

The **Results** module

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

Table of contents

Section 1	<u>Table of contents</u>
Section 2	<u>Opening the Results module</u>
Section 3	<u>Creating a results file in Equilib</u>
Section 4	<u>Opening a results file and defining Axes</u>
Section 5	<u>Selecting Species/Phases</u>
Section 6	<u>Specify the Graphical Output and display a Figure</u>
Section 7	<u>Advanced output selection (phase distribution)</u>

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

The screenshot shows the 'Equilib' menu window in FactSage 5.0. The window title is 'F Menu - Equilib'. The menu bar includes 'File', 'Units', 'Parameters', and 'Help'. The main input area shows 'Reactants (2)' as $\text{SiO}_2 + 1.8 \text{ C}$. The 'Products' section has 'Compound species' (gas, liquid, aqueous, solid) and 'Solution species' (FACT-LMLQ, Lite-Liq). The 'Final Conditions' section shows a temperature range of 1800 to 3200 K at 1 atm, with 10 steps and 57 calculations. The 'Equilibrium' section has radio buttons for 'normal', 'predominant', 'transitions', and 'open', with 'transitions' selected. A 'Calculate >>' button is highlighted.

Reactants (2): $\text{SiO}_2 + 1.8 \text{ C}$

Products:

- Compound species: gas (ideal), liquid, aqueous, solid
- Solution species: FACT-LMLQ, Lite-Liq

Final Conditions:

<A>		T(K)	P(atm)	Product H(J)
		1800 3200 25	1	

Equilibrium: normal, predominant, transitions, open

Calculate >>

Input window for a **carbothermic reduction of silica** ($\text{SiO}_2 + 1.8 \text{ C}$) in the range $1800 < T/\text{K} < 3200$ and $p=1 \text{ atm}$. 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...**

The screenshot shows the 'Results - Equilib 2000 K' window. The 'Output' menu is open, and 'Save Results file ...' is selected. The main window displays the following text:

```
SiO2 + 1.8 C =  
  
1.4969 mol ( 0.85116 CO  
+ 0.14875 SiO  
+ 0.84823E-04 CO2  
+ 0.96298E-05 Si  
+ 0.26041E-06 Si2C  
+ 0.23341E-07 Si2  
+ 0.20715E-07 SiC2  
+ 0.11757E-08 Si3  
+ 0.46189E-09 C2O  
+ 0.80127E-10 O  
+ 0.54983E-10 C3O2  
+ 0.39965E-10 SiC  
+ 0.64170E-11 C  
+ 0.45067E-12 C3  
+ 0.76435E-13 C2  
+ 0.15457E-13 O2  
+ 0.65488E-17 C4  
+ 0.27040E-17 C5  
+ 0.97764E-28 O3)  
( 1995.99 K, 1.0000 atm, gas_ideal)
```

Enter a file number and a description

The dialog box is titled 'Save File in C:\FactSage\Equi*.res'. It contains the following text and controls:

Enter the file number (1 - 9999)

and add any comments (optional)

Opening a **results** file and defining **axes**

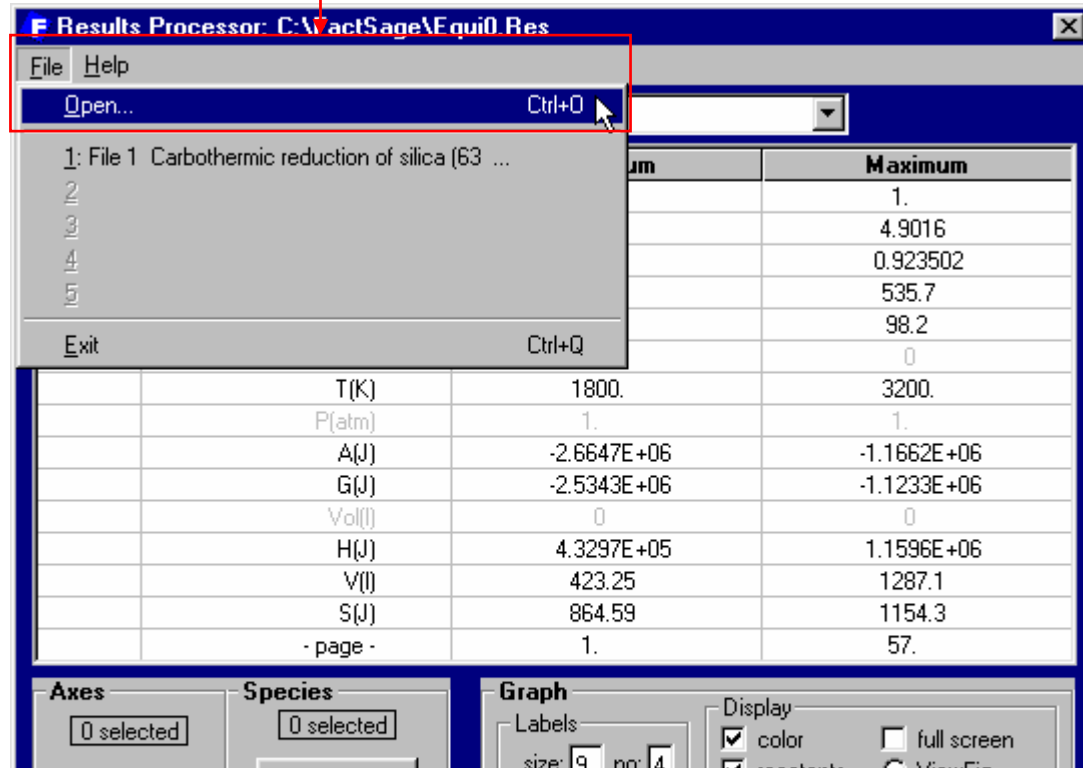
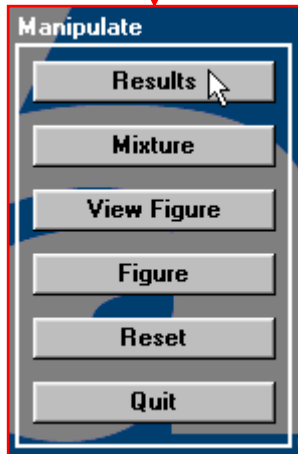
The following slides show how an already stored **Equi*.RES** file is opened and what **information on the contents of the file** is made available to the user in order to **select properly axes variable** etc.

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**.

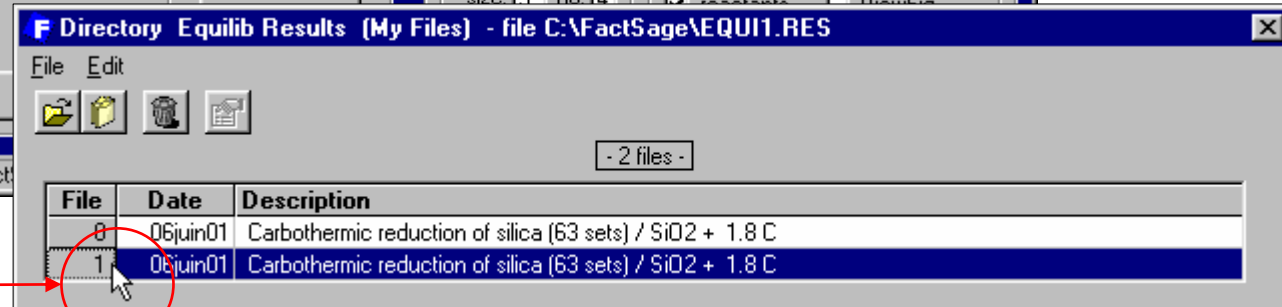
Opening a **results** file in the **Results** program

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

Open a results file: **F**ile > **O**pen...

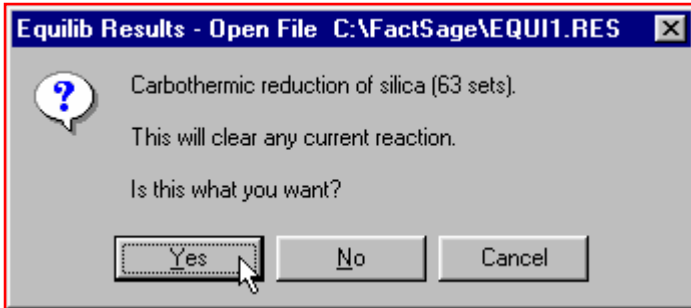


Select and double-click on the chosen file.



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.

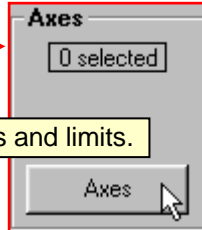
Click on «Axes» to define
the diagram axes.

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

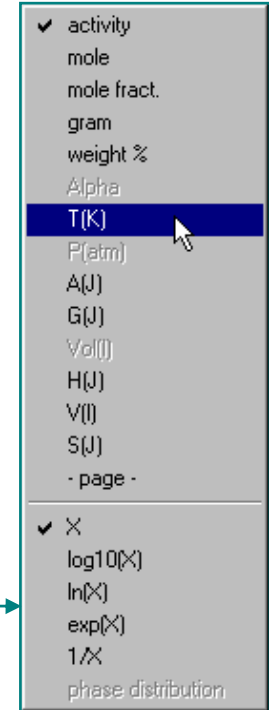
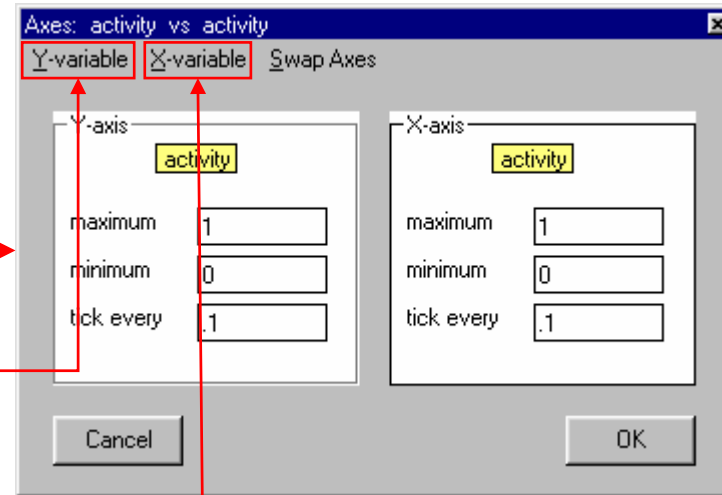
Axis	Variable	Minimum	Maximum
	activity	0	1.
	mole	0	2.6095
	mole fract.	0	0.993366
	gram	0	81.704
	weight %	0	99.315
	Alpha	0	0
	T(K)	1800.	3200.
	P(atm)	1.	1.
	A(J)	-2.0805E+06	-1.1831E+06
	G(J)	-2.0111E+06	-1.1650E+06
	Vol(l)	0	0
	H(J)	-3.9344E+05	3.2212E+05
	V(l)	178.81	685.24
	S(J)	428.63	729.12
	- page -	1.	63.

Axes Window

1. Click on «**Axes**».



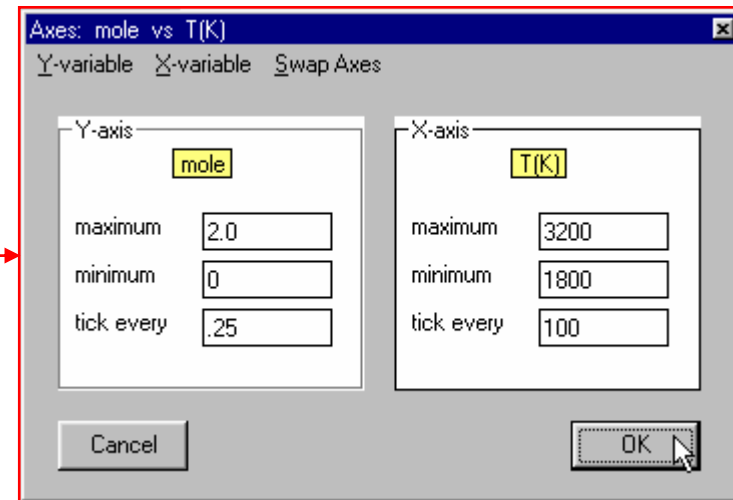
Define X & Y-axes and limits.



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

Plot: mole vs T(K)

File Help

SiO2 + 1.8 C

Axis	Variable	Minimum	Maximum
Y-axis	activity	0	1.
	mole	0	2.6095
	mole fract.	0	0.993366
	gram	0	81.704
	weight %	0	99.315
X-axis	Alpha	0	0
	T(K)	1800.	3200.
	P(atm)	1.	1.
	A(J)	-2.0805E+06	-1.1831E+06
	G(J)	-2.0111E+06	-1.1650E+06
	Vol(l)	0	0
	H(J)	-3.9344E+05	3.2212E+05
	V(l)	178.81	685.24
	S(J)	428.63	729.12
	- page -	1.	63.

Axes: mole vs T(K)

Species: 0 selected

Graph: Labels: mole vs T(K), size: 9, no: 4, Display: color, reactants, full screen, ViewFig, Figure

FactSage 5.0 C:\FactSage\EQUI1.RES 6juin01 63 sets

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

Select species and phases to be plotted.

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

F Species Selection - EQUILIB Results

File

+	#	Species	Mole (min)	Mole (max)	Fract. (min)	Fract. (max)	Act. (min)	Act. (max)
	GAS							
	1	C(g)	2.8102E-13	1.7659E-04	2.3214E-13	6.7672E-05	2.3214E-13	6.7672E-05
	2	C2(g)	6.3203E-15	2.4763E-05	5.2211E-15	9.4897E-06	5.2211E-15	9.4897E-06
	3	C3(g)	1.9131E-13	5.0061E-05	1.5804E-13	1.9184E-05	1.5804E-13	1.9184E-05
	4	C4(g)	3.7371E-18	3.3820E-08	3.0871E-18	1.2960E-08	3.0871E-18	1.2960E-08
	5	C5(g)	2.8550E-18	1.7424E-08	1.4275E-18	6.8341E-09	1.4275E-18	6.8341E-09
	6	O(g)	2.4495E-12	8.7881E-07	2.0235E-12	3.3677E-07	2.0235E-12	3.3677E-07
	7	O2(g)	3.3917E-16	6.4541E-12	2.8018E-16	2.4733E-12	2.8018E-16	2.4733E-12
	8	O3(g)	1.1111E-31	1.4215E-23	9.1787E-32	5.4476E-24	9.1787E-32	5.4476E-24
	9	CO(g)	1.2025	1.727	0.64595	0.993366	0.64595	0.993366
	10	C2O(g)	1.8680E-10	8.2861E-06	1.5431E-10	3.1754E-06	1.5431E-10	3.1754E-06
	11	CO2(g)	3.7668E-06	1.3669E-04	1.4774E-06	9.0665E-05	1.4774E-06	9.0665E-05
	12	C3O2(g)	6.1042E-11	2.8016E-09	3.0522E-11	1.3066E-09	3.0522E-11	1.3066E-09
	13	Si(g)	9.9505E-08	0.503335	8.2199E-08	0.192885	8.2199E-08	0.192885
	14	Si2(g)	1.5830E-11	2.1367E-02	1.3077E-11	8.3794E-03	1.3077E-11	8.3794E-03
	15	Si3(g)	9.8608E-14	2.9329E-03	8.1458E-14	1.1503E-03	8.1458E-14	1.1503E-03
	16	SiC(g)	2.8349E-13	8.0859E-04	2.3419E-13	3.0986E-04	2.3419E-13	3.0986E-04
	17	SiC2(g)	1.2250E-09	3.5492E-02	1.0119E-09	1.3921E-02	1.0119E-09	1.3921E-02
	18	Si2C(g)	1.0595E-09	7.5722E-02	8.7520E-10	2.9699E-02	8.7520E-10	2.9699E-02

Click on the "+" column or use {Ins} and {Del} to add and remove species.

Mass
 mole
 gram

Order
 integer #
 mass (maximum)
 fraction (maximum)
 activity (maximum)

Select Top 0 species selected

Clear Refresh OK

Summary of species

List ordered with respect to:

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

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

Click on the "+" column or use {Ins} and {Del} to add and remove species.

Mass

- mole
- gram

Order

- integer #
- mass (maximum)
- fraction (maximum)
- activity (maximum)

Select Top

0 species selected

Refresh

OK

Species Window after selection

SiC(s2) = 0 to 0.59739 mole

Species Selection - EQUILIB Results

	#	Species	Mole (min)	Mole (max)	Fract. (min)	Fract. (max)	Act. (min)	Act. (max)
+	9	CO(g)	1.2025	1.727	0.64595	0.993366	0.64595	0.993366
+	21	Si	0	0.602919	0.742555	0.990684	2.5978E-02	0.984329
+	19	SiO(g)	7.9299E-03	0.599901	6.5507E-03	0.299962	6.5507E-03	0.299962
+	27	SiC(s2)	0	0.59739	0	0	0.182577	1.
+	13	Si(g)	9.9505E-08	0.503335	8.2199E-08	0.192885	8.2199E-08	0.192885
+	33	SiO2(s6)	0	0.39468	0	0	3.0086E-07	1.
+	22	SiO2(liq)	0	0.25151	0	0	3.7386E-07	1.
	18	Si2C(g)	1.0595E-09	7.5722E-02	8.7520E-10	2.9699E-02	8.7520E-10	2.9699E-02
	20	C	0	3.6279E-02	9.3161E-03	0.257445	7.4892E-03	0.115513
	17	SiC2(g)	1.2250E-09	3.5492E-02	1.0119E-09	1.3921E-02	1.0119E-09	1.3921E-02
	14	Si2(g)	1.5830E-11	2.1367E-02	1.3077E-11	8.3794E-03	1.3077E-11	8.3794E-03
	15	Si3(g)	9.8608E-14	2.9329E-03	8.1458E-14	1.1503E-03	8.1458E-14	1.1503E-03
	16	SiC(g)	2.8349E-13	8.0859E-04	2.3419E-13	3.0986E-04	2.3419E-13	3.0986E-04
	1	C(g)	2.8102E-13	1.7659E-04	2.3214E-13	6.7672E-05	2.3214E-13	6.7672E-05
	11	CO2(g)	3.7668E-06	1.3669E-04	1.4774E-06	9.0665E-05	1.4774E-06	9.0665E-05
	3	C3(g)	1.9131E-13	5.0061E-05	1.5804E-13	1.9184E-05	1.5804E-13	1.9184E-05
	2	C2(g)	6.3203E-15	2.4763E-05	5.2211E-15	9.4897E-06	5.2211E-15	9.4897E-06
	10	C2O(g)	1.8680E-10	8.2861E-06	1.5431E-10	3.1754E-06	1.5431E-10	3.1754E-06
	6	O(g)	2.4495E-12	8.7881E-07	2.0235E-12	3.3677E-07	2.0235E-12	3.3677E-07

Click on the "+" column or use {Ins} and {Del} to add and remove species.

Clear

Mass
 mole
 gram

Order
 integer #
 mass (maximum)
 fraction (maximum)
 activity (maximum)

Select Top 7 7 species selected

Refresh OK

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).

Labels

size: no:

chemical
 integer #
 none

No labels.

Label appears as the # number.

Label appears as a chemical formula.

Select the display properties.

Plot: mole vs T(K)

SiO2 + 1.8 C

Axis	Variable	Minimum	Maximum
Y-axis	activity	0	1.
	mole	0	2.6095
	mole fract.	0	0.993366
	gram	0	81.704
	weight %	0	99.315
X-axis	Alpha	0	0
	T(K)	1800.	3200.
	P(atm)	1.	1.
	A(J)	-2.0805E+06	-1.1831E+06
	G(J)	-2.0111E+06	-1.1650E+06
	Vol(l)	0	0
	H(J)	-3.9344E+05	3.2212E+05
	V(l)	178.81	685.24
	S(J)	428.63	729.12
	- page -	1.	63.

Species: 7 selected

Graph Labels: size: no:
 chemical
 integer #
 none

Display:
 color full screen
 reactants ViewFig
 file name Figure

Plot >>

Plot the graph.

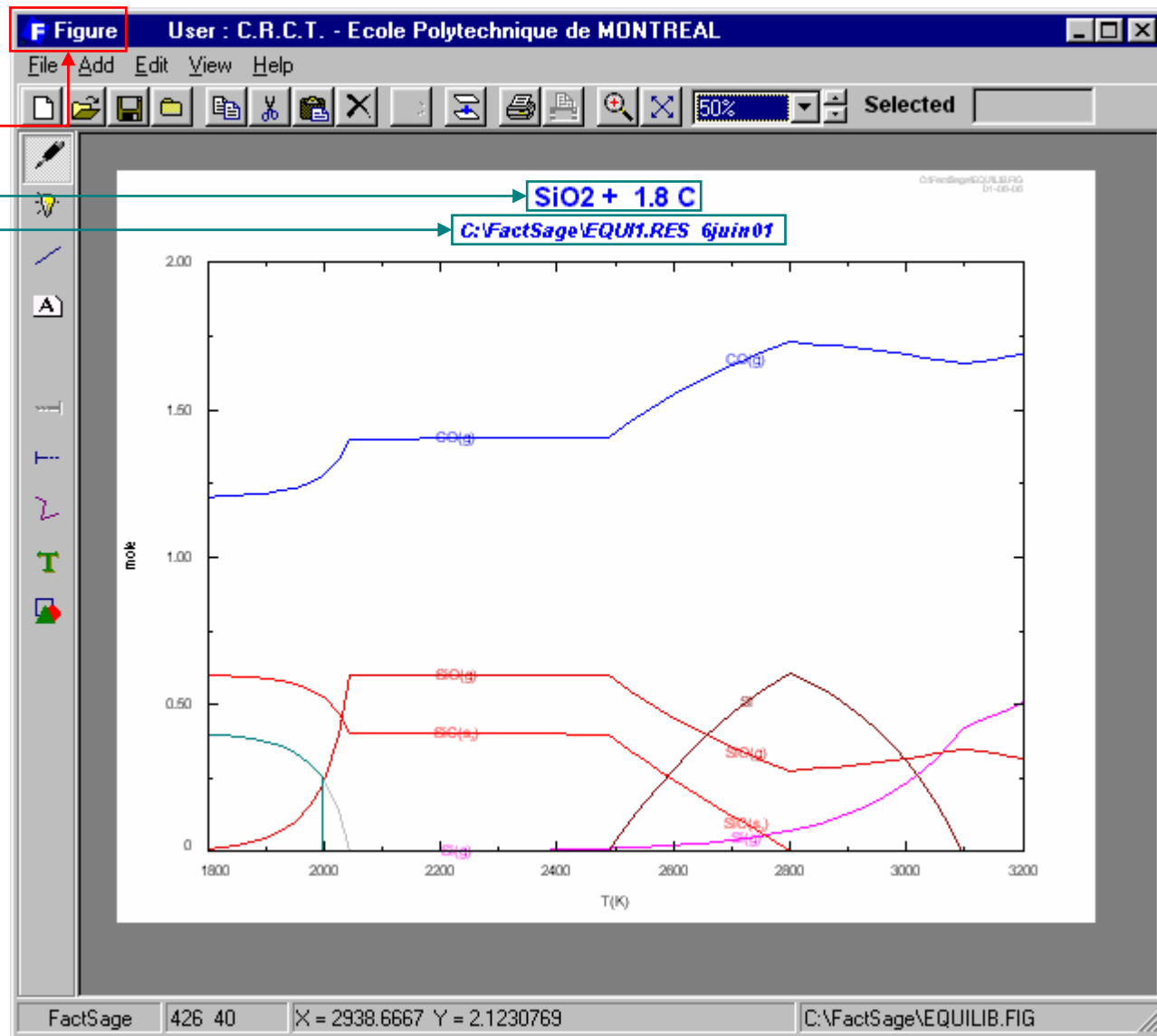
FactSage 5.0 C:\FactSage\Equi0.Res 6jun01 63 sets

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

Figure Output

Display

- color
- full screen
- reactants
- ViewFig
- file name
- Figure



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

Advanced output selection (**phase distribution**)

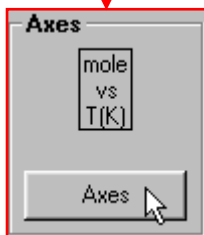
The following two slides show an advanced use of the **Results** module.

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

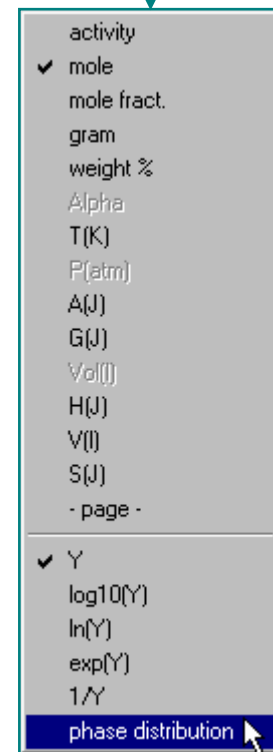
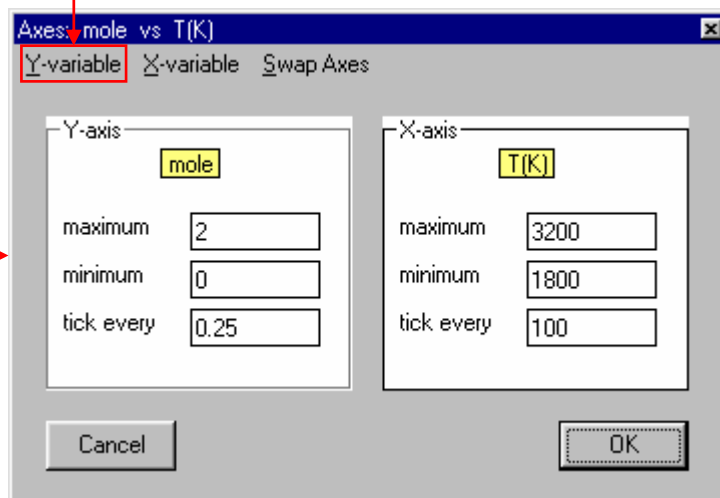
The resulting diagram is shown.

Specifying **phase distribution**

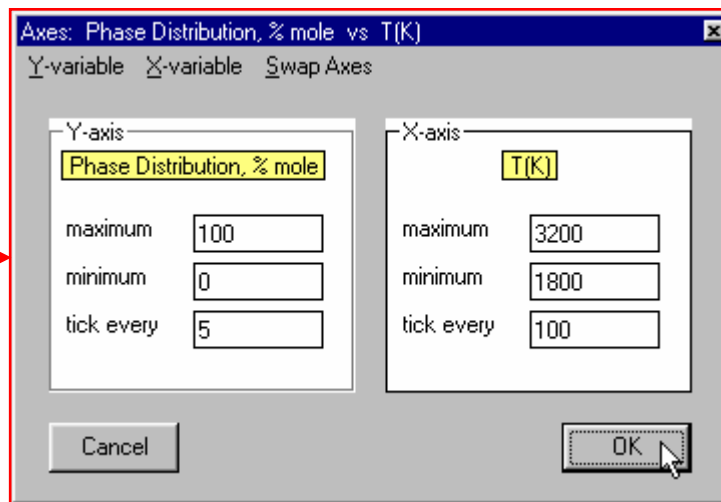
1. Click on «**Axes**».



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

