

The *Reaction* module

Use *Reaction* to calculate the thermochemical properties of a species or a chemical reaction.

Reaction accesses only compound type databases.

Note that *Reaction* assumes all gases to be 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.



Pure substance property calculations (Pure Cu)

The **simplest** possible **application** of the **Reaction** module is the calculation of **thermodynamic properties of a pure substance**.

In order to do that the input in the Reactants window is **not a balanced reaction** but a single line with **one substance** name.

The properties of this substance are calculated as a function of temperature depending upon the choice of the **phase state** given in the Reactants window. If a particular phase state is chosen, the properties of this phase are calculated, if the **option most stable** is used, the phase state that corresponds to the temperature that is used in the calculation is chosen.

A graph is given which shows the **Gibbs energy minimum principle** in order to determine the **most stable** state.

Reactants window - entry of a species

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

- Add a Product
- Add a Reactant
- Open
- New Reaction

Mass(mol)	Species	Phase	T(K)	P(atm)**	Activity	Data
1	Cu	most stable	T	1.0	1.0	

non standard states

Next >>

FactSage 5.1 Compound: FACT ELEM SGPS SGSL

Entry of reactant species

Compound databases available

Go to the Table window

Table window – calculating thermodynamic properties of a species

Open New Reaction Save Stop Calculation

Summary of the **Reactants** window entry

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

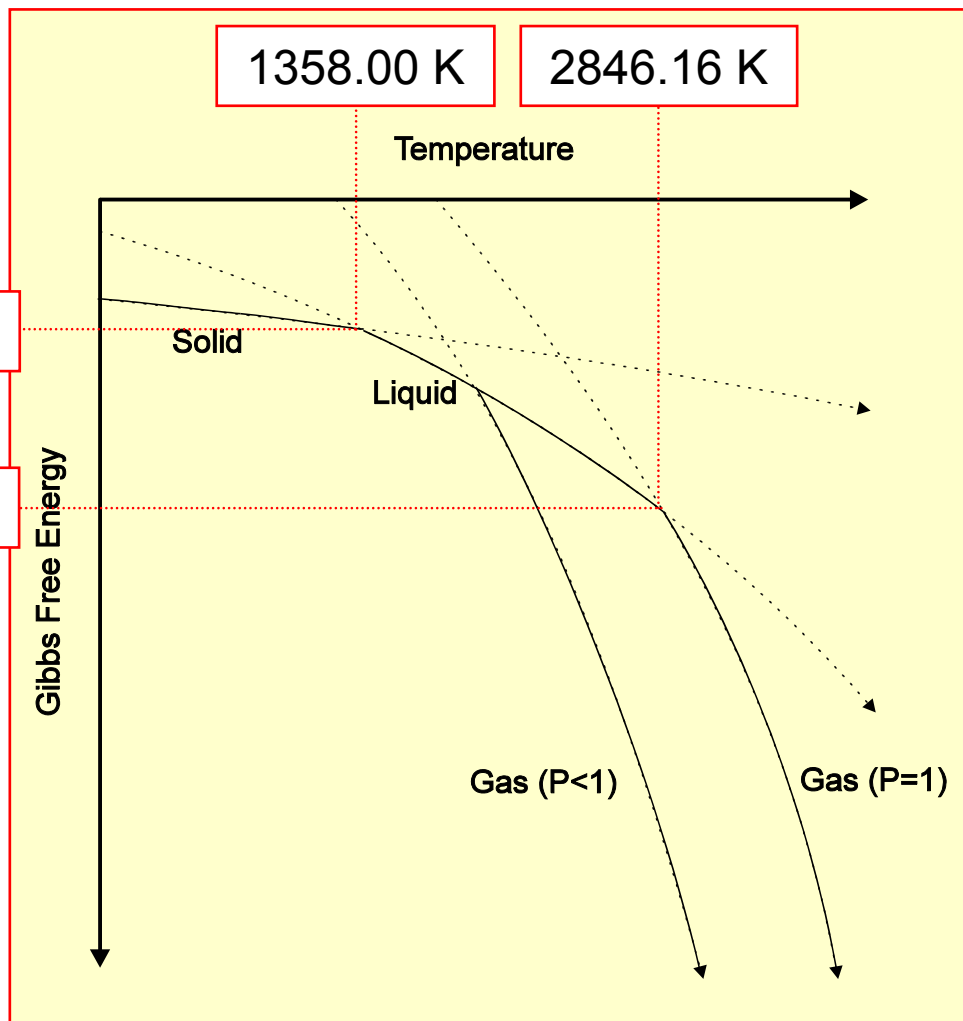
<< Back Clear

A multiple entry for **T**: **min**, **max** and **step**.
This results in the computation of the **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.

Isothermal standard state reactions (**oxidation of copper**)

The **classical use** of the **Reaction** module is the determination of the **isothermal reaction properties of a stoichiometric reaction**.

From the names of the reactants and products as well as their respective stoichiometric coefficients it is possible to calculate from the data stored in a **Compound** type database the values for **ΔH , ΔS , ΔG , ΔV , ΔA and K** (the equilibrium constant) as functions of temperature.

The results are shown in a table (but can also be plotted using the **Figure** module, see **Figure Help, section 8**).

As an example the reaction $4 \text{Cu} + \text{O}_2 = 2 \text{Cu}_2\text{O}$ is used.

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

Entry of an isothermal standard state reaction: **$4 \text{ Cu} + \text{O}_2 = 2 \text{ Cu}_2\text{O}$**

An alternative way to enter this data is from the **Slide Show Examples Directory**. Go to the **menu bar** and click on: **File > Directories... > Slide Show Examples** and **double-click** on a file.

Isothermal means same "**T**" throughout

Non-standard states checkbox is **not** selected

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	most stable	T	1.0	1.0	
+ 1	O2	most stable	T	1.0	1.0	
= 2	Cu2O	most stable	T	1.0	1.0	

non standard states

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FactSage 5.1 Compound: FACT ELEM SGPS SGSL

Oxidation of copper at various temperatures

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

F Table Reaction

File Units Output Figure Help

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

Reactants

4 Cu + O2 = 2 Cu2O
 (T) (T) (T)

T(K)	Delta H(J)	Delta G(J)	Delta Vol(l)	Delta S(J/K)	Delta Cp(J/K)	Keq	T
-----	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	

300 2000 300

Calculate << Back Clear

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

Using **non-standard states** in equilibrium reaction

A more advanced application of the **Reaction** module is the **use of non-standard states** for the **reactants** and/or **products** of a reaction.

This option permits to fix certain activities or partial pressures of the species and to resolve the equation $\Delta G^\circ = -RT \ln K_{eq}$ for a suitable variable.

It is for example possible to **fix all activities/partial pressures** of the reactants and products and **thus fix K**, set the equilibrium condition $\Delta G=0$ and then **resolve for the temperature** that fits the fixed value of K.

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	

non standard states

*** 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.

Select non standard state

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

$$P_{\text{O}_2(\text{g})} = \text{"P"}$$

Standard state reaction:
 $P_{\text{O}_2(\text{g})} = 1.0 \text{ atm}$
 $a_{\text{Cu(s)}} = 1.0$

F Table Reaction

File Units Output Figure Help

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	

Specifying an extensive property change to deal with chemical equilibrium

For simple chemical equilibrium: $\Delta G = \Delta G^0 + RT \ln \left(\frac{a_{\text{Cu}_2\text{O}}^2}{a_{\text{Cu}}^4 \cdot P_{\text{O}_2}} \right)$ 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 $\Delta G = 0$.

Table Reaction

File Units Output Figure Help

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

Reactants

$$4 \text{ Cu} + \text{O}_2 = 2 \text{ Cu}_2\text{O}$$

(T,s,X) (T,P,g) (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	
1000.00	1.0359E-10	1.0000E+00	-335381.1	0.0	-7.9216E+11	-335.381	
1000.00	1.0000E+00	3.1903E-03	-335381.1	0.0	-8.2039E+01	-335.381	
897.01	1.0000E-12	1.0000E+00	-336673.3	0.0	-7.3607E+13	-375.327	T

1e-12 1 0

Calculate << Back Clear

Specify 3 variables.

For the last entry:

- $P_{\text{O}_2(\text{g})} = 10^{-12}$
- $a_{\text{Cu}(\text{s})} = 1$
- $\Delta G = 0$, equilibrium

Non-isothermal non-equilibrium calculation (**heating of pure (Al)**)

A further use of the **Reaction** module lies in the calculation of non-isothermal non-equilibrium balances of the **extensive property changes** ΔH , ΔS , ΔG , ΔV , ΔF for a given reaction.

It is assumed that this reaction does **not** represent **an equilibrium but a complete transition** from the reactants to the products. Under this condition it is possible to attribute the reactants one temperature and the products another.

Thus the above mentioned extensive property changes from one state (**reactants at reactant temperature**) to the other (**products at product temperature**) can be calculated using data from a **Compound** type database.

As an example the heating of Al is demonstrated by use of the reaction $\text{Al}(300\text{K}) = \text{Al}(T)$.

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

phase transition, $\text{Al}_{(s)} \rightarrow \text{Al}_{(l)}$
 (i.e. *fusion*) at 933.45 K
 $\Delta H^{\circ}_{\text{fusion}} = T_{\text{fusion}} \cdot \Delta S^{\circ}_{\text{fusion}}$
 $= 28649.1\text{J} - 17938.1\text{J}$
 $= 10711.0\text{J}$

F Reactants - Reaction

File Edit Units Data Search Help

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

Mass(mol)	Species	Phase	T(K)	P(atm)**	Activity	Data
1	Al	most stable	300	1.0	1.0	
= 1	Al	most stable	T	1.0	1.0	

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F Table Reaction

File Units Output Figure Help

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

Reactants

Al = Al
(300K) (T)

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

Calculate << Back Clear

Heating Al: setting 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 you wish to plot.

Table Reaction

File Units Output Figure Help

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

Reactants

Al = Al
(300K) (T)

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

Y-variable X-variable Swap Axes

Y-axis

Delta H(J)

maximum 42500

minimum 0

tick every 2500

X-axis

T(K)

maximum 1300

minimum 300

tick every 50

Cancel OK

T(K)

Delta H(J)

Delta G(J)

Delta Vol(l)

Delta S(J/K)

Delta Cp(J/K)

Delta A (J)

Y

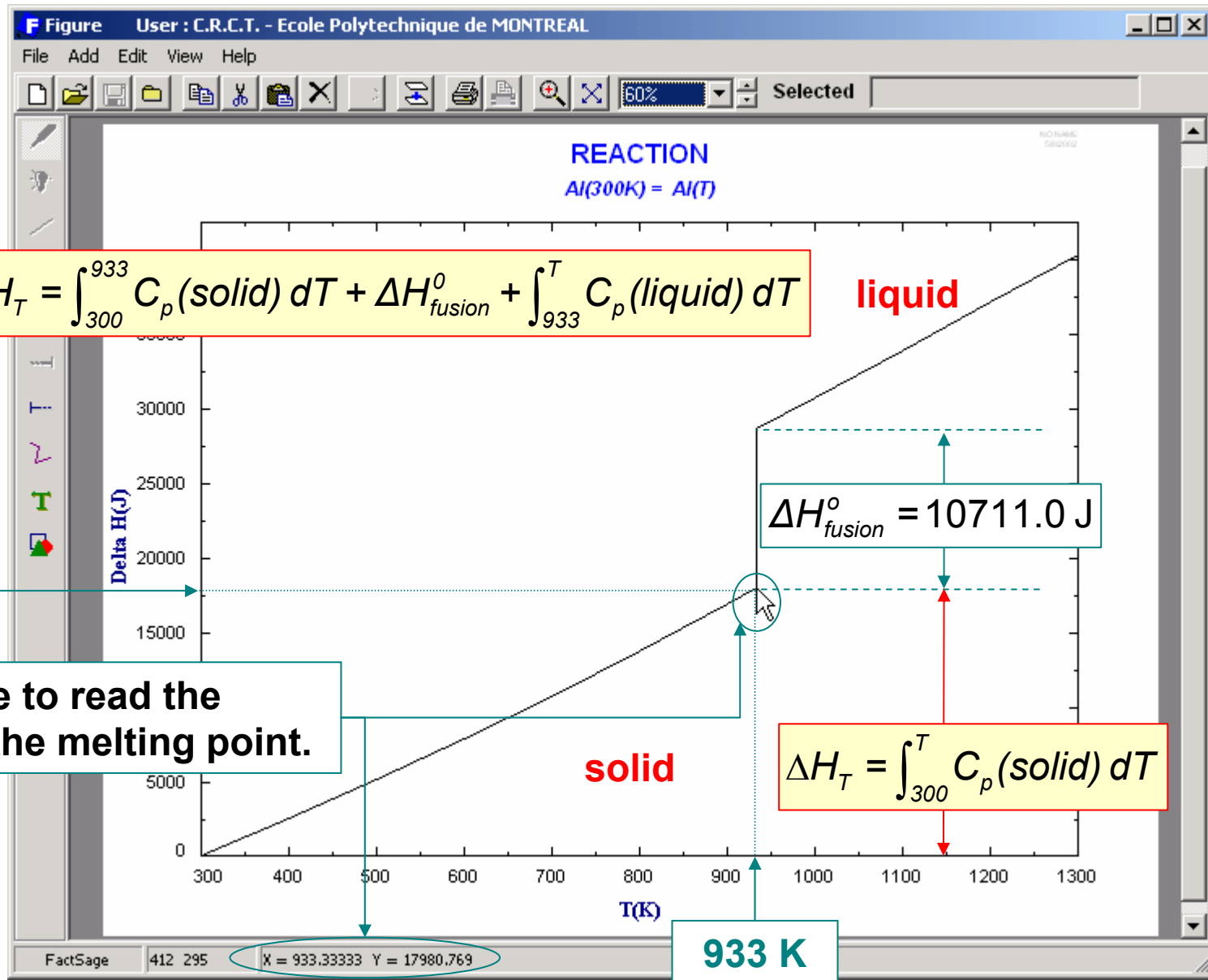
log10(Y)

ln(Y)

exp(Y)

1/Y

Heating Al: a few thermodynamic considerations



Two phase single component equilibrium (ideal binary system)

An thermodynamically more advanced application of the **Reaction** module is its use in the calculation of the **equilibrium of pure solid with its liquid** under the assumption that this liquid is dissolved in a solvent (some other liquid which is not explicitly given) **under the condition of ideal mixing**.

This situation is reflected in an equilibrium of the type:

$$Me(\text{pure solid}, T) = Me(\text{liquid}, a(\text{Me}) = x(\text{Me}), T)$$

In the example **Cu** is used. A **graph for the phase boundary** of the ideal liquid in equilibrium with the pure solid is given.

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

Cu(solid) = Cu(liquid)

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

$a_{\text{Cu(liquid)}} = X$

Mass(mol)	Species	Phase	T(K)	P(atm)**	Activity	Data
1	Cu	solid-FACT	T	1	1.0	FACT
= 1	Cu	liquid-FACT	T	1	X	FACT

*** 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

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Compound: **FACT** ELEM SGPS SGSL

Your choice of phases:

- **liquid** phase from the **FACT** database;
- **2 compound databases** are included in your data search.

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

1. To connect databases, click on the **Data Search** menu, select **Databases...** to open the Databases dialog box.

2. Follow the instructions if you want to **include** or **exclude** a **database** in the **data search**.

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

Click on "+" column to include/exclude database in the data search. Click on the "Name" column for "Information" on that database.

To Add a Database to the List
If a database does not appear in the list click on the menu bar (top left corner) "File > Add a database to the list ...".
To remove a database from the list click on its "Name" column and then click on the menu bar "File > Remove database from the list". Note, this does not delete the database.

+	Database	Name
+	FS50BASE.CDB	FACT
	ELEMBASE.CDB	ELEM
+	SGPSBASE.CDB	SGPS
	SGSLBASE.CDB	SGSL

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

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

For an ideal solution:
 $a_{\text{Cu(liquid)}} = X_{\text{Cu(liquid)}}$

Table Reaction

File Units Output Figure Help

T(K) P(atm)

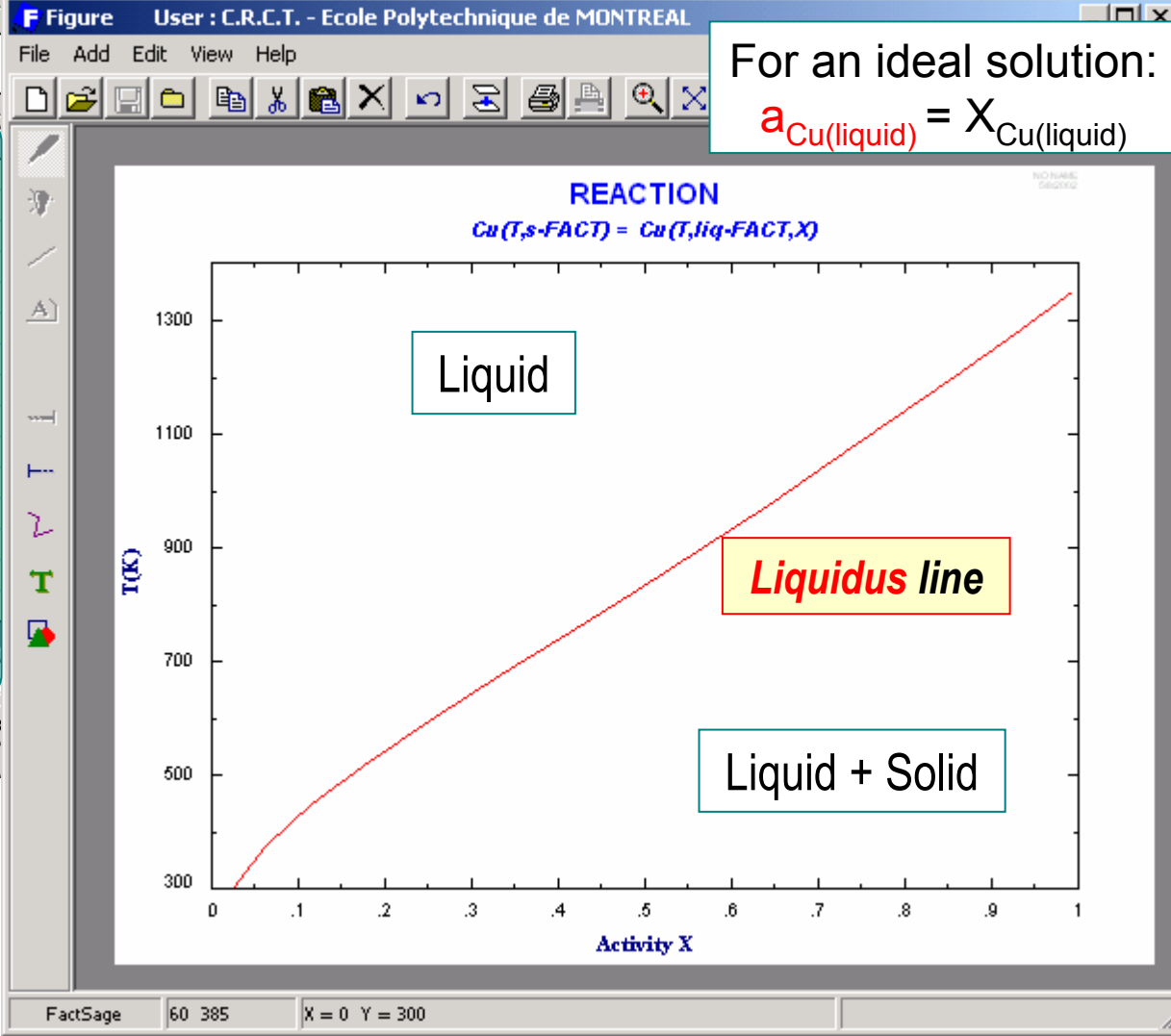
Reactants

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

Calculate Specify 2 variables. << Back



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

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

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

As an example the combustion reaction



is used. The **Alpha** variable is introduced to handle the **excess** amount.

In the example is also shown how the **autobalance feature** can be used to generate stoichiometric coefficient that satisfy the mass-balances automatically.

Combustion of methane in excess **<Alpha>** O₂ – data entry

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

Mass(mol)	Species	Phase	T(K)	P(atm)**	Activity	Data
1	CH4	gas	298	1.0	1.0	
+ <A>	O2	gas	298	1.0	1.0	
= 1	CO2	gas	T	1.0	1.0	
+ 2	H2O	gas steam	T	1.0	1.0	
+ <A-2>	O2	gas	T	1.0	1.0	

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FactSage 5.1 Compound: FACT ELEM SGPS SGSL

Variable quantity
<Alpha>

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

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

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

Combustion of methane in excess $\langle A \rangle$ O₂ – **adiabatic** reactions

Stoichiometric reaction ($A = 2$):
 $\text{CH}_4 + 2 \text{O}_2 = \text{CO}_2 + 2 \text{H}_2\text{O}$

Reaction with **excess** O₂ ($A > 2$):
 $\text{CH}_4 + (2 + \text{excess}) \text{O}_2 = \text{CO}_2 + 2 \text{H}_2\text{O} + (\text{excess}) \text{O}_2$

Exothermic reaction

Table Reaction

File Units Output Figure Help

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

Reactants

CH4 + $\langle A \rangle$ O2 = CO2 + 2 H2O + $\langle A-2 \rangle$ O2
 (298K,g) (298K,g) (T,g) (T,g) (T,g)

$\langle A \rangle$	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	T
10.0000	2196.28	0.0	-5991619.2	1.7135E+03	795.161	141.768	T

10 0

Calculate << Back Clear

Adiabatic reaction: $\Delta H = 0$

Product flame temperature

As $\langle A \rangle$ increases, the flame temperature decreases.
 Energy is required to heat the **excess** O₂.

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

The screenshot displays the FactSage software interface for defining a chemical reaction. The main window is titled "Reactants - Reaction" and contains a table for defining reaction components. The table has columns for Mass(mol), Species, Phase, T(K), P(atm), and Activity. The reaction is defined as:

Mass(mol)	Species	Phase	T(K)	P(atm)	Activity
1	CO2	gas	298	1.0	1.0
2	H2O	gas steam	298	1.0	1.0
6	O2	gas	298	1.0	1.0
1	CO2	gas	T	1.0	1.0
2	H2O	gas steam	T	1.0	1.0
6	O2	gas	T	1.0	1.0

The "Unbalanced Reaction" dialog box is open, asking: "The reaction is not balanced. Do you want the program to automatically balance the reaction?" with "Yes", "No", and "Cancel" buttons. The "Balanced Reaction" dialog box is also open, displaying: "- reaction balanced" with an "OK" button. Red arrows point from the "Unbalanced Reaction" dialog to the "6" in the O2 row of the reactants table. Blue arrows point from the "Balanced Reaction" dialog to the "6" in the O2 row of the products table. The "Next >>" button is visible at the bottom of the main window.

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

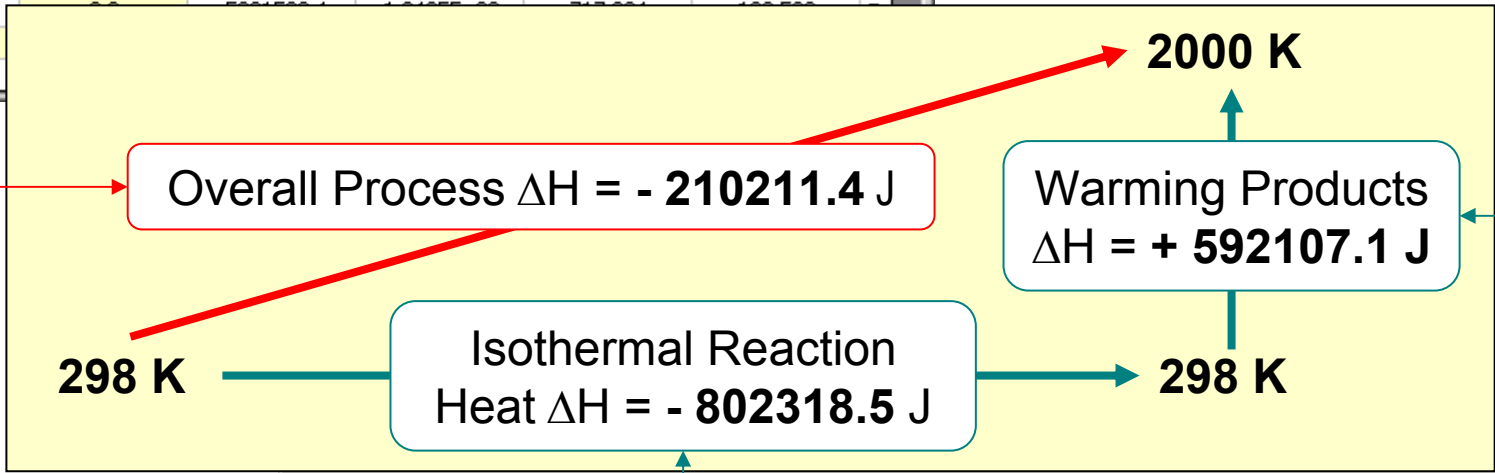
T(K) P(atm) Energy(J) Mass(mol) Vol(l)

Reactants

$$\text{CH}_4 + \langle A \rangle \text{O}_2 = \text{CO}_2 + 2 \text{H}_2\text{O} + \langle A-2 \rangle \text{O}_2$$

(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						



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

Reactants

$$\text{CO}_2 + 2 \text{H}_2\text{O} + 6 \text{O}_2 = \text{CO}_2 + 2 \text{H}_2\text{O} + 6 \text{O}_2$$

(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	

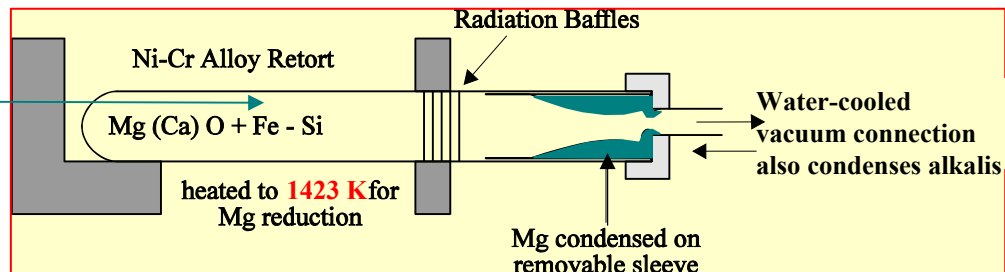
Pidgeon Process for the Production of Magnesium

The following five slides show how various aspects of the **Pidgeon process** (production of Mg vapor from MgO in a redox reaction with Si) can be treated using reaction thermochemistry.

Pidgeon Process for the Production of Magnesium

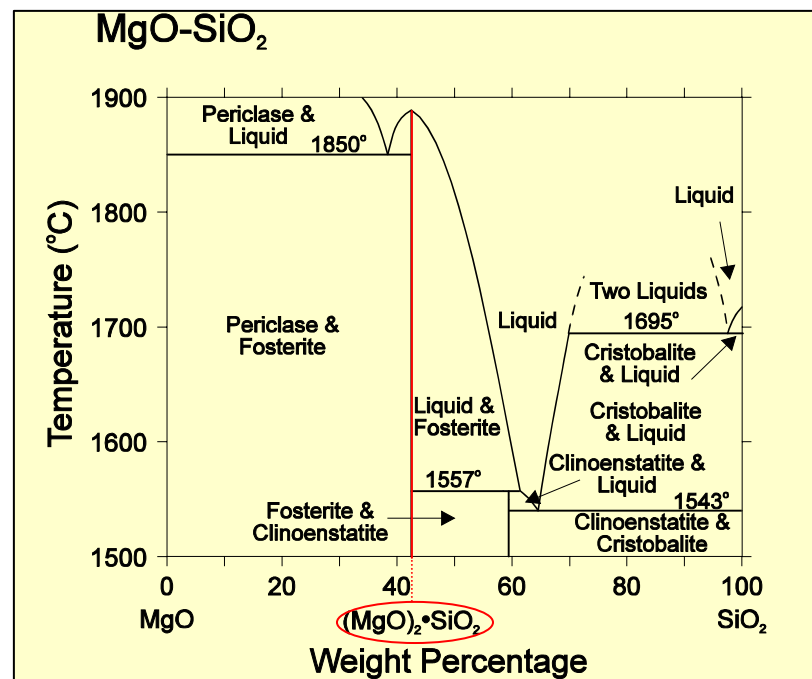
Apparatus Schema:

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



MgO-SiO₂ phase diagram:

Note: MgO(s) and SiO₂(s) can **not** coexist.



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

In the reaction, the hydrostatic pressure above the condensed phases: MgO(s), Si(s) and SiO₂(s2) is 1 atm – i.e. has no effect.

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

Mass(mol)	Species	Phase	T(K)	P(atm)**	Activity	Data
2	MgO	solid periclase	T	1.0	1.0	
+ 1	Si	solid	T	1.0	1.0	
= 2	Mg	gas	T	P	1.0	
+ 1	SiO2	solid-2 quartz(h)	T	1.0	X	

** 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 'M_DP' term

non standard states

Next >>

The activity of SiO₂ is: $a_{\text{SiO}_2} = X$.

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

Allotrope s2(solid-2) has been selected for **SiO₂** 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 ($P_{Mg(g)}$, $a_{SiO_2(s)}$) which satisfy K_{eq} . Here we select 3 special cases.

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

F Table Reaction

File Units Output Figure Help

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

Reactants

$$2\ MgO + Si = 2\ Mg + SiO_2$$

(T,s) (T,s) (T,P,g) (T,s2X)

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 ($\Delta G=0$), when $a_{SiO_2(s)} = 1.0$ and $T=1423\ K$, $P_{Mg\ eq} = 8.6443 \times 10^{-5}\ atm$

At equilibrium ($\Delta G=0$), when $P_{Mg\ eq} = 1\ atm$ and $T=1423\ K$, $a_{SiO_2(s)\ eq} = 7.4723 \times 10^{-9}$

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

Computation of SiO₂ activity when MgO coexists with (MgO)₂•SiO₂

F Reactants - Reaction

File Edit Units Data Search Help

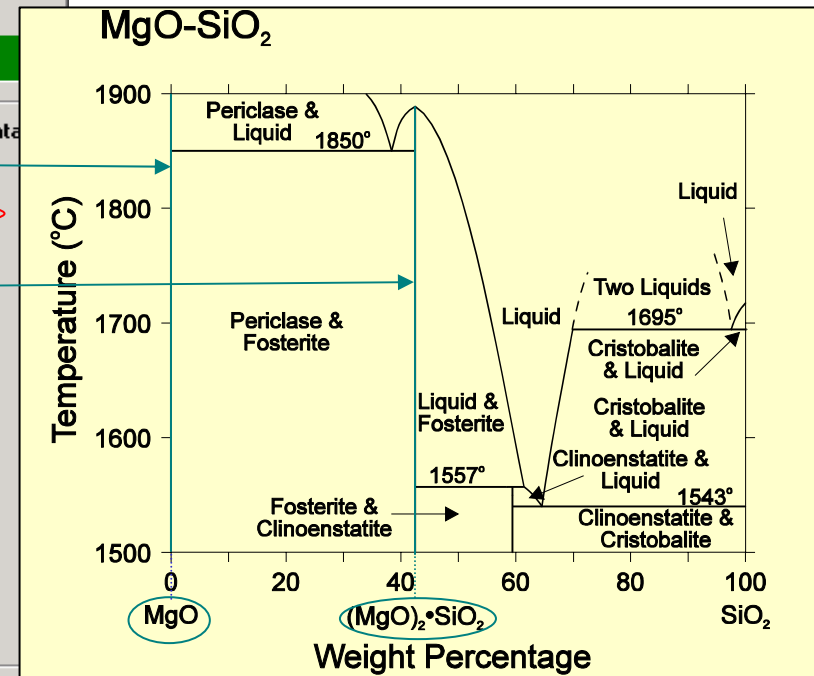
T(K) P(atm) Energy(J) Mass(mol) Vol(l)

Mass(mol)	Species	Phase	T(K)	P(atm) ^{**}	Activity	Data
2	MgO	solid periclase	T	1.0	1.0	
+ 1	SiO2	solid-2 quartz(h)	T	1.0	X	
= 1	(MgO)2SiO2	solid-1 forsterite	T	1.0	1.0	

Pure MgO → T(K) = T, P(atm) = 1.0, Activity = 1.0
Pure (MgO)₂•SiO₂ → T(K) = T, P(atm) = 1.0, Activity = 1.0
SiO₂(s2) at activity X → T(K) = T, P(atm) = 1.0, Activity = X

** 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



Gives the equilibrium value of the **activity of SiO₂(s2)** at 1423 K: **$a_{\text{SiO}_2(\text{s}2)} = 0.006317$**

F Table Reaction

File Units Output Figure Help

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

Reactants

$$2 \text{ MgO} + \text{ SiO}_2 = (\text{MgO})_2\text{SiO}_2$$

(T,s)
(T,s2X)
(T,s1)

T(K)	Activity X	Delta H(J)	Delta G(J)	De
1423.00	6.3170E-03	-63559.7	0.0	-1.

Isothermal... → T(K) = 1423.00
Activity X = 6.3170E-03
...and at equilibrium → Delta G(J) = 0.0

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

Remember, $\Delta G = 0$ (equilibrium) calculations are only meaningful for isothermal reactions («T» throughout).

Reactants - Reaction

Mass(mol)	Species	Phase	T(K)	P(atm)**	Activity	Data
4	MgO	solid periclase	T	1	1.0	
+ 1	Si	solid	T	1	1.0	
- 2	Mg	gas	T	P	1.0	
+ 1	Mg2SiO4	solid-1 forsterite	T	1	1.0	

Table Reaction

Reactants

$$4 \text{ MgO} + \text{Si} = 2 \text{ Mg} + \text{Mg}_2\text{SiO}_4$$

(T,s) (T,s) (T,P,g) (T,s1)

T(K)	P(atm)	Delta H(J)	Delta G(J)	Delta Vol(l)	Delta S(J/K)	Delta Cp(J/K)	T
1423.00	1.0876E-03	506709.7	0.0	2.1472E+05	356.086	-12.832	

FactSage 5.1 Compound: FACT ELEM SGPS SGSI

Magnesium production is enhanced by:

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

Aqueous applications

In the following two slides examples are given for the use of the **Reaction** module in aqueous thermochemistry.

It should be noted however, that ideal behaviour of the aqueous species is assumed since **Reaction** accesses **Compound** type databases. If a system requires non-ideal behaviour of the aqueous phase the **Equilib** module must be used.

Hydrogen reduction of aqueous copper ion - **Reactants** and **Table** windows

The standard Gibbs energy change underlined yields standard reduction potential of Cu^{2+} when divided by -2 Faradays. (Remember: $\Delta G^\circ = -nFE^\circ$, where F ($= 96485 \text{ C/mol}$) is the Faraday constant)

F Reactants - Reaction

File Edit Units Data Search Help

1 - 4

Mass[mol]	Species	Phase	T(K)	P[atm]**	Activity	Data
1	Cu(++)	aqueous	T	1.0	X	
+	1	H2	gas	T	P	1.0
=	1	Cu	solid	T	1.0	1.0
+	2	H(+)	aqueous	T	1.0	1.0

Standard state reaction at **298.15 K**

** 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

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

$\text{H}_2(\text{g})$ pressure is "P" atm.

F Table Reaction

File Units Output Figure Help

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

Reactants

Cu(++) + H2 = Cu + 2 H(+)

(T,aq)X (T,P,g) (T,s) (T,aq)

T(K)	P(atm)	Activity X	Delta H(J)	Delta G(J)	Delta Vol(l)	Delta S(J/K)	T
298.15	1.0000E+00	1.0000E+00	-64852.0	-65499.8	-2.4458E+01	2.173	
308.15	1.0000E+00	1.0000E+00	-65088.5	-65517.5	-2.5279E+01	1.392	
318.15	1.0000E+00	1.0000E+00	-65301.1	-65528.0	-2.6100E+01	0.713	
328.15	1.0000E+00	1.0000E+00	-65491.3	-65532.1	-2.6920E+01	0.124	
338.15	1.0000E+00	1.0000E+00	-65660.1	-65530.7	-2.7741E+01	-0.383	
348.15	1.0000E+00	1.0000E+00	-65808.6	-65524.7	-2.8561E+01	-0.816	
358.15	1.0000E+00	1.0000E+00	-65937.8	-65514.6	-2.9382E+01	-1.182	
368.15	1.0000E+00	1.0000E+00	-66048.4	-65501.2	-3.0202E+01	-1.486	
370.00	1.0000E+00	1.0000E+00	-66066.9	-65498.4	-3.0354E+01	-1.536	
315.00	1.0000E+00	1.3633E-11	-65236.6	0.0	-2.5841E+01	-207.100	
315.00	2.0000E+00	6.8163E-12	-65236.6	0.0	-1.2917E+01	-207.100	
315.00	3.0000E+00	4.5442E-12	-65236.6	0.0	-8.6089E+00	-207.100	
315.00	4.0000E+00	3.4081E-12	-65236.6	0.0	-6.4549E+00	-207.100	
315.00	5.0000E+00	2.7265E-12	-65236.6	0.0	-5.1625E+00	-207.100	
315.00	6.0000E+00	2.2721E-12	-65236.6	0.0	-4.3009E+00	-207.100	
315.00	7.0000E+00	1.9475E-12	-65236.6	0.0	-3.6855E+00	-207.100	

315 1 71 0

Calculate << Back Clear

Standard state reaction at various temperatures

Equilibrium molality at various P_{H_2}

Thermal balance for leaching of zinc oxide

F Reactants - Reaction

File Edit Units Data Search Help

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

1 - 9

Mass(mol)	Species	Phase	T(K)	P(atm)**	Activity	Data
55.55	H2O	liquid	294.7	1.0	1.0	
+ 1.2952	H(+)	aqueous	294.7	1.0	1.0	
+ 1.2952	HSO4(-)	aqueous-1	294.7	1.0	1.0	
+ 0.25246	ZnO	solid zincite	294.7	1.0	1.0	
= 55.802	H2O	liquid	T	1.0	1.0	
+ 1.1167	HSO4(-)	aqueous	T	1.0	1.0	
+ 0.9687	H(+)	aqueous	T	1.0	1.0	
+ 0.1785	ZnSO4	aqueous	T	1.0	1.0	
+ 0.0740	Zn(++)	aqueous	T	1.0	1.0	

non standard states

FactSage 5.1 Compound: FACT ELEM SGPS S

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

F Table Reaction

File Units Output Figure Help

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

Reactants

55.55 H2O + 1.2952 H(+) + 1.2952 HSO4(-) + 0.25246 ZnO = 55.802 H2O + 1.1167 HSO4(-) + 0.9687 H(+) + 0.1785 ZnSO4 + 0.0740 Zn(++)

(294.7K,liq) (294.7K,aq) (294.7K,aq1) (294.7K,s) (T,liq) (T,aq) (T,aq) (T,aq) (T,aq)

T(K)	Delta H(J)	Delta G(J)	Delta Vol(l)	Delta S(J/K)	Delta Cp(J/K)	Delta A (J)	T
294.70	-23372.4	-16327.8	8.7457E-04	-23.904	-36.676	-16327.9	T
300.06	0.0	-37929.7	8.7457E-04	54.693	-41.902	-37929.8	T

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

The following two slides show how **Reaction** is used on a system with **polymer formation in the gas** phase ($\text{Na(l)} \leftrightarrow \text{Na}_1 + \text{Na}_2$) and on a pure substance system that is submitted to **very high pressure (C)**.

Computation of P_{Na} and P_{Na_2} partial pressure in equilibrium with liquid Na

Both reactions are **isothermal**, hence $\Delta G=0$ gives **equilibrium**.

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	0	

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

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

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

non standard states

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	0	

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

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

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

Table Reaction

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	T

Table Reaction

Reactants

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	T

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: $P_{Na} + P_{Na_2}$ ($0.888 + 0.111 \cong 1$).

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

Where available, **density** (i.e. molar volume) data for solids and liquids are employed in **REACTION** (the “**VdP**” term) although their effect only becomes significant at high pressures. (However, unlike **EQUILIB**, compressibility and expansivity data are **NOT** employed.)

1 - 2

Mass(mol)	Species	Phase	T(K)	P(atm)**	Activity	Data
1	C	solid-1 graphite	T	P	1.0	
1	C	solid-2 diamond	T	P	1.0	

Here, carbon **density** data are employed to calculate the high pressure required to convert **graphite to diamond at 1000 K**.

** 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

At **1000 K** and **30597 atm**, graphite and **diamond** are at equilibrium ($\Delta G=0$)

Table Reaction

Reactants

C = C
(T,P,s1) (T,P,s2)

T(K)	P(atm)	Delta H(J)	Delta G(J)	Delta Vol(l)	Delta S(J/K)	Delta Cp(J/K)	T
1000.00	1.0000E+04	-574.7	3926.0	-1.8812E-03	-4.501	-0.581	
1000.00	2.0000E+04	-2480.8	2019.9	-1.8812E-03	-4.501	-0.581	
1000.00	3.0000E+04	-4386.9	113.8	-1.8812E-03	-4.501	-0.581	
1000.00	4.0000E+04	-6293.0	-1792.3	-1.8812E-03	-4.501	-0.581	
1000.00	5.0000E+04	-8199.0	-3698.4	-1.8812E-03	-4.501	-0.581	
1000.00	3.0597E+04	-4500.7	0.0	-1.8812E-03	-4.501	-0.581	

The volume of diamond is smaller than graphite. Hence, at high pressures, the “**VdP**” term creates a **favorable negative contribution to the enthalpy change** associated with the **graphite → diamond** transition.