

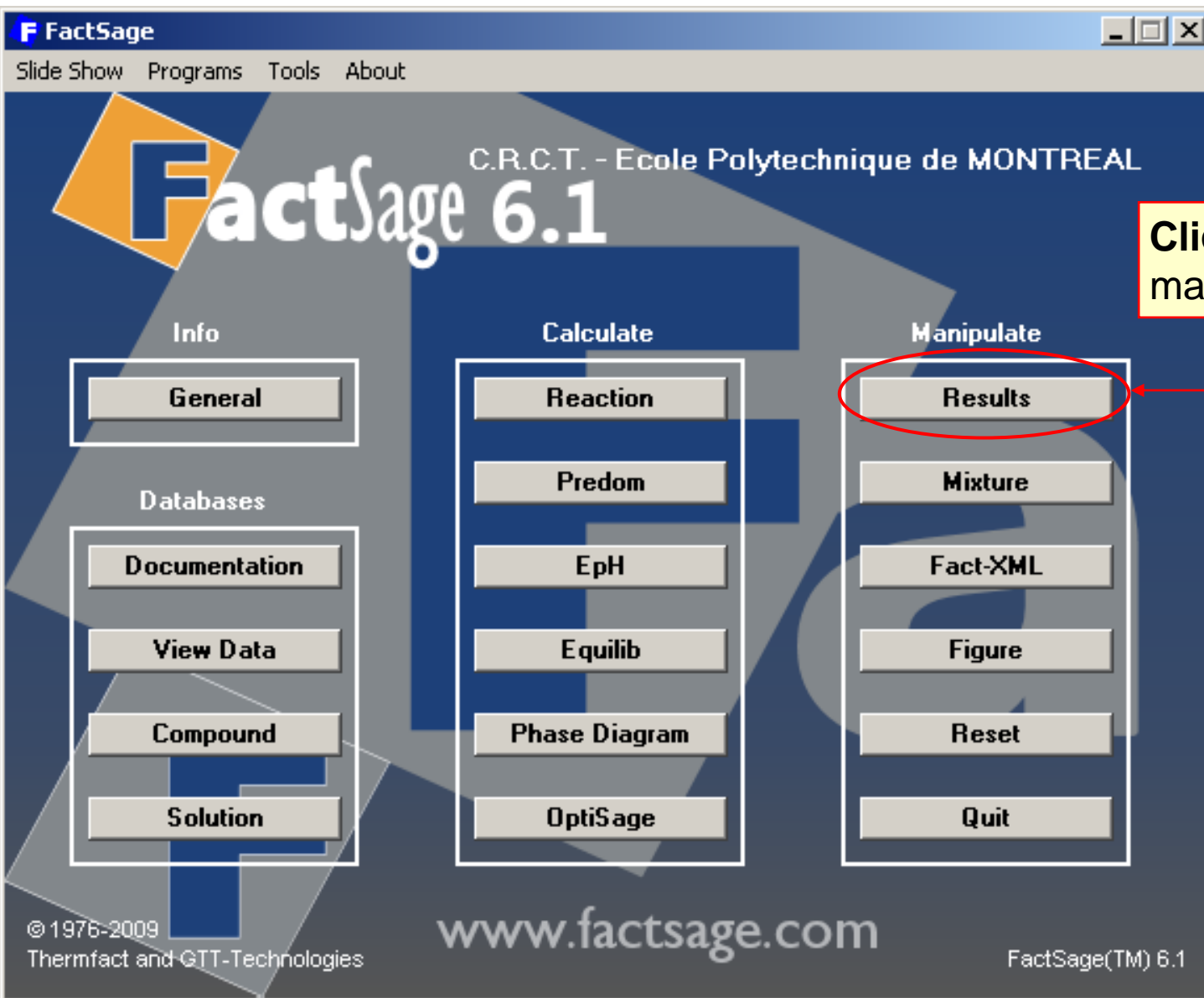
The **Results** module

- **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

The screenshot shows the 'Equilib' menu window in FactSage. The title bar reads 'F Menu - Equilib: last system'. The menu includes 'File', 'Units', 'Parameters', and 'Help'. The main input area shows 'Reactants (2)' as $\text{SiO}_2 + 1.8 \text{ C}$. The 'Products' section is divided into 'Compound species' and 'Solution species'. 'Compound species' includes options for gas, aqueous, pure liquids, and pure solids, with a total of 34 species. 'Solution species' shows a table with 'Base-Phase' and 'Full Name' columns, with 'FACT-LMLQ' and 'Lite-Liq' selected. The 'Final Conditions' section shows a temperature range of 1800 to 3200 K and a pressure of 1 atm. The 'Equilibrium' section has 'normal' and 'transitions' options selected. A 'Calculate >>' button is visible at the bottom right.

*	+	Base-Phase	Full Name
	+	FACT-LMLQ	Lite-Liq

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

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

The screenshot shows the 'Results - Equilib 1995.99 K (page 9/63)' window. The 'Output' menu is open, and 'Save Results file ...' is highlighted. The main window displays a list of chemical species and their amounts at 1995.99 K and 1 atm. The species list includes CO, SiO, CO2, Si, Si2C, Si2, SiC2, Si3, C2O, O, C3O2, SiC, C, C3, C2, O2, C4, C5, and O3.

Species	Amount
CO	0.85116
SiO	0.14875
CO2	8.4823E-05
Si	9.6298E-06
Si2C	2.6041E-07
Si2	2.3341E-08
SiC2	2.0715E-08
Si3	1.1757E-09
C2O	4.6189E-10
O	8.0127E-11
C3O2	5.4983E-11
SiC	3.9965E-11
C	6.4170E-12
C3	4.5067E-13
C2	7.6435E-14
O2	1.5457E-14
C4	6.5488E-18
C5	2.7040E-18
O3	9.7764E-29

Enter a file number and a description

The dialog box prompts the user to enter a file number (1-9999) or a file name. The file name '1 Carbothermic reduction of silica' is entered in the text field.

Save File in c:\FactSage\Equi*.res

Enter the file number (1 - 9999)

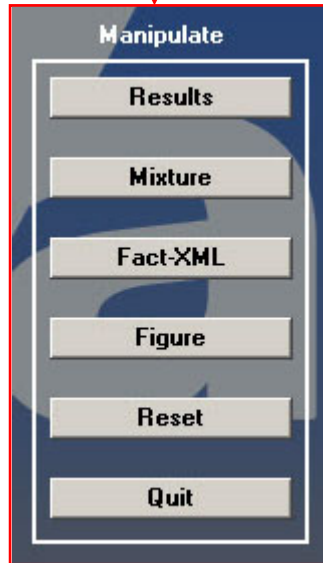
or enter the file name, for example

My very favorite results

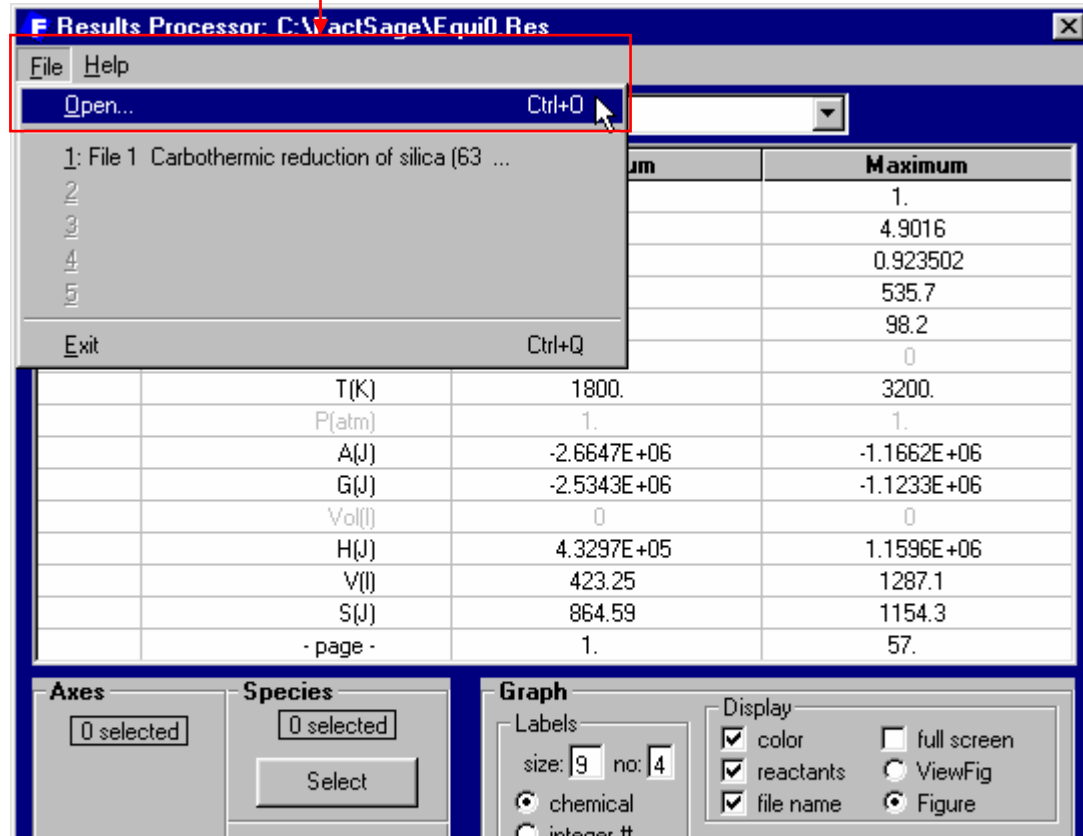
- avoid the special characters ?@/!\~.,"*%+;<>()\

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

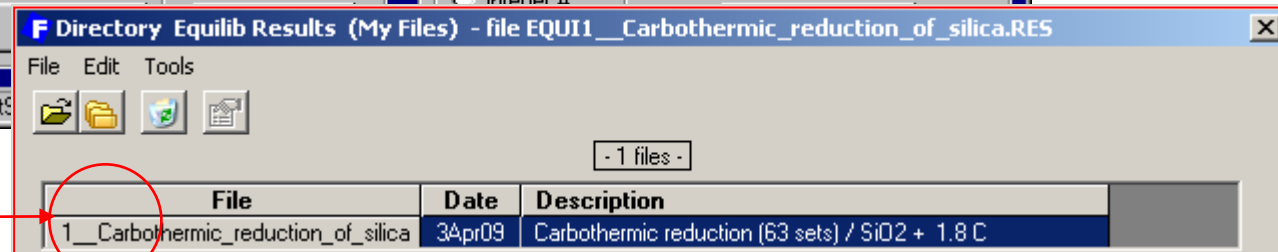
Now you can initiate the **Results** Program.



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

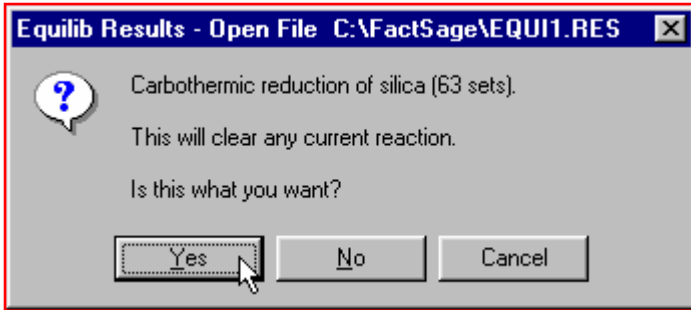


Select and double-click on the file.



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.

Results Processor: c:\FactSage\EQUI1_Carbothermic_reduction_of_silica.RES

File Help

SiO₂ + 1.8 C

activity	0	1.
mole	0	2.6095
mole fract.	0	0.993366
gram	0	81.704
weight %	0	99.599
Alpha	0	0
T(K)	1800.	3200.
P(atm)	1.	1.
Cp(J)	95.361	3993.
G(J)	-2.0111E+06	-1.1650E+06
Vol(litre)	0	0
H(J)	-3.9344E+05	3.2212E+05
V(litre)	178.81	685.22
S(J)	428.63	729.12
- page -	1.	63.

Axes 0 selected **Species** 0 selected

Graph

Labels: size: 9 no: 4

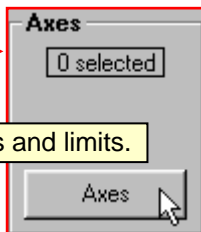
Display: color full screen
 reactants Viewer
 file name Figure

Plot >>

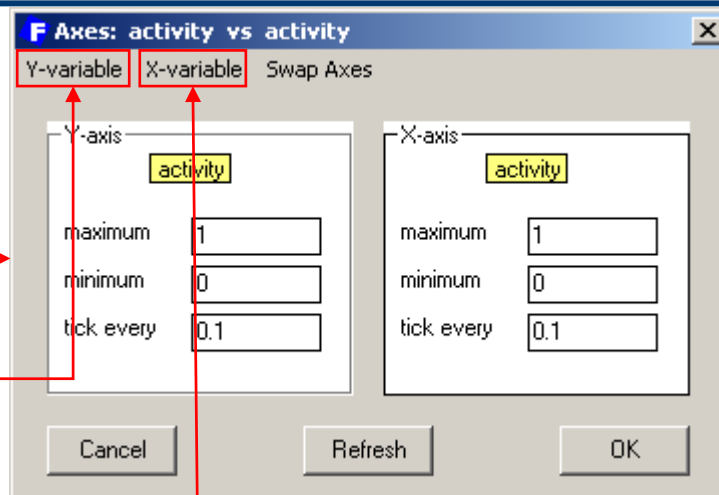
FactSage c:\FactSage\EQUI1_Carbothermic_reduction_of_silica.RES 3Apr09 63 sets

Axes Window

1. Click on «**Axes**».



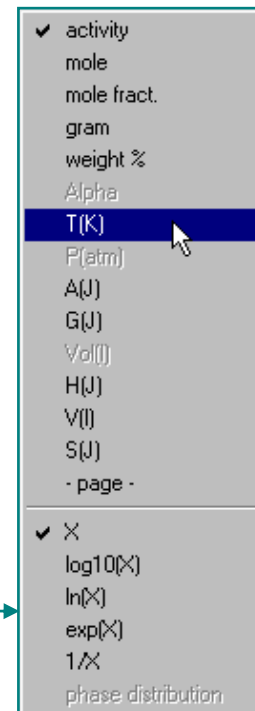
Define X & Y-axes and limits.



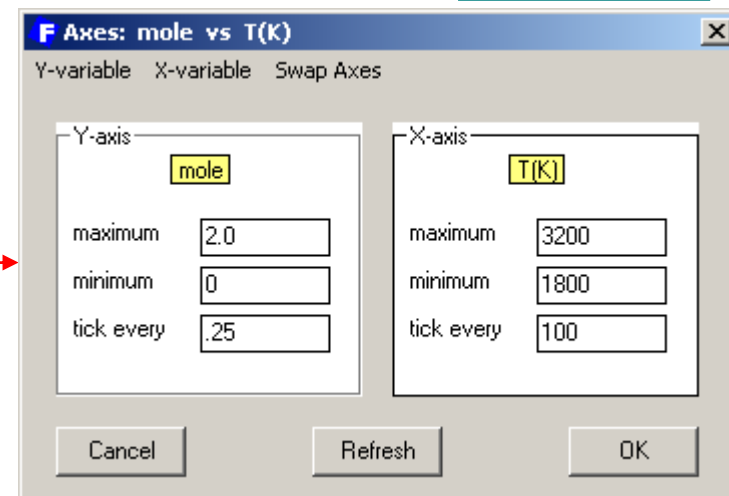
2. Click on «**Y-variable**». Define the **Y-axis** in the **pop-up** menu.



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

	activity	0	1.
Y-axis	mole	0	2.6095
	mole fract.	0	0.993366
	gram	0	81.704
	weight %	0	99.599
	Alpha	0	0
X-axis	T(K)	1800.	3200.
	P(atm)	1.	1.
	Cp(J)	95.361	3993.
	G(J)	-2.0111E+06	-1.1650E+06
	Vol(litre)	0	0
	H(J)	-3.9344E+05	3.2212E+05
	V(litre)	178.81	685.22
	S(J)	428.63	729.12
	- page -	1.	63.

Axes mole vs T(K) **Species** 0 selected

Buttons: Axes, Repeat, Select

Graph

Labels: size: 9 no: 4

Display: color full screen
 reactants Viewer
 file name Figure

Plot >>

FactSage | c:\FactSage\EQUI1_Carbothermic_reduction_of_silica.RES | 3Apr09 | 63 sets

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

Species Selection - EQUILIB Results: mole vs T(K)

File

+ #	Species	Mole (min)	Mole (max)	Fract. (min)	Fract. (max)	Act. (min)	Act. (max)
	Gas Phase						
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	0.645949	0.993366	0.645949	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

Mass: mole gram source

Order: integer # mass (max) fraction (max) activity (max)

Select Top: 15 0 species selected

Clear Refresh OK

Click on the "+" column to add or remove species.

Summary of species

List ordered with respect to:

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

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

Mass: mole gram source

Order: integer # mass (max) fraction (max) activity (max)

Select Top: 7 0 species selected

Clear Refresh OK

Click on the "+" column to add or remove species.

Species Window after selection

SiC(s2) = 0 to 0.59739 mole

Species Selection - EQUILIB Results: mole vs T(K)

	#	Species	Mole (min)	Mole (max)	Fract. (min)	Fract. (max)	Act. (min)	Act. (max)
+	9	CO(g)	1.2025	1.727	0.645949	0.993366	0.645949	0.993366
+	21	Si(LMLQ)	0	0.602919	0.728018	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
+	28	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
+	34	SiO2(s6)	0	0.39468	0	0	3.0086E-07	1.
+	23	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(LMLQ)	0	3.6279E-02	9.3161E-03	0.271982	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

Mass: mole gram source

Order: integer # mass (max) fraction (max) activity (max)

Select Top: 7 7 species selected

Clear Refresh OK

Click on the "+" column to add or remove species.

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).

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

	activity	0	1.
Y-axis	mole	0	2.6095
	mole fract.	0	0.993366
	gram	0	81.704
	weight %	0	99.599
	Alpha	0	0
X-axis	T(K)	1800.	3200.
	P(atm)	1.	1.
	Cp(J)	95.361	3993.
	G(J)	-2.0111E+06	-1.1650E+06
	Vol(litre)	0	0
	H(J)	-3.9344E+05	3.2212E+05
	V(litre)	178.81	585.22
	S(J)	428.63	729.12
	- page -	1.	63.

Axes: mole vs T(K) Species: 7 selected

Graph: Labels size: 9 no: 2
 chemical
 integer #
 none

Display:
 color full screen
 reactants Viewer
 file name Figure

Plot >>

Plot the graph.

FactSage c:\FactSage\EQUI1_Carbothermic_reduction_of_silica.RES 3Apr09 63 sets

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

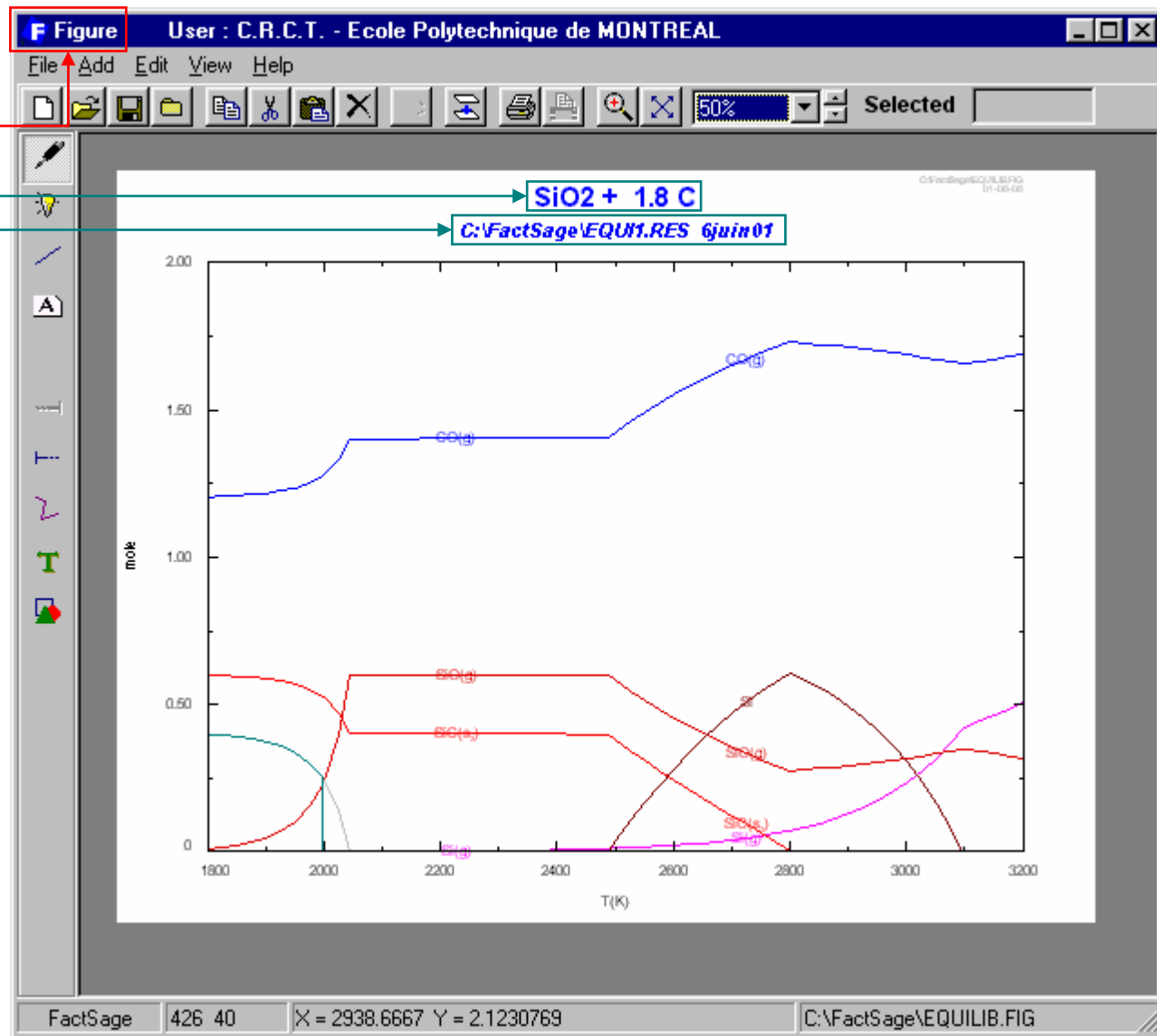
Figure Output

Display

color full screen

reactants ViewFig

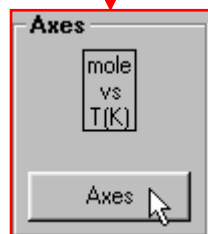
file name Figure



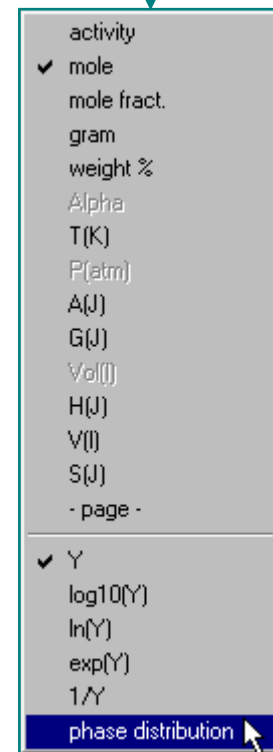
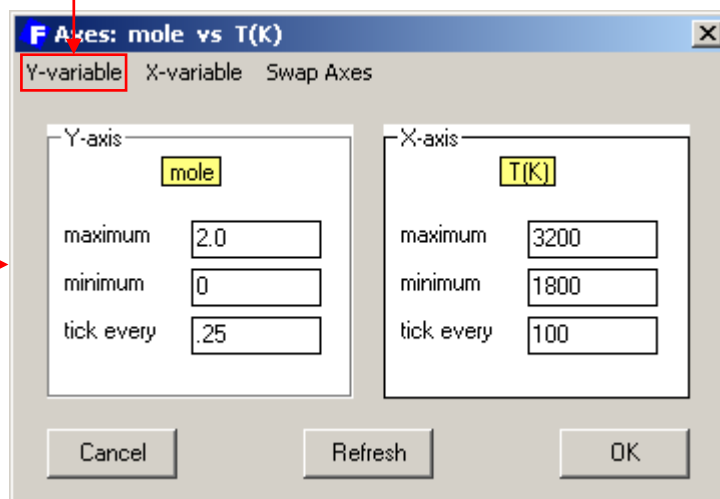
In **Figure**, you can edit and save the graph.

Specifying **phase distribution**

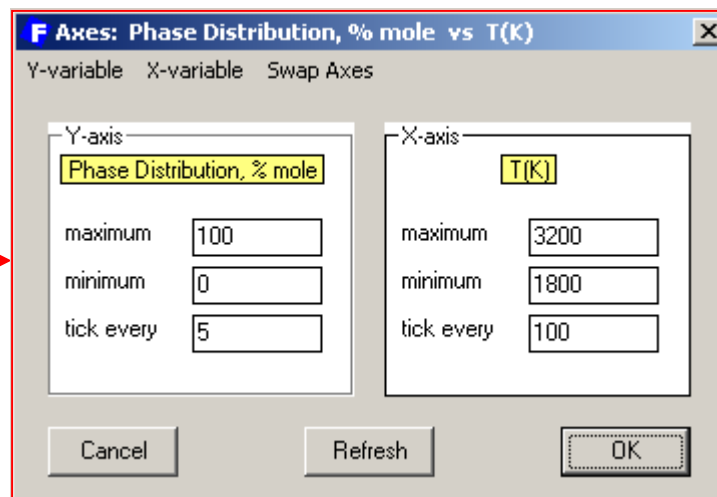
1. Click on «**Axes**».



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

