The ***Results*** module

- ***Results*** generates graphs from Equilib Results (Equi*.Res) files.

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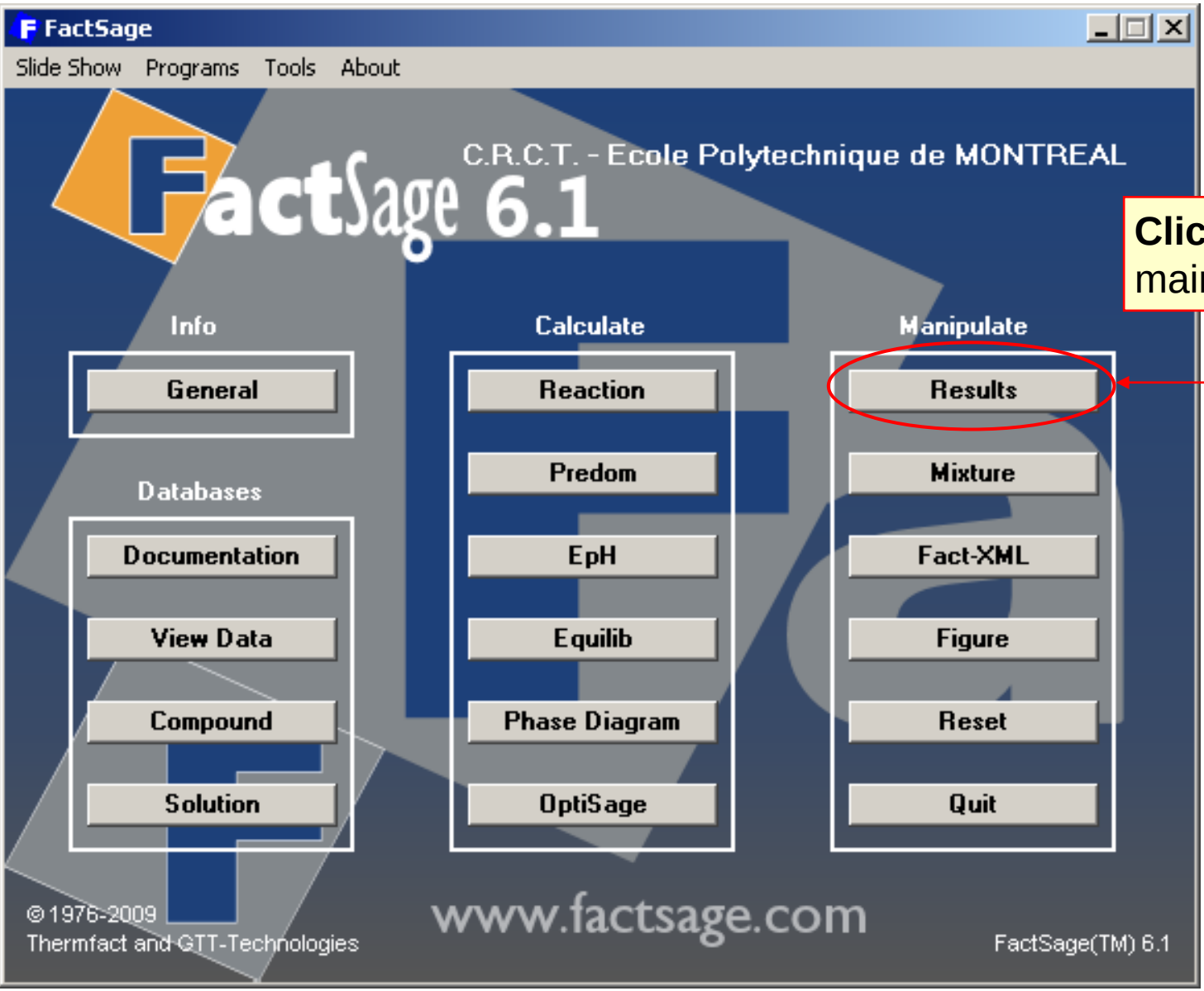
The ***Results*** module



Click on ***Results*** in the main ***FactSage*** window.

Creating a **Results** file in ***Equilib***

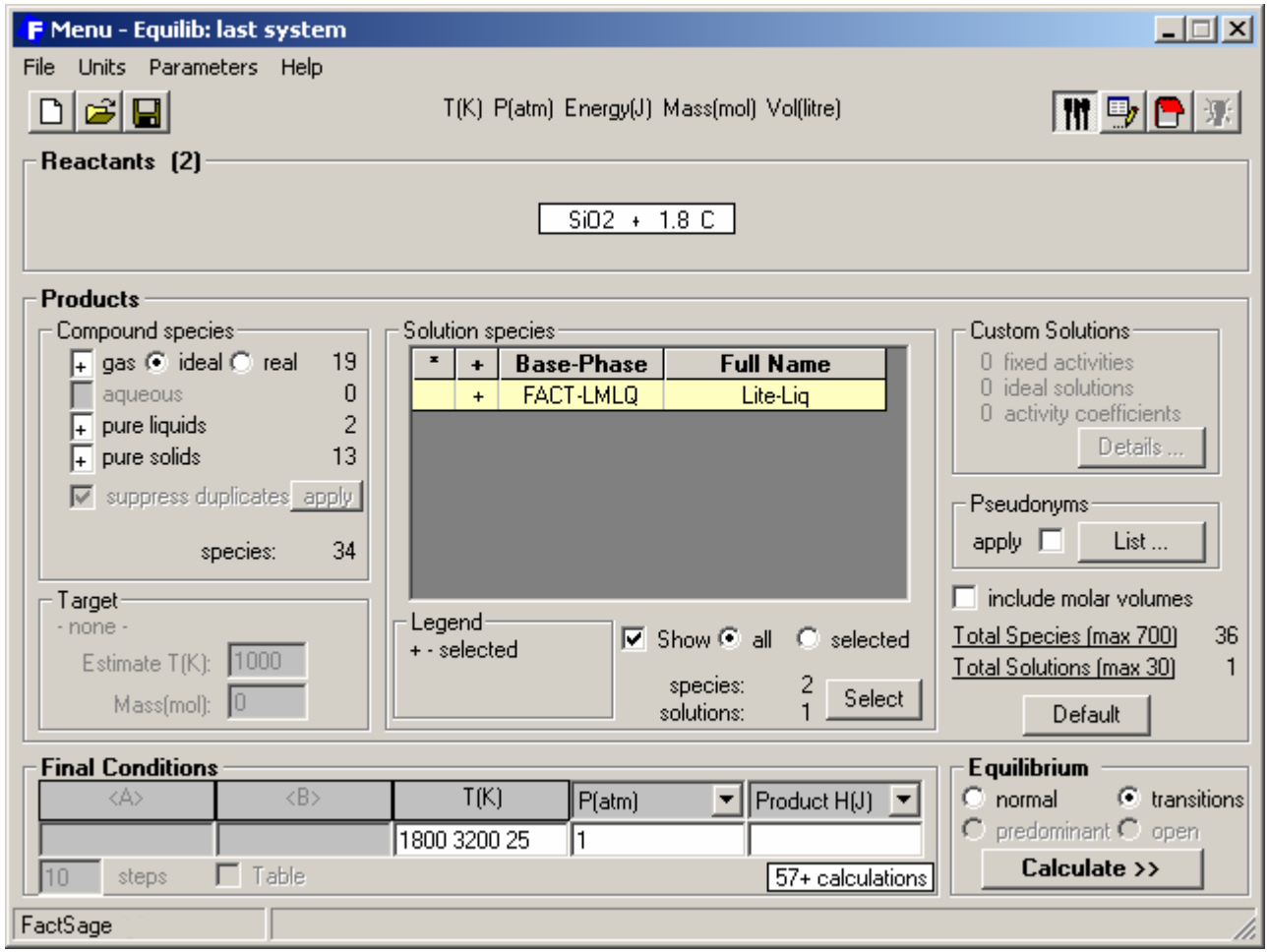
The ***Results*** module is used to post-process the output of complex equilibrium calculations performed with ***Equilib***.

There are two methods by which this post-processing can be initiated: Immediately after the execution of the calculation or at a later stage. In both cases the Results Window in Equilib is used to start the appropriate action.

In the present example it is assumed that the user has chosen the second method, i.e. he has stored the Equilib results in an Equi*.RES file and opened it later on in the Results module.

All the actions with the Results module which are shown here can also be performed in Equilib by using the Equilib Results file option (see slide 3.2).

Creating a **Results** file: the ***Equilib*** Menu window

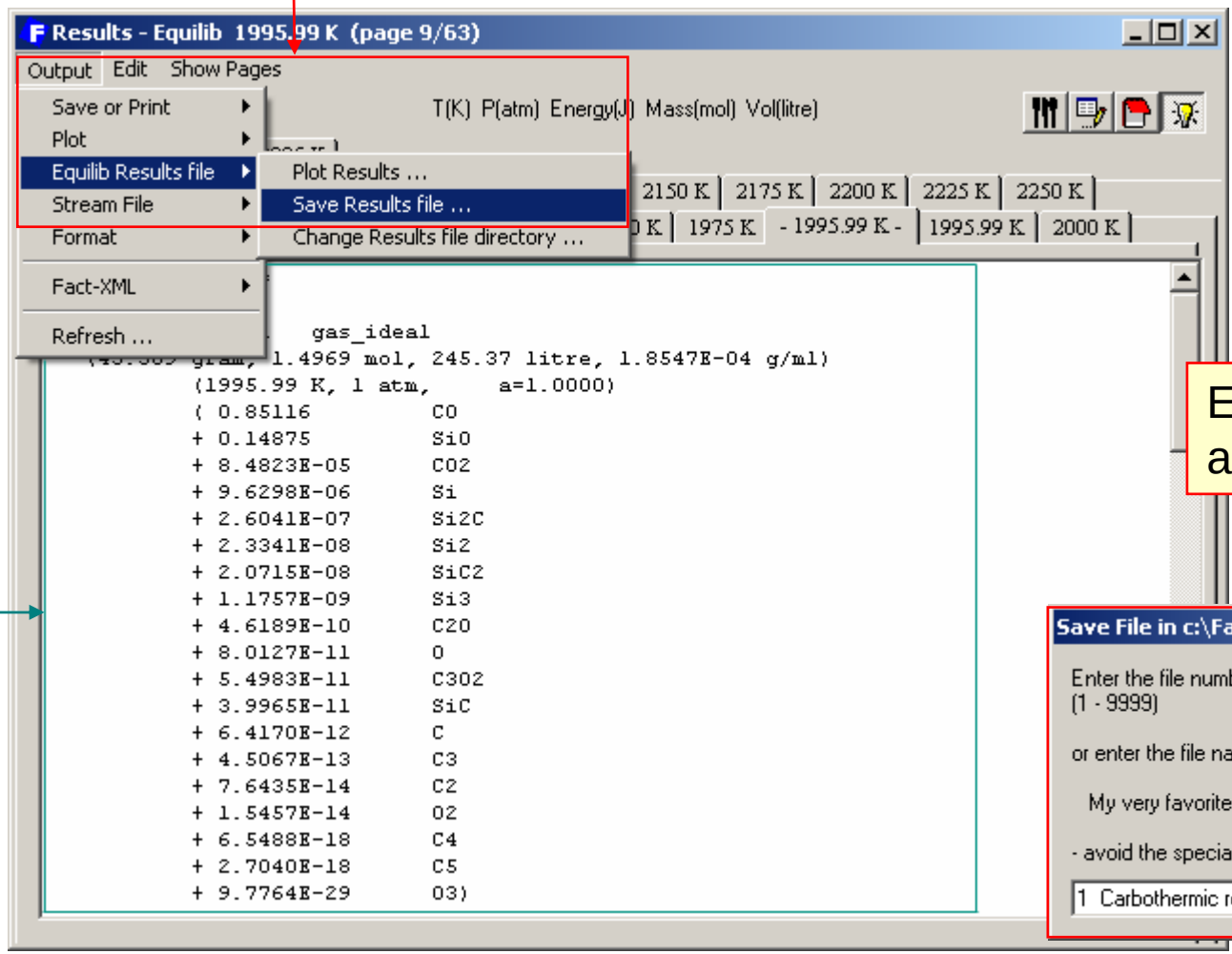


Input window for a **carbothermic reduction of silica** (**SiO_2 + 1.8 C**) in the range **1800 < T/K < 3200** and **p=1 atm**. All data are taken from the FACT databases.

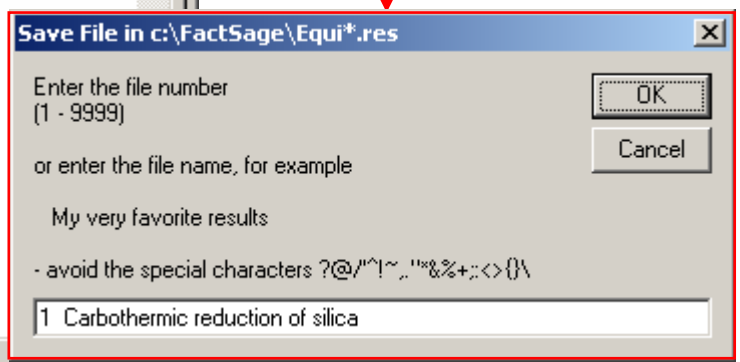
Creating a **Results** file: the ***Equilib*** Results window

Results window for carbothermic reduction of silica (see previous slide)

To create a results file: Output > Equilib Results file > Save Results file…

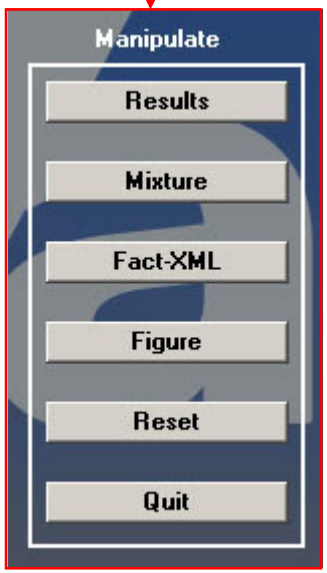


Enter a file number and a description

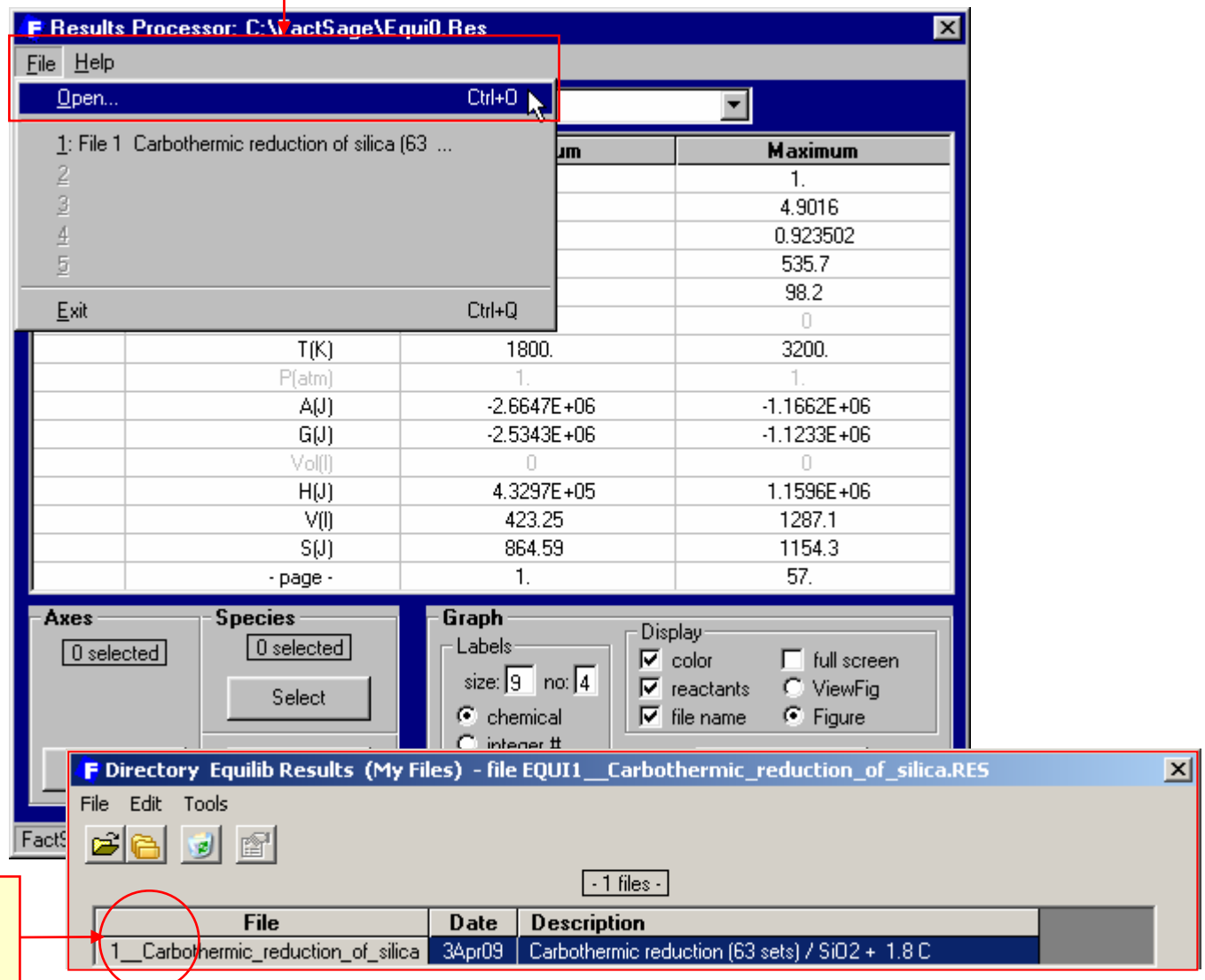


Opening a results file in the ***Results*** program

Now you can initiate the ***Results*** Program.

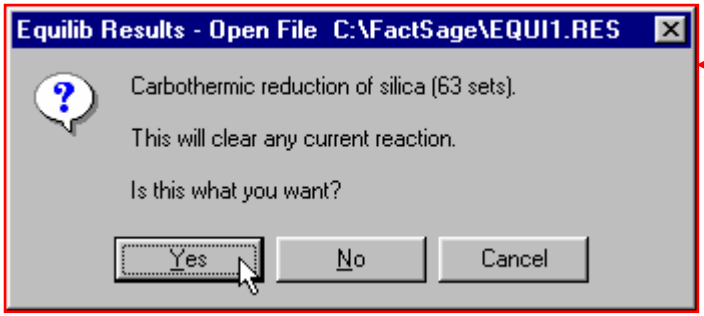


Open a results file: File > Open…



Select and double-click on the file.

Results Window



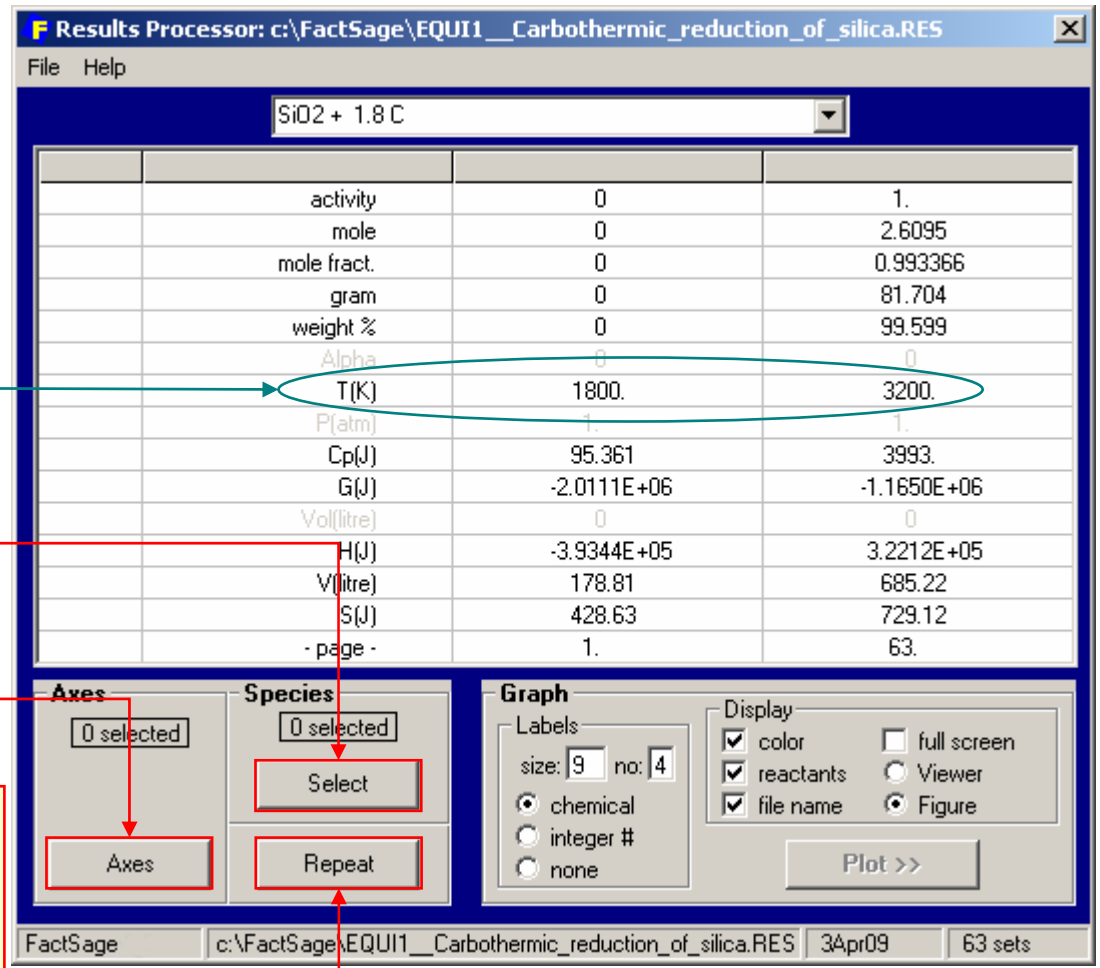
Press «**Yes**» to open the ***Results*** window.

Summary of **results**, **T(K)** = **1800** to **3200**

Click on «Select» to define the species in the graph.

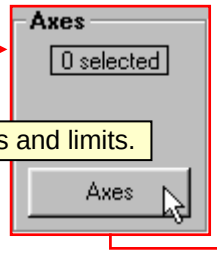
Click on «Axes» to define the diagram axes.

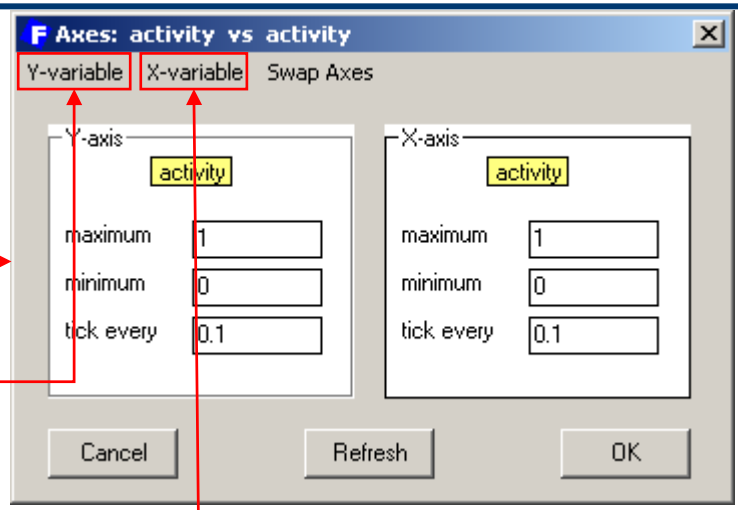
Click on «Repeat» to use the same axes and species as in the last plot.



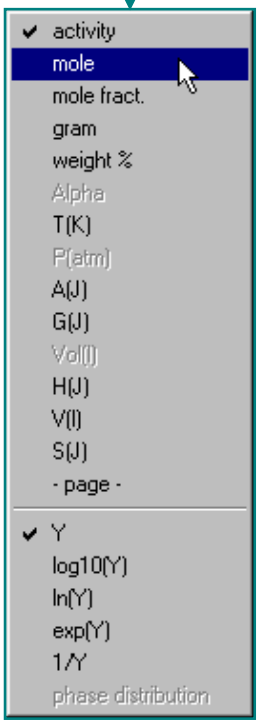
Axes Window

1. Click on «**Axes**».

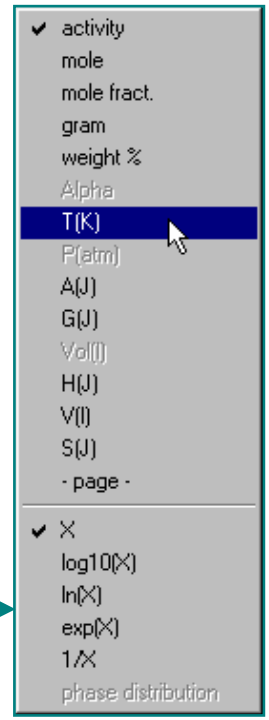




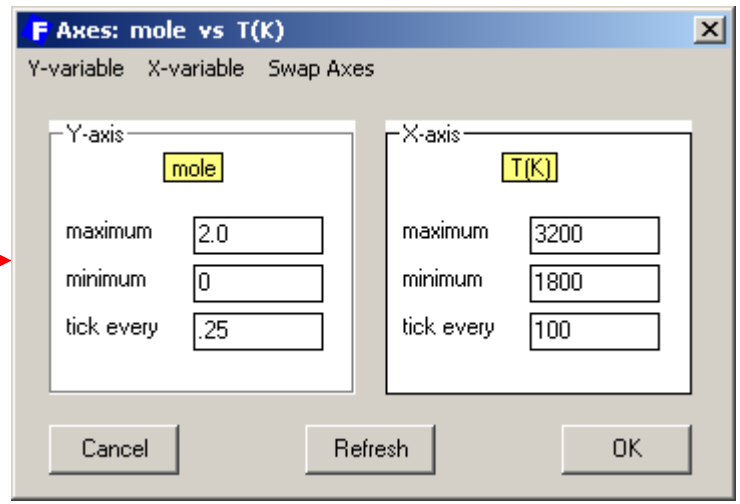
2. Click on «**Y-variable**». Define the Y-axis in the **pop-up** menu.



3. Click on «**X-variable**». Define the X-axis in the **pop-up** menu.

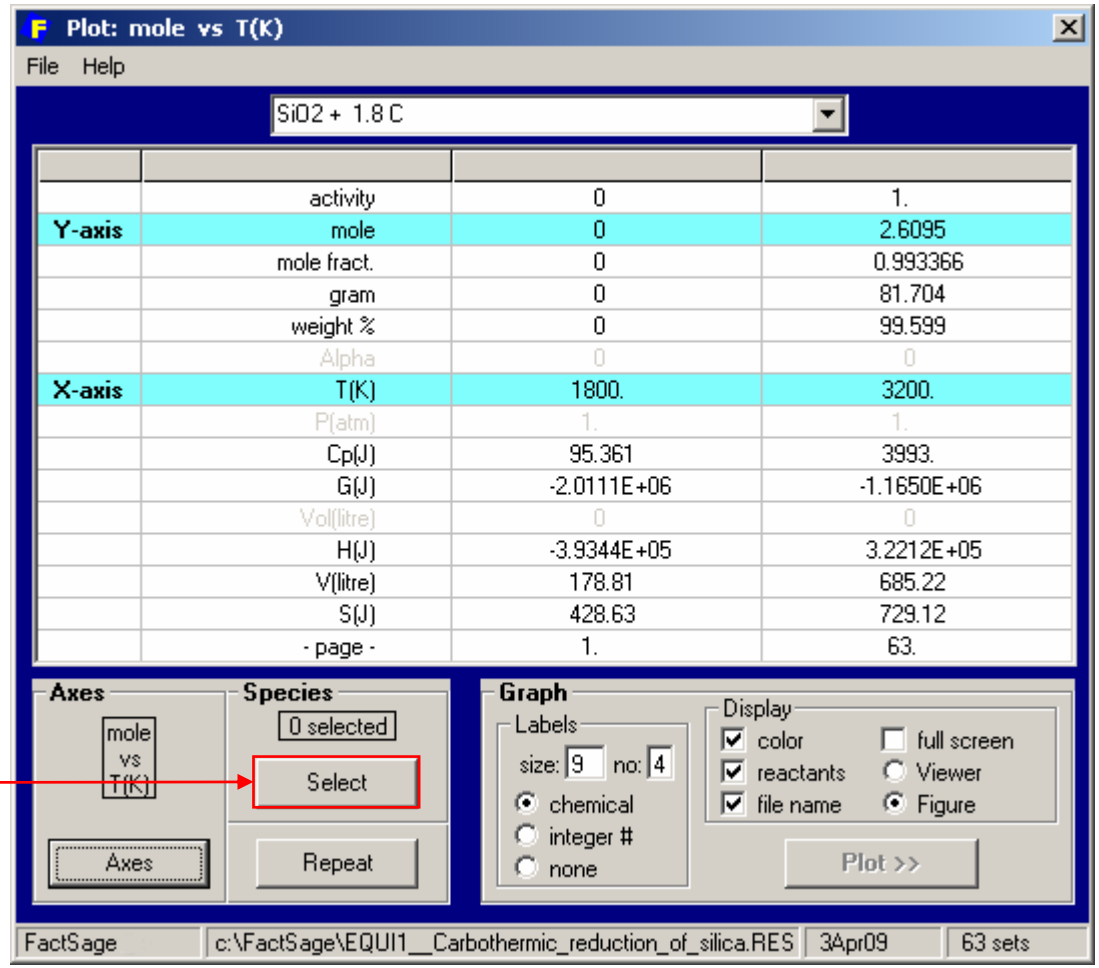


4. Enter the limits of both axes and press «**OK**».



Results Window after axes definition

Press on «**Select**» to open the Species window.



Selecting species and/or phase for a plot

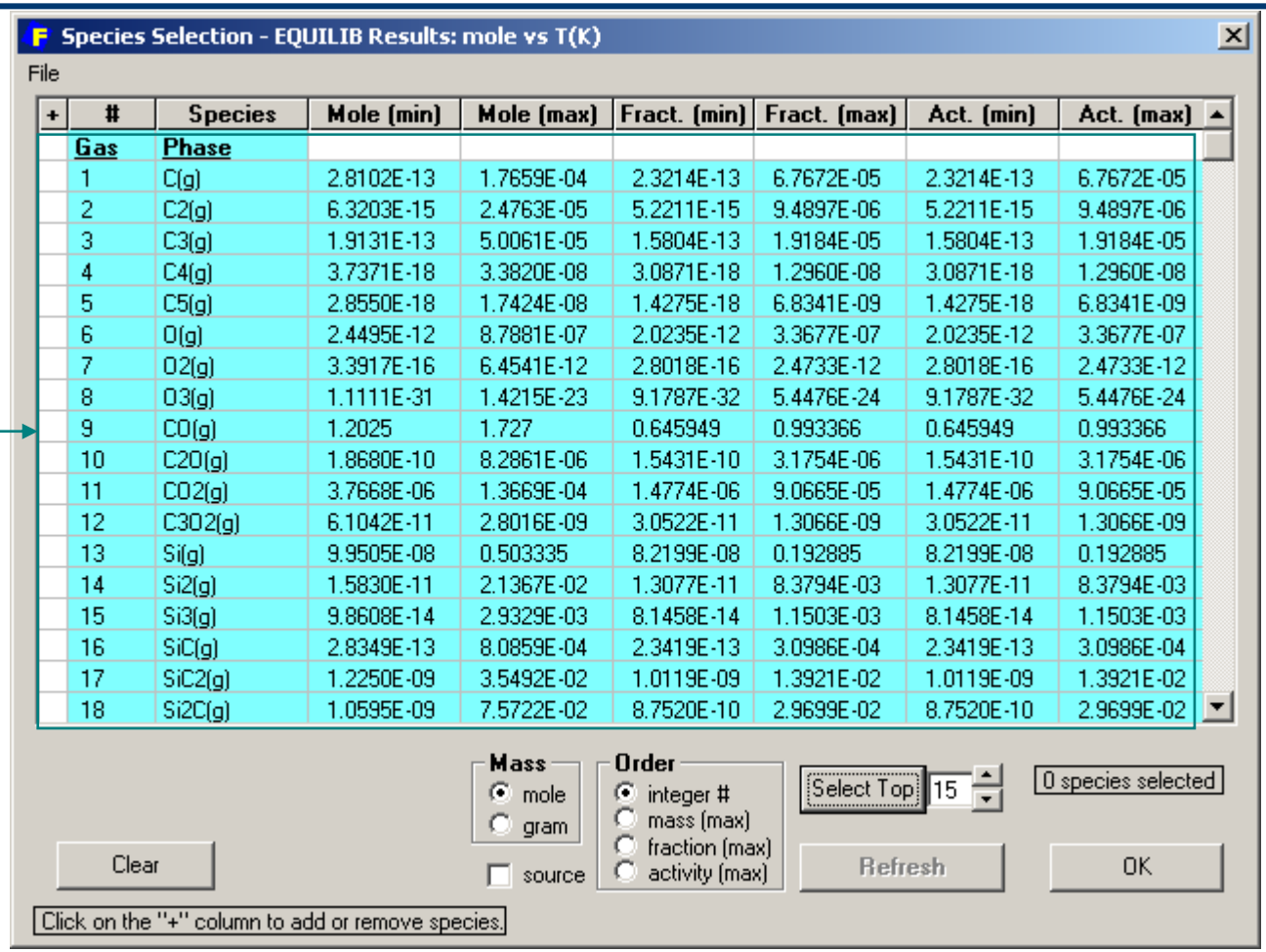
Depending upon the selected axis variable(s) it may be necessary to specify in addition to the variable itself a species or phase to which this variable is related.

For example Amount, Activity or Weight% must always be coupled to a species or phase, while Enthalpy, Entropy, Gibbs energy, Volume are calculated as extensive properties of the entire system and therefore do not need to be coupled to any substance.

In the present example note that both gaseous species (SiO, CO) and condensed stoichiometric phases (Si, SiO2, SiC) are selected.

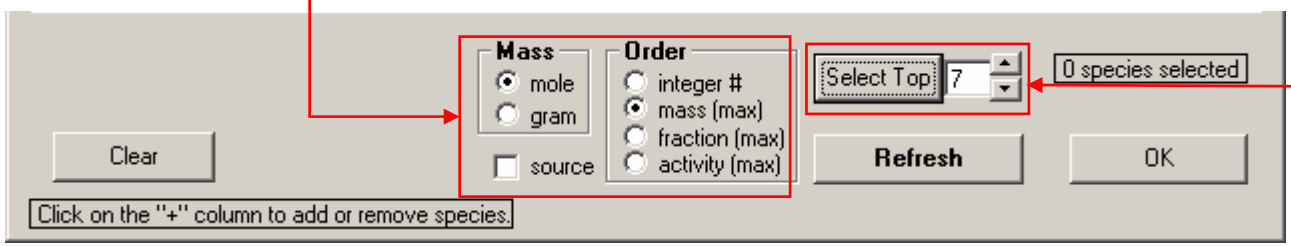
Species Window

Summary of species



List **order**ed with respect to:

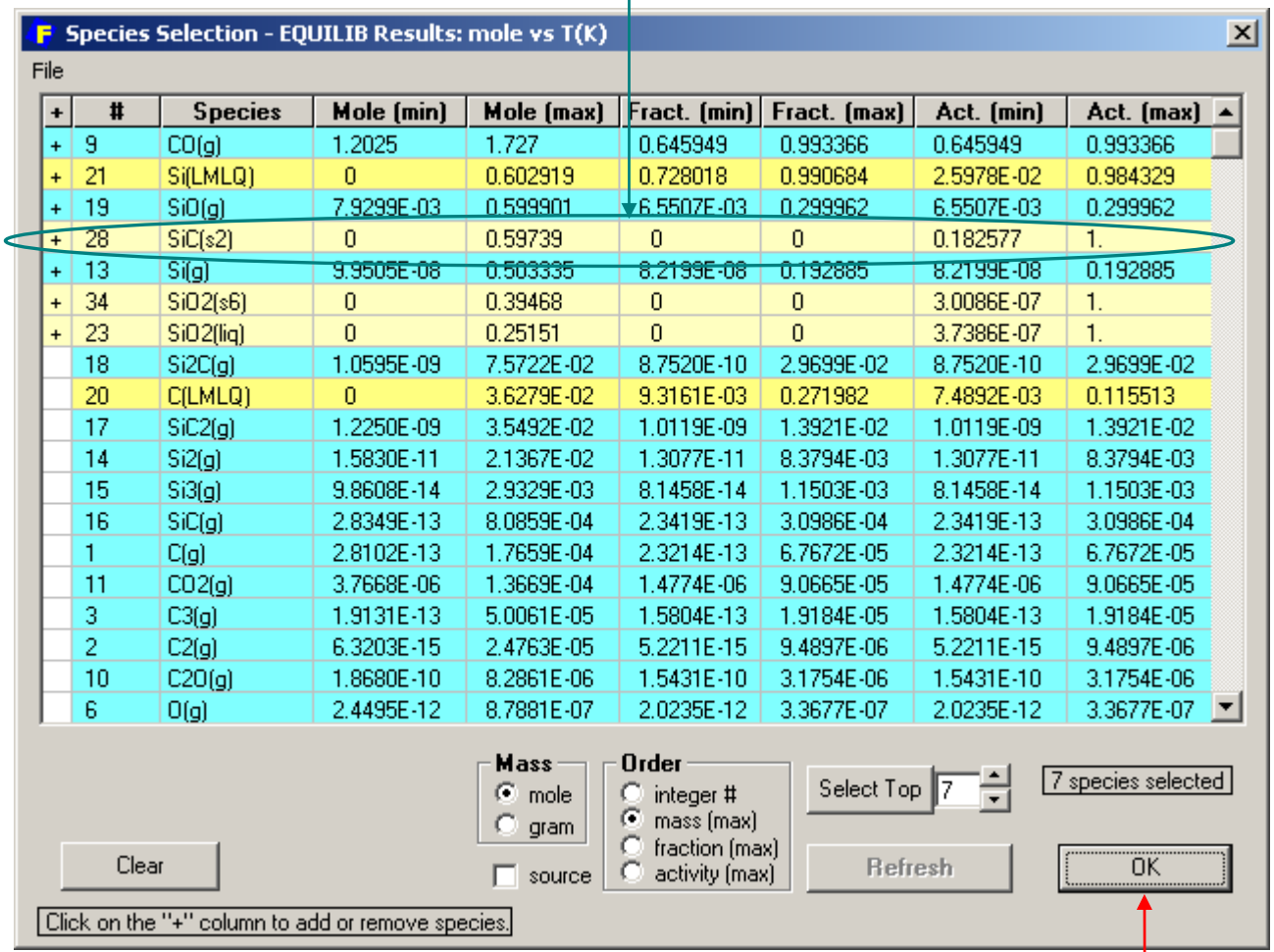
- **Mass**: mole
- **Order**: mass



Click on «**Select Top**» to select the **7** most prominent (mass) species.

Species Window after selection

SiC(s2) = 0 to 0.59739 mole



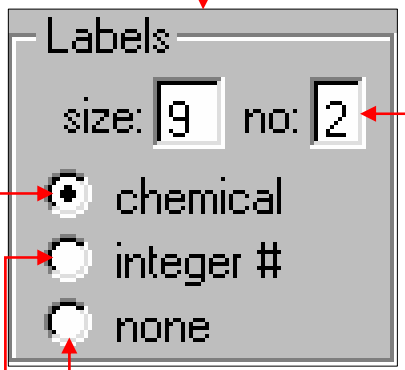
Click on «OK» when finished.

Specifying the **Graphical** Output

Select the size and type of labels.

Number of labels per line (1-9).

Label size (2-24).

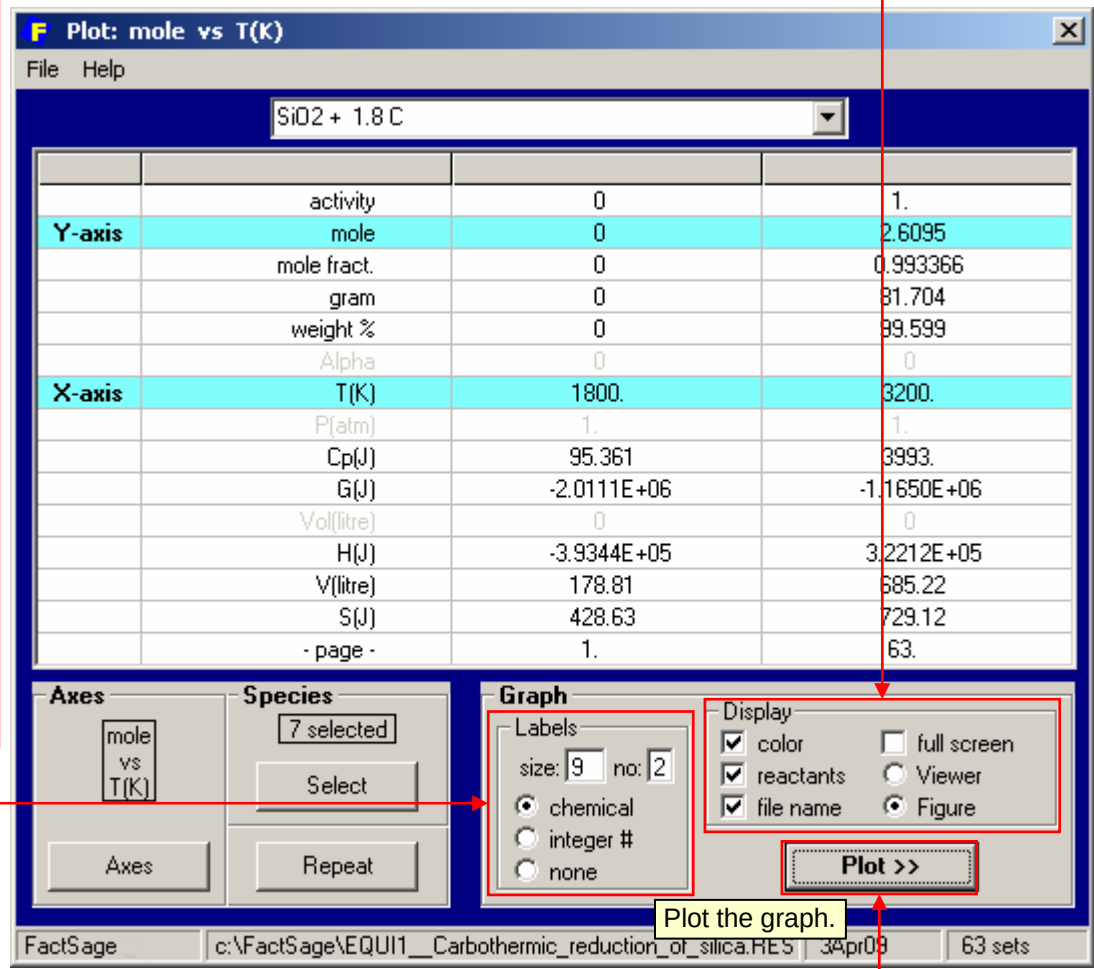


No labels.

Label appears as the # number.

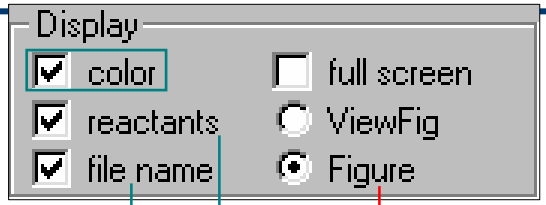
Label appears as a chemical formula.

Select the display properties.

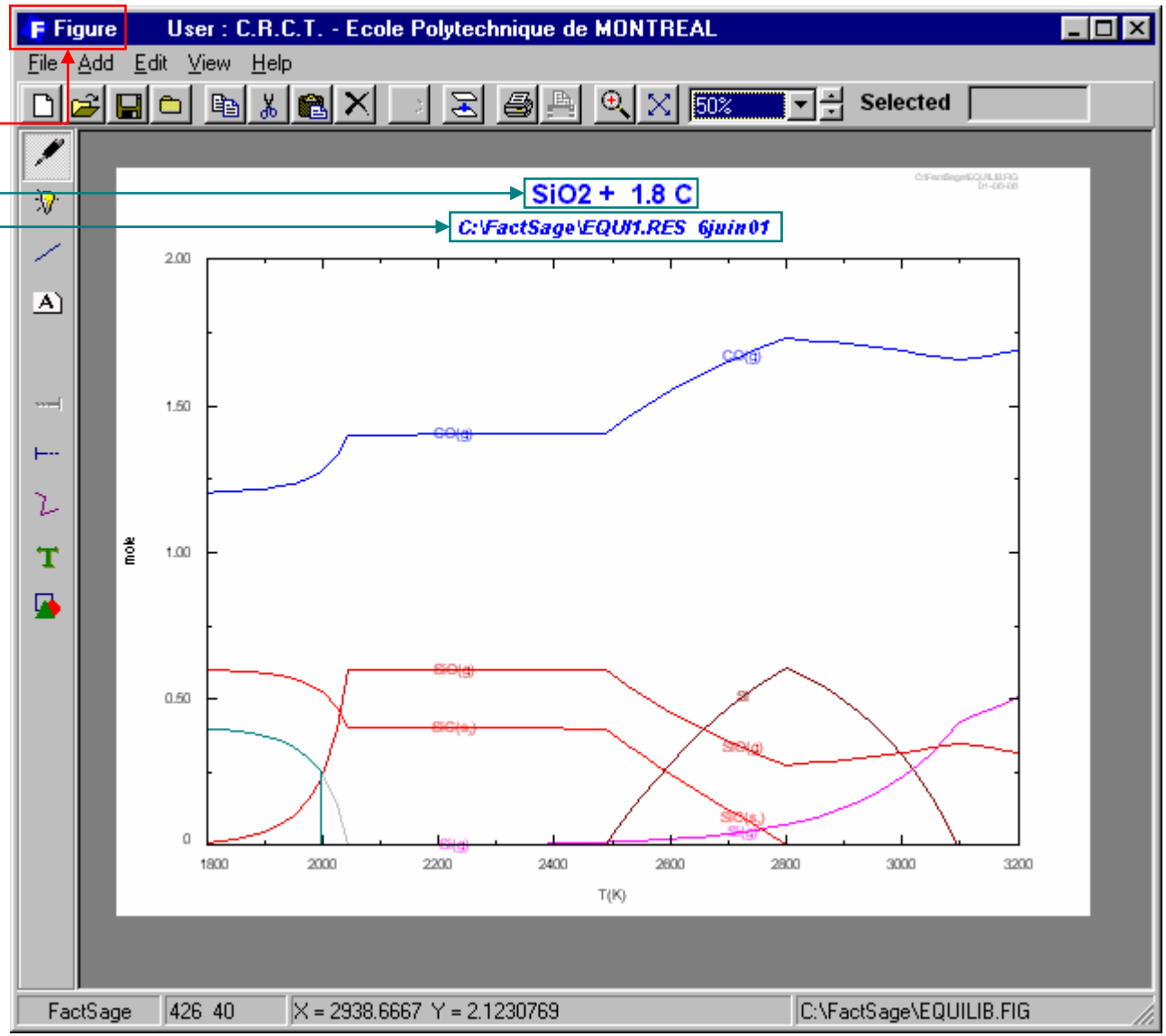


Click on «**Plot >>**» when ready for the graph.

Figure Output

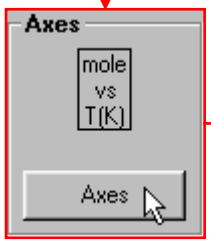


In ***Figure***, you can edit and save the graph.

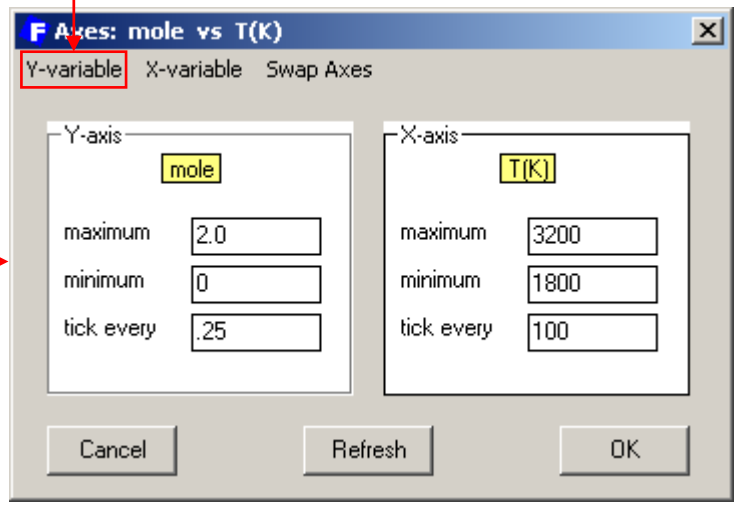


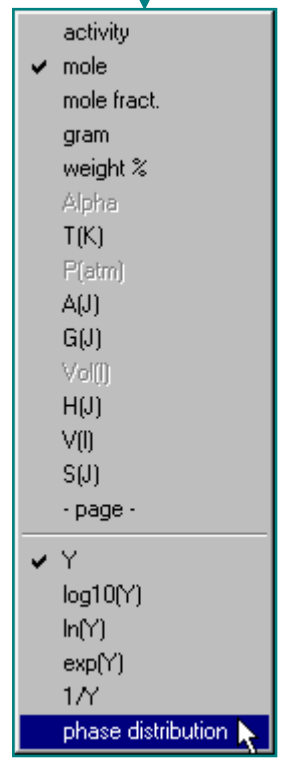
Specifying **phase distribution**

1. Click on «**Axes**».

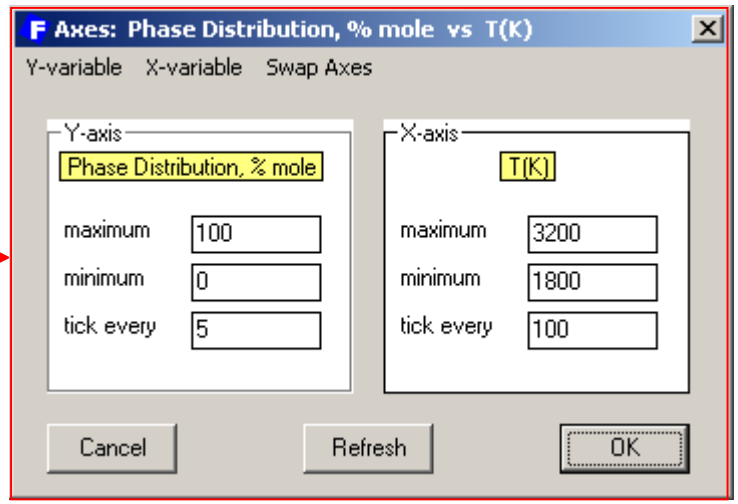


2. Click on «**Y-variable**». Define the Y-axis by checking **phase distribution** in the **pop-up** menu.





3. Enter the limits of both axes and click on «**OK**».



Phase distribution vs Temperature