



Aalto University
School of Engineering

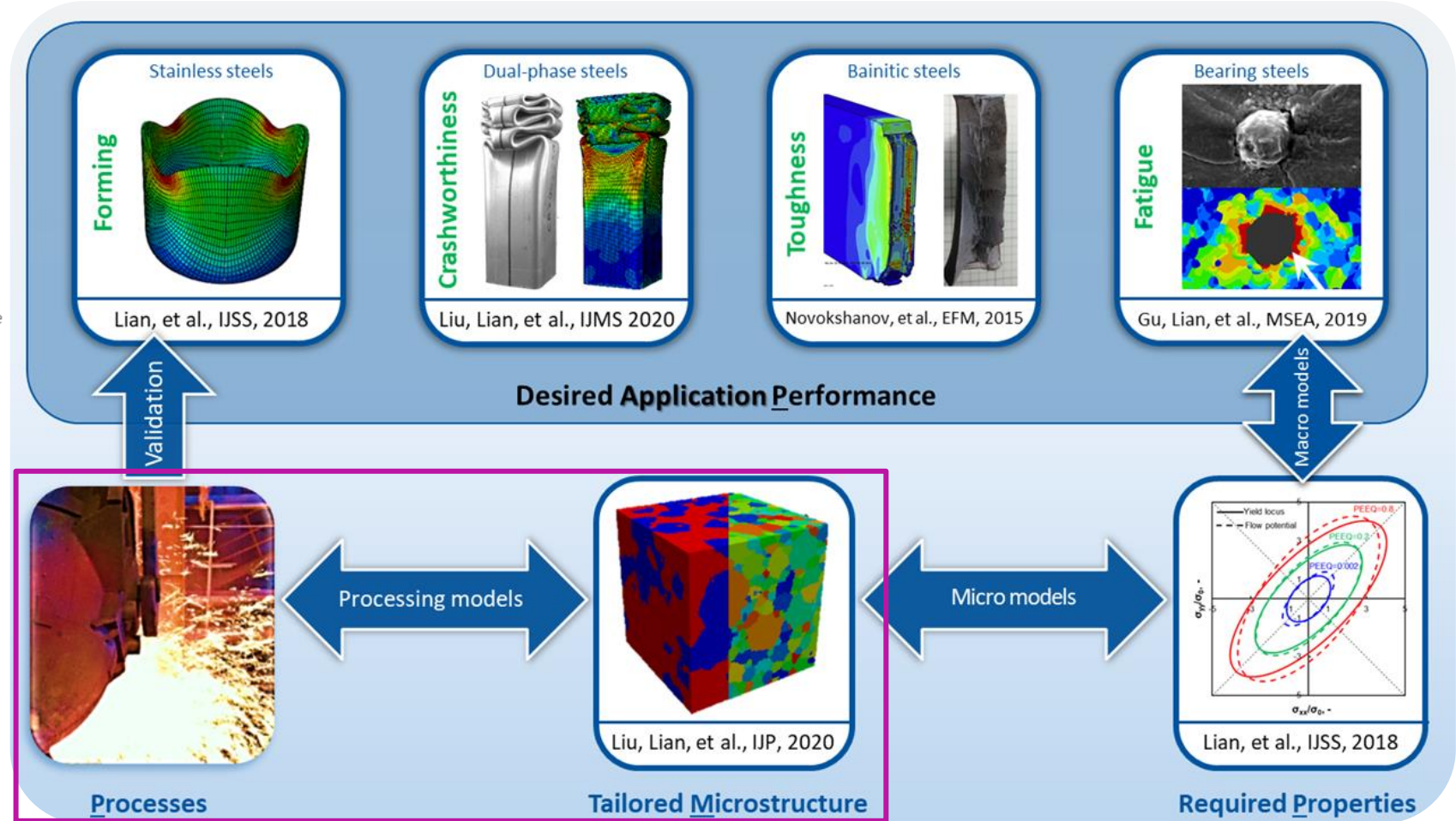
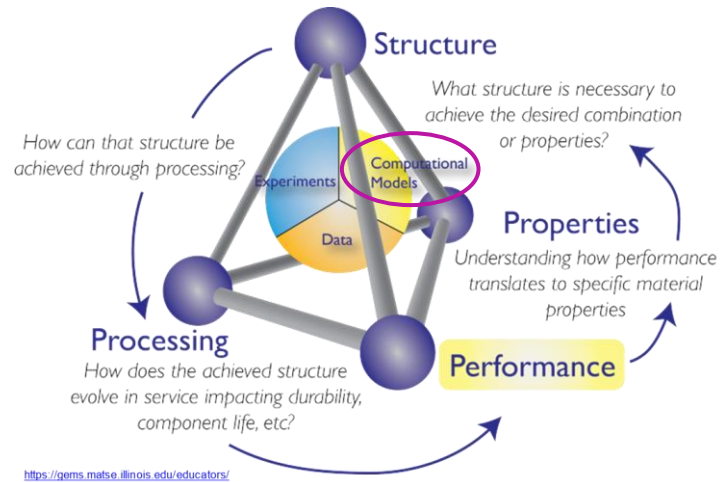
COE-C2004 - Materials Science and Engineering

Exercise 4

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Integrated computational materials engineering (ICME)



<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)

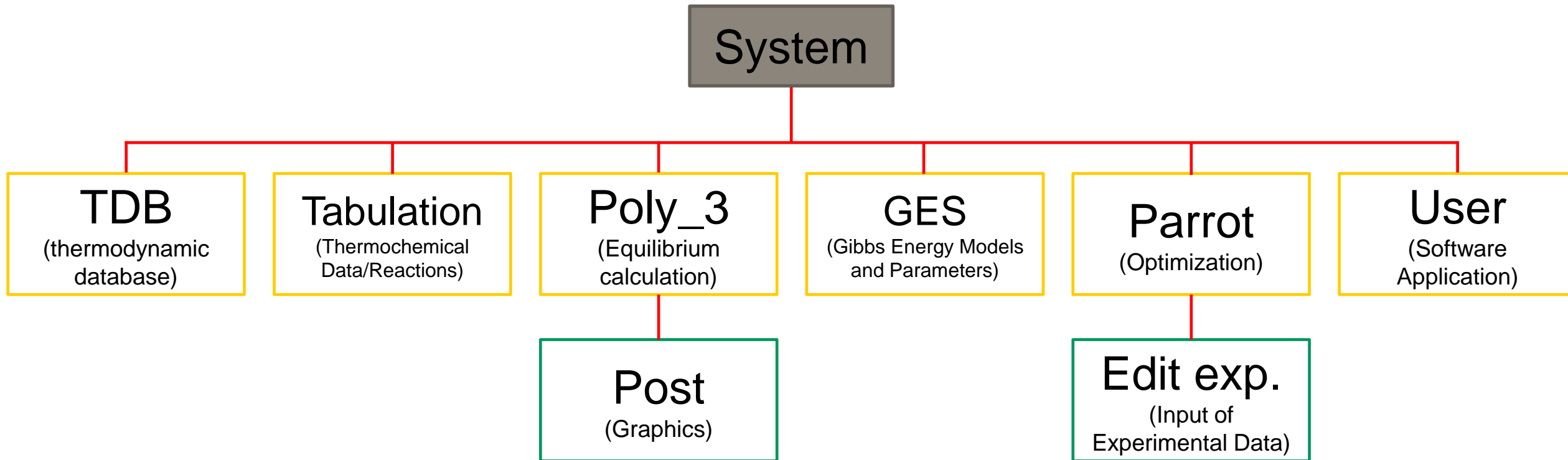
Thermo-CalC overview (cont.)

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).

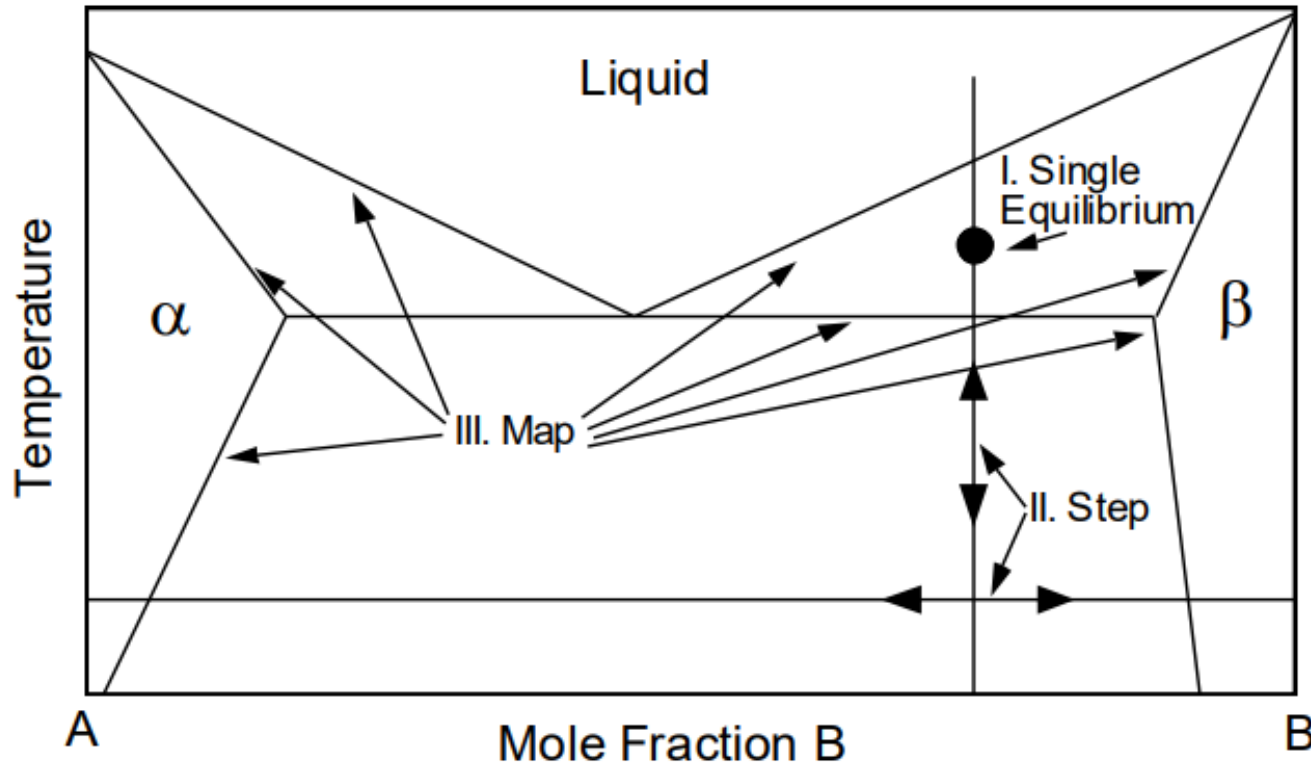
Components: The smallest possible division of matter required to describe a given phase.

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

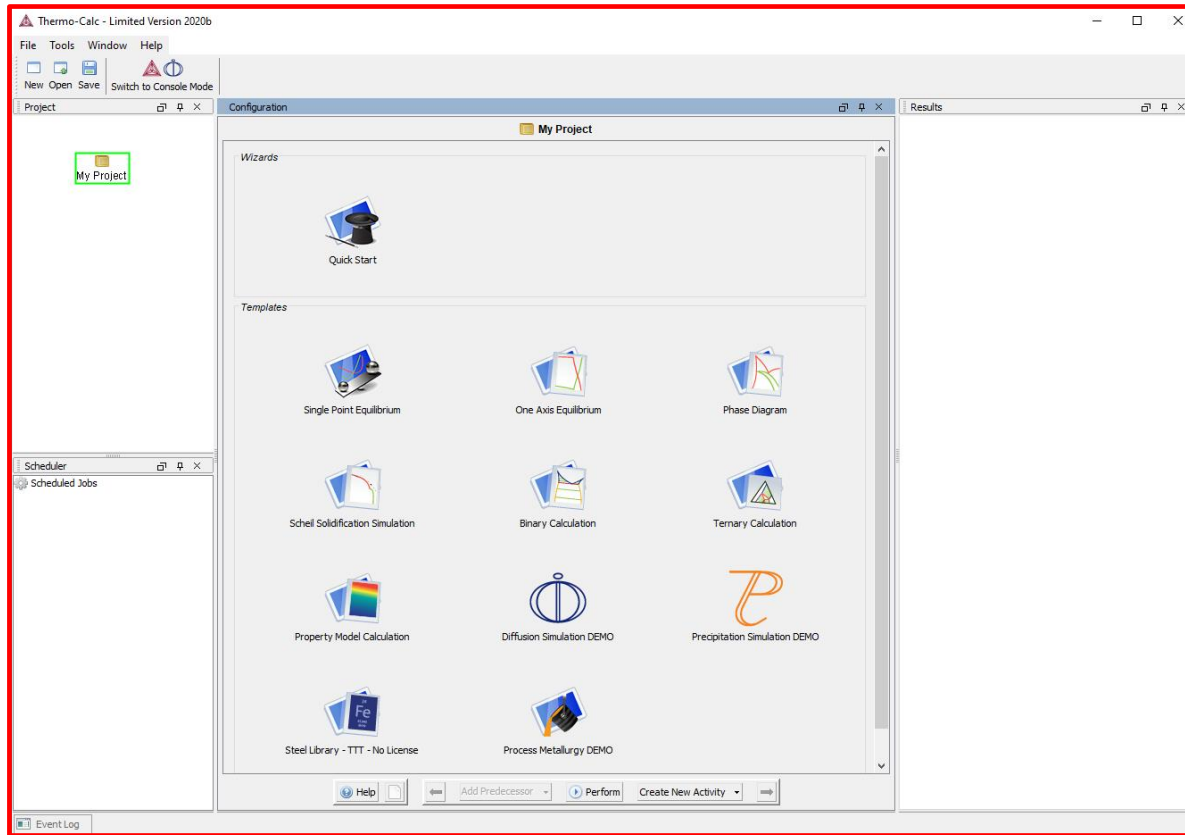
Tasks: Three types of calculations



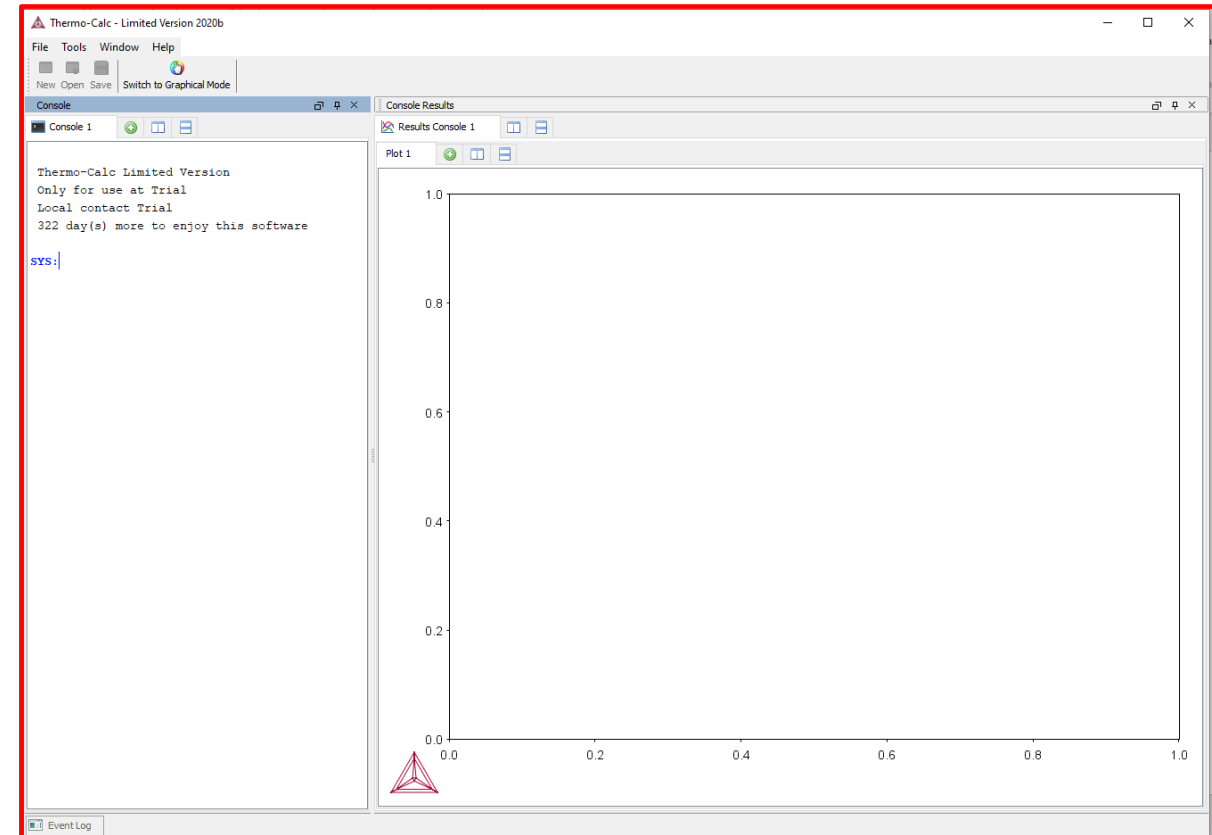
- I. Single Equilibrium (Single Point Calculation): **Nothing is varied**
- II. Step Calculation (Property Diagram): **One state variable is varied**
- III. Map Calculation (Phase Diagram): **Two state variables are varied**

Thermo-Calc operations

Thermo-CalC graphical user interface



GUI mode

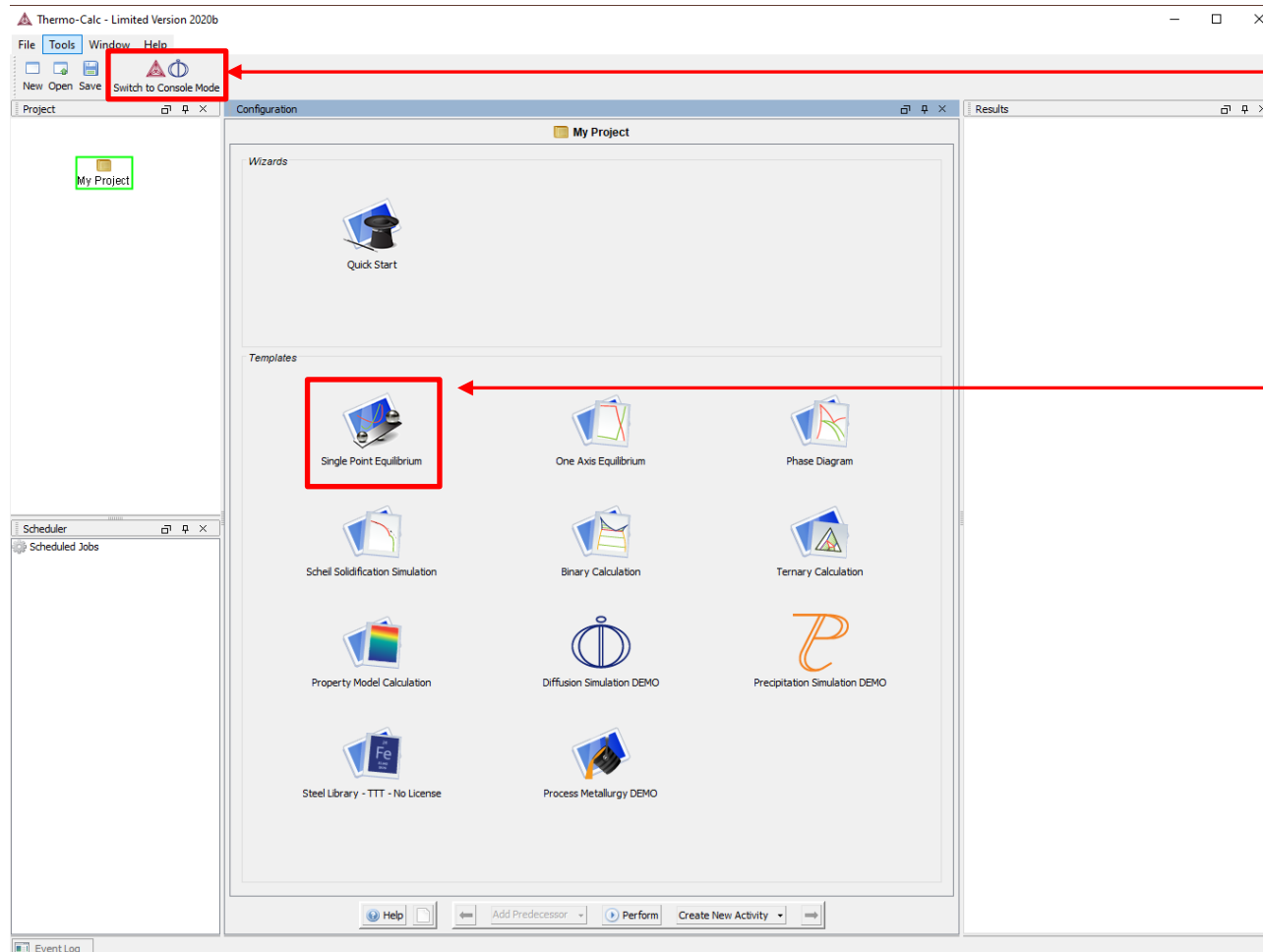


Console mode

Task: #1 Single point calculation of Fe-0.02C at $T=820^{\circ}\text{C}$

Determine phase fraction and compositions at a given temperature

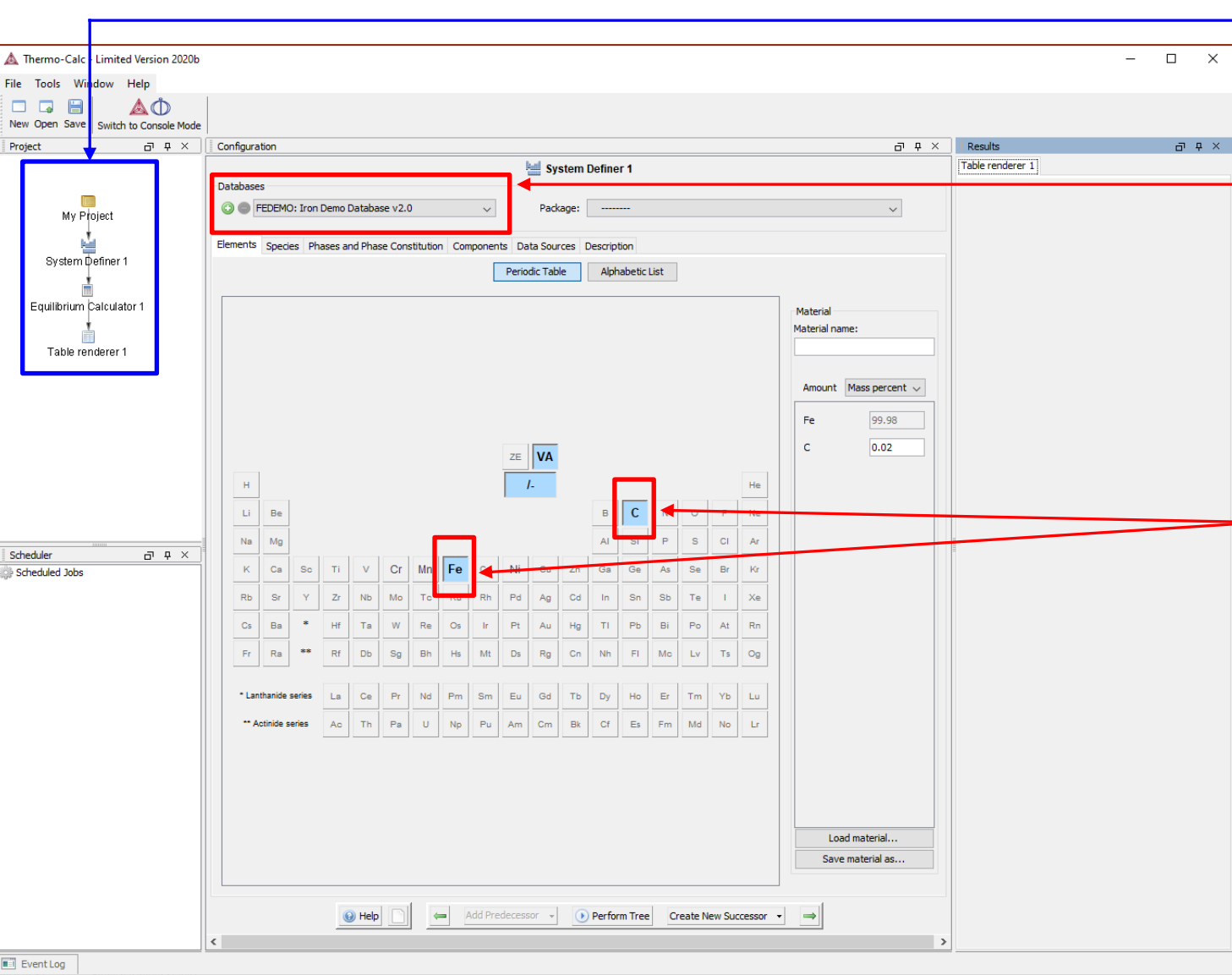
Step 1: Open Thermo-Calc 2020b and enter GUI mode. Select `Single Point Equilibrium`



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

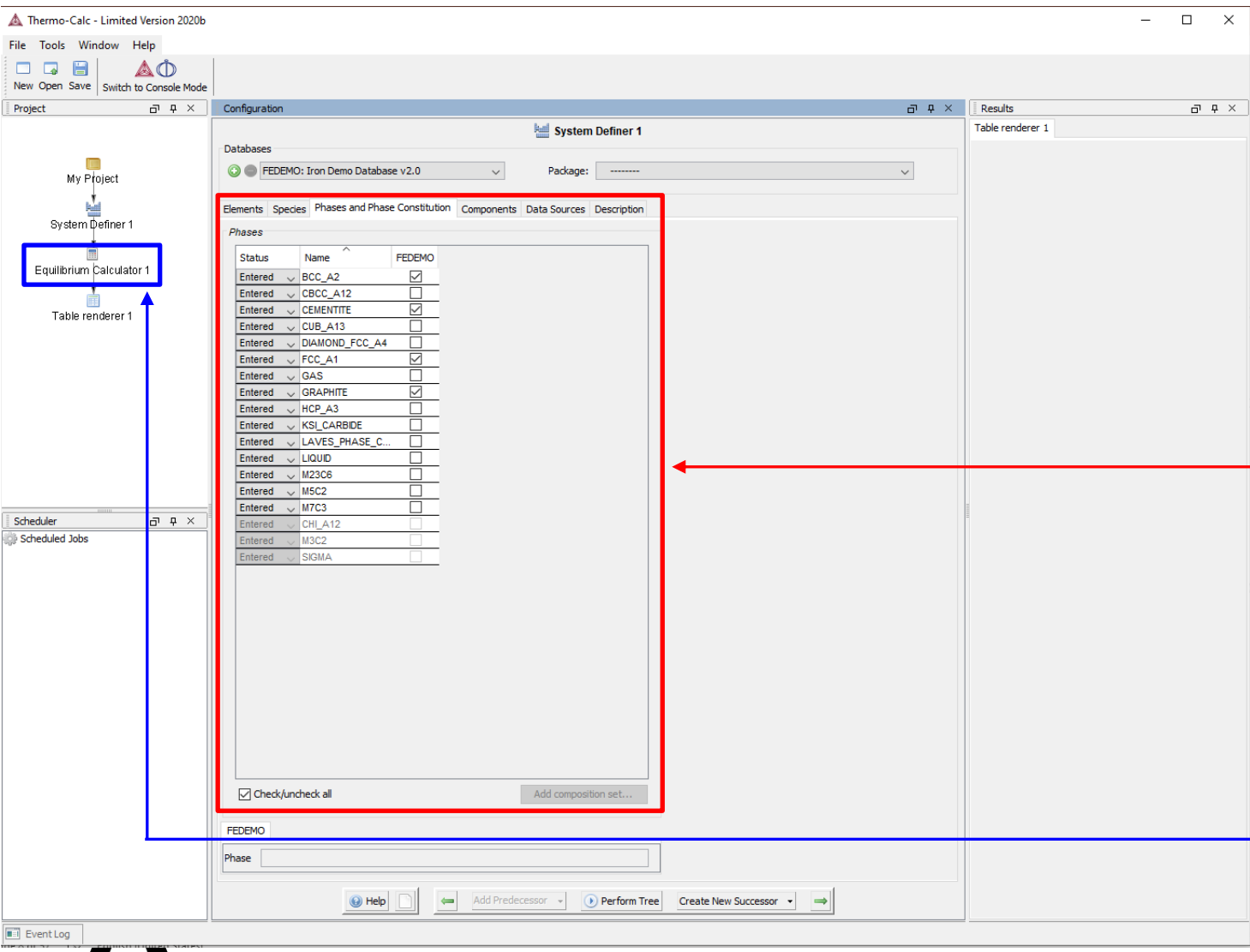


The Project Tree structure will populate. We begin the System Definer 1

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

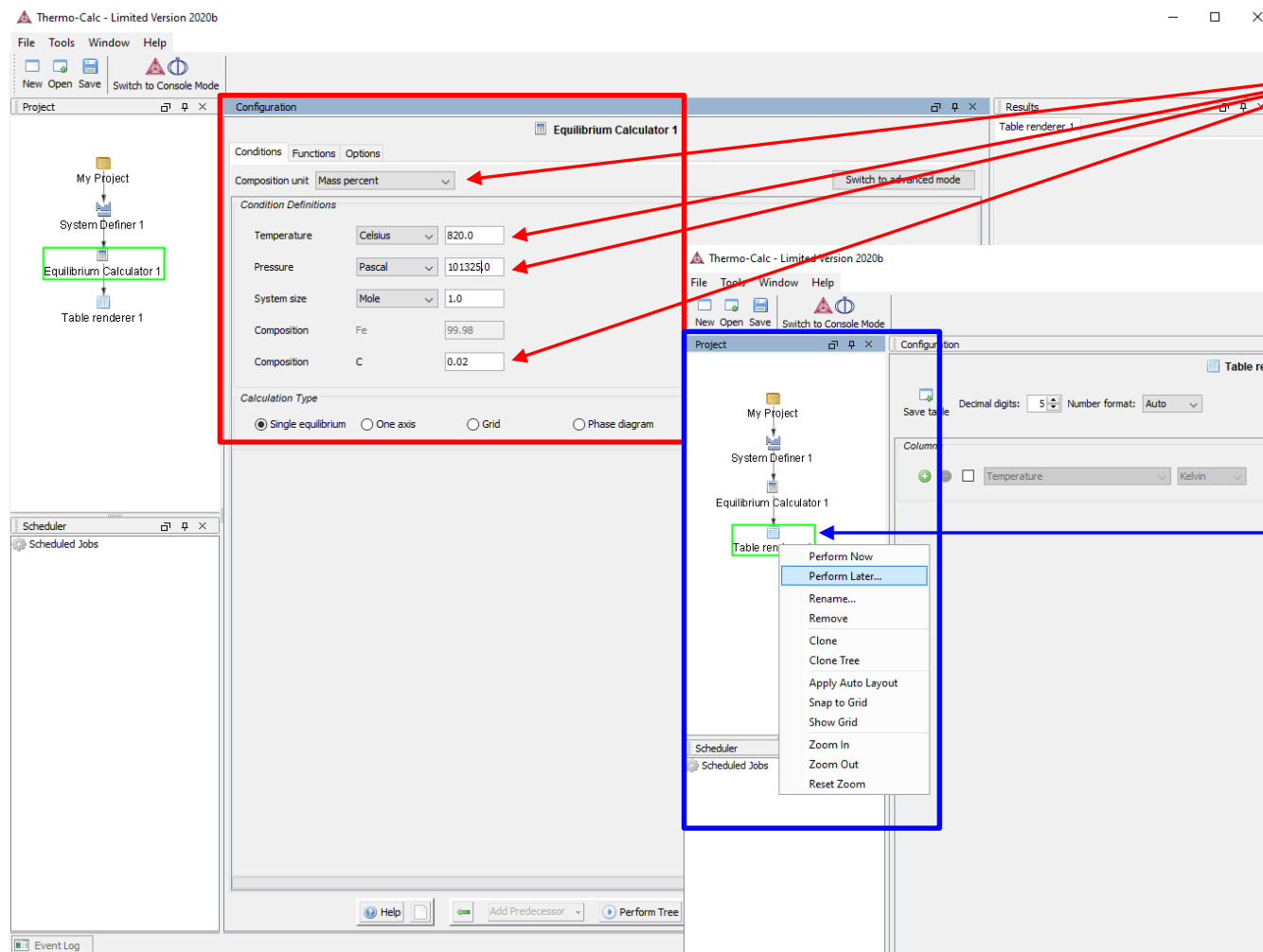
Add **Fe** and **C** to the system by clicking on the list

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

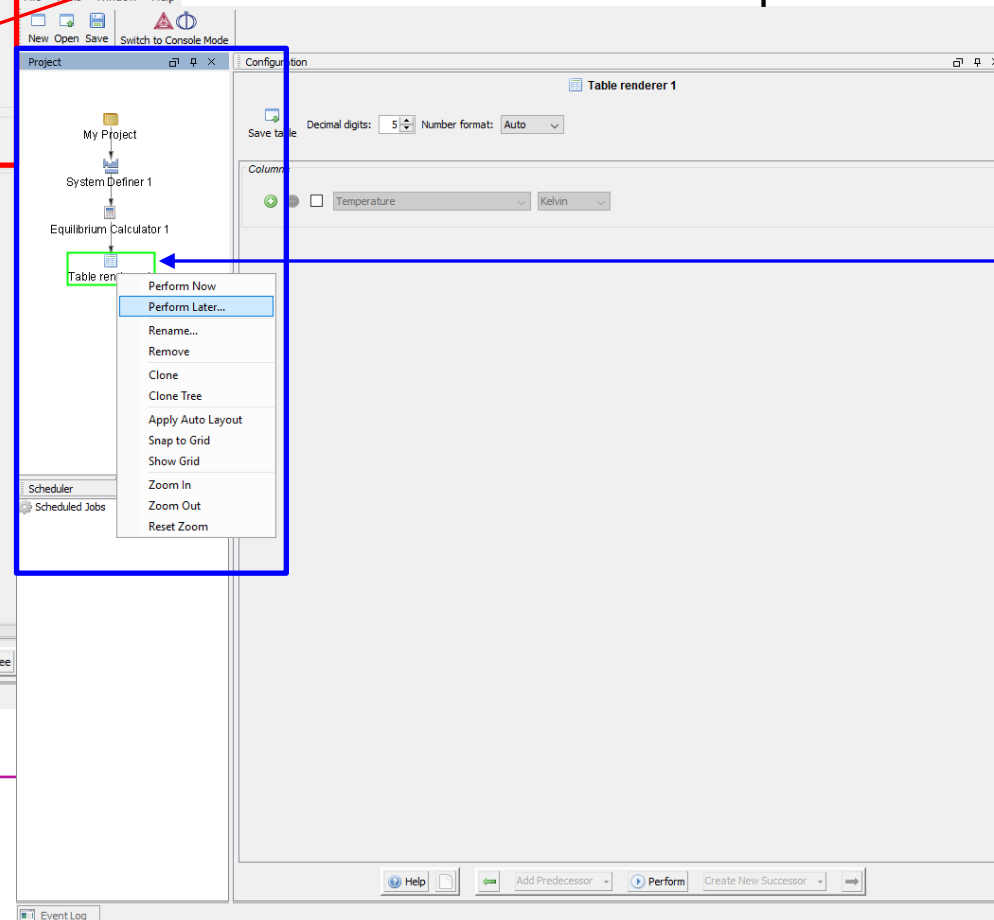


1. Click [Phases and Phase Constitution] Tab.
Uncheck all phases except:
**BCC_A2,CEMENTITE,
FCC_A1, GRAPHITE**
Only the checked phases are `Entered` and are allowed in the calculation.
Unchecked phases are `Suspended`
2. Click the [Equilibrium Calculator 1] in the `Project` window to proceed to set 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

The screenshot shows the Thermo-Calc software interface. The 'Table renderer 1' window is highlighted with a red box, showing the results of the calculation. The 'Event Log' window is also visible, showing the sequence of events during the calculation.

Table Renderer 1

System

Moles	1.00000
Mass	55.80627 [g]
Temperature	1093.15000 [K]
Total Gibbs Energy	-48726.52792 [J]
Enthalpy	29719.13772 [J]
Volume	7.34142E-6 [m³]

Component Mole Fraction Mass Fraction Activity Potential

C	0.00093	0.00020	0.04103	-29026.00477
Fe	0.99907	0.99980	0.00469	-48744.85171

Stable Phases

	Moles	Mass	Volume Fraction	
BCC_A2#1	0.95966	53.57448	0.96043	Composition
Composition				
Component	Mole Fraction	Mass Fraction		
Fe	0.99953	0.99990		
C	0.00047	0.00010		
FCC_A1#1	0.04034	2.23179	0.03957	Composition
Composition				
Component	Mole Fraction	Mass Fraction		
Fe	0.98805	0.99741		
C	0.01195	0.00259		

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

Event Log

```
00:37:27,447 INFO Gobblid: 00:37:27,446 INFO Koermann, T. Hickel, J. Neugebauer, CALPHAD, 34, 129 -33(2010); Fe-C'  
00:37:27,447 INFO Gobblid: 00:37:27,446 INFO 'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121 -127; Molar  
00:37:27,448 INFO Gobblid: 00:37:27,446 INFO volumes'  
00:37:27,635 INFO The activity System Definer 1 executed in 1488 ms  
00:37:27,644 INFO Performing general equilibrium calculation  
00:37:27,812 INFO *** Invoking Gibbs Energy System v6 ***  
00:37:28,087 INFO The subprocess completed normally  
00:37:28,354 INFO The activity Equilibrium Calculator 1 executed in 717 ms  
00:37:28,476 INFO The activity Table renderer 1 executed in 121 ms
```

Table renderer 1				
System				
Moles	1.00000			
Mass	55.80627	[g]		
Temperature	1093.15000	[K]		
Total Gibbs Energy	-48726.52792	[J]		
Enthalpy	29719.13772	[J]		
Volume	7.34142E-6	[m³]		
 Component Mole Fraction Mass Fraction Activity Potential				
C	0.00093	0.00020	0.04103	-29026.00477
Fe	0.99907	0.99980	0.00469	-48744.85171
 Stable Phases				
	Moles	Mass	Volume Fraction	
BCC_A2#1	0.95966	53.57448	0.96043	Composition
 Composition				
Component	Mole Fraction	Mass Fraction		
Fe	0.99953	0.99990		
C	0.00047	0.00010		
 FCC_A1#1				
	Moles	Mass	Volume Fraction	
FCC_A1#1	0.04034	2.23179	0.03957	Composition
 Composition				
Component	Mole Fraction	Mass Fraction		
Fe	0.98805	0.99741		
C	0.01195	0.00259		

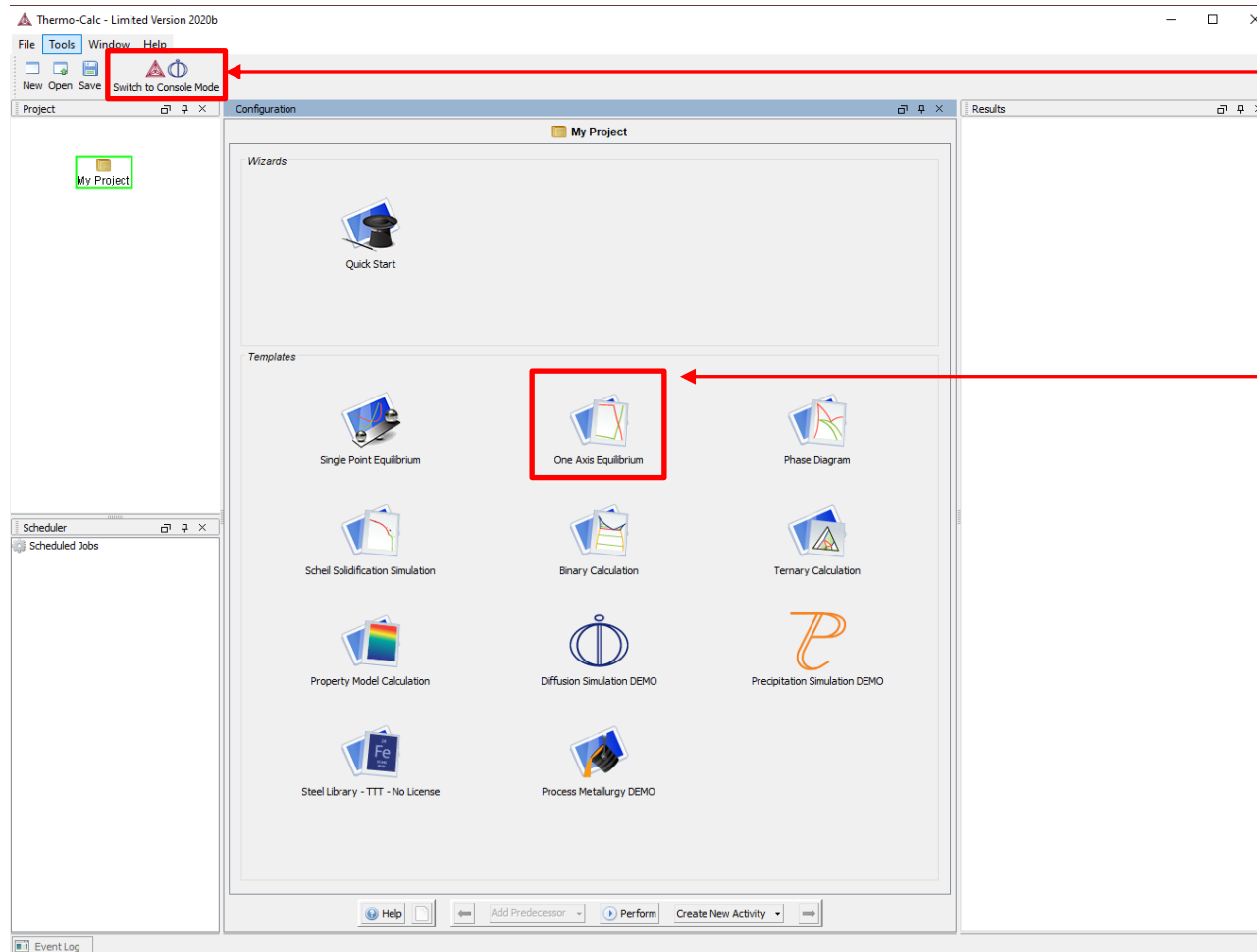
The Stable Phases are listed with Mole, Mass, Volume fractions and Compositions

The results should match what you calculate from Lever Rule.

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.

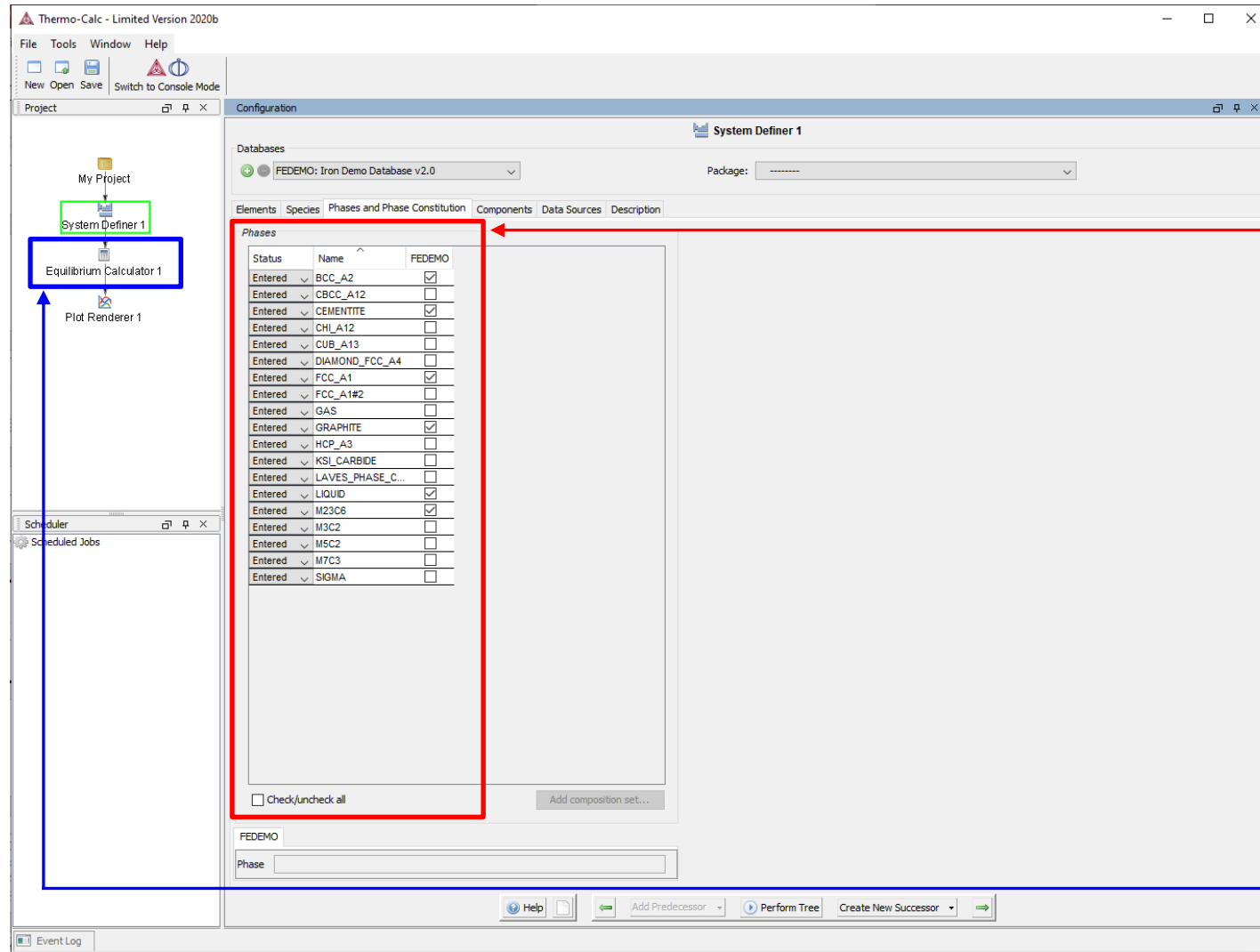
The screenshot shows the Thermo-Calc software interface. The main window is titled 'System Definer 1'. The 'Databases' dropdown menu is set to 'FEDEMO: Iron Demo Database v2.0'. The 'Phases and Phase Constitution' tab is selected. The periodic table is displayed, with elements Fe, C, and Cr highlighted. The material name is empty, and the amount is set to mass percent. The interface also includes a 'Scheduler' window on the left and an 'Event Log' at the bottom.

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.

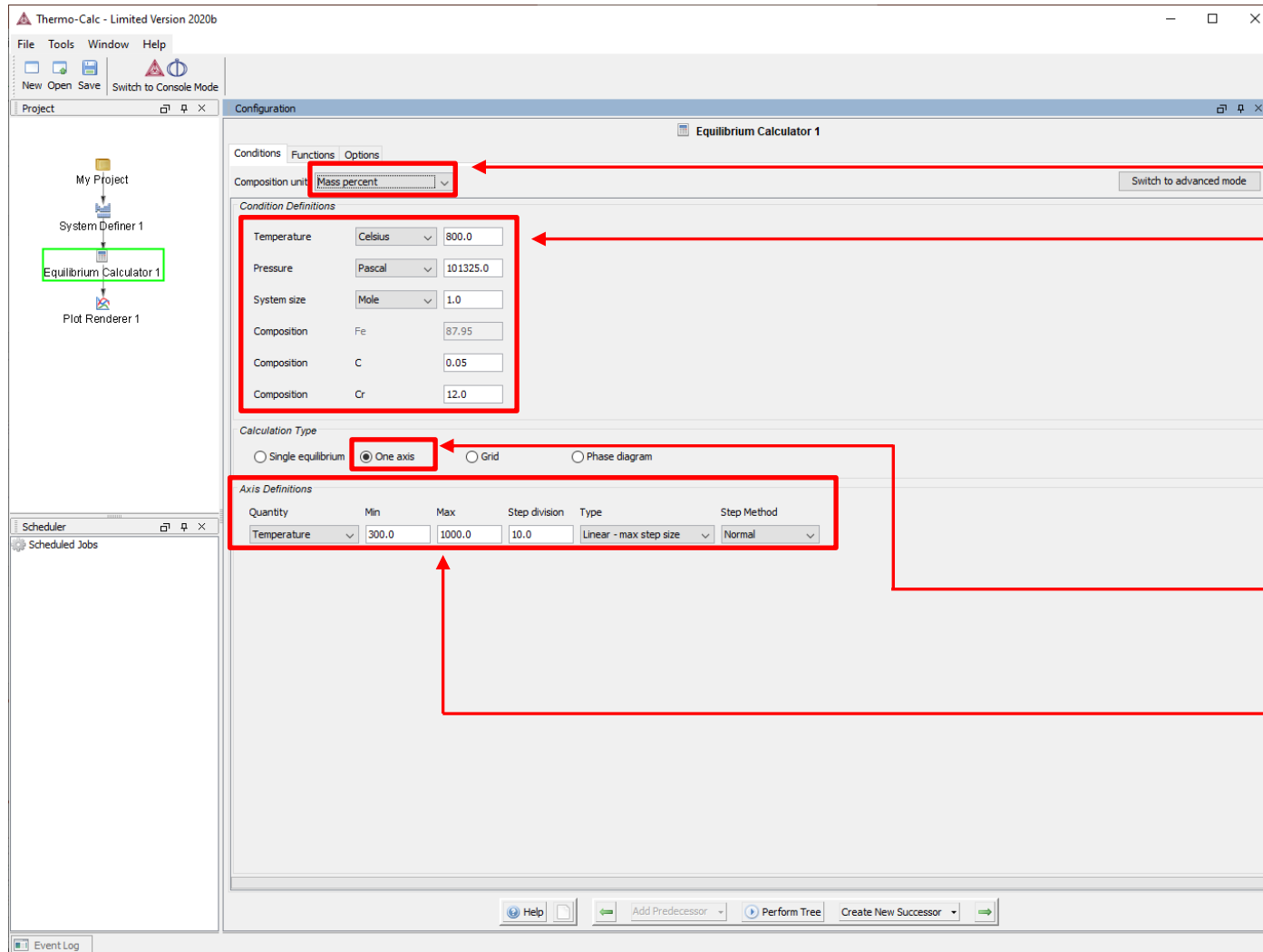
2. Check the following phases: **BCC_A2, CEMENTITE, FCC_A1, GRAPHITE, LIQUID, M23C6**

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.

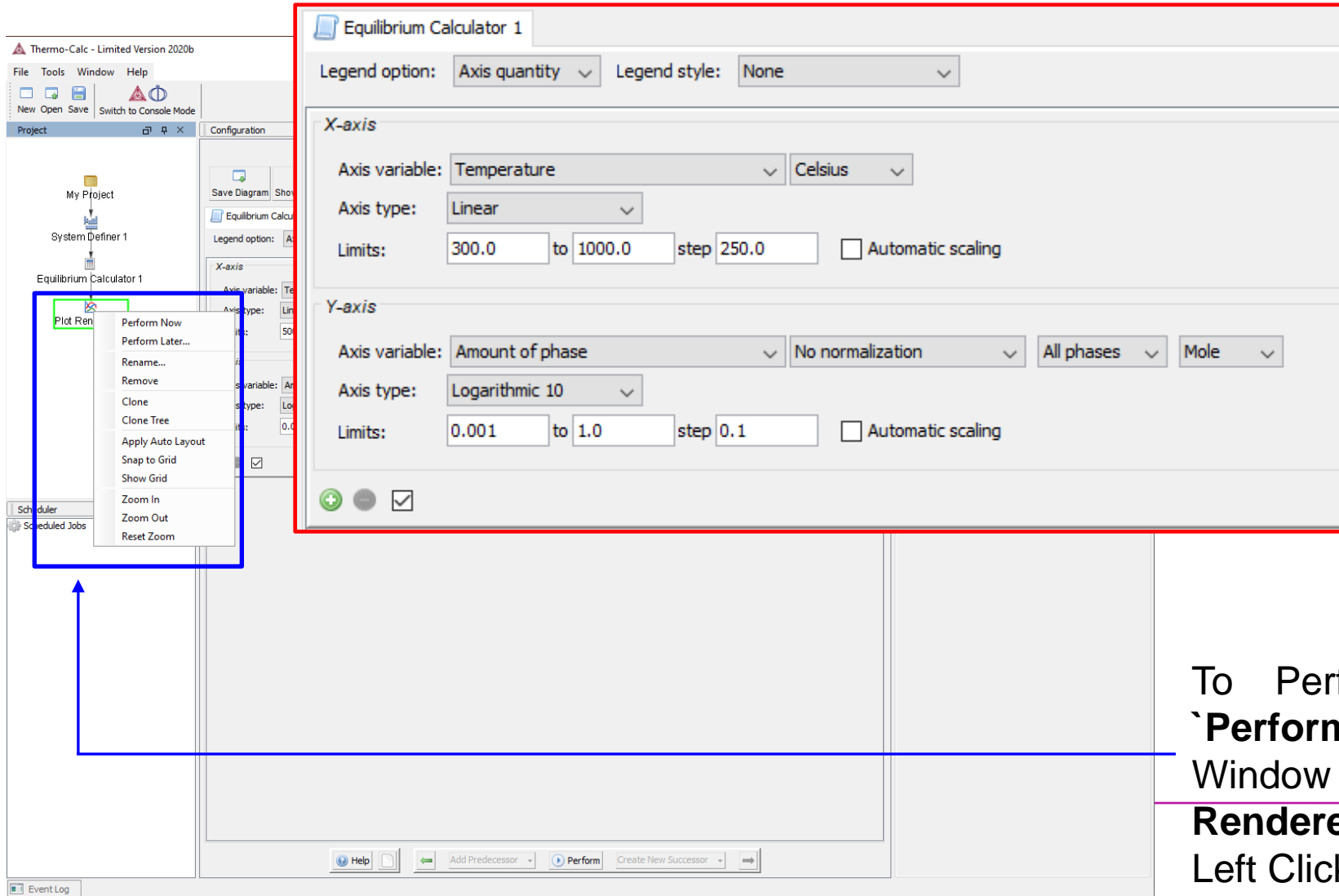
Under **`Axis Definitions`** (This defines the step calculation):

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**

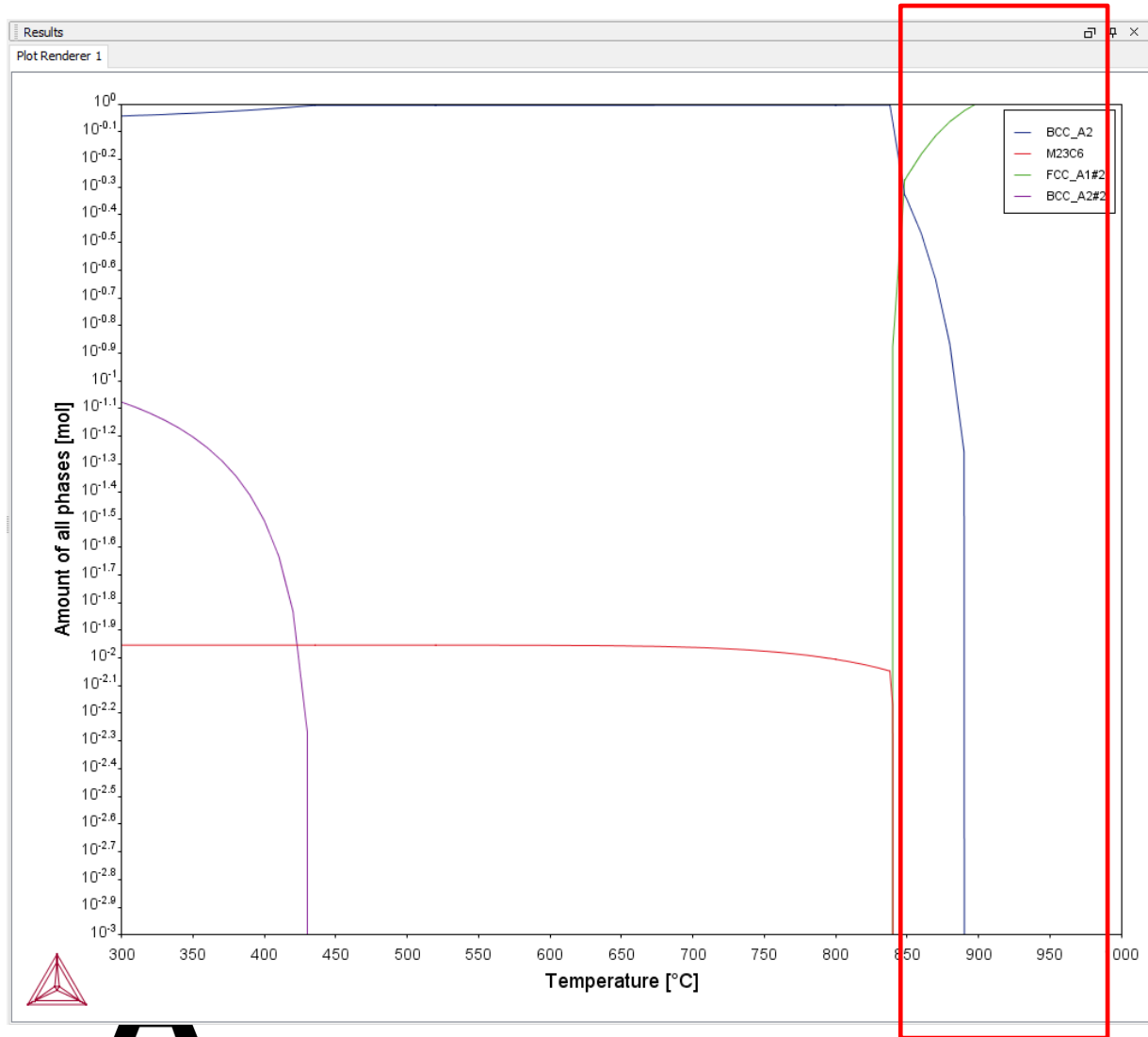
Y-Axis: Make Axis Type “Logarithmic 10”. **Adjust Limits to Min: 0.001, Max: 1.0**

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.

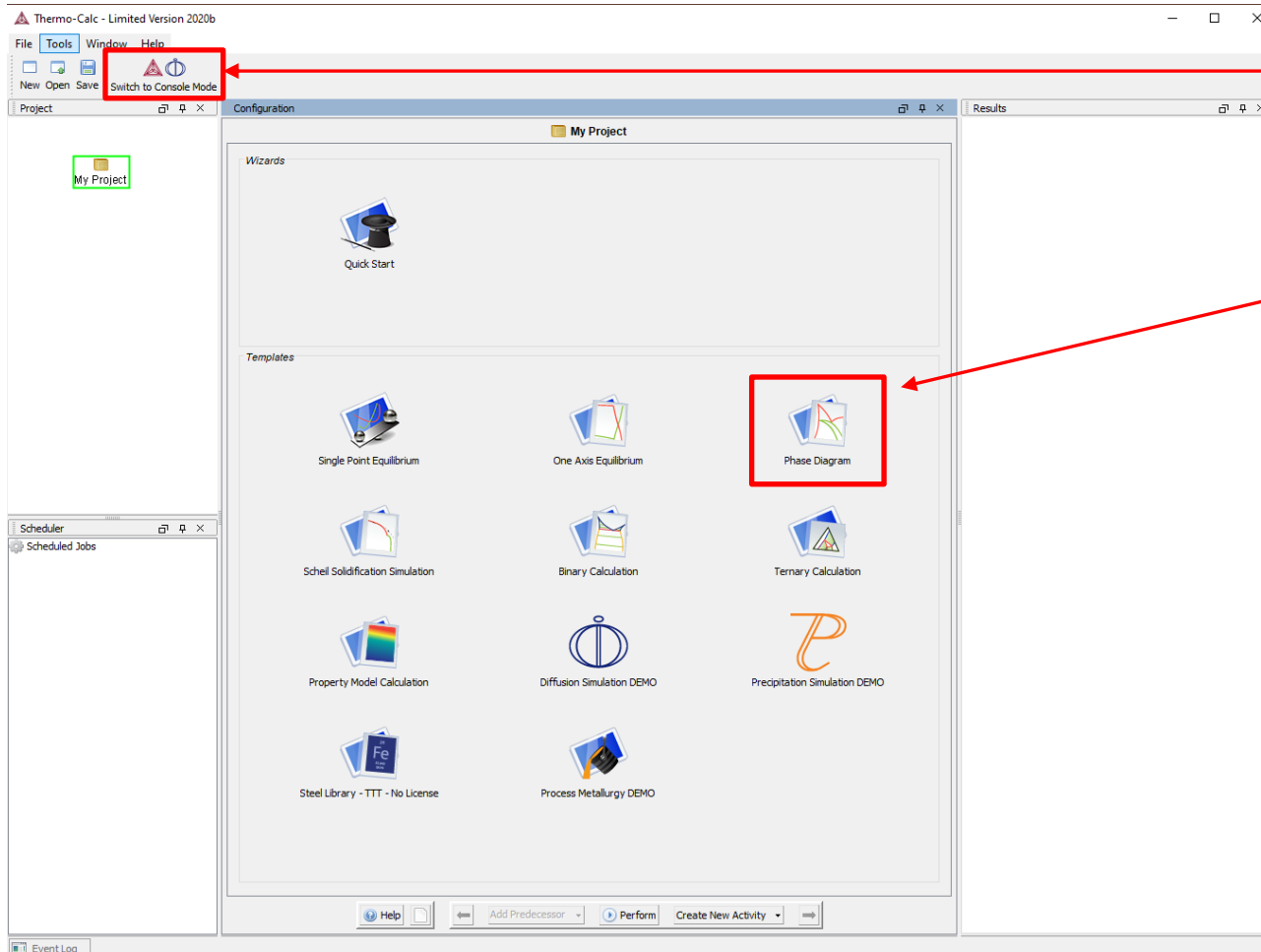
The phase line color matches the legend. The diagram can be saved by Right-Click **Save As**

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 calculation (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

The screenshot shows the Thermo-Calc software interface. The 'Configuration' window is active, displaying the 'System Definer 1' configuration. The 'Databases' dropdown menu is set to 'FEDEMO: Iron Demo Database v2.0'. The 'Elements' tab is selected, showing a periodic table with 'Fe' and 'C' highlighted. The 'Amount' column shows 'Fe' at 99.98 and 'C' at 0.02. The 'Phases and Phase Constitution' tab is also visible. The 'Material' name field is empty. The 'Load material...' and 'Save material as...' buttons are at the bottom right. The 'Scheduler' window is visible on the left, showing 'My Project' and 'System Definer 1'.

Thermo-Calc - Limited Version 2020b

File Tools Window Help

New Open Save Switch to Console Mode

Project

My Project

System Definer 1

Equilibrium Calculator 1

Plot Renderer 1

Scheduler

Scheduled Jobs

Configuration

System Definer 1

Databases: FEDEMO: Iron Demo Database v2.0

Package: -----

Elements Species Phases and Phase Constitution Components Data Sources Description

Periodic Table Alphabetic List

Material

Material name:

Amount Mass percent

Fe 99.98

C 0.02

Load material...

Save material as...

Help Add Predecessor Perform Tree Create New Successor

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.

Configuration

Databases

FEDEMO: Iron Demo Database v2.0

Elements Species Phases and Phase Constitution Com

Phases

Status	Name ^	FEDEMO
Entered	BCC_A2	<input checked="" type="checkbox"/>
Entered	CBCC_A12	<input type="checkbox"/>
Entered	CEMENTITE	<input checked="" type="checkbox"/>
Entered	CUB_A13	<input type="checkbox"/>
Entered	DIAMOND_FCC_A4	<input type="checkbox"/>
Entered	FCC_A1	<input checked="" type="checkbox"/>
Entered	GAS	<input type="checkbox"/>
Dormant	GRAPHITE	<input checked="" type="checkbox"/>
Entered	HCP_A3	<input type="checkbox"/>
Entered	KSI_CARBIDE	<input type="checkbox"/>
Entered	LAVES_PHASE_C...	<input type="checkbox"/>
Entered	LIQUID	<input checked="" type="checkbox"/>
Entered	M23C6	<input type="checkbox"/>
Entered	M5C2	<input type="checkbox"/>
Entered	M7C3	<input type="checkbox"/>
Entered	CHI_A12	<input type="checkbox"/>
Entered	M3C2	<input type="checkbox"/>
Entered	SIGMA	<input type="checkbox"/>

Change GRAPHITE to 'DORMANT' with dropdown menu

☐ Check/uncheck all

Add composition set...

FEDEMO

Phase

Help Add Predecessor Perform Tree Create New Successor

Uncheck all phases and then Click to add:

BCC_A2, CEMENTITE, FCC_A1, GRAPHITE, LIQUID

Step 4: Step Map Conditions in Equilibrium Calculator

Equilibrium Calculator 1

Conditions Functions Options

Composition unit: Mass fraction

Switch to advanced mode

Condition Definitions

Temperature: Celsius 1200.0

Pressure: Pascal 101325.0

System size: Mole 1.0

Composition: Fe 0.98

Composition: C 0.02

Calculation Type

☐ Single equilibrium ☐ One axis ☐ Grid ☒ Phase diagram

Axis Definitions

Quantity	Min	Max	Step division	Type
Mass fraction C	0.0	1.0	50.0	Linear - min no. of steps
Temperature	500.0	2000.0	10.0	Linear - max step size

Help Add Predecessor Perform Tree Create New Successor

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 deviation** = 50.0

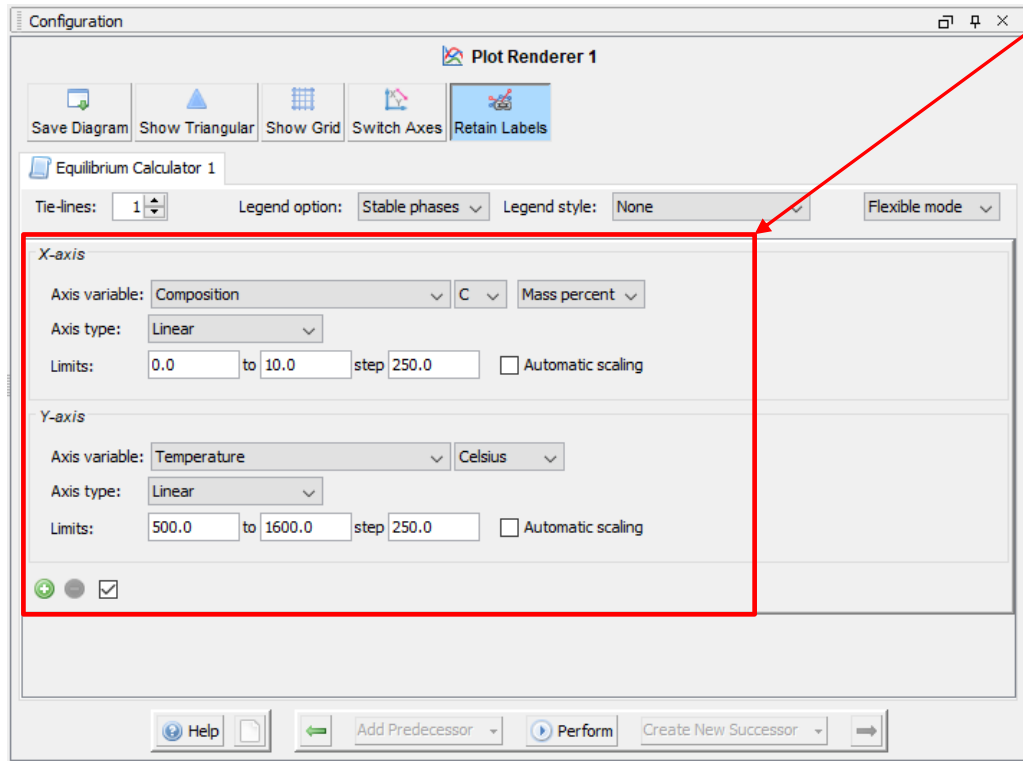
Type = Linear min No. of steps

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

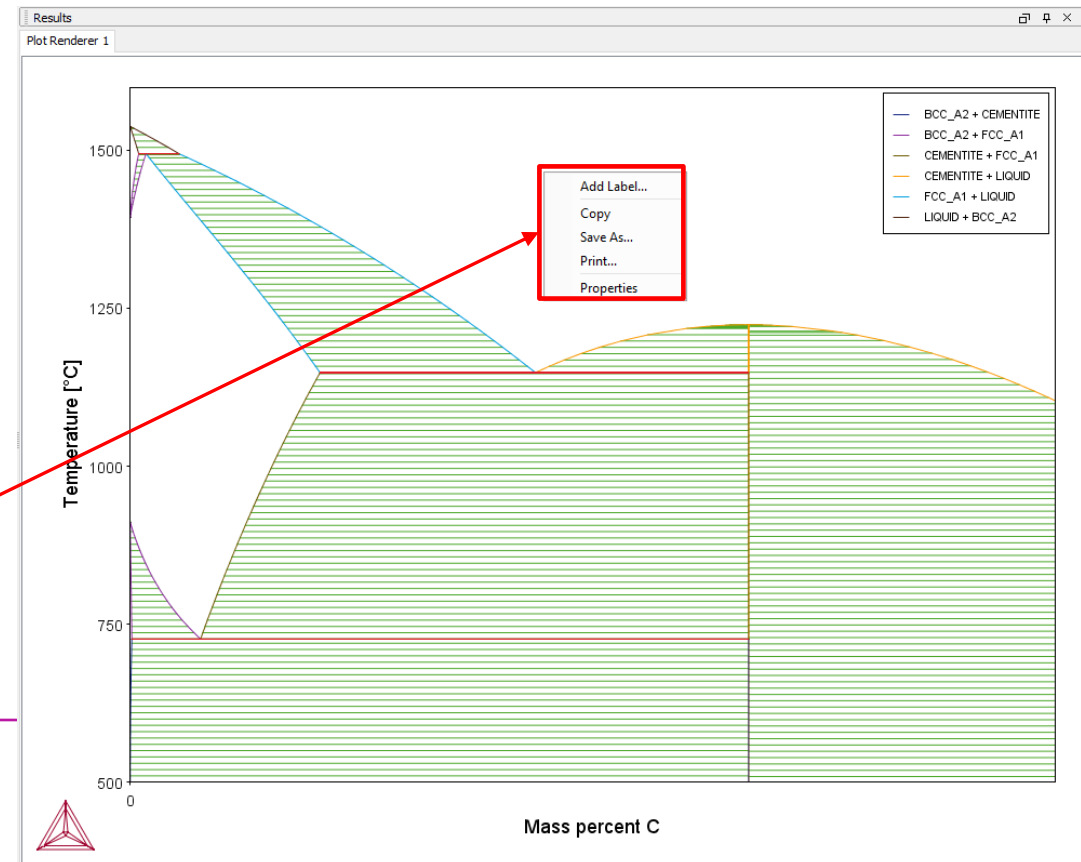


Change Limits:

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

Add Label

Label: LIQUID Plain text

Font: AaBbCc123 AaBbγγ

Rotation angle: 0.0

☒ Show anchor ☒ Hide details

Equilibrium Information

5

LIQUID (4.55200, 1459.67)

Quantities

Mass percent C	4.55200	[Mass percent]
Temperature	1459.66550	[°C]

System

Moles	1.00000
Mass	47.89080 [g]
Temperature	1732.81550 [K]
Total Gibbs Energy	-93955.47061 [J]
Enthalpy	65652.86395 [J]
Volume	7.03249E-6 [m³]

Component Mole Fraction Mass Fraction Activity Potential

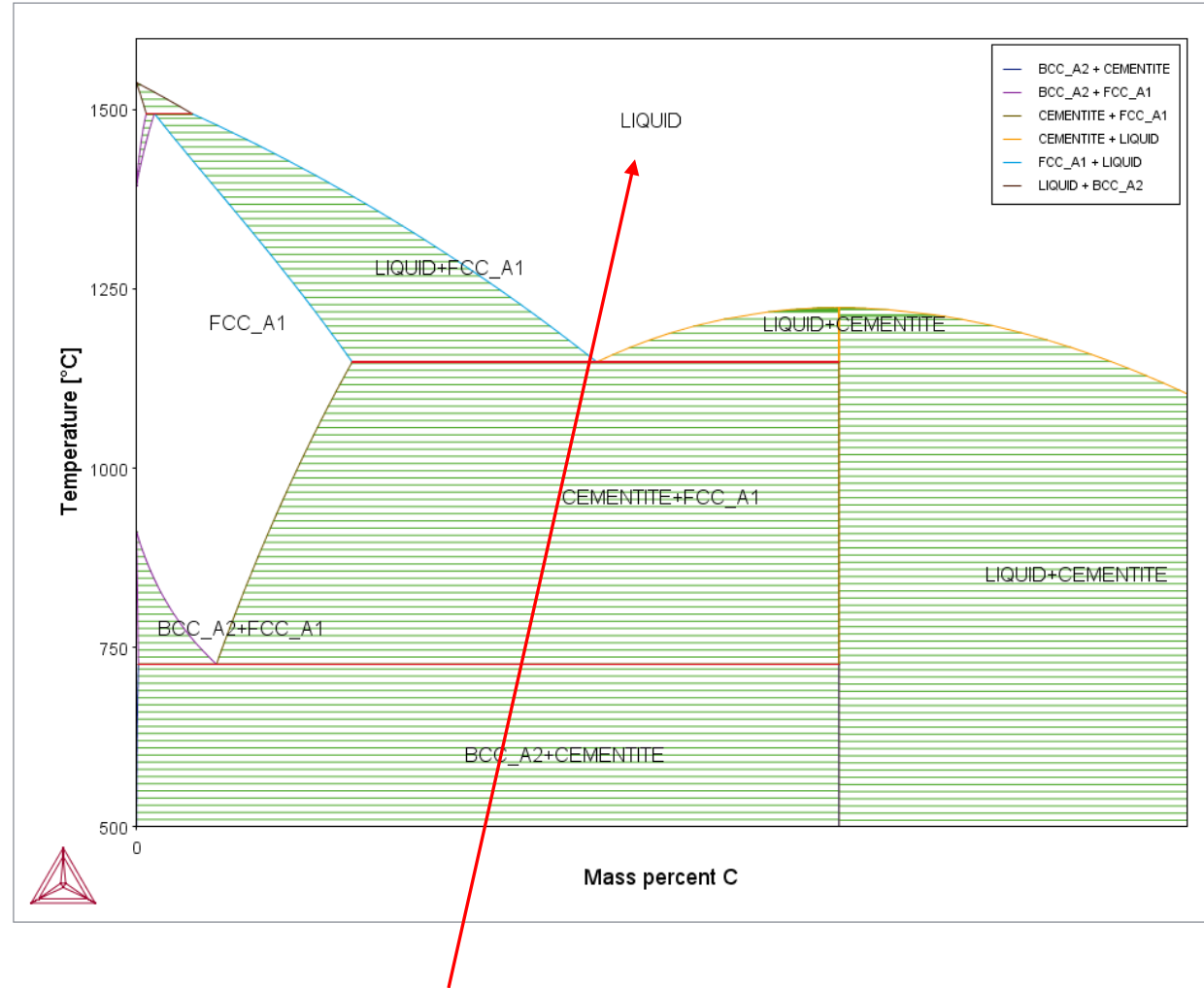
C	0.18150	0.04552	0.06301	-39828.07226
Fe	0.81850	0.95448	0.00064	-1.05958E5

Stable Phases

	Moles	Mass	Volume Fraction	
LIQUID#1	1.00000	47.89080	1.00000	Composition

Composition

Component	Mole Fraction	Mass Fraction
C	0.18150	0.04552
Fe	0.81850	0.95448



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 Exercises

- 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**