The ***Results*** module

- Use ***Results*** to generate graphs from Equilib Results (Equi*.Res) files.

Table of contents

The ***Results*** module

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

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

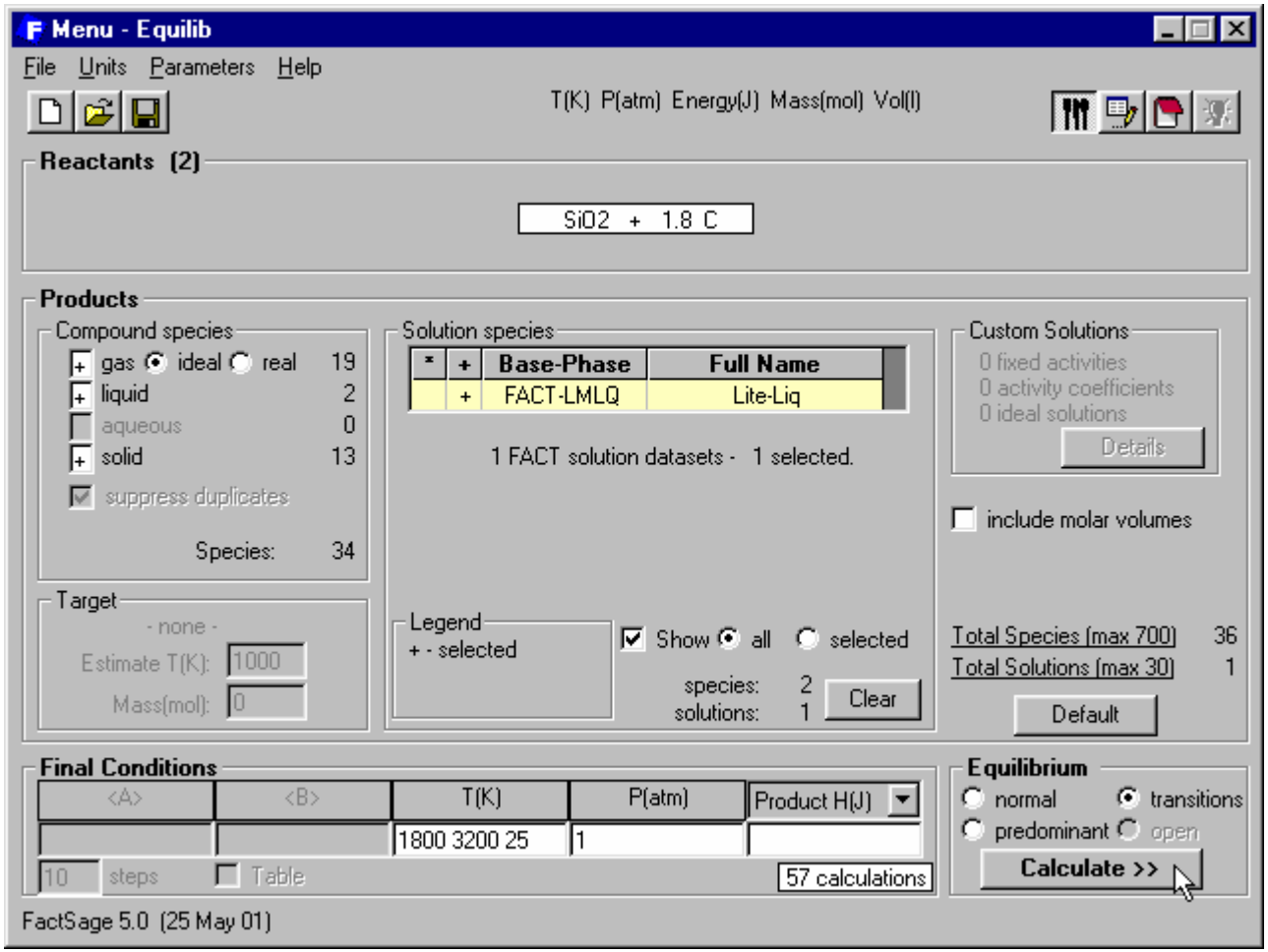
The ***Results*** module is used to post-process the output of complex equilibrium calculations performed with ***Equilib***.

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 screen in Equilib is used to start the appropriate action.

In the present example shown in the following two slides it is assumed that the user has chosen the second method, i.e. he stores the Equilib result on an intermediate file Equi*.RES and opens this at a later stage in the Results module.

HOWEVER, all the actions with the Results module which are shown in the slides of this file can also be performed in immediate sequence to an Equilib calculation. Instead of using the Equilib Results file option in the Equilib Results screen simply use the Plot option (see slide 3.2) for direct transfer to the Results module.

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

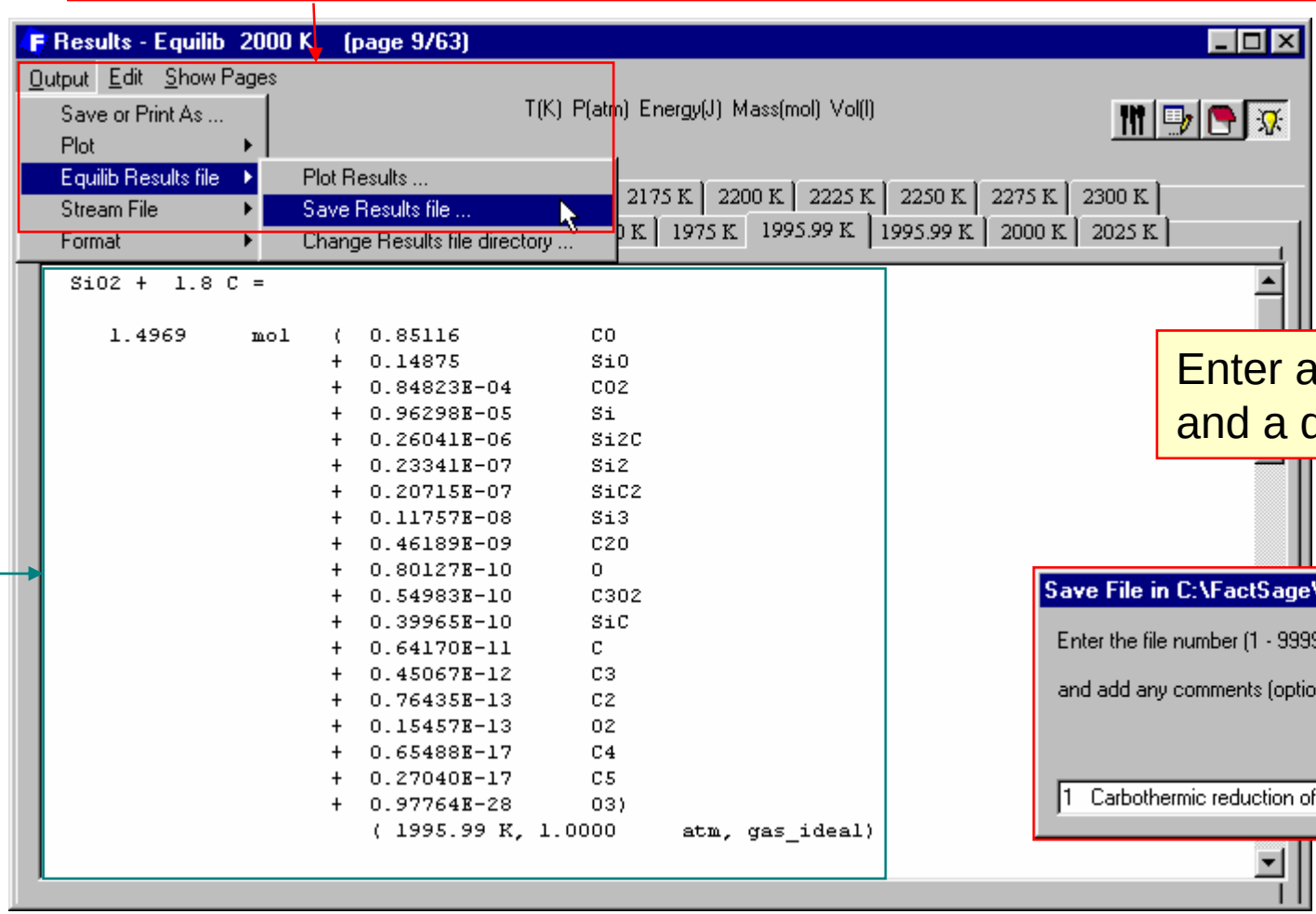


Input window for a **carbothermic reduction of silica** (**SiO_2 + 1.8 C**) in the range **1800 < T/K < 3200** and **p=1 atm**. Result (see next slide) is used for plot.

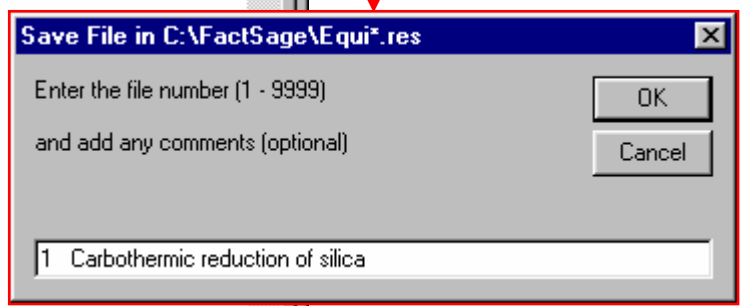
Creating a **Results** file: the ***Equilib*** Results window

Results screen 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



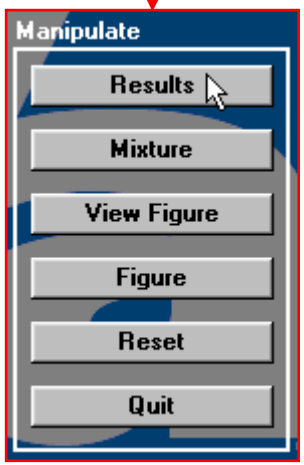
Opening a results file and defining axes

The following slides show how an already stored Equi*.RES file is opened and what information on the contents of the file is made available to the user in order to select properly axes variable etc.

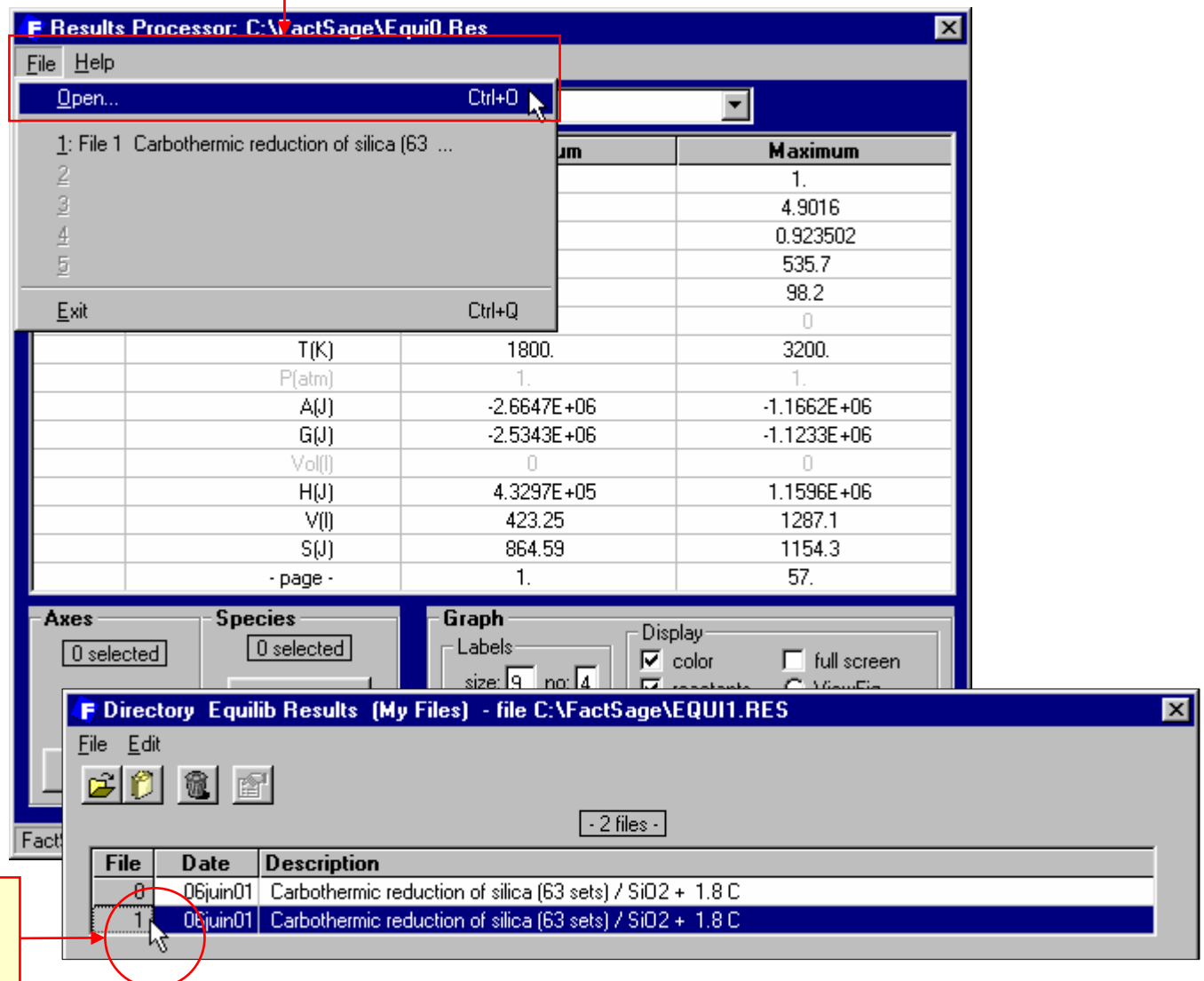
NOTE that the set of slides 4.2 to 4.4 is completely identical to what a user would see if he had transferred control from the Equilib Results screen directly to the ***Results*** module using the Plot option.

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

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

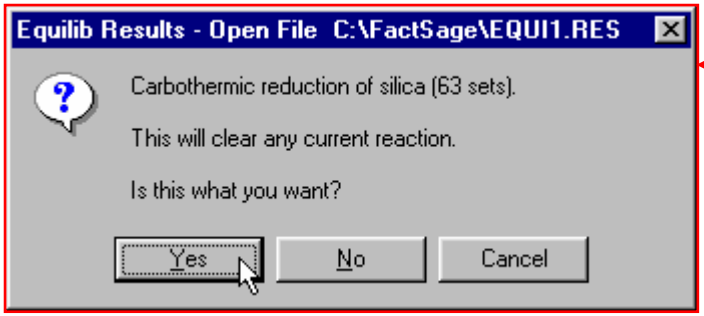


Open a results file: File > Open…

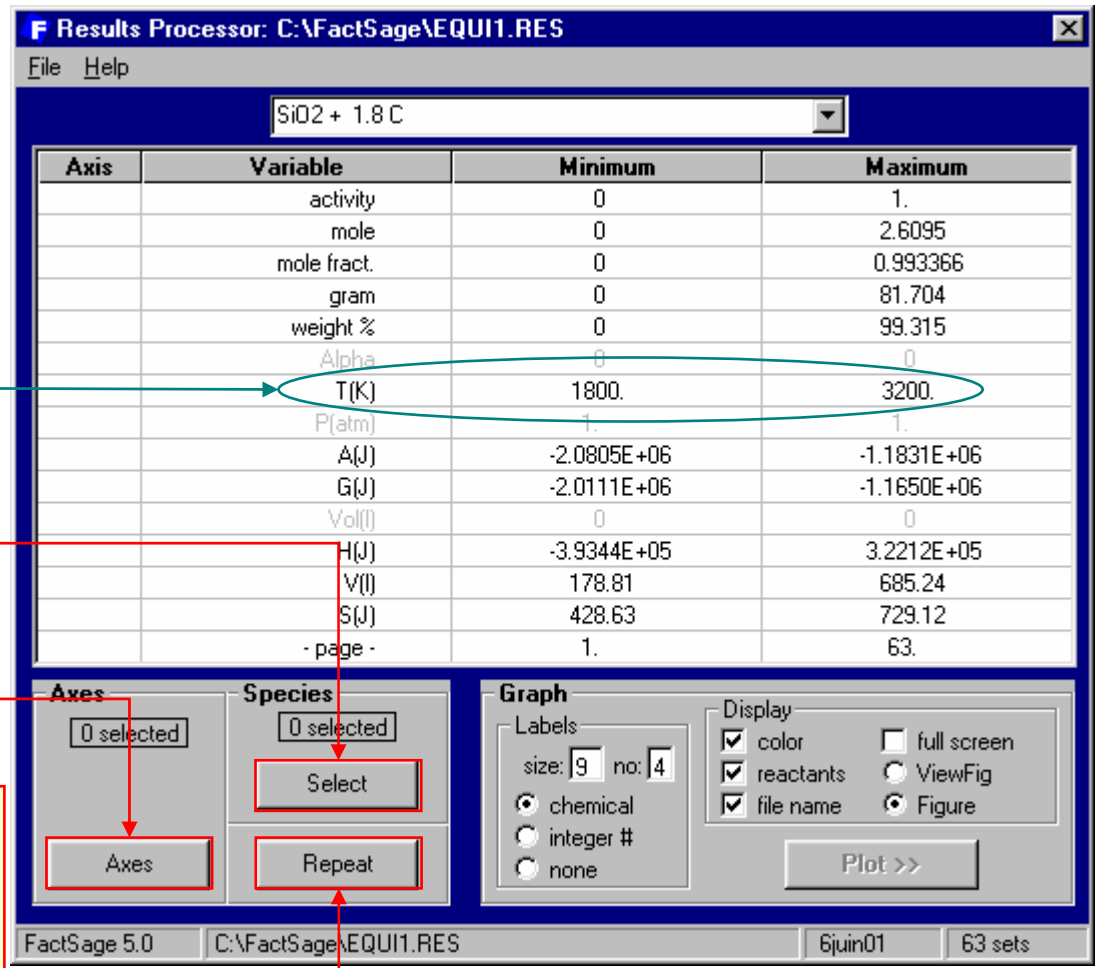


Select and double-click on the chosen file.

Results Window



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



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

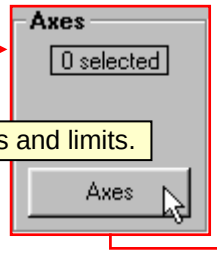
Click on «Select» to define the species in the graph.

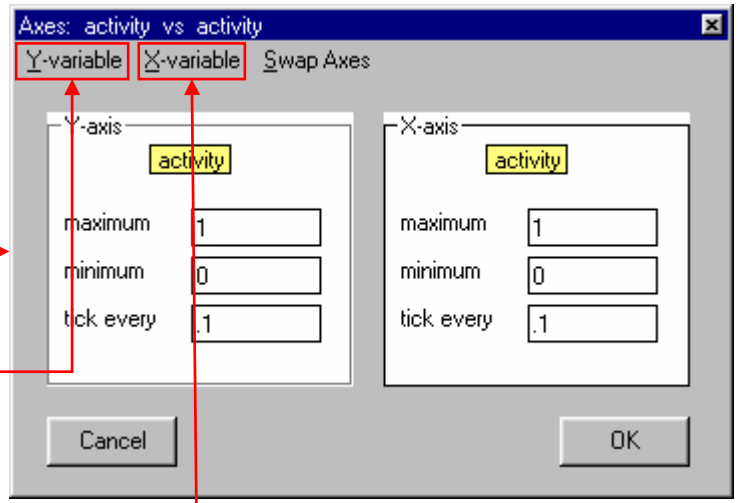
Click on «Axes» to define the diagram axes.

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

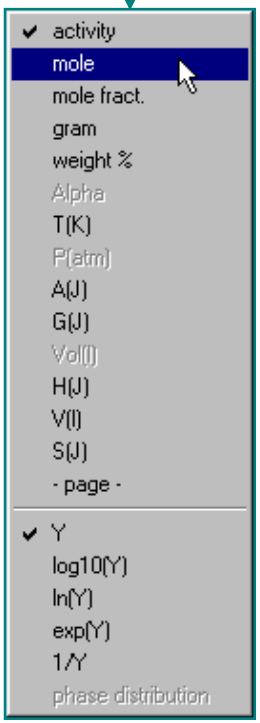
Axes Window

1. Click on «**Axes**».

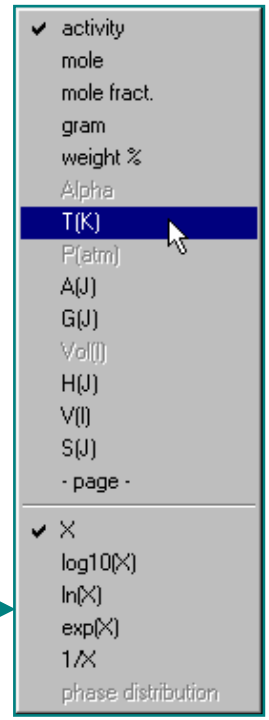




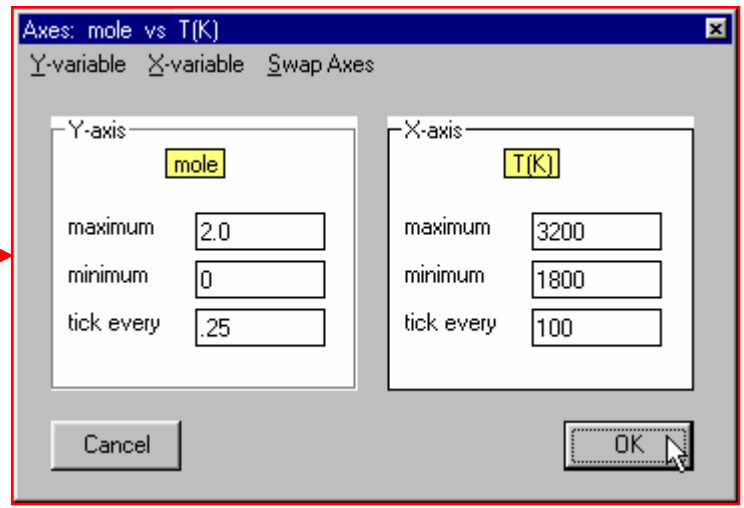
2. Click on «**Y-variable**». Define the Y-axis in the **pop-up** menu.



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

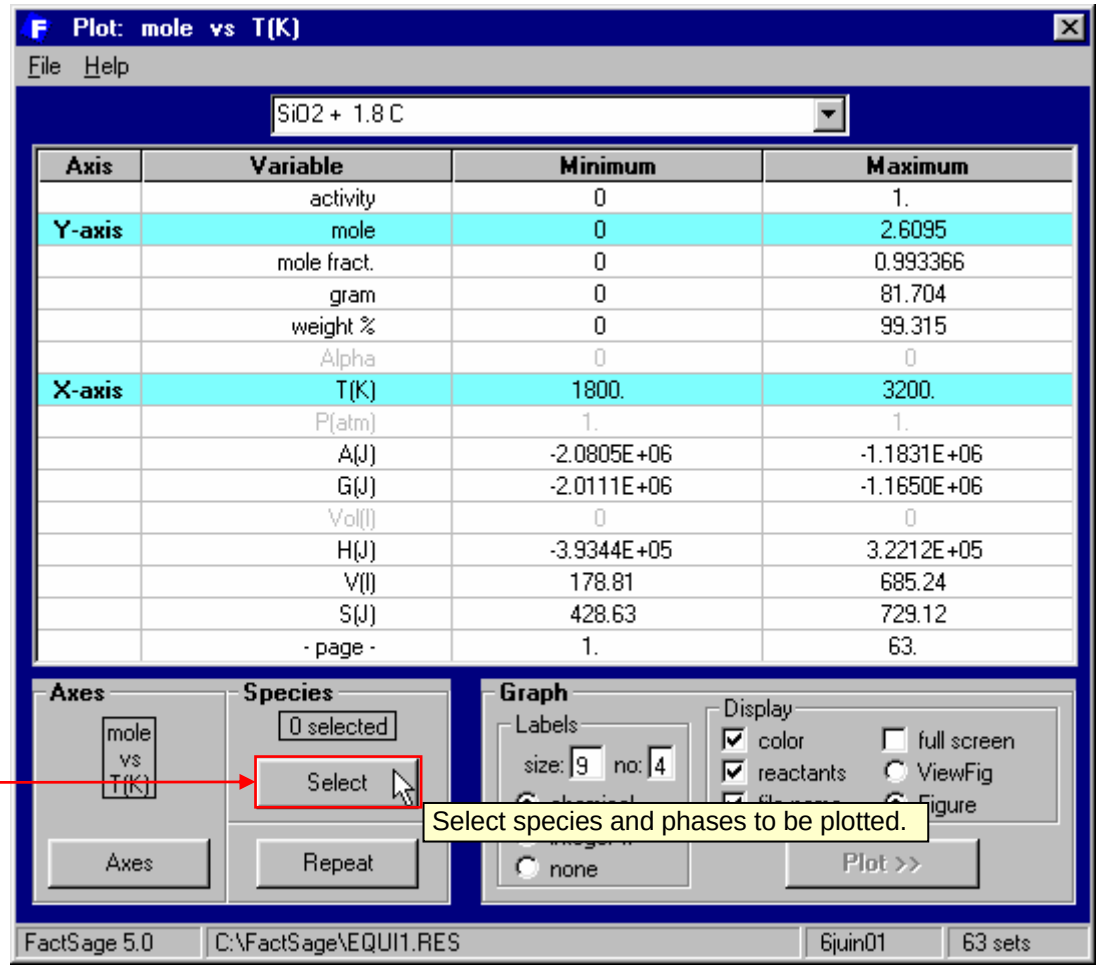


4. Enter the limits of both axes and press «**OK**».



Results Window after axes definition

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



Selecting species and/or phase for a plot

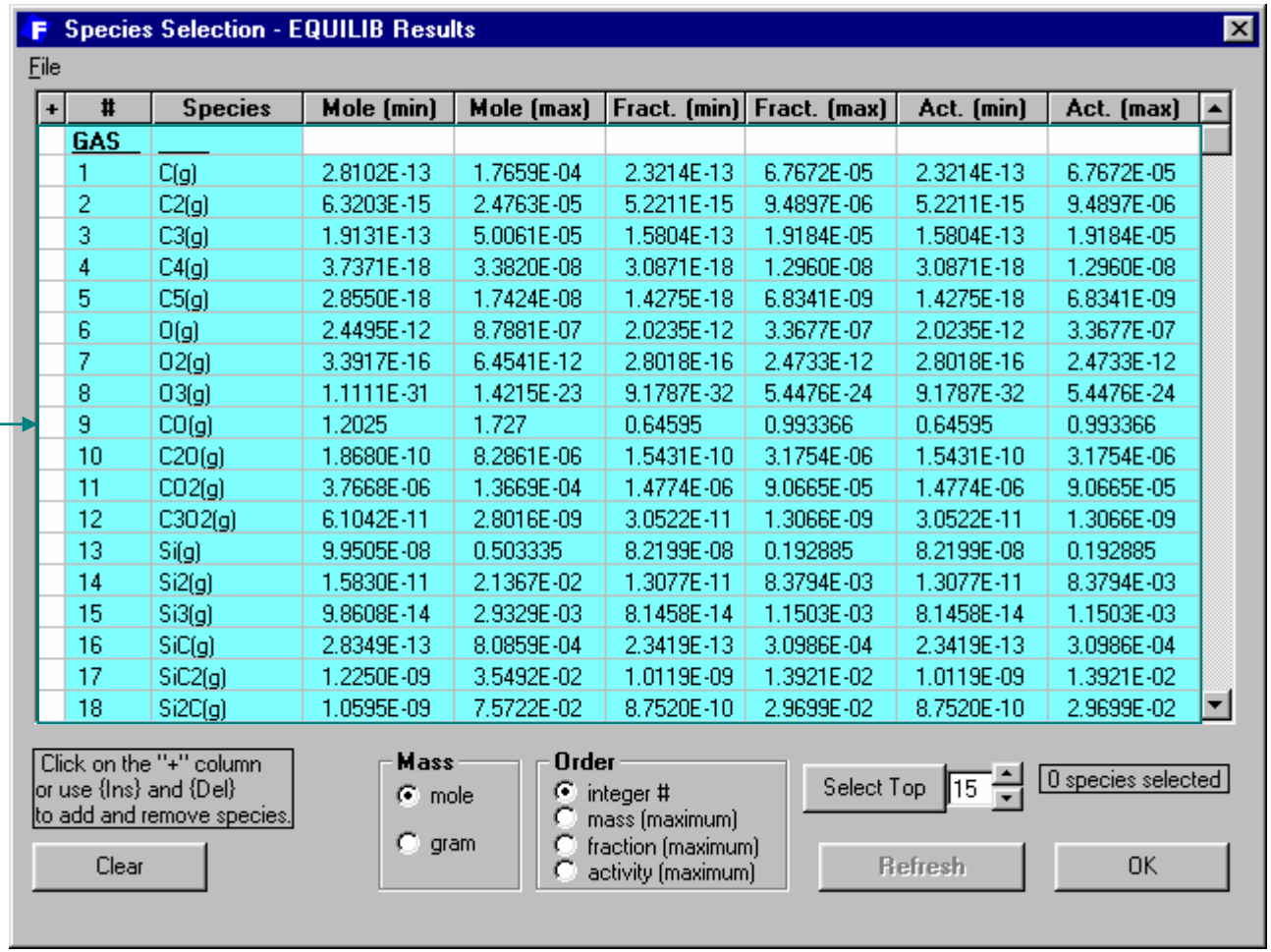
Depending upon the chosen axis variable(s) it may be necessary to specify in addition to the variable itself also a species or phase to which this variable is related.

For example Amount, Activity or Weight% must always be related 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 related to any substance.

In the present example note that both gaseous species (SiO, CO) and condensed stoichiometric phases (Si, SiO2, SiC) are chosen. Whether or not a substance is a species in a phase or a condensed stoichiometric phase can be seen from the color coding of the list (see slide 5.2).

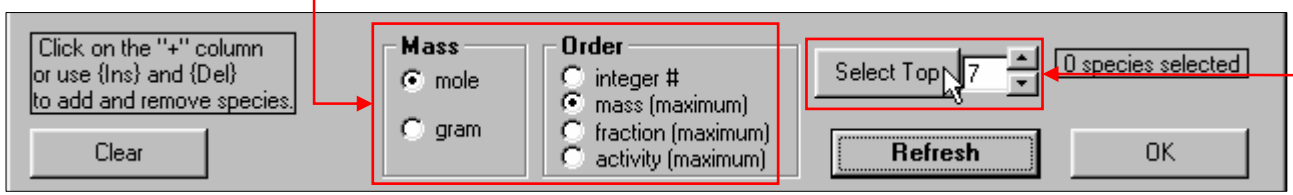
Species Window

Summary of species



List **order**ed with respect to:

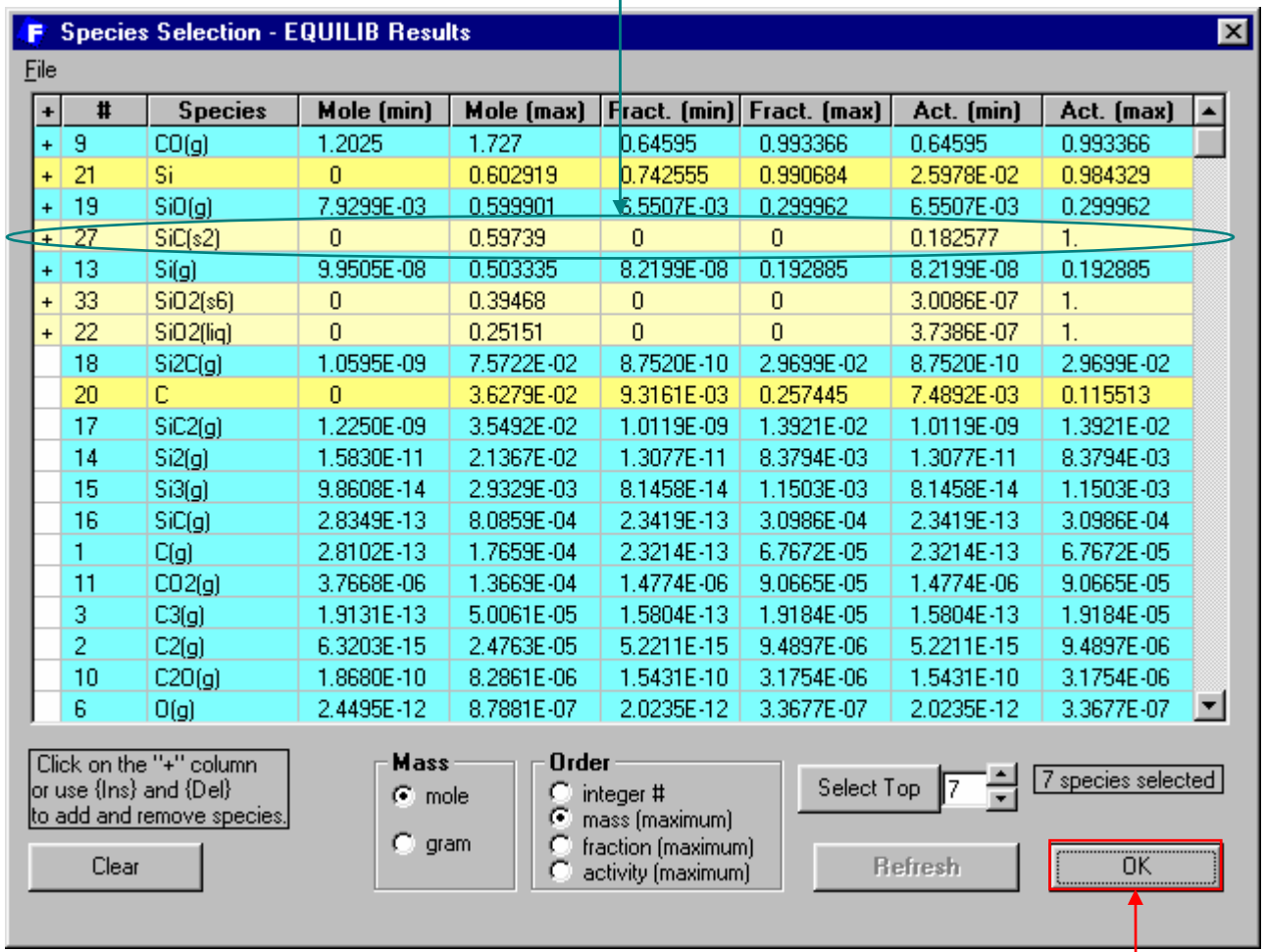
- **Mass**: mole
- **Order**: mass



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.

Specify the **Graphical** Output and display a Figure

In the following two slides is shown how the module for graphical display is selected (***View Figure*** or ***Figure***) and how the resulting diagram is displayed on screen.

In the present case the ***Figure*** module is used.

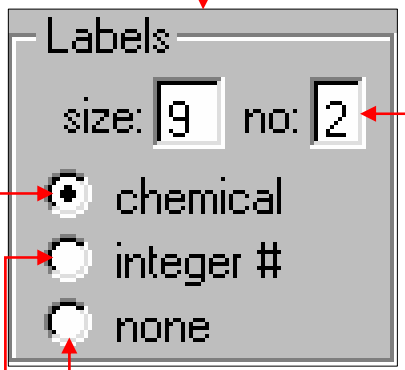
Note that the choice of the graphical module is used as default for the next time.

Specifying the **Graphical** Output

Select the size and type of labels.

Number of labels per line (1-9).

Label size (2-24).

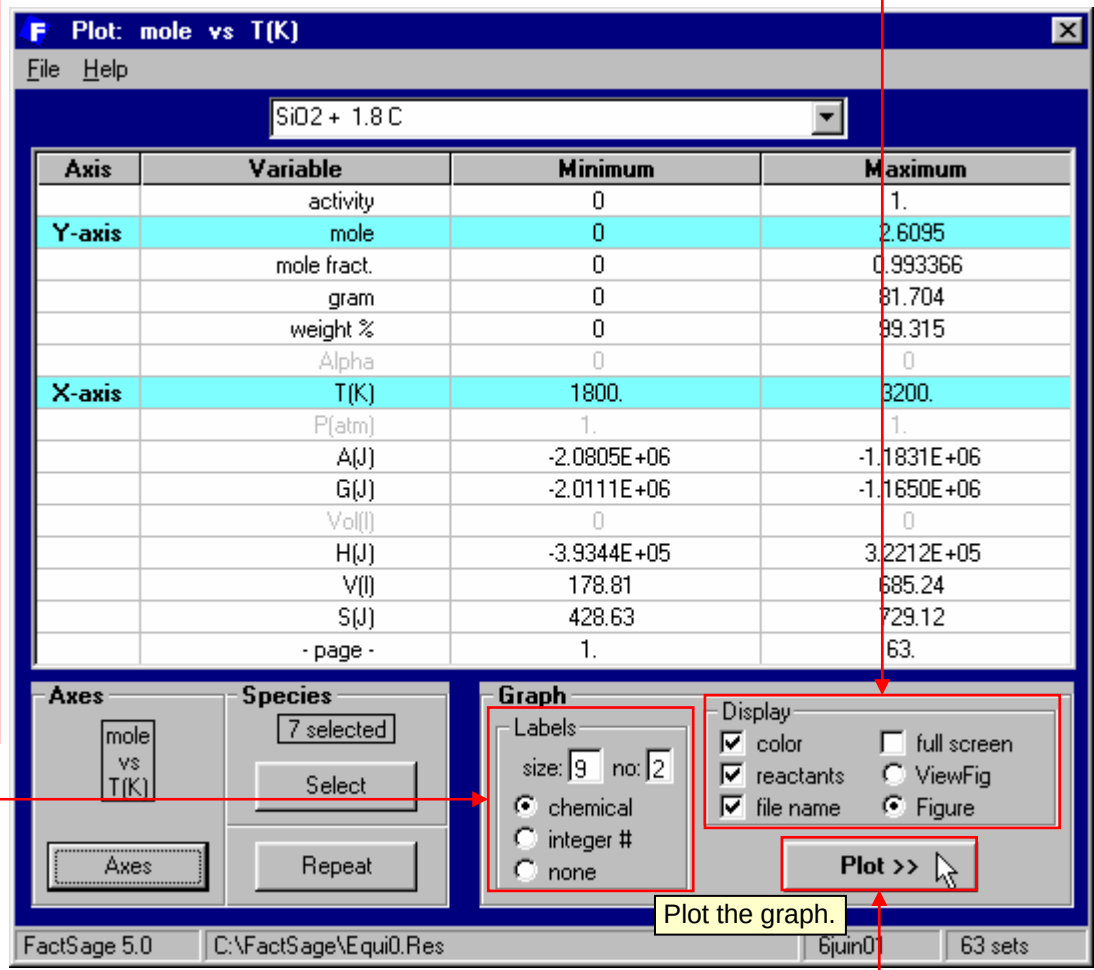


No labels.

Label appears as the # number.

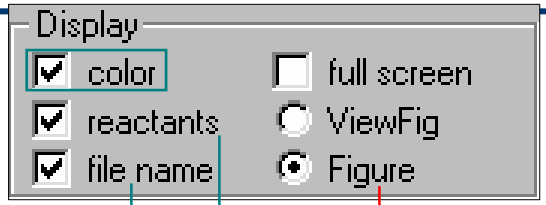
Label appears as a chemical formula.

Select the display properties.

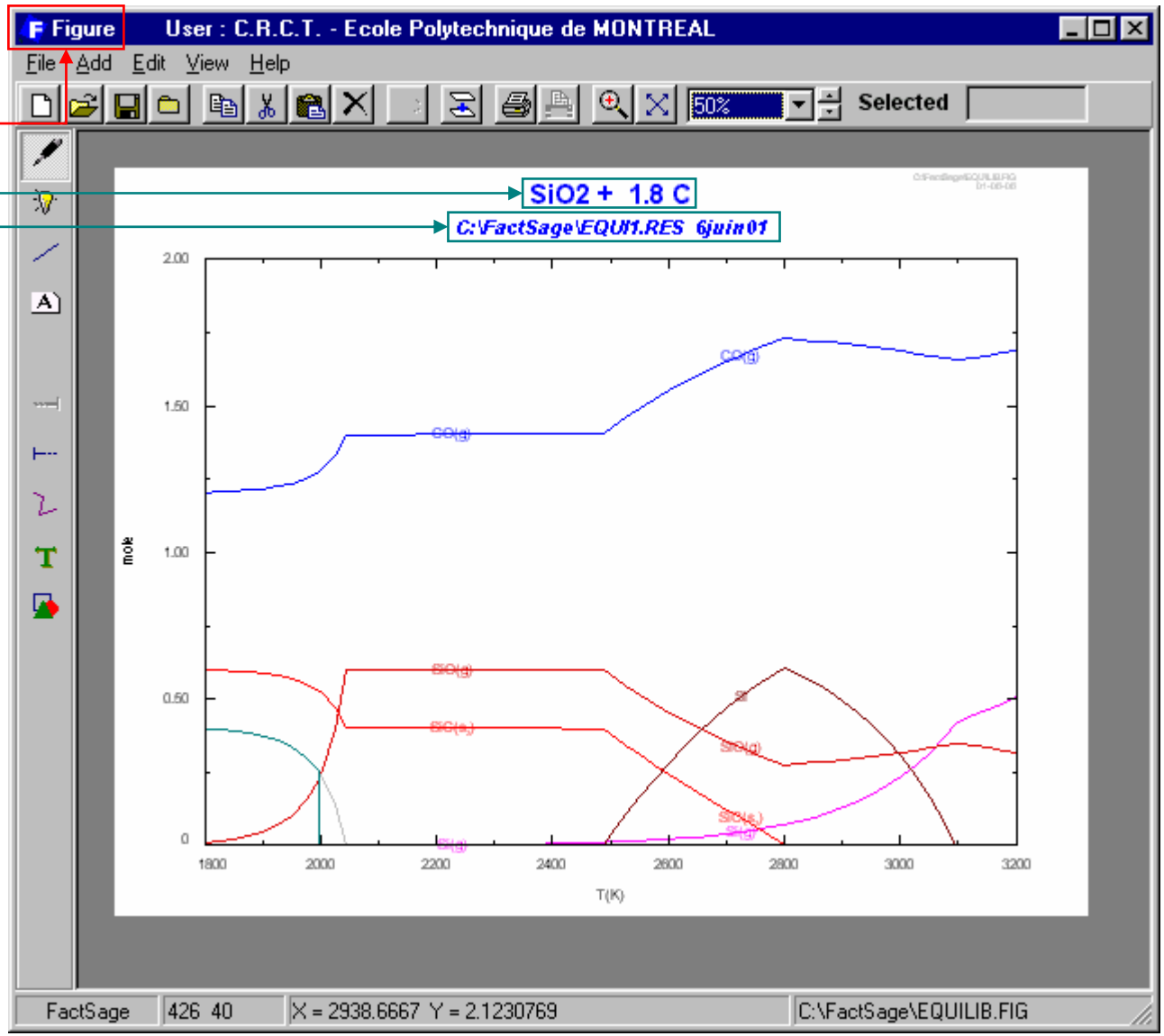


Click on «**Plot >>**» when ready for the graph.

Figure Output



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



Advanced output selection (**phase distribution)**

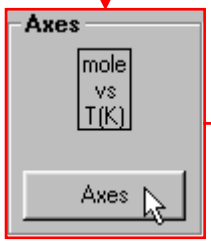
The following two slides show an advanced use of the ***Results*** module.

In addition to the variable Amount the option Phase Distribution is selected.

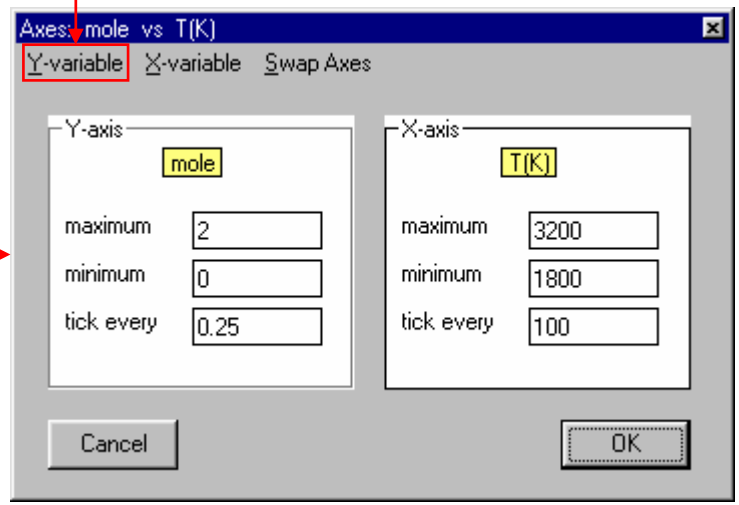
The resulting diagram is shown.

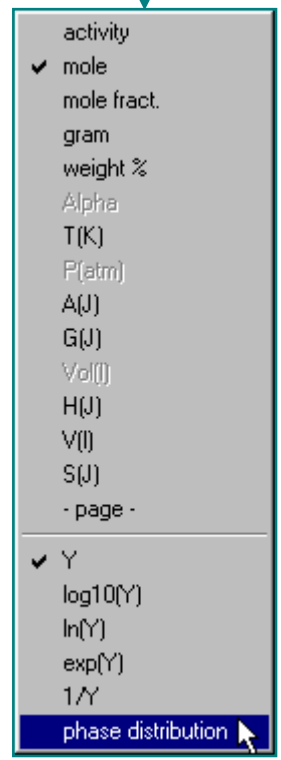
Specifying **phase distribution**

1. Click on «**Axes**».

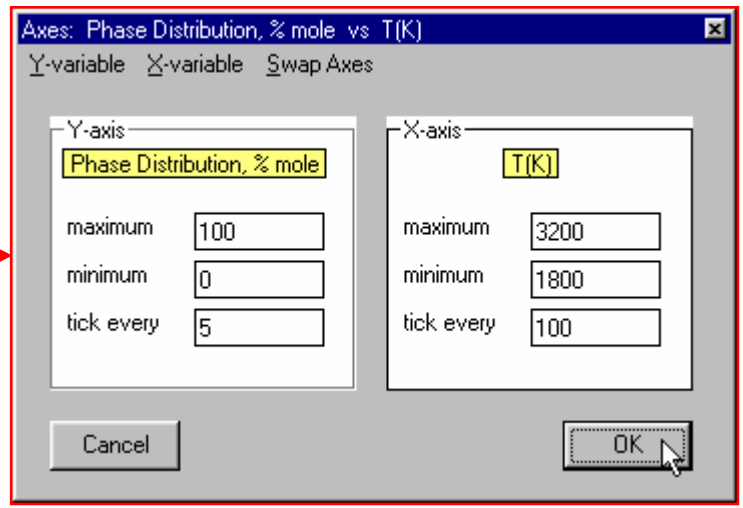


2. Click on «**Y-variable**». Define the Y-axis by checking **phase distribution** in the **pop-up** menu.





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



Phase distribution vs Temperature