The *Reaction* module

Reaction calculates the thermochemical properties of a species, a mixture of species or a chemical reaction.

Reaction accesses only compound databases.

Reaction assumes all gases are ideal and ignores expansivities and compressibilities of solids and liquids.

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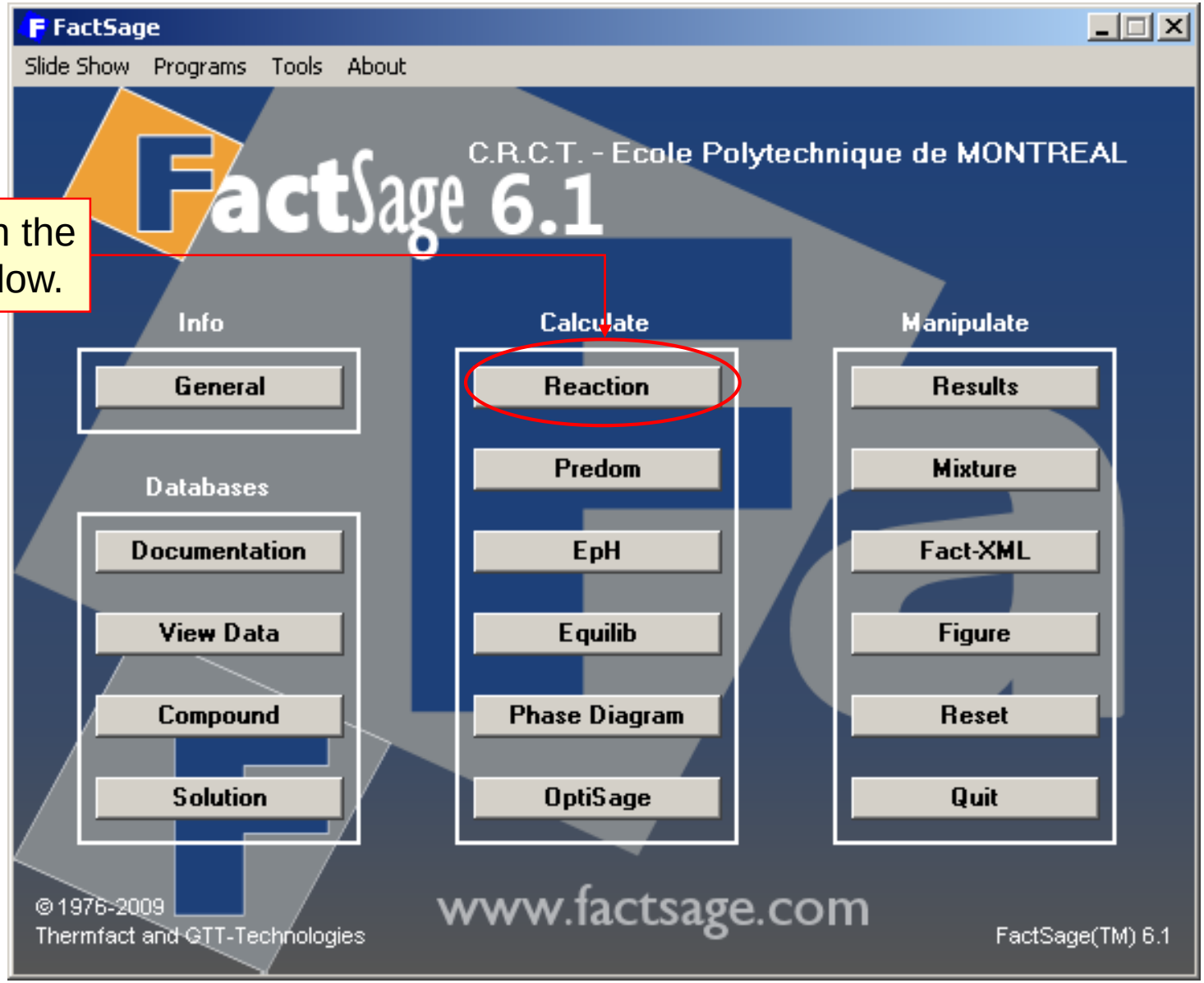
The *Reaction* module

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



Reactants window - entry of a species (pure Cu)

Add a Product

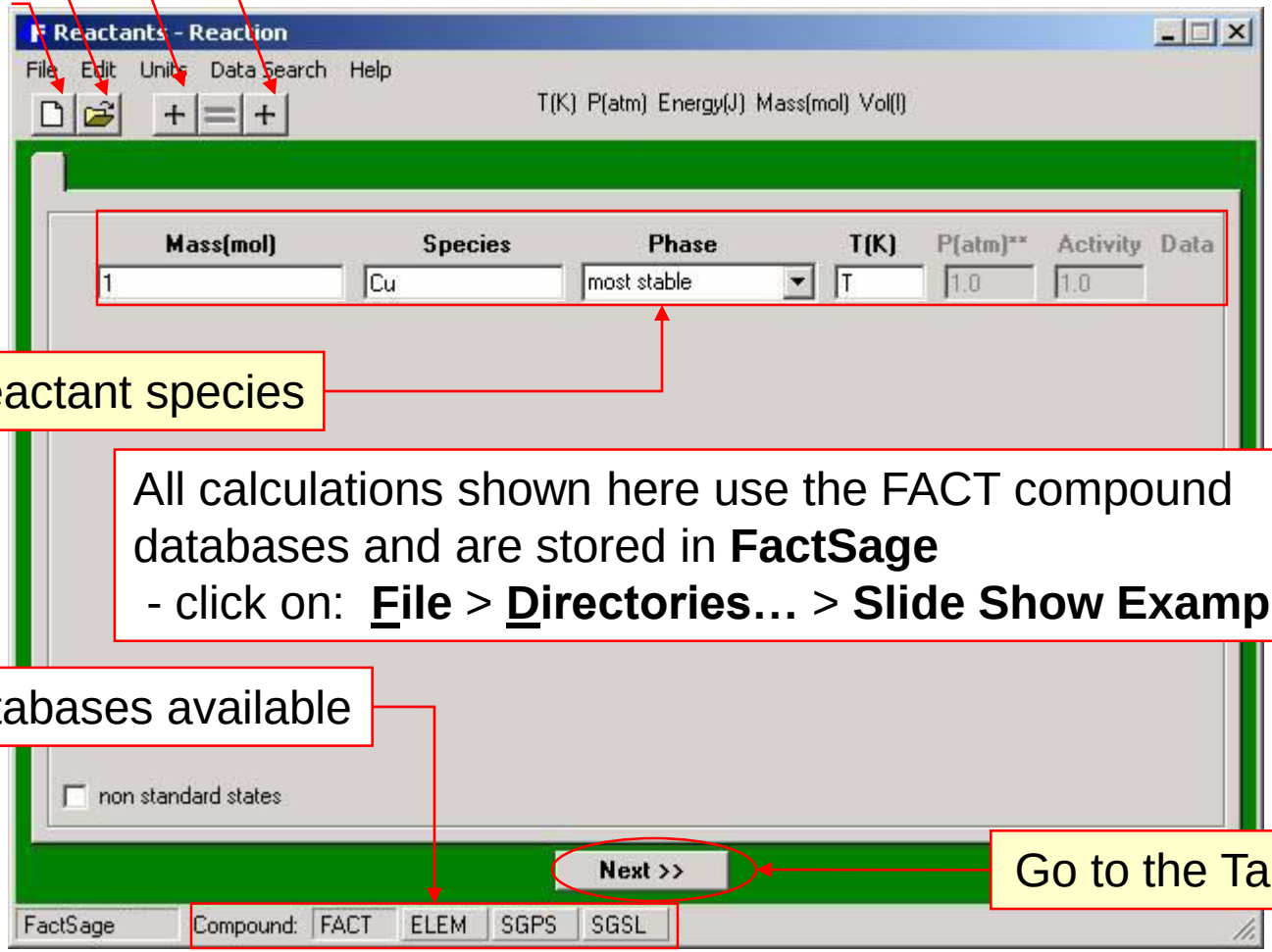
Add a Reactant

Open

New Reaction

Reaction has two windows – **Reactants** and **Table**

Reaction can only access compounds (not solutions)



Entry of reactant species

All calculations shown here use the FACT compound databases and are stored in **FactSage**
- click on: **File** > **Directories…** > **Slide Show Examples** …

Compound databases available

Go to the Table window

Table window – thermodynamic properties of a species

Open

Save

New Reaction

Stop Calculation

Table Reaction

File Units Output Figure Help

T(K) P(atm) Energy(J) Mass(mol) Vol(l)

Reactants

Cu (T)

Summary of the **Reactants** window

T(K)	H(J)	G(J)	Vol(l)	S(J/K)	Cp(J/K)	A (J)	T
------	Cu(s)	------					
300.00	45.3	-9949.3	7.1240E-03	33.315	24.468	-9950.1	
800.00	13120.4	-33868.0	7.1240E-03	58.736	27.481	-33868.8	
1300.00	27758.9	-66968.6	7.1240E-03	72.867	32.201	-66969.4	
1358.00	29659.9	-71236.5	7.1240E-03	74.298	33.362	-71237.2	
------	Cu(l)	------					
Cu(1 mol):	DH = 13138.0	DG = 0	------	DS = 9.674			
1358.00	42797.9	-71236.5	7.1240E-03	83.972	32.844	-71237.2	
1800.00	57314.9	-110493.4	7.1240E-03	93.227	32.844	-110494.1	
2300.00	73736.9	-159201.7	7.1240E-03	101.278	32.844	-159202.4	
2800.00	90158.9	-211508.6	7.1240E-03	107.738	32.844	-211509.4	
2846.16	91675.0	-216494.2	7.1240E-03	108.275	32.844	-216494.9	
------	Cu(g)	------					
Cu(1 mol):	DH = 300653.1	DG = 0	------	DS = 105.635			
2846.16	392328.1	-216494.2	2.3355E+02	213.910	24.400	-240158.6	
3300.00	403914.1	-314439.8	2.7079E+02	217.683	26.675	-341877.7	

300 3300 500

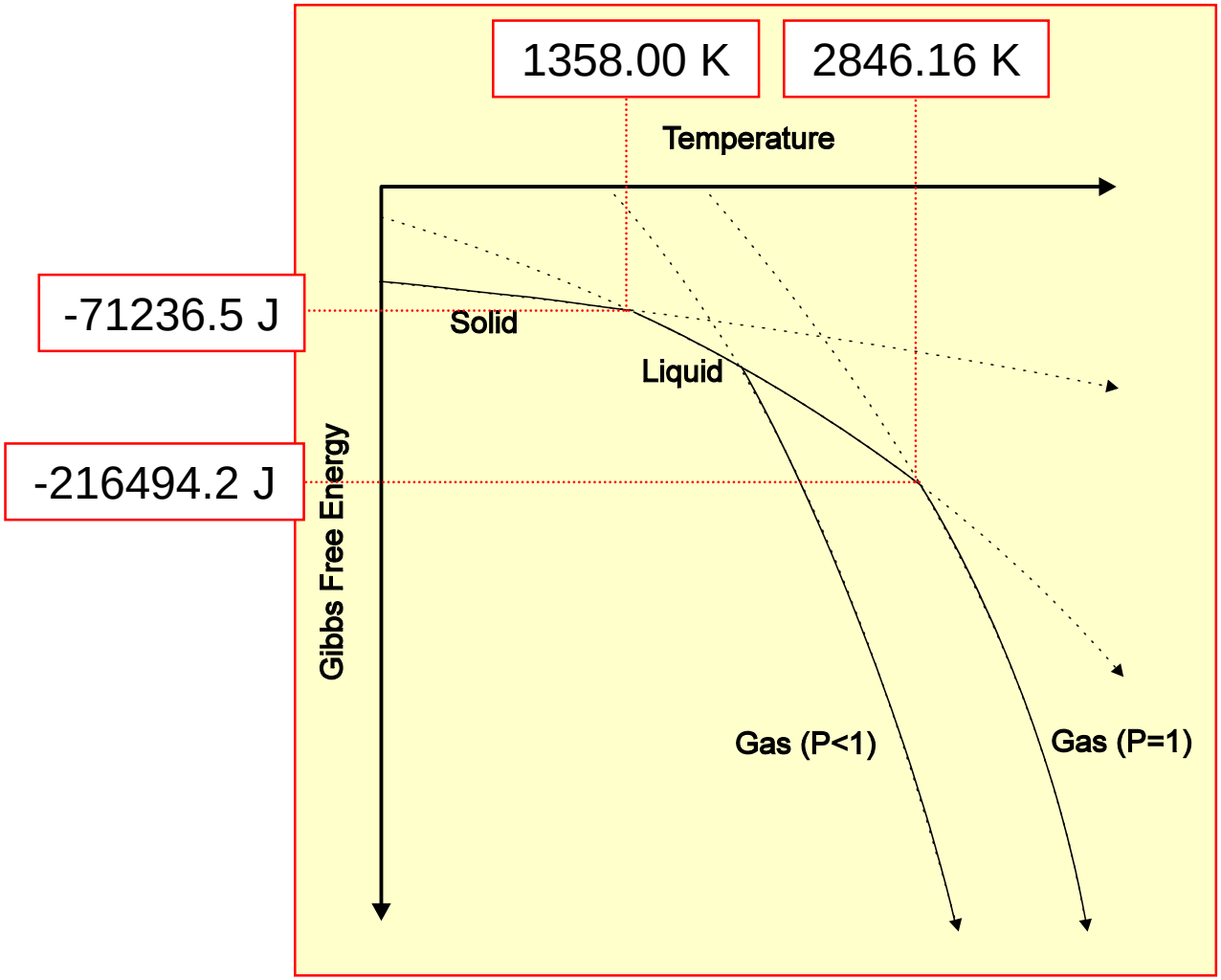
Calculate << Back Clear

A multiple entry for **T**: **min**, **max** and **step**. The results also display the calculated **transition temperatures**.

Return to the **Reactants** window

Determination of most stable phase by **Gibbs energy minimization**

Phase with **lowest** Gibbs energy is the **most** stable.



Points on the solid lines for **P = 1 atm** are given in column «**T**» and «**G**» of the previous figure for copper.

Simple isothermal standard state reaction: **oxidation of copper**

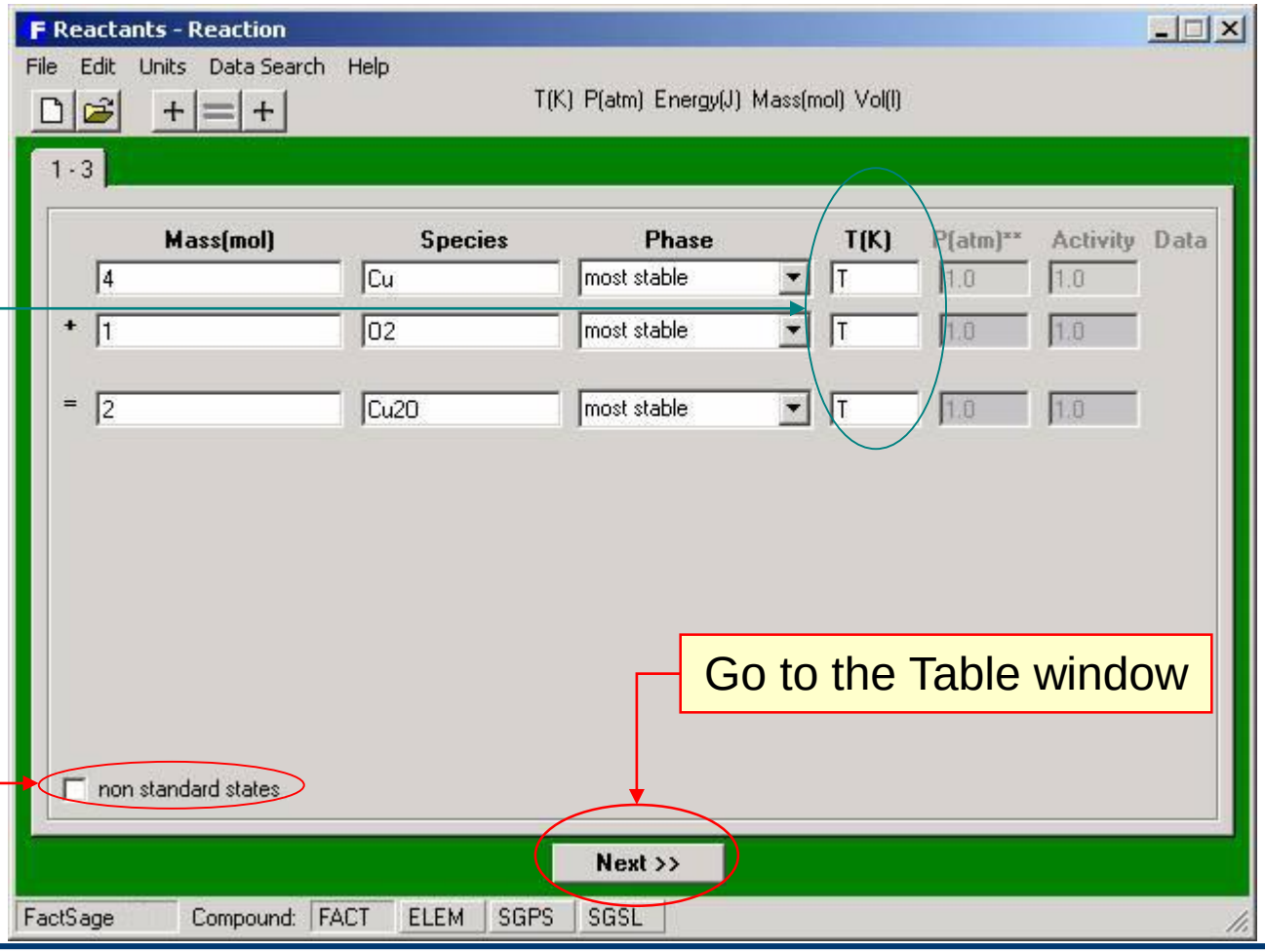
Entry of an isothermal standard state reaction: **$4\ Cu + O_2 = 2\ Cu_2O$**

This example is stored in **FactSage**. Go to the **menu bar** and click on: **File** > **Directories…** > **Slide Show Examples** and **select** file 2.

Isothermal "**T**" throughout

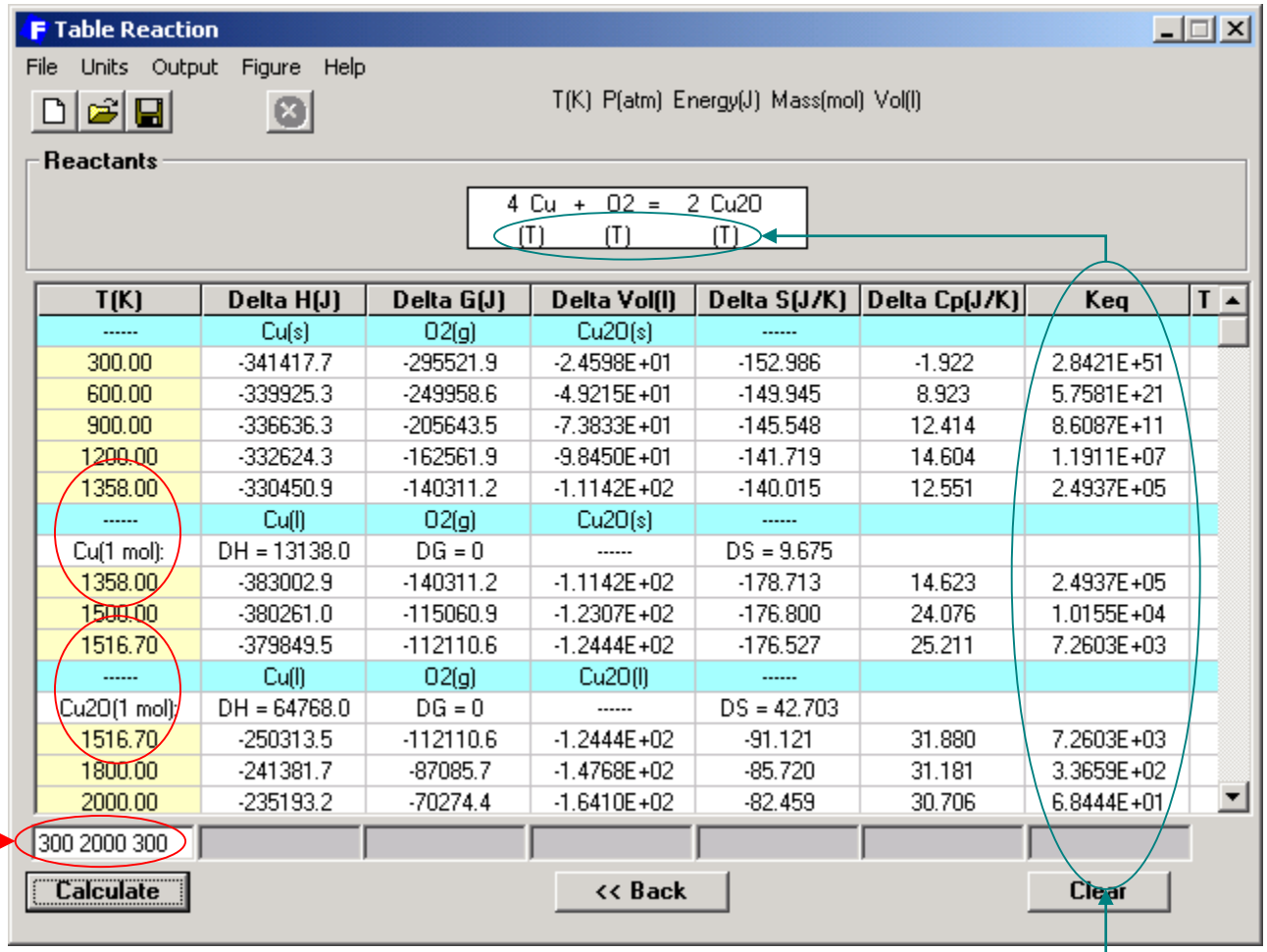
Non standard states checkbox is **not** selected

Go to the Table window



Oxidation of copper at various temperatures

Entry: T_{min}=**300K**, T_{max}=**2000K** and **step=300K.** Note the **transition temperatures**.



T(K)	Delta H(J)	Delta G(J)	Delta Vol(l)	Delta S(J/K)	Delta Cp(J/K)	Keq
------	Cu(s)	O2(g)	Cu2O(s)	------		
300.00	-341417.7	-295521.9	-2.4598E+01	-152.986	-1.922	2.8421E+51
600.00	-339925.3	-249958.6	-4.9215E+01	-149.945	8.923	5.7581E+21
900.00	-336636.3	-205643.5	-7.3833E+01	-145.548	12.414	8.6087E+11
1200.00	-332624.3	-162561.9	-9.8450E+01	-141.719	14.604	1.1911E+07
1358.00	-330450.9	-140311.2	-1.1142E+02	-140.015	12.551	2.4937E+05
------	Cu(l)	O2(g)	Cu2O(s)	------		
Cu(1 mol):	DH = 13138.0	DG = 0	------	DS = 9.675		
1358.00	-383002.9	-140311.2	-1.1142E+02	-178.713	14.623	2.4937E+05
1500.00	-380261.0	-115060.9	-1.2307E+02	-176.800	24.076	1.0155E+04
1516.70	-379849.5	-112110.6	-1.2444E+02	-176.527	25.211	7.2603E+03
------	Cu(l)	O2(g)	Cu2O(l)	------		
Cu2O(1 mol):	DH = 64768.0	DG = 0	------	DS = 42.703		
1516.70	-250313.5	-112110.6	-1.2444E+02	-91.121	31.880	7.2603E+03
1800.00	-241381.7	-87085.7	-1.4768E+02	-85.720	31.181	3.3659E+02
2000.00	-235193.2	-70274.4	-1.6410E+02	-82.459	30.706	6.8444E+01

The equilibrium constant column appears for an **isothermal** standard state reaction. $\Delta G^o = -RT \ln K$. For the values of the gas constant ***R***, click on the **Units** menu.

Simple chemical equilibrium: **non standard state** oxidation of copper

F Reactants - Reaction

File Edit Units Data Search Help

T(K) P(atm) Energy(J) Mass(mol) Vol(l)

1 - 3

	Mass(mol)	Species	Phase	T(K)	P(atm)**	Activity	Data
	4	Cu	solid	T	1.0	X	
+	1	O2	gas	T	P		
=	2	Cu2O	solid	T	1.0	1.0	

$a_{Cu(s)}$ = "X"

$P_{O_2(g)}$ = "P"

Select non standard state

** For a gas species, P(atm/bar/psi) is its ideal partial pressure.
For a liquid or solid, P is the hydrostatic pressure above the phase
- molar volume (but not compressibility) data are employed in the 'VdP' term.

☑ non standard states

Next >>

FactSage Compound: FACT ELEM SGPS SGSL

T(K) P(atm) Energy(J) Mass(mol) Vol(l)

Reactants

4 Cu (T,s,X)	+	O2 (T,P,g)	=	2 Cu2O (T,s)

T(K)	P(atm)	Activity X	Delta H(J)	Delta G(J)	Delta Vol(l)	Delta S(J/K)	T
1000.00	1.0000E+00	1.0000E+00	-335381.1	-191155.7	-8.2039E+01	-144.225	

Standard state reaction:

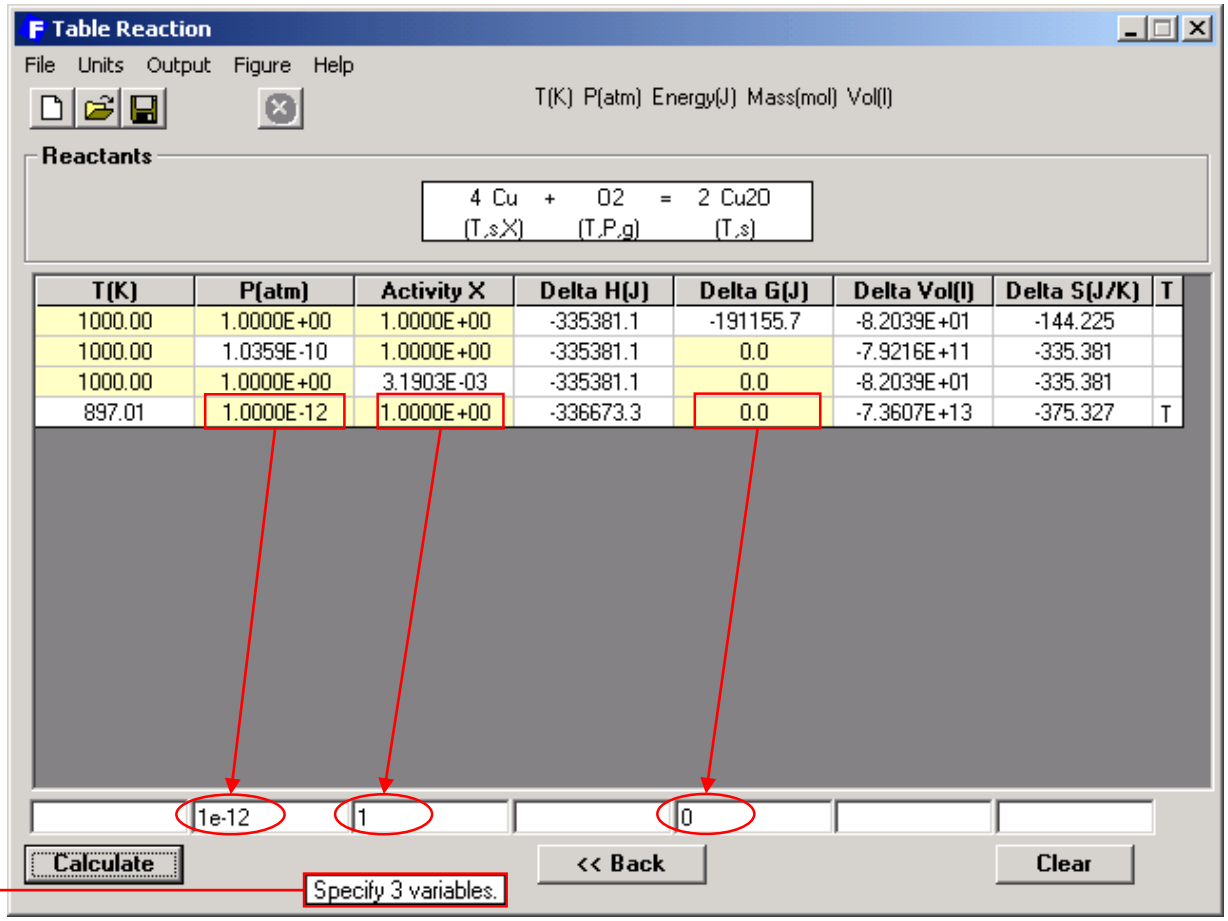
$P_{O_2(g)}$ = **1.0 atm**

$a_{Cu(s)}$ = **1.0**

Specifying an extensive property change to deal with chemical equilibrium

For simple chemical equilibrium: $\Delta G = \Delta G^0 + RT \ln\left(\frac{a^2_{Cu_2O}}{a^4_{Cu} \cdot P_{O_2}}\right)$ and $\Delta G^0 = -RT \ln K_{eq}$

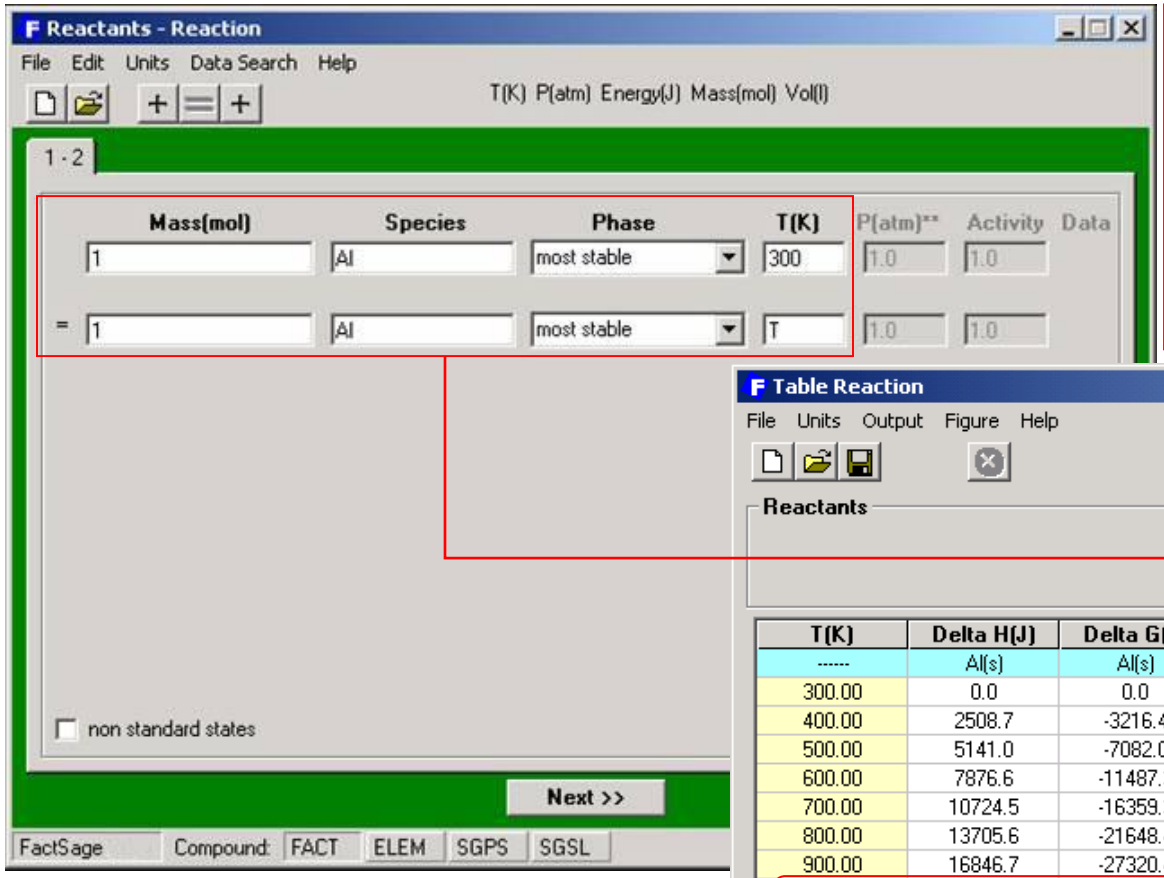
Table provides ΔG using: $\Delta G = \Delta G^0 + RT \ln\left(\frac{1}{X^4 \cdot P}\right)$ and $K_{eq} = \frac{1}{X^4 \cdot P}$ when $\Delta G = 0$.



For the last entry:

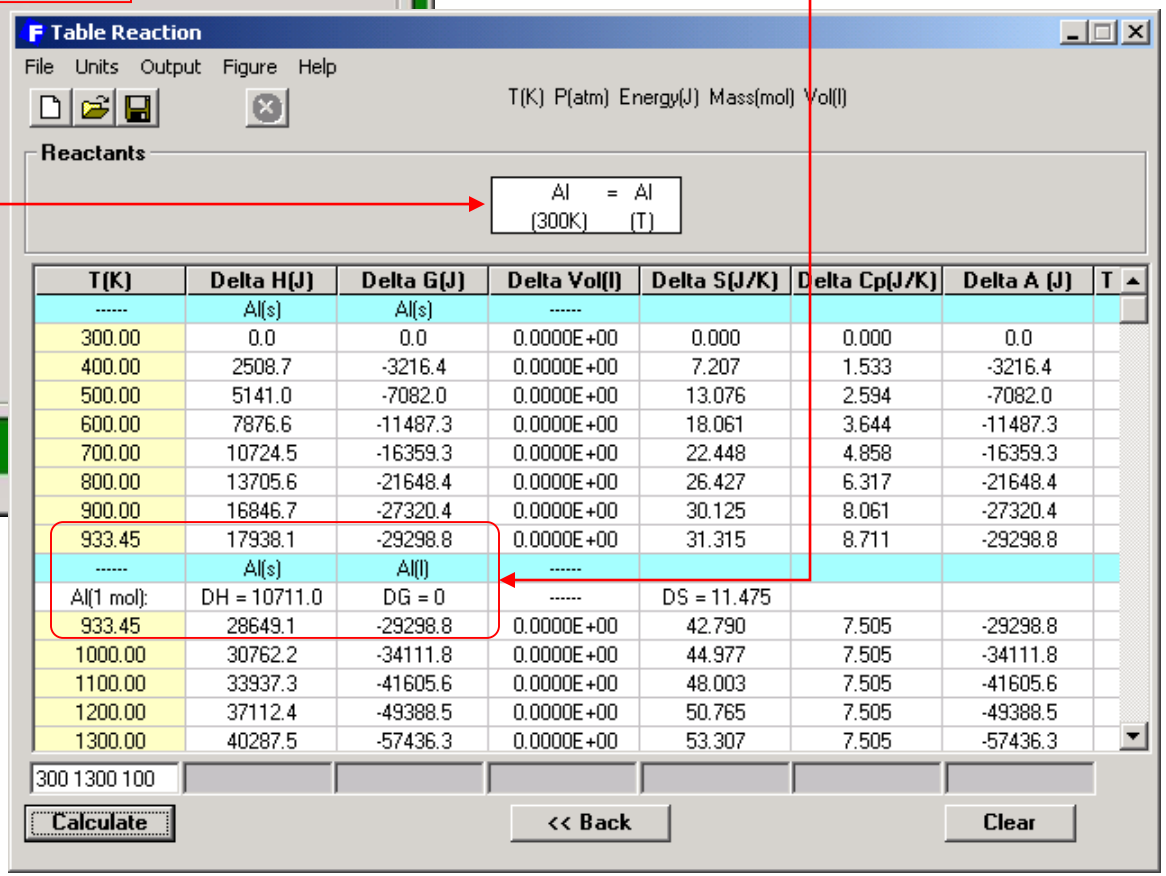
- $P_{O_2(g)}$ = **10^{-12}**
- $a_{Cu(s)}$ = **1**
- ΔG = **0**, equilibrium

Heating **Al** from **300 K** to the temperature **T**



phase transition, $\mathbf{Al}_{(s)} \rightarrow \mathbf{Al}_{(l)}$ (i.e. *fusion*) at 933.45 K

$$\Delta H^\circ_{fusion} = T_{fusion} \bullet \Delta S^\circ_{fusion}$$
$$= 28649.1\text{J} - 17938.1\text{J}$$
$$= 10711.0\ \text{J}$$



T(K)	Delta H(J)	Delta G(J)	Delta Vol(l)	Delta S(J/K)	Delta Cp(J/K)	Delta A (J)
------	Al(s)	Al(s)	------			
300.00	0.0	0.0	0.0000E+00	0.000	0.000	0.0
400.00	2508.7	-3216.4	0.0000E+00	7.207	1.533	-3216.4
500.00	5141.0	-7082.0	0.0000E+00	13.076	2.594	-7082.0
600.00	7876.6	-11487.3	0.0000E+00	18.061	3.644	-11487.3
700.00	10724.5	-16359.3	0.0000E+00	22.448	4.858	-16359.3
800.00	13705.6	-21648.4	0.0000E+00	26.427	6.317	-21648.4
900.00	16846.7	-27320.4	0.0000E+00	30.125	8.061	-27320.4
933.45	17938.1	-29298.8	0.0000E+00	31.315	8.711	-29298.8
------	Al(s)	Al(l)	------			
Al(1 mol):	DH = 10711.0	DG = 0	------	DS = 11.475		
933.45	28649.1	-29298.8	0.0000E+00	42.790	7.505	-29298.8
1000.00	30762.2	-34111.8	0.0000E+00	44.977	7.505	-34111.8
1100.00	33937.3	-41605.6	0.0000E+00	48.003	7.505	-41605.6
1200.00	37112.4	-49388.5	0.0000E+00	50.765	7.505	-49388.5
1300.00	40287.5	-57436.3	0.0000E+00	53.307	7.505	-57436.3

300 1300 100

The equilibrium constant is **not** displayed because this is a **non-isothermal non-equilibrium calculation**.

Heating Al: creating the graphical display with *Figure*

1. Click on the menu **Figure** and select **Axes...**

2. A dialog box opens and provides you with a choice of **axes** for the figure.

F Table Reaction

File Units Output Figure Help

Axes...
Plot
Save Figure

T(K) P(atm) Energy(J) Mass(mol) Vol(l)

Reactants

Al (300K) = Al (T)

T(K)	Delta H(J)	Delta G(J)	Delta Vol(l)	Delta S(J/K)	Delta Cp(J/K)	Delta A (J)
------	Al(s)	Al(s)	------			
300.00	0.0	0.0	0.0000E+00	0.000	0.000	0.0
400.00	2508.7	-3216.4	0.0000E+00	7.207	1.533	-3216.4
500.00	5141.0	-7082.0	0.0000E+00	13.076	2.594	-7082.0
600.00	7876.6	-11487.3	0.0000E+00	18.061	3.644	-11487.3
700.00	10724.5	-16359.3	0.0000E+00	22.448	4.858	-16359.3
800.00	13705.6	-21648.4	0.0000E+00	26.427	6.317	-21648.4
900.00	16846.7	-27320.4	0.0000E+00	30.125	8.061	-27320.4
933.45	17938.1	-29298.8	0.0000E+00	31.315	8.711	-29298.8
------	Al(s)	Al(l)	------			
Al(1 mol):	DH = 10711.0	DG = 0	------	DS = 11.475		
933.45	28649.1	-29298.8	0.0000E+00	42.790	7.505	
1000.00	30762.2	-34111.8	0.0000E+00	44.977	7.505	
1100.00	33937.3	-41605.6	0.0000E+00	48.003	7.505	
1200.00	37112.4	-49388.5	0.0000E+00	50.765	7.505	
1300.00	40287.5	-57436.3	0.0000E+00	53.307	7.505	

300 1300 100

Calculate << Back

F Axes: Delta H(J) vs T(K)

Y-variable X-variable Swap Axes

T(K)
✔ Delta H(J)
Delta G(J)
Delta Vol(l)
Delta S(J/K)
Delta Cp(J/K)
Delta A (J)

✔ Y
log10(Y)
ln(Y)
exp(Y)
1/Y

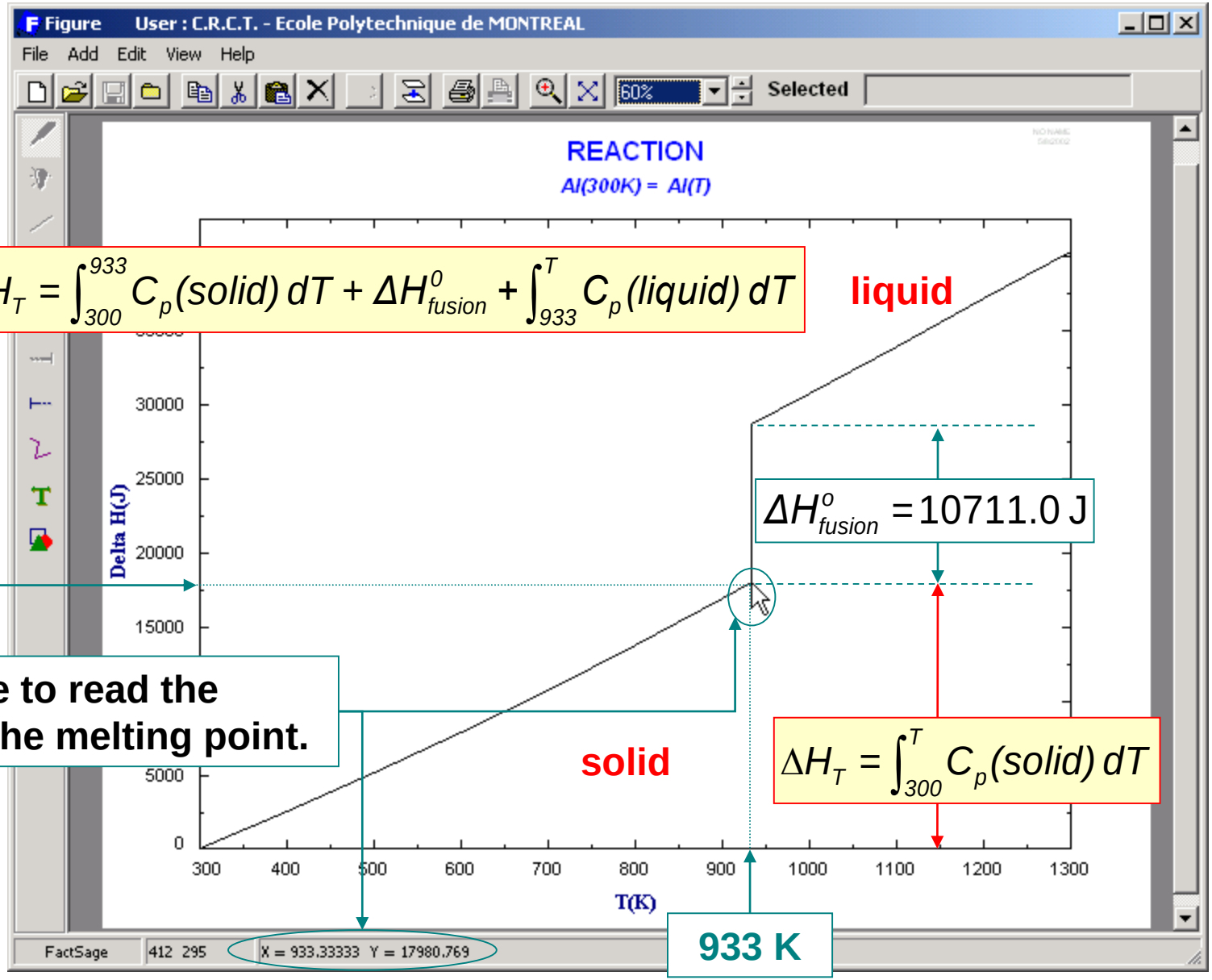
Y-axis: Delta H(J)
maximum 42500
minimum 0
tick every 2500

X-axis: T(K)
maximum 1300
minimum 300
tick every 50

Cancel Refresh OK

Click on **Refresh** for the default settings

Heating Al: graphical display of thermodynamic properties

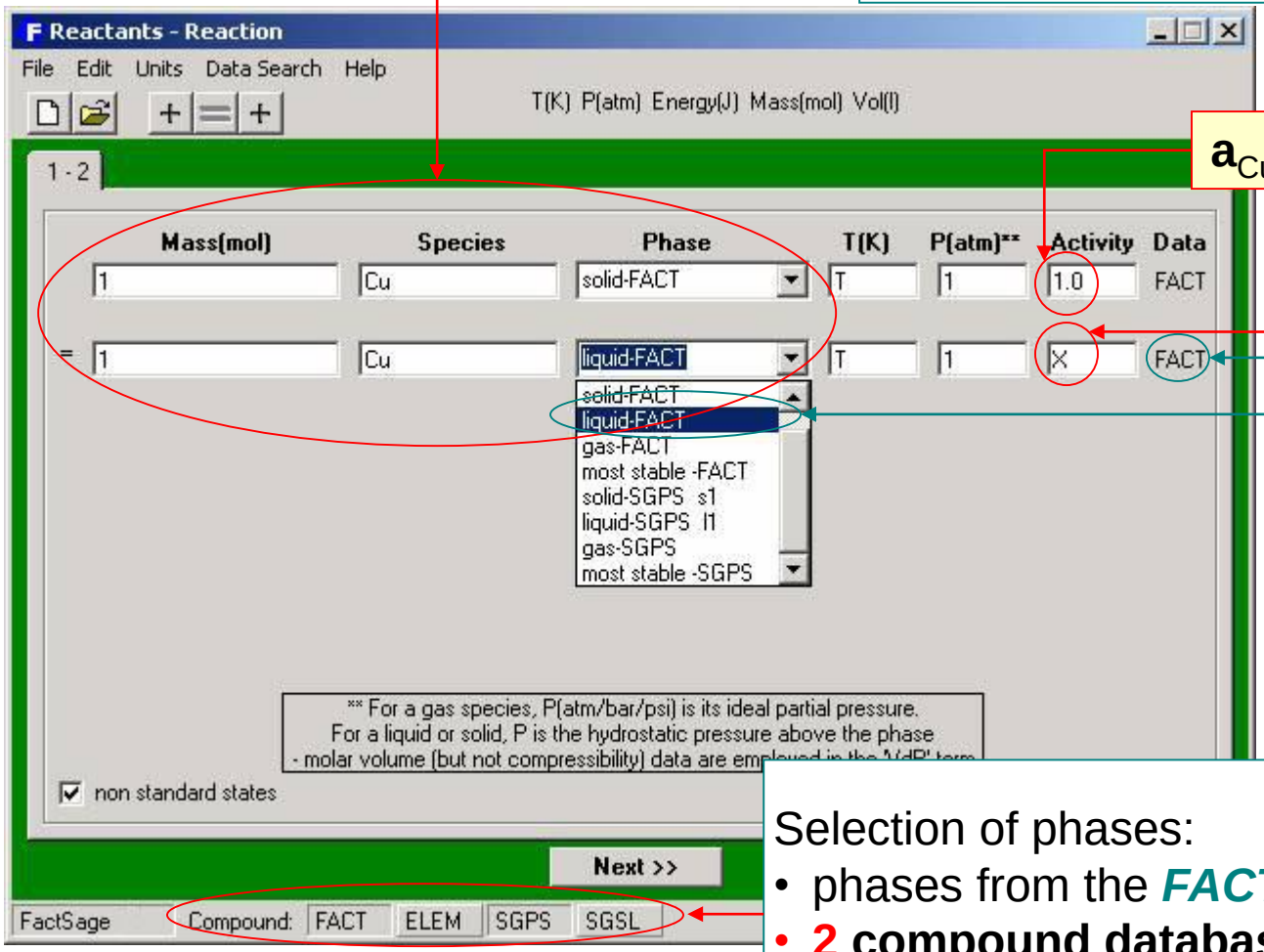


Point the mouse to read the coordinates of the melting point.

Computation of Cu **liquidus** in an ideal binary system: **data entry**

Cu(solid) = **Cu**(liquid)

Equilibrium of the type:
Me(pure solid,T) = Me (liquid,a(Me) = x(Me),T)



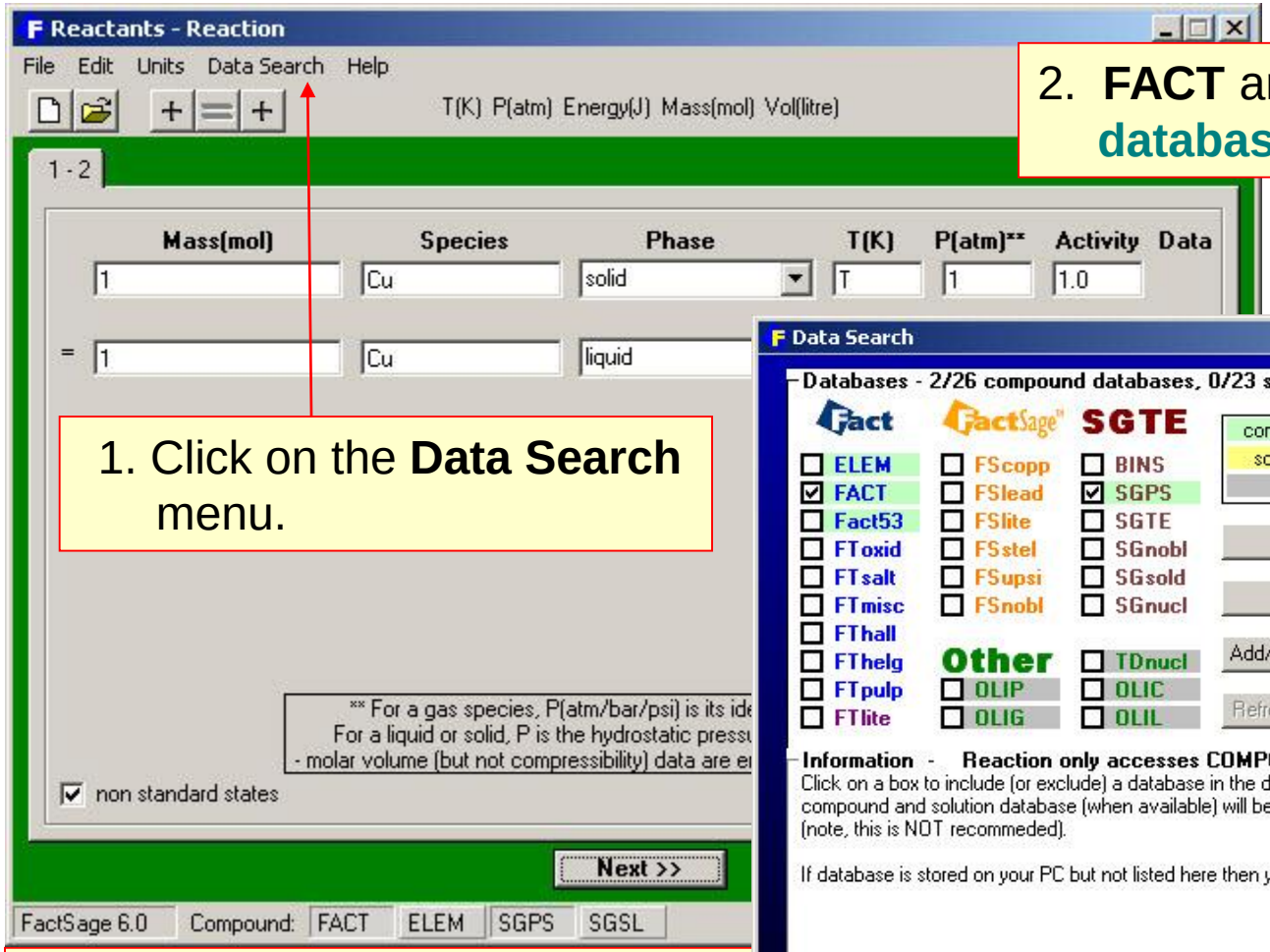
$a_{Cu(solid)}$ = **1**, pure solid copper

$a_{Cu(liquid)}$ = **X**

Selection of phases:

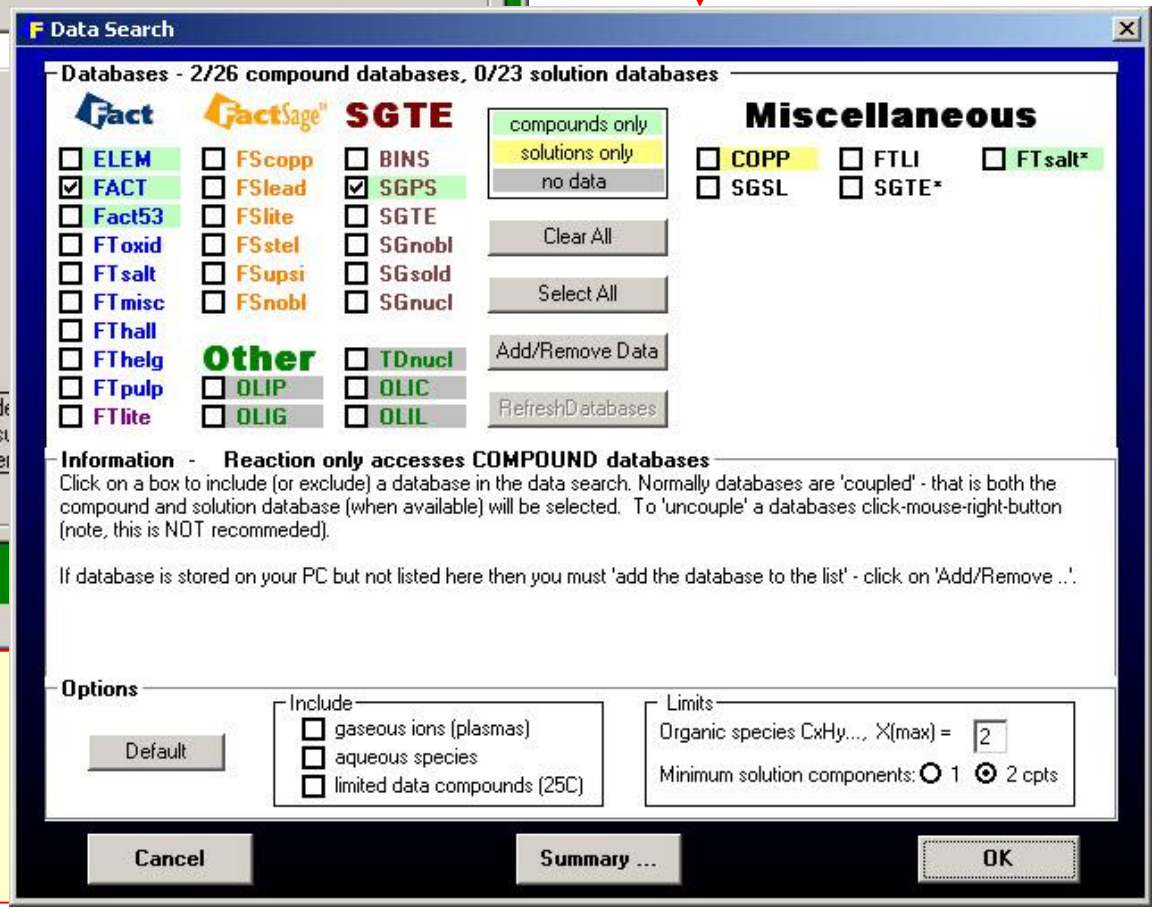
- phases from the ***FACT*** database;
- **2 compound databases** are included in the **Data Search** but here only **FACT** data are selected.

Computation of Cu **liquidus** in an **ideal solution**: **mixing databases**



1. Click on the **Data Search** menu.

2. **FACT** and **SGPS** compound **databases** are selected



3. Follow the instructions if you want to **add** (or **remove** - this does not delete) a **database** to (or from) your **list**.

Computation of Cu **liquidus** in an **ideal binary system**: tabular and graphical output

Calculated activity of **Cu**(liquid) in **equilibrium (ΔG=0)** with pure **Cu**(solid) at **various temperatures T**.

Table Reaction

File Units Output Figure Help

T(K) P(atm)

Reactants

Cu = (T,s-FACT) (T

T(K)	Activity X	Delta H(J)	Delta G(J)
300.00	2.3836E-02	11856.1	0.0
375.00	6.1674E-02	11857.4	0.0
450.00	1.1625E-01	11857.4	0.0
525.00	1.8280E-01	11855.7	0.0
600.00	2.5669E-01	11854.3	0.0
675.00	3.3426E-01	11854.5	0.0
750.00	4.1288E-01	11856.1	0.0
825.00	4.9078E-01	11858.2	0.0
900.00	5.6684E-01	11858.8	0.0
975.00	6.4144E-01	12200.3	0.0
1050.00	7.1519E-01	12503.8	0.0
1125.00	7.8763E-01	12766.1	0.0
1200.00	8.5840E-01	12979.5	0.0
1275.00	9.2706E-01	13112.0	0.0
1350.00	9.9313E-01	13141.5	0.0

300 1350 75 | | | 0

Calculate | Specify 2 variables. | << Back

The 2 specified variables, **T** and **ΔG**, are highlighted.

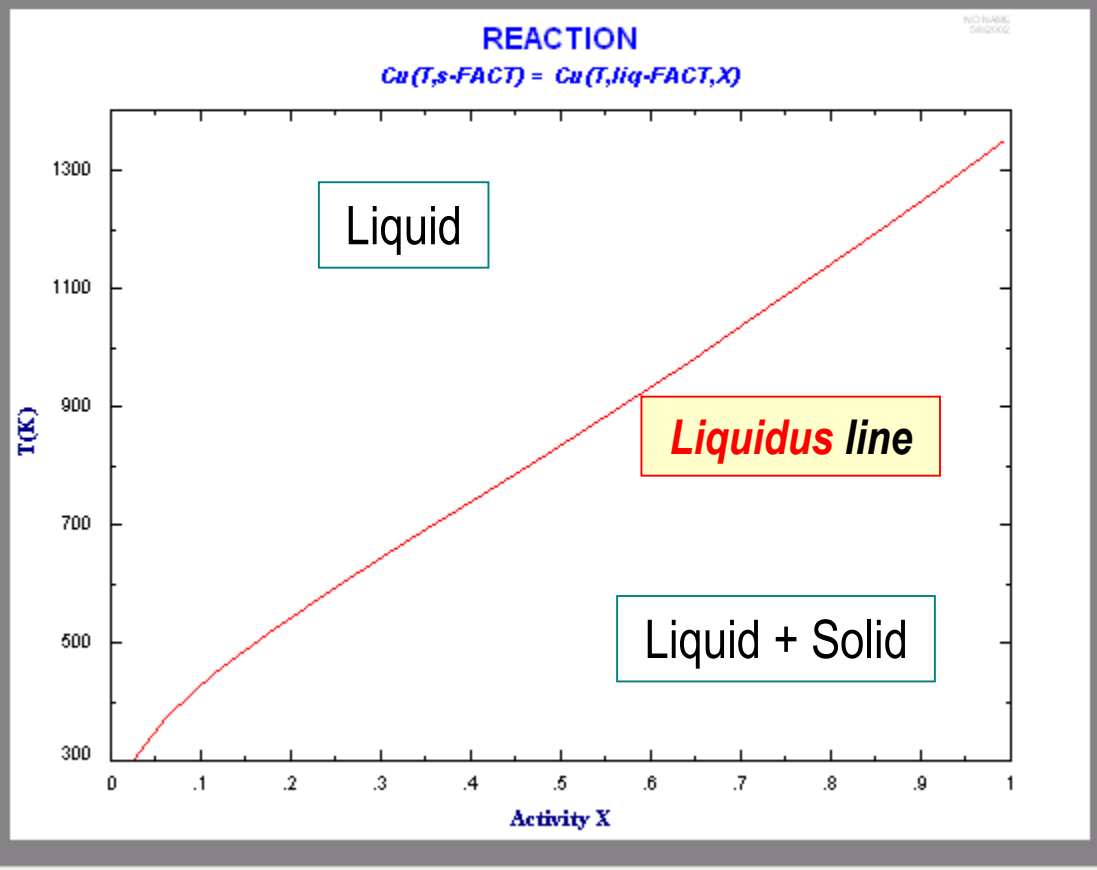
Note: When **$\Delta G = 0$**, the reaction must be isothermal.

Figure User : C.R.C.T. - Ecole Polytechnique de MONTREAL

File Add Edit View Help

For an ideal solution:

$a_{Cu(liquid)} = X_{Cu(liquid)}$



FactSage 60 385 X = 0 Y = 300

The following example shows how a variable amount of a reactant can be used to simulate an excess of this substance, i.e. its appearance among both the reactants and the products.

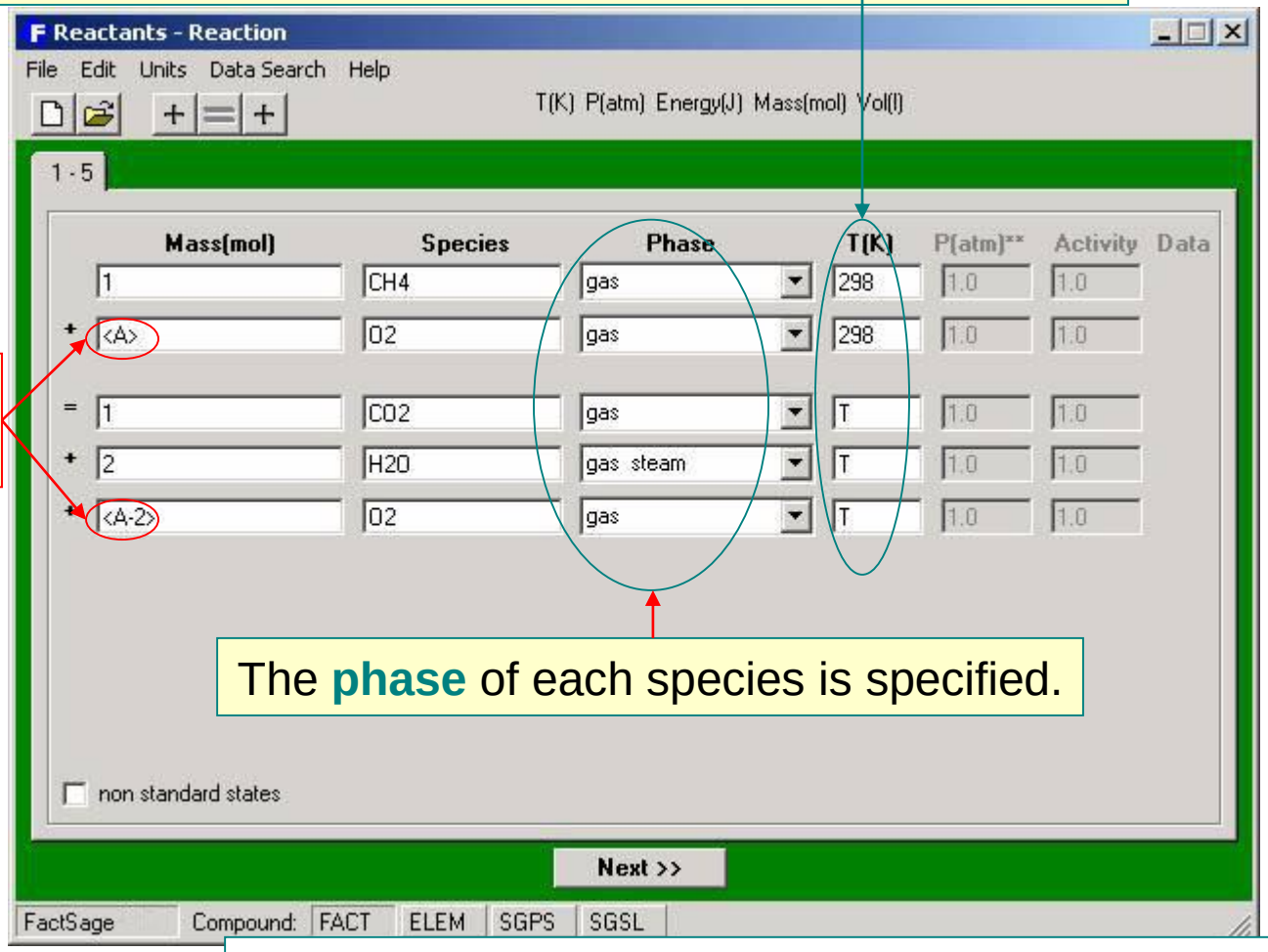
A simple combustion reaction:

$$CH_4 + \langle A \rangle\ O_2 = CO_2 + 2\ H_2O + \langle A\text{-}2 \rangle\ O_2$$

The **A**lpha variable, <A>, is used to define the quantity of O_2.

Combustion of CH_4 in variable amount <Alpha> O_2 – data entry

The **reactants** are at **298 K** but the **products** are at an unspecified **T**.



Variable quantity
<Alpha>

The **phase** of each species is specified.

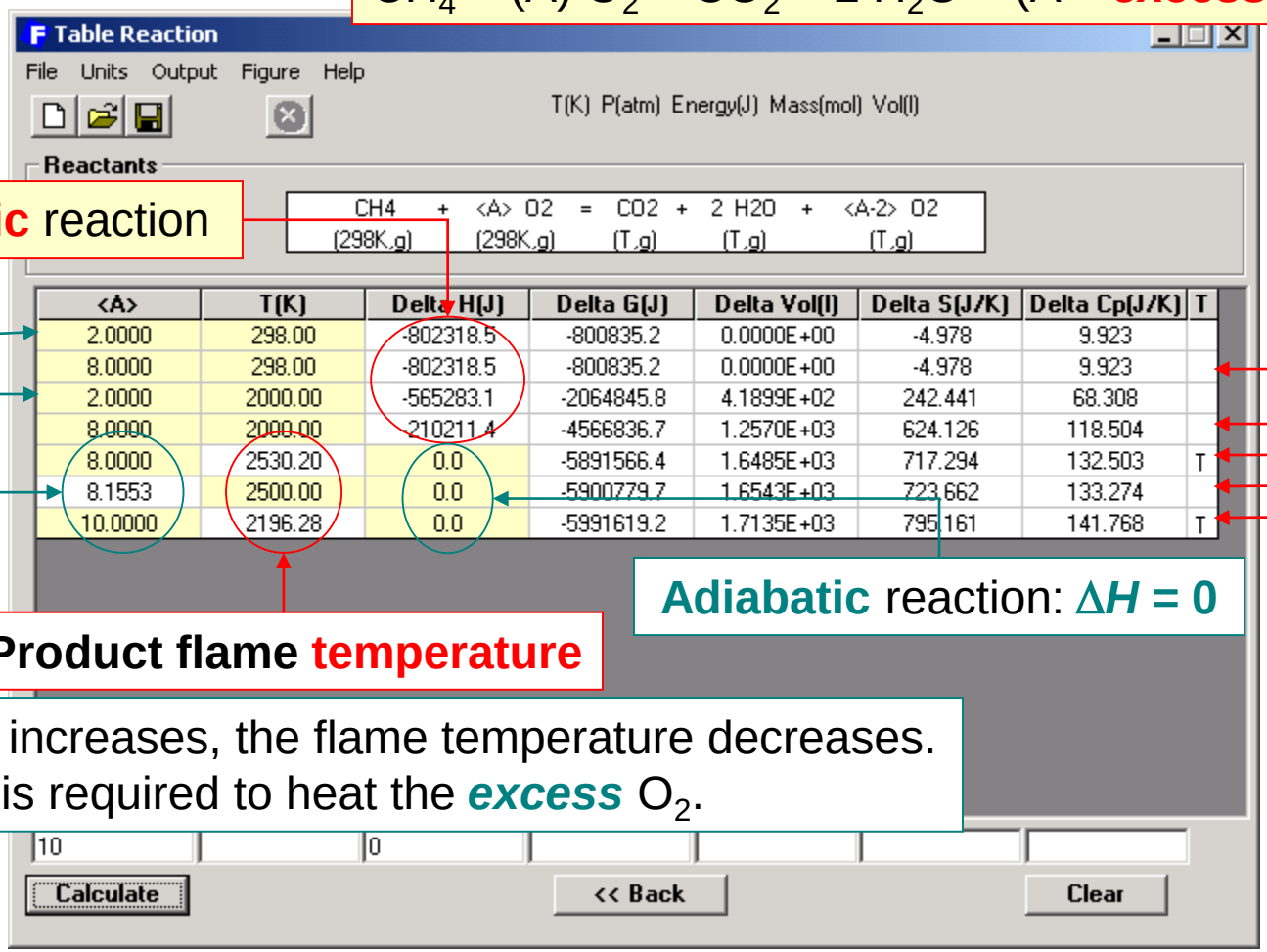
The reaction is **non-isothermal** (except when T = 298 K). Hence:

- $\mathbf{K_{eq}}$ will not appear as a column in the **Table** window.
- Setting **ΔG = 0** is meaningless (except when T = 298 K).

Combustion of CH_4 in variable amount <Alpha> O_2 – adiabatic reactions

Stoichiometric reaction (**A = 2**):
$CH_4 + 2\ O_2 = CO_2 + 2\ H_2O$

Reaction with ***variable amount*** O_2 (**A > 2**):
$CH_4 + (A)\ O_2 = CO_2 + 2\ H_2O + (A + \textit{excess})\ O_2$



<A>	T(K)	Delta H(J)	Delta G(J)	Delta Vol(l)	Delta S(J/K)	Delta Cp(J/K)	T
2.0000	298.00	-802318.5	-800835.2	0.0000E+00	-4.978	9.923	
8.0000	298.00	-802318.5	-800835.2	0.0000E+00	-4.978	9.923	
2.0000	2000.00	-565283.1	-2064845.8	4.1899E+02	242.441	68.308	
8.0000	2000.00	-210211.4	-4566836.7	1.2570E+03	624.126	118.504	
8.0000	2530.20	0.0	-5891566.4	1.6485E+03	717.294	132.503	T
8.1553	2500.00	0.0	-5900779.7	1.6543E+03	723.662	133.274	
10.0000	2196.28	0.0	-5991619.2	1.7135E+03	795.161	141.768	T

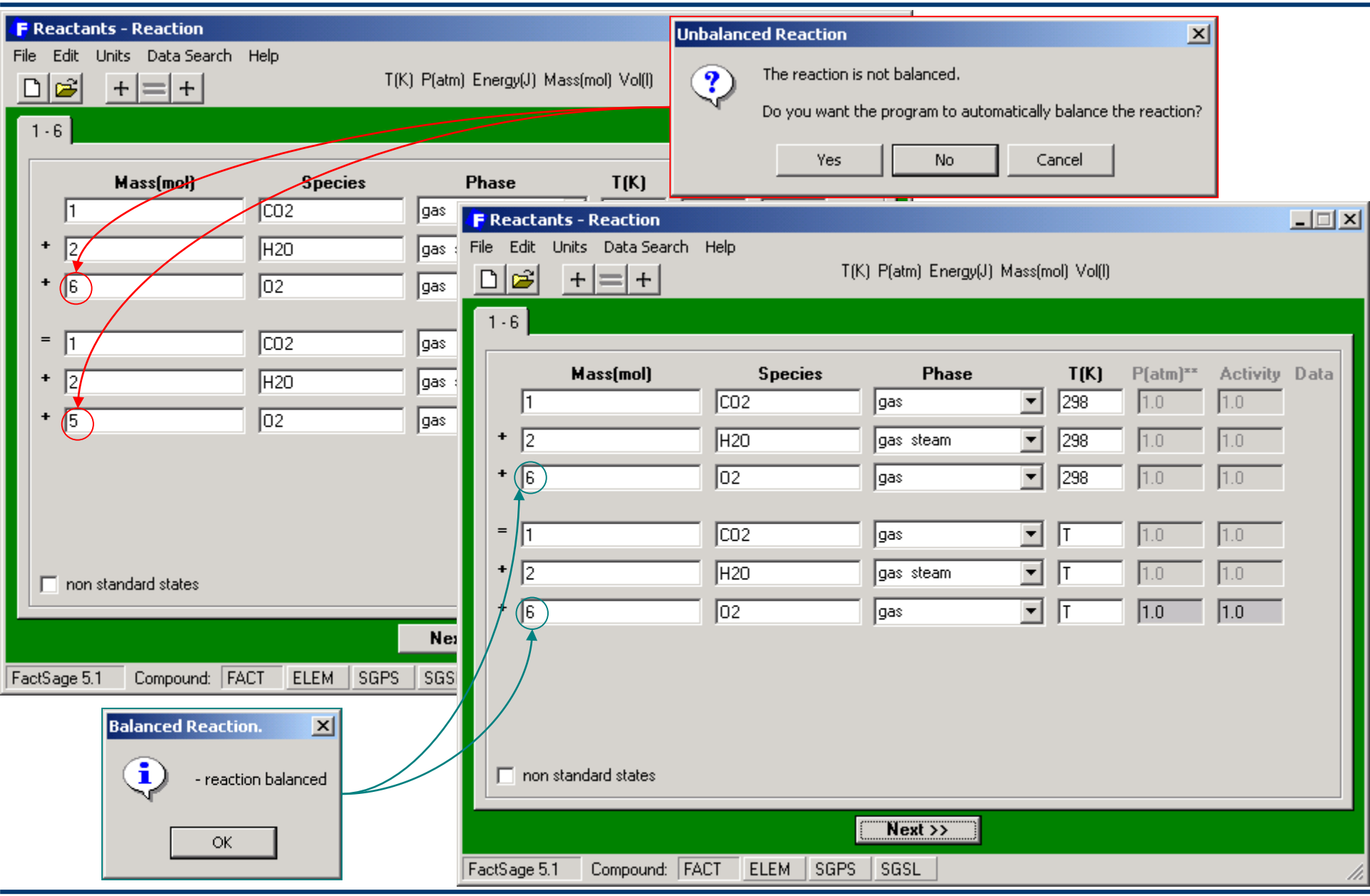
Exothermic reaction

Adiabatic reaction: $\Delta H = 0$

Product flame temperature

As **<A>** increases, the flame temperature decreases.
Energy is required to heat the ***excess*** O_2.

Heating the products of the methane combustion. *Reaction* «auto-balance» feature



Step wise heat balance in treating methane combustion

Different thermodynamic paths, **same** variation of **extensive** properties (here **ΔH**).

Table Reaction

File Units Output Figure Help

T(K) P(atm) Energy(J) Mass(mol) Vol(l)

Reactants

CH4	+	<A> O2	=	CO2	+	2 H2O	+	<A-2> O2
(298K,g)		(298K,g)		(T,g)		(T,g)		(T,g)

<A>	T(K)	Delta H(J)	Delta G(J)	Delta Vol(l)	Delta S(J/K)	Delta Cp(J/K)	T
2.0000	298.00	-802318.5	-800835.2	0.0000E+00	-4.978	9.923	
8.0000	298.00	-802318.5	-800835.2	0.0000E+00	-4.978	9.923	
2.0000	2000.00	-565283.1	-2064845.8	4.1899E+02	242.441	68.308	
8.0000	2000.00	-210211.4	-4566836.7	1.2570E+03	624.126	118.504	
8.0000	2530.20						
8.1553	2500.00						
10.0000	2196.28						

2000 K

Overall Process ΔH = **- 210211.4** J

Warming Products ΔH = **+ 592107.1 J**

298 K

Isothermal Reaction Heat ΔH = **- 802318.5** J

298 K

T(K) P(atm) Energy(J) Mass(mol) Vol(l)

Reactants

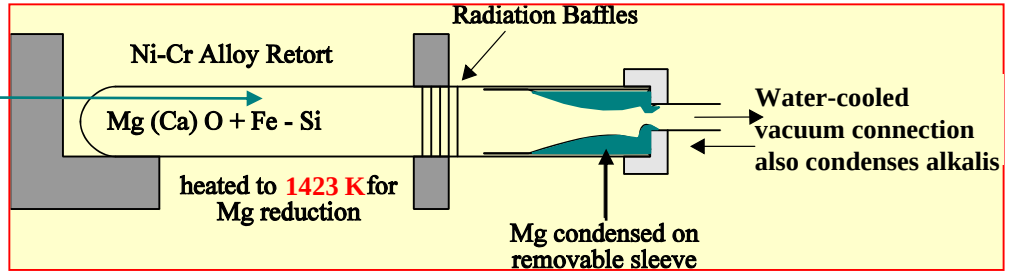
CO2	+	2 H2O	+	6 O2	=	CO2	+	2 H2O	+	6 O2
(298K,g)		(298K,g)		(298K,g)		(T,g)		(T,g)		(T,g)

T(K)	Delta H(J)	Delta G(J)	Delta Vol(l)	Delta S(J/K)	Delta Cp(J/K)	Delta A (J)	T
2000.00	592107.1	-3766001.5	1.2570E+03	629.104	108.581	-3893363.2	
2530.20	802320.1	-5090741.2	1.6485E+03	722.272	122.580	-5257778.0	

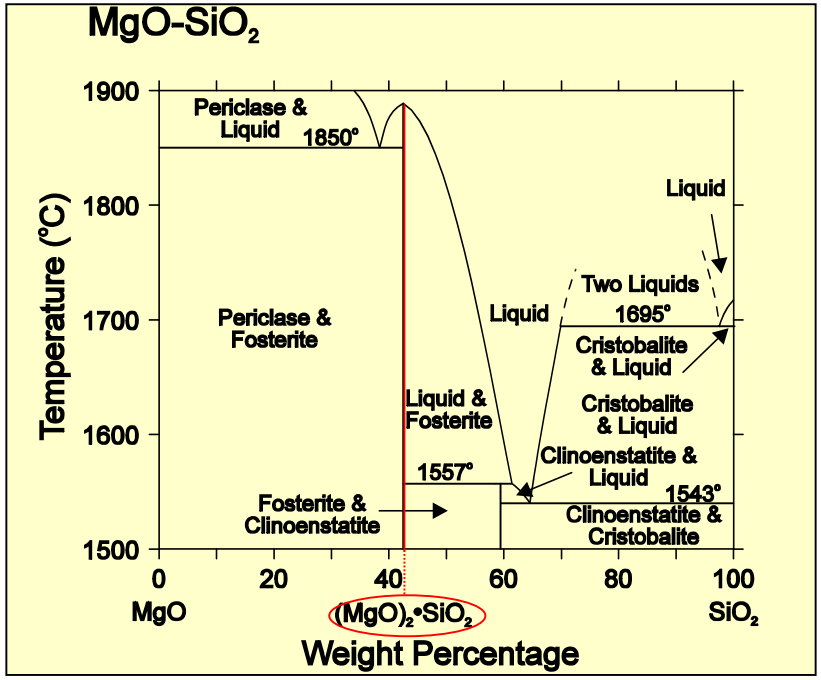
Pidgeon Process for the Production of Magnesium

Apparatus Schema:

Equilibrium **Mg partial pressure** developed at the hot end of the retort



$MgO\text{-}SiO_2$ phase diagram:

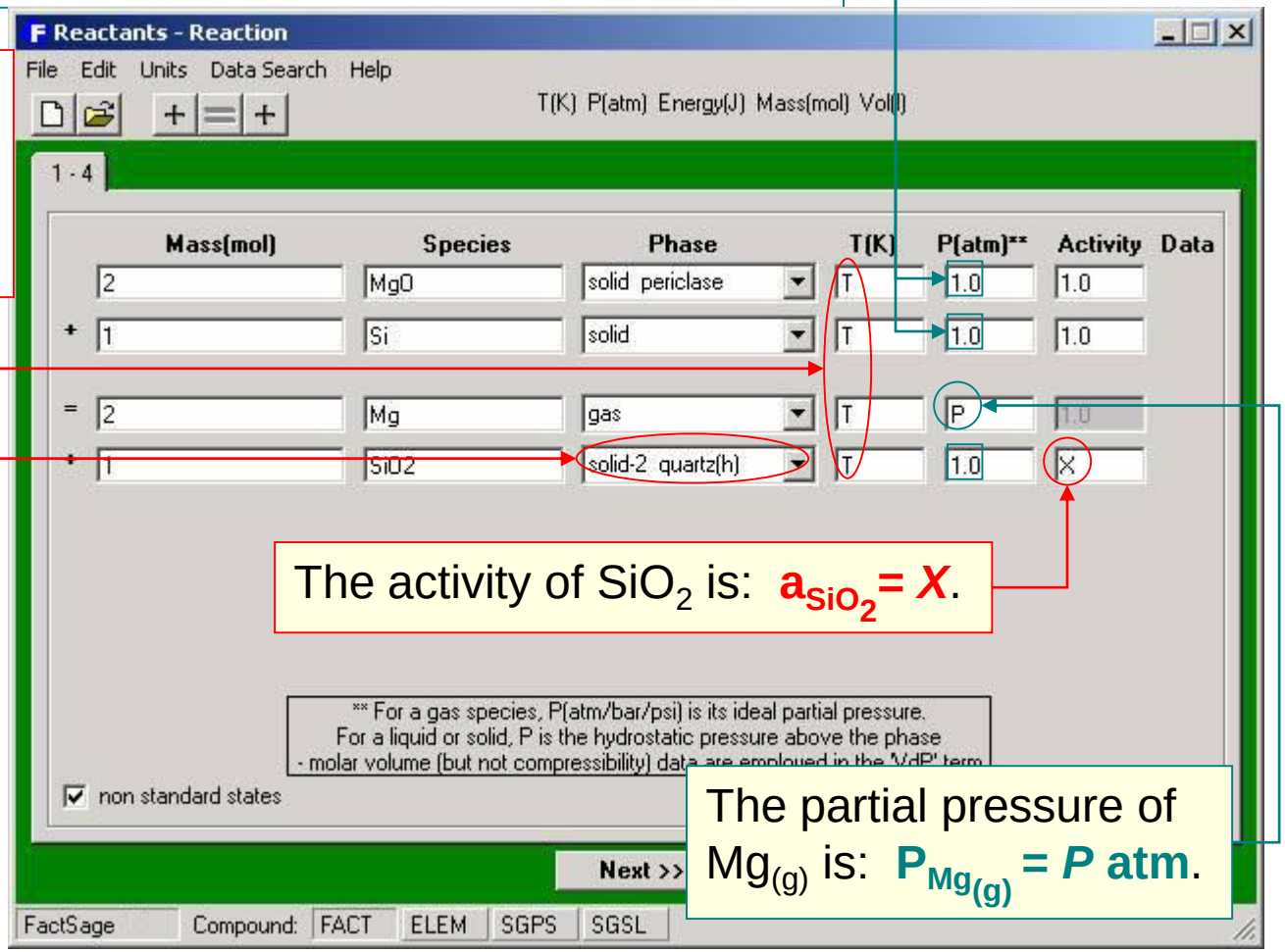


Note: MgO(s) and SiO_2(s) can **not** coexist – they react to form $(MgO)_2 \cdot SiO_2$.

Pidgeon Process for the Production of Magnesium: **Data Entry**

In the reaction, the hydrostatic pressure above the condensed phases: MgO(s), Si(s) and SiO_2(s2) is 1 atm – i.e. has no effect.

The reaction is **isothermal** (same "***T***" throughout), hence $\Delta G = 0$ gives equilibrium.



The activity of SiO_2 is: $a_{SiO_2} = X$.

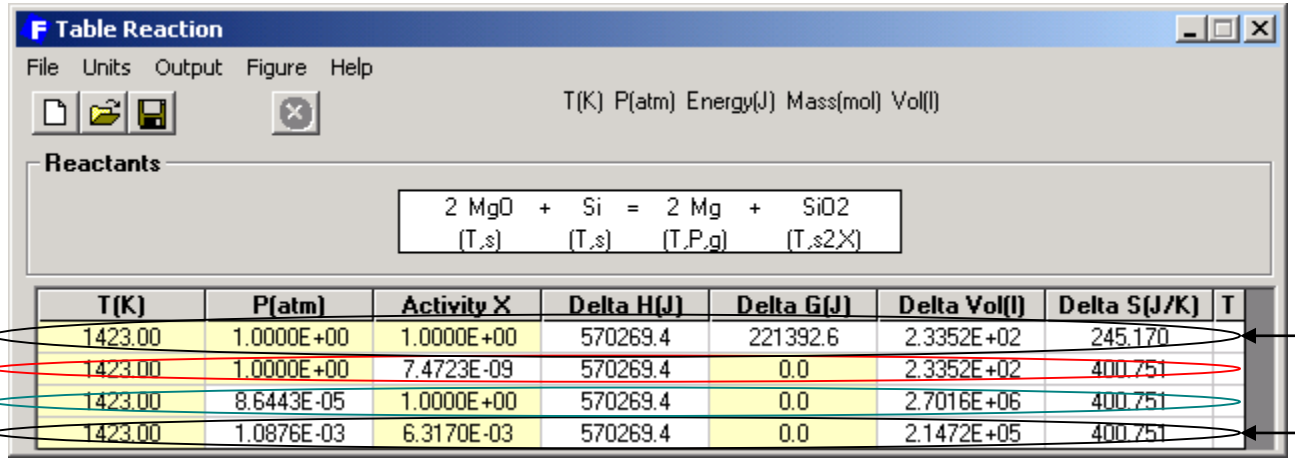
The partial pressure of $Mg_{(g)}$ is: $P_{Mg_{(g)}} = P$ atm.

Allotrope s2(solid-2) has been selected for **SiO_2** in order to fully specify the phase – **if the phase is not completely specified, equilibrium calculations ($\Delta G = 0$) can not be performed**.

Equilibrium **Mg partial pressure** developed at the hot end of the retort

Note: There are an infinite number of values of ($P_{Mg(g)}$, $a_{SiO_2(s2)}$) which satisfy K_{eq} . Here we select 3 special cases.

Standard state reaction at **1423 K**: $P_{Mg\ eq}$ = **1 atm** and $a_{SiO_2(s2)}$ = **1**
ΔG^o = 221.39 kJ = $-RT \ln K_{eq}$, hence $K_{eq} = 7.4723 \times 10^{-9}$ $\Delta G^o > 0$ but Mg can be produced by reducing $P_{Mg(g)}$ and/or a_{SiO_2}.



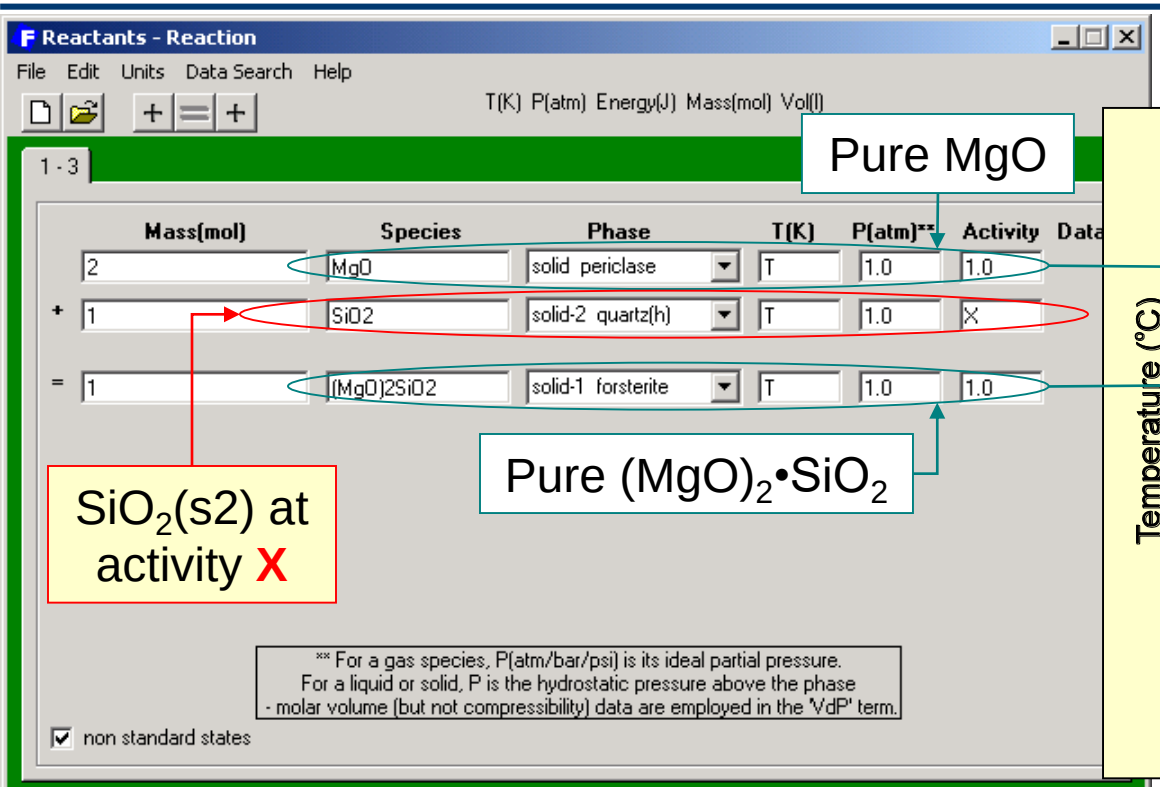
T(K)	P(atm)	Activity X	Delta H(J)	Delta G(J)	Delta Vol(l)	Delta S(J/K)	T
1423.00	1.0000E+00	1.0000E+00	570269.4	221392.6	2.3352E+02	245.170	
1423.00	1.0000E+00	7.4723E-09	570269.4	0.0	2.3352E+02	400.751	
1423.00	8.6443E-05	1.0000E+00	570269.4	0.0	2.7016E+06	400.751	
1423.00	1.0876E-03	6.3170E-03	570269.4	0.0	2.1472E+05	400.751	

At equilibrium(ΔG=**0**), when $a_{SiO_2(s2)}$=**1.0** and T=**1423 K**, $P_{Mg\ eq}$=**8.6443 × 10^{-5}** atm

At equilibrium(ΔG=**0**), when $P_{Mg\ eq}$=**1atm** and T=**1423 K**, $a_{SiO_2(s2)\ eq}$=**7.4723 × 10^{-9}**

When ΔG=**0**, T=**1423 K** and $a_{SiO_2(s2)}$=**0.006317** then $P_{Mg(g)\ eq}$=**1.0876 × 10^{-3} atm**.
This value of $a_{SiO_2(s2)}$ is taken from the next page calculation.

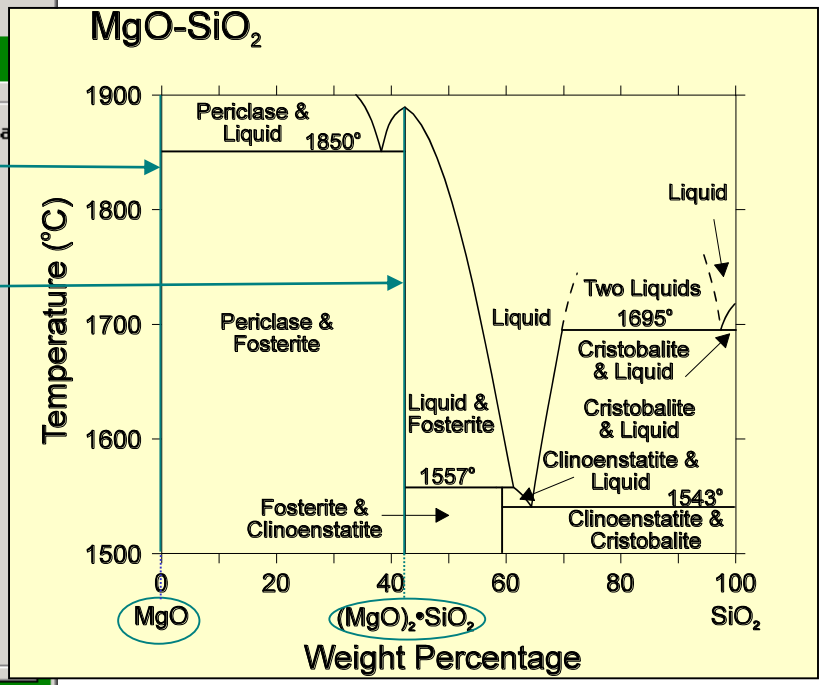
Computation of SiO_2 activity when MgO coexists with $(MgO)_2 \bullet SiO_2$



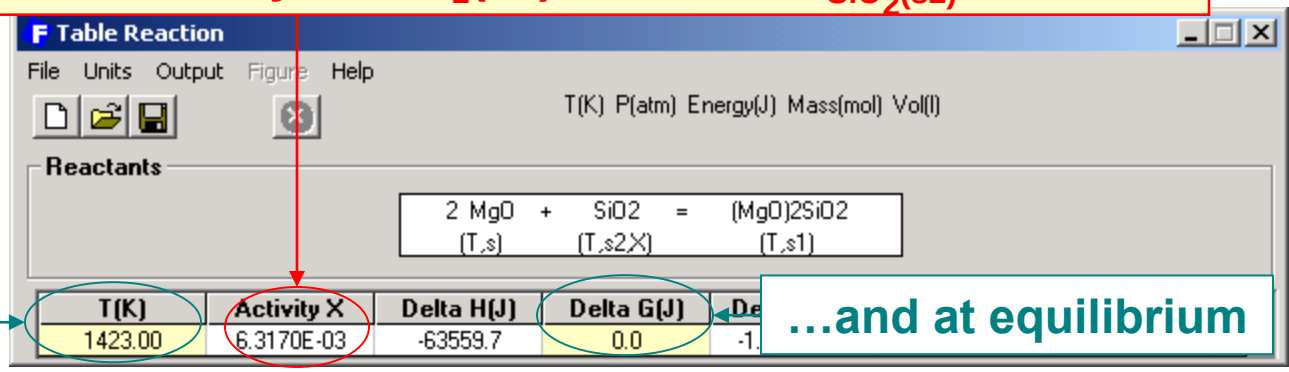
Pure MgO

Pure $(MgO)_2 \bullet SiO_2$

SiO_2(s2) at activity **X**



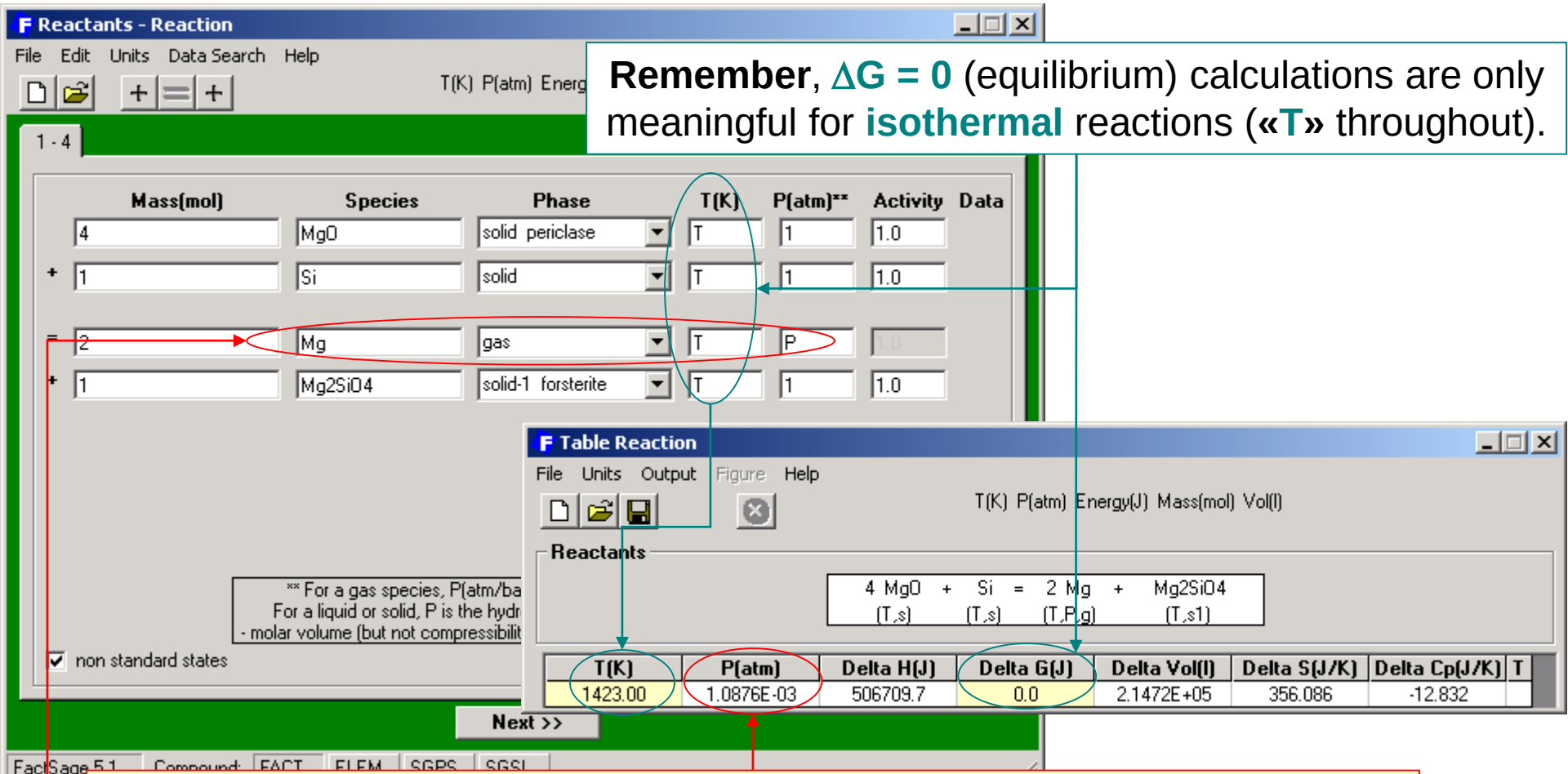
Gives the equilibrium value of the **activity of SiO_2(s2)** at 1423 K: **$a_{SiO_2(s2)}$=0.006317**



Isothermal…

…and at equilibrium

Alternative way to calculate equilibrium **Mg partial pressure**

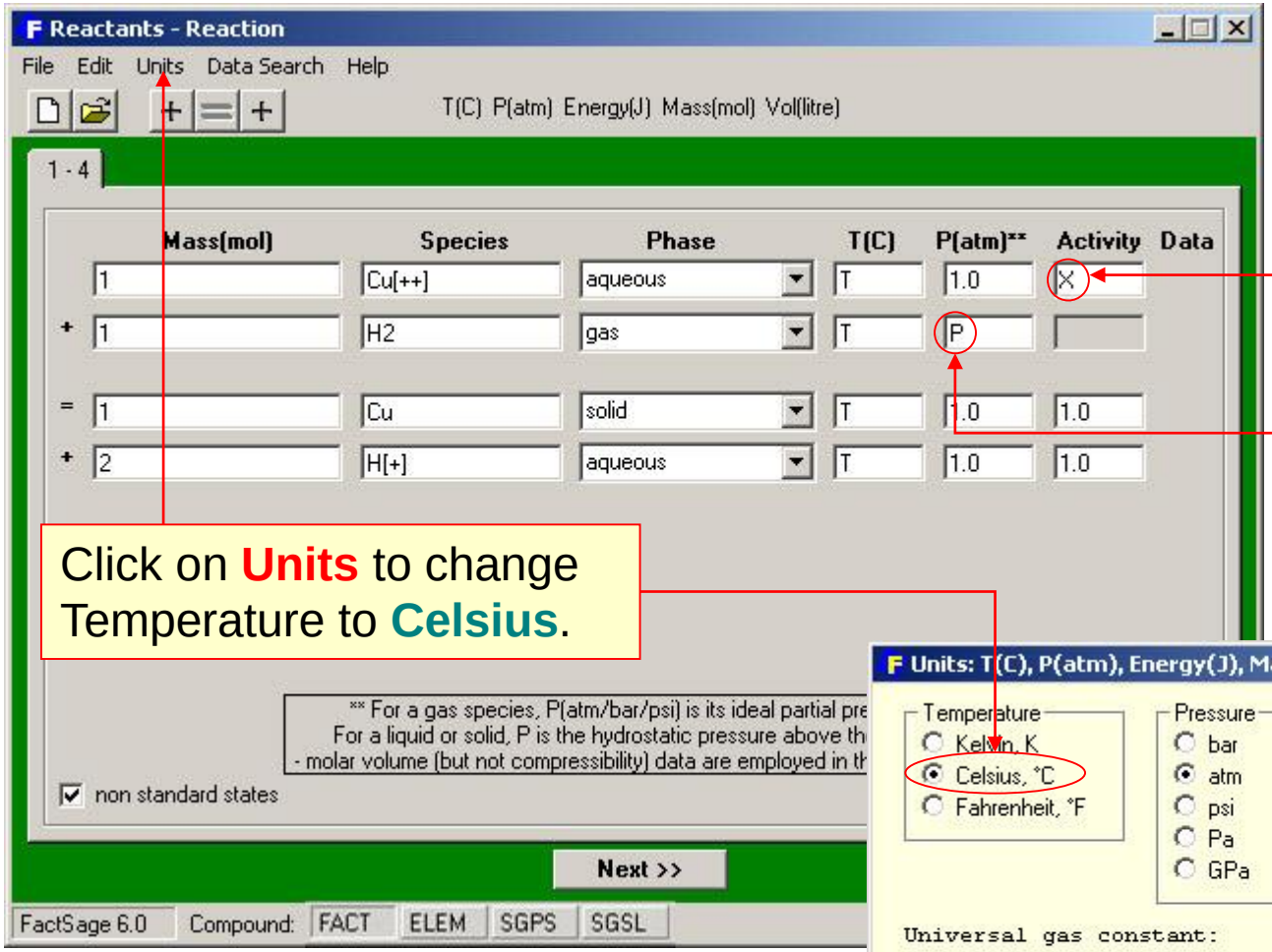


Remember, **ΔG = 0** (equilibrium) calculations are only meaningful for **isothermal** reactions (**«T»** throughout).

Magnesium production is enhanced by:

- reducing the total pressure (**<0.0010876 atm**);
- reducing a_{SiO_2} – this is done automatically due to $(MgO)_2\,SiO_2$ formation, but the addition of say CaO (slag formation) reduces a_{SiO_2} further.

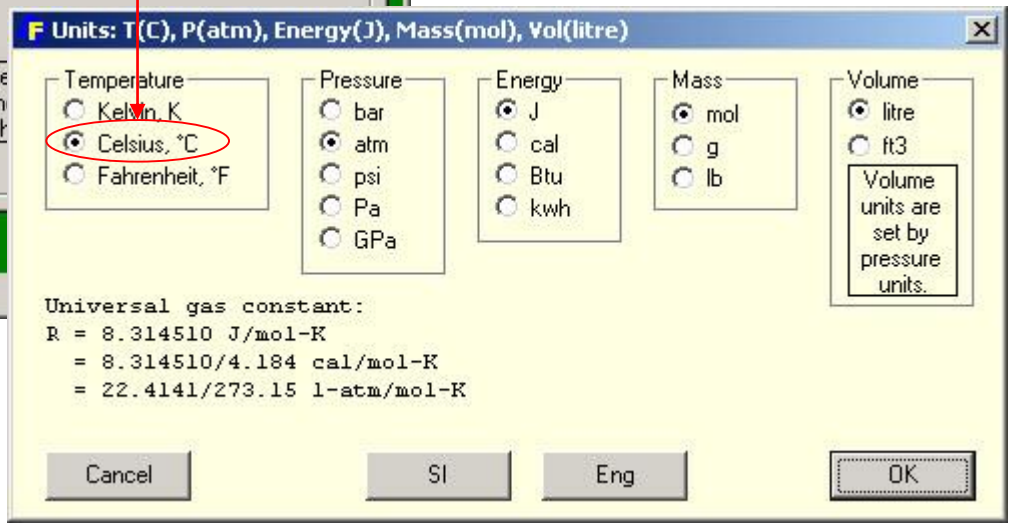
Aqueous applications – hydrogen reduction of aqueous copper ion



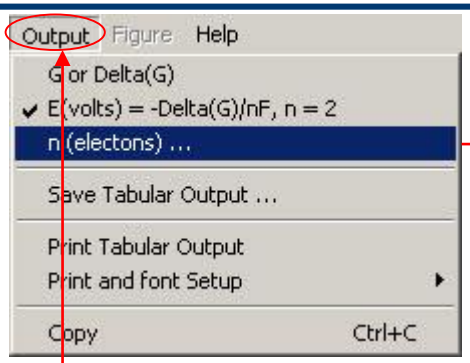
The molality of Cu^{2+} is given by "**X**".

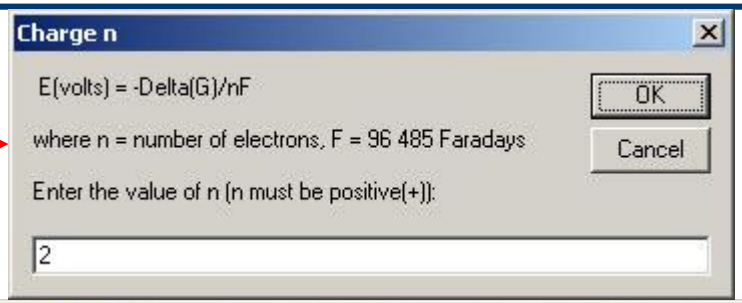
$H_2(g)$ pressure is "**P**" atm.

Click on **Units** to change Temperature to **Celsius**.



Aqueous applications – hydrogen reduction of aqueous copper ion



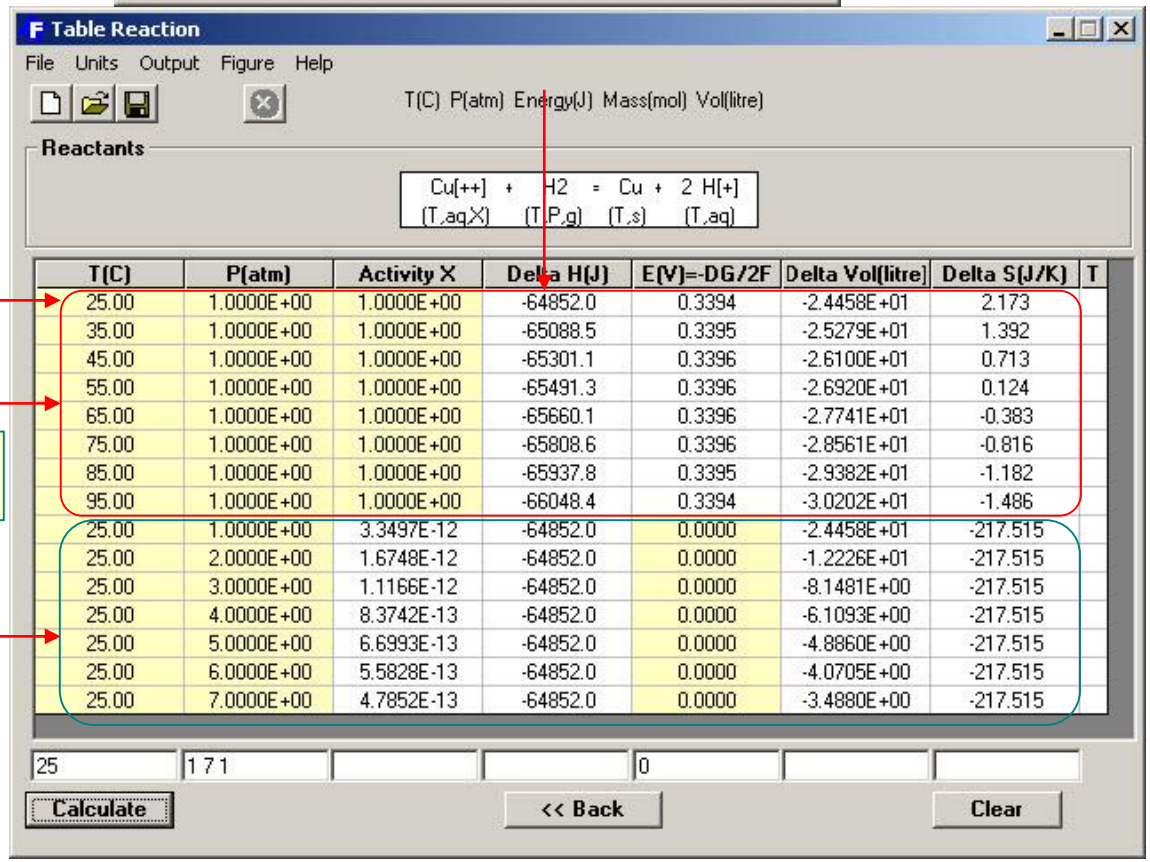


Click on **Output** to change display to **E(volts)** and define **n**, the number of **electrons**

Standard state reaction at **25° C**

Equilibrium molality at various P_{H_2}

Standard state reaction at various temperatures



T(C)	P(atm)	Activity X	Delta H(J)	E(V)=-DG/2F	Delta Vol(litre)	Delta S(J/K)	T
25.00	1.0000E+00	1.0000E+00	-64852.0	0.3394	-2.4458E+01	2.173	
35.00	1.0000E+00	1.0000E+00	-65088.5	0.3395	-2.5279E+01	1.392	
45.00	1.0000E+00	1.0000E+00	-65301.1	0.3396	-2.6100E+01	0.713	
55.00	1.0000E+00	1.0000E+00	-65491.3	0.3396	-2.6920E+01	0.124	
65.00	1.0000E+00	1.0000E+00	-65660.1	0.3396	-2.7741E+01	-0.383	
75.00	1.0000E+00	1.0000E+00	-65808.6	0.3396	-2.8561E+01	-0.816	
85.00	1.0000E+00	1.0000E+00	-65937.8	0.3395	-2.9382E+01	-1.182	
95.00	1.0000E+00	1.0000E+00	-66048.4	0.3394	-3.0202E+01	-1.486	
25.00	1.0000E+00	3.3497E-12	-64852.0	0.0000	-2.4458E+01	-217.515	
25.00	2.0000E+00	1.6748E-12	-64852.0	0.0000	-1.2226E+01	-217.515	
25.00	3.0000E+00	1.1166E-12	-64852.0	0.0000	-8.1481E+00	-217.515	
25.00	4.0000E+00	8.3742E-13	-64852.0	0.0000	-6.1093E+00	-217.515	
25.00	5.0000E+00	6.6993E-13	-64852.0	0.0000	-4.8860E+00	-217.515	
25.00	6.0000E+00	5.5828E-13	-64852.0	0.0000	-4.0705E+00	-217.515	
25.00	7.0000E+00	4.7852E-13	-64852.0	0.0000	-3.4880E+00	-217.515	

$E^o = -\Delta G^o/nF$, where **F** (= 96485 C/mol) is the Faraday constant.

Thermal balance for leaching of zinc oxide

Reactants - Reaction

File Edit Units Data Search Help

T(C) P(atm) Energy(J) Mass(mol) Vol(litre)

1 - 9

	Mass(mol)	Species	Phase	T(C)	P(atm)**	Activity	Data
	55.55	H2O	liquid	25			
+	1.2952	H[+]	aqueous	25			
+	1.2952	HSO4[-]	aqueous	25			
+	0.25246	ZnO	solid zincite	25			
=	55.802	H2O	liquid	T			
+	1.1167	HSO4[-]	aqueous	T			
+	0.9687	H[+]	aqueous	T			
+	0.1785	ZnSO4	aqueous	T			
+	0.0740	Zn[++]	aq				

non standard states

FactSage 6.0 Compound: FACT ELEM SGPS SG

The reaction is exothermic: $\Delta H < 0$.

Table Reaction

File Units Output Figure Help

T(C) P(atm) Energy(J) Mass(mol) Vol(litre)

Reactants

55.55 H2O (25C,liq) + 1.2952 H[+] (25C,aq) + 1.2952 HSO4[-] (25C,aq) + 0.25246 ZnO (25C,s) = 55.802 H2O (T,liq) + 1.1167 HSO4 (T,aq)

T(C)	Delta H(J)	Delta G(J)	Delta Vol(litre)	Delta S(J/K)	Delta Cp(J/K)	Delta A (J)	T
25.00	-23494.7	-16244.6	8.7457E-04	-24.317	-34.210	-16244.7	
30.39	0.0	-38246.5	8.7457E-04	53.781	-38.135	-38246.6	T

This entry calculates the product temperature for an adiabatic reaction: $\Delta H = 0$.

Computation of Na and Na_2 partial pressure in equilibrium with liquid Na

Both reactions are **isothermal**, hence **ΔG=0** gives **equilibrium**.

F Reactants - Reaction

File Edit Units Data Search

1 - 2

Mass(mol)	Species	Phase	T(K)	P(atm)**	Activity	Data
1	Na	liquid	T	1.0	1.0	
= 1	Na	gas	T	P		

$Na_{(l)} \rightarrow Na_{(g)}$ (monomer)

1. Calculate **T** when P_{Na} **= 1 atm**

- molar volume (but not compressibility) data are employed in the 'VdP' term.

non standard states

2. Calculate P_{Na} when **T = 1158 K**

FactSage Com

F Reactants - Reaction

1 - 2

Mass(mol)	Species	Phase	T(K)	P(atm)**	Activity	Data
2	Na	liquid	T	1.0	1.0	
= 1	Na2	gas	T	P		

$2\ Na_{(l)} \rightarrow Na_{2(g)}$ (dimer)

** For a gas species, P(atm/bar/psi) is its ideal partial pressure.
For a liquid or solid, P is the hydrostatic pressure above the phase
- molar volume (but not compressibility) data are employed in the 'VdP' term.

non standard states

Next >>

FactSage 5.1 Compound: FACT ELEM SGPS SGSL

F Table Reaction

File Units Output Figure Help

T(K) P(atm) Energy(J) Mass(mol) Vol(l)

Reactants

Na = Na
(T,liq) (T,P,g)

T(K)	P(atm)	Delta H(J)	Delta G(J)	Delta Vol(l)	Delta S(J/K)	Delta Cp(J/K)	T
1171.80	1.0000E+00	97012.3	0.0	9.6132E+01	82.789	-8.871	T
1158.00	8.8805E-01	97134.3	0.0	1.0698E+02	83.881	-8.802	

F Table Reaction

File Units Output

Reactants

3. Calculate P_{Na_2} when **T=1158 K**

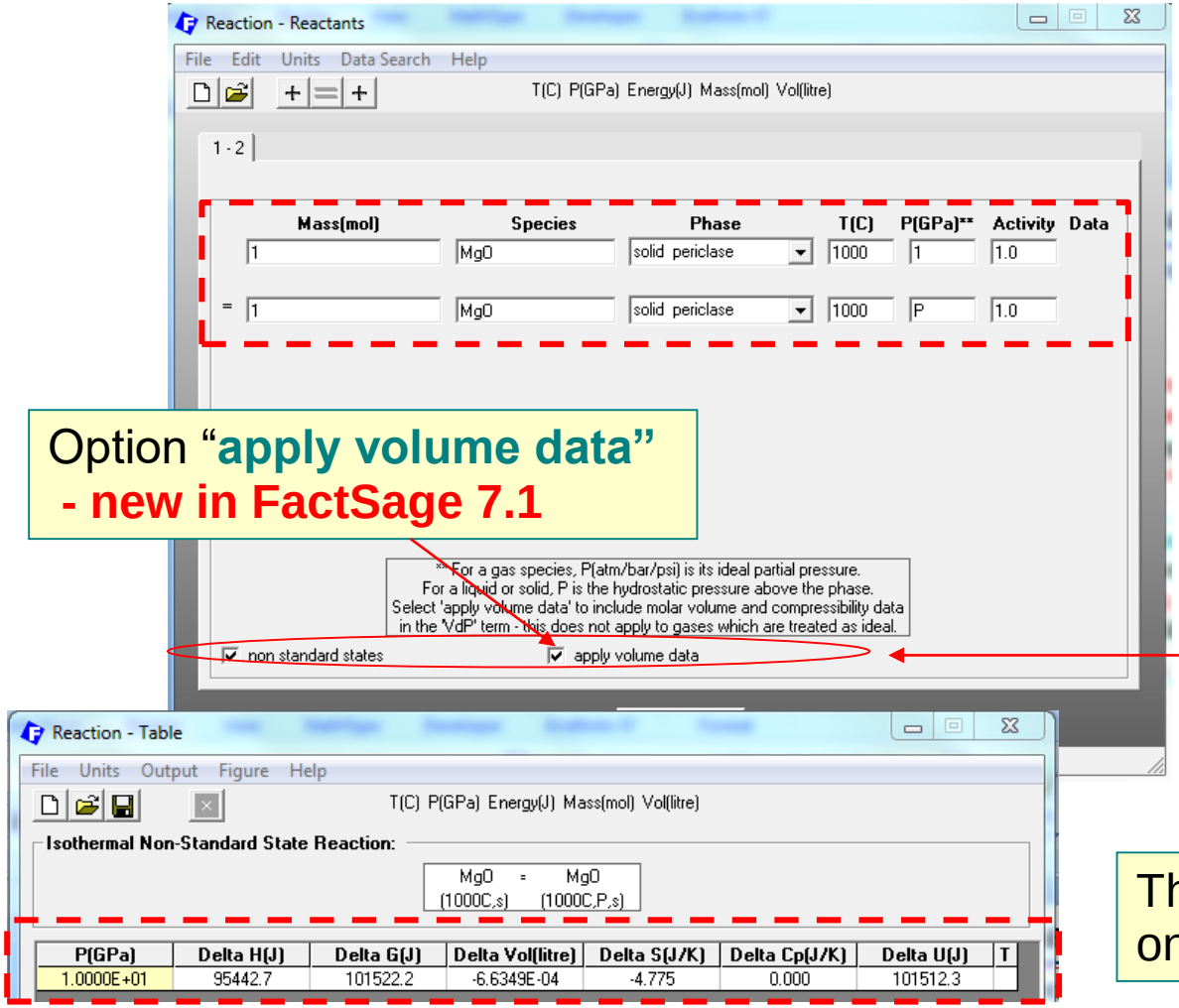
2 Na = Na2
(T,liq) (T,P,g)

T(K)	P(atm)	Delta H(J)	Delta G(J)	Delta Vol(l)	Delta S(J/K)	Delta Cp(J/K)	T
1158.00	1.1067E-01	119358.8	0.0	8.5854E+02	103.073	-20.353	

Na also forms a gaseous dimer **Na_2(g)**. The proportion of **Na_2/Na** near the boiling point (**1171.8 K**) of **Na** is: **0.111/0.888** at **1158 K**; and the total vapor pressure over **Na(l)** would be: P_{Na} **+** P_{Na_2} **(0.888 + 0.111 ≅ 1)**.

Effect of **high pressure** on **condensed phases**

Option "**apply volume data**" includes molar volume data for solids and liquids as well as any compressibility and expansivity data, in order to calculate the "**VdP**" term. At high pressures this can effect phase stability.



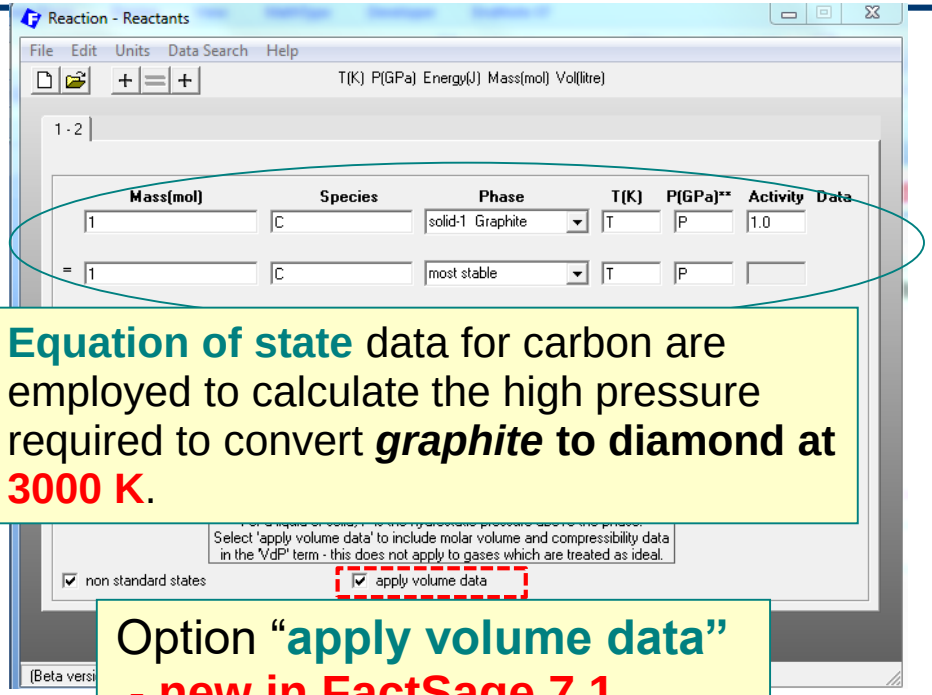
Option "**apply volume data**" **- new in FactSage 7.1**

The **pressure dependence** of **MgO (periclase) properties at 1000°C** and **10 GPa**,

Here, **volume** data are employed to calculate **the ∫Vdp contribution to the Gibbs energy at 1000 °C**.

The effect of 10 GPa pressure on V, G, H, S and U at 1000 K

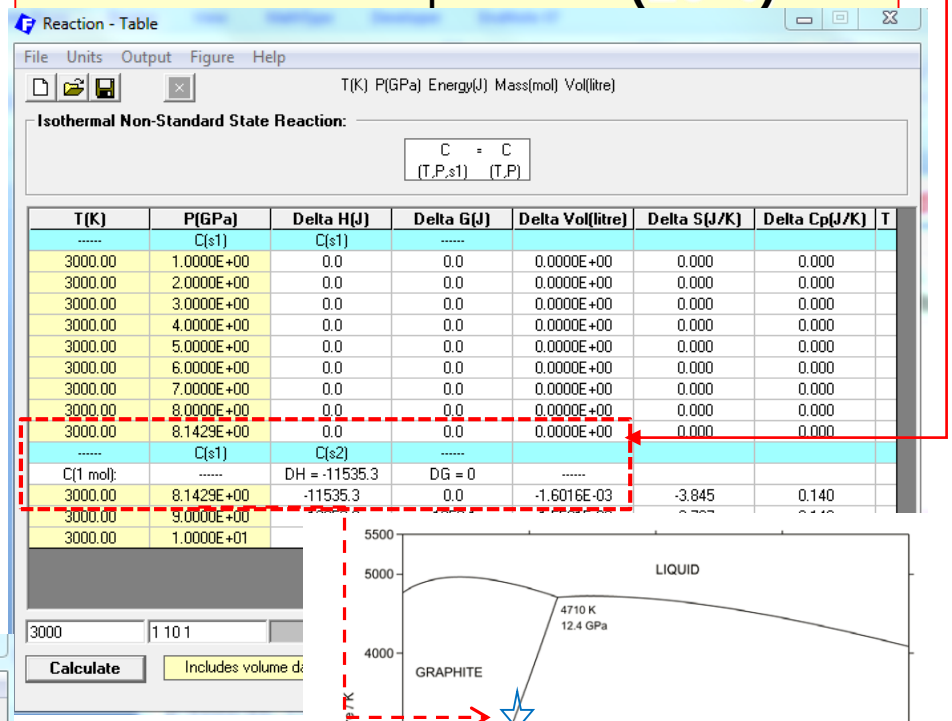
Effect of **high pressure** on the **graphite** to **diamond** transition



Equation of state data for carbon are employed to calculate the high pressure required to convert ***graphite*** **to diamond at 3000 K**.

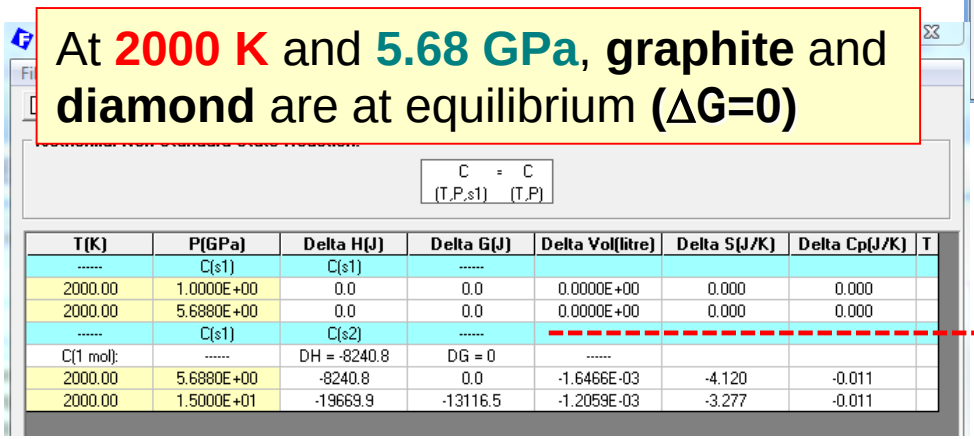
Option "**apply volume data**" **- new in FactSage 7.1**

At **3000 K** and **8.14 GPa**, **graphite** and **diamond** are at equilibrium **(ΔG=0)**

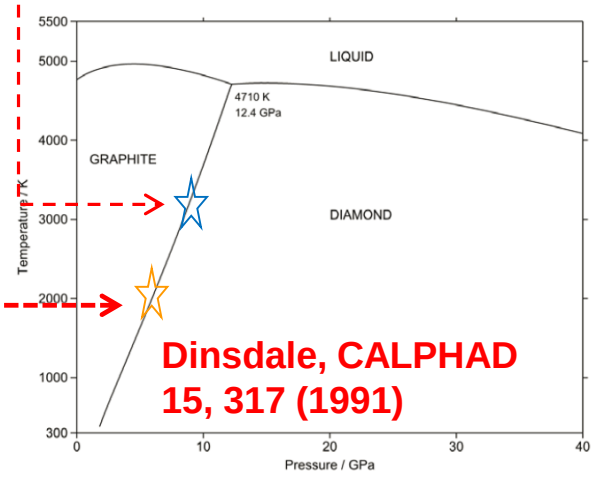


T(K)	P(GPa)	Delta H(J)	Delta G(J)	Delta Vol(litre)	Delta S(J/K)	Delta Cp(J/K)	T
------	C(s1)	C(s1)	------				
3000.00	1.0000E+00	0.0	0.0	0.0000E+00	0.000	0.000	
3000.00	2.0000E+00	0.0	0.0	0.0000E+00	0.000	0.000	
3000.00	3.0000E+00	0.0	0.0	0.0000E+00	0.000	0.000	
3000.00	4.0000E+00	0.0	0.0	0.0000E+00	0.000	0.000	
3000.00	5.0000E+00	0.0	0.0	0.0000E+00	0.000	0.000	
3000.00	6.0000E+00	0.0	0.0	0.0000E+00	0.000	0.000	
3000.00	7.0000E+00	0.0	0.0	0.0000E+00	0.000	0.000	
3000.00	8.0000E+00	0.0	0.0	0.0000E+00	0.000	0.000	
3000.00	8.1429E+00	0.0	0.0	0.0000E+00	0.000	0.000	
------	C(s1)	C(s2)	------				
C(1 mol):	------	DH = -11535.3	DG = 0	------			
3000.00	8.1429E+00	-11535.3	0.0	-1.6016E-03	-3.845	0.140	
3000.00	9.0000E+00						
3000.00	1.0000E+01						

At **2000 K** and **5.68 GPa**, **graphite** and **diamond** are at equilibrium **(ΔG=0)**



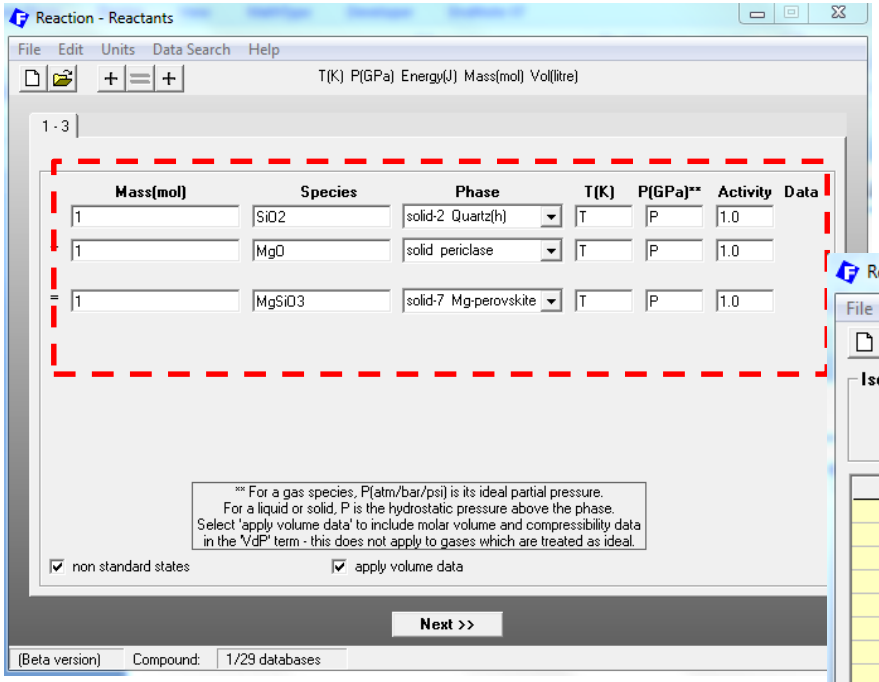
T(K)	P(GPa)	Delta H(J)	Delta G(J)	Delta Vol(litre)	Delta S(J/K)	Delta Cp(J/K)	T
------	C(s1)	C(s1)	------				
2000.00	1.0000E+00	0.0	0.0	0.0000E+00	0.000	0.000	
2000.00	5.6880E+00	0.0	0.0	0.0000E+00	0.000	0.000	
------	C(s1)	C(s2)	------				
C(1 mol):	------	DH = -8240.8	DG = 0	------			
2000.00	5.6880E+00	-8240.8	0.0	-1.6466E-03	-4.120	-0.011	
2000.00	1.5000E+01	-19669.9	-13116.5	-1.2059E-03	-3.277	-0.011	



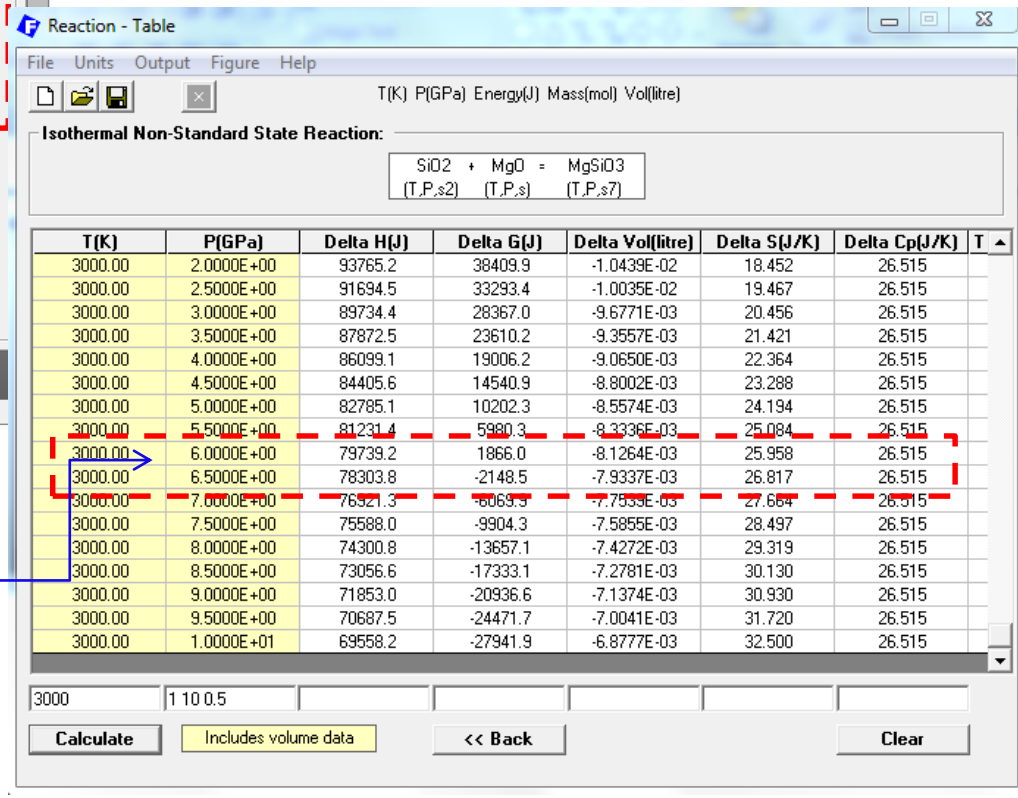
Dinsdale, CALPHAD 15, 317 (1991)

P-T phase diagram for C

Effect of **high pressure** on the SiO_2+MgO→$MgSiO_3$ reaction



At which pressure does the formation of $MgSiO_3$(s7) from SiO2(s2) and MgO(s) at 3000 K occur?



T(K)	P(GPa)	Delta H(J)	Delta G(J)	Delta Vol(litre)	Delta S(J/K)	Delta Cp(J/K)
3000.00	2.0000E+00	93765.2	38409.9	-1.0439E-02	18.452	26.515
3000.00	2.5000E+00	91694.5	33293.4	-1.0035E-02	19.467	26.515
3000.00	3.0000E+00	89734.4	28367.0	-9.6771E-03	20.456	26.515
3000.00	3.5000E+00	87872.5	23610.2	-9.3557E-03	21.421	26.515
3000.00	4.0000E+00	86099.1	19006.2	-9.0650E-03	22.364	26.515
3000.00	4.5000E+00	84405.6	14540.9	-8.8002E-03	23.288	26.515
3000.00	5.0000E+00	82785.1	10202.3	-8.5574E-03	24.194	26.515
3000.00	5.5000E+00	81231.4	5980.3	-8.3336E-03	25.084	26.515
3000.00	6.0000E+00	79739.2	1866.0	-8.1264E-03	25.958	26.515
3000.00	6.5000E+00	78303.8	-2148.5	-7.9337E-03	26.817	26.515
3000.00	7.0000E+00	76921.3	-6069.5	-7.7535E-03	27.664	26.515
3000.00	7.5000E+00	75588.0	-9904.3	-7.5855E-03	28.497	26.515
3000.00	8.0000E+00	74300.8	-13657.1	-7.4272E-03	29.319	26.515
3000.00	8.5000E+00	73056.6	-17333.1	-7.2781E-03	30.130	26.515
3000.00	9.0000E+00	71853.0	-20936.6	-7.1374E-03	30.930	26.515
3000.00	9.5000E+00	70687.5	-24471.7	-7.0041E-03	31.720	26.515
3000.00	1.0000E+01	69558.2	-27941.9	-6.8777E-03	32.500	26.515

Between 6 GPa and 6.5 Gpa ΔG becomes negative showing that the reaction is thermodynamically favorable.