

Beginner's Introduction to TC 3.0

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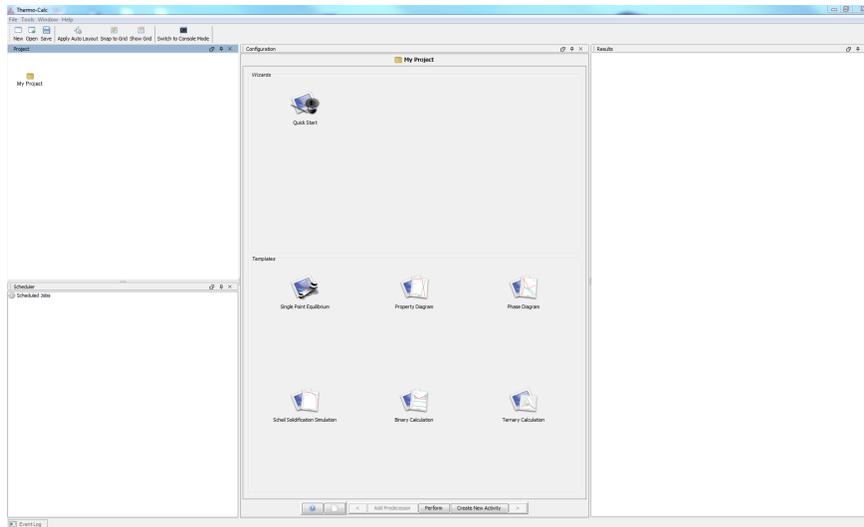


Figure 1: The default view when starting TC 3.0.

1 Beginner’s Introduction to TC 3.0

The default view when starting the program should be as shown in Fig. 1. If the windows have been rearranged they can be reset to the default view by choosing Window -> Reset Windows from the top menu.

2 Calculating a single point equilibrium using the Quick Start wizard

The easiest way to start is to use the “Quick Start” – press this. The windows that appear will guide you through all necessary steps.

- The first window show different project types. Among the options available are “Single point equilibrium”. Choose this and press **next**.
- In the second window the database and the system is selected (or a Material file if created previously). Choose, for example, the PTERN database and elements Fe and C and press **next**.



Figure 2: The GUI layout

- In the third window the equilibrium conditions are selected. Set, for example, the temperature to 1000 K and the composition to 1 mass-% C. One should normally also specify pressure and system size, but these are set to default values when the Quick Start wizard is used. Press **Finish**.

The result from the calculation is in the default view shown to the right. The System and the Stable Phases are listed in a “Table Renderer”.

3 GUI (graphical user interface) Layout

The basic components are shown in Fig. 2.

1. Project window

The purpose of the project window is to create, manipulate and navigate between the activities that make up a project. By left-clicking on an activity it is selected. Right-clicking on an activity yields a menu that shows the options available for that particular activity.

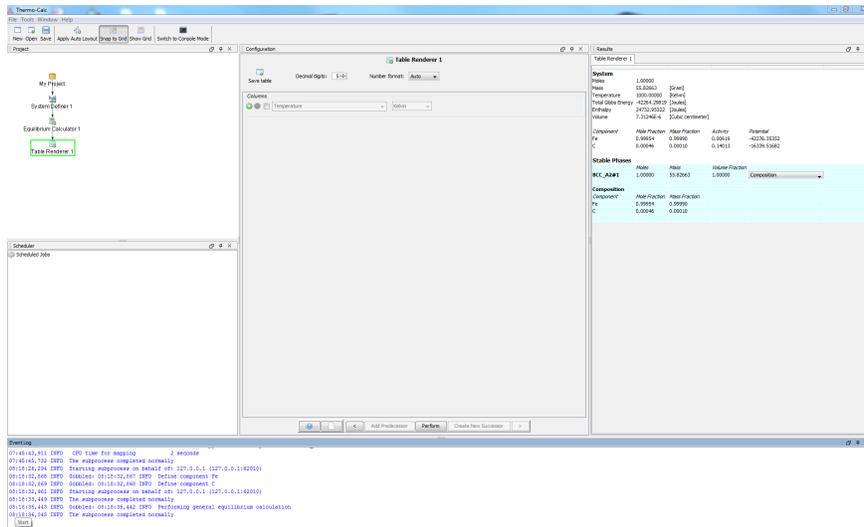


Figure 3: Output from a single-point equilibrium

2. Configuration window

This shows the settings of the currently selected activity.

3. Results window

This shows the results of the last activity that was selected that produce graphic or text output.

4. Scheduler window

This window show information of jobs, i.e. calculations, that are being performed or that are scheduled to be performed.

5. Event log window (hidden by default)

This window is by default hidden, but, also by default, pops up during calculations to yield progress information.

4 Calculating a single-point equilibrium step by step

All the necessary activities can be set up by the program if the *Single Point Equilibrium Template* is used. Alternatively, the activities can be created one at a time by selecting and right-clicking the appropriate predecessor.

1. Define the thermodynamic system
 - If there isn't one already, first create a System Definer activity by right clicking the default My Project activity in the top left Project window and choose **Create New Activity -> System Definer** in the menu that appear.
 - Select the System Definer activity by left clicking its icon in the Project window.
 - In the middle Configuration window, which now shows the settings for the selected System Definer, do the following.
 - Make sure that the view is of the Elements tab.
 - Select the thermodynamic database PTERN.
 - The elements present in the selected database are shown either as an alphabetic list or highlighted in a periodic table. Select carbon, C and iron, Fe. Vacancy, VA, is pre-selected and should be disregarded.
 - Click the Perform button at the bottom of the Configuration window to read thermodynamic data from file.
2. Set the thermodynamic conditions
 - If there isn't one already, first create an Equilibrium Calculator activity by right clicking the icon of the previously used System Definer activity in Project window and choose **Create New Successor -> Equilibrium Calculator**.
 - Select the Equilibrium Calculator activity by left clicking its icon.
 - In the middle Configuration window, which now shows the settings for the selected Equilibrium Calculator, do the following.
 - Make sure that the view in the Configuration window is of the simplified mode; the text in the button in the upper right hand part should read "Switch to advanced mode".
 - Set Composition unit to Mole fraction.
 - Set Temperature to 1000 [K].
 - Set Pressure to 100000 [Pa].
 - Set System size to 2 [mol].

- The composition is specified by entering the mole fraction of either carbon or iron; one of these is dependent since the overall size of the system has been specified as 2 [mol]. Either set Composition C to 0.05 or Composition Fe to 0.95; the value for the other, dependent, composition will show up automatically.
- Make sure that the Axis definitions are un-selected since only a single equilibrium calculation will be performed.
- Click the Perform button to perform the equilibrium calculation

3. View results

- If there isn't one already, first create a Table Renderer activity by right clicking the Equilibrium Calculator icon and choose **Create New Successor -> Table Renderer**.
- Select the Table Renderer activity by left clicking its icon.
- In the middle Configuration window, which now shows the settings for the selected Table Renderer, do the following.
 - Since only a single equilibrium is calculated, make sure that all check boxes are un-selected.
 - Click the Perform button at the bottom.
- The equilibrium is now displayed in the right-most Results window. At the top are some general information about the system corresponding to the selected data and the thermodynamic conditions. Below are the stable phases listed along with their amount and composition.

5 Calculating a binary phase diagram step-by-step

As in the previous example there is a template that set up all the necessary activities.

1. Define the thermodynamic system

- If there isn't one already, first create a System Definer activity by right clicking the default My Project activity in the top left Project window and choose **Create New Activity -> System Definer** in the menu that appears.
- Select the System Definer activity by left clicking its icon in the Project window.

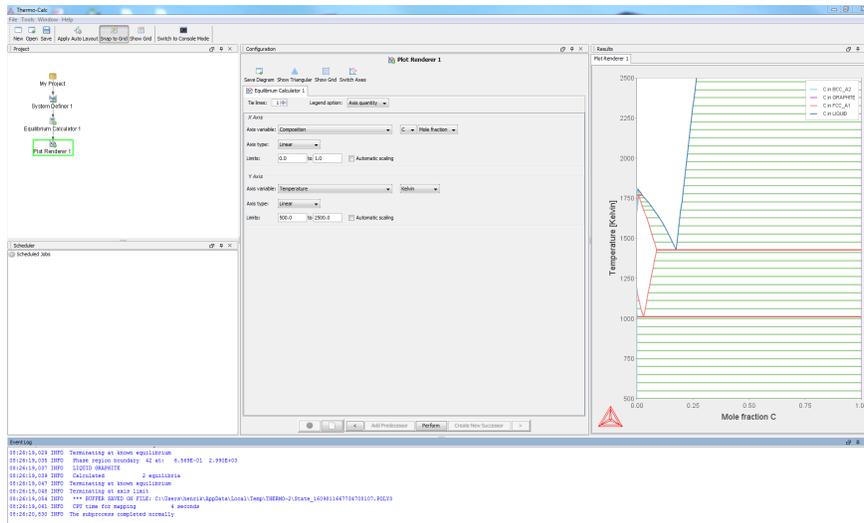


Figure 4: Output from a phase diagram calculation.

- In the middle Configuration window, which now shows the settings for the selected System Definer, do the following.
 - Make sure that the Elements tab is selected.
 - Select the thermodynamic database PTERN.
 - The elements present in the selected database are shown either as an alphabetic list or highlighted in a periodic table. Select carbon, C and iron, Fe. Vacancy, VA, is pre-selected and should be disregarded.
- Click the Perform button at the bottom of the Configuration window to read thermodynamic data from file.

2. Set the thermodynamic conditions

- If there isn't one already, first create an Equilibrium Calculator activity by right clicking the icon of the previously used System Definer activity in Project window and choose **Create New Successor -> Equilibrium Calculator**.
- Select the Equilibrium Calculator activity by left clicking its icon.
- In the middle Configuration window, which now shows the settings for the selected Equilibrium Calculator, do the following.

- Make sure that the view in the Configuration window is of the simplified mode; the text in the button in the upper right hand part should read Switch to advanced mode.
- Set Composition unit to Mole fraction.
- Set Temperature to 1000 [K].
- Set Pressure to 100000 [Pa].
- Set System size to 1 [mol].
- The composition is specified by entering the mole fraction of either carbon or iron; one of these is dependent since the overall size of the system has been specified as 1 [mol]. Either set Composition C to 0.05 or Composition Fe to 0.95; the value for the other, dependent, composition will show up automatically.
- Tick both the check boxes of the Axis definitions.
- One Axis definition should correspond to the the composition variable, i.e. mole fraction C or Fe and the other axis should be for temperature. Let the composition range be between 0.0 and 1.0 and the temperature range 500.0 to 2500.0. Let the other options for the axis definitions retain their default values.
- Click the Perform button to compute the phase diagram.

3. View results

- If there isn't one already, first create a Plot Renderer activity by right clicking the Equilibrium Calculator icon and choose **Create New Successor -> Plot Renderer**.
- Select the Plot Renderer activity by left clicking its icon.
- In the middle Configuration window, which now shows the settings for the selected Plot Renderer, do the following.
 - The settings for the X axis variable should be Composition, C, Mole fraction. The X axis type should be set to Linear and the X limits should be set to 0.0 and 1.0 with the Automatic scaling check box un-ticked.
 - The settings for the Y axis variable should be Temperature, Kelvin. The Y axis type should be set to Linear and the Y limits should be set to 500.0 and 2500.0 with the Automatic scaling check box un-ticked.
- Click the Perform button
- The Fe-C binary phase diagram should now be displayed in the right-most Results window.