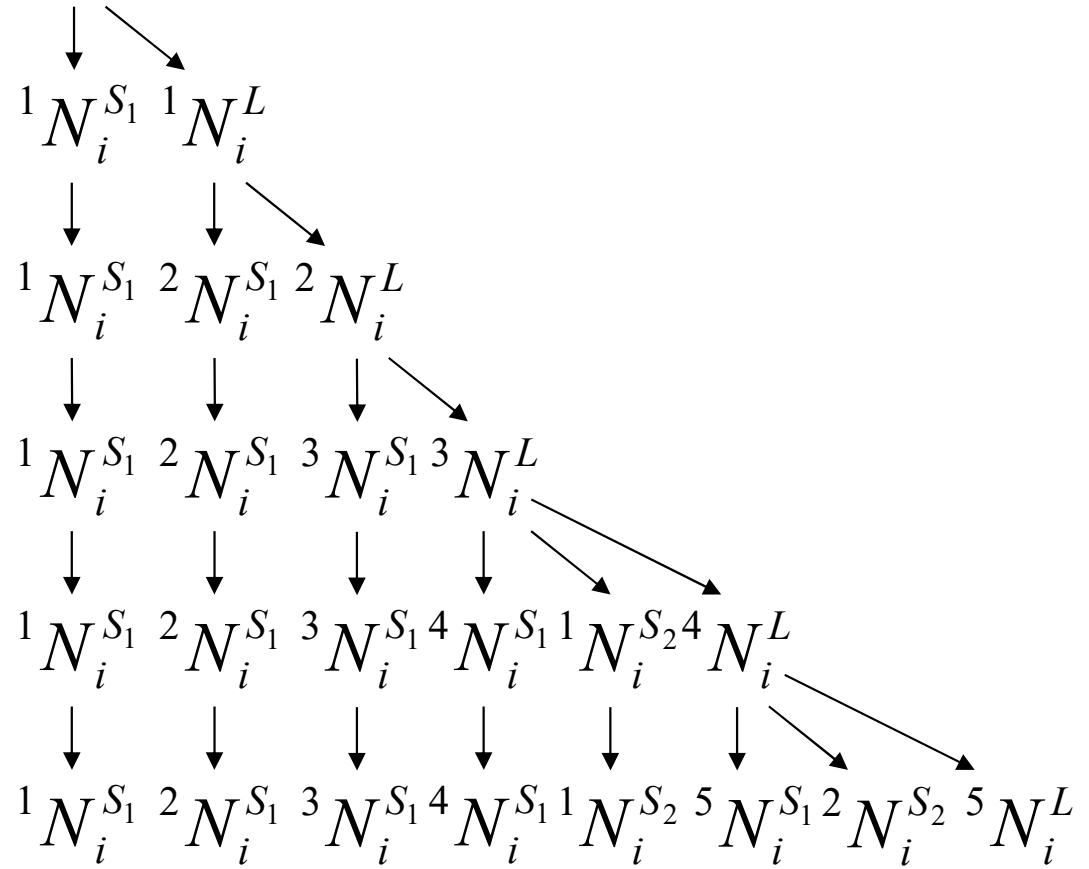
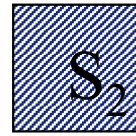
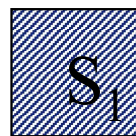
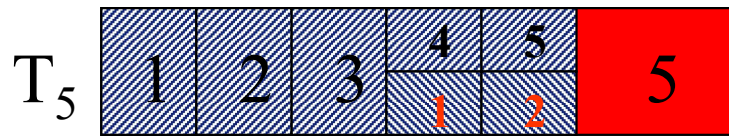
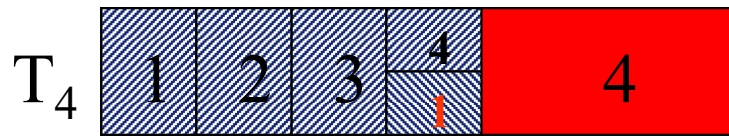
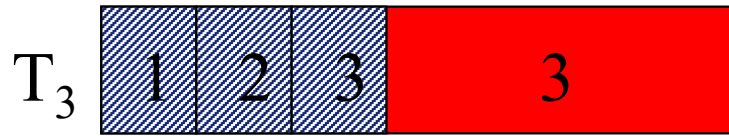
Scheil model

Assumptions in traditional Scheil:

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

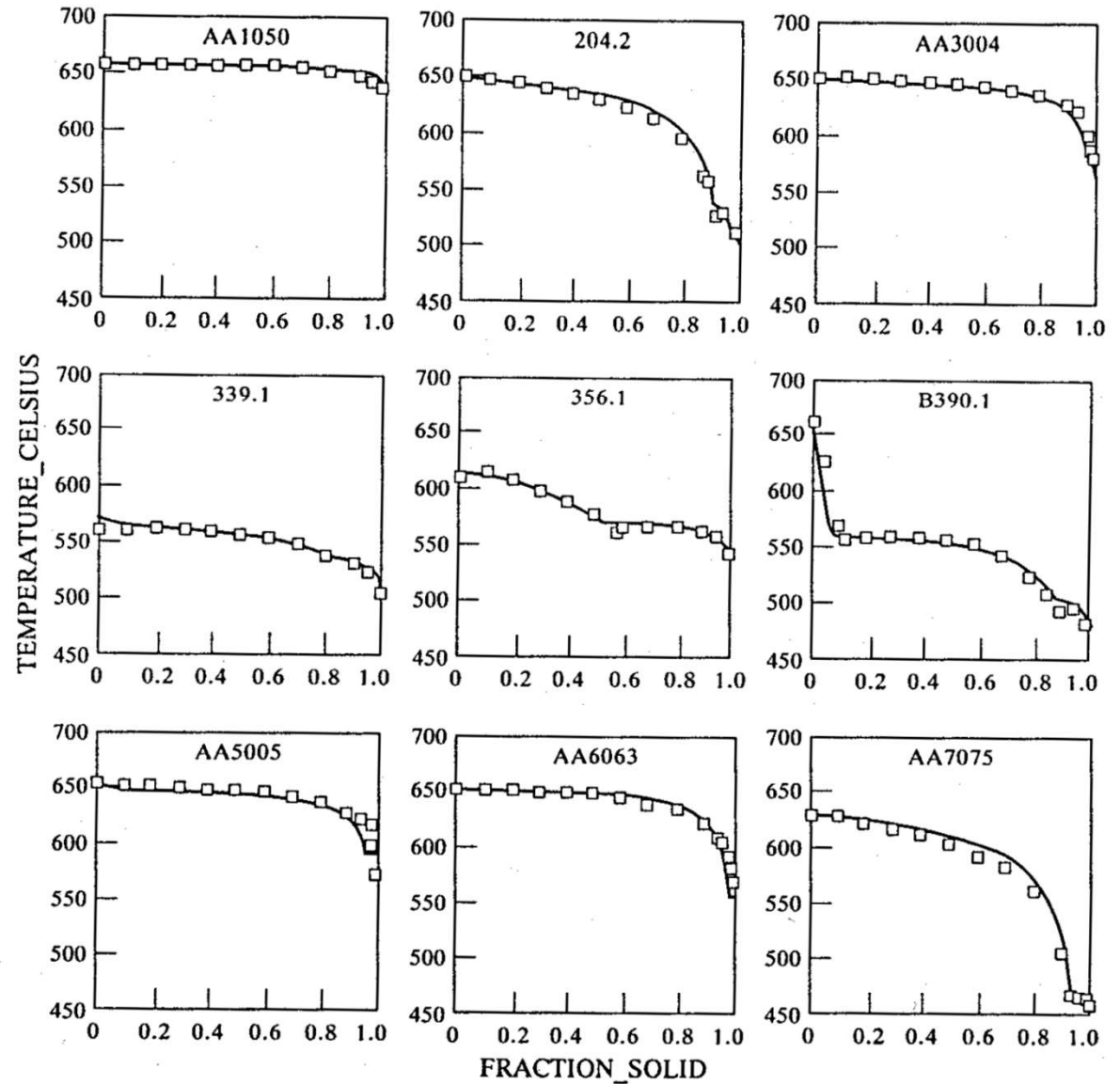


Algorithm in traditional Scheil



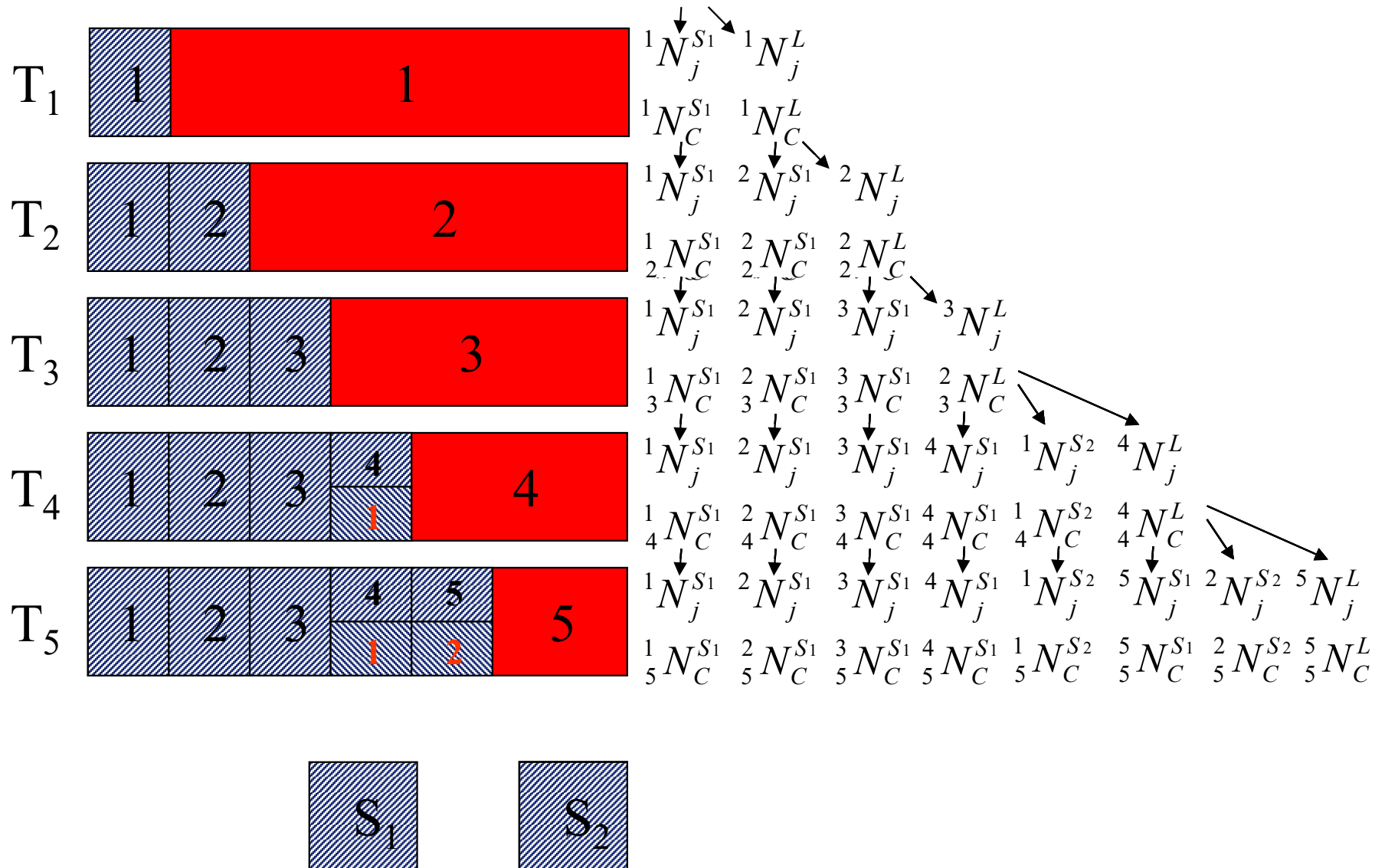
Some Examples

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

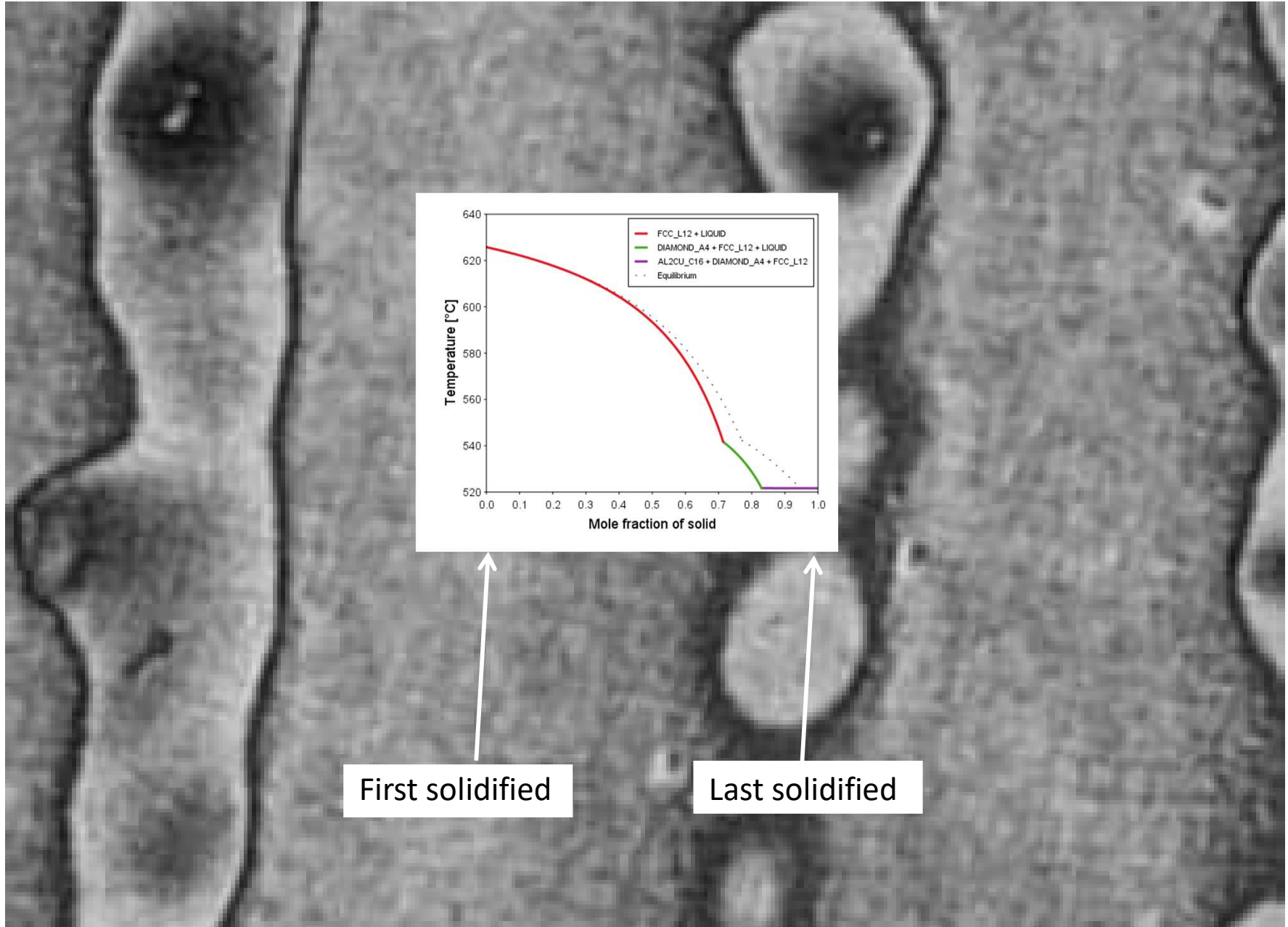


From: Saunders & Miedownik: "Calphad -a comprehensive review"

Algorithm in modified Scheil (partial eq.)



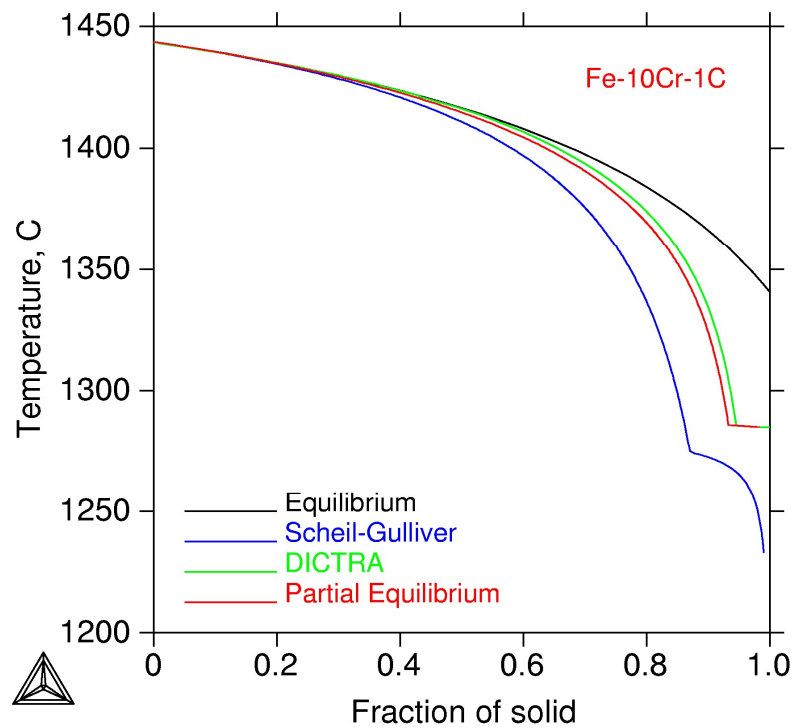
Translating the Scheil to Microstructure



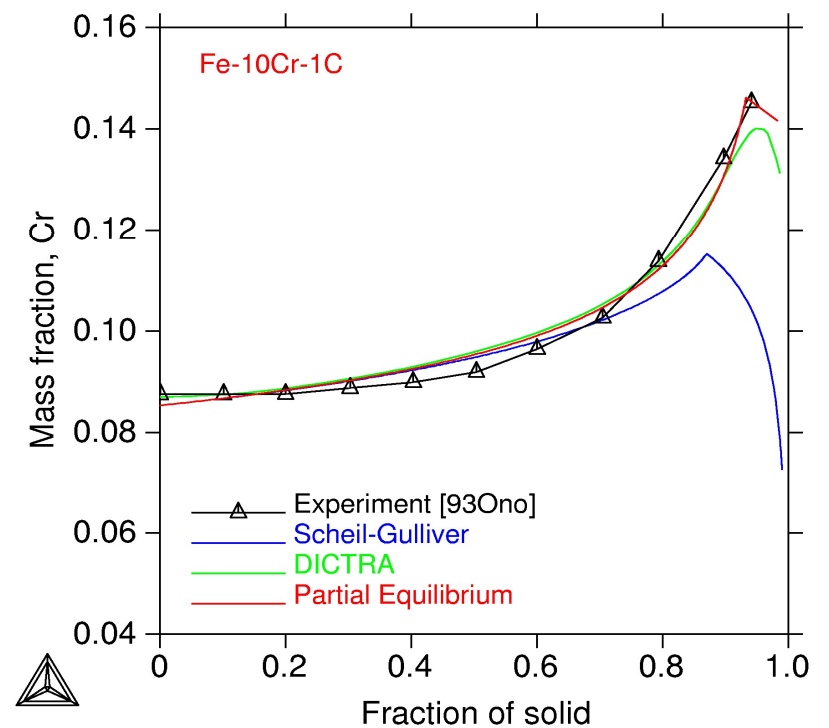
Some results: Fe-10Cr-1C

Comparison of equilibrium, Scheil, and partial eq

Freezing Range



Microsegregation



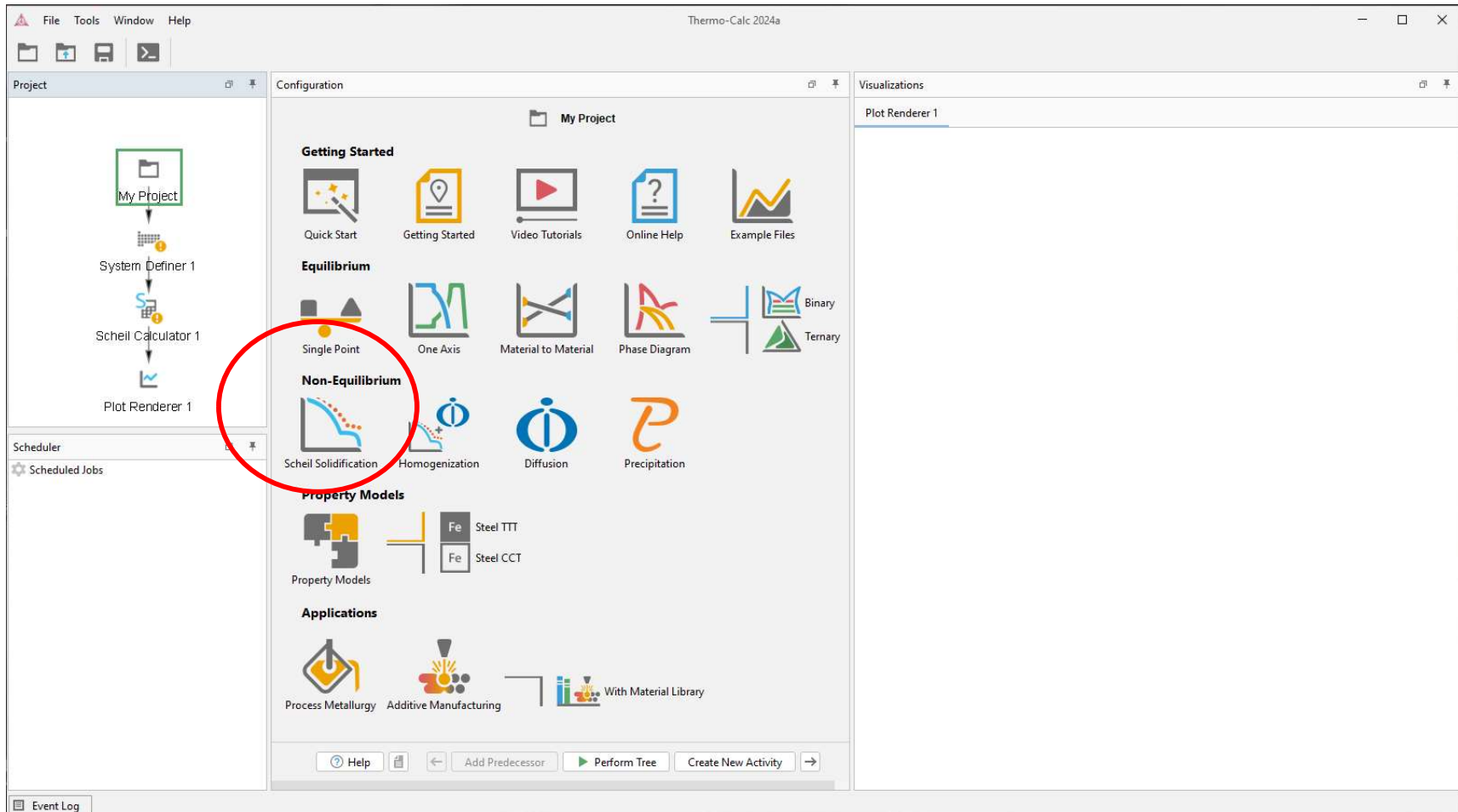
Q. Chen & B. Sundman, Materials Transactions, 43(3)551(2002).

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?



The screenshot displays the Thermo-Calc 2024a software interface. The main window is divided into several panes:

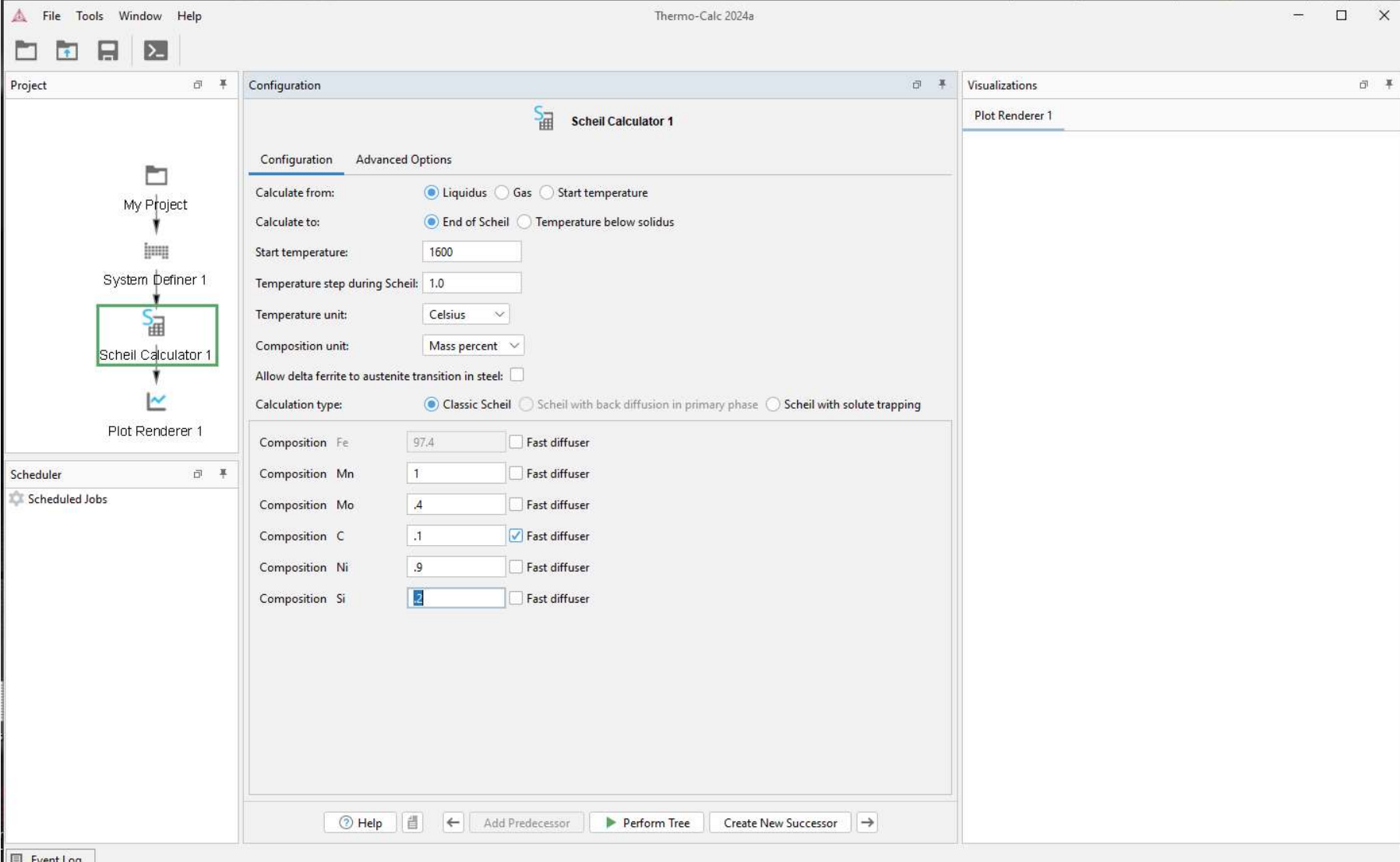
- Project:** Shows a workflow tree with steps: My Project, System Definer 1, Scheil Calculator 1, and Plot Renderer 1.
- Configuration:** Contains a central menu for "My Project" with categories:
 - Getting Started:** Quick Start, Getting Started, Video Tutorials, Online Help, Example Files.
 - Equilibrium:** Single Point, One Axis, Material to Material, Phase Diagram, Binary, Ternary.
 - Non-Equilibrium:** Scheil Solidification (highlighted with a red circle), Homogenization, Diffusion, Precipitation.
 - Property Models:** Steel TTT, Steel CCT.
 - Applications:** Process Metallurgy, Additive Manufacturing, With Material Library.
- Scheduler:** Shows "Scheduled Jobs".
- Visualizations:** Shows "Plot Renderer 1".

At the bottom of the Configuration pane, there are buttons for "Help", "Add Predecessor", "Perform Tree", and "Create New Activity".

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 "Scheil Calculator 1" and is divided into several panes:

- Project:** A tree view showing the project structure: "My Project" (folder icon), "System Definer 1" (grid icon), "Scheil Calculator 1" (calculator icon, highlighted with a green box), and "Plot Renderer 1" (checkmark icon).
- Scheduler:** A section labeled "Scheduled Jobs" with a star icon.
- Configuration:** The main settings area for the Scheil Calculator, divided into "Configuration" and "Advanced Options" tabs. The "Configuration" tab is active, showing:
 - Calculate from: Liquidus Gas Start temperature
 - Calculate to: End of Scheil Temperature below solidus
 - Start temperature: 1600
 - Temperature step during Scheil: 1.0
 - Temperature unit: Celsius
 - Composition unit: Mass percent
 - Allow delta ferrite to austenite transition in steel:
 - Calculation type: Classic Scheil Scheil with back diffusion in primary phase Scheil with solute trapping
- Visualizations:** A section labeled "Plot Renderer 1" which is currently empty.

At the bottom of the configuration pane, the alloy composition is listed with input fields and checkboxes for "Fast diffuser":

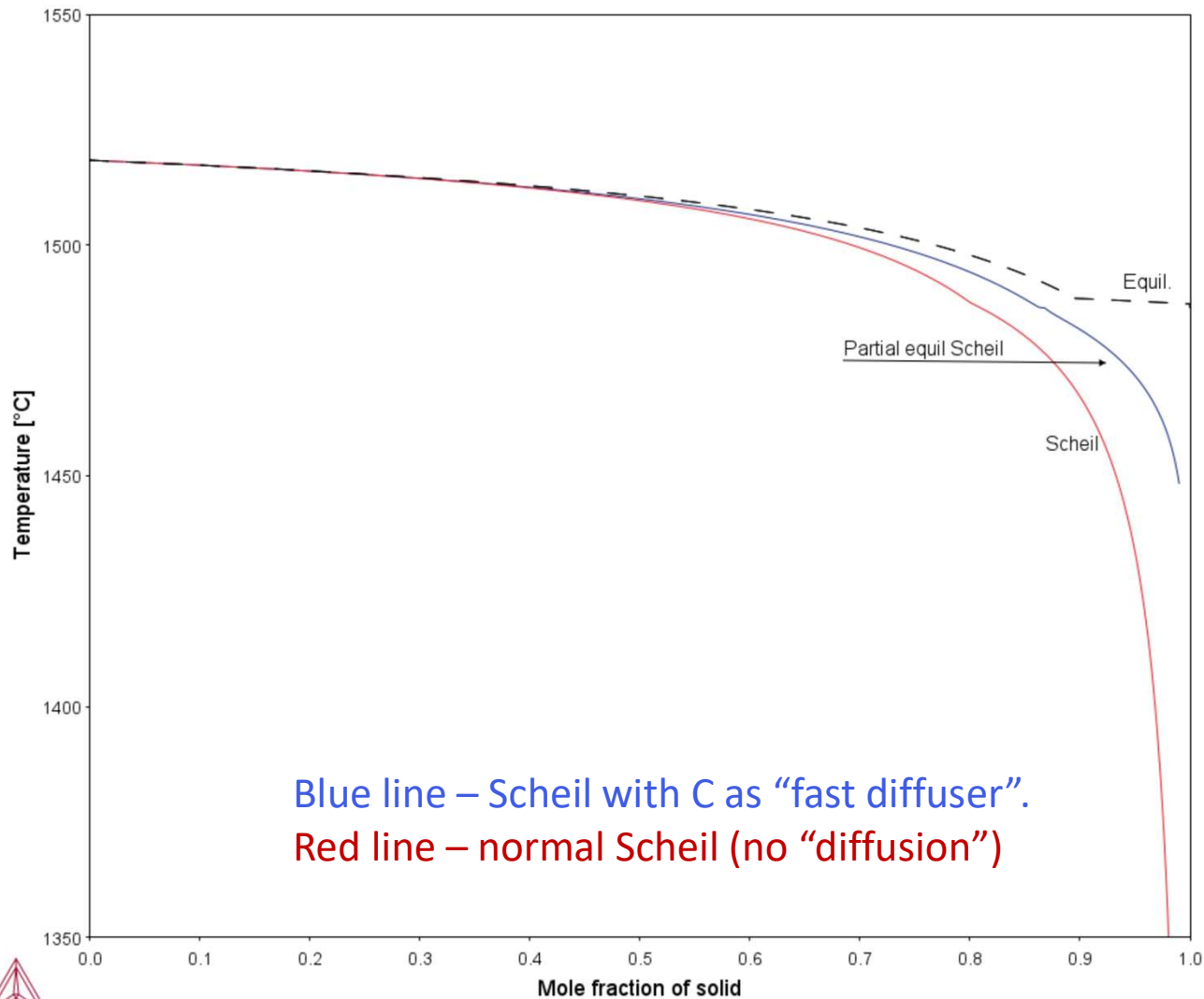
Composition	Value	Fast diffuser
Fe	97.4	<input type="checkbox"/>
Mn	1	<input type="checkbox"/>
Mo	.4	<input type="checkbox"/>
C	.1	<input checked="" type="checkbox"/>
Ni	.9	<input type="checkbox"/>
Si	.2	<input type="checkbox"/>

Navigation buttons at the bottom include: Help, Add Predecessor, Perform Tree, and Create New Successor.

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-number for duplex stainless steel

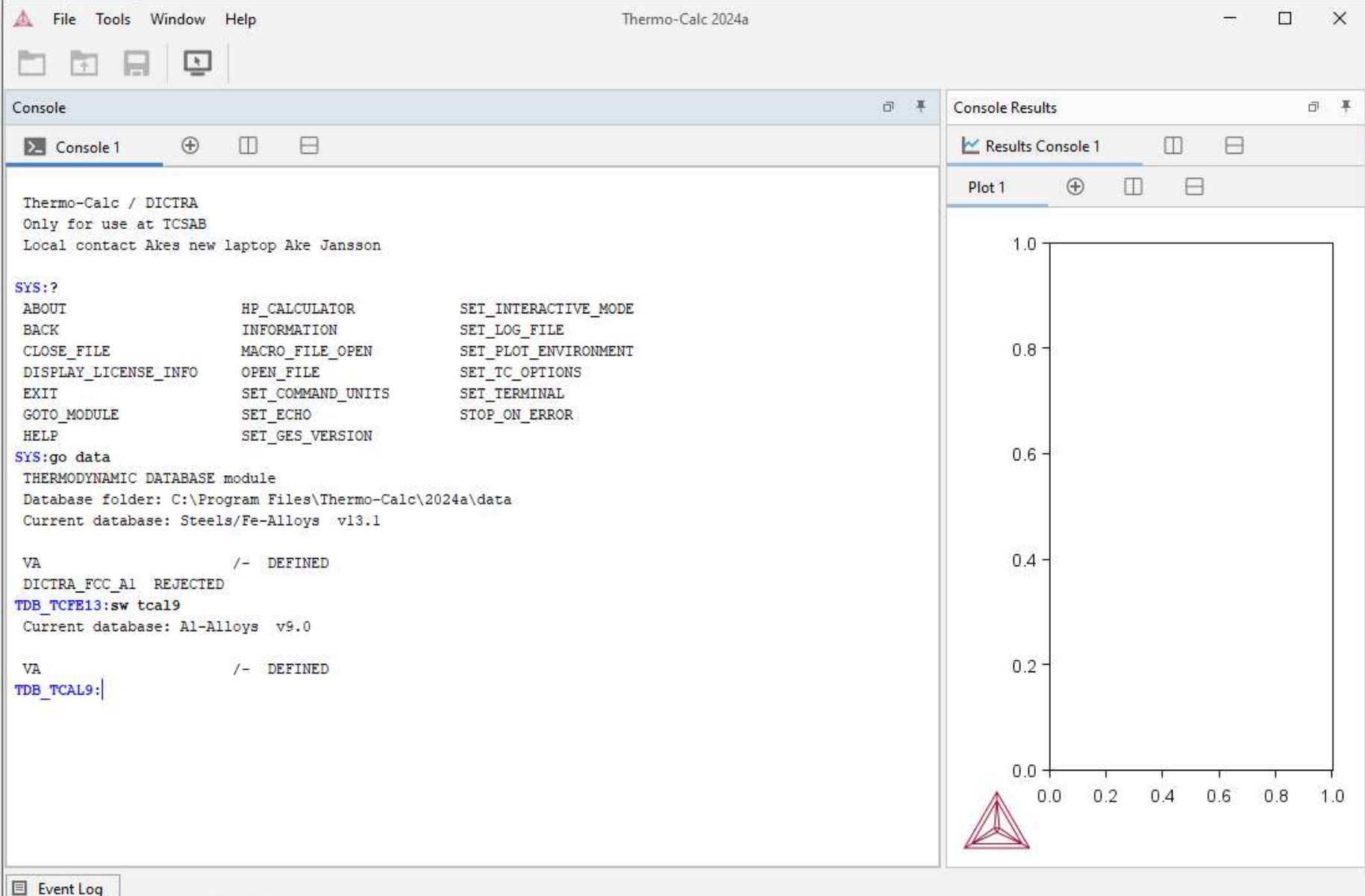
- PRE (Pitting Resistance Equivalence) is an empirical measure for corrosion resistance in stainless steels.
- PRE can be defined as:
$$\text{PRE} = w\% \text{Cr} + 3 * w\% \text{Mo} + 16 * w\% \text{N}$$
- For duplex stainless steels, it is desirable to have a high and balanced PRE-numbers in ferrite 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. The interface is divided into two main panels: "Console" on the left and "Console Results" on the right.

The "Console" panel shows the following text:

```
Thermo-Calc / DICTRA
Only for use at TCSAB
Local contact Akes 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

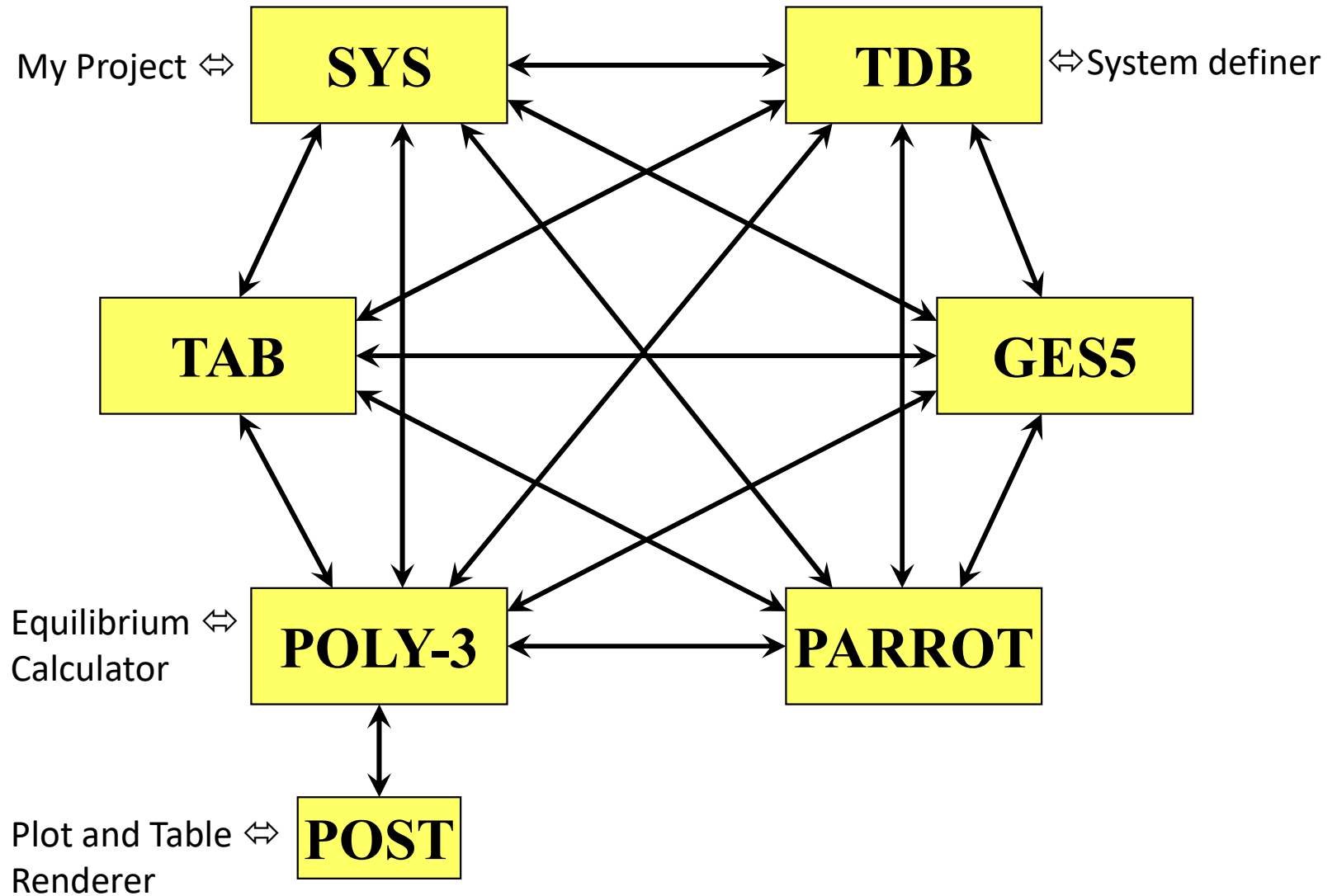
VA              /- DEFINED
DICTRA_FCC_A1  REJECTED
TDB_TCFE13:sw tcal9
Current database: Al-Alloys v9.0

VA              /- DEFINED
TDB_TCAL9:|
```

The "Console Results" panel shows a plot titled "Plot 1". The plot is a square with both axes ranging from 0.0 to 1.0. The y-axis is labeled from 0.0 to 1.0 in increments of 0.2. The x-axis is also labeled from 0.0 to 1.0 in increments of 0.2. The plot area is currently empty. A small Thermo-Calc logo is visible in the bottom-left corner of the plot area.

At the bottom of the interface, there is an "Event Log" button.

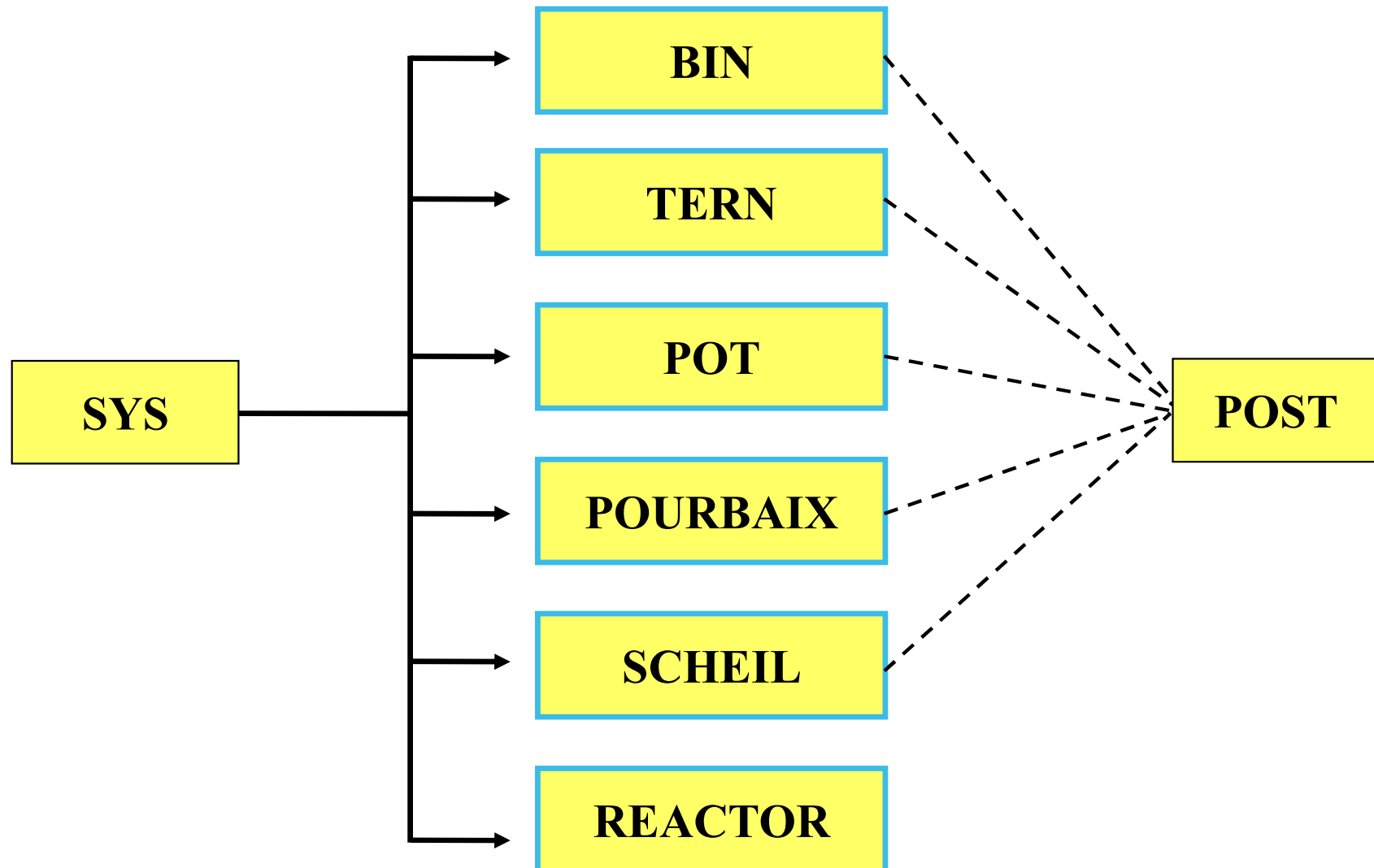
Modules in Thermo-Calc Console mode



Special modules in Console mode

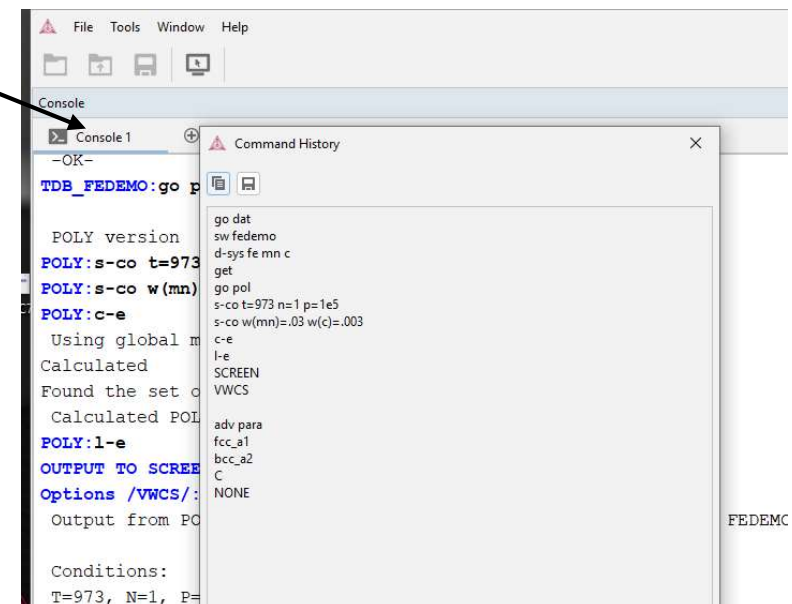
These modules* are very automatic and after entering a few conditions, the calculation will start and end with a plotted diagram.

*) 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,,

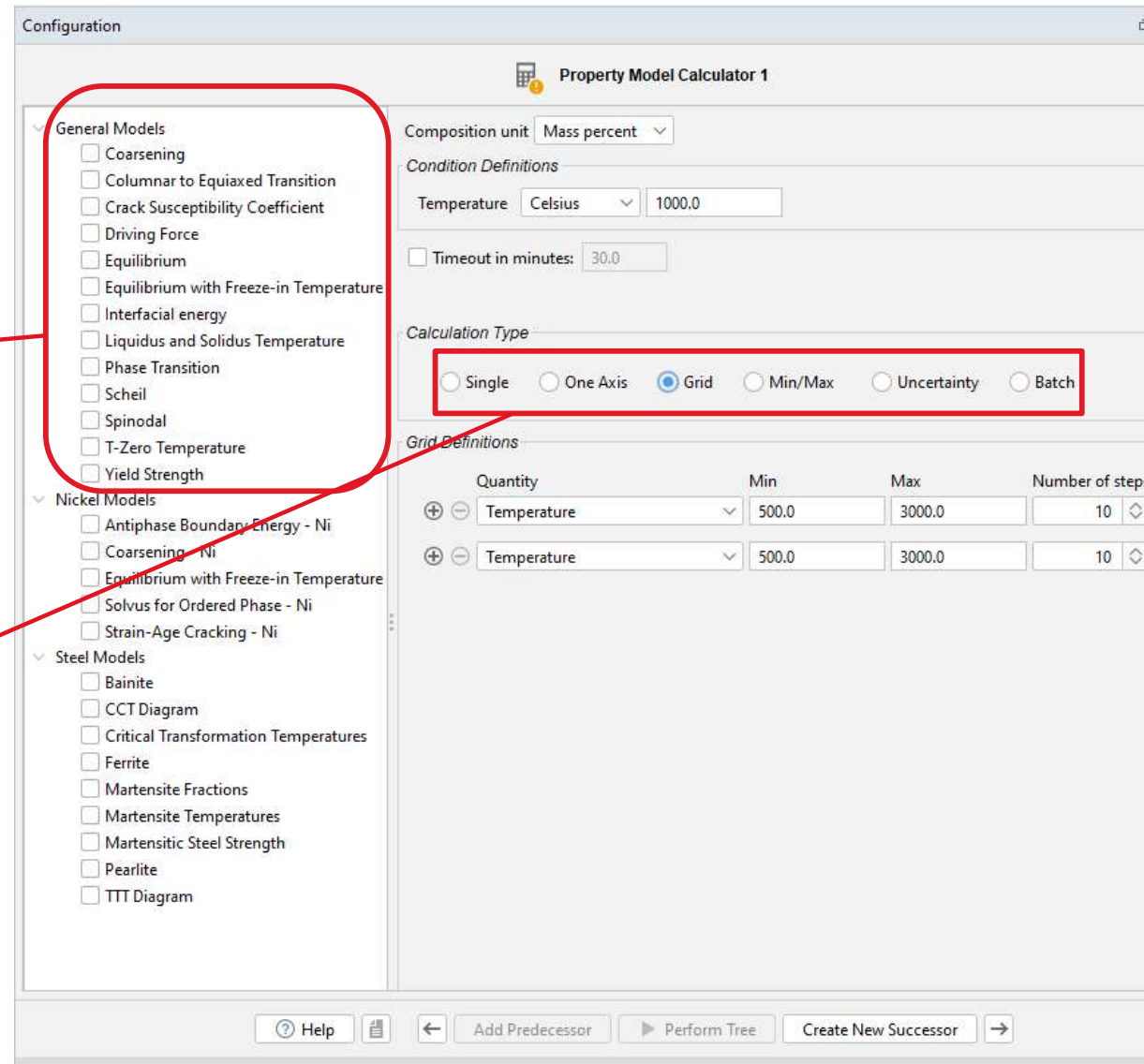
set-interact
```

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.



Variation of A1 over a composition range

Composition of this steel:

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

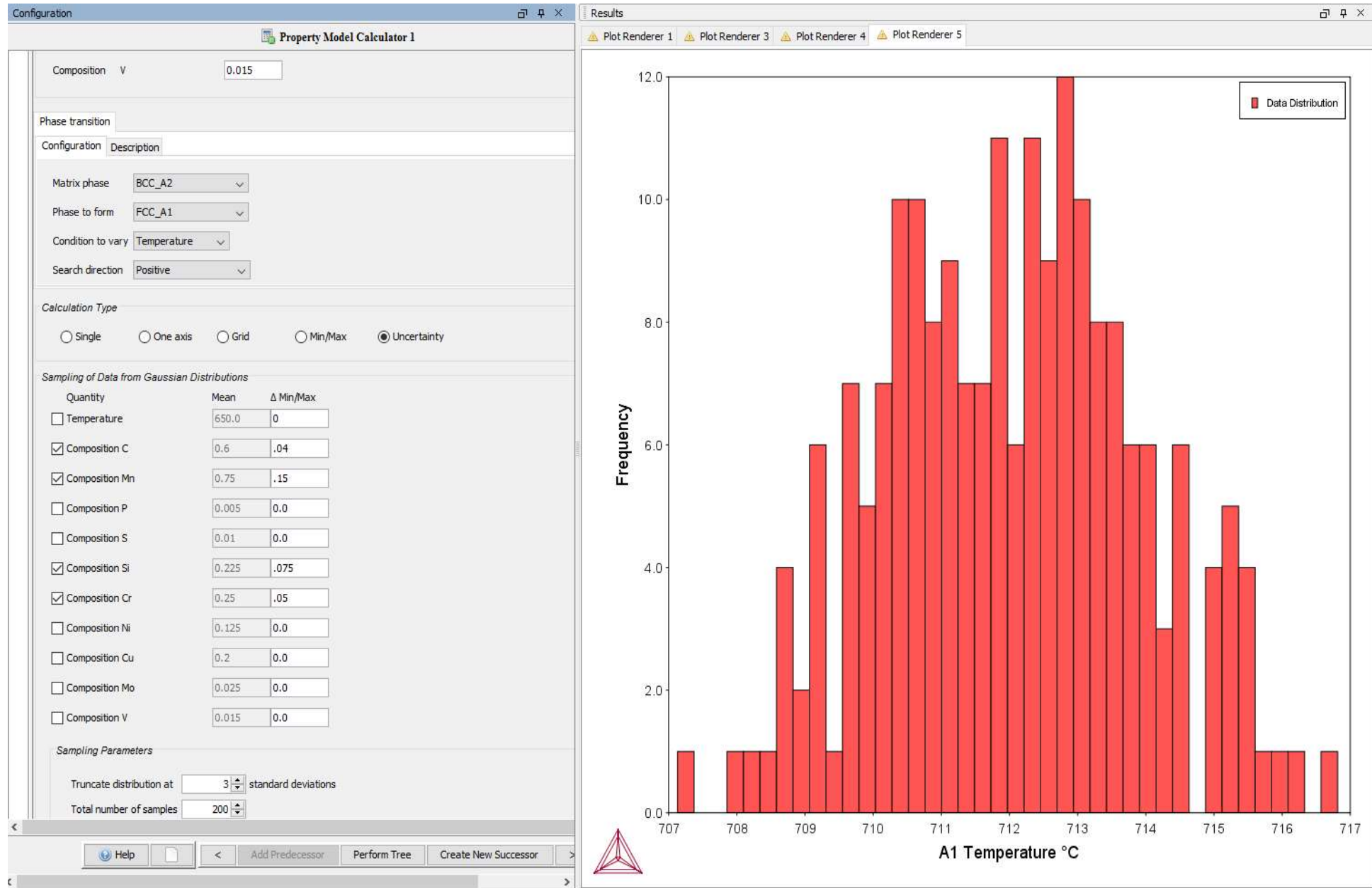
200 random samples, where
4 elements were varied:

C Mn Si Cr

The other elements were
constant at their nominal
composition.

<input type="checkbox"/> Temperature	650.0	0
<input checked="" type="checkbox"/> Composition C	0.6	.04
<input checked="" type="checkbox"/> Composition Mn	0.75	.15
<input type="checkbox"/> Composition P	0.005	0.0
<input type="checkbox"/> Composition S	0.01	0.0
<input checked="" type="checkbox"/> Composition Si	0.225	.075
<input checked="" type="checkbox"/> Composition Cr	0.25	.05
<input type="checkbox"/> Composition Ni	0.125	0.0
<input type="checkbox"/> Composition Cu	0.2	0.0
<input type="checkbox"/> Composition Mo	0.025	0.0
<input type="checkbox"/> Composition V	0.015	0.0

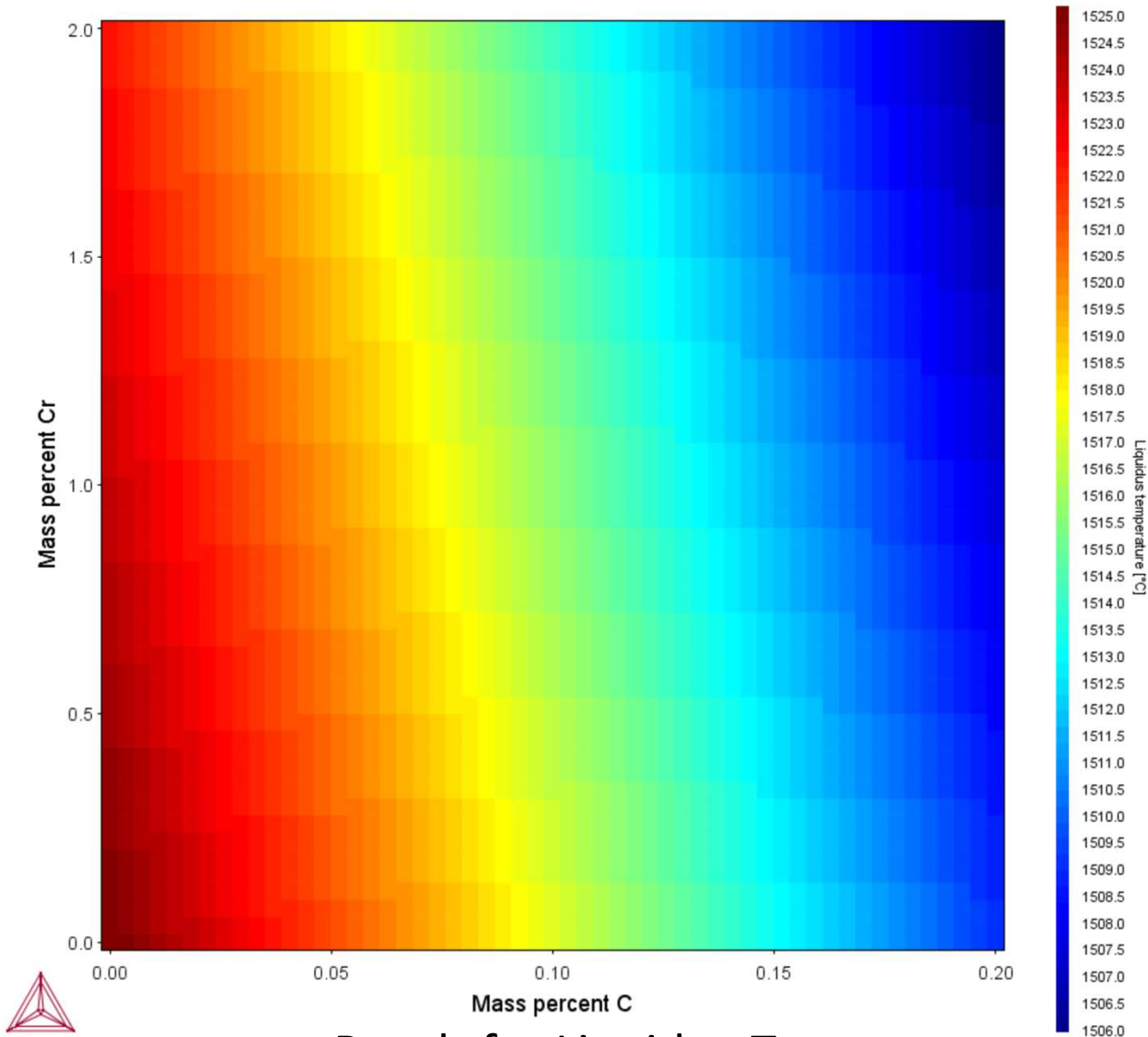
Variation of A1 over a composition range - result



Property Model Calculator result – Liquidus/(Solidus)

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

2020.10.16.08.35.43



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.

General Models

- Coarsening
- Crack Susceptibility Coefficient
- Driving Force
- Equilibrium
- Equilibrium with Freeze-in Temperature

Material

Material name: UNS_A94032

Amount: Mass percent

Al	85.0
Si	12.2
Mg	1.0
Ni	0.9
Cu	0.9

Composition unit: Mass percent

Condition Definitions

Temperature: Celsius, 20

Composition: Al 85.0, Si 12.2, Mg 1.0, Ni 0.9, Cu 0.9

Timeout in minutes: 30.0

Equilibrium with Freeze-in Temperature

Configuration	Description
Freeze-in-temperature	350.0
Equilibrium above freeze-in temperature	<input checked="" type="checkbox"/>
Evaluate for a single phase only	<input type="checkbox"/>
Equilibrium minimization strategy	Global minimization only
Homogenization function	Inverse rule of mixtures (lower Wiener bound)
Account for phase interface scattering	<input type="checkbox"/>
Set reference temperature for technical CTE	20.0
Define user functions	<input type="checkbox"/>

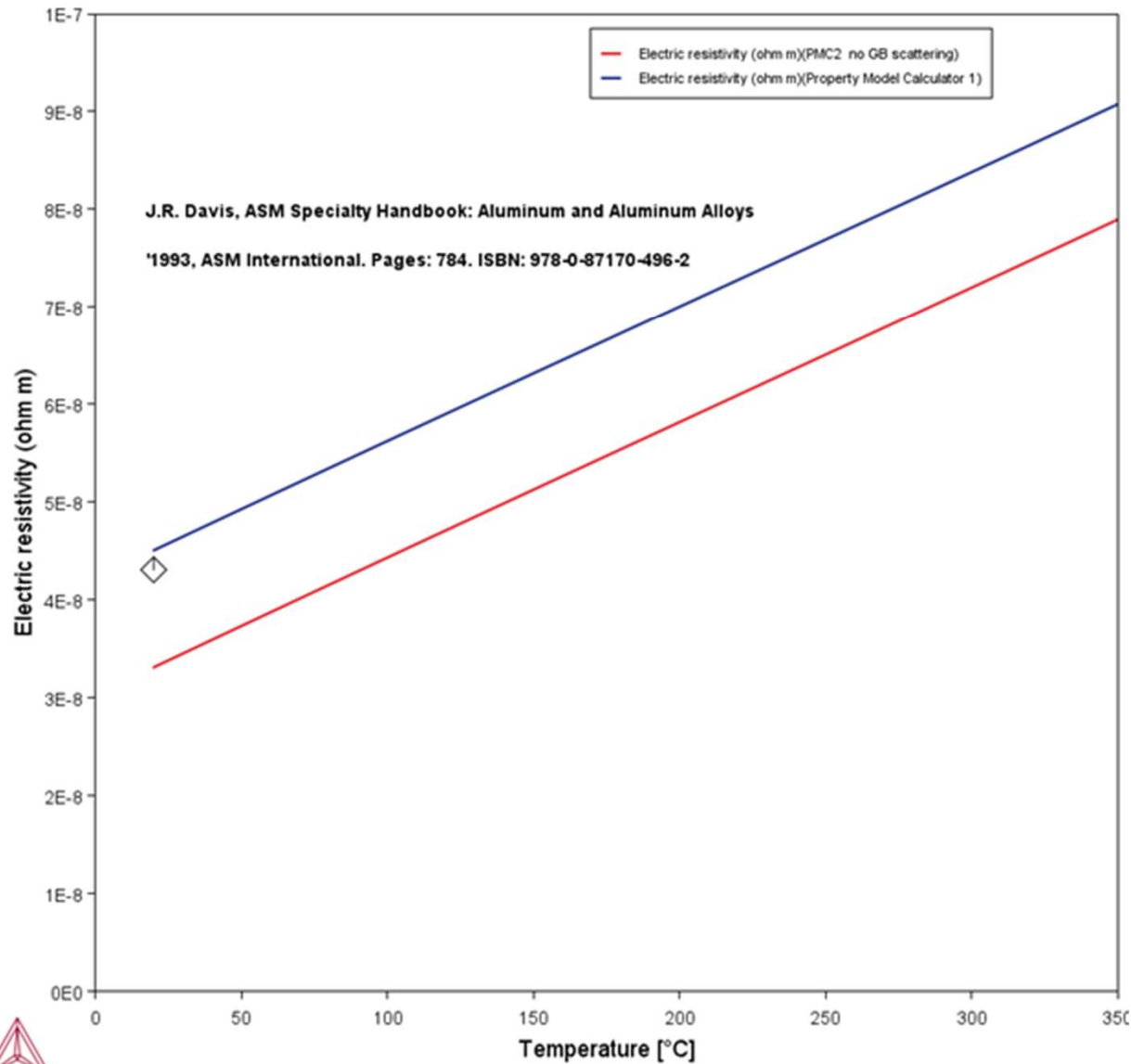
Calculation Type

Single One Axis Grid Min/Max Uncertainty Batch

Grid Definitions

Quantity	Min	Max	Number of steps
Temperature	20.0	350.0	30

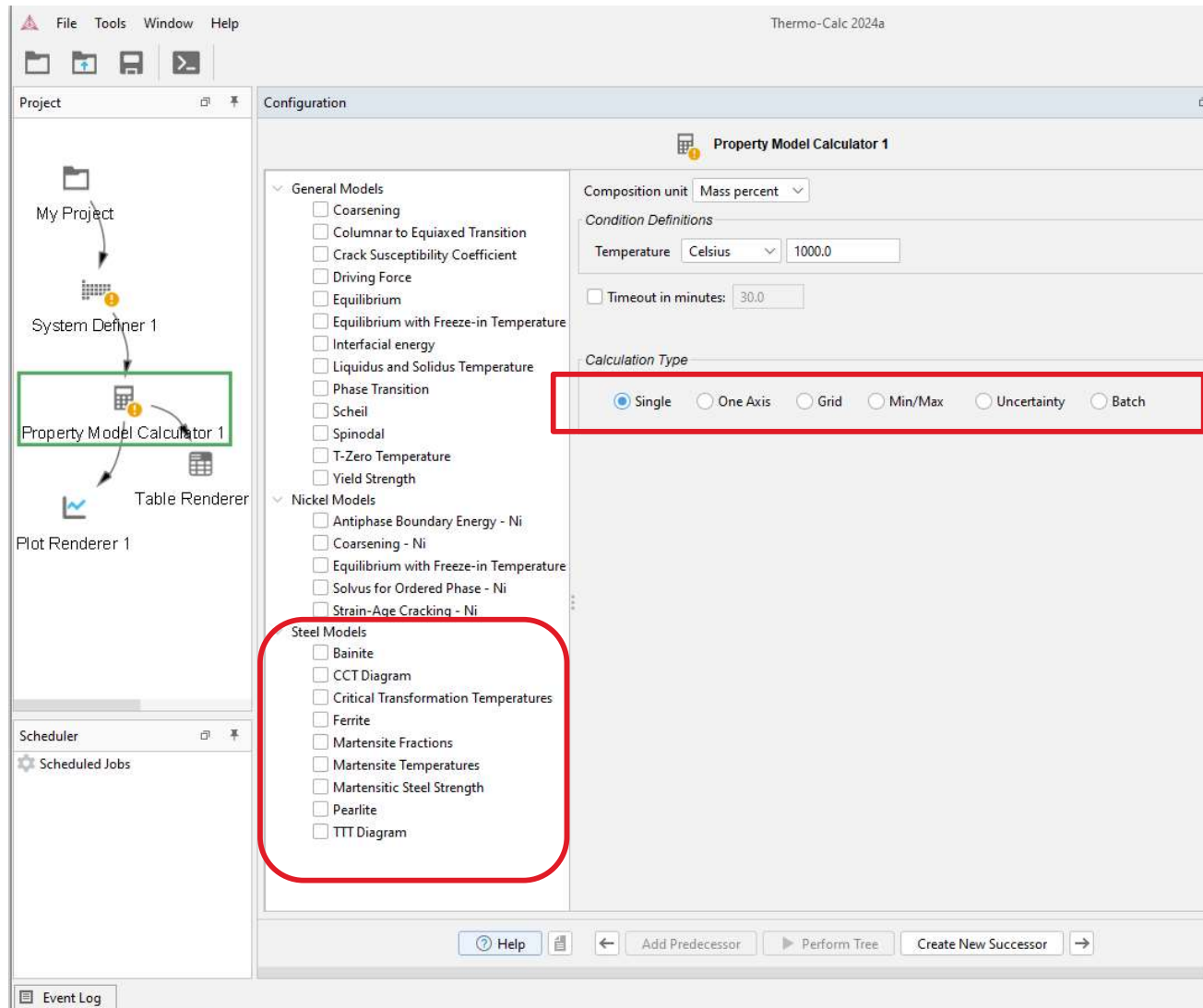
Property Model Calculator result – Electrical resistivity, freeze-in



Steel Model Library

Steel Model Library

- ❑ Advanced models for formation of structures in steel.
- ❑ Introduced in 2019, 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.



The screenshot displays the Thermo-Calc 2024a software interface. The main window is titled "Property Model Calculator 1". The left sidebar shows a project tree with "My Project" containing "System Definer 1", "Property Model Calculator 1", and "Table Renderer". The "Property Model Calculator 1" node is highlighted with a green box. The main configuration area is divided into several sections:

- General Models:** A list of checkboxes for various models including 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, and Yield Strength.
- Nickel Models:** A list of checkboxes for models like Antiphase Boundary Energy - Ni, Coarsening - Ni, Equilibrium with Freeze-in Temperature, Solvus for Ordered Phase - Ni, and Strain-Age Cracking - Ni.
- Steel Models:** A list of checkboxes for models including Bainite, CCT Diagram, Critical Transformation Temperatures, Ferrite, Martensite Fractions, Martensite Temperatures, Martensitic Steel Strength, Pearlite, and TTT Diagram. This section is highlighted with a red rounded rectangle.

On the right side of the configuration window, there are settings for "Composition unit" (Mass percent), "Condition Definitions" (Temperature: Celsius, 1000.0), and "Timeout in minutes" (30.0). The "Calculation Type" section at the bottom right is highlighted with a red rectangle and contains radio buttons for "Single" (selected), "One Axis", "Grid", "Min/Max", "Uncertainty", and "Batch".

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

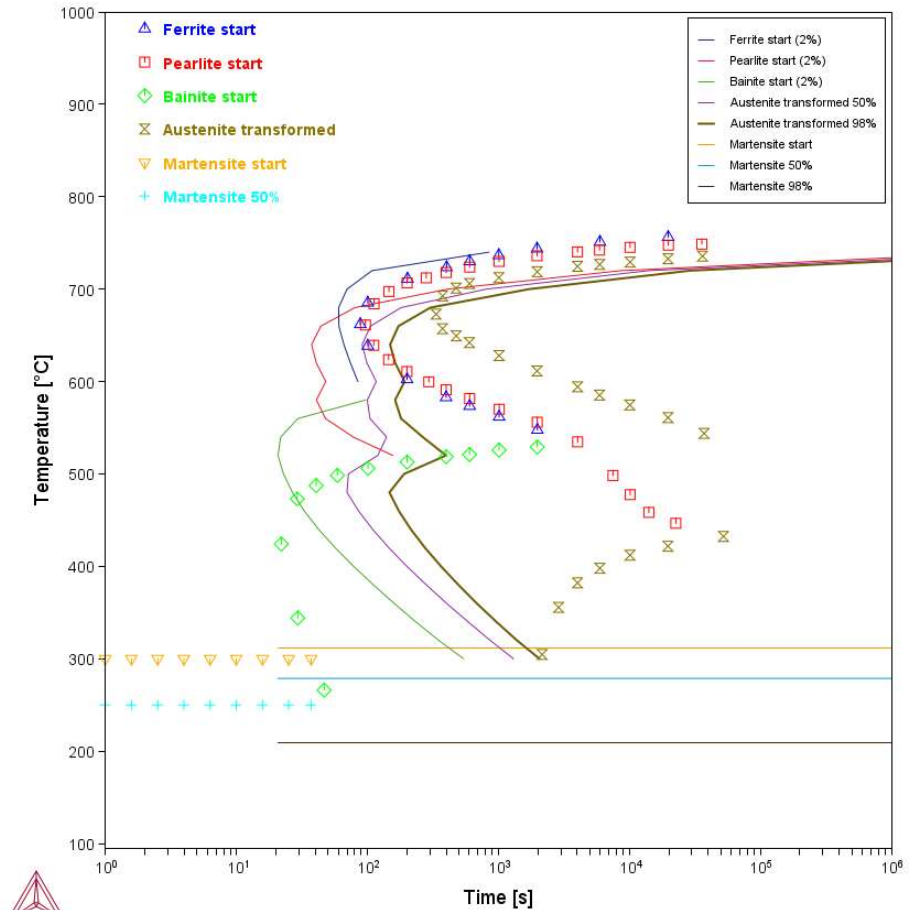
Timeout in minutes: 30.0

TTT Diagram

Configuration	Description
Austenite composition from	Equilibrium composition at austenizing temperature
Austenizing temperature	1050.0
Grain size [um]	89.8
Calculation setting	Custom
Ferrite selected	<input checked="" type="checkbox"/>
Pearlite selected	<input checked="" type="checkbox"/>
Bainite selected	<input checked="" type="checkbox"/>
Martensite selected	<input checked="" type="checkbox"/>
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	<input checked="" type="checkbox"/>
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

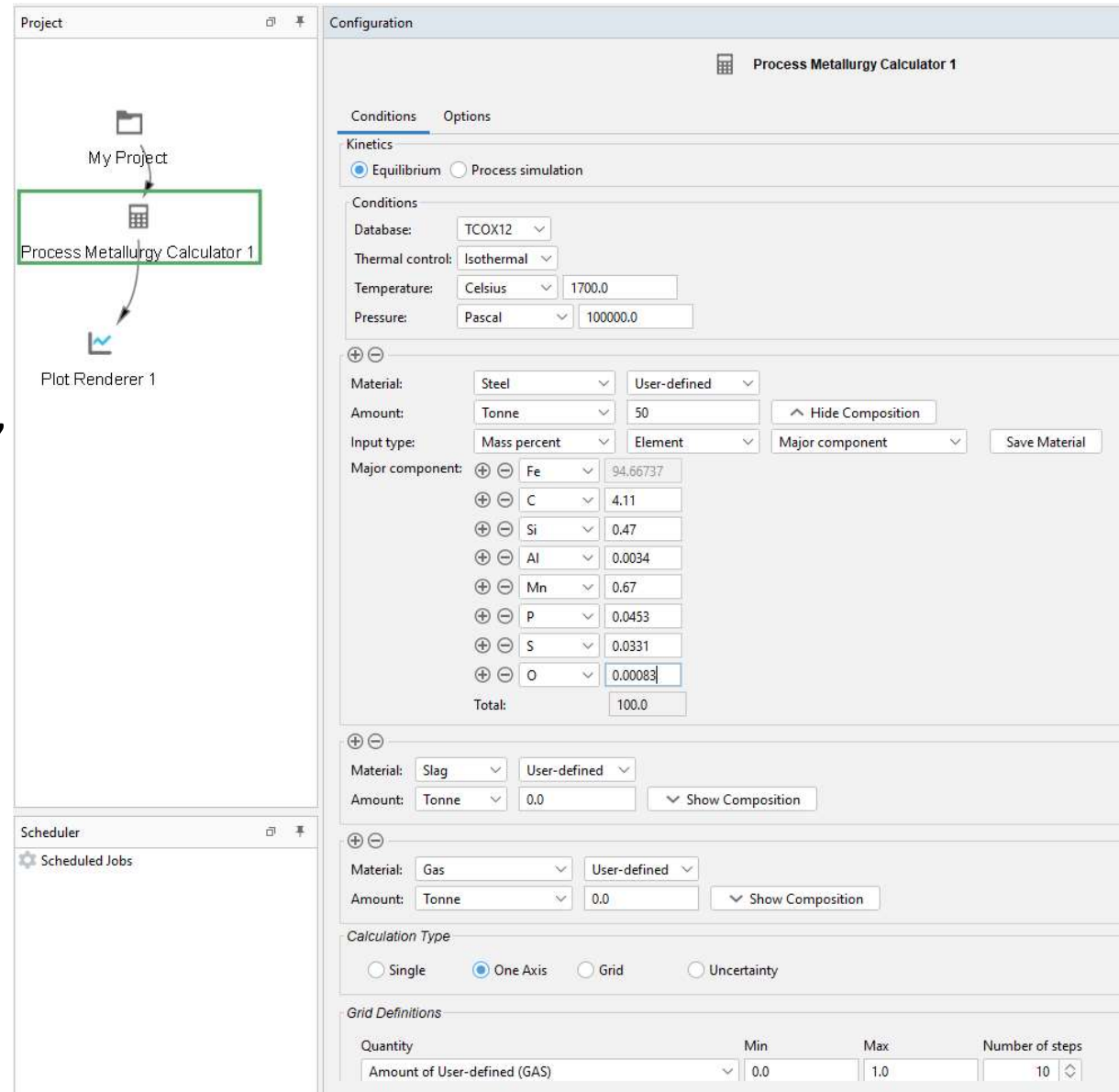
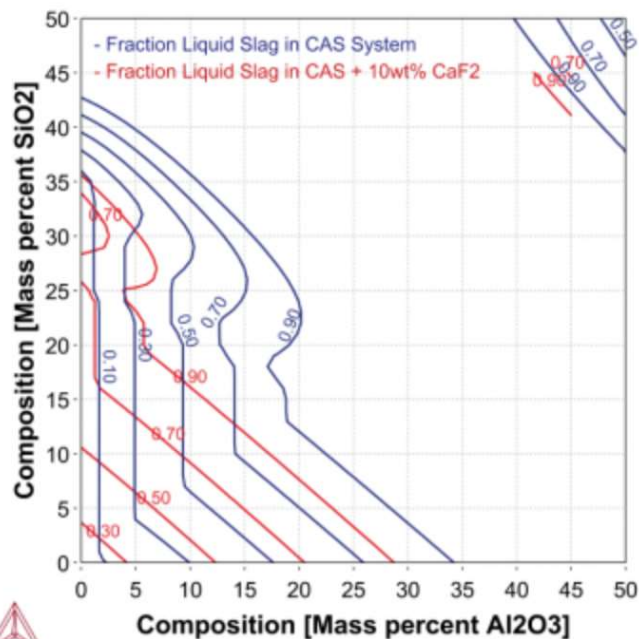
Single
 One axis
 Grid
 Min/Max
 Uncertainty
 Batch



Process Metallurgy Module

Process Metallurgy Module (PMM)

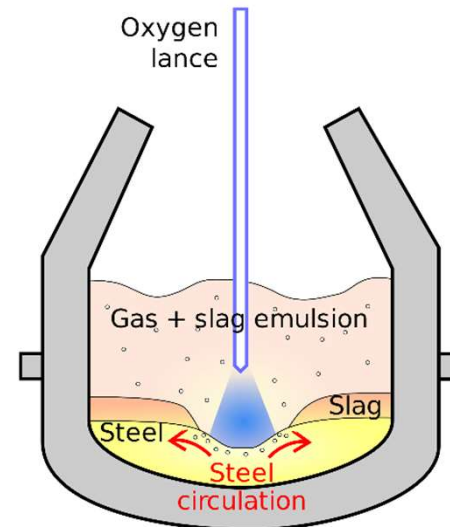
- ❑ Module for easy set-up of Steel-Slag-Gas equilibria.
- ❑ New in 2019.
- ❑ Designed for steel making and steel refining processes, BOF, EAF, LF and more.



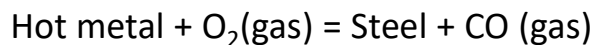
The screenshot displays the Thermo-Calc software interface. The 'Project' window shows a tree view with 'My Project' containing 'Process Metallurgy Calculator 1' and 'Plot Renderer 1'. The 'Configuration' window is open, showing settings for 'Process Metallurgy Calculator 1'. The 'Conditions' tab is active, with 'Equilibrium' selected under 'Kinetics'. The 'Conditions' section includes: Database: TCOX12, Thermal control: Isothermal, Temperature: Celsius, 1700.0, Pressure: Pascal, 100000.0. The 'Major component' list includes Fe (94.66737), C (4.11), Si (0.47), Al (0.0034), Mn (0.67), P (0.0453), S (0.0331), and O (0.00083). The 'Material' section shows 'Steel' and 'User-defined' material types with 'Tonne' and '50' amount. The 'Slag' section shows 'Slag' and 'User-defined' material types with 'Tonne' and '0.0' amount. The 'Gas' section shows 'Gas' and 'User-defined' material types with 'Tonne' and '0.0' amount. The 'Calculation Type' section has 'One Axis' selected. The 'Grid Definitions' section shows 'Amount of User-defined (GAS)' with Min: 0.0, Max: 1.0, and Number of steps: 10.

PMM Example

Calculation of decarburization (steelmaking)

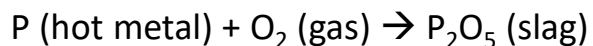


The hot metal from a blast furnace contains about 4.5 wt% Carbon. This makes it brittle and unsuitable for forging and rolling. The carbon content therefore needs to be reduced. This is termed steel-making and is mostly carried out in a converter (basic oxygen furnace, BOF) by blowing oxygen into the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

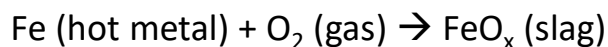


This reaction is highly exothermic and results in a temperature increase in the converter from $\sim 1450^\circ\text{C}$ to over 1650°C .

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

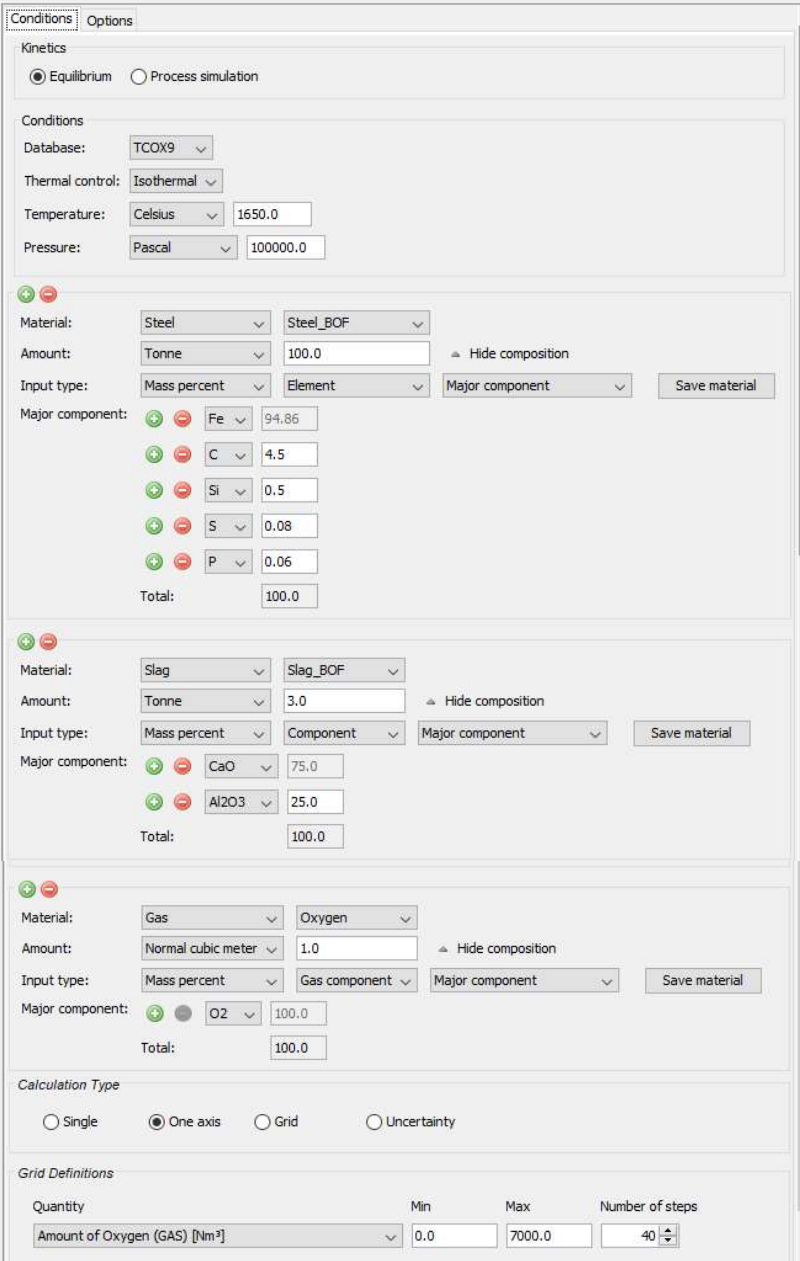


Other oxidation reactions are not desirable, such as the oxidation of the iron itself, that results in a reduced yield of the process:



PMM Example 1

Calculation of decarburization EQUILIBRIUM



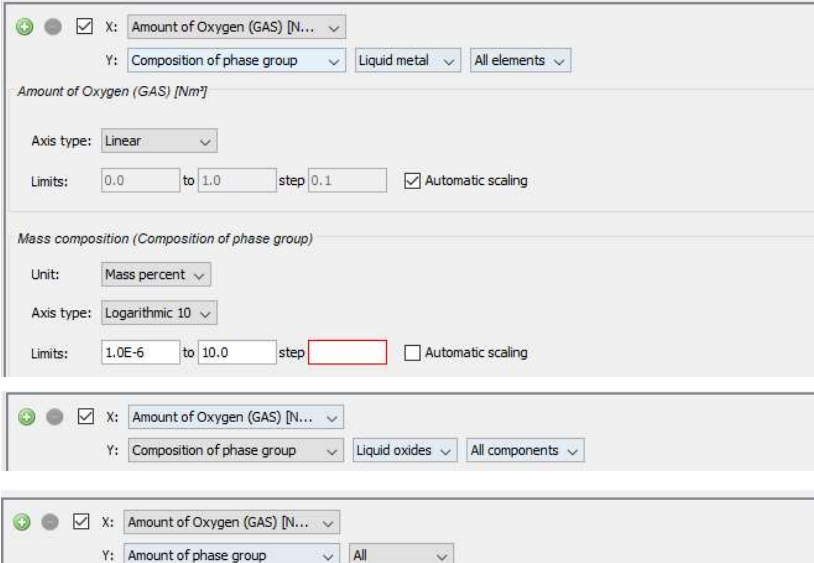
The screenshot shows the 'Conditions' and 'Options' tabs of the Thermo-Calc software. The 'Equilibrium' radio button is selected under 'Kinetics'. The 'Database' is set to 'TCOx9'. 'Thermal control' is 'Isothermal', 'Temperature' is 'Celsius' at '1650.0', and 'Pressure' is 'Pascal' at '100000.0'. There are three material definitions: 1) 'Steel' (Steel_BOF) with 100.0 Tonne, composed of Fe (94.86%), C (4.5%), Si (0.5%), S (0.08%), and P (0.06%). 2) 'Slag' (Slag_BOF) with 3.0 Tonne, composed of CaO (75.0%) and Al2O3 (25.0%). 3) 'Gas' (Oxygen) with 1.0 Normal cubic meter, composed of O2 (100.0%). The 'Calculation Type' is set to 'One axis'. The 'Grid Definitions' table is as follows:

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:



The three screenshots show different plot configurations:

- Plot 1: X-axis: Amount of Oxygen (GAS) [Nm³], Y-axis: Composition of phase group (Liquid metal), All elements. Axis type: Linear. Limits: 0.0 to 1.0, step 0.1. Automatic scaling is checked.
- Plot 2: X-axis: Amount of Oxygen (GAS) [Nm³], Y-axis: Composition of phase group (Liquid oxides), All components. Unit: Mass percent. Axis type: Logarithmic 10. Limits: 1.0E-6 to 10.0, step [red box]. Automatic scaling is unchecked.
- Plot 3: X-axis: Amount of Oxygen (GAS) [Nm³], Y-axis: Amount of phase group, All.

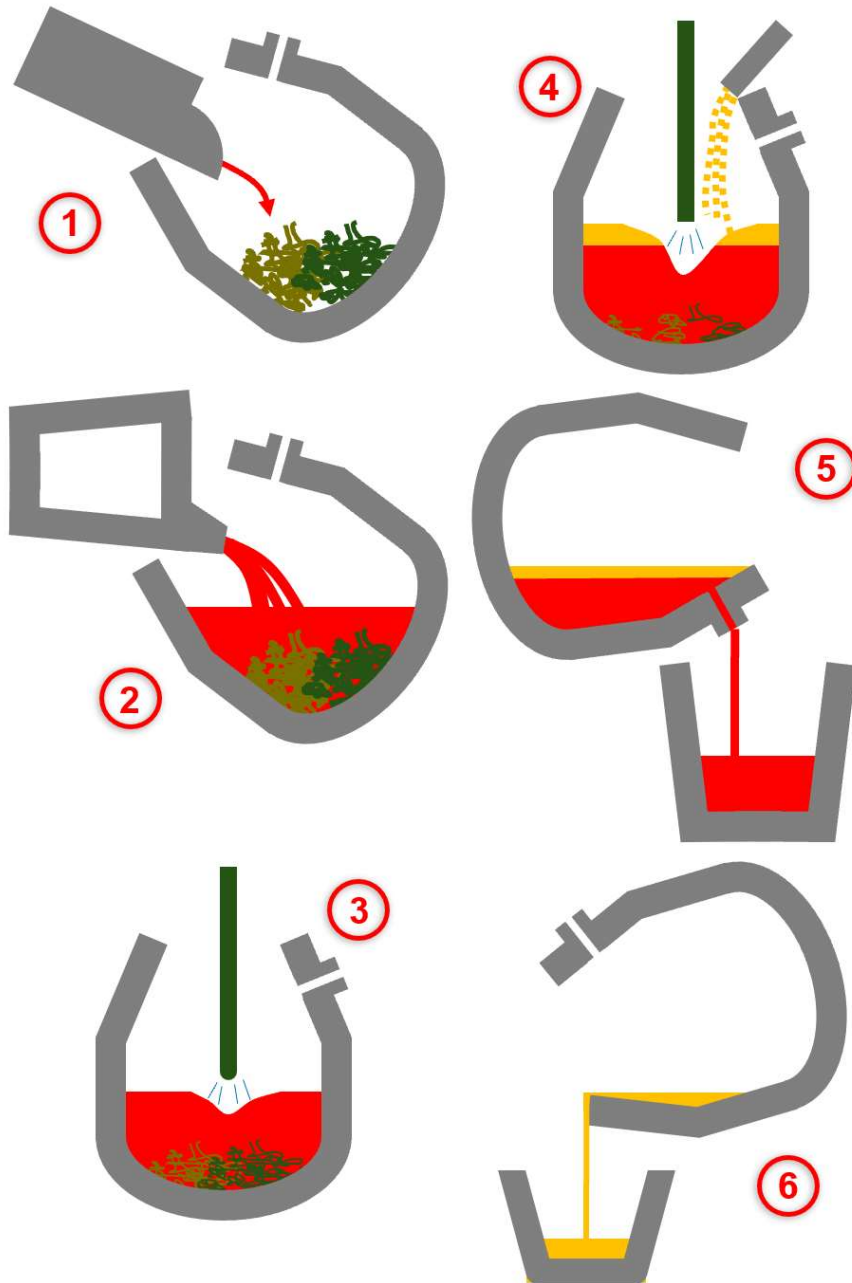
or
or

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



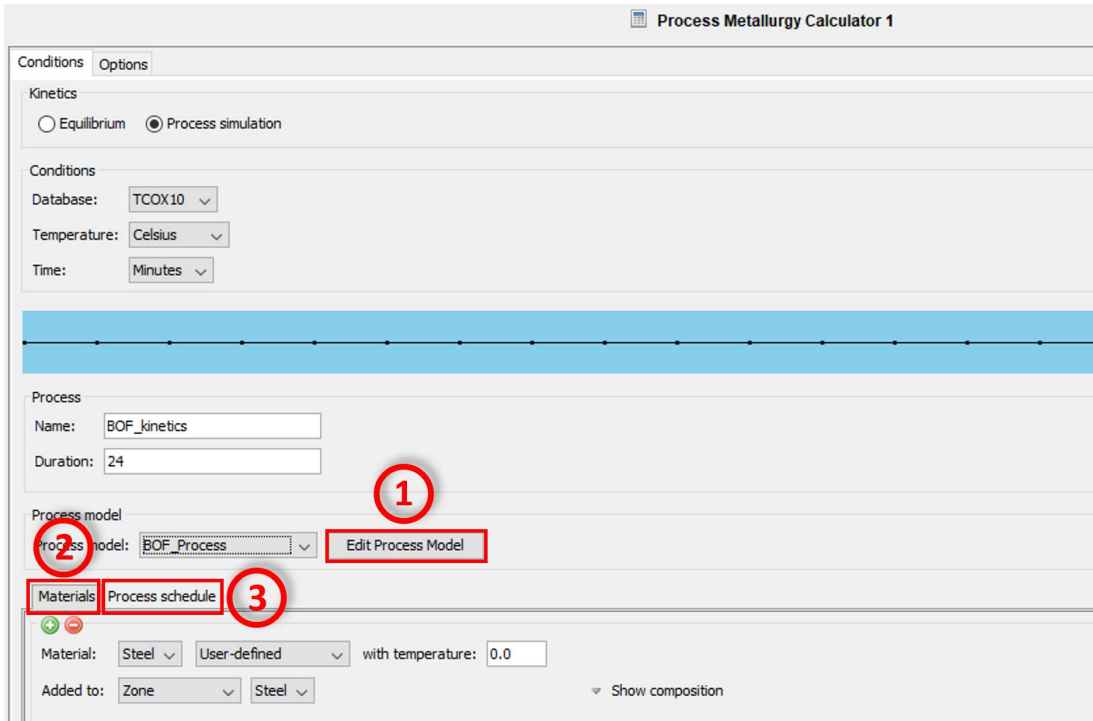
Setting up equilibrium calculation

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

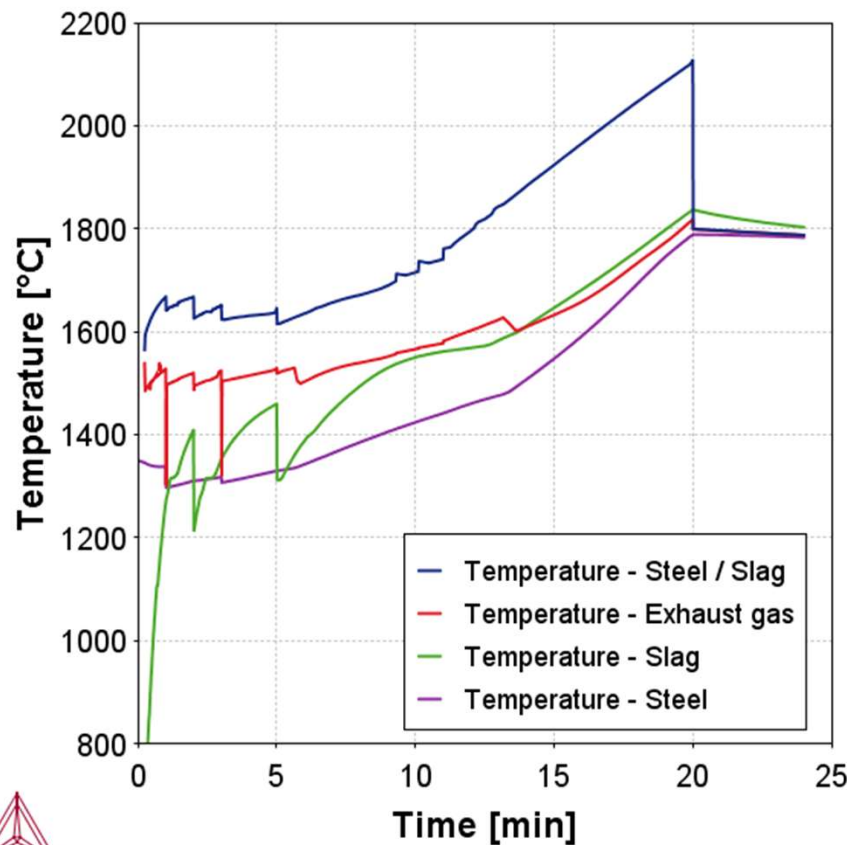
Note: Calculation times for a full process simulation can be 30 min or more

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

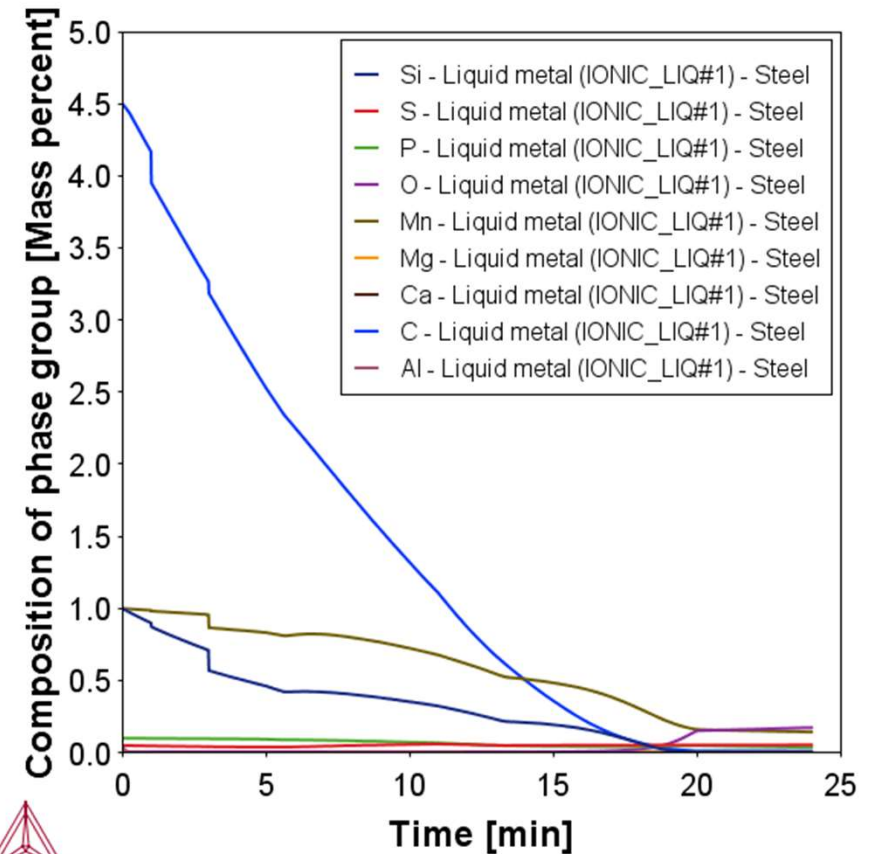
PMM Example 2

Calculation of decarburization PROCESS SIMULATION

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.



You are here: [Thermo-Calc](#) > Welcome



Welcome to the Thermo-Calc Help

This help contains the same documentation that is also installed in folders with your software. The advantage is you can browse the menus and search for key words and phrases. Click the links below to learn about navigating the help and how to contact our offices.



When in Thermo-Calc, press <F1> on the keyboard to open this help. You can also open the documentation folder (which has all the PDFs) from the main menu in Thermo-Calc: **Help → Manuals Folder.**

- [Search](#)
- [Browse](#)
- [Software Updates](#)
- [Training and Contact Information](#)
- Get started with [About the Thermo-Calc Software](#)



There are several resources available on our website to help you learn how to use Thermo-Calc and other Add-on Modules. Go to the [Getting Started Guides](#) page and choose one of the guides that provides new users an introduction to setting up simple calculations in Graphical Mode. The information there is also in this help documentation.

Thermo-Calc

Welcome

- Search
- Browse
- Software Updates
- Training and Contact Information
- Introduction
- Graphical Mode
- Console Mode
- General Reference
- Installation

The Online Help

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



Thermo-Calc Diffusion Module (DICTRA) Precipitation Module (TC-PRISMA) Databases SDKs

Search 

You are here: [Thermo-Calc](#) > [Console Mode](#) > [Working in Console Mode](#) > 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		In(Activity)	Component	R
	LNAC (sp,ph) ²			Species relative to a solution phase	R

Thermodynamic Variables

Intensive Variables

Extensive Variables

Special Quantities

The u-Fraction Variable

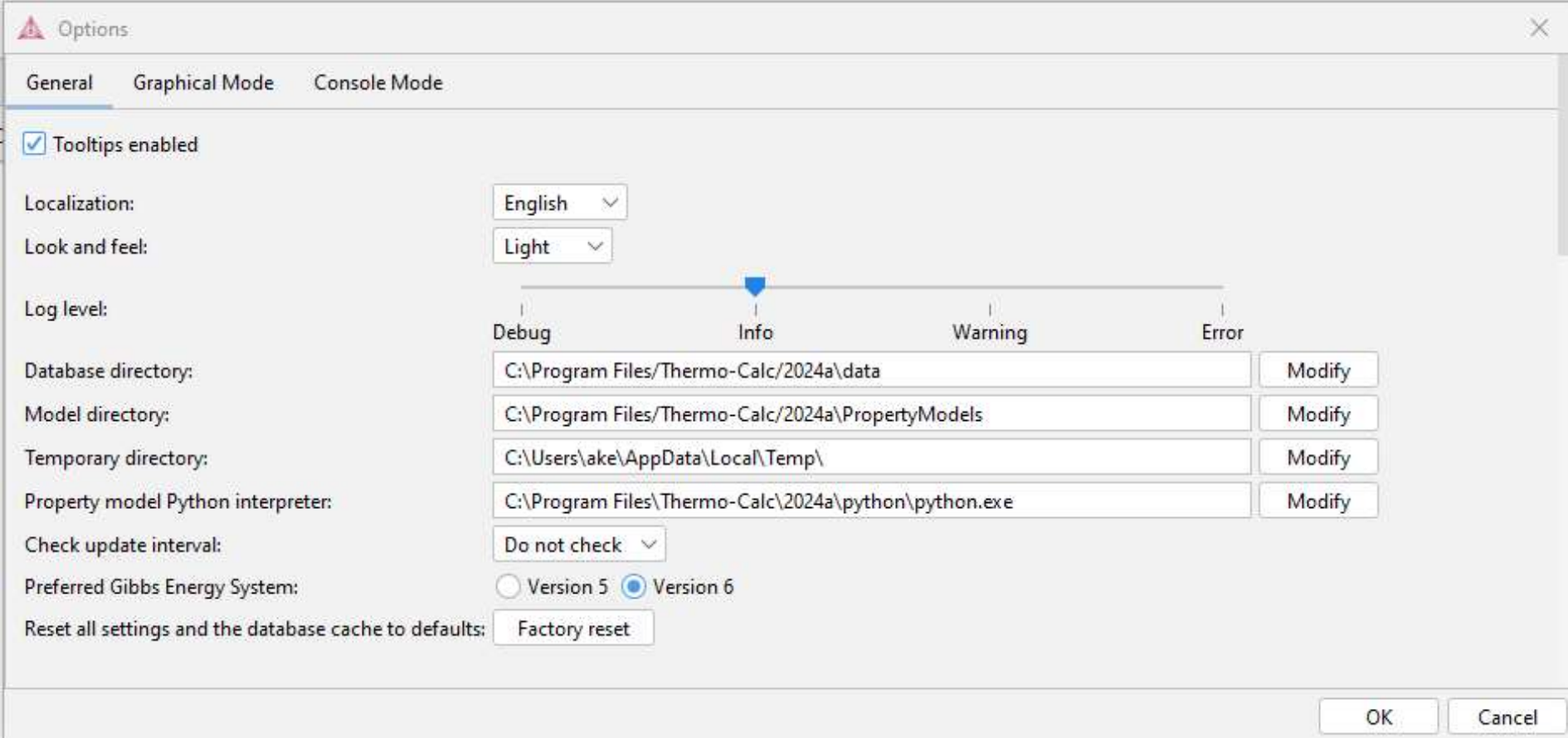
Suffixes

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)

Tools -> Options

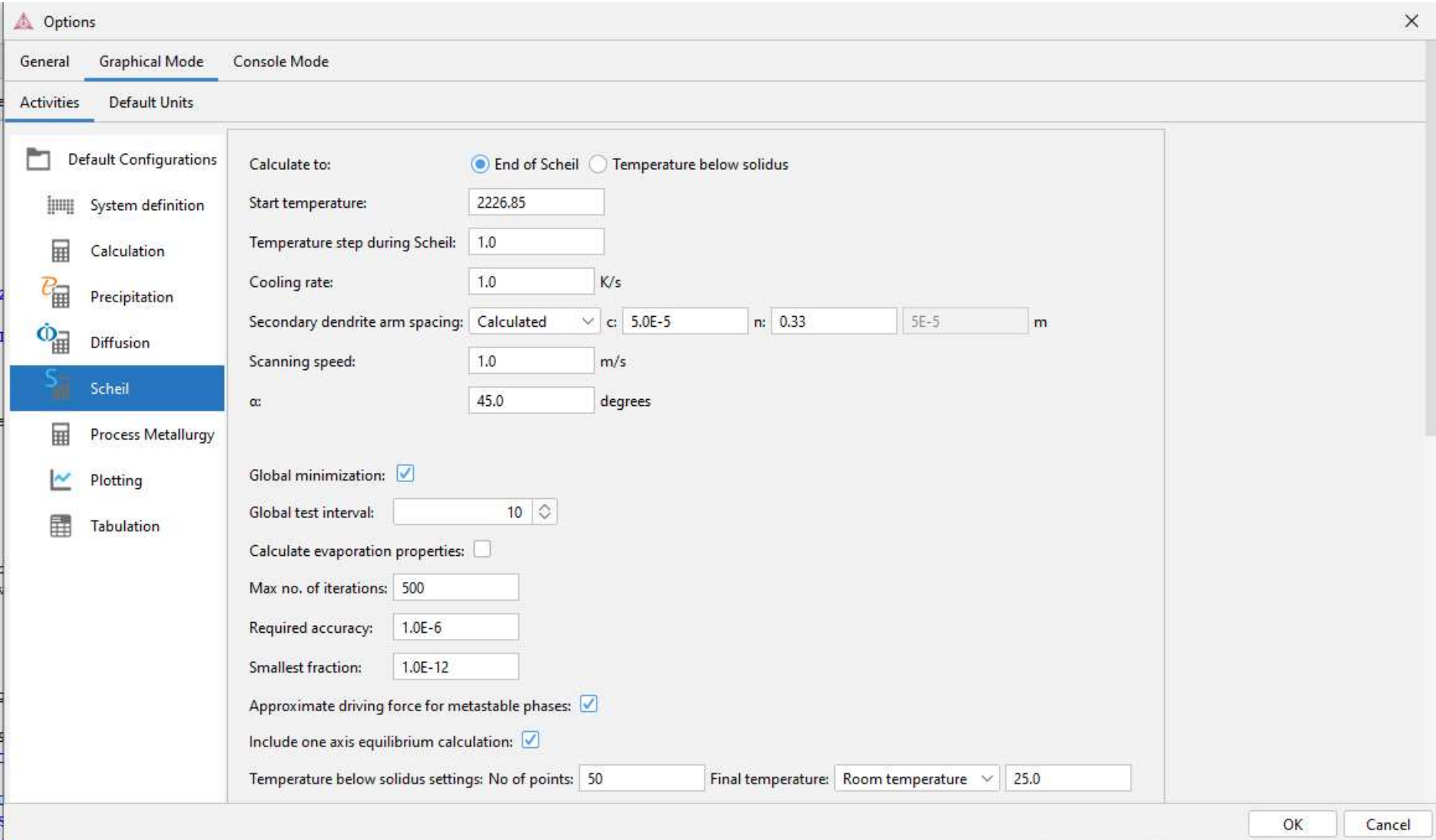


The screenshot shows the 'Options' dialog box with the 'General' tab selected. The dialog has a title bar with a warning icon and the text 'Options'. Below the title bar are three tabs: 'General', 'Graphical Mode', and 'Console Mode'. The 'General' tab contains the following settings:

- Tooltips enabled
- Localization: English (dropdown)
- Look and feel: Light (dropdown)
- Log level: Info (slider between Debug and Error)
- Database directory: C:\Program Files\Thermo-Calc\2024a\data (Modify)
- Model directory: C:\Program Files\Thermo-Calc\2024a\PropertyModels (Modify)
- Temporary directory: C:\Users\ake\AppData\Local\Temp\ (Modify)
- Property model Python interpreter: C:\Program Files\Thermo-Calc\2024a\python\python.exe (Modify)
- Check update interval: Do not check (dropdown)
- Preferred Gibbs Energy System: Version 5 Version 6
- Reset all settings and the database cache to defaults: Factory reset (button)

At the bottom right of the dialog are 'OK' and 'Cancel' buttons.

Tools -> Options -> Graphical mode



The screenshot shows the 'Options' dialog box in Thermo-Calc, with the 'Graphical Mode' tab selected. The 'Scheil' option is highlighted in the left-hand navigation pane. The main area contains various settings for the Scheil calculation, including temperature, cooling rate, and dendrite arm spacing.

Options [X]

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

Global minimization:

Global test interval: 10

Calculate evaporation properties:

Max no. of iterations: 500

Required accuracy: 1.0E-6

Smallest fraction: 1.0E-12

Approximate driving force for metastable phases:

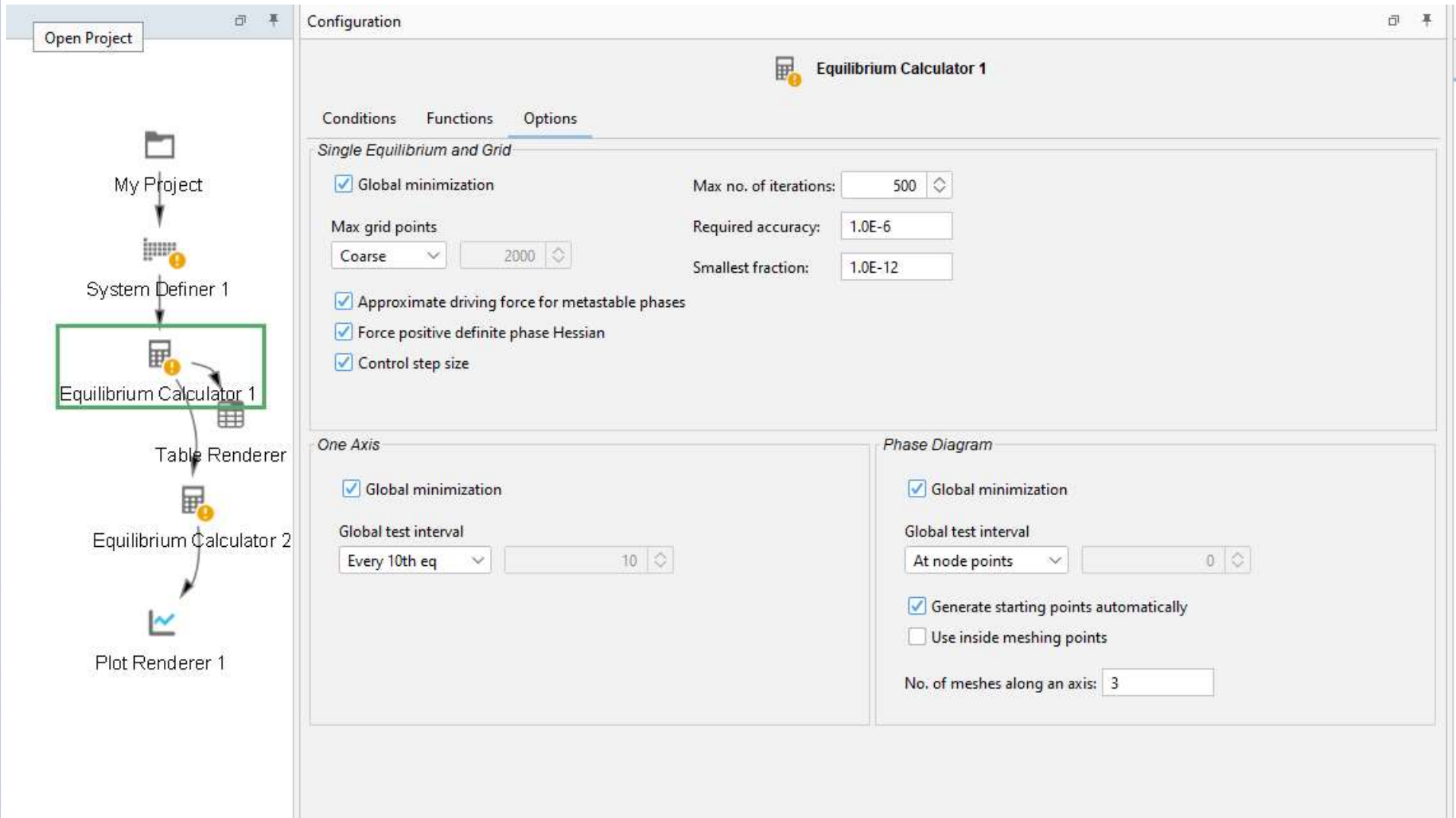
Include one axis equilibrium calculation:

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

OK Cancel

Settings

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



The screenshot displays the Thermo-Calc software interface. On the left, a project workflow diagram shows the sequence: My Project → System Definer 1 → Equilibrium Calculator 1 (highlighted with a green box) → Table Renderer → Equilibrium Calculator 2 → Plot Renderer 1. The main window is titled "Configuration" and shows the settings for "Equilibrium Calculator 1". The "Options" tab is selected, and the settings are organized into three sections:

- Single Equilibrium and Grid**
 - Global minimization
 - Max no. of iterations: 500
 - Max grid points: Coarse (dropdown), 2000
 - 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
- Phase Diagram**
 - Global minimization
 - Global test interval: At node points (dropdown), 0
 - Generate starting points automatically
 - Use inside meshing points
 - No. of meshes along an axis: 3

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.