Aalto University
School of Engineering

COE-C2004 - Materials Science and Engineering

Exercise 4

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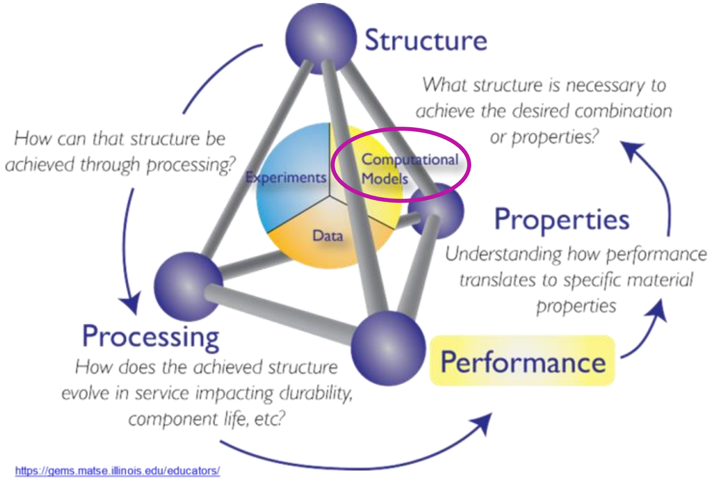
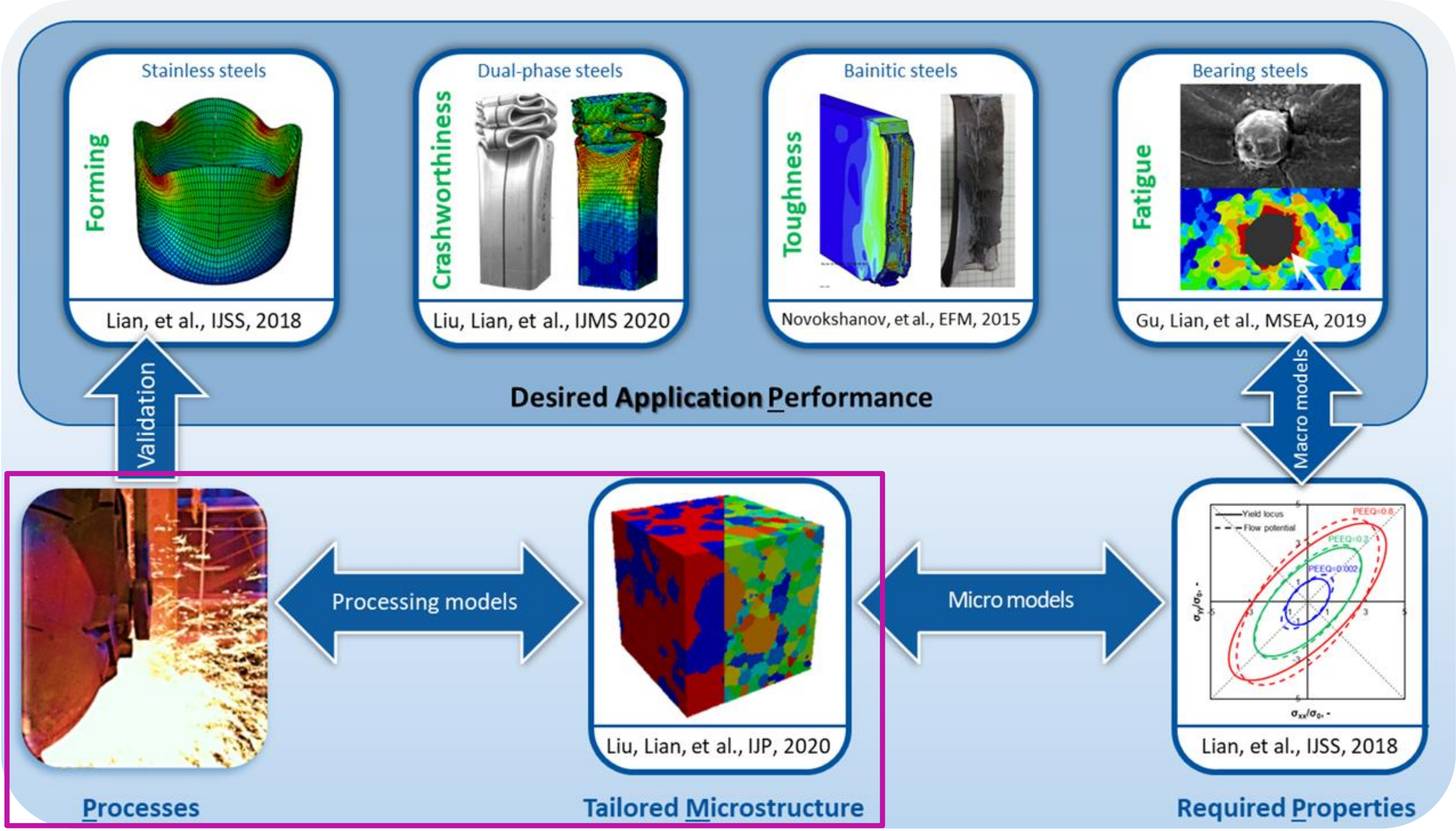
Theerawat Kumnorkaew

Integrated computational materials engineering (ICME)



https://gems.matse.illinois.edu/educators/

Thermo-Calc Software



https://www.researchgate.net/lab/Junhe-Lian-Lab

Thermo-CalC overview

What is Thermo-CalC?

- Software/Database package for thermodynamic calculation
- Originated from Royal Institute of Technology, Stockholm (www.thermocalc.com)

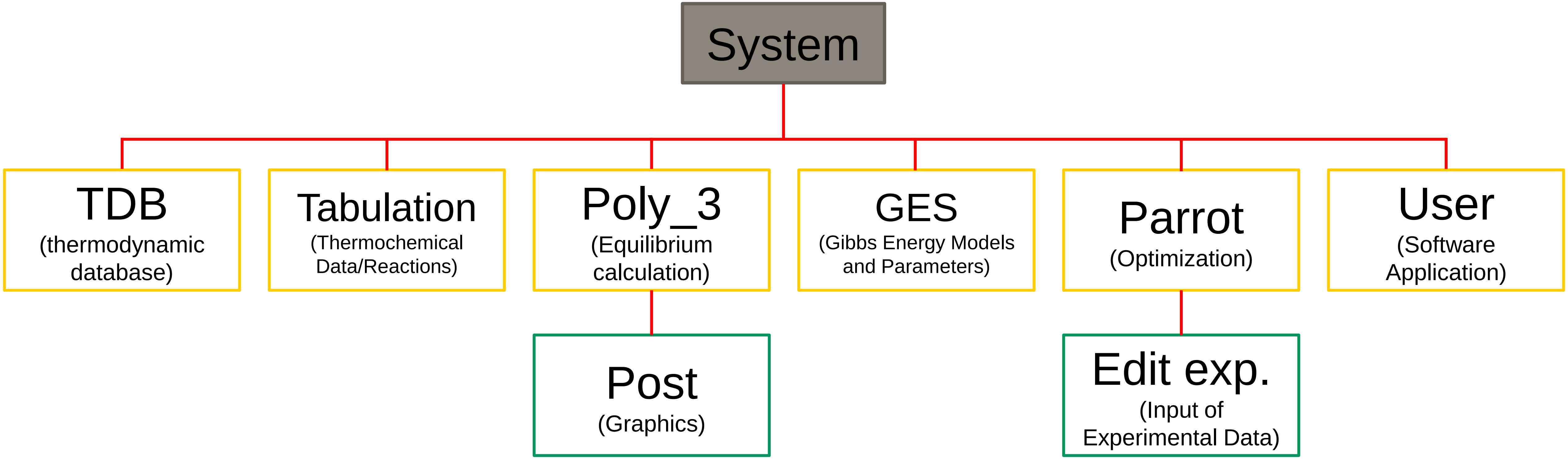
Thermo-CalC overview (cont.)

What can Thermo-CalC do?

- Amounts of phases and their compositions
- Stable and meta-stable heterogeneous phase equilibria
- Thermochemical data such as enthalpies, heat capacity and activity
- Transformation temperatures, such as liquidus and solidus
- Driving force for phase transformations
- Phase diagrams (binary, ternary and multi-component)
- Solidification applying the Scheil-Gulliver model
- Thermodynamic properties of chemical reactions
- ...effect of stress, interfacial energy *etc.*

Applications?
- Material processing
- Material design

The organization of Thermo-calC modules



Definitions Relevant to Thermo-CalC

System: A region (defined in terms of composition, temperature and pressure) of interest that can be closed or open to the exchange of matter, heat and work to its surroundings. In ThermoCalc all equilibrium calculations are performed with the assumption that the system is closed.

Phases: A region in the system that is homogeneous (uniform) and physically distinct and has the same structure and property everywhere.

Equilibrium State: A stable state against internal fluctuations in a number of variables.

Gibbs Phase Rule: States the number of degrees of freedom in a system is equal to the number of components in the system minus the number of stable phases plus 2 (temperature and pressure).

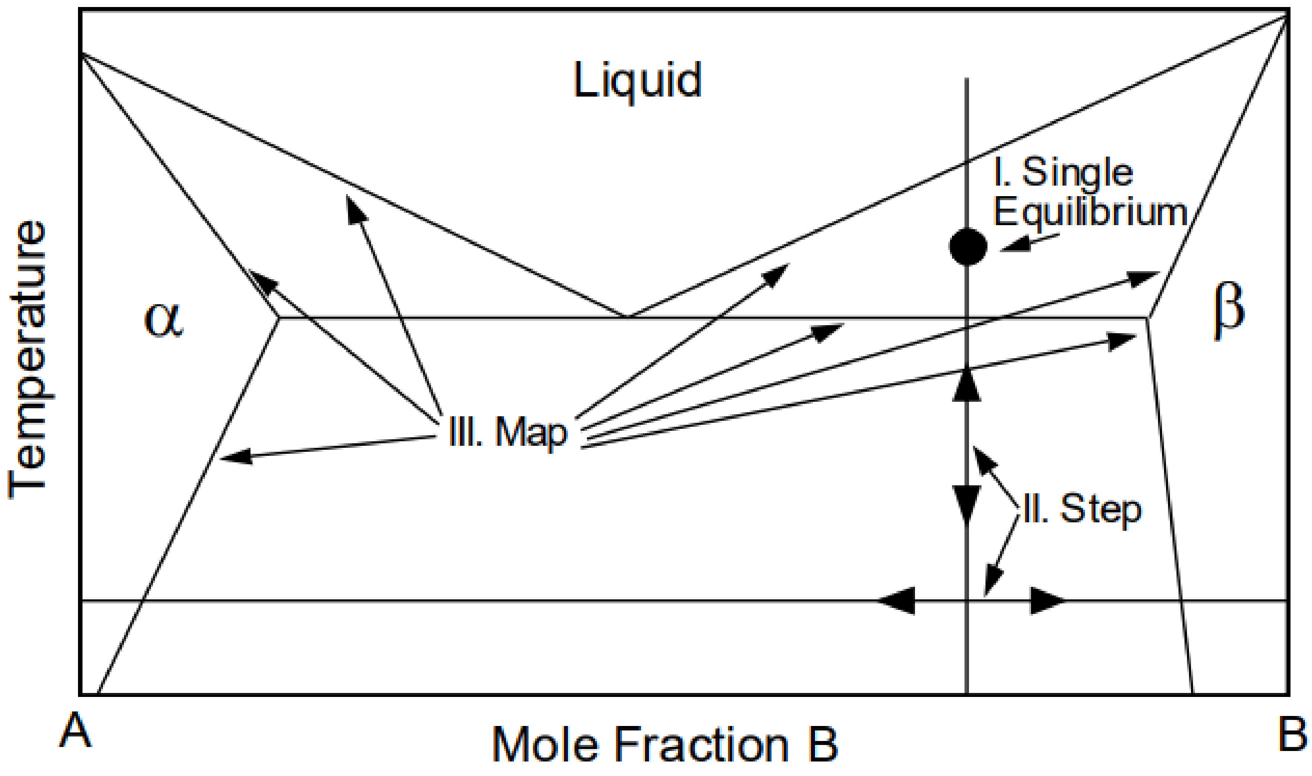
Components: The smallest possible division of matter required to describe a given phase.

Constituents: Determine the composition dependence of the properties of the phase and can reflect additional internal degrees of freedom.

Species: The collection of all constituents for the phases in a given system and can be elements, molecular aggregates, charged or neutral.

Tasks

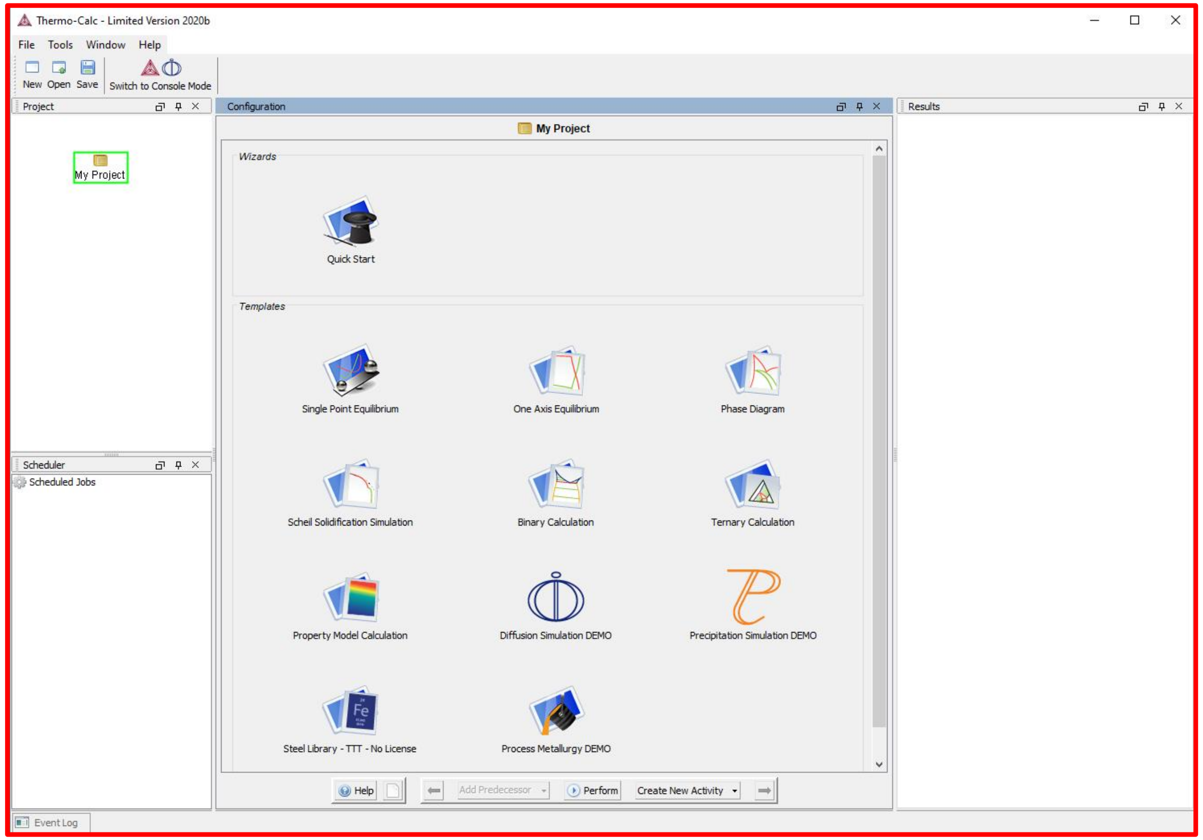
Tasks: Three types of calculations

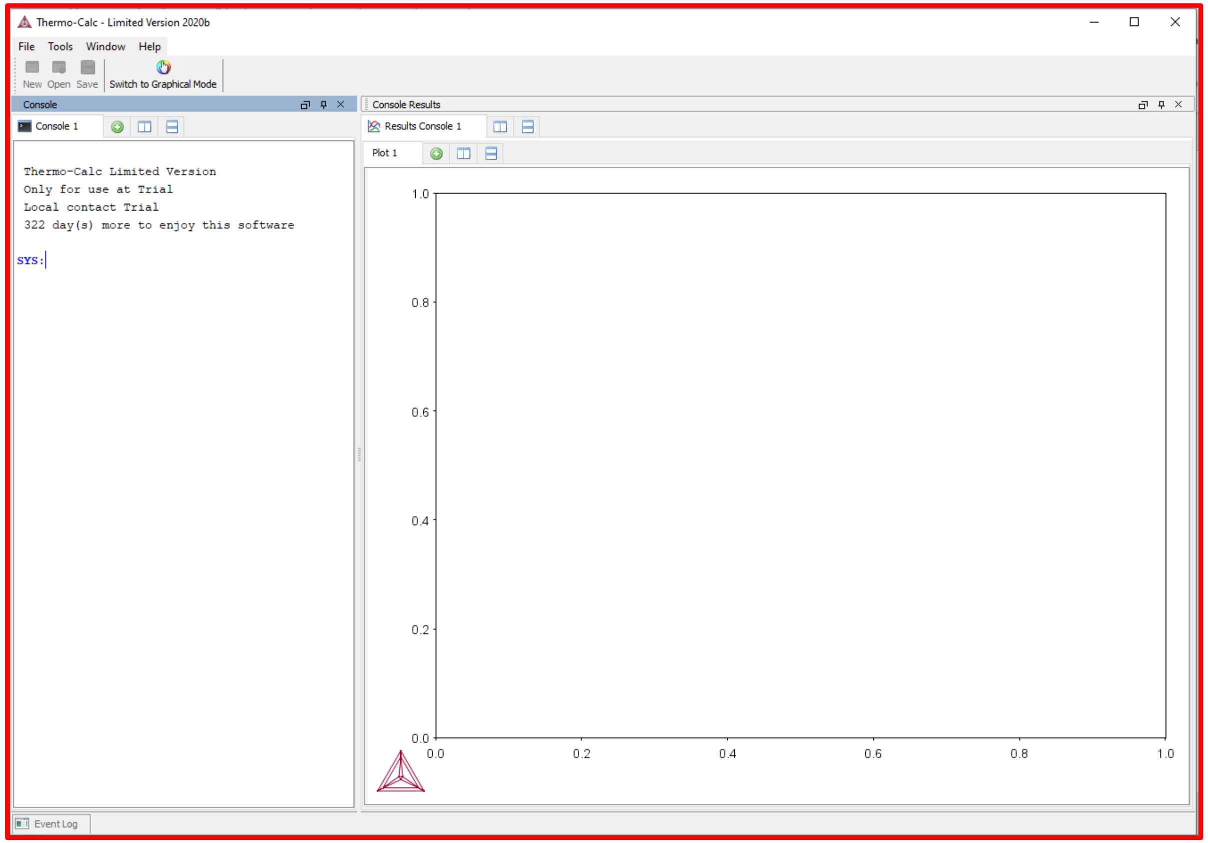


I. Single Equilibrium (Single Point Calculation): Nothing is varied
II. Step Calculation (Property Diagram): One state variable is varied
III. Map Calculation (Phase Diagram): Two state variables are varied

Thermo-CalC operations

Thermo-CalC graphical user interface



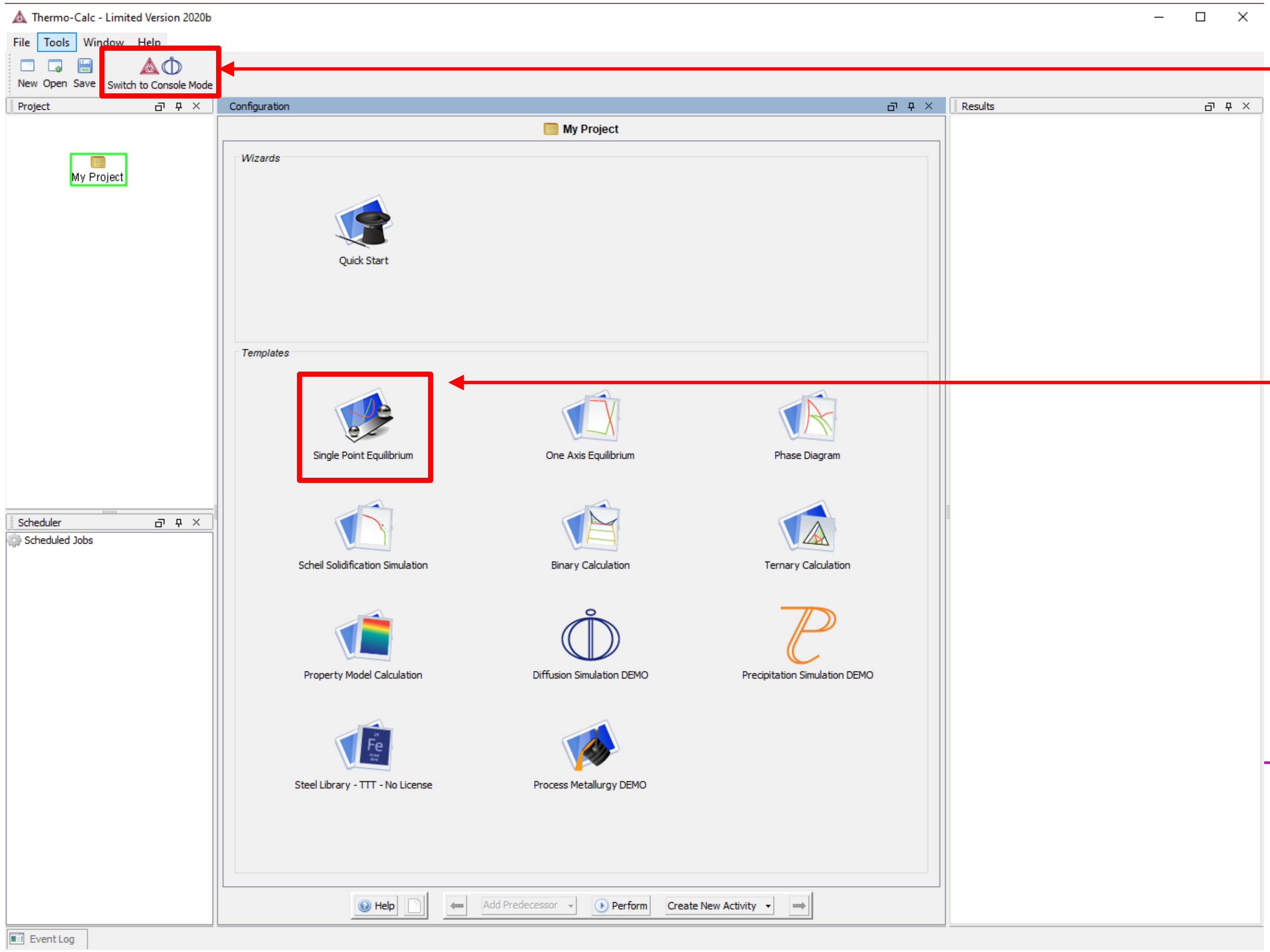


GUI mode **Console mode**

Task: #1 Single point calculation of Fe-0.02C at T=820°C

Determine phase fraction and compositions at a given temperature

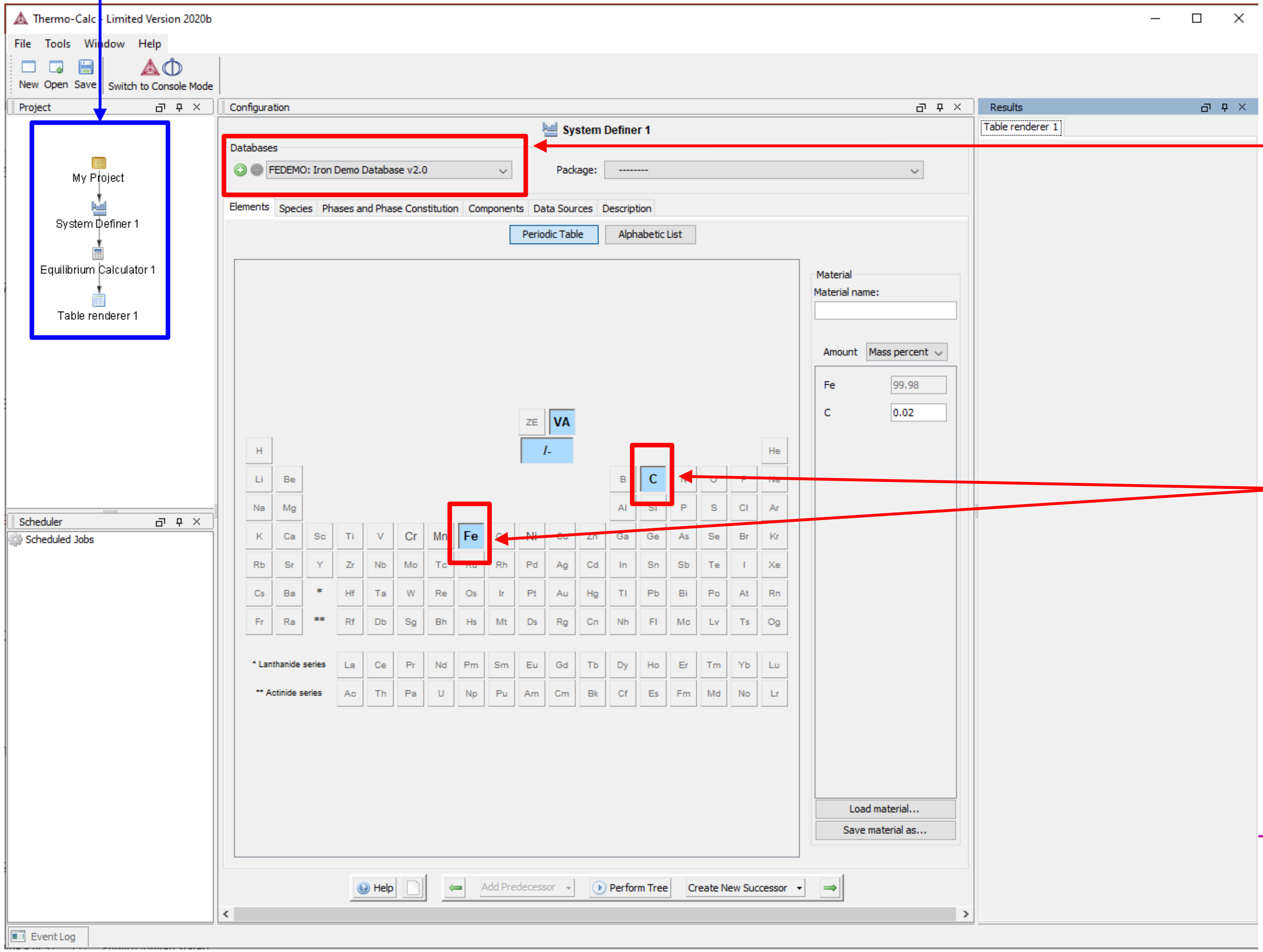
Step 1: **Open Thermo-CalC 2020b and enter GUI mode. Select `Single Point Equilibrium`**



Make sure we are in GUI mode (as pictured), if not, click **[Switch to Graphical Mode]** to get to this screen

Click **[Single Point Equilibrium]** to begin the calculation

Step 2: System Definer 1. Pick Database and Elements in the system

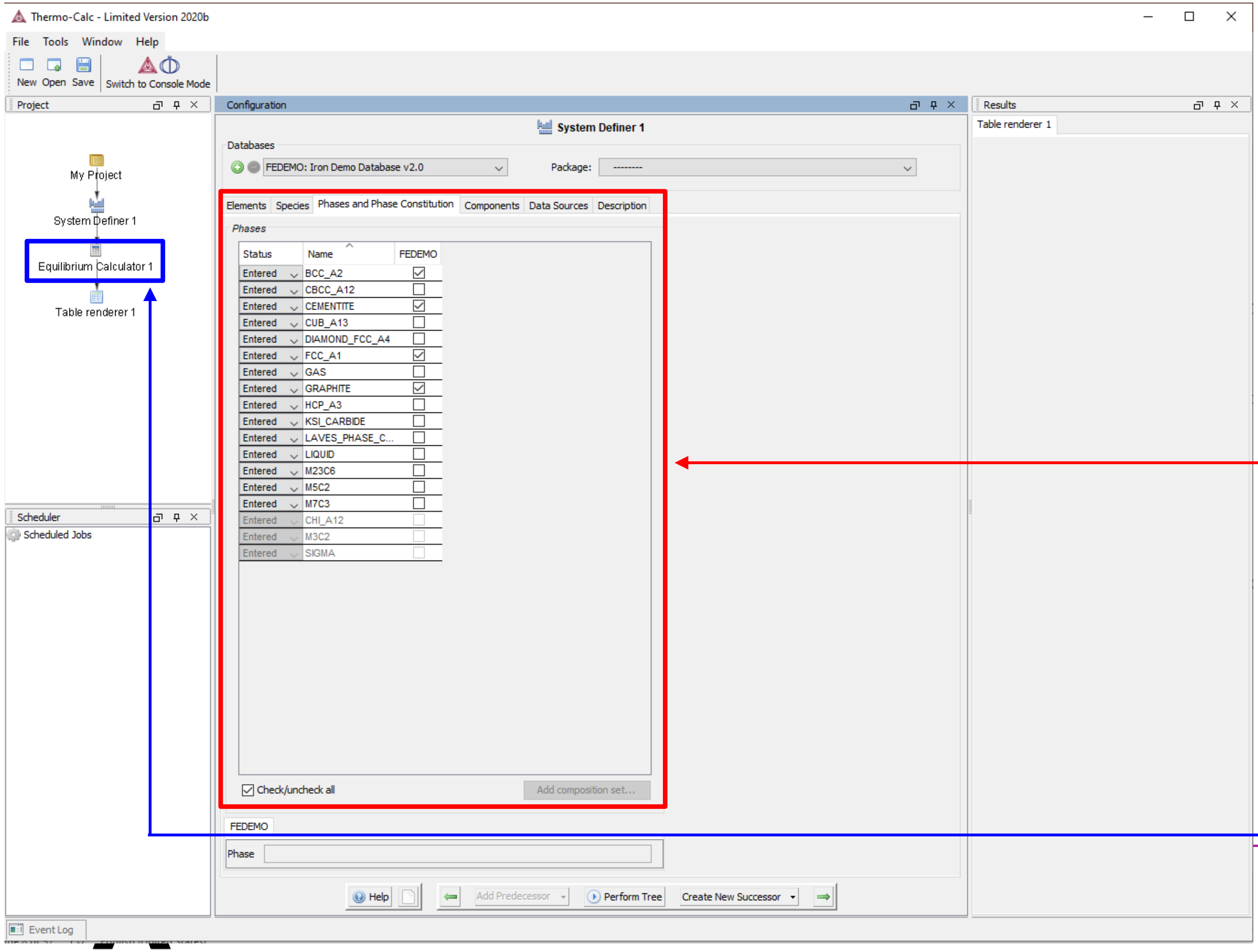


The Project Tree structure will populate. We begin the System Definer 1

In the Configuration Windows, pick `**FEDEMO**` from the Database dropdown menu.

Add `**Fe**` and `**C**` to the system by clicking on the list

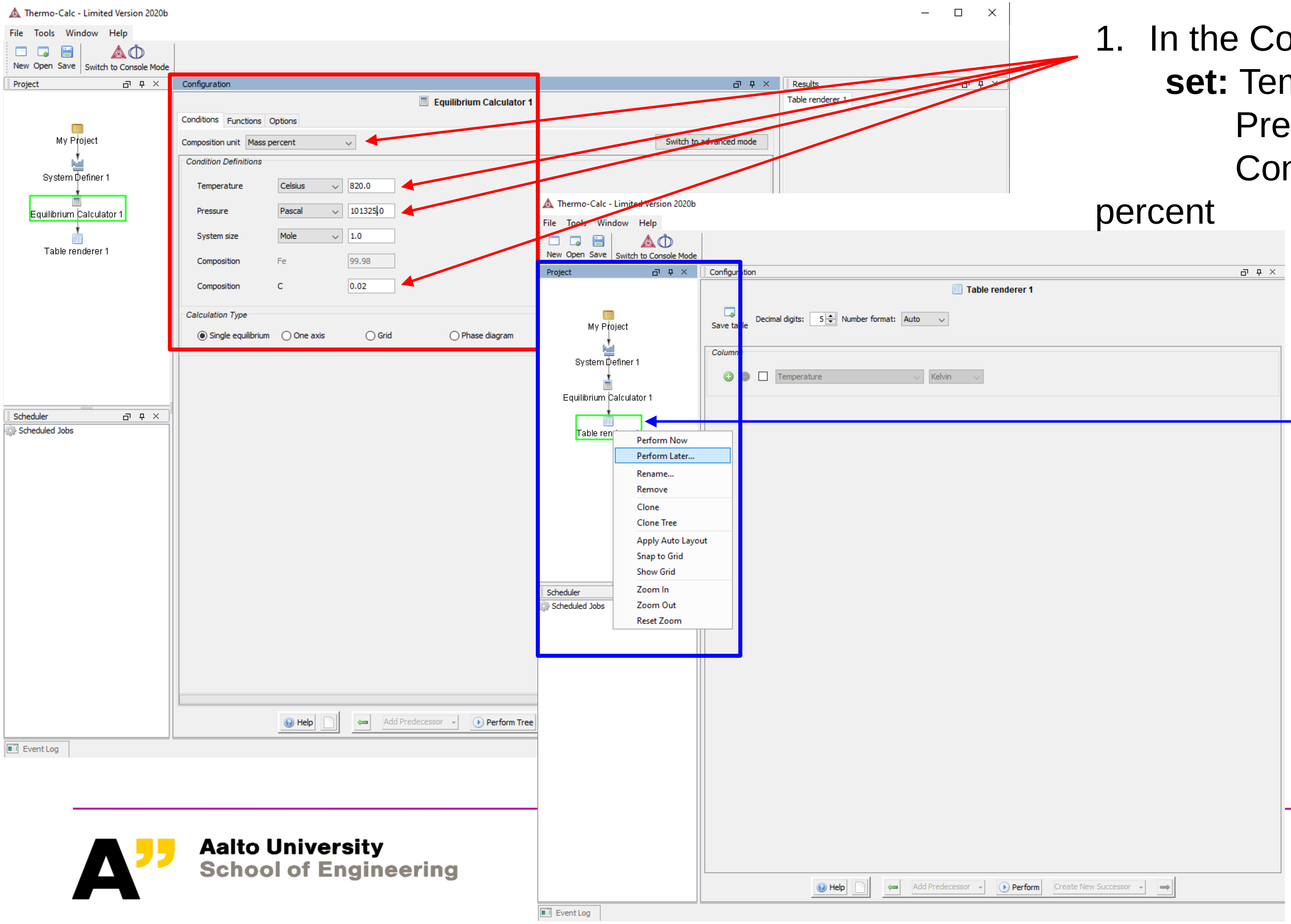
Step 3: System Definer 1. Identify phases and phase constitution in system



1. Click [Phases and Phase Constitution] Tab.
   Uncheck all phases except:
   BCC_A2,CEMENTITE,
   FCC_A1, GRAPHITE
   Only the checked phases are `Entered` and are
   allowed in the calculation.
   Unchecked phases are `Suspended`

2. Click the [Equilibrium Calculator 1] in the `Project`
   window to proceed to set the conditions of the
   equilibrium calculation

Step 4: Equilibrium Definer 1. Set temperature and Composition. Then perform calculation



1. In the Configuration Window,
   set: Temperature (Celsius) = 820.0
   Pressure (Pascal) = 101325.0
   Composition (C) = 0.02 ***in mass percent

2. Right-Click on **[Table Renderer]** and then Left-Click **[Perform Now]**

Step 5: Table Renderer Results

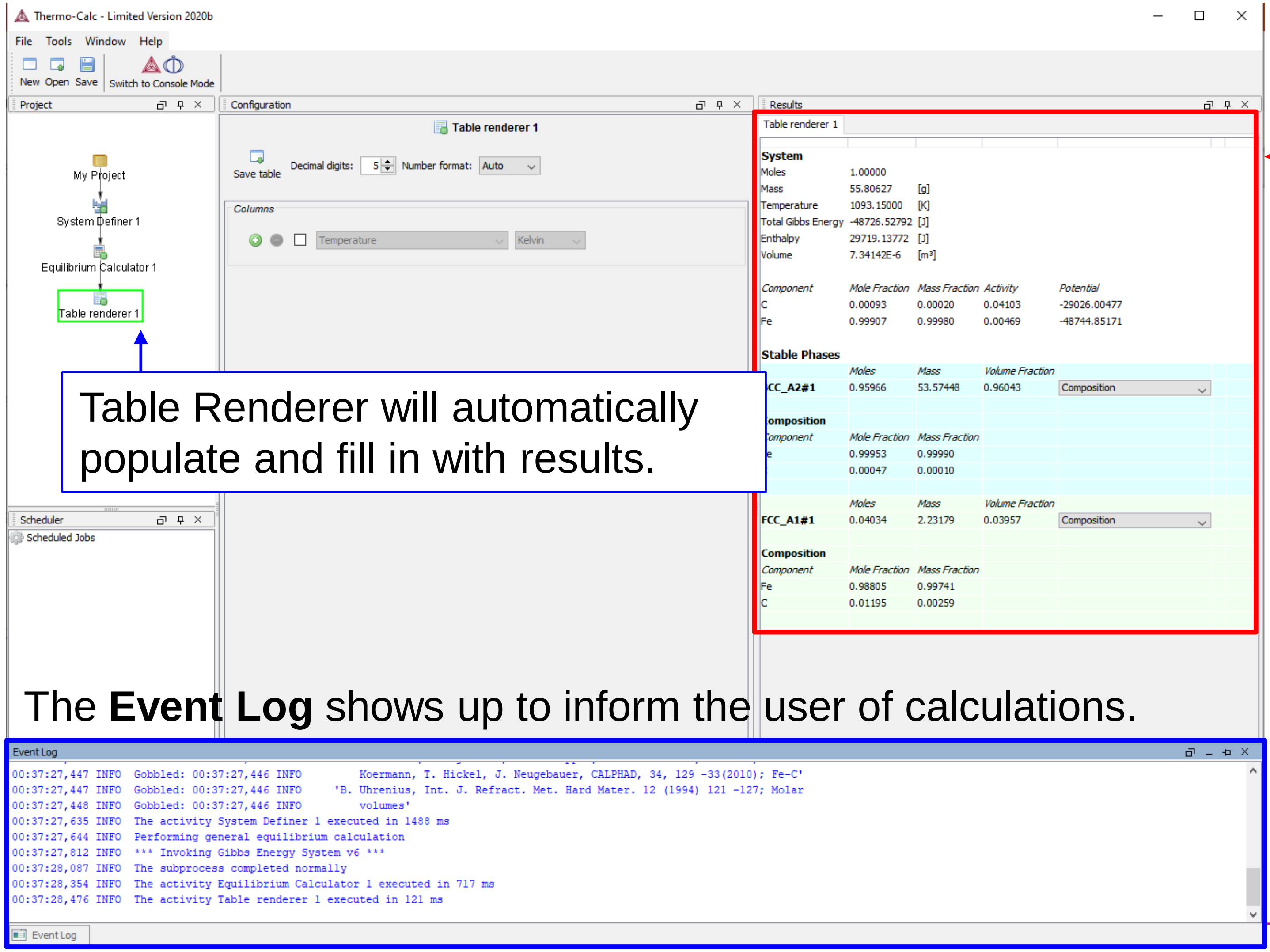
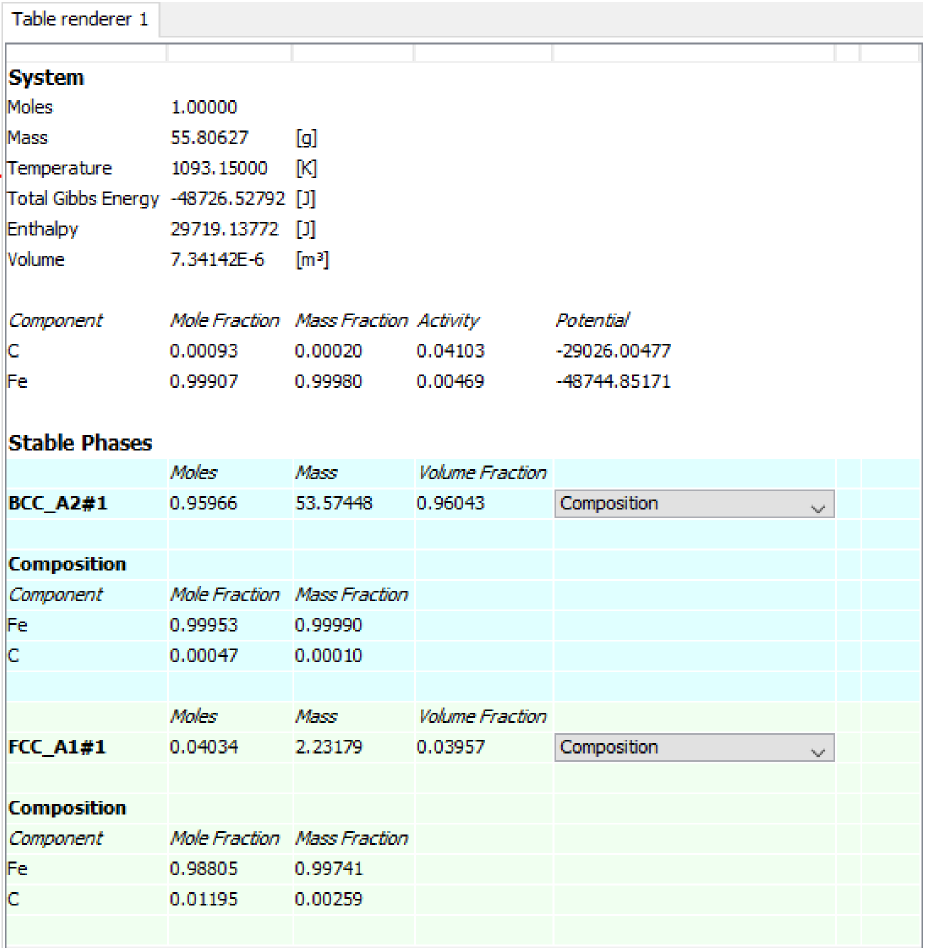


Table Renderer will automatically populate and fill in with results.

The **Event Log** shows up to inform the user of calculations.



The Stable Phases are listed with Mole, Mass, Volume fractions and Compositions

The results should match what you calculate from Lever Rule.

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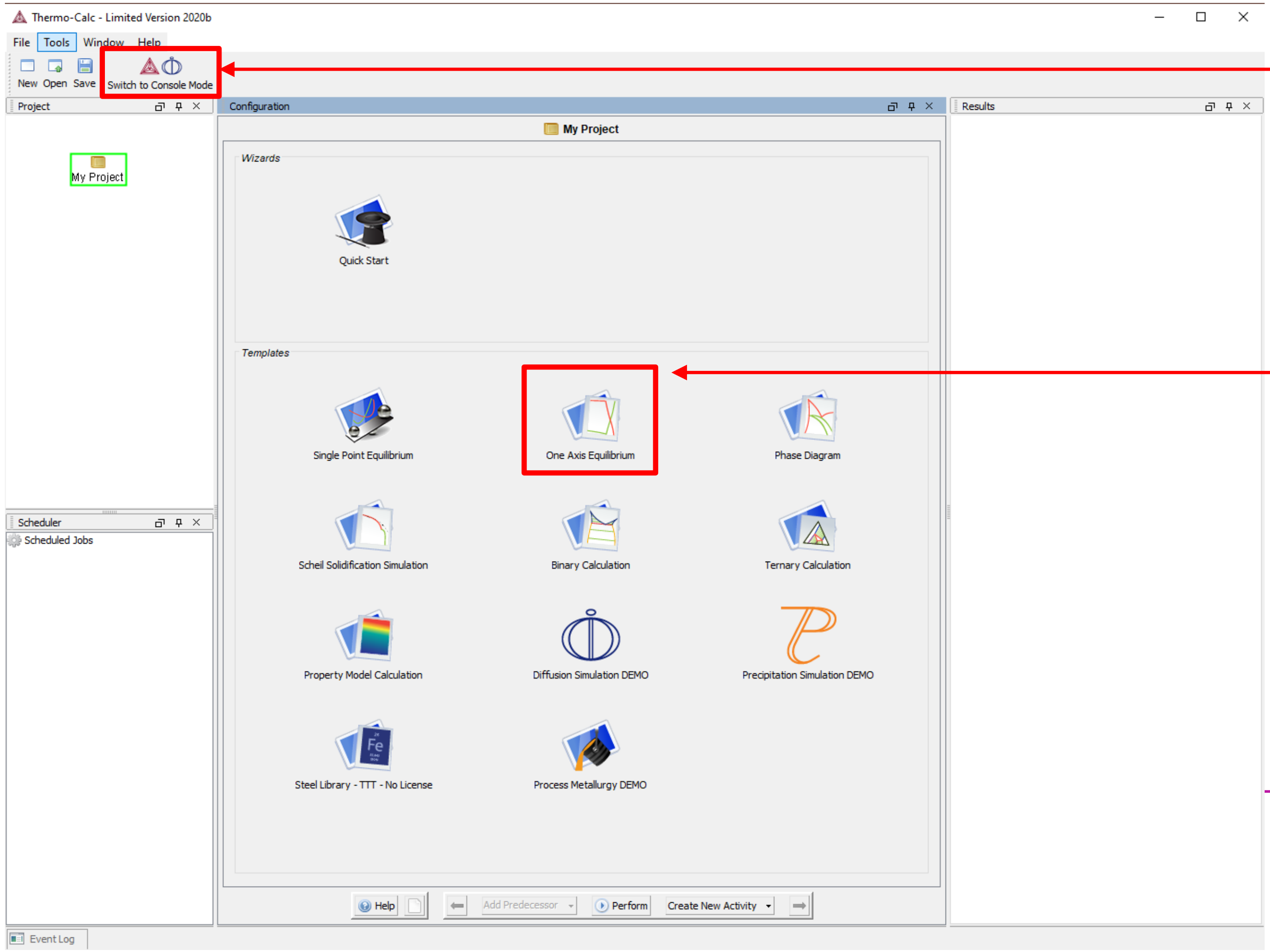
Task: #2 Step calculation (Calculation through a single variable after initiating a point equilibrium)

Determine the optimum temperature for processing for a given alloy

Step 1: **Open Thermo-CalC 2020b and enter GUI mode. Start by clicking `One Axis Equilibrium` or `Property Diagram`**

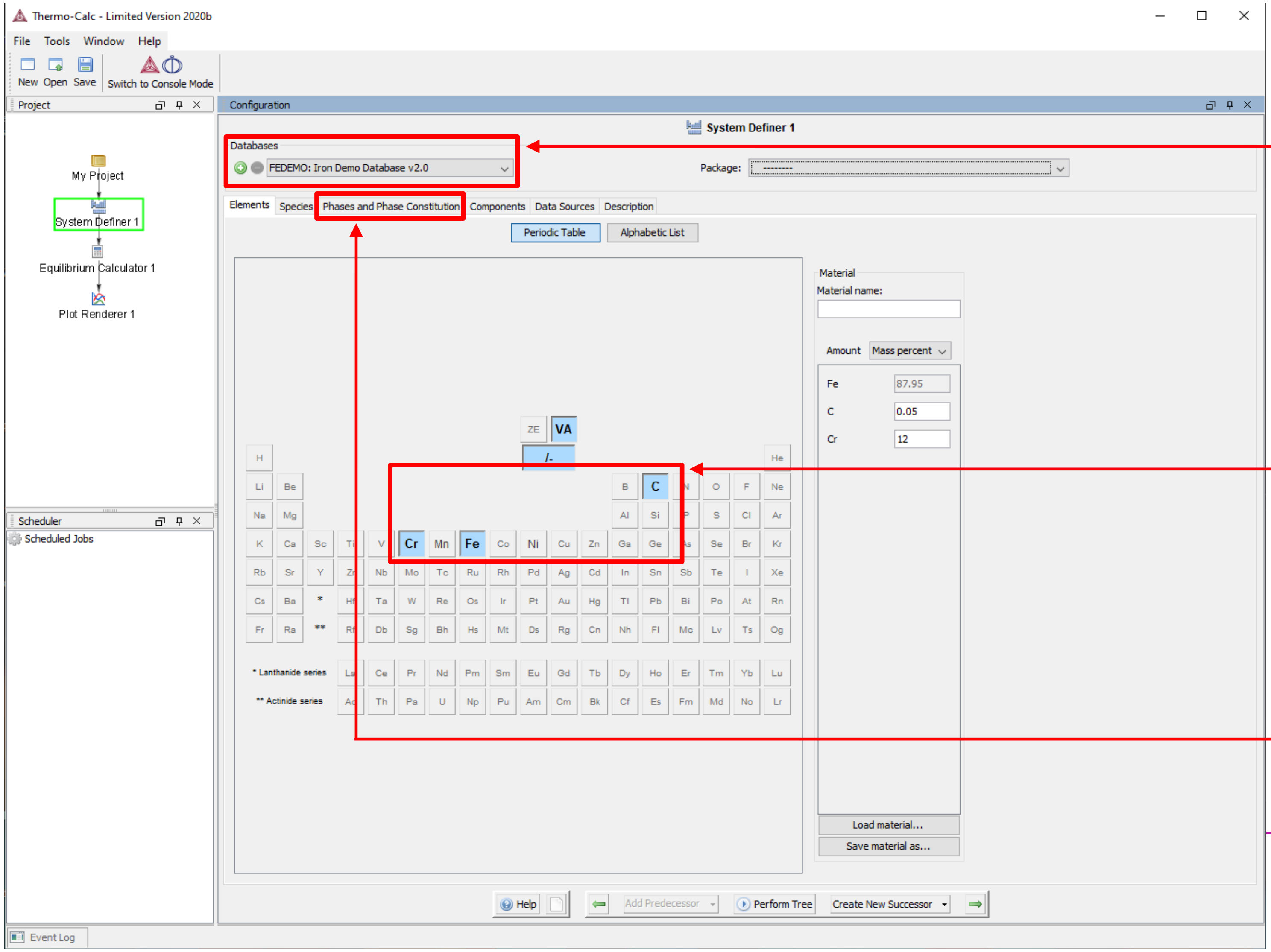


Make sure we are in GUI mode (as pictured), if not, click **[Switch to Graphical Mode]** to get to this screen

Click **[One Axis Equilibrium]** to begin the calculation

In this example, we will use an Fe-0.58C-1.5Cr. We want to find out what is its solution treatment temperature (i.e., the temperature at which all solutes are dissolved in Fe). We also want to know what the equilibrium phase(s) are at various tempering temperatures.

Step 2: Change the database, add the correct elements, go to the Phases tab.

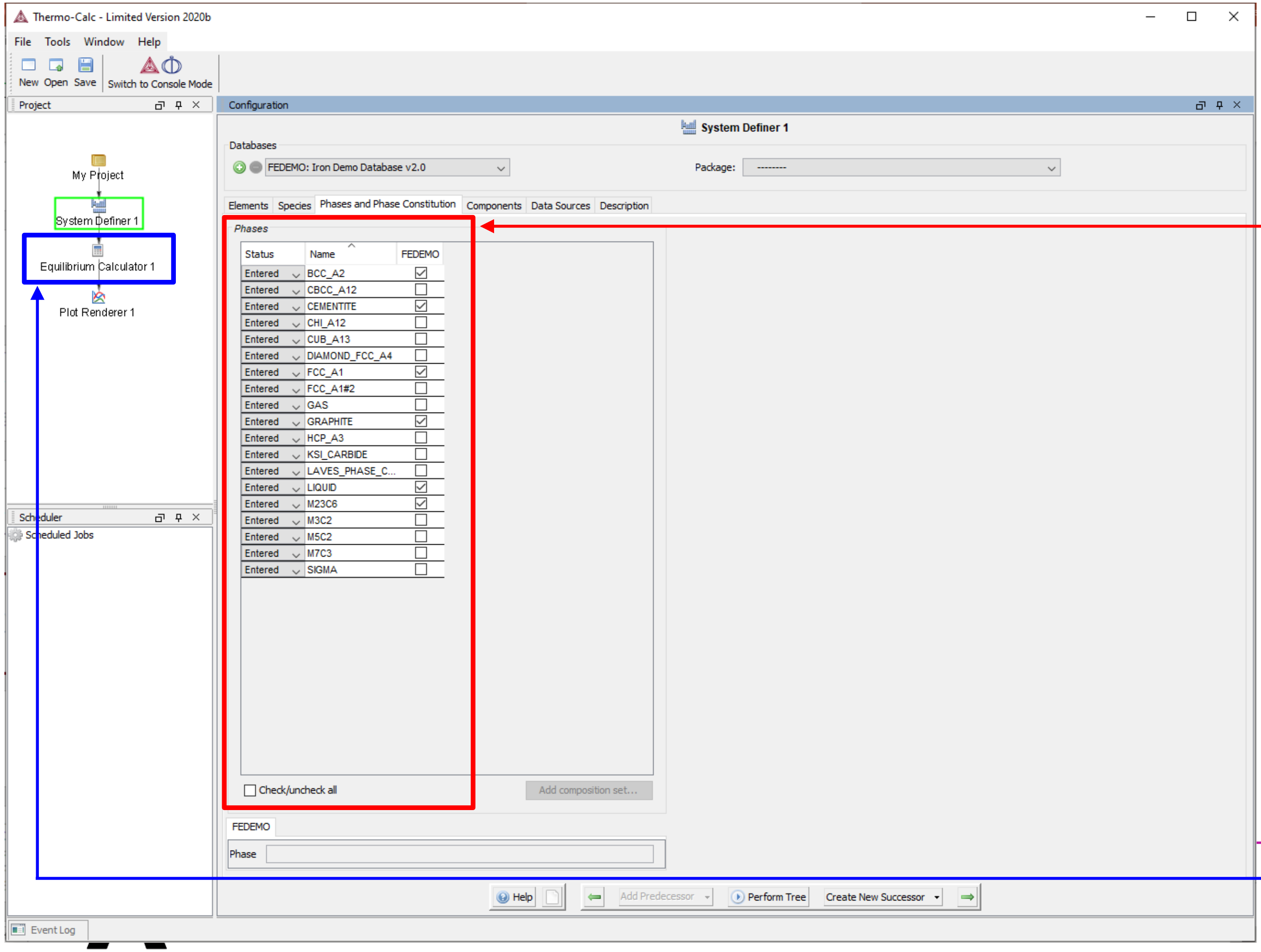


Select the Database `**FEDEMO**` for the calculation

In the Configuration Window, add the elements
Fe, C, Cr, respectively.

Then click the **Phases and Phase Constitution** Tab

Step 3: Choose the appropriate phases to participate in the calculation

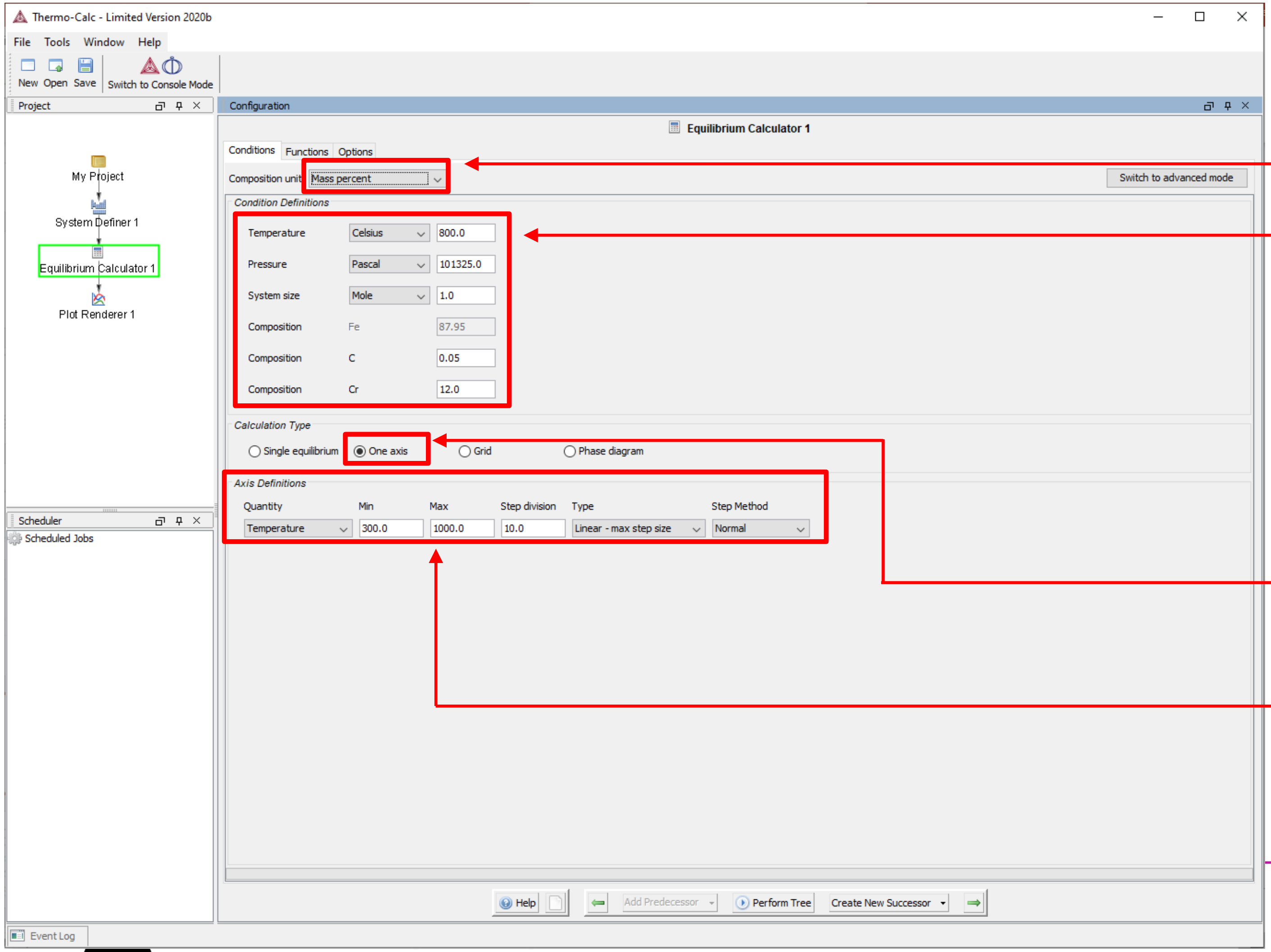


1. Click **`Check/Uncheck All`** to remove all phases.
2. Check the following phases: **BCC_A2, CEMENTITE, FCC_A1, GRAPHITE, LIQUID, M23C6**

Only phases checked will be considered as `Entered` phases participating in the calculation.

3. Click the **Equilibrium Calculator** in the Project Window to move to set calculation conditions.

Step 4: **In the Equilibrium Calculator, set the conditions of the calculation.**



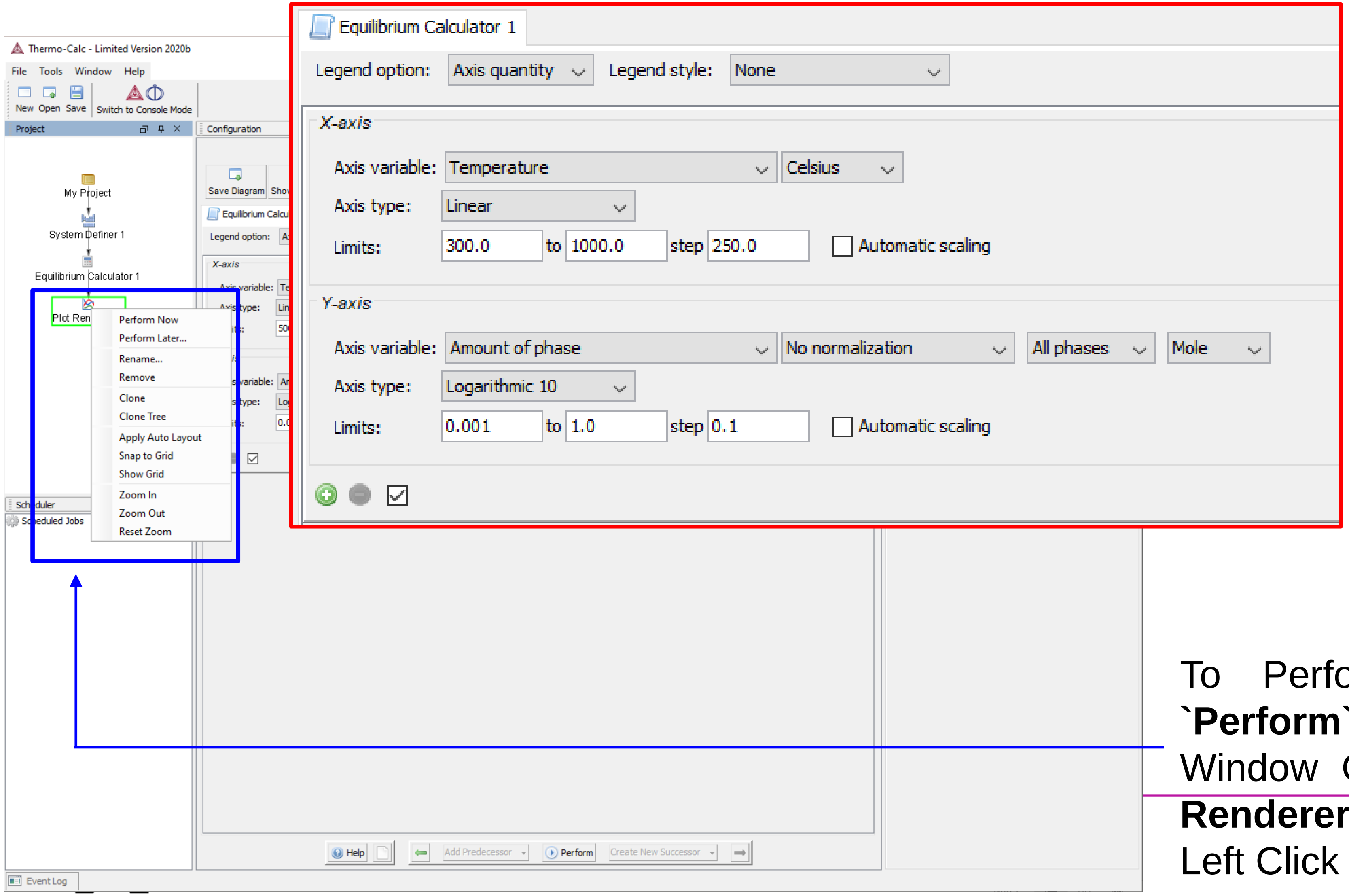
Change the composition unit to `**Mass Fraction**`

Set the conditions as follows:
Temperature = 800.0 ° C
Pressure = 101325.0 Pa
System size = 1 Mole
Composition of C = 0.05
Composition of Cr = 12

Make sure the `**One axis**` calculation is checked.

Under `**Axis Definitions**` (This defines the step calculation):
Quantity = Temperature; **Min** = 300.0, **Max** = 1000.0
Step Division = 10.0
Type = `Linear-max step size`

Step 5: Proceed to Plot Renderer



Change your plotting conditions when the job is complete.

X-Axis: Put Temperature in Celsius. **Adjust Limits to Min**: 300, **Max**:1000

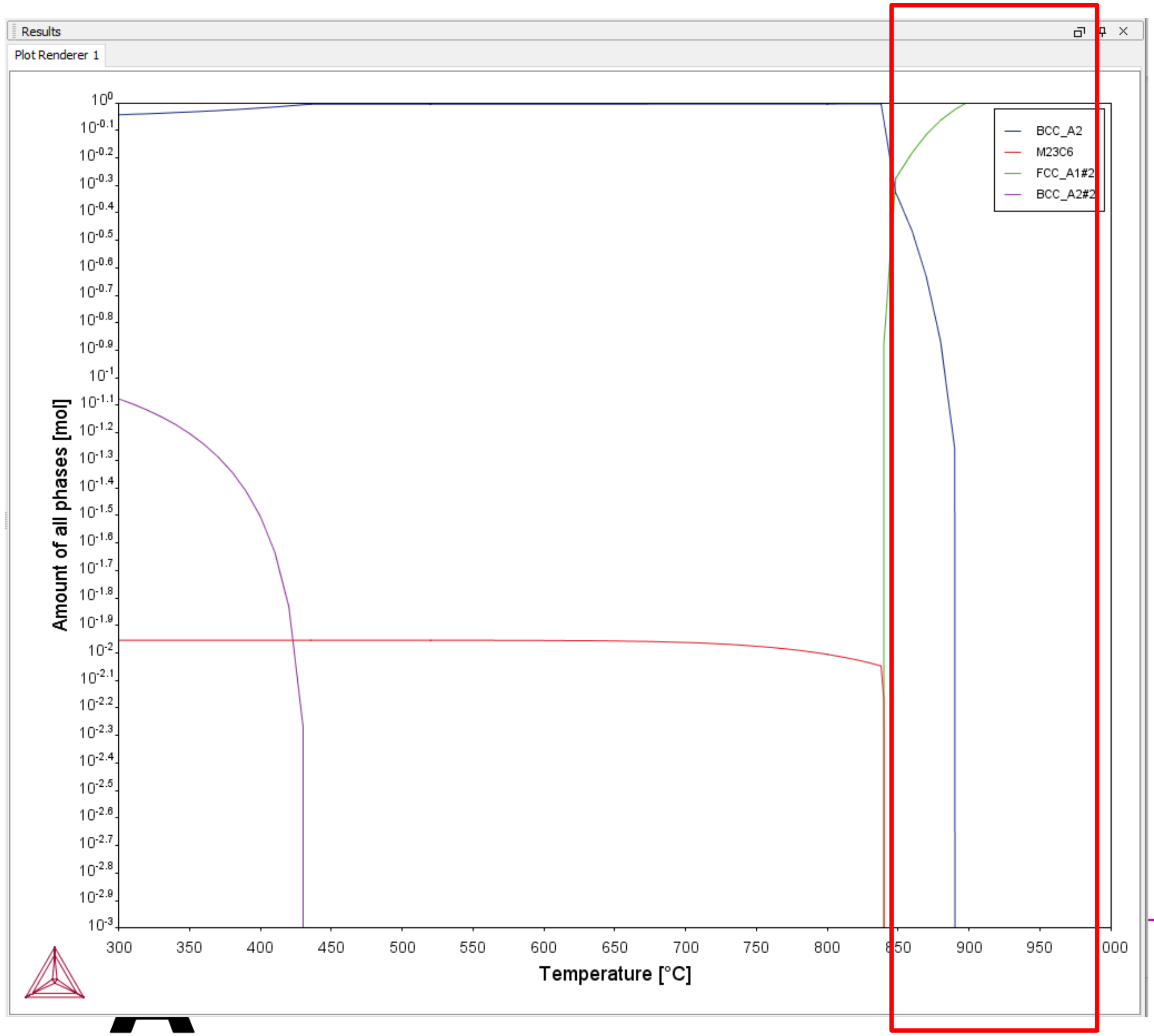
Y-Axis: Make Axis Type “Logarithmic 10”. **Adjust Limits to Min**: 0.001, **Max**: 1.0

To execute these changes, use **Perform** button or **Perform Now** from the Project tree.

NOTE: This will be much faster since the solution is already in the computer memory.

To Perform the calculation, either: Click `**Perform**` at the bottom of the Configuration Window OR (more reliably) Right-Click `**Plot Renderer 1**` in the Project Window and then Left Click **Perform Now.**

Step 6: Save the diagram or create a corresponding data table



Plot Renderer 1 shows the results of the **`Step Calculation`**

This is commonly called a Step Diagram. It shows equilibrium phase fractions of phases present in the system at a given temperature. It is best to plot phase fraction in Log base 10.

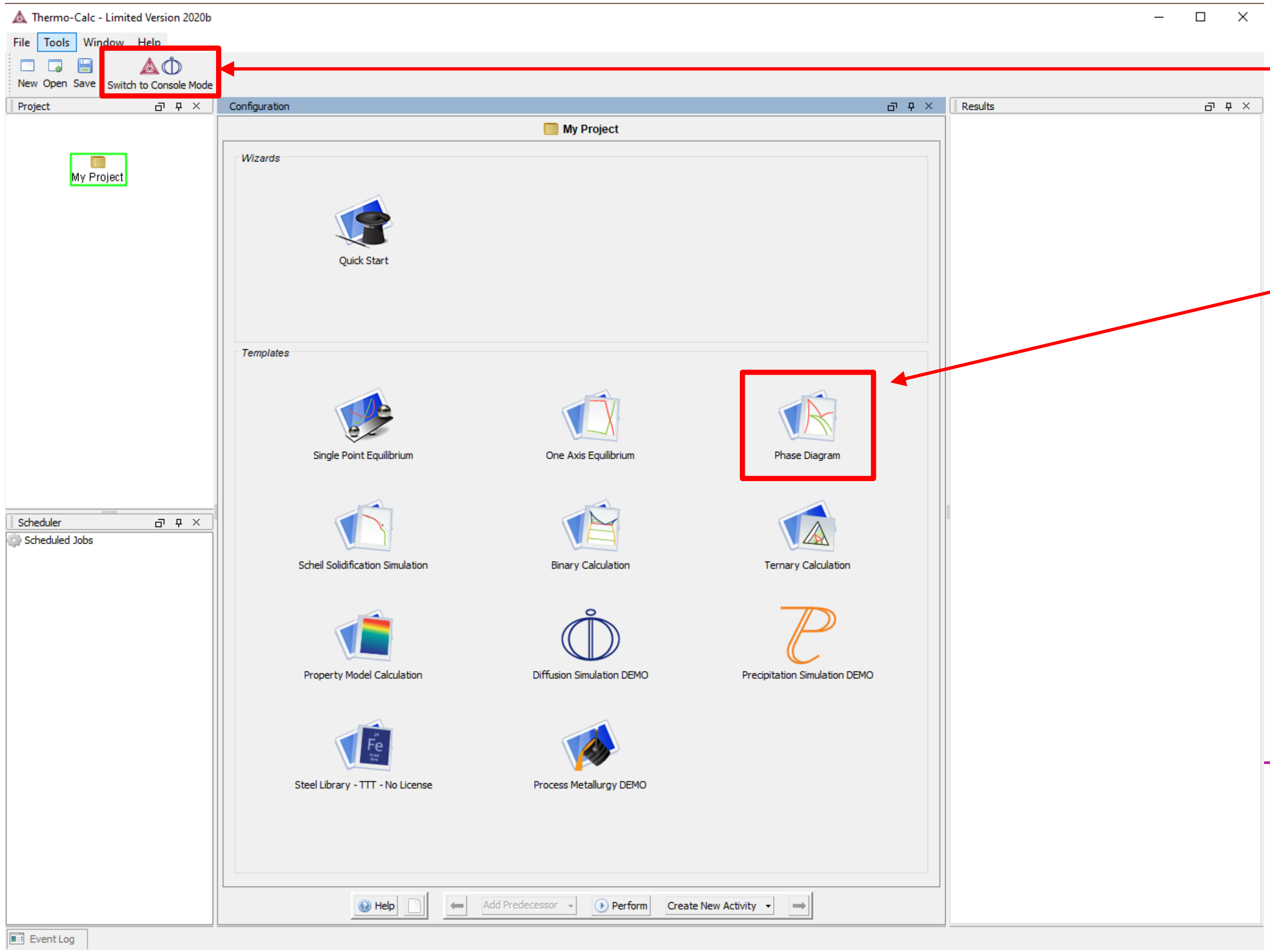
The phase line color matches the legend. The diagram can be saved by Right-Click **`Save As´**

A table with the data calculated can be created using **`Table Renderer`**. Right-Click **`Equilibrium Calculator`** in the Project Tree. Right-Click **`Create New Successor>Table Renderer`**. Right-Click your **`Table Renderer>Perform Now`** to generate the corresponding table. You can copy all data or save all as a text, xls, or html file.

Task : #3 Map calulation (Equilibrium Phase Diagram)

Calculate an equilibrium phase diagram of Fe-C

Step 1: Start the GUI calculation by clicking `Phase diagram`

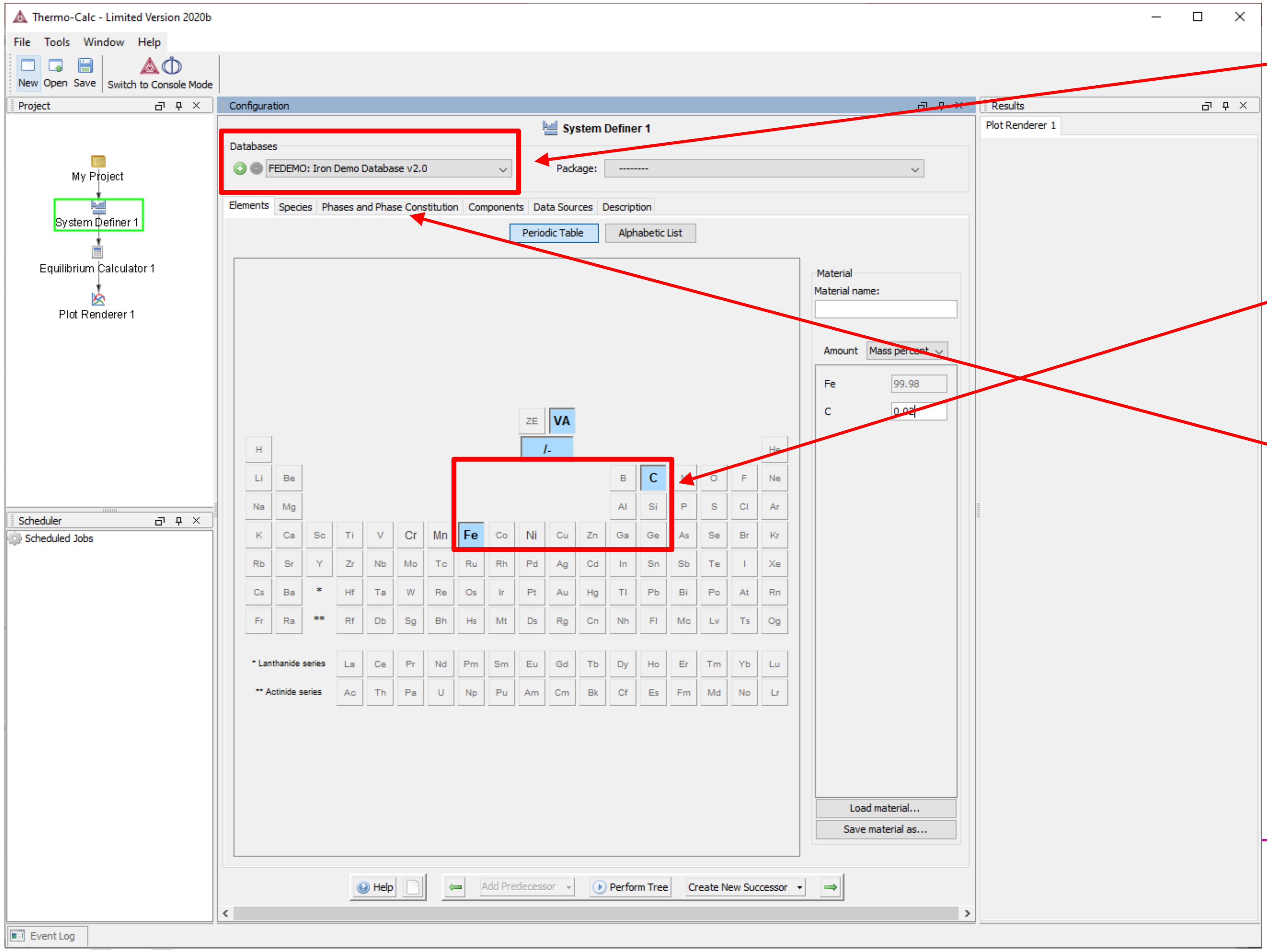


Make sure we are in GUI mode (as pictured), if not, click **[Switch to Graphical Mode]** to get to this screen

Start the GUI and click on **`Phase diagram`** Even if you aren't making a classical equilibrium phase diagram, this will allow for you to do a map calculation.

For mapping calculations allow variation of two variable (varying Temperature and Composition).
These enable the calculation of phase diagrams.

Step 2: Choose the Correct Database and add Elements

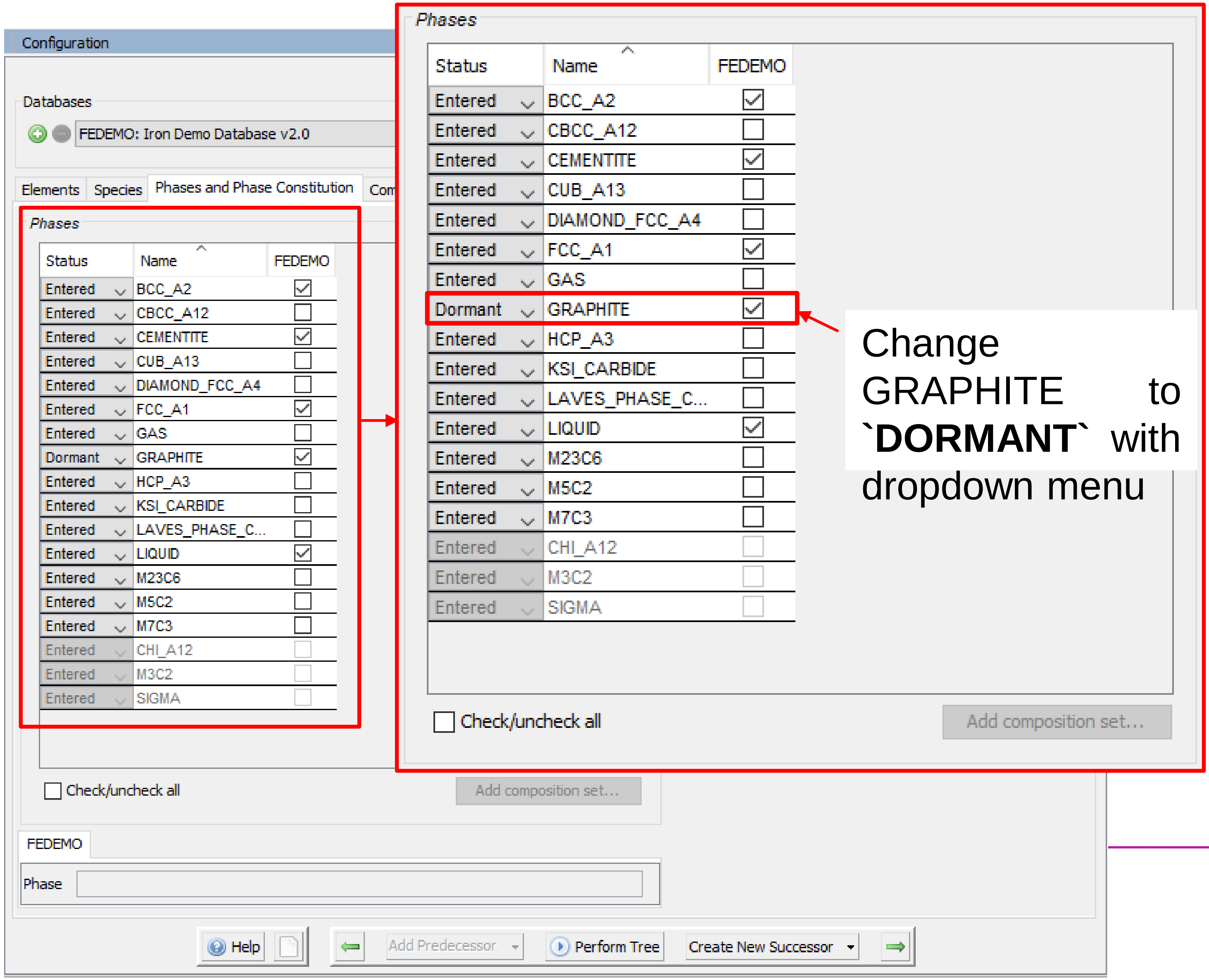


Select the Database of `**FEDEMO**` for iron

Select elements: **FE and C**.

Follow by clicking **Phases and Phase Constitution Tab**

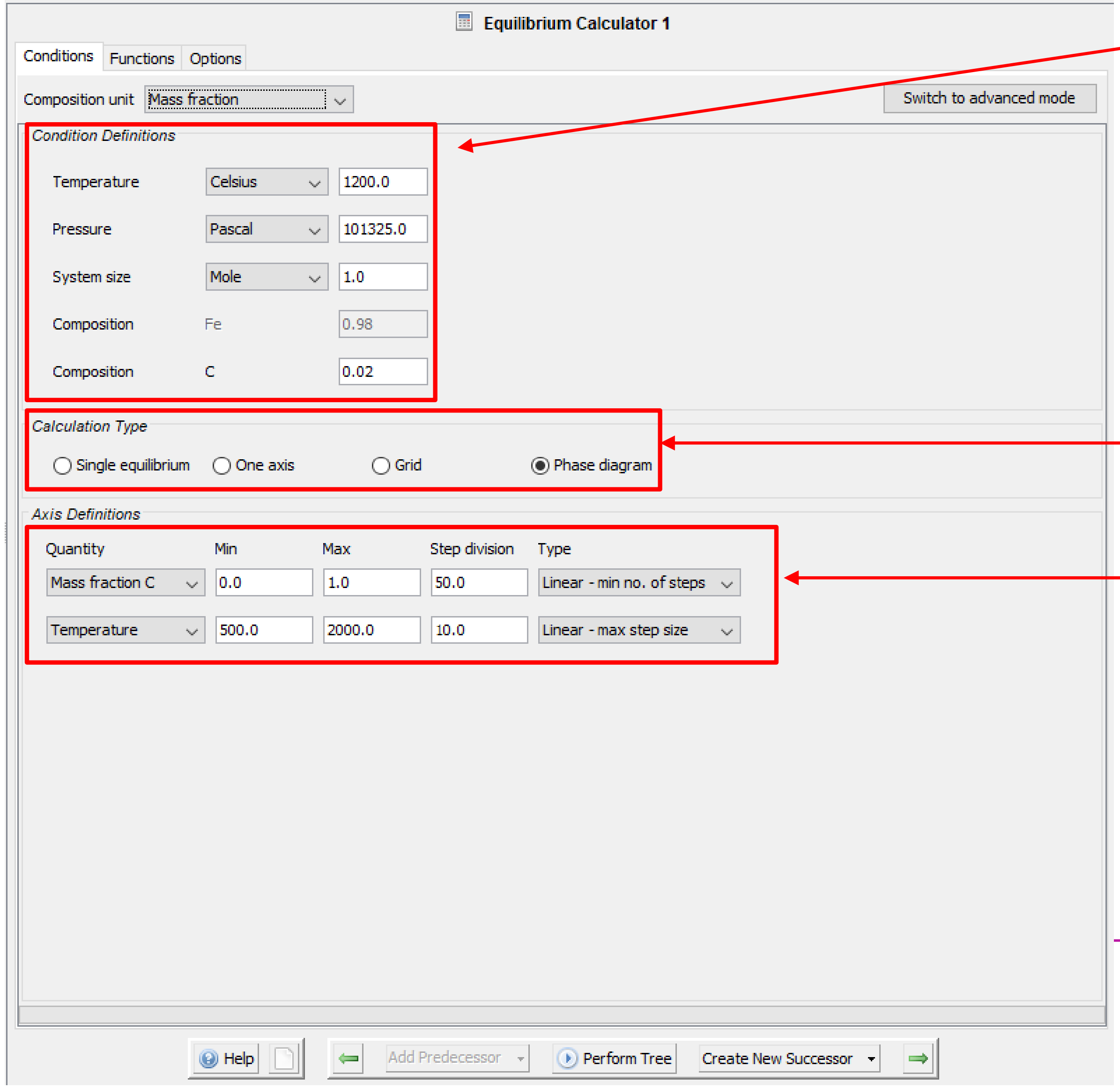
Step 3: Add Phases and Make Graphite Dormant.



Change GRAPHITE to `**DORMANT**` with dropdown menu

Uncheck all phases and then Click to add:
BCC_A2, CEMENTITE, FCC_A1, GRAPHITE, LIQUID

Step 4: Step Map Conditions in Equilibrium Calculator



Click **Equilibrium Calculator 1** in the Project Window and set the following conditions:

Composition Unit: Mass fraction

Temperature : 1200.0 ° C

Pressure : 101325 Pa

System size : 1 Mole

Composition of C : 0.02

Make sure **`Phase Diagram`** is checked under the Calculation Type

These conditions could be set as follows:

Mass fraction C: Min = 0.0, **Max** = 1.0, **Step diviation** = 50.0

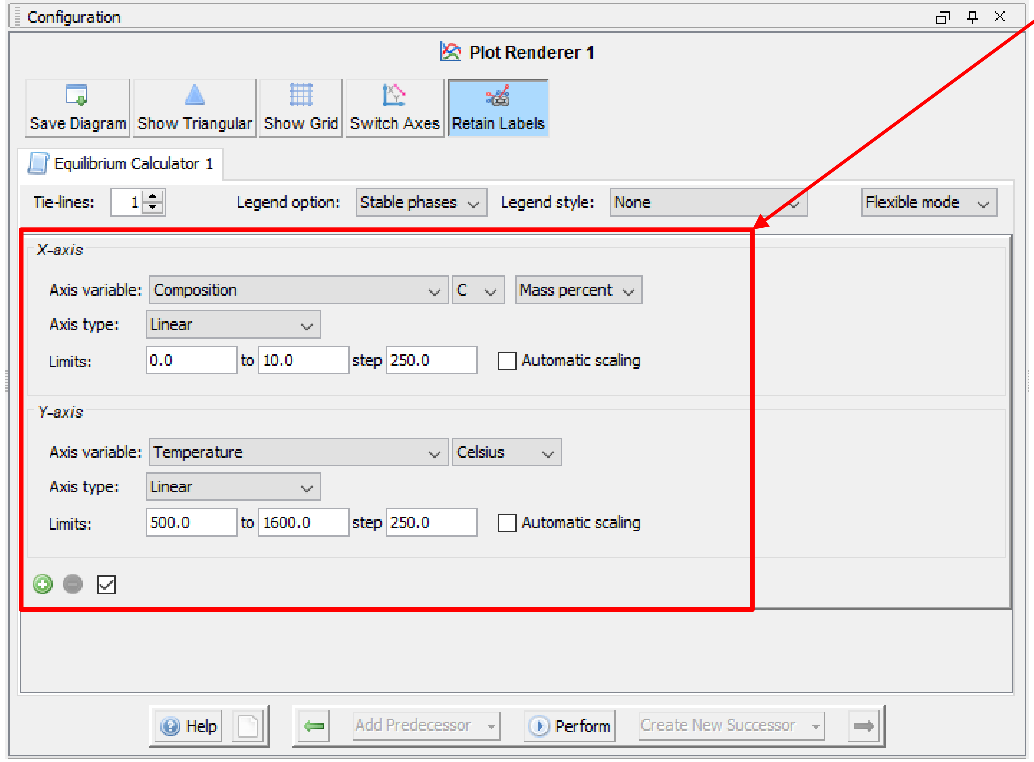
Type = Linear min No. of steps

Temperature: Min = 500.0, **Max** = 2000.0, **Step deviation** = 10.0

Type = Linear max Step Size

Follow by clicking **`Plot Renderer`** in the Project Window

Step 5: **Change axis limits and insert labels**

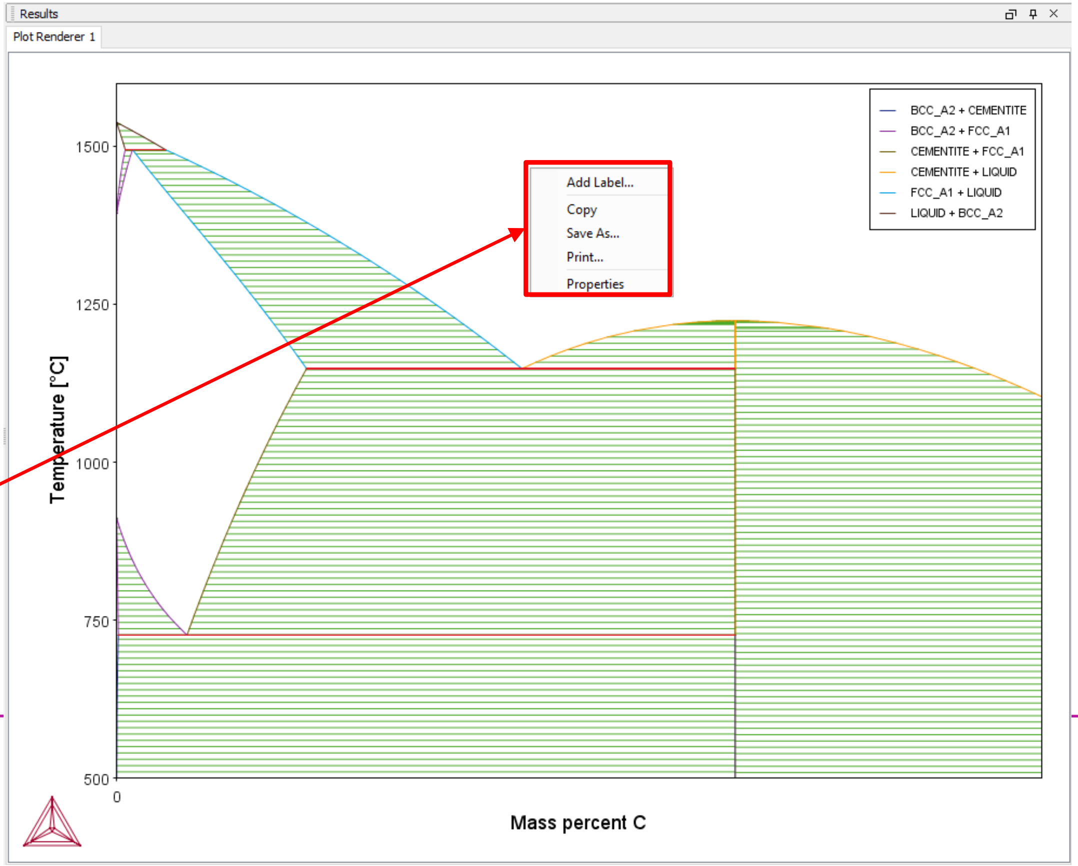


Change Limits:

X-Axis: Composition C in Mass percent, **Min** = 0.0, **Max** = 10, **Step** = 250.0

Y-Axis: Temperature in Celsius, **Min** = 500.0, **Max** = 1600.0, **Step** = 250.0

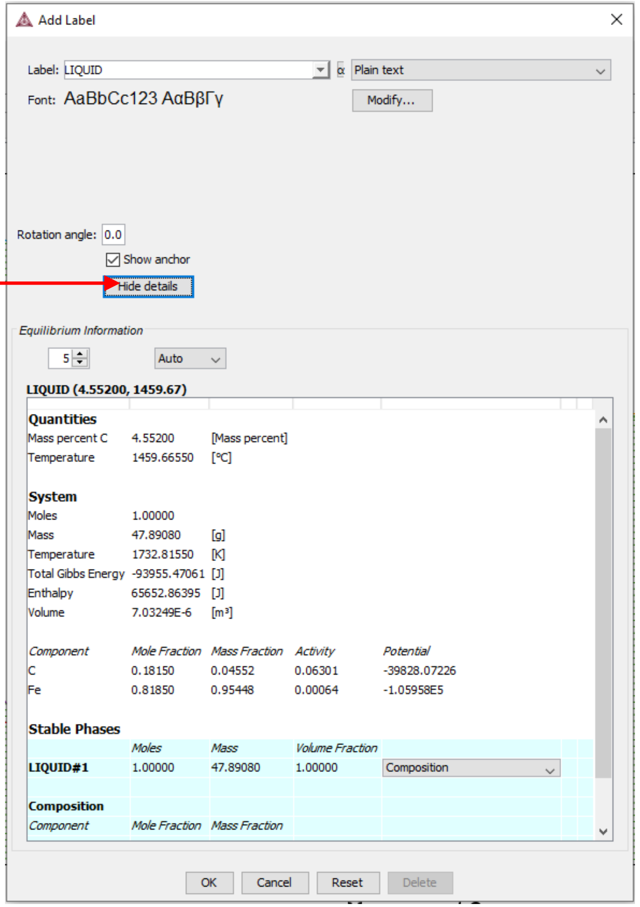
Perform the calculation by Right-clicking on `**Plot Renderer**`. Left-click `**Perform Now**` to start the calculation.

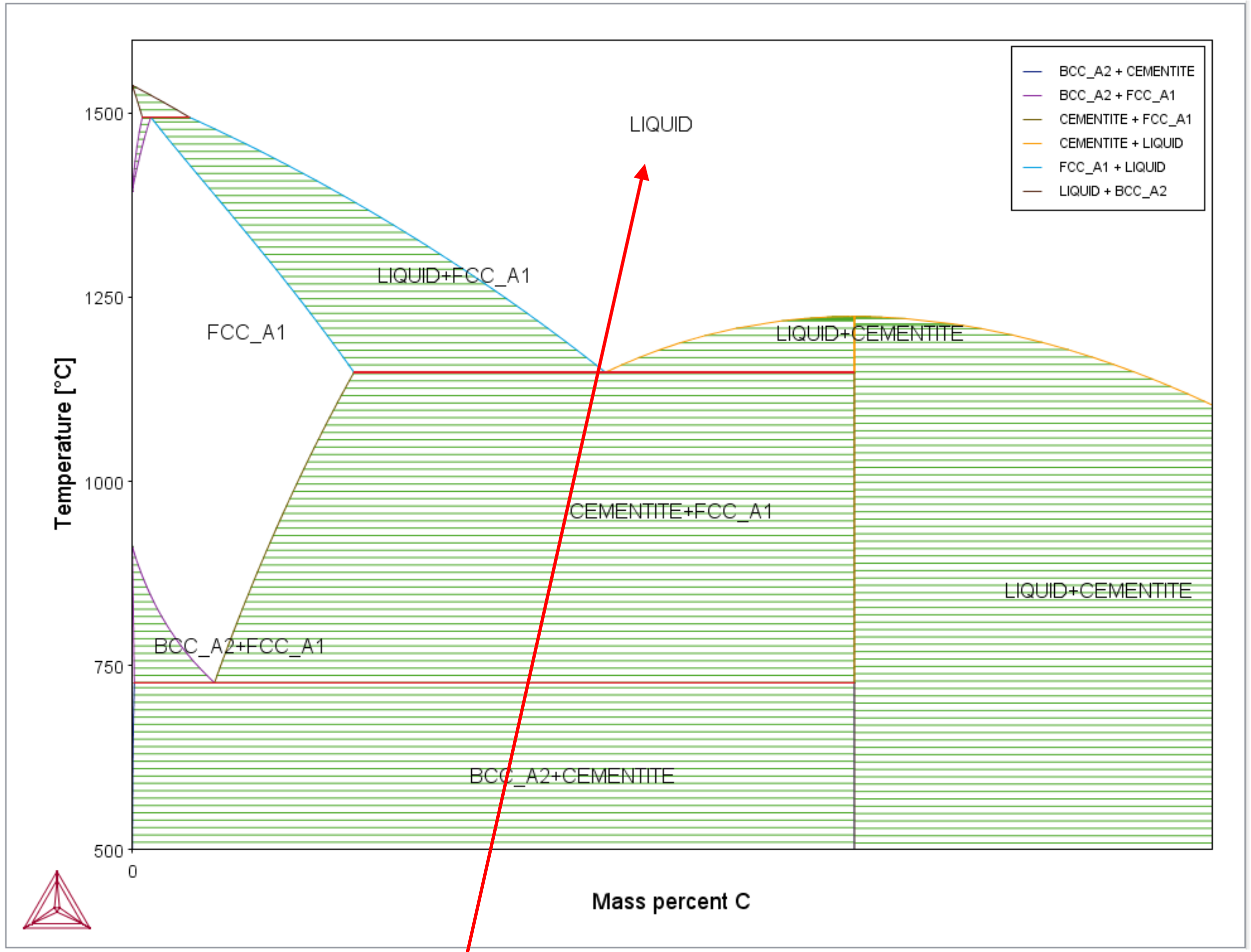


Right-Click on a Phase space and Left-Click to

Add Label

Step 6: Labeling Phase fields





Before adding the Label, Click ´**Details**´ A Point Calculation Result will appear, showing the results of that phase space. Clicking `**OK**` adds the label. Repeat for all significant fields.

Videos for Excercises

- Task1_TC_Single point calculation
- https://vimeo.com/485758585

- Task2_TC_Step calculation
- https://vimeo.com/485758485

- Task3_TC_Map calculation (Equilibrium Phase Diagram)
- https://vimeo.com/485758400

Questions?

- **Contact: MyCourses ‘General discussion’ channel**