

Slide show
revised:
2012-09-21



Reaction-Web^{Plus} is part of the **Fact-Web** series of internet modules that offer free access to the **FactSageTM** thermochemical software and databases.

Reaction-Web^{Plus} accesses only compound data stored in **FactPS** – the **Fact** pure substances database. It assumes all gases are ideal and ignores expansivities and compressibilities of solids and liquids.

In the **Reaction** module of the full **FactSageTM** package data may also be retrieved from private and other databases. Spreadsheets can be generated and figures plotted that then may be exported into other applications such as Excel. For details visit www.factsage.com.

Reactants Window : entry of a pure species -1

Reaction-Web has two windows – **Reactants Window** and **Table Window**

Here in the **Reactants Window** the reactant is 1 mol Cu

Select the units of temperature, mass, energy, pressure, volume

Add a Reactant

Add a Product

Amount	Species	Phase	T	P	Activity
1	Cu	most stable	T	1.0	1.0

Entry of reactant species

Cu phases are in their standard states i.e. pure at unit P.

Go to the **Table Window**

Reaction-Web can only access compounds (not solutions). All calculations shown here use the **FactPS** compounds database.

Table Window : thermodynamic properties of a species - 2

Reaction
1 Cu
(T)

Summary of the **Reactants Window**

A multiple entry for T:
min, max and **step**.

T(K)	P(ATM)	Activity X	H (J)	G (J)	Vol (l)	S (J/K)	Cp (J/K)	T
300 3300 500								
----- Cu(s) -----								
300.00			45.3	-9949.3	7.1240E-03	33.315	24.468	
800.00			13120.4	-33868.0	7.1240E-03	58.736	27.481	
1300.00			27758.9	-66968.6	7.1240E-03	72.867	32.201	
1358.00			29659.9	-71236.5	7.1240E-03	74.298	33.362	
----- 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	
1800.00			57314.9	-110493.4	7.1240E-03	93.227	32.844	
2300.00			73736.9	-159201.7	7.1240E-03	101.278	32.844	
2800.00			90158.9	-211508.6	7.1240E-03	107.738	32.844	
2846.16			91675.0	-216494.2	7.1240E-03	108.275	32.844	
----- 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	
3300.00			403914.1	-314439.8	2.7079E+02	217.683	26.675	

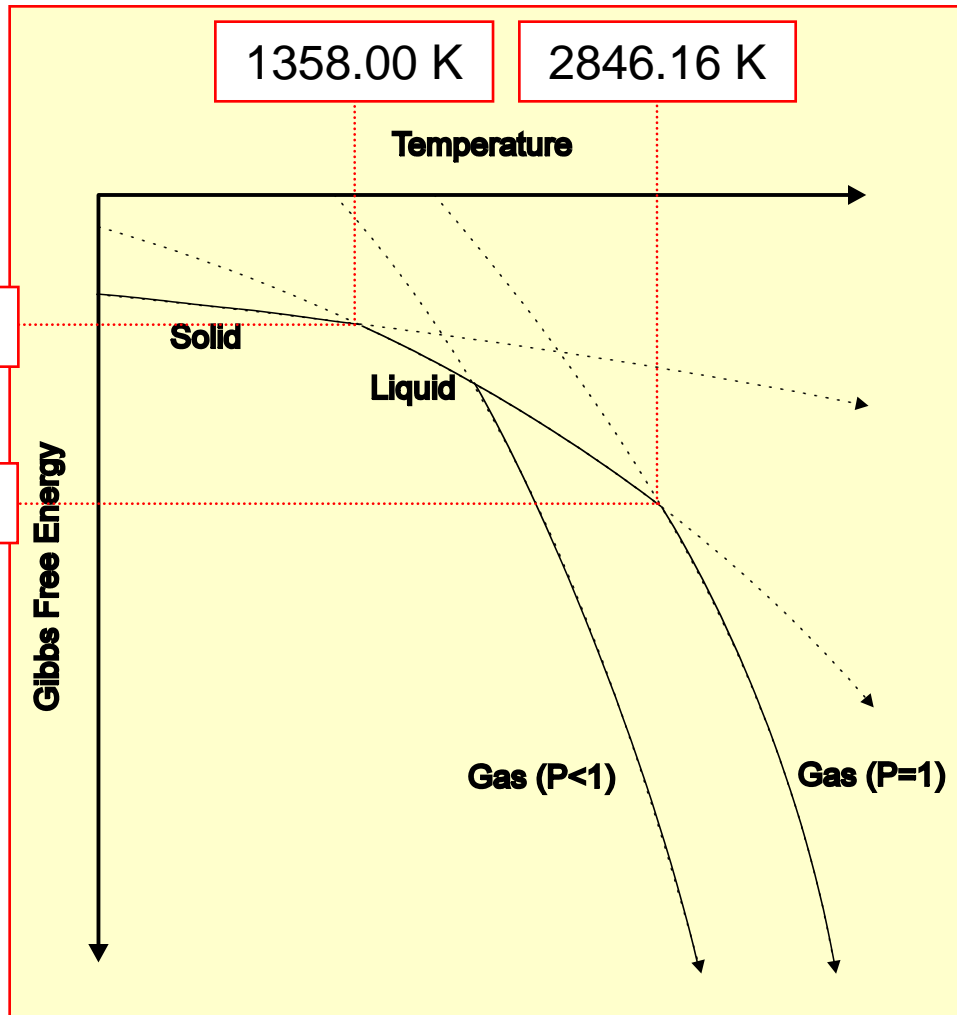
<< Back Clear

The table also display **transitions**

Return to the **Reactants Window**

Most stable phase : **Gibbs energy minimization** - 3

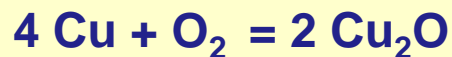
Phase with **lowest** Gibbs energy is the **most** stable.



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

Isothermal standard state reaction : **oxidation of copper** - 1

Entry of an isothermal standard state reaction:



Add reactant O2

Add product Cu2O

Units

K mole joule atm litre

Reactants

+ = +

Amount	Species	Phase	T	P	Activity
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

Next >>

Isothermal "T" throughout

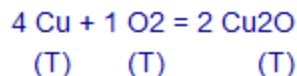
Non-standard states checkbox is **not** selected

Go to the Table window

Oxidation of copper at various temperatures - 2

Entry: $T_{\min} = 300\text{K}$,
 $T_{\max} = 2000\text{K}$, step = 300K.

Reaction



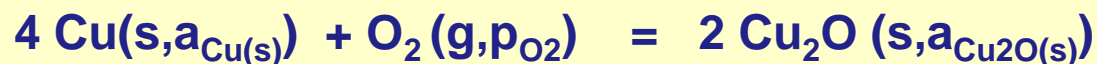
T(K)	P(ATM)	Activity X	Delta H (J)	Delta G (J)	Delta Vol (l)	Delta S (J/K)	Delta Cp (J/K)	Keq	T
300 2000 300									
----- Cu(s) O2(g) Cu2O(s) -----									
300.00			-341417.7	-295521.9	-2.4598E+01	-152.986	-1.922	2.8421E+51	
600.00			-339925.3	-249958.6	-4.9215E+01	-149.945	8.923	5.7581E+21	
900.00			-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	

Calculate

<< Back

Clear

The equilibrium constant column appears for an **isothermal** standard state reaction.
 $\Delta G^{\circ} = -RT \ln K$. At 1500K, $K = 1.0155 \times 10^4$, $\Delta G^{\circ} = -8.3145 \times 1500 \times \ln(K) = -115.06 \text{ kJ}$



Units

K ▾
mole ▾
joule ▾
atm ▾
litre ▾

Reactants

+ = +

Amount	Species	Phase	T	P	Activity
4	Cu	S solid-1 ▾	T	1.0	X
+	1	O2	G gas	P	1.0
=	2	Cu2O	S solid-1 ▾	1	1

Non standard states
 Next >>

For "Activity" enter a value or "X".
For "Pressure" enter a value or "P".

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

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

$$a_{\text{Cu}_2\text{O(s)}} = 1$$

Non-standard states

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 $\Delta G^0 = -RT \ln K_{eq}$

Chemical equilibrium : isothermal **non-standard state** oxidation - 2

Standard state
T = 1000 K
P_{O₂(g)} = 1.0 atm
a_{Cu(s)} = 1.0

At 1000 K,
ΔG° = -191.16 kJ

a_{Cu(s)} = "X"

P_{O₂(g)} = "P"

Reaction: 4 Cu + 1 O₂ = 2 Cu₂O
 (T, X, s) (T, P, g) (T, s)

T(K)	P(ATM)	Activity X	Delta H (J)	Delta G (J)	Delta Vol (l)	Delta S (J/K)	Delta Cp (J/K)	T
1000	1.0	1	-335381.1	-191155.7	-8.2039E+01	-144.225		
1000.00	1.0000E+00	1.0000E+00						

Buttons: Calculate, << Back, Download TXT file, Clear

Equilibrium
T = 1000 K
a_{Cu(s)} = 1.0
ΔG = 0

T(K)	P(ATM)	Activity X	Delta H (J)	Delta G (J)	Delta Vol (l)	Delta S (J/K)	Delta Cp (J/K)	T
1000		1		0				
1000.00	1.0359E-10	1.0000E+00	-335381.1	0.0	-7.9216E+11	-335.381		

Buttons: Calculate, << Back, Clear

Equilibrium: ΔG = 0, T = 1000 K,
P_{O₂(g)} (equilib) = 1.0359x10⁻¹⁰ atm, a_{Cu(s)} (equilib) = 1.0

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

Chemical equilibrium : isothermal **non standard state** oxidation - 3

Standard state
T = 1000 K
P_{O₂(g)} = 1.0 atm
a_{Cu(s)} = 1.0

At 1000 K,
ΔG° = -191.16 kJ

a_{Cu(s)} = "X"

P_{O₂(g)} = "P"

Reaction
 4 Cu + 1 O₂ = 2 Cu₂O
 (T, X) (T, P) (T)

T(K)	P(ATM)	Activity X	Delta H (J)	Delta G (J)	Delta Vol (l)	Delta S (J/K)	Delta Cp (J/K)	T
1000	1.0	1						
1000.00	1.0000E+00	1.0000E+00	-335381.1	-191155.7	-8.2039E+01	-144.225		

Buttons: Calculate, << Back, Clear

Equilibrium
T = 500 - 1000K
P_{O₂(g)} = 1.0 atm
ΔG = 0

T(K)	P(ATM)	Activity X	Delta H (J)	Delta G (J)	Delta Vol (l)	Delta S (J/K)	Delta Cp (J/K)	T
500 1000 100	1			0				
500.00	1.0000E+00	1.1979E-07	-340720.5	0.0	-4.1010E+01	-681.441		
600.00	1.0000E+00	3.6302E-06	-339925.3	0.0	-4.9215E+01	-566.542		
700.00	1.0000E+00	4.1248E-05	-338951.7	0.0	-5.7421E+01	-484.217		
800.00	1.0000E+00	2.5385E-04	-337842.3	0.0	-6.5627E+01	-422.303		
900.00	1.0000E+00	1.0382E-03	-336636.3	0.0	-7.3833E+01	-374.040		
1000.00	1.0000E+00	3.1903E-03	-335381.1	0.0	-8.2039E+01	-335.381		

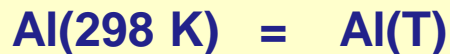
Buttons: Calculate, << Back, Clear

Two requirements for **equilibrium**:
ΔG = 0 and **Isothermal Reaction**

Equilibrium: ΔG = 0, T = 500 - 1000 K,
P_{O₂(g)} (equilib) = 1 atm, a_{Cu(s)} (equilib) = calculated

Heating **Al** from **298 K** to the temperature **T** - 1

Here in the **Reactants Window** the reactant is 1 mol Al at 298 K and the product is 1 mol Al at temperature “T”



Amount	Species	Phase	T	P	Activity
1	Al	most stable	298	1.0	1.0
= 1	Al	most stable	T	1.0	1.0

For “Temperature” enter a value or “T”.

$T_{(\text{initial})} = \text{“298”}$

$T_{(\text{final})} = \text{“T”}$

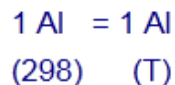
The Al phases are in their standard states (pure, 1 atm)

Reaction-Web accesses the Al phases stored in the **FactPS** compounds database.

Heating Al from 298 K to the temperature T - 2

Entry: $T_{\min}=300\text{K}$,
 $T_{\max}=1300\text{K}$, step=100K.

Reaction



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

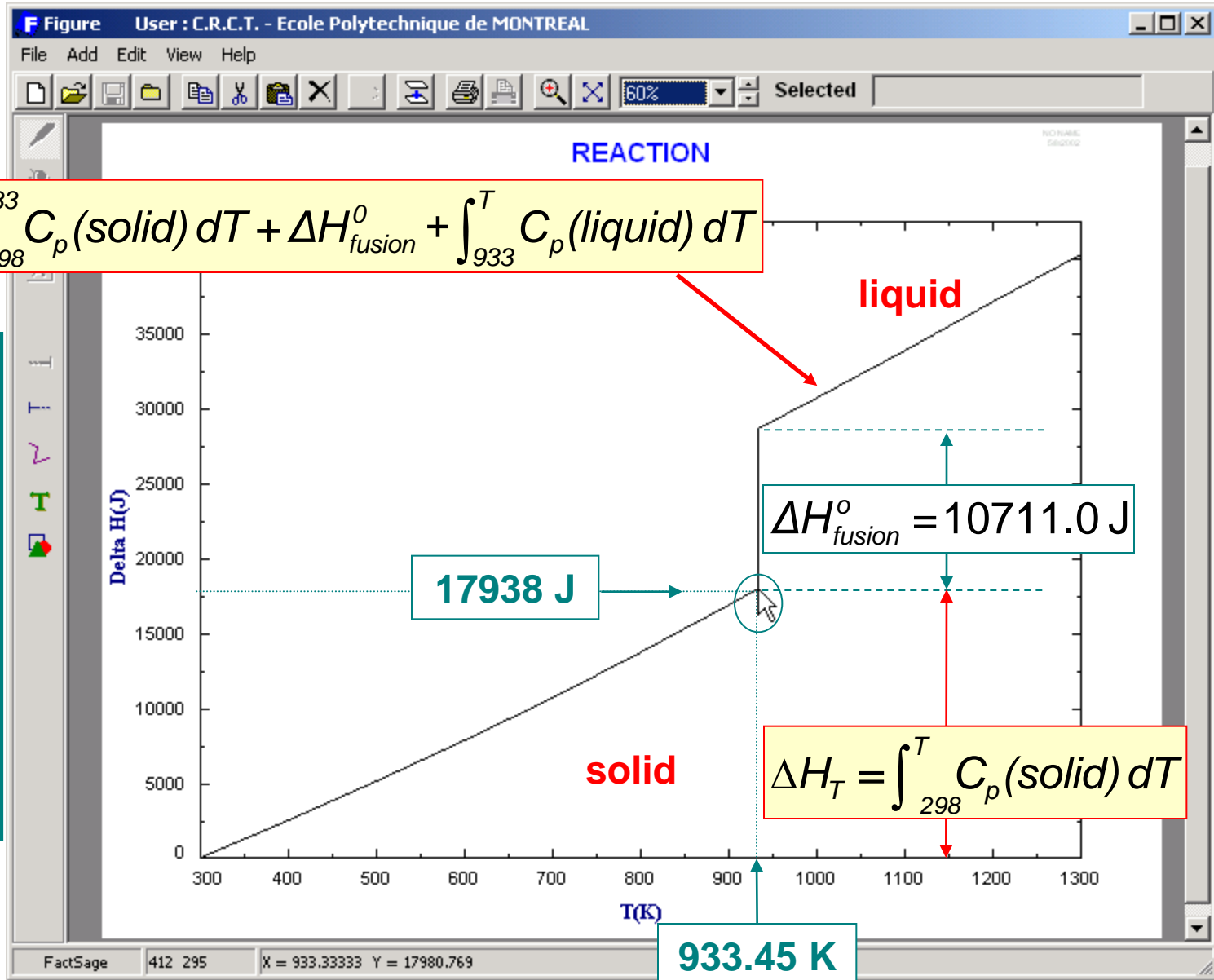
T(K)	P(ATM)	Activity X	Delta H (J)	Delta G (J)	Delta Vol (l)	Delta S (J/K)	Delta Cp (J/K)	T
300 1300 100								
----- Al(s) Al(s) -----								
300.00			48.4	-56.7				
400.00			2557.2	-3273.1				
500.00			5189.5	-7138.7	0.0000E+00	13.238	2.637	
600.00			7925.1	-11544.0	0.0000E+00	18.223	3.686	
700.00			10773.0	-16416.0	0.0000E+00	22.610	4.901	
800.00			13754.1	-21705.1	0.0000E+00	26.589	6.360	
900.00			16895.1	-27377.1	0.0000E+00	30.287	8.103	
933.45			17986.6	-29355.5	0.0000E+00	31.477	8.754	
----- Al(s) Al(l) -----								
Al(1 mol): DH° = 10711.0 DG° = 0 ----- DS° = 11.475								
933.45			28697.6	-29355.5	0.0000E+00	42.952	7.547	
1000.00			30810.6	-34168.5	0.0000E+00	45.139	7.547	
1100.00			33985.7	-41662.3	0.0000E+00	48.165	7.547	
1200.00			37160.8	-49445.2	0.0000E+00	50.927	7.547	
1300.00			40335.9	-57493.0	0.0000E+00	53.469	7.547	

Reference data for Al(s):
 table of $H_T - H_{\text{ref}(298)}$

Fusion : $\text{Al}_{(s)} \rightarrow \text{Al}_{(l)}$ at 933.45 K
 $\Delta H^{\circ}_{\text{fusion}} = T_{\text{fusion}} \cdot \Delta S^{\circ}_{\text{fusion}}$
 $= 933.45 \times 11.475 = 10711.0 \text{ J}$

At 933.45 K $G(\text{Al}_{(s)}) = G(\text{Al}_{(l)})$
 $\text{Al}_{(s)}$ is in equilibrium with $\text{Al}_{(l)}$.

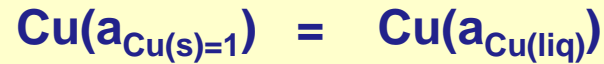
Heating AI : FactSage graphical display - 3



Reaction-Web

is not equipped to plot the results. Here the graphical display is created by running **Reaction** in **FactSage**.

Computation of Cu **liquidus** in an **ideal binary system** - 1



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

Amount	Species	Phase	T	P	Activity
1	Cu	S solid-1	T	1.0	1.0
= 1	Cu	L liquid-1	T	1.0	X

Non standard states Next >>

For "Activity" enter a value or "X"

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

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

Non-standard states

Computation of Cu **liquidus** in an **ideal binary system** - 2



Two requirements for **equilibrium**:
Isothermal Reaction and $\Delta G = 0$

Entry: **T = 500 - 1000K**, $\Delta G = 0$

Reaction

1 Cu = 1 Cu
(T, s) (T, X, l)

“T” appearing in this column indicates the Cp(T) data have been extrapolated outside the reported Cp(T) range – see **Compound-Web** for Cp(T).

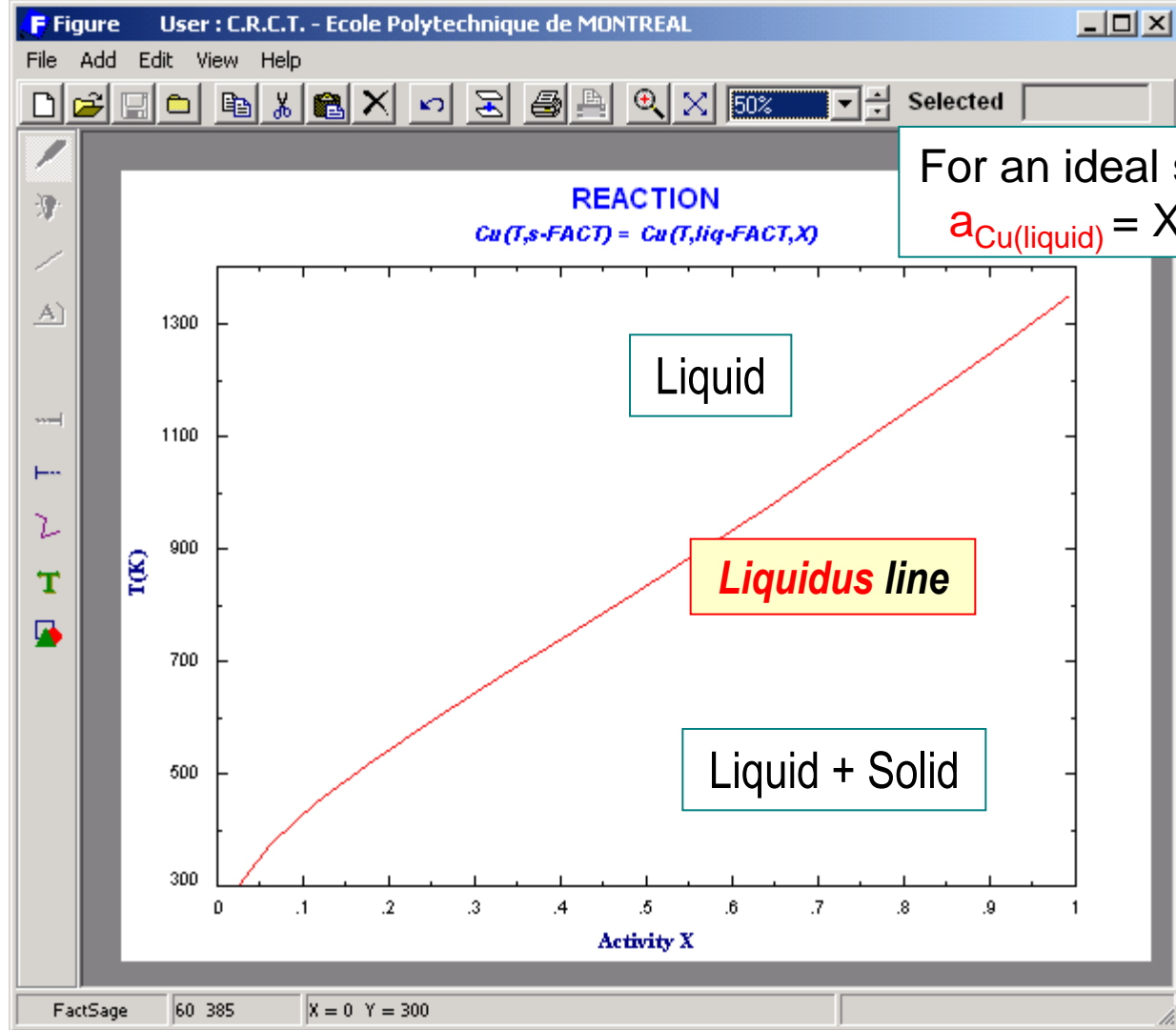
T(K)	P(ATM)	Activity X	Delta H (J)	Delta G (J)	Delta Vol (l)	Delta S (J/K)	Delta Cp (J/K)	T
300 1300 100				0				
300.00		2.3836E-02	11856.1	0.0	0.0000E+00	39.520	-0.005	
400.00		7.8222E-02	11857.7	0.0	0.0000E+00	29.644	0.004	
500.00		1.5959E-01	11856.3	0.0	0.0000E+00	23.713	-0.025	
600.00		2.5669E-01	11854.3	0.0	0.0000E+00	19.757	-0.009	
700.00		3.6045E-01	11854.9	0.0	0.0000E+00	16.936	0.020	
800.00		4.6498E-01	11857.6	0.0	0.0000E+00	14.822	0.028	
900.00		5.6684E-01	11858.8	0.0	0.0000E+00	13.176	4.790	
1000.00		6.6614E-01	12305.9	0.0	0.0000E+00	12.306	4.137	
1100.00		7.6366E-01	12683.1	0.0	0.0000E+00	11.530	3.391	
1200.00		8.5840E-01	12979.5	0.0	0.0000E+00	10.816	2.370	
1300.00		9.4940E-01	13134.0	0.0	0.0000E+00	10.103	0.643	

Calculate << Back Download TXT file Clear

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

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

Reaction-Web is not equipped to plot the results. Here the graphical display is created by running **Reaction** in **FactSage**.



For an ideal solution:

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

Adiabatic reaction : **combustion of CH₄** - 1



The **Phase** of each **Species** is specified

Amount	Species	Phase	T	P	Activity
1	CH4	G gas-1	25	1.0	1.0
+	2	O2	25	1.0	1.0
=	2	H2O	T	1.0	1.0
+	1	CO2	T	1.0	1.0

Non standard states Next >>

The **Reactants** are at 25°C .
The **Products** are unspecified at T.

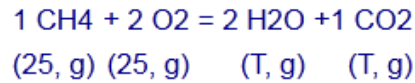
The reaction is **non-isothermal** (except when $T = 25^\circ\text{C}$). Hence K_{eq} will not appear as a column in the **Table Window**

This a simple combustion reaction with H₂O and CO₂ products. At high T other species may be more stable.

Adiabatic reaction : **combustion of CH₄** - 2

Entry: T_{min} = 1000°C,
T_{max} = 7000°C , step = 1000°C

Reaction



The assumed products of combustion are H₂O and CO₂. At high temperatures other gas species will be stable – use **Equilib**.

T(C)	P(ATM)	Activity X	Delta H (J)	Delta G (J)	Delta Vo	(J/C)
1000 7000 1000						
1000.00			-678227.8	-1479158.6	2.40	
2000.00			-520300.2	-2296752.3	4.86	
3000.00			-348655.9	-3189310.1	7.32	
4000.00			-170464.8	-4136170.5	9.78	
5000.00			11653.1	-5125576.4	1.22	
6000.00			196879.6	-6150046.6	1.17	
7000.00			382970.4	-7204211.0	1.71	

Exothermic : ΔH < 0
 - heat is given off

Endothermic : ΔH > 0
 - heat is required

T(C)	Delta H (J)	Delta G (J)	Delta Vol (l)	Delta S (J/C)	Delta Cp (J/C)	T
	0					
4936.54	0.0	-5061684.7	1.2091E+03	409.495	89.141	T

Adiabatic flame temperature = 4936.54°C

Adiabatic reaction: ΔH = 0

Setting **ΔG = 0** serves no useful purpose. The reaction is non-isothermal and so equilibrium is not possible.

“T” denotes extrapolated Cp(T) data

Aqueous applications : H_2 reduction of aqueous Cu ion - 1



Units

C mole joule atm litre

Reactants

Amount	Species	Phase	T	P	Activity
1	Cu[++]	Aq aqueous	T	1.0	X
+ 1	H2	G gas-1	T	P	1.0
= 1	Cu	S solid-1	T	1.0	1.0
+ 2	H[+]	Aq aqueous	T	1.0	1.0

Non standard states

Next >>

The **phase** of each species is specified

Non-standard states

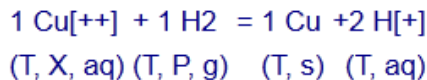
The molality of Cu^{2+} is given by "X".

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

Aqueous applications : H_2 reduction of aqueous Cu ion - 2

Entry: $T = 25^\circ C$, $P = 1$ atm
 $m_{Cu^{++}} = 0.2 - 1$, step = 0.2

Reaction



T(C)	P(ATM)	Activity X	Delta H (J)	E(v) = -DG/2F	Delta G (J)	Delta S (J/C)	Delta Cp (J/C)
25	1	0.2 1 0.2					
25.00	1.0000E+00	2.0000E-01	-64852.0	0.3188	-2.4458E+01	-217.515	
25.00	1.0000E+00	4.0000E-01	-64852.0	0.3277	-2.4458E+01	-217.515	
25.00	1.0000E+00	6.0000E-01	-64852.0	0.3329	-2.4458E+01	-217.515	
25.00	1.0000E+00	8.0000E-01	-64852.0	0.3366	-2.4458E+01	-217.515	
25.00	1.0000E+00	1.0000E+00	-64852.0	0.3394	-2.4458E+01	-217.515	

EMF of Cu/Cu⁺⁺ electrode with respect to standard H₂/H⁺ electrode at 25° C

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

Entry: $T = 25^\circ C$,
 $P = 0.2 - 1$ atm, $DG = 0$

T(C)	P(ATM)	Activity X	Delta H (J)	E(v) = -DG/2F	Delta Vol (l)	Delta S (J/C)	Delta Cp (J/C)
25	0.2 1 0.2			0			
25.00	2.0000E-01	1.6748E-11	-64852.0	0.0000	-1.2232E+02	-217.515	
25.00	4.0000E-01	8.3742E-12	-64852.0	0.0000	-6.1157E+01	-217.515	
25.00	6.0000E-01	5.5828E-12	-64852.0	0.0000	-4.0769E+01	-217.515	
25.00	8.0000E-01	4.1871E-12	-64852.0	0.0000	-3.0575E+01	-217.515	
25.00	1.0000E+00	3.3497E-12	-64852.0	0.0000	-2.4458E+01	-217.515	

Equilibrium molality $m_{Cu^{++}}$ at various P_{H_2}

Effect of high pressure : **graphite to diamond transition** - 1

Where available, **density** data for solids and liquids are employed in **Reaction** (the “**VdP**” term) although their effect only becomes significant at high pressures.



Amount	Species	Phase	T	P	Activity
1	C	S1 graphite	T	P	1.0
= 1	C	S2 diamond	T	P	1.0

Non standard states

Next >>

The **phase** of each species is specified

Non-standard states

The **Reactants** and **Products** are unspecified at “**T**” and “**P**”

Here “**P**” is the hydrostatic pressure above the solids.

The reaction is **isothermal**. Hence **equilibrium** can be calculated by setting $\Delta G = 0$ in the **Table Window**

Effect of high pressure : **graphite to diamond transition** - 2

Entry: $T = 1500\text{K}$, $P_{\min} = 10000$,
 $P_{\max} = 90000$, $\text{step} = 1000$ atm.

In **Reaction** compressibility and expansivity data are **NOT** employed.

T(K)	P(ATM)	Activity X	Delta H (J)	Delta G (J)	Delta Vol (l)	Delta S (J/K)	D
1500	1e4 9e4 1e4						
1500.00	1.0000E+04		-796.6	6231.0	-1.8811E-03	-4.685	-0.275
1500.00	2.0000E+04		-2702.7	4324.9	-1.8811E-03		
1500.00	3.0000E+04		-4608.7	2418.9	-1.8811E-03		
1500.00	4.0000E+04		-6514.7	512.8	-1.8811E-03		
1500.00	5.0000E+04		-8420.8	-1393.2	-1.8811E-03		
1500.00	6.0000E+04		-10326.8	-3299.2	-1.8811E-03		
1500.00	7.0000E+04		-12232.9	-5205.3	-1.8811E-03		
1500.00	8.0000E+04		-14138.9	-7111.3	-1.8811E-03		
1500.00	9.0000E+04		-16044.9	-9017.3	-1.8811E-03	-4.685	-0.275

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At **1500 K** as **P** increases ΔG becomes more negative and the transition of graphite to diamond becomes thermodynamically more favorable.

T(K)	P(ATM)	Activity X	Delta H (J)	Delta G (J)	Delta Vol (l)	Delta S (J/K)	Delta Cp (J/K)	T
1500				0				
1500.00	4.2691E+04		-7027.6	0.0	-1.8811E-03			

Calculate << Back Clear

At **1500 K** and **42691 atm**, graphite and **diamond** are at equilibrium ($\Delta G = 0$)

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