The *Equilib* module – Regular Features

- ***Equilib*** calculates the conditions for multiphase, multicomponent equilibria, with a wide variety of tabular and graphical output modes, under a large range of constraints.
- ***Equilib*** accesses both compound and solution databases.

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(continued)

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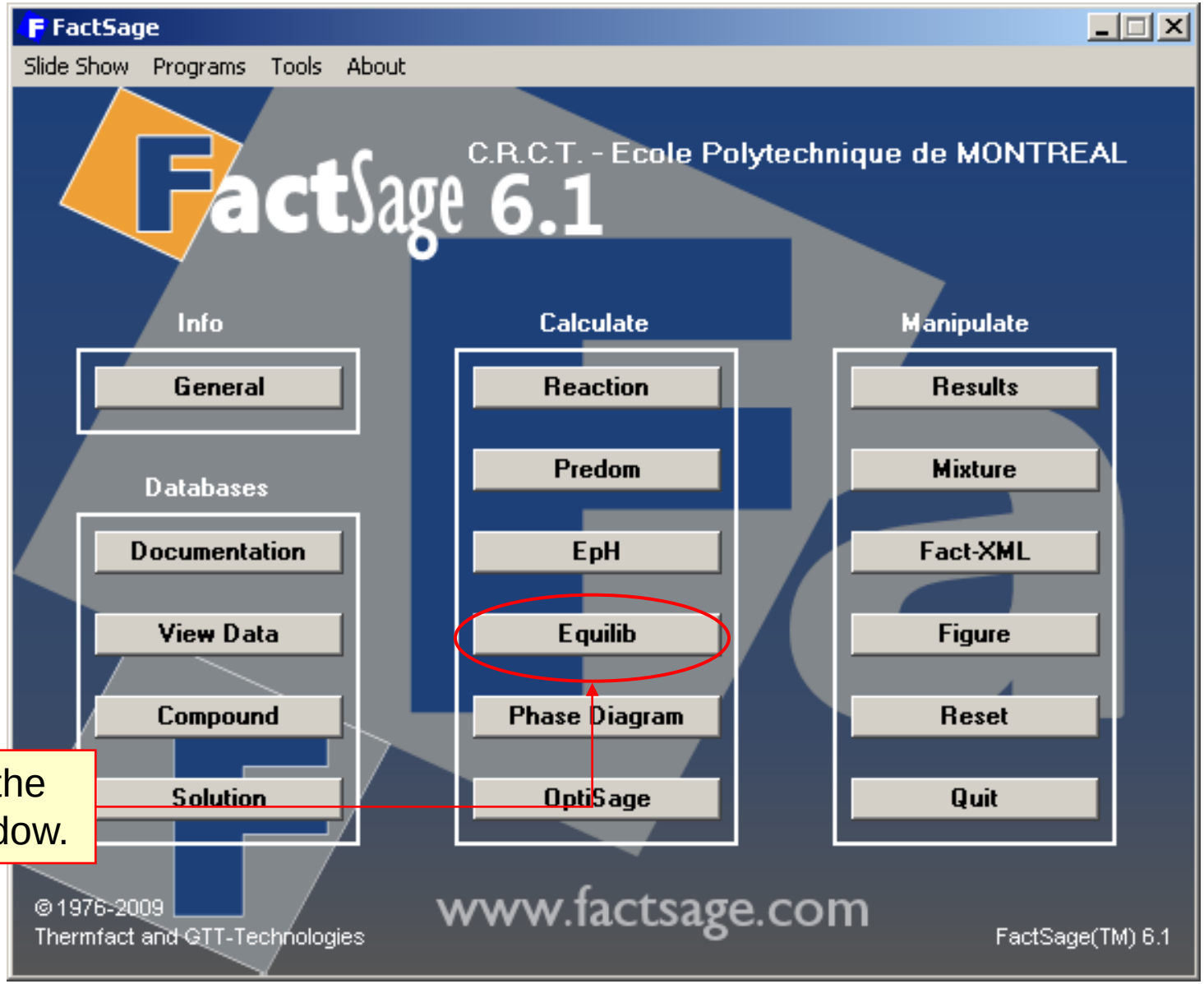
The *Equilib* module



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

Using ***Reaction*** and ***Equilib*** modules to identify the most probable reaction

What are the products of the following chemical reaction at 25°C:

$Mg + 3\ Cu_2O + 2\ Fe_3C + Ar$?

We will assume that only pure stoichiometric compounds can be formed and we will ignore kinetic considerations. Using the Reaction program, we see (on the following page) there are many possibilities. For example:

1 **$MgO + 6\ Cu + 4.5\ Fe + 2\ C + 0.5\ Fe_3O_4 + Ar$**

2 **$MgO + 6\ Cu + 4.667\ Fe + 2\ C + 0.667\ Fe_2O_3 + Ar$**

3 **$MgCO_3 + 6\ Cu + 6\ Fe + 1\ C + Ar$**

4 **$6\ Cu + 4.667\ Fe + 2\ C + 0.667\ MgFe_2O_4 + 0.333\ MgO + Ar$**

etc…

According to the ***Reaction*** program, **reaction 1** has the most negative Gibbs energy change. Hence, according to thermodynamic laws, this is the most probable reaction.

By the method of Gibbs energy minimization, in a single calculation module ***Equilib*** identifies this most probable reaction.

Reaction module: 4 possible **isothermal isobaric** reactions and 4 values of ΔG

Table Reaction

File Units Output Figure Help

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

Most negative ΔG

Reaction 1

Reactants

Mg (T,s) + 3 Cu2O (T,s) + 2 Fe3C (T,s1) + Ar (T,g) = MgO (T,s) + 6 Cu (T,s) + 4.5 Fe (T,s1) + 2 C (T,s1) + 0.5 Fe3O4 (T,s1) + Ar (T,g)

T(C)	Delta H(J)	Delta G(J)	Delta Vol(l)	Delta S(J/K)	Delta Cp(J/K)	Keq	T
25.00	-693267.6	-669706.1	-1.3366E-02	-79.026	-38.225	2.1221+117	

$\Delta G_1 \approx -670$ kJ

Reaction 2

Reactants

Mg (T,s) + 3 Cu2O (T,s) + 2 Fe3C (T,s1) + Ar (T,g) = MgO (T,s) + 6 Cu (T,s) + 4.667 Fe (T,s1) + 2 C (T,s1) + 0.667 Fe2O3 (T,s1) + Ar (T,g)

T(C)	Delta H(J)	Delta G(J)	Delta Vol(l)	Delta S(J/K)	Delta Cp(J/K)	Keq	T
25.00	-685259.8	-658662.9	-1.4253E-02	-89.206	-40.503	2.4666+115	

$\Delta G_2 \approx -659$ kJ

Reaction 3

Reactants

Mg (T,s) + 3 Cu2O (T,s) + 2 Fe3C (T,s1) + Ar (T,g) = MgCO3 (T,s) + 6 Cu (T,s) + 6 Fe (T,s1) + C (T,s1) + Ar (T,g)

T(C)	Delta H(J)	Delta G(J)	Delta Vol(l)	Delta S(J/K)	Delta Cp(J/K)	Keq	T
25.00	-644755.4	-621499.5	-1.3484E-02	-78.001	-46.243	7.6100+108	

$\Delta G_3 \approx -621$ kJ

Reaction 4

Reactants

Mg (T,s) + 3 Cu2O (T,s) + 2 Fe3C (T,s1) + Ar (T,g) = 6 Cu (T,s) + 4.667 Fe (T,s1) + 2 C (T,s1) + 0.667 MgFe2O4 (T,s1) + 0.333 MgO (T,s) + Ar (T,g)

T(C)	Delta H(J)	Delta G(J)	Delta Vol(l)	Delta S(J/K)	Delta Cp(J/K)	Keq	T
25.00	-692539.1	-667823.0	-4.1941E-02	-82.898	-42.565	9.9281+116	

$\Delta G_4 \approx -668$ kJ

Gibbs Energy Minimization

$$
\begin{aligned}
G = & \sum_{\substack{ideal\\gas}} n_i (g_i^o + RT \ln P_i) \\
& + \sum_{\substack{pure\\condensed\\phases}} n_i g_i^o \\
& + \sum_{solution-1} n_i (g_i^o + RT \ln X_i + RT \ln \gamma_i) \\
& + \sum_{solution-2} n_i (g_i^o + RT \ln X_i + RT \ln \gamma_i) \\
& + \cdots \\
& + \cdots
\end{aligned}
$$

Where,

n_i : moles

P_i : gas partial pressure

X_i : mole fraction

γ_i : activity coefficient

g_i^o : standard molar Gibbs energy

Equilib determines the combination of n_i, P_i and X_i which minimizes the total Gibbs energy ***G*** of the system.

In the present example the equilibrium products are an ideal gas and pure solid compounds

Reactants window – entering a new reaction

Reactants window

Add a New Reactant

Reaction Table

***Equilib* has 4 windows:**

Reactants window

Menu window

List window

Results window

1st entry: Click on New Reaction

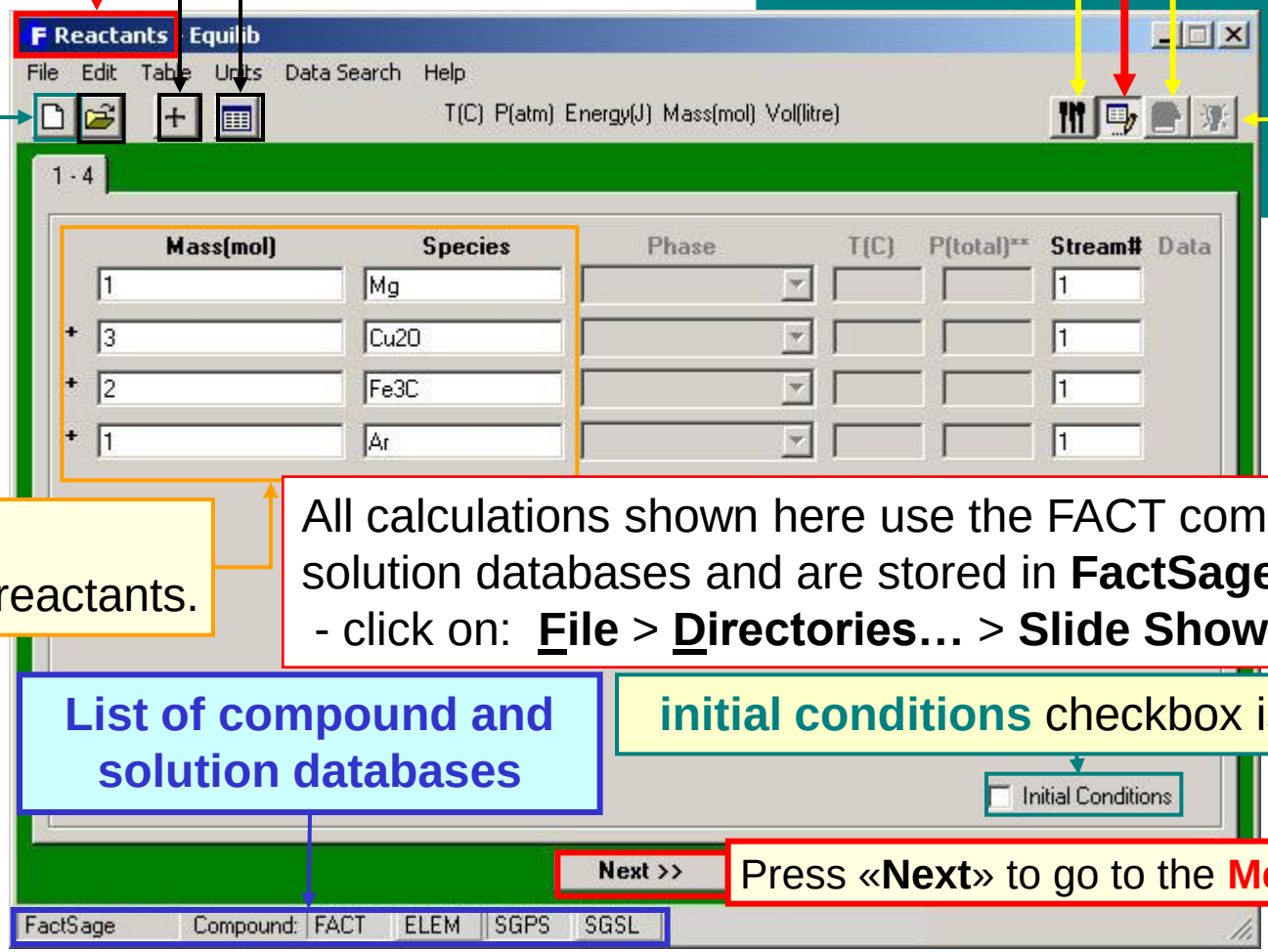
2nd entry: Define the reactants.

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

List of compound and solution databases

initial conditions checkbox is not selected

Press «**Next**» to go to the **Menu** window



Menu window – possible products, final T and P, and calculating the equilibrium

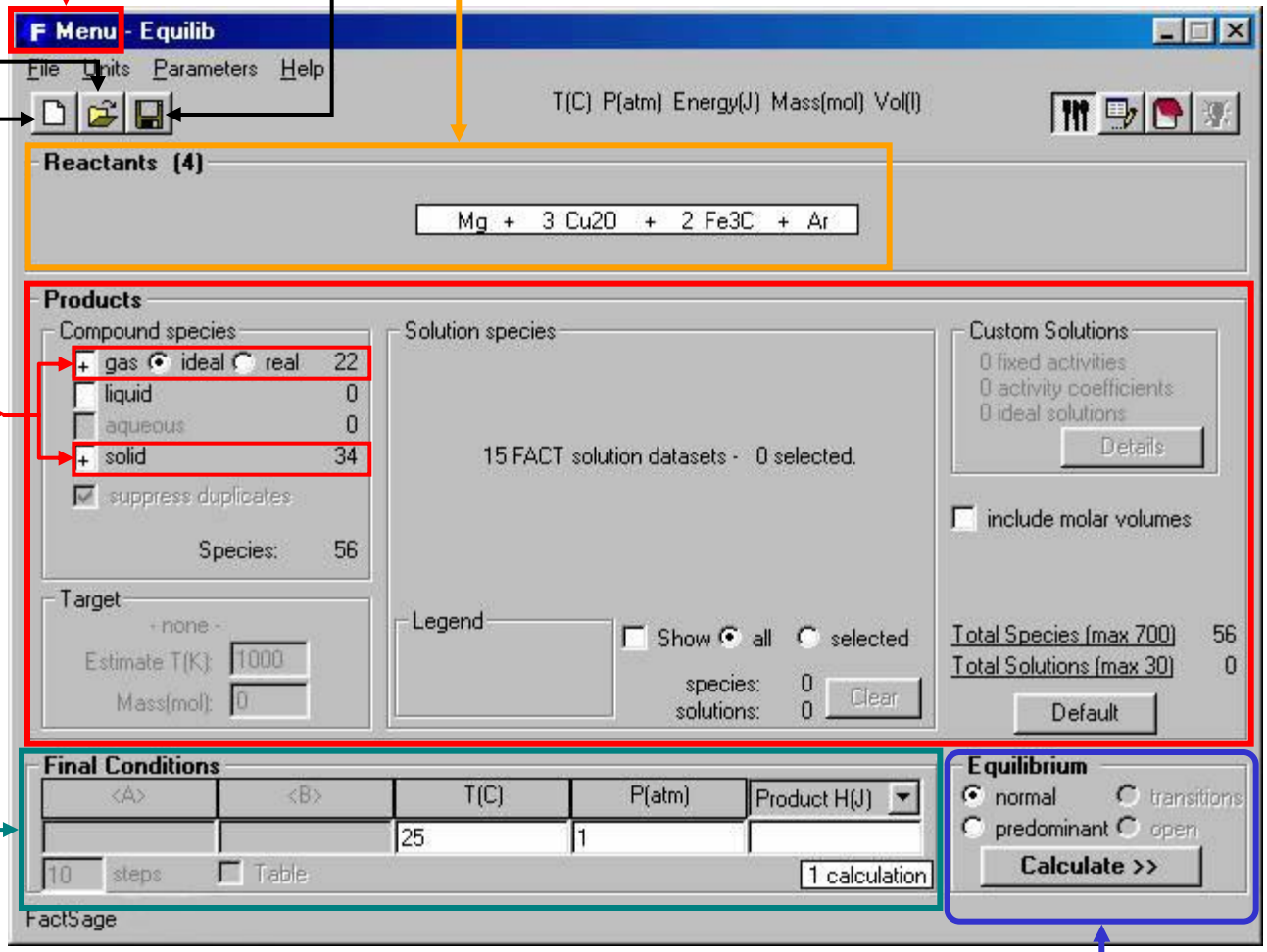
Menu window

Save

Open

New Reaction

Summary of the **Reactants**.



3rd entry:
Selection of compound products: **ideal gas phase** and **pure solids**.

4th entry:
Final conditions: **25°C**, **1 atm**.

5th. Press to **calculate** equilibrium.

Results window – *FACT* format output.

Results window

The equilibrium products: **Cu**, **Fe**, **C**, **MgO**, **Fe_3O_4** and **Ar** satisfy the **mass balance** and minimize the Gibbs energy.

1 mol (39.948g) of product **ideal** gas at 1 atm: mainly **Ar**.

Note the pure stable stoichiometric solids: activity = 1.0

Solids beyond this point are not formed: **0 mol** and **activity < 1.0** They are ordered with regard to activity.

F Results Equilib 25 C

Output Edit Show Pages

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

```
 Mg +  3 Cu2O +  2 Fe3C +  Ar =

 1.0000      mol    gas_ideal
  (39.948 gram, 1.0000 mol, 24.466 litre, 1.63
          (25.00 C, 1 atm,      a=1.0000)
          ( 1.0000              Ar
          + 1.7814E-20          CO2
          + 4.0065E-21          CO
          + 6.4396E-53          Cu
          + 2.7902E-64          Fe
          + 2.2972E-70          C3O2)

+ 6.0000      mol    Cu_solid
  (381.28 gram, 6.0000 mol)
          (25.00 C, 1 atm, S1, a=1.0000)

+ 4.5000      mol    Fe_bcc
  (251.31 gram, 4.5000 mol)
          (25.00 C, 1 atm, S1, a=1.0000)

+ 2.0000      mol    C_graphite
  (24.022 gram, 2.0000 mol)
          (25.00 C, 1 atm, S1, a=1.0000)

+ 1.0000      mol    MgO_periclase
  (40.304 gram, 1.0000 mol)
          (25.00 C, 1 atm, S1, a=1.0000)

+ 0.50000     mol    Fe3O4_magnetite
  (115.77 gram, 0.50000 mol)
          (25.00 C, 1 atm, S1, a=1.0000)

+ 0.00000     mol    C_diamond
          (25.00 C, 1 atm, S2, a=0.31007)

+ 0.00000     mol    (MgO)(Fe2O3)_solid
          (25.00 C, 1 atm, S1, a=0.26830)
```

These are mole fractions X_i , in an ideal gas: $P_i = X_i \times P_{total}$ or $P(CO_2)_{eq} = 0.17814 \times 10^{-19}$ atm.

6 mol **Cu(s1)**

4.5 mol **Fe(s1)**

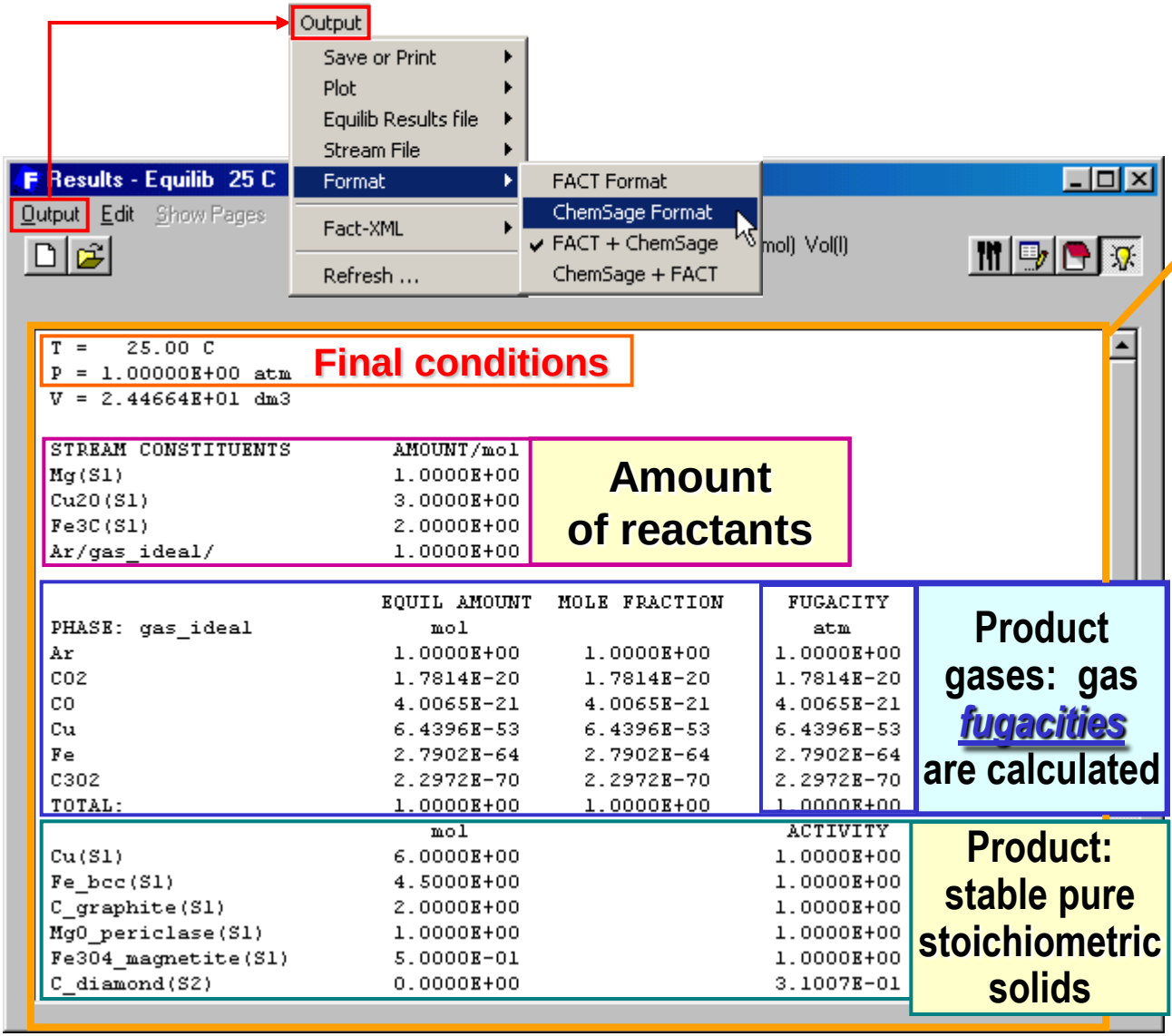
2 mol **C(s1)** [graphite]

1 mol **MgO(s1)**

0.5 mol **Fe_3O_4(s1)**

Results window – *ChemSage* format output

Menu bar: Output > Format > *ChemSage* Format




```
T =   25.00 C
P = 1.00000E+00 atm
V = 2.44664E+01 dm3

STREAM CONSTITUENTS          AMOUNT/mol
Mg(S1)                       1.0000E+00
Cu2O(S1)                     3.0000E+00
Fe3C(S1)                     2.0000E+00
Ar/gas_ideal/                1.0000E+00

                             EQUIL AMOUNT  MOLE FRACTION     FUGACITY
PHASE: gas_ideal                mol                           atm
Ar                           1.0000E+00    1.0000E+00     1.0000E+00
CO2                          1.7814E-20    1.7814E-20     1.7814E-20
CO                           4.0065E-21    4.0065E-21     4.0065E-21
Cu                           6.4396E-53    6.4396E-53     6.4396E-53
Fe                           2.7902E-64    2.7902E-64     2.7902E-64
C3O2                         2.2972E-70    2.2972E-70     2.2972E-70
TOTAL:                       1.0000E+00    1.0000E+00     1.0000E+00
                                mol                        ACTIVITY
Cu(S1)                       6.0000E+00                   1.0000E+00
Fe_bcc(S1)                   4.5000E+00                   1.0000E+00
C_graphite(S1)               2.0000E+00                   1.0000E+00
MgO_periclase(S1)            1.0000E+00                   1.0000E+00
Fe3O4_magnetite(S1)          5.0000E-01                   1.0000E+00
C_diamond(S2)                0.0000E+00                   3.1007E-01
(MgO)(Fe2O3)(S1)             0.0000E+00                   2.6830E-01
Fe_fcc(S2)                   0.0000E+00                   1.1313E-01
Fe3O4_magnetite(S2)          0.0000E+00                   3.0146E-02
FeO_wustite(S1)              0.0000E+00                   2.9862E-02
Fe2O3_hematite(S1)           0.0000E+00                   1.0536E-03
Fe3C(S1)                     0.0000E+00                   5.7017E-04
Fe3C(S2)                     0.0000E+00                   4.8652E-04
Fe2O3_hematite(S2)           0.0000E+00                   1.3826E-04
CuFeO2(S1)                   0.0000E+00                   5.1316E-09
MgCO3_magnesite(S1)          0.0000E+00                   3.5860E-09
FeCO3_siderite(S1)           0.0000E+00                   1.8979E-13
(Cu2O)(Fe2O3)(S2)            0.0000E+00                   8.9883E-17
Fe2O3_high-pressure-(S3)     0.0000E+00                   6.0428E-17
(Cu2O)(Fe2O3)(S1)            0.0000E+00                   3.8423E-17
Fe2O3_high-pressure-(S4)     0.0000E+00                   7.9278E-18
Cu2O(S1)                     0.0000E+00                   3.0689E-19
CuO_tenorite(S1)             0.0000E+00                   1.1332E-22
(CuO)(Fe2O3)(S2)             0.0000E+00                   1.8465E-26
(CuO)(Fe2O3)(S1)             0.0000E+00                   3.5212E-27
(CuO)(Fe2O3)(S3)             0.0000E+00                   9.0684E-28
Fe3O4_high-pressure-(S3)     0.0000E+00                   6.7678E-29
Fe3O4_high-pressure-(S4)     0.0000E+00                   2.0390E-30
CuCO3(S1)                    0.0000E+00                   4.7043E-43
Cu2Mg(S1)                    0.0000E+00                   6.4758E-50
Mg(S1)                       0.0000E+00                   5.0150E-56
*************************************************************************
  Cp_EQUIL       H_EQUIL        S_EQUIL        G_EQUIL        V_EQUIL
   J.K-1           J             J.K-1            J             dm3
*************************************************************************
 4.09293E+02  -1.16020E+06   5.87967E+02  -1.33550E+06   2.44664E+01

Mole fraction of the system components:
                gas_ideal
Cu               6.4396E-53
Fe               2.7902E-64
Ar               1.0000E+00
O                3.9635E-20
C                2.1821E-20

The cutoff limit for phase or gas constituent activities is 1.00E-70
```

List window – manipulating the results

List window

Final conditions

Click on **List Window**

choice of phases:

solid

and

GAS

Sorry – diamond is not formed

$a_{diamond} < 1$

Display of gas **fugacities**, for example:

$f_{CO_2} = 1.7814 \times 10^{-20}$ atm.

In an ideal gas, the **fugacity** is equal to the **partial pressure**. Hence:

$P_{CO_2} = X_{CO_2} \times P_T =$

$f_{CO_2} = 1.7814 \times 10^{-20}$ atm

format and **order***ed* with respect to moles

F List Equilib T(C) = 25, P(atm) = 1 (Page 1/1)

File Edit Help

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

+	Code	Species	Data	Phase	Mole	Fraction	Activity	Range	T	V
+	55	Cu(s)	FACT	solid	6.000		1.0000E+00	25 - 1728		
+	41	Fe(s)	FACT	bcc	4.500		1.0000E+00	25 - 1539		
+	34	C(s)	FACT	graphite	2.000		1.0000E+00	25 -		
+	16	Ar(g)	FACT	gas	1.000	1.000	1.0000E+00	25 -		
+	39	MgO(s)	FACT	periclase	1.000		1.0000E+00	25 -		
+	49	Fe3O4(s)	FACT	magnetite	0.5000		1.0000E+00	25 -		
+	11	CO2(g)	FACT	gas	1.7814E-20	1.7814E-20	1.7814E-20	25 -		
+	9	CO(g)	FACT	gas	4.0065E-21	4.0065E-21	4.0065E-21	25 -		
+	20	Cu(g)	FACT	gas	6.4396E-53	6.4396E-53	6.4396E-53	25 -		
+	17	Fe(g)	FACT	gas	2.7902E-64	2.7902E-64	2.7902E-64	25 -		
+	12	C3O2(g)	FACT	gas	2.2972E-70	2.2972E-70	2.2972E-70	25 -		
+	1	C(g)	FACT	gas			2.534E-118	25 -		
+	2	C2(g)	FACT	gas			1.108E-137	25 -		
+	3	C3(g)	FACT				6.589E-133	25 -		
+	4	C4(g)					4.622E-160	25 -		
+	5						4.092E-161	25 -		
+	6						9.4351E-86	25 -		
							1.4173E-89	25 -		
+							1.386E-162	25 -		
+							3.7908E-89	25 -		
							9.5887E-76	25 -		
							1.374E-152	25 - 5728		
+							1.444E-106	25 - 5728		
+				gas			2.7958E-83	25 - 5728		
+	15			gas			4.293E-102	25 - 5728		
+	21		FACT	gas			1.3413E-76	25 - 5728		
+	22		FACT	gas			1.2078E-93	25 - 5728		
+	35	C(s2)	FACT	diamond			3.1007E-01	25 - 2728	V	

Show
Species
gas 22 — duplicate
liquid 0 — selected 55
aqueous 0
solid 33 — All/Clear
solution 0
properties

Format: mole, gram, pound, data, distribution

Order: code, amount, fraction, activity

Post-Calculate: activity

Refresh

List window – distribution format

For example, Fe is distributed in: a gas phase: 0% as Fe(g) | 2 solid phases: 75% as Fe(s) and 25% as Fe_3O_4(s)

F List - Equilib T(C) = 25, P(atm) = 1 (Page 1/1)

File Edit Help

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

	Code		Data		Mole	Gram	Per Cent	Cumulate	T
Cu		ELEMENT Cu							
		GAS PHASE							
	20	Cu(g)			6.4396E-53	4.0921E-51	1.073E-51 %	1.073E-51 %	
				Totals	6.4396E-53	4.0921E-51	1.073E-51 %		
		PURE SPECIES							
	56	Cu(s)			6.000	381.3	100.0 %	100. %	
				Totals	6.000	381.3	100.0 %		
		TOTAL Cu			6.000	381.3			
Fe		ELEMENT Fe							
		GAS PHASE							
	17	Fe(g)			2.7902E-64	1.5582E-62	4.6503E-63 %	4.650E-63 %	
				Totals	2.7902E-64	1.5582E-62	4.6503E-63 %		
		PURE SPECIES							
	41	Fe(s)			4.500	251.3	75.00 %	75.0 %	
	50	Fe3O4(s)			1.500	83.77	25.00 %	100. %	
				Totals	6.000	335.1	100.0 %		
		TOTAL Fe			6.000	335.1			
Ar		ELEMENT Ar							
		GAS PHASE							
	16	Ar(g)			1.000	39.95	100.0 %	100. %	
				Totals	1.000	39.95	100.0 %		
		PURE SPECIES							
				Totals	0.0000	0.0000	0.0000 %		
		TOTAL Ar			1.000	39.95			

Show Specie: ga, liq, ad, so, solution 0; All None; properties

Format: mole, gram, data, distribution

Order: code, amount, fraction, activity

Post-Calculate: activity

Refresh

1. Select **distribution format**

2. Press **Refresh**

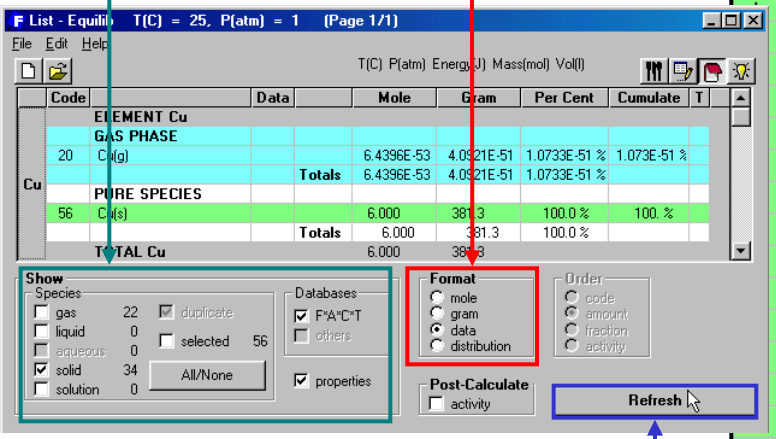
3. Scroll

	Code		Data		Mole	Gram	Per Cent	Cumulate	T
Cu		ELEMENT Cu							
		GAS PHASE							
	20	Cu(g)			6.4396E-53	4.0921E-51	1.0733E-51 %	1.073E-51 %	
				Totals	6.4396E-53	4.0921E-51	1.0733E-51 %		
		PURE SPECIES							
	56	Cu(s)			6.000	381.3	100.0 %	100. %	
				Totals	6.000	381.3	100.0 %		
		TOTAL Cu			6.000	381.3			
Fe		ELEMENT Fe							
		GAS PHASE							
	17	Fe(g)			2.7902E-64	1.5582E-62	4.6503E-63 %	4.650E-63 %	
				Totals	2.7902E-64	1.5582E-62	4.6503E-63 %		
		PURE SPECIES							
	41	Fe(s)			4.500	251.3	75.00 %	75.0 %	
	50	Fe3O4(s)			1.500	83.77	25.00 %	100. %	
				Totals	6.000	335.1	100.0 %		
		TOTAL Fe			6.000	335.1			
Ar		ELEMENT Ar							
		GAS PHASE							
	16	Ar(g)			1.000	39.95	100.0 %	100. %	
				Totals	1.000	39.95	100.0 %		
		PURE SPECIES							
				Totals	0.0000	0.0000	0.0000 %		
		TOTAL Ar			1.000	39.95			
Mg		ELEMENT Mg							
		GAS PHASE							
				Totals	0.0000	0.0000	0.0000 %		
		PURE SPECIES							
	39	MgO(s)			1.000	24.31	100.0 %	100. %	
				Totals	1.000	24.31	100.0 %		
					1.000	24.31			
O					4.0065E-21	6.4101E-20	1.3355E-19 %	1.335E-19 %	
	11	CO2(g)			3.5628E-20	5.7003E-19	1.1876E-18 %	1.321E-18 %	
	12	C3O2(g)			4.5943E-70	7.3506E-69	1.5314E-68 %	1.321E-18 %	
				Totals	3.9635E-20	6.3413E-19	1.3212E-18 %		
		PURE SPECIES							
	39	MgO(s)			1.000	16.00	33.33 %	33.3 %	
	50	Fe3O4(s)			2.000	32.00	66.67 %	100. %	
				Totals	3.000	48.00	100.0 %		
		TOTAL O			3.000	48.00			
C		ELEMENT C							
		GAS PHASE							
	9	CO(g)					0032E-19 %	2.003E-19 %	
	11	CO2(g)					9071E-19 %	1.091E-18 %	
	12	C3O2					4457E-68 %	1.091E-18 %	
				Totals	2.1821E-20	2.6209E-19	1.0910E-18 %		
		PURE SPECIES							
	34	C(s)			2.000	24.02	100.0 %	100. %	
				Totals	2.000	24.02	100.0 %		
		TOTAL C			2.000	24.02			

List window – thermodynamic data format

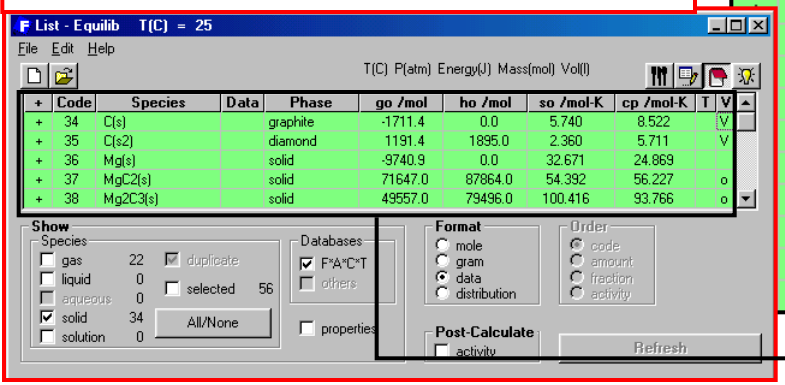
Selection:

1. **Show:** pure **solid** phases
2. **Format:** thermodynamic **data**



3. And press **Refresh**

4. To obtain the thermodynamic data format



+	Code	Species	Data	Phase	go /mol	ho /mol	so /mol-K	cp /mol-K	T	V
+	34	C(s)		graphite	-1711.4	0.0	5.740	8.522		V
+	35	C(s2)		diamond	1191.4	1895.0	2.360	5.711		V
+	36	Mg(s)		solid	-9740.9	0.0	32.671	24.869		
+	37	MgC2(s)		solid	71647.0	87864.0	54.392	56.227		o
+	38	Mg2C3(s)		solid	49557.0	79496.0	100.416	93.766		o
	39	MgO(s)		periclase	-609535.6	-601500.0	26.951	37.189		V
	40	MgCO3(s)		magnesite	-1131323.4	-1111689.0	65.854	76.208		V
	41	Fe(s)		bcc	-8133.5	0.0	27.280	24.845		
	42	Fe(s2)		fcc	-2731.2	7972.9	35.902	25.198		
	43	Fe3C(s)		solid-a	-7594.9	22593.0	101.253	107.123		
	44	Fe3C(s2)		solid-b	-7201.6	23684.5	103.593	110.936	T	
	45	FeO(s)		wustite	-283570.9	-265832.2	59.496	49.526		V
	46	Fe2O3(s)		hematite	-851696.8	-825627.4	87.437	103.980		V
	47	Fe2O3(s2)								
	48	Fe2O3(s3)								
	49	Fe2O3(s4)								
	50	Fe3O4(s)								
+	51	Fe3O4(s2)								
+	52	Fe3O4(s3)								
+	53	Fe3O4(s4)								
+	54	FeCO3(s)								
+	55	(MgO)(Fe2O								
+	56	Cu(s)								
+	57	CuO(s)								
	58	Cu2O(s)								
	59	CuCO3(s)								
	60	CuC2O4(s)								
	61	Cu2Mg(s)								
	62	CuFeO2(s)								
	63	(CuO)(Fe2O								
	64	(CuO)(Fe2O3)(s2)		solid-b	-1015832.1	-983007.1	110.096	227.191	T	o
	65	(CuO)(Fe2O3)(s3)		solid-c	-1008361.3	-963708.0	149.768	178.246	T	o
	66	(Cu2O)(Fe2O3)(s)		solid-a	-1078908.9	-1025916.8	177.736	159.991		o
	67	(Cu2O)(Fe2O3)(s2)		solid-b	-1081015.7	-1031945.3	164.583	191.990	T	o

«Absolute» values of Gibbs energy G°.

$\Delta G°$ for the reaction:

$$3\,Fe(s) + C(s) = Fe_3C(s)$$

is given by:

$$\Delta G° = G°_{Fe_3C} - [\,3G°_{Fe} + G°_{C}\,]$$

$$= -7594.9 - [\,3(-8133.5) + (-1711.4)]$$

$$= 18517 \text{ J/mol}$$

Comparison of Gibbs energy values obtained by the ***Reaction*** and the ***Equilib*** programs

F Reactants - Equilib

F Results - Equilib 25 C

Output Edit Show Pages

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

```
 Mg +  3 Cu2O +  2 Fe3C +  Ar =
 (25,l,s,#1) (25,l,s,#1) (25,l,sl,#1) (25,l,g,#1)

  1.0000     mol   gas_ideal
  (39.948 gram, 1.0000 mol, 24.466 litre, 1.6328E-03 g/ml)
          (25.00 C, 1 atm,     a=1.0000)
          ( 1.0000          Ar
          + 1.7814E-20      CO2
          + 4.0065E-21      CO
          + 6.4396E-53      Cu
          + 2.7902E-64      Fe
          + 2.2972E-70      C3O2)

+ 6.0000     mol   Cu_solid
  (381.28 gram, 6.0000 mol)
          (25.00 C, 1 atm, Sl, a=1.0000)

+ 4.5000     mol   Fe_bcc
  (251.31 gram, 4.5000 mol)
          (25.00 C, 1 atm, Sl, a=1.0000)

+ 2.0000     mol   C_graphite
  (24.022 gram, 2.0000 mol)
          (25.00 C, 1 atm, Sl, a=1.0000)

+ 1.0000     mol   MgO_periclase
  (40.304 gram, 1.0000 mol)
          (25.00 C, 1 atm, Sl, a=1.0000)

+ 0.50000    mol   Fe3O4_magnetite
  (115.77 gram, 0.50000 mol)
          (25.00 C, 1 atm, Sl, a=1.0000)

+ 0.00000    mol   C_diamond
          (25.00 C, 1 atm, S2, a=0.31007)
```

+ . . .

DELTA H (J)	DELTA G (J)	DELTA V (litre)	DELTA S (J/K)	DELTA Cp (J/K)
-6.93268E+05	-6.69706E+05	0.00000E+00	-7.90256E+01	-3.82247E+01

Specify the phase of each reactant at 25ºC and 1 atm pressure…

Thermodynamic functions: **ΔH**, **ΔG**, **ΔV**, **ΔS**, **ΔU**, **ΔA** and **Prod V**. The value of **ΔG** is the same as the ***Reaction*** program **(Reaction 1, page 3)**

tm) Energy(J) Mass(mol) Vol(l)

	T(C)	P(total)**	Stream#	Data
	25	1.0	1	FACT
	25	1.0	1	FACT
u-1 solid-a	25	1.0	1	FACT
	25	1.0	1	FACT

ic pressure above the phase.
am this is the sum of the
he species in that stream.

initial conditions

ext >>

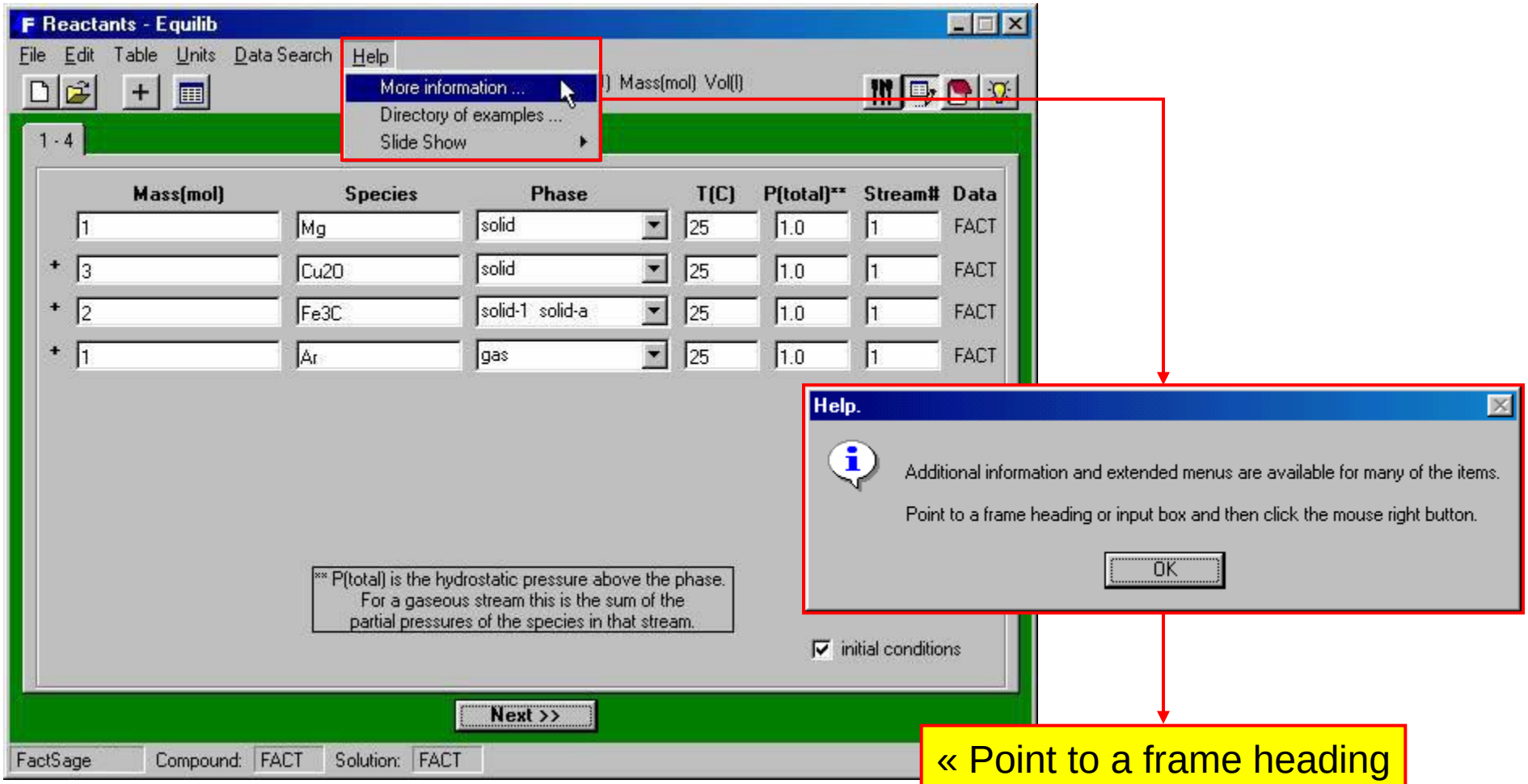
Select the initial conditions

A spontaneous isobaric isothermal chemical reaction takes place (**ΔG<0**) and the reaction is exothermic:

ΔH = - 693.3 kJ

Reactants window – Help > More information...

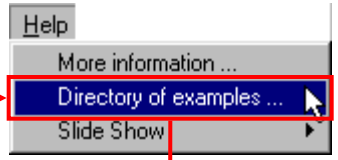
Menu bar: Help > More information...



« Point to a frame heading or input box and then click the **mouse right button**. »

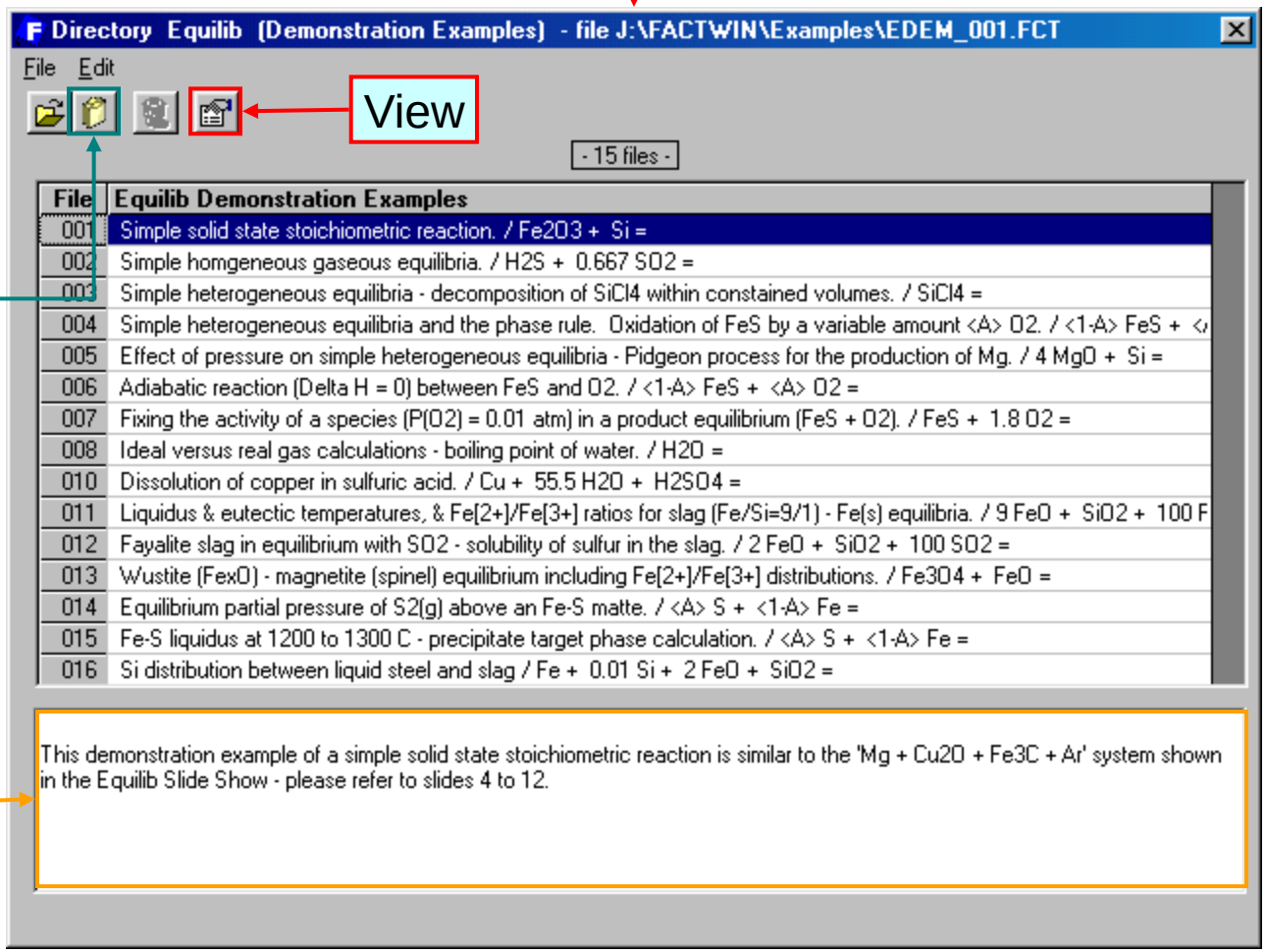
Reactants or Menu window - Help > Directory of examples...

Reactants or Menu window menu bar:
Help > **Directory of examples...**



If you want to Change Directory then go to **File > Directory >**

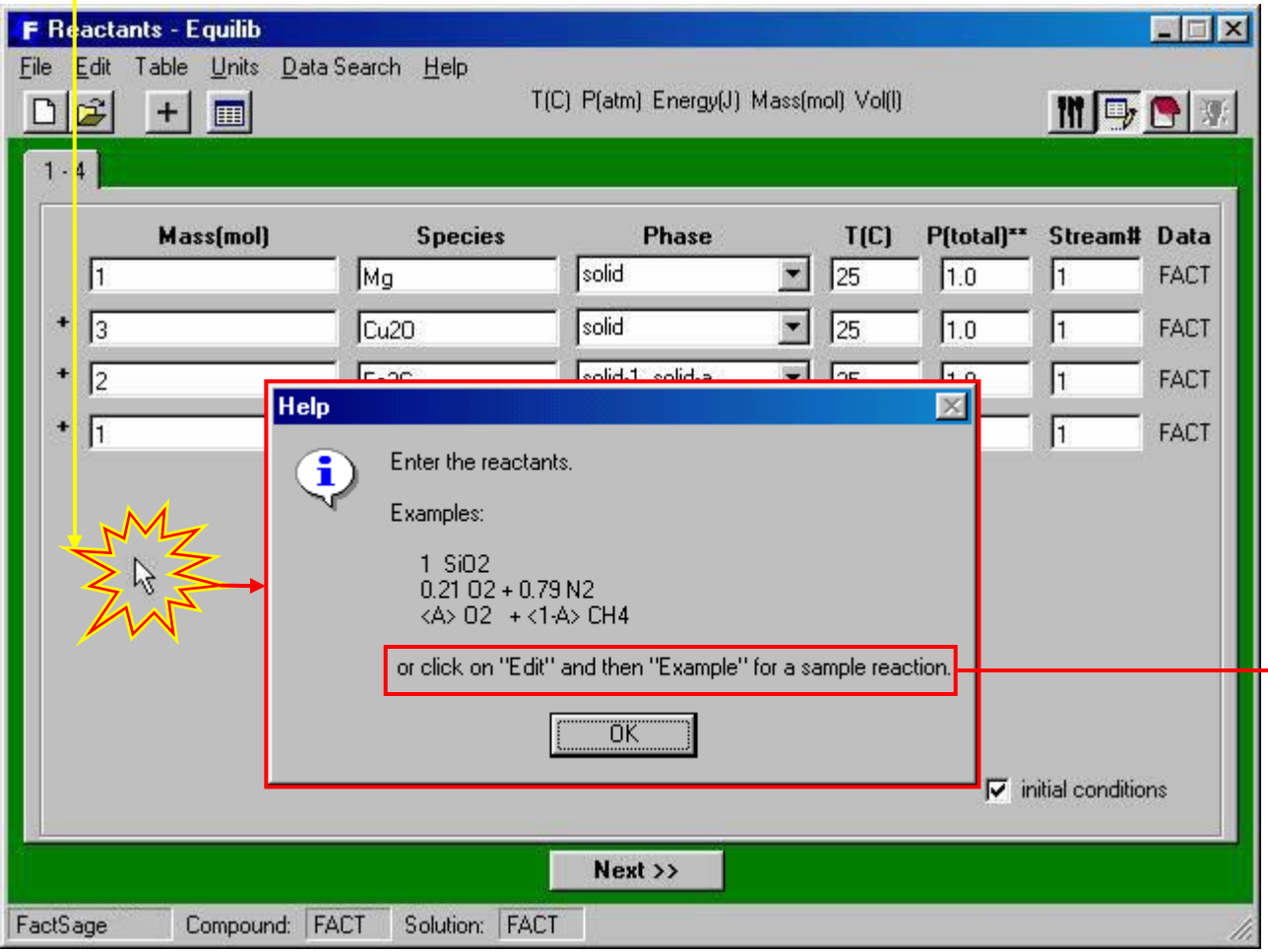
[Select a directory] or press on

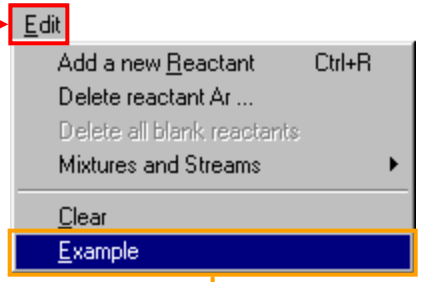


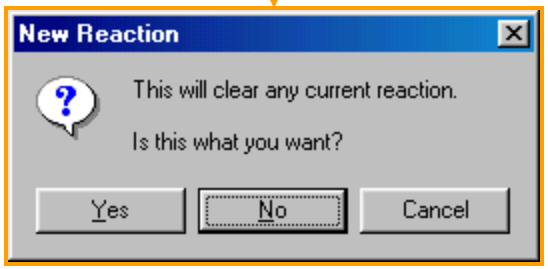
Short description of the example

The mouse right button - Reactants

Click with the mouse right button

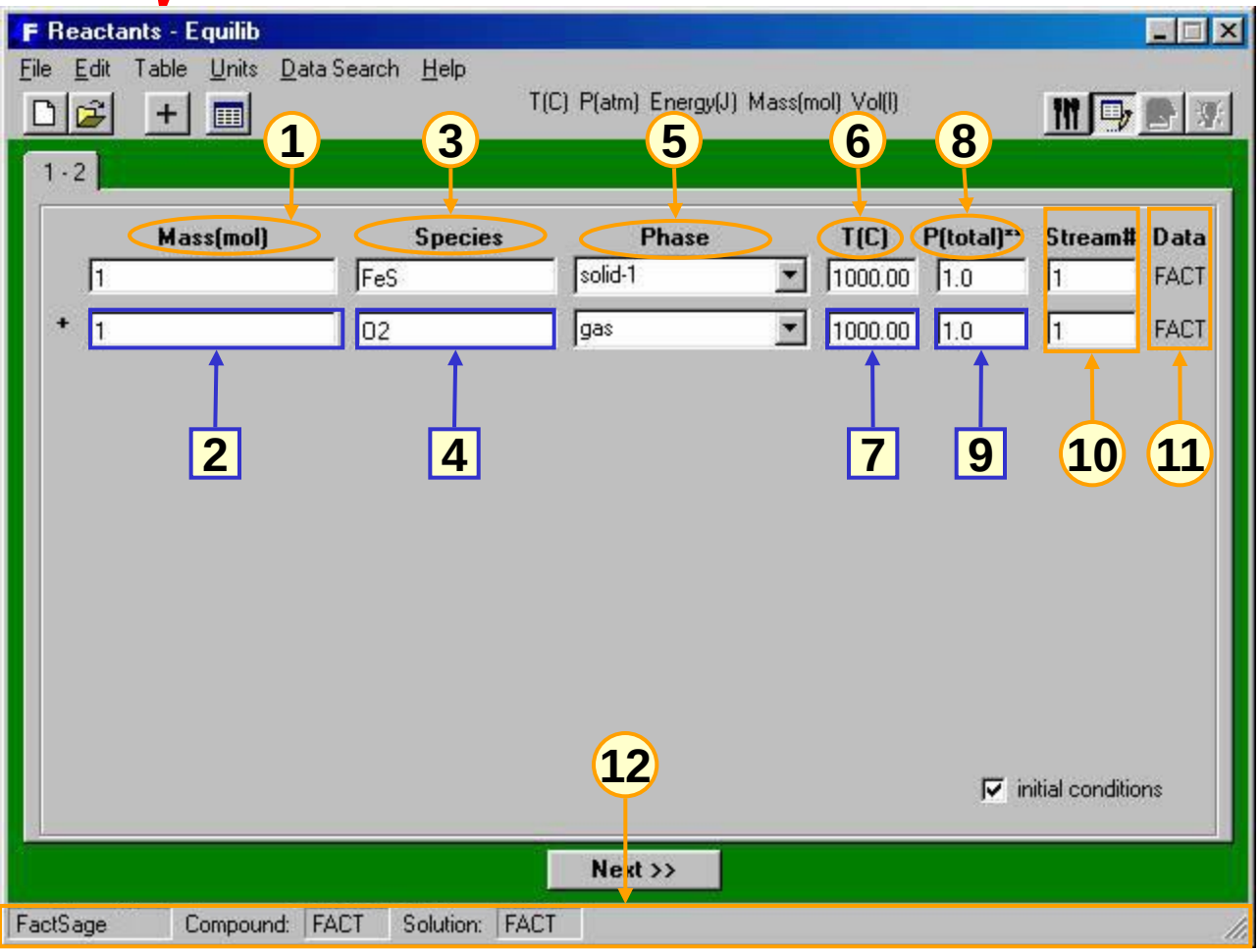






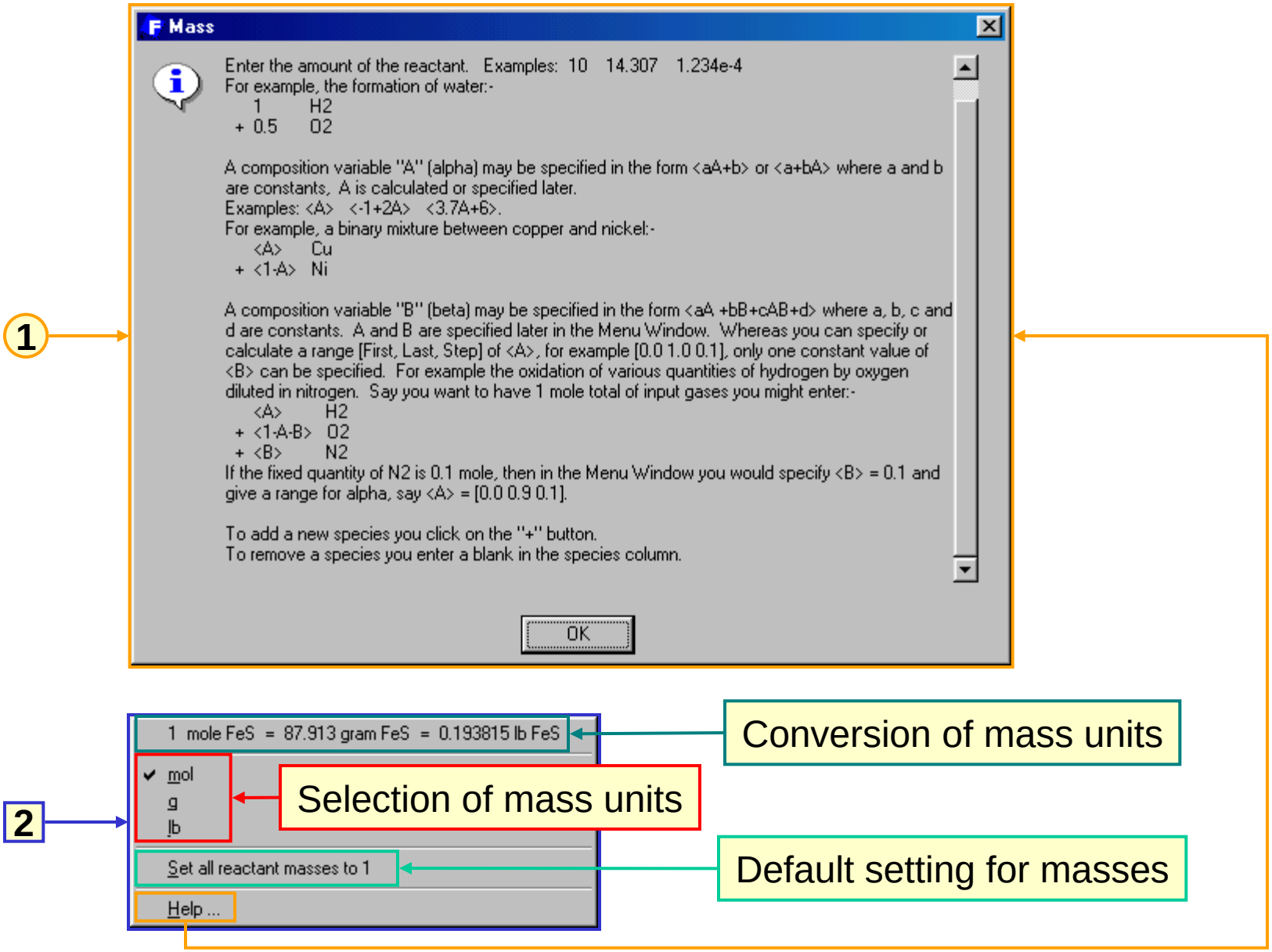
Help: – the **mouse right button**

Click with the **mouse right button** in the enclosed areas: header or input box and information boxes will appear.



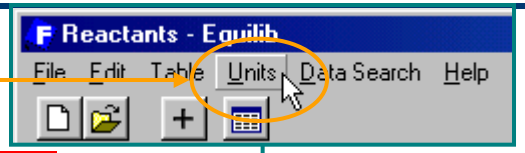
1. **Mass** info
2. **Mass** units
3. **Species** info
4. **Species** access to ViewData
5. **Phase**
6. **Temperature** info
7. **Temperature** units
8. **Pressure** info
9. **Pressure** units
10. **Stream number** info
11. **Data** info
12. **Databases** info

Help – Example of mouse right button, Mass: 1. Header and 2. Input Box



Units window: T,P, Energy, Mass and Volume

Reactants Menu bar: Units >



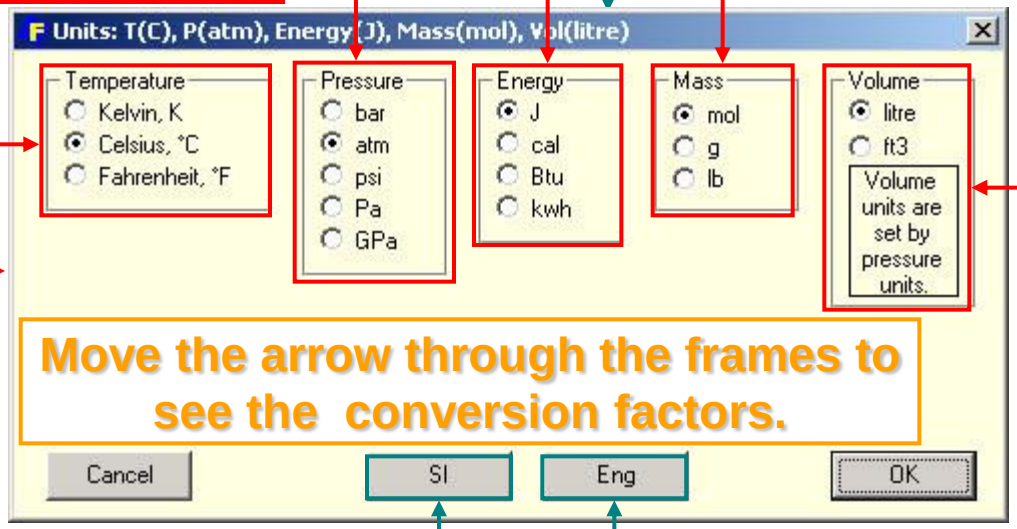

```
Energy:
1 J       = 1/4.184 cal        = 1/1055.06 BTU      = 1/3.6e6 kwh
4.184 J   = 1 cal              = 4.184/1055.06 BTU  = 4.184/3.6e6 kwh
1055.06J  = 1055.06/4.184 cal  = 1 BTU              = 1055.06/3.6e6 kwh
3.60e6 J  = 3.60e6/4.184 cal   = 3.6e6/1055.06 BTU  = 1 kwh
```

```
Mass:
1 gram   =  0.00220462262 lb
1 lb     =  453.59237 gram
```

```
Pressure:          1 GPa        = 10^9 Pa
1 bar            = 100000 Pa    = 1/1.01325 atm      = 1/0.06894757 psi
0.00001 bar      = 1 Pa         = 1/101325 atm       = 1/6894.757   psi
1.01325 bar      = 101325 Pa    = 1 atm        = 1.01325/0.06894745 psi
0.06894757 bar   = 6894.757 Pa  = 0.06894757/1.01325 atm        = 1 psi
```

```
Volume:
1 litre              = 1/28.316847 Ft3
28.316847 litre      = 1 Ft3
```

```
Temperature:
TK                    = TC + 273.15   = (TF - 32)/1.8 + 273.15
TK - 273.15           = TC            = (TF - 32)/1.8
1.8*(TK-273.15) +32   = 1.8*TC + 32   =  TF
```




```
Universal gas constant:
R = 8.314510 J/mol-K
  = 8.314510/4.184 cal/mol-K
  = 22.4141/273.15 l-atm/mol-K
```

Move the arrow through the frames to see the conversion factors.

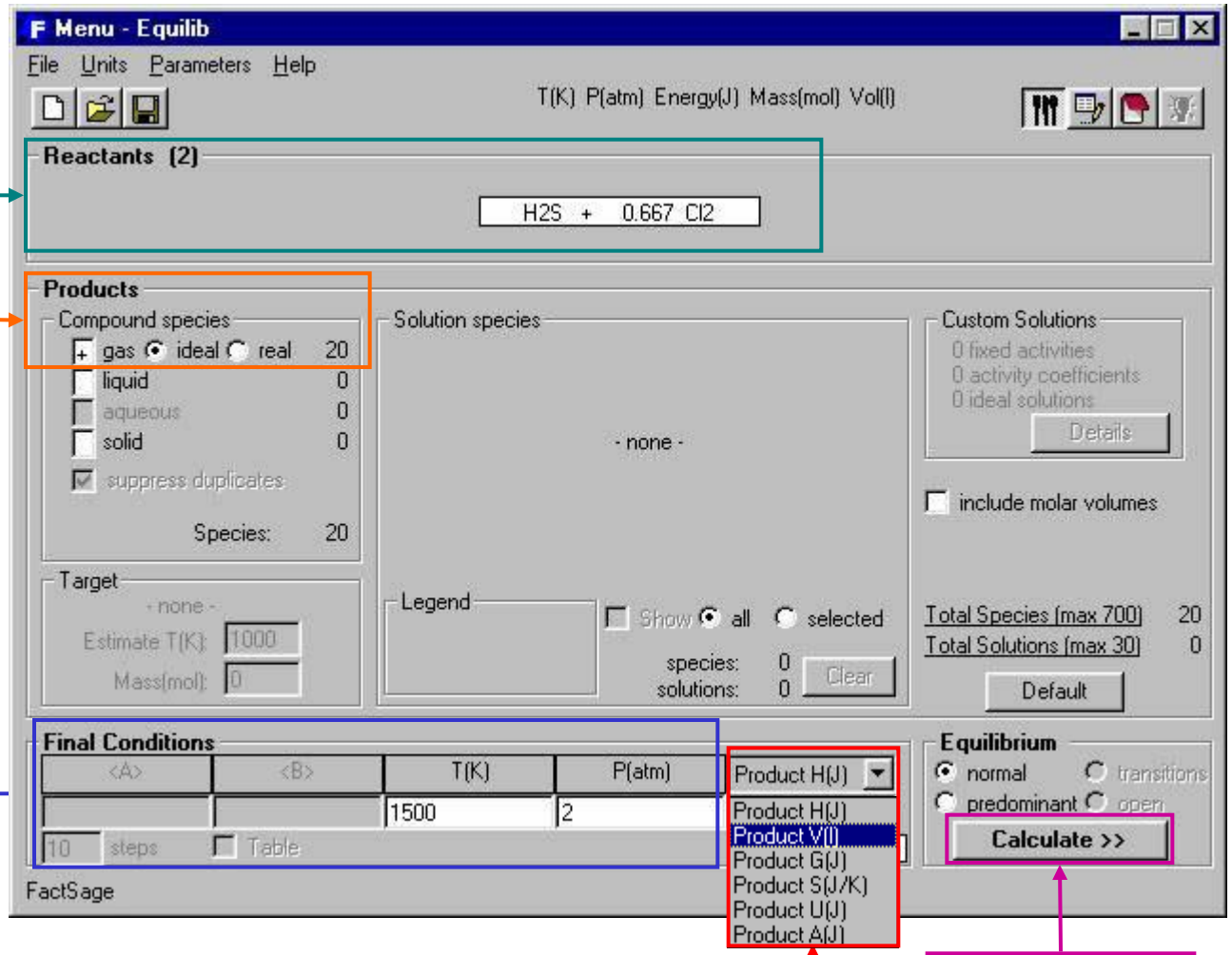
```
SI units:

T(K), P(bar), Energy(J), Mass(mol), Volume(litre)
```

```
English units:

T(F), P(psi), Energy(BTU), Mass(lb), Volume(Ft3)
```

Homogeneous Gaseous Equilibria

Reacting H_2S with Cl_2

Products selection: **ideal gas** solution phase



Product **T= 1500 K** and **P=2 atm**

Drop-down menu for **extensive property**

Press «**Calculate**»

$H_2S + Cl_2 =$ Results window, *FACT* Format Output

F Results - Equilib 1500 K

Output Edit Show Pages

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

```
H2S +  0.667 Cl2 =

 2.0492      mol    gas_ideal
 (81.376 gram, 2.0492 mol, 126.11 litre, 6.4525E-04 g/ml)
         (1500.00 K, 2.0000 atm,      a=1.0000)
         ( 0.65092          HCl
         + 0.18447          S2
         + 0.11109          H2S
         + 4.9336E-02       H2
         + 1.5653E-03       HS
         + 1.3313E-03       H2S2                                   T
         + 1.1825E-03       S3
         + 3.8066E-05       S2Cl
         + 2.9188E-05       Cl
         + 2.3553E-05       S4
         + 1.2399E-05       S
         + 2.7491E-06       H
         + 9.7369E-07       SCl
         + 5.0530E-07       Cl2
         + 3.1353E-07       SCl2
         + 7.4550E-08       S5
         + 1.5872E-08       ClSSCl
         + 6.7778E-09       S6
         + 3.4417E-10       S7
         + 3.2114E-12       S8)

The cutoff concentration has been specified to 1.0000E-75

Data on 1 product species identified with "T" have been extrapolated

*****************************************************************
      H            G            V            S            Cp
     (J)          (J)        (litre)      (J/K)        (J/K)
*****************************************************************
 4.48414E+03 -7.62454E+05  1.26115E+02  5.11292E+02  1.08034E+02
```

Total pressure P_{total} = 2.0 atm

Mole fraction X_{HCl} = 0.65092

$\Rightarrow P_{HCl} = X_{HCl} \times P_{total} = 1.30184$ atm

List window – Help >

List - Equilib T(K) = 1500, P(atm) = 2 (Page 1/1)

File Edit Help

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

+	Code	Species	Data	Phase	Mole	Fraction	Activity	Range	T	V
+	1	H(g)		gas	5.6334E-06	2.7491E-06	5.4981			
+	2	H2(g)		gas	0.1011	4.9336E-02	9.8672			
+	3	S(g)		gas	2.5409E-05	1.2399E-05	2.4799			
+	4	S2(g)		gas	0.3780	0.1845	3.6895			
+	5	S3(g)		gas	2.4231E-03	1.1825E-03	2.3649			
+	6	S4(g)		gas	4.8265E-05	2.3553E-05	4.7106			
+	7	S5(g)		gas	1.5277E-07	7.4550E-08	1.4910			
+	8	S6(g)		gas	1.3889E-08	6.7778E-09	1.3556			
+	9	S7(g)		gas	7.0527E-10	3.4417E-10	6.8834			
+	10	S8(g)		gas	6.5808E-12	3.2114E-12	6.4228E-12	298 - 6001		
+	11	HS(g)		gas	3.2077E-03	1.5653E-03	3.1307E-03	298 - 6001		
+	12	H2S(g)		gas	0.2276	0.1111	2.2217E-01	298 - 6001		v
+	13	H2S2(g)		gas	2.7282E-03	1.3313E-03	2.6627E-03	298 - 1001	T	
+	14	Cl(g)		gas	5.9812E-05	2.9188E-05	5.8376E-05	298 - 6001		
+	16	HCl(g)		gas	1.334	0.6509	1.3018E+00	298 - 6001		v
+	17	SCl(g)		gas	1.9953E-06	9.7369E-07	1.9474E-06	298 - 6001		
+	18	S2Cl(g)		gas	7.8004E-05	3.8066E-05	7.6131E-05	298 - 6001		
+	19	SCl2(g)		gas	6.4248E-07	3.1353E-07	6.2705E-07	298 - 6001		
+	20	ClSSCl(g)		gas	3.2524E-08	1.5872E-08	3.1743E-08	298 - 1501		
	21	S(liq)		liquid				298 - 1500		
	22	H2S2(liq)		liquid				240 - 314	T	

"+" denotes species or phase is selected as a possible product. Other options are available. Click right button for more …

Show

Species

- ☑ gas 20
- ☑ liquid 0
- ☐ aqueous 0
- ☑ solid 0
- ☑ solution 0

☑ duplicate

☐ selected 20

All/None

☑ properties

Format

- (•) mole
- ( ) gram
- ( ) pound
- ( ) data
- ( ) distribution

Order

- (•) code
- ( ) amount
- ( ) fraction
- ( ) activity

Post-Calculate

☐ activity

Refresh

Help

Additional information and extended menus are available.

Point to a frame heading ("Show", "Format" etc.) then click the mouse right button.

OK

…and go to the next slide

Point to a frame heading or input box, a message box appears and then click the **mouse right button**

Help – Another example of the use of the **mouse right button**

"+" Column

" + " denotes the species or phase is selected as a possible product.

To add or remove species, set target phases, define activities, specify ideal solutions, etc. go to Menu Window, point to the gas, liquid, aqueous or solid compound group or to the solution "+" column, and then click with the mouse right button to get the extended menu.

OK

1

Menu - Equilib

File Units Parameters Help

T(K) P(atm) Energy(

Reactants (2)

H2S + 0.667 Cl2

Products

Compound species

+ gas ideal real 20

liquid 0

suppress duplicates

Species: 20

Solution species

Click mouse right button to custom select species for gas species

2

3

12 H2S(g)

- clear

✔ + - select

✔ - standard stable phase

! - dormant (metastable) phase

F - formation target phase

P - precipitate target phase

S - Scheil cooling gas phase

C - composition target ...

Ideal Solution

a Activity

Help ...

Equilibrium Values

Miscellaneous data

Standard State Data

✔ activity

mole

gram

mole fraction

wt. per cent

All equilibrium values

T(K) = 1500, P(atm) = 2 (Page 1/1)

File Edit Show Sort

Selected: 20/20

GAS

+	Code	Species	Data	Phase	T	V	Activity
+	1	H(g)		gas			5.4981E-06
+	2	H2(g)		gas			9.8672E-02
+	3	S(g)		gas			2.4799E-05
+	4	S2(g)		gas			0.3689
+	5	S3(g)		gas			2.3649E-03
+	6	S4(g)		gas			4.7106E-05
+	7	S5(g)		gas			1.4910E-07
+	8	S6(g)		gas			1.3556E-08
+	9	S7(g)		gas			6.8834E-10
+	10	S8(g)		gas			6.4228E-12
+	11	HS(g)		gas			3.1307E-03
+	12	H2S(g)		gas			0.2222
+	13	H2S2(g)		gas	T		2.6627E-03
+	14	Cl(g)		gas			5.8376E-05
+	15	Cl2(g)		gas			[illegible]
+	16	[illegible]		[illegible]			[illegible]
+	17	SCl(g)		gas			1.9474E-06
+	18	S2Cl(g)		gas			7.6131E-05
+	19	SCl2(g)		gas			6.2705E-07

Click mouse right button for extended menu on H2S(g)

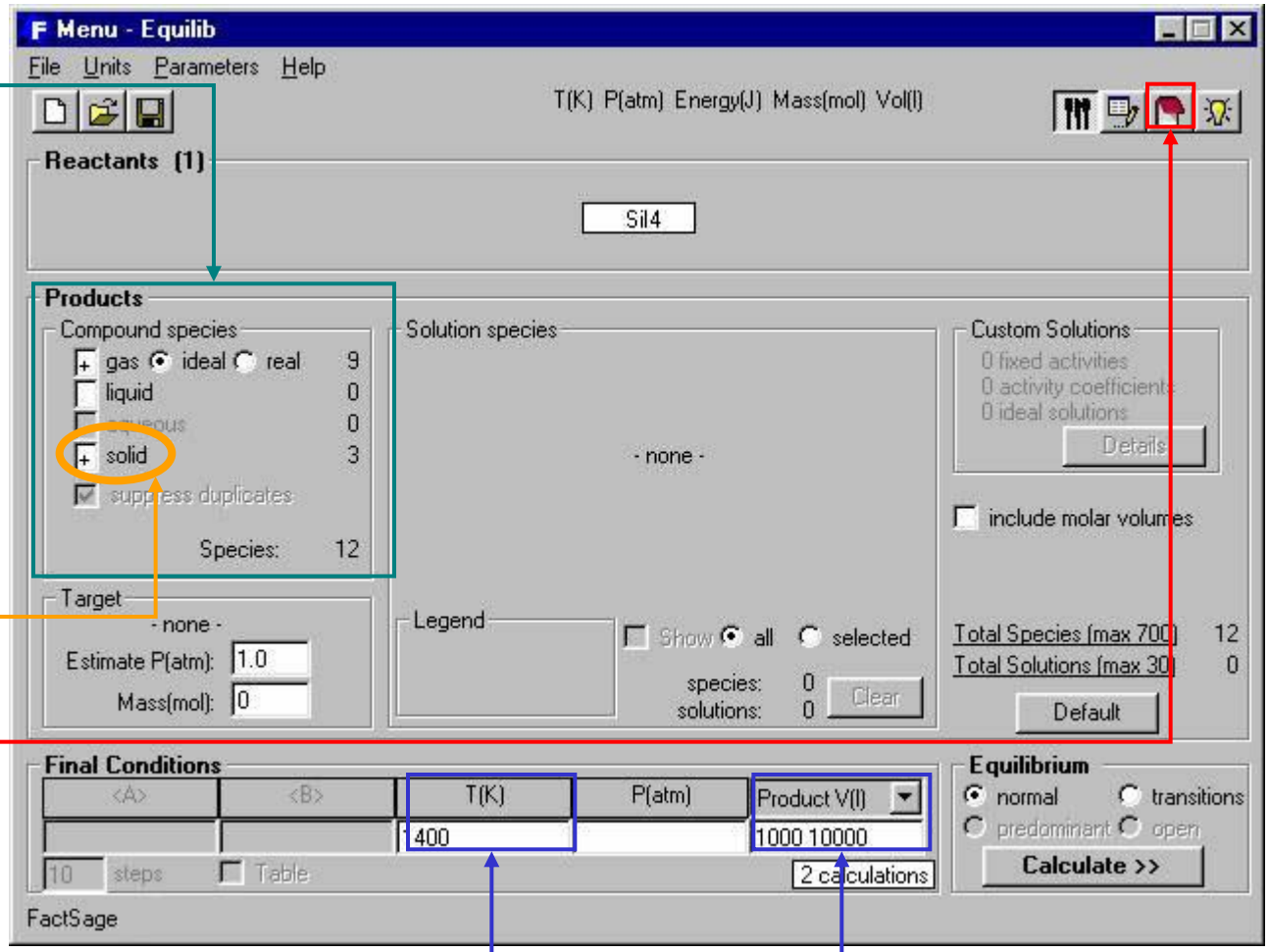
Click ... species. For a ... or {Del}.

To get all the information you need about the extended menu

Simple heterogeneous **equilibrium**: thermal decomposition of SiI_4

Species selection for the thermal decomposition of SiI_4: an **ideal** solution **gas** phase and **pure solids** are selected as possible **products**.

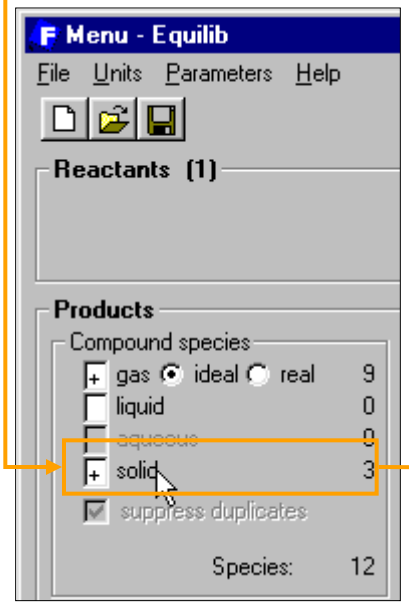
To view a list of the species selected before computation and specify a **pure solid Si** phase instead of **3 pure solids**, **click the mouse right button** at a «**Compound species**» **input box** or press the «**List Window**» **button**

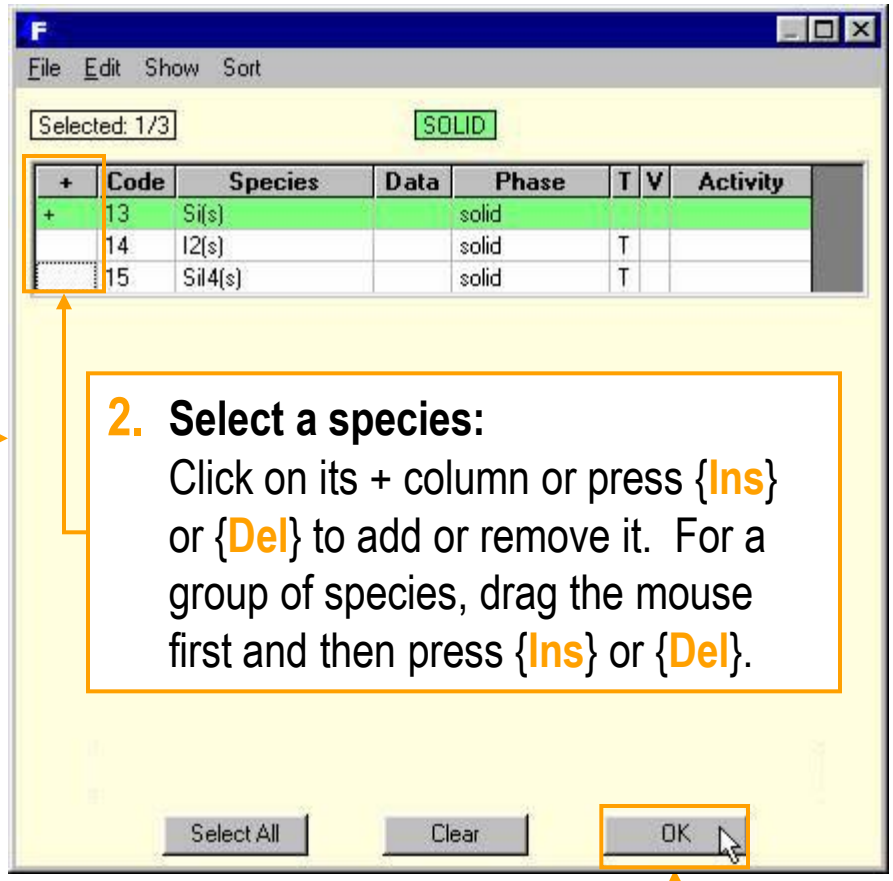


Computations are at **1400 K** for two fixed volumes: **1000** and **10000 litres**.

Custom selection of product species: a short-cut

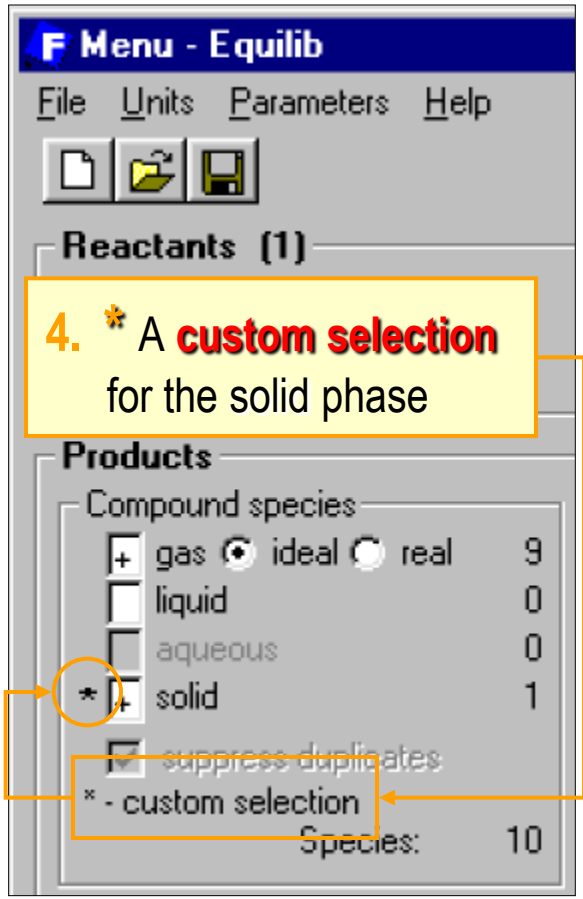
1. Click with mouse right button.





2. Select a species:
Click on its + column or press {Ins} or {Del} to add or remove it. For a group of species, drag the mouse first and then press {Ins} or {Del}.

3. Press «OK»



4. * A **custom selection** for the solid phase

The **Selection** Window

File
- Save As ... Ctrl+S
- Print Ctrl+P
- Print Setup ...
- Print Font ...
- Close

Edit
- Copy Ctrl+C
- Find Ctrl+F
- Find Next F3

File Edit Show Sort

Selected: 1/3 SOLID

+	Code	Species	Data	Phase	T	V	Activity
+	13	Si(s)		solid			
	14	I2(s)		solid	T		
	15	SiI4(s)		solid	T		

Click on its + column (or press {Ins} or {Del}) to add or remove a species.
For a group of species 'drag' the mouse first and then press {Ins} or {Del}.

Select All Clear OK

Sort
- Descending order
- Ascending order
  - Code
  - Activity

You can also double click on the column header to sort the list.

Add columns to the list filled with the data you have requested or calculated.

Show
- ✔ Tips
- Equilibrium Values
- Standard State Data
- Miscellaneous data

Equilibrium Values
- ✔ activity
- mole
- gram
- mole fraction
- wt. per cent
- All equilibrium values

Miscellaneous data
- Cp(TK)
- density
- molar volume
- molecular weight
- All miscellaneous data

Standard State Data
- T(K) = 1400
- Specify T(K) ...
- go J/mol
- ho J/mol
- so J/mol-K
- cp J/mol-K
- All standard state data

Standard State Temperature

Enter the temperature (K)

OK Cancel

Note: Your last selection becomes a default setting.

Results window – 1400 K, 1000 L for SiI_4

First tab [page 1/2] (**selected**): 0.2281 atm

F Results - Equilib 0.228 atm, V = 1.000E+03 (page 1/2)

Output Edit Show Pages

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

0.228 atm, V = 1.000E+03 | 3.529E-02 atm, V = 1.000E+04

```
SiI4 =

 1.9858      mol    gas_ideal
 (535.70 gram, 1.9858 mol, 1000.0 litre, 5.3570E-04 g/ml)
         (1400.00 K, 0.22813 atm,      a=1.0000)
         ( 0.42828          I
         + 0.27390          SiI2
         + 0.21293          SiI4
         + 6.8138E-02       I2
         + 1.6751E-02       SiI3
         + 2.0181E-06       SiI
         + 1.9315E-09       Si
         + 6.2299E-13       Si2
         + 4.9018E-14       Si3)

+ 0.00000     mol    Si_solid
         (1400.00 K, 0.22813 atm, Sl, a=0.53366)

The cutoff concentration has been specified to 1.0000E-75

*****************************************************************************
      H            G            V            S            Cp
     (J)          (J)        (litre)      (J/K)        (J/K)
*****************************************************************************
 2.16076E+05 -8.40003E+05  1.00000E+03  7.54342E+02  1.61507E+03

Total mass/gram = 535.70
```

Fixed volume: **1000 L**

Second tab: 3.529E-02 atm [page 2/2]

Decomposition of SiI_4 at **lower vapor pressures**

V = **1000 L**
T = **1400 K**, P = 0.22813 atm
0 mol (no Si(s) formed)
activity < 1

F Results - Equilib 0.228 atm, V = 1.000E+03 (page 1/2)

Output Edit Show Pages

T(K) P(atm) Energy(J) Mass(mol) V

0.228 atm, V = 1.000E+03 | 3.529E-02 atm, V = 1.000E+04

```
SiI4 =

 1.9858      mol    gas_ideal
 (535.70 gram, 1.9858 mol, 1000.0 litre, 5.3570E-04
          (1400.00 K, 0.22813 atm,      a=1.0000)
          ( 0.42828          I
          + 0.27390          SiI2
          + 0.21293          SiI4
          + 6.8138E-02       I2
          + 1.6751E-02       SiI3
          + 2.0181E-06       SiI
          + 1.9315E-09       Si
          + 6.2299E-13       Si2
          + 4.9018E-14       Si3)

+ 0.00000     mol    Si_solid
          (1400.00 K, 0.22813 atm, Sl, a=0.53366)

The cutoff concentration has been specified to 1.0000E-75

*****************************************************************
      H            G            V            S            Cp
     (J)          (J)        (litre)      (J/K)        (J/K)
*****************************************************************
 2.16076E+05 -8.40003E+05  1.00000E+03  7.54342E+02  1.61507E+03

Total mass/gram = 535.70
```

F Results - Equilib 3.529E-02 atm, V = 1.000E+04 (page 2/2)

Output Edit Show Pages

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

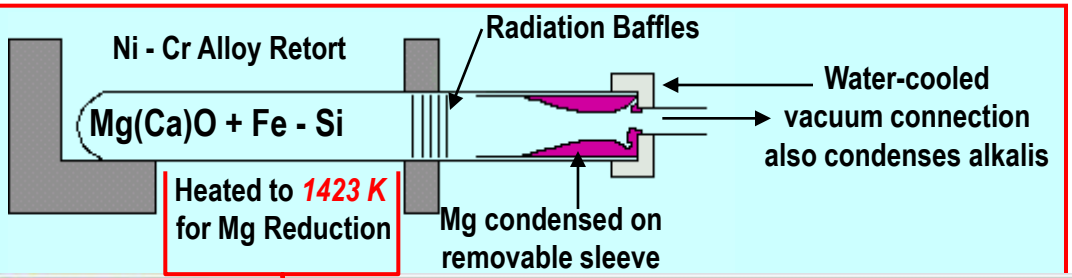
0.228 atm, V = 1.000E+03 | - 3.529E 02 atm, V = 1.000E+04 -

```
SiI4 =

 3.0718      mol    gas_ideal
 (528.66 gram, 3.0718 mol, 10000. litre, 5.2866E-05 g/ml)
          (1400.00 K, 3.5290E-02 atm,      a=1.0000)
          ( 0.72583          I
          + 0.22804          SiI2
          + 3.0275E-02       I2
          + 1.2185E-02       SiI4
          + 3.6564E-03       SiI3
          + 6.4089E-06       SiI
          + 2.3397E-08       Si
          + 1.4141E-11       Si2
          + 2.0849E-12       Si3)

+ 0.25082     mol    Si_solid
 (7.0444 gram, 0.25082 mol)
          (1400.00 K, 3.5290E-02 atm, Sl, a=1.0000)

The cutoff concentration has been specified to 1.0000E-75

*****************************************************************
      H            G            V            S            Cp
     (J)          (J)        (litre)      (J/K)        (J/K)
*****************************************************************
 4.16535E+05 -8.95027E+05  1.00000E+04  9.36830E+02  8.95592E+02
```

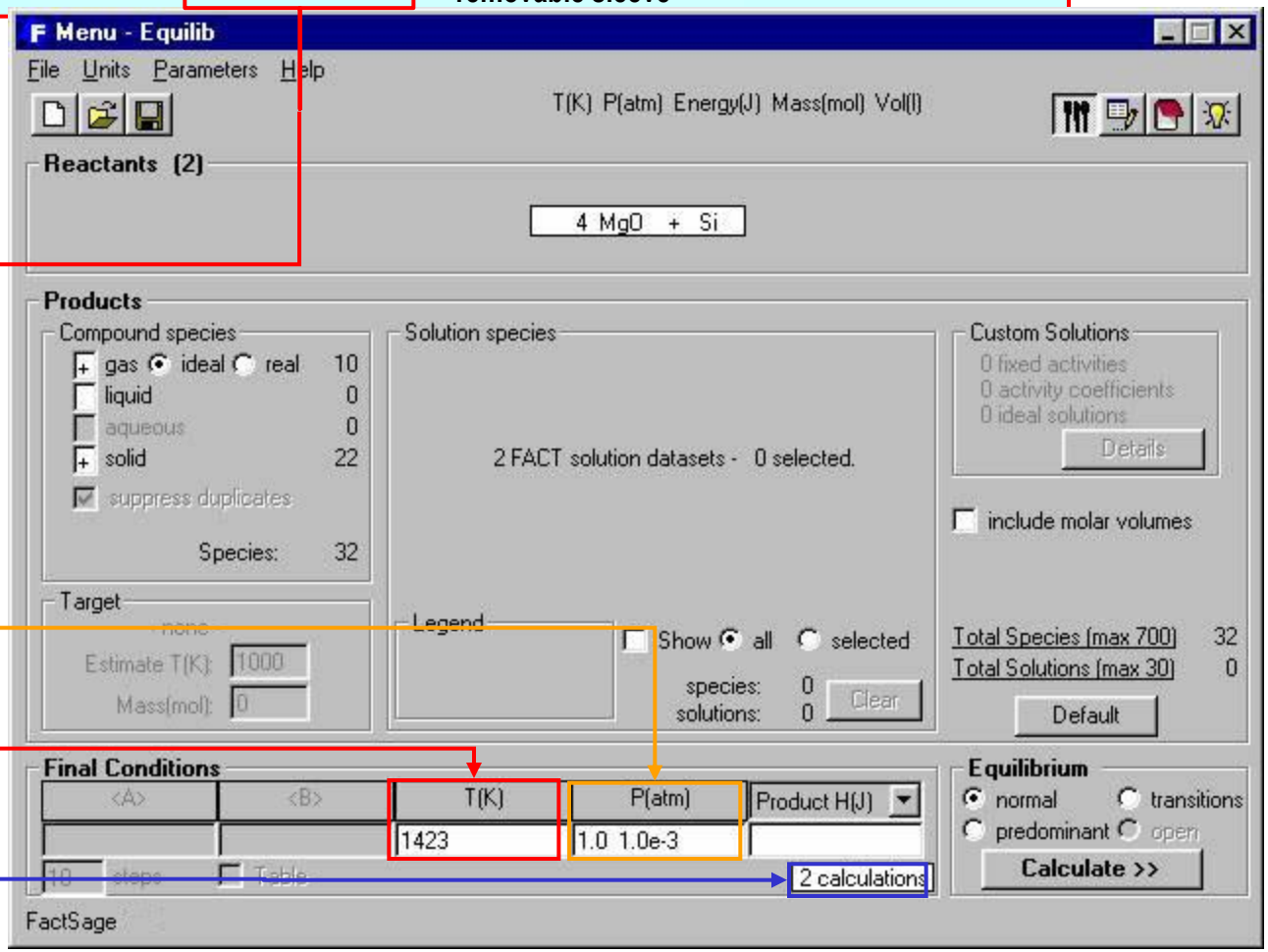
V = **10000 L**
T = **1400 K**, P = 0.03529 atm
0.25082 mol Si(s) formed
activity = 1

Effect of Pressure on Simple Heterogeneous Equilibria:

Pidgeon Process for the Production of Magnesium:
Apparatus Schema



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



Final Conditions:

two different pressures
and
one temperature
result in
2 calculations

Reacting MgO with Si at 1 atm – no reaction

Reactants

0 mol of gas, however X_{Mg} = **1.0876×10^{-3}** and P_{total} = **1 atm**, hence $P_{Mg_{eq}}$ = **1.0876×10^{-3} atm**

F Results - Equilib 1 atm (page 1/2)

Output Edit Show Pages

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

1 atm | 1.000E-03 atm

```
4 MgO +  Si  =

  0.00000     mol    gas_ideal
            (1423.00 K, 1 atm,
            ( 1.0876E-03        Mg
            + 9.3098E-06        SiO
            + 1.5326E-09        Si
            + 3.5933E-10        Mg2
            + 1.1163E-12        Si2
            + 1.7377E-13        Si3
            + 2.2478E-15        MgO
            + 9.2704E-20        O
            + 4.7988E-27        O2
            + 4.9979E-49        O3)

+ 4.0000      mol    MgO_periclase
  (161.22 gram, 4.0000 mol)
            (1423.00 K, 1 atm, S1, a=1.0000)

+ 1.0000      mol    Si_solid
  (28.086 gram, 1.0000 mol)
            (1423.00 K, 1 atm, S1, a=1.0000)

+ 0.00000     mol    Mg2SiO4_forsterite
            (1423.00 K, 1 atm, S1, a=1.0000)

+ 0.00000     mol    MgSiO3_proto-enstatite
            (1423.00 K, 1 atm, S3, a=9.1316E-02)
```

a=1.0969E-03)

Products

$\Sigma P_{gas\ species}$ = **1.0969×10^{-3} atm**

No reaction takes place because the pressure (1 atm) is too *high* for the gas phase

Note: **Unit** activity but **0 mol**. i.e. it is **«thermodynamically ready»** to form.

MgO and Si reaction at a reduced total pressure

The gas phase is stable under a reduced total pressure.

X_{Mg}= 0.99151 and P_{total}= 0.001 atm, hence $P_{Mg_{eq}}$= 9.91×10^{-4} atm

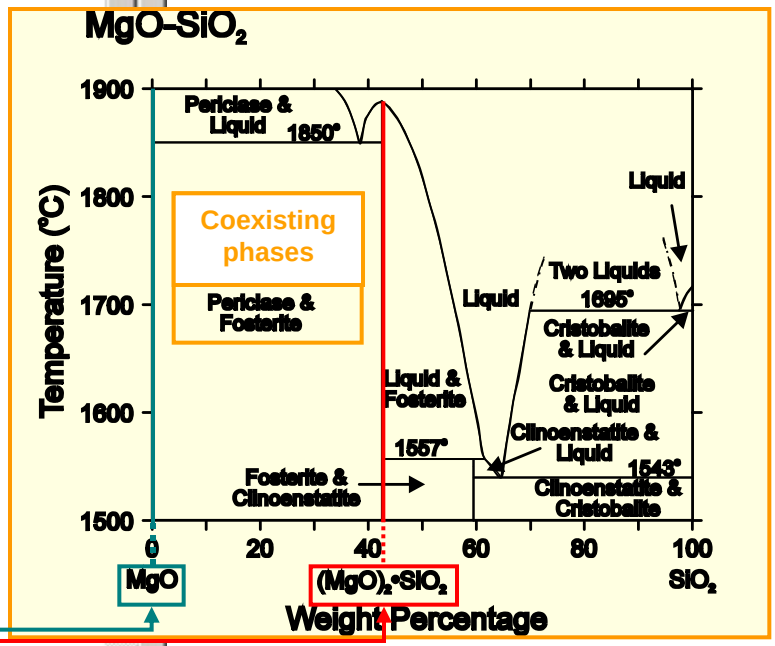
F Results - Equilib 1.000E-03 atm (p

Output Edit Show Pages

1 atm - 1.000E-03 atm -

```
4 MgO +  Si =

 2.0000      mol    gas_ideal
 (48.946 gram, 2.0000 mol, 2.3354E+05 litre, 2.0958E-07 g/ml)
         (1423.00 K, 1.0000E-03 atm,      a=1.0000)
         ( 0.99151          Mg
         + 8.4873E-03       SiO
         + 1.2737E-06       Si
         + 2.9864E-07       Mg2
         + 7.7103E-10       Si2
         + 9.9754E-11       Si3
         + 2.2478E-12       MgO
         + 1.0169E-16       O
         + 5.7741E-24       O2
         + 6.5965E-46       O3)

+ 0.98302     mol    Mg2SiO4_forsterite
  (138.30 gram, 0.98302 mol)
         (1423.00 K, 1.0000E-03 atm, Sl, a=1.0000)

+ 5.0934E-02 mol    MgO_periclase
  (2.0528 gram, 5.0934E-02 mol)
         (1423.00 K, 1.0000E-03 atm, Sl, a=1.0000)

+ 0.00000     mol    Si_solid
         (1423.00 K, 1.0000E-03 atm, Sl, a=0.83109)

+ 0.0         mol    MgSiO3_proto-enstatite
```

Gas phase: numbers are mole fractions



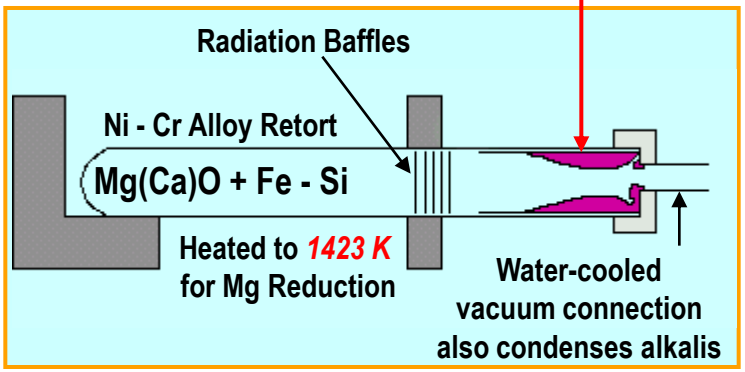
Compare the formation of the gas phase here at 10^{-3} atm with the previous page where pressure is 1 atm.

Refer to the next page for the distribution of elements in the products.

Pidgeon Process for the Production of Magnesium: **Results**

T = 1423 K
P_{total}= 0.001 atm

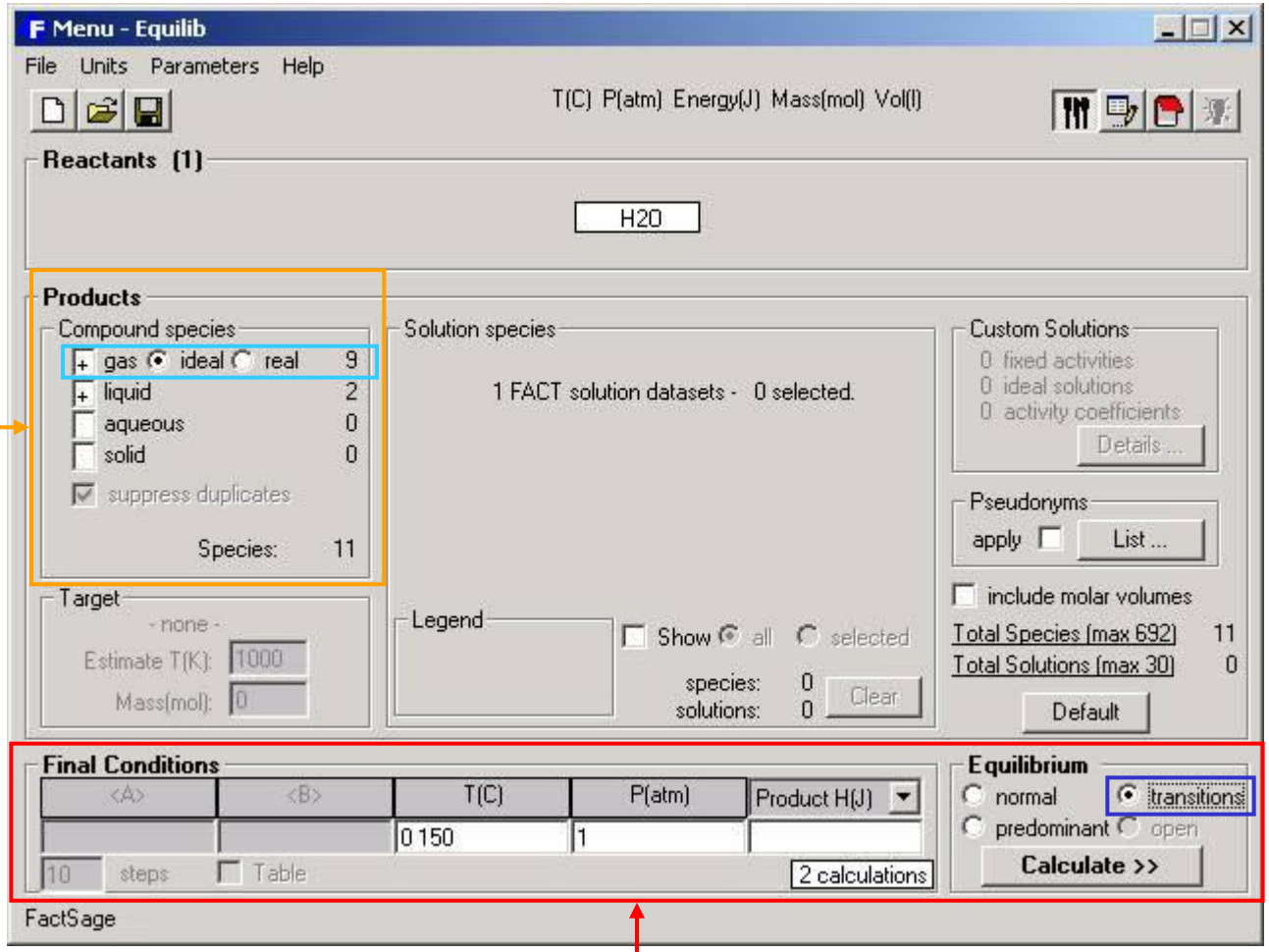
Mg(g) condenses on water-cooled removable sleeve



	Code		Data		Mole	Gram	Per Cent	Cumulate	T
		ELEMENT Mg			Mole	Gram	Per Cent	Cumulate	
		GAS PHASE							
	4	Mg(g)	FACT		1.983	48.20	49.58 %	49.6 %	
	5	Mg2(g)	FACT		1.1945E-06	2.9033E-05	2.9864E-05 %	49.6 %	
	6	MgO(g)	FACT		4.4955E-12	1.0926E-10	1.1239E-10 %	49.6 %	
Mg				Totals	1.983	48.20	49.58 %		
		PURE SPECIES							
	18	MgO(s)	FACT		5.0934E-02	1.238	1.273 %	50.8 %	
	36	Mg2SiO4(s)	FACT		1.966	47.78	49.15 %	100. %	
				Totals	2.017	49.02	50.42 %		
		TOTAL Mg			4.000	97.22			
		ELEMENT O			Mole	Gram	Per Cent	Cumulate	
		GAS PHASE							
	1	O(g)	FACT		2.0338E-16	3.2539E-15	5.0845E-15 %	5.084E-15 %	
	2	O2(g)	FACT		2.3096E-23	3.6953E-22	5.7741E-22 %	5.084E-15 %	
	3	O3(g)	FACT		3.9579E-45	6.3324E-44	9.8947E-44 %	5.084E-15 %	
	6	MgO(g)	FACT		4.4955E-12	7.1926E-11	1.1239E-10 %	1.124E-10 %	
O	10	SiO(g)	FACT		1.6974E-02	0.2716	0.4244 %	0.424 %	
				Totals	1.6974E-02	0.2716	0.4244 %		
		PURE SPECIES							
	18	MgO(s)	FACT		5.0934E-02	0.8149	1.273 %	1.70 %	
	36	Mg2SiO4(s)	FACT		3.932	62.91	98.30 %	100. %	
				Totals	3.983	63.73	99.58 %		
		TOTAL O			4.000	64.00			
		ELEMENT Si			Mole	Gram	Per Cent	Cumulate	
		GAS PHASE							
	7	Si(g)	FACT		2.5474E-06	7.1545E-05	2.5474E-04 %	2.547E-04 %	
	8	Si2(g)	FACT		3.0841E-09	8.6619E-08	3.0841E-07 %	2.550E-04 %	
	9	Si3(g)	FACT		5.9853E-10	1.6810E-08	5.9853E-08 %	2.551E-04 %	
Si	10	SiO(g)	FACT		1.6974E-02	0.4767	1.697 %	1.70 %	
				Totals	1.6977E-02	0.4768	1.698 %		
		PURE SPECIES							
	36	Mg2SiO4(s)	FACT		0.9830	27.61	98.30 %	100. %	
				Totals	0.9830	27.61	98.30 %		
		TOTAL Si			1.000	28.09			

Boiling Point of Water: Ideal Gas Calculation Settings

Products:
- a **liquid phase**;
- an **ideal gas** phase



Final Conditions:
T = 0°C and **150°C**;
P = 1atm;
and any **transition** point in the temperature interval

Boiling Point of Water: Ideal Gas Calculation; Results: T_b(water) = 100.35°C

The asterisk in front of **T = 100.35°C** indicates the calculated value …

Results - Equilib 100.35 C (page 2/4)

Output Edit Show Pages

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

0 C | - 100.35 C - | 100.35 C | 150 C |

```
*T = 100.35 C
P = 1.00000E+00 atm
V = 0.00000E+00 dm3

STREAM CONSTITUENTS          AMOUNT/mol
H2O                          1.0000E+00

                            EQUIL AMOUNT   MOLE FRACTION      FUGACITY
PHASE: gas_ideal               mol                            atm
H2O                         0.0000E+00     1.0000E+00      1.0000E+00
H2                          0.0000E+00     1.2793E-21      1.2793E-21
O2                          0.0000E+00     6.3963E-22      6.3963E-22
OH                          0.0000E+00     2.1382E-26      2.1382E-26
HOOH                        0.0000E+00     3.6636E-29      3.6636E-29
HOO                         0.0000E+00     7.9014E-35      7.9014E-35
H                           0.0000E+00     4.4771E-39      4.4771E-39
O                           0.0000E+00     4.1454E-43      4.1454E-43
O3                          0.0000E+00     4.5857E-56      4.5857E-56
TOTAL:                      0.0000E+00     1.0000E+00      1.0000E+00
                               mol                          ACTIVITY
H2O_liquid(liq)             1.0000E+00                      1.0000E+00
HOOH_liquid(liq)            0.0000E+00                      2.1885E-28
*******************************************************************
  Cp_EQUIL        H_EQUIL        S_EQUIL        G_EQUIL        V_EQUIL
   J.K-1            J             J.K-1            J             dm3
*******************************************************************
 7.60017E+01  -2.80143E+05   8.69534E+01  -3.12620E+05   0.00000E+00
```

Results - Equilib 100.35 C (page 3/4)

Output Edit Show Pages

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

0 C | 100.35 C | - 100.35 C - | 150 C |

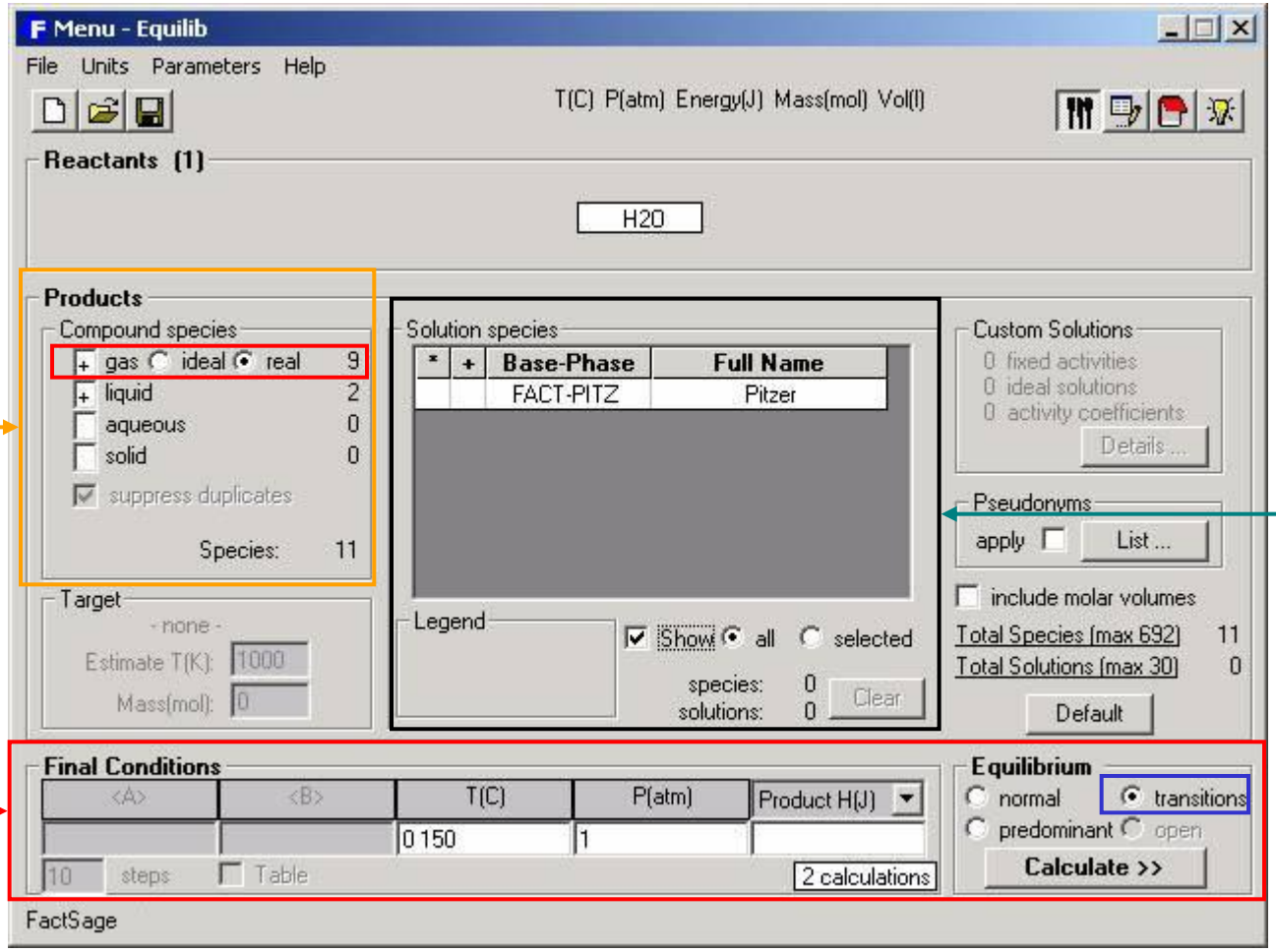
```
*T = 100.35 C
P = 1.00000E+00 atm
V = 3.06490E+01 dm3

STREAM CONSTITUENTS          AMOUNT/mol
H2O                          1.0000E+00

                            EQUIL AMOUNT   MOLE FRACTION      FUGACITY
PHASE: gas_ideal               mol                            atm
H2O                         1.0000E+00     1.0000E+00      1.0000E+00
H2                          1.2793E-21     1.2793E-21      1.2793E-21
O2                          6.3967E-22     6.3967E-22      6.3967E-22
OH                          2.1384E-26     2.1384E-26      2.1384E-26
HOOH                        3.6638E-29     3.6638E-29      3.6638E-29
HOO                         7.9020E-35     7.9020E-35      7.9020E-35
H                           4.4775E-39     4.4775E-39      4.4775E-39
O                           4.1458E-43     4.1458E-43      4.1458E-43
O3                          4.5862E-56     4.5862E-56      4.5862E-56
TOTAL:                      1.0000E+00     1.0000E+00      1.0000E+00
                               mol                          ACTIVITY
H2O_liquid(liq)             0.0000E+00                      9.9999E-01
HOOH_liquid(liq)            0.0000E+00                      2.1886E-28
*******************************************************************
  Cp_EQUIL        H_EQUIL        S_EQUIL        G_EQUIL        V_EQUIL
   J.K-1            J             J.K-1            J             dm3
*******************************************************************
 3.40522E+01  -2.39287E+05   1.96339E+02  -3.12620E+05   3.06490E+01
```

Compare the final **volume** of the phase

… for the equilibrium temperature between H_2O(g) [**ideal gas phase**] and H_2O(L1) [i.e., the **ideal** boiling point]

Boiling Point of Water: Real Gas Calculation Settings

Products:
- a **liquid phase**;
- an **real gas** phase



Final Conditions:
T = 0°C and **150°C**;
P = 1atm;
and any **transition** point in the temperature interval

Possible selection of solution species (the box Show and the radio button all are checked).

Boiling Point of Water, Real Gas Calculation Results T_b = 100°C [*ChemSage* Output]

Results - Equilib 100 C (page 2/4)

Output Edit Show Pages

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

0 C | - 100 C - | 100 C | 150 C

```
*T = 100.00 C
P = 1.00000E+00 atm
V = 0.00000E+00 dm3

STREAM CONSTITUENTS          AMOUNT/mol
H2O                          1.0000E+00

                            EQUIL AMOUNT  MOLE FRACTION     FUGACITY
PHASE: gas_real                  mol                          atm
H2O                         0.0000E+00     1.0000E+00     9.8754E-01
H2                          0.0000E+00     1.1937E-21     1.2087E-21
O2                          0.0000E+00     5.9683E-22     6.0207E-22
OH                          0.0000E+00     2.0176E-26     1.9925E-26
HOOH                        0.0000E+00     3.4412E-29     3.3983E-29
HOO                         0.0000E+00     7.3173E-35     7.2261E-35
H                           0.0000E+00     4.1210E-39     4.0696E-39
O                           0.0000E+00     3.7721E-43     3.7251E-43
O3                          0.0000E+00     3.9962E-56     4.0086E-56
TOTAL:                      0.0000E+00     1.0000E+00     1.0000E+00
                                 mol                       ACTIVITY
H2O_liquid(liq)             1.0000E+00                    1.0000E+00
HOOH_liquid(liq)            0.0000E+00                    2.0601E-28
*******************************************************************
  Cp_EQUIL        H_EQUIL        S_EQUIL        G_EQUIL        V_EQUIL
    J.K-1            J             J.K-1            J             dm3
*******************************************************************
 7.59935E+01  -2.80170E+05   8.68810E+01  -3.12589E+05   0.00000E+00

Mole fraction of system components:
                 gas_real
O                0.33333
H                0.66667
```

The asterisk in front of **T = 100°C** indicates the calculated value …

Results - Equilib 100 C (page 3/4)

Output Edit Show Pages

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

0 C | 100 C | - 100 C - | 150 C

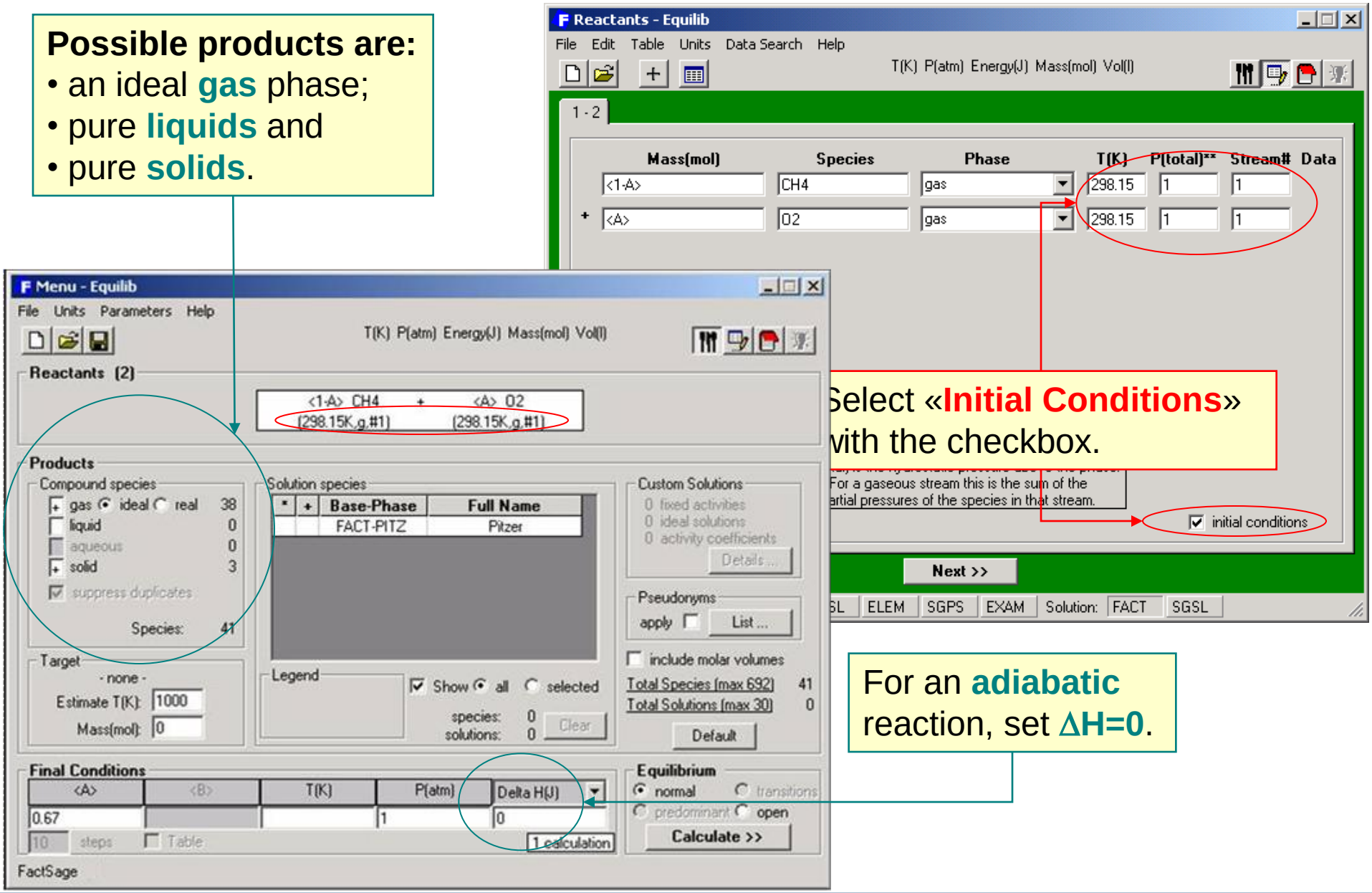
```
*T = 100.00 C
P = 1.00000E+00 atm
V = 3.02358E+01 dm3

STREAM CONSTITUENTS          AMOUNT/mol
H2O                          1.0000E+00

                            EQUIL AMOUNT  MOLE FRACTION     FUGACITY
PHASE: gas_real                  mol                          atm
H2O                         1.0000E+00     1.0000E+00     9.8754E-01
H2                          1.1937E-21     1.1937E-21     1.2088E-21
O2                          5.9687E-22     5.9687E-22     6.0210E-22
OH                          2.0178E-26     2.0178E-26     1.9926E-26
HOOH                        3.4414E-29     3.4414E-29     3.3985E-29
HOO                         7.3179E-35     7.3179E-35     7.2267E-35
H                           4.1214E-39     4.1214E-39     4.0700E-39
O                           3.7725E-43     3.7725E-43     3.7255E-43
O3                          3.9967E-56     3.9967E-56     4.0091E-56
TOTAL:                      1.0000E+00     1.0000E+00     1.0000E+00
                                 mol                       ACTIVITY
H2O_liquid(liq)             0.0000E+00                    9.9999E-01
HOOH_liquid(liq)            0.0000E+00                    2.0602E-28
*******************************************************************
  Cp_EQUIL        H_EQUIL        S_EQUIL        G_EQUIL        V_EQUIL
    J.K-1            J             J.K-1            J             dm3
*******************************************************************
 3.61170E+01  -2.39471E+05   1.95950E+02  -3.12589E+05   3.02358E+01

Mole fraction of system components:
                 gas_real
O                0.33333
H                0.66667
```

Compare the final **volume** of the phase

… for the equilibrium temperature between $H_2O(g)$ [**real gas phase**] and $H_2O(L1)$ [i.e., the **real** boiling point]

Adiabatic Reaction between CH_4 and O_2 – Specifying an Extensive Property, $\Delta H=0$

Possible products are:
- an ideal **gas** phase;
- pure **liquids** and
- pure **solids**.



Select «**Initial Conditions**» with the checkbox.

For an **adiabatic** reaction, set $\Delta H=0$.

Equilibrium **Products** and Final **T** of the **Adiabatic** Reaction between CH_4 and O_2

F Results - Equilib 3052.94 K

Output Edit Show Pages

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

```
<1-A> CH4 +  <A> O2 =
(298.15,1,g,#1) (298.15,1,g,#1)

 1.2374     mol    gas_ideal
 (26.733 gram, 1.2374 mol, 309.99 litre, 8.6238E-05 g/ml)
        (3052.94 K, 1 atm,      a=1.0000)
        ( 0.39022          H2O
        + 0.15179          CO
        + 0.11490          CO2
        + 9.5707E-02       OH
        + 8.7708E-02       O2
        + 7.0753E-02       H2
        + 4.9018E-02       H
        + 3.9835E-02       O
        + 7.2878E-05       HOO
        + 2.0256E-06       HOOH                                T
        + 5.4383E-07       HCO
        + 2.7914E-08       O3
        + 6.1629E-09       H2CO)

+ 0.00000    mol    C_graphite
        (3052.94 K, 1 atm, S1, a=2.2229E-07)

+ 0.00000    mol    C_diamond                                   T
        (3052.94 K, 1 atm, S2, a=1.2094E-07)

where "A" on the reactant side is 0.67000

The cutoff concentration has been specified to 1.0000E-09

Data on 3 product species identified with "T" have been extrapolated

*****************************************************************
  DELTA H        DELTA G        DELTA V        DELTA S        DELTA Cp
    (J)            (J)           (litre)         (J/K)          (J/K)
*****************************************************************
 0.00000E+00 -1.02592E+06  2.85527E+02  1.51899E+02  3.23684E+02
```

Product T is **3053 K**. Clearly a very high temperature. It can be used for flame spectroscopic applications.

No condensed phases

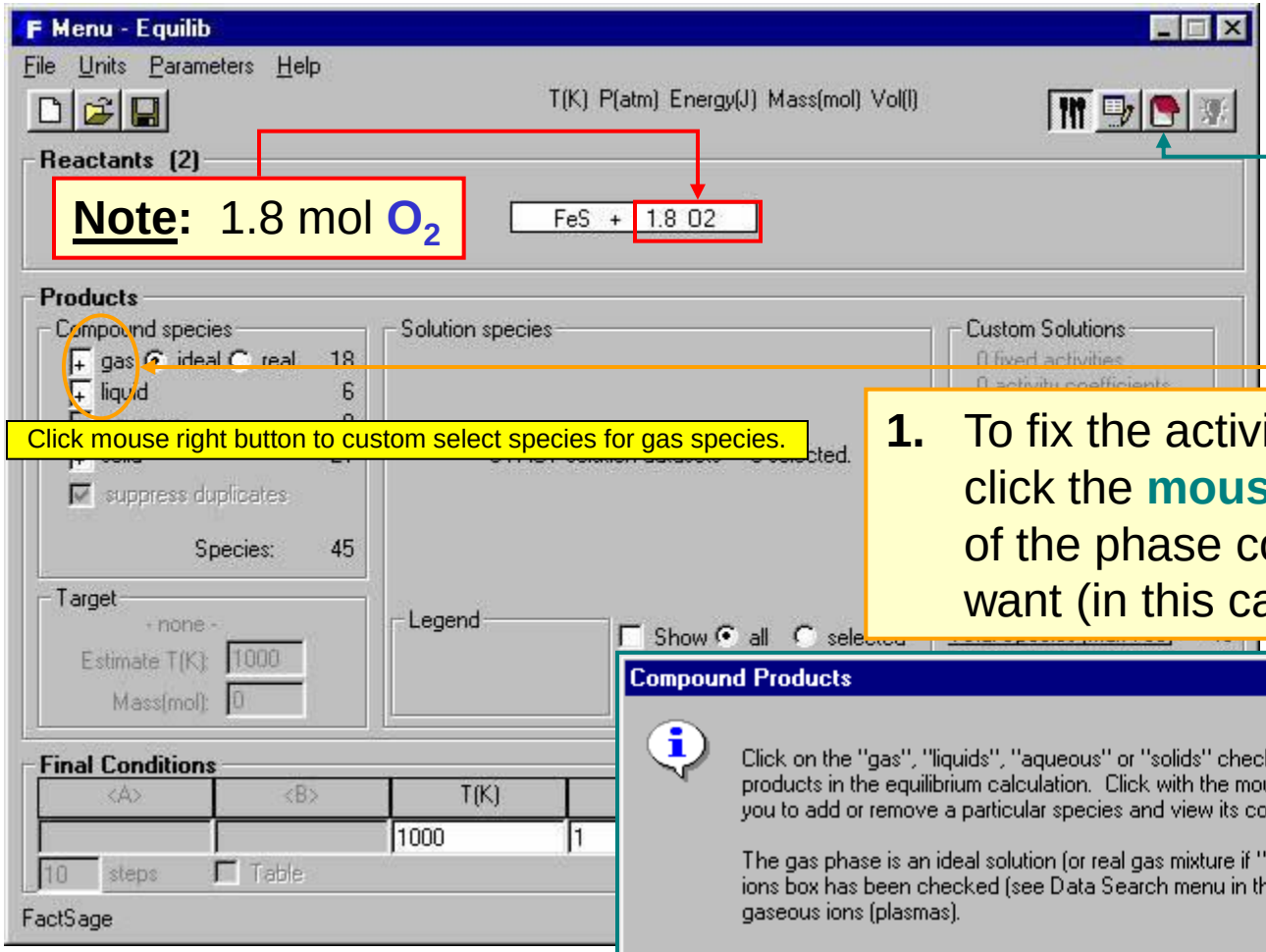
Note:
ΔH=0;
ΔS is a maximum for specified input conditions

Fixing the activity of a component in the equilibrium state

In the following four slides is shown how the ***Equilib*** module can be used in order to perform calculations which do not use an amount of a substance but rather its chemical potential, here the partial pressure of a gas species.

As an example FeS is considered in a gas atmosphere with a given O_2 partial pressure.

Fixing the Activity of a Species $O_2(g)$ in the Product Equilibrium FeS and O_2

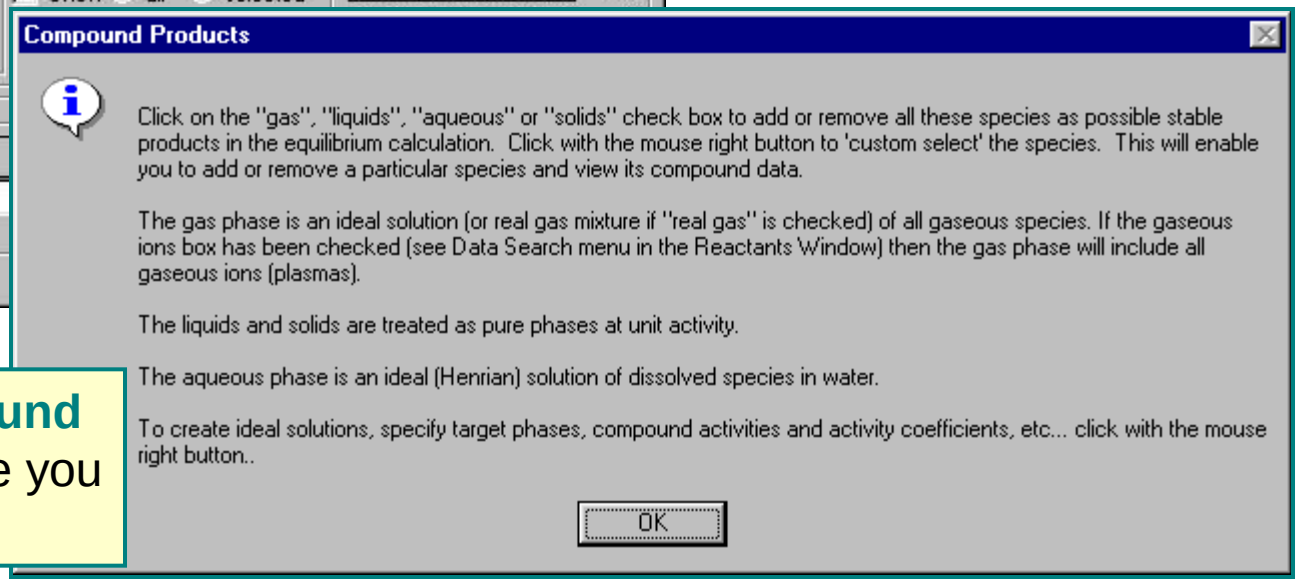


Note: 1.8 mol O_2

Click mouse right button to custom select species for gas species.

To view a list of the species selected before computation, press the «List Window» button.

1. To fix the activity of a species as $O_2(g)$, click the **mouse right button** on the name of the phase containing the species you want (in this case, the **gas** phase).



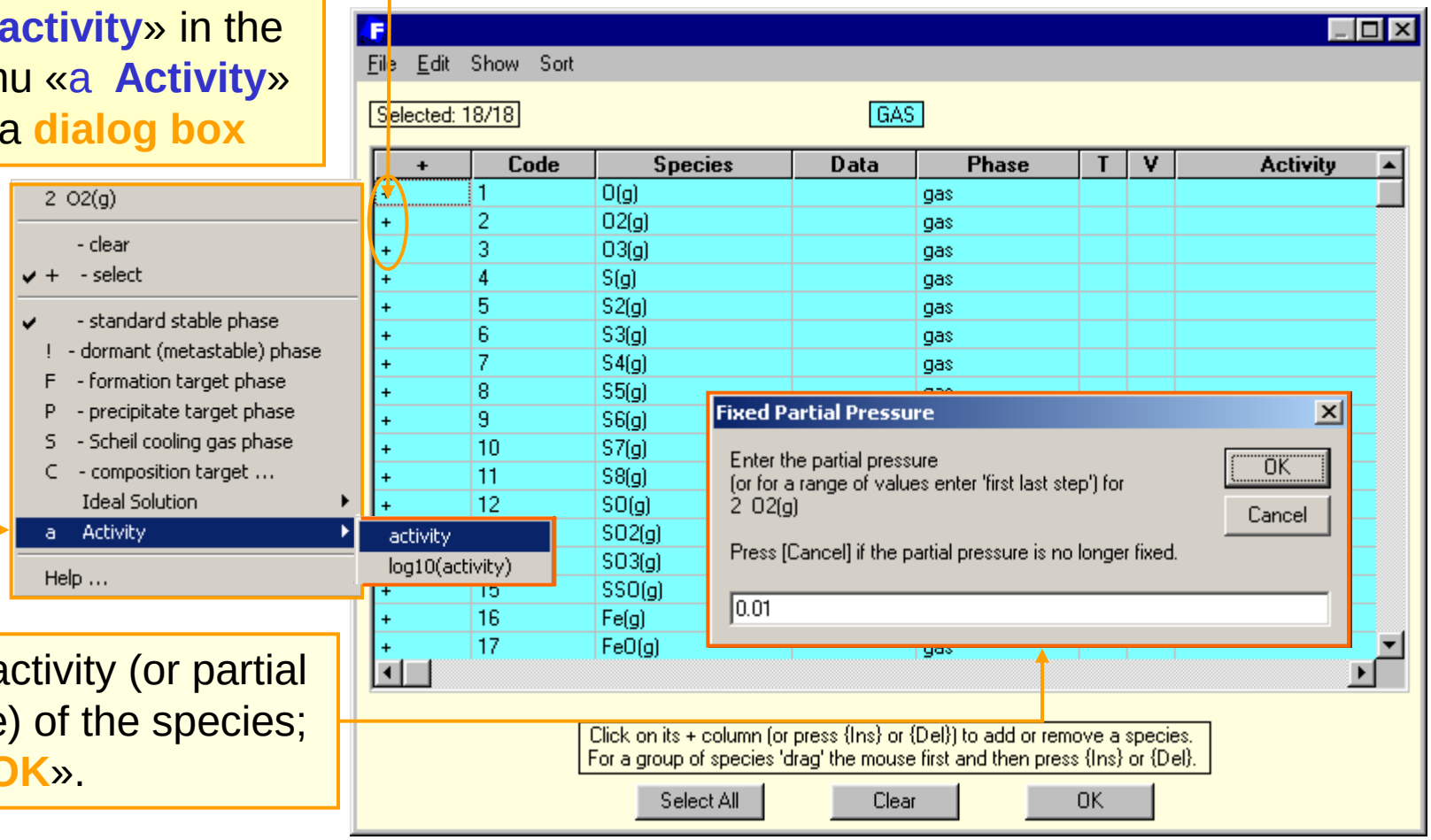
A right click in the «**compound species**» frame will provide you some information

Fixing the Activity of a Species

2. Click the **mouse right button** in the first column of the line containing **O_2(g)** species, **a context menu opens…**

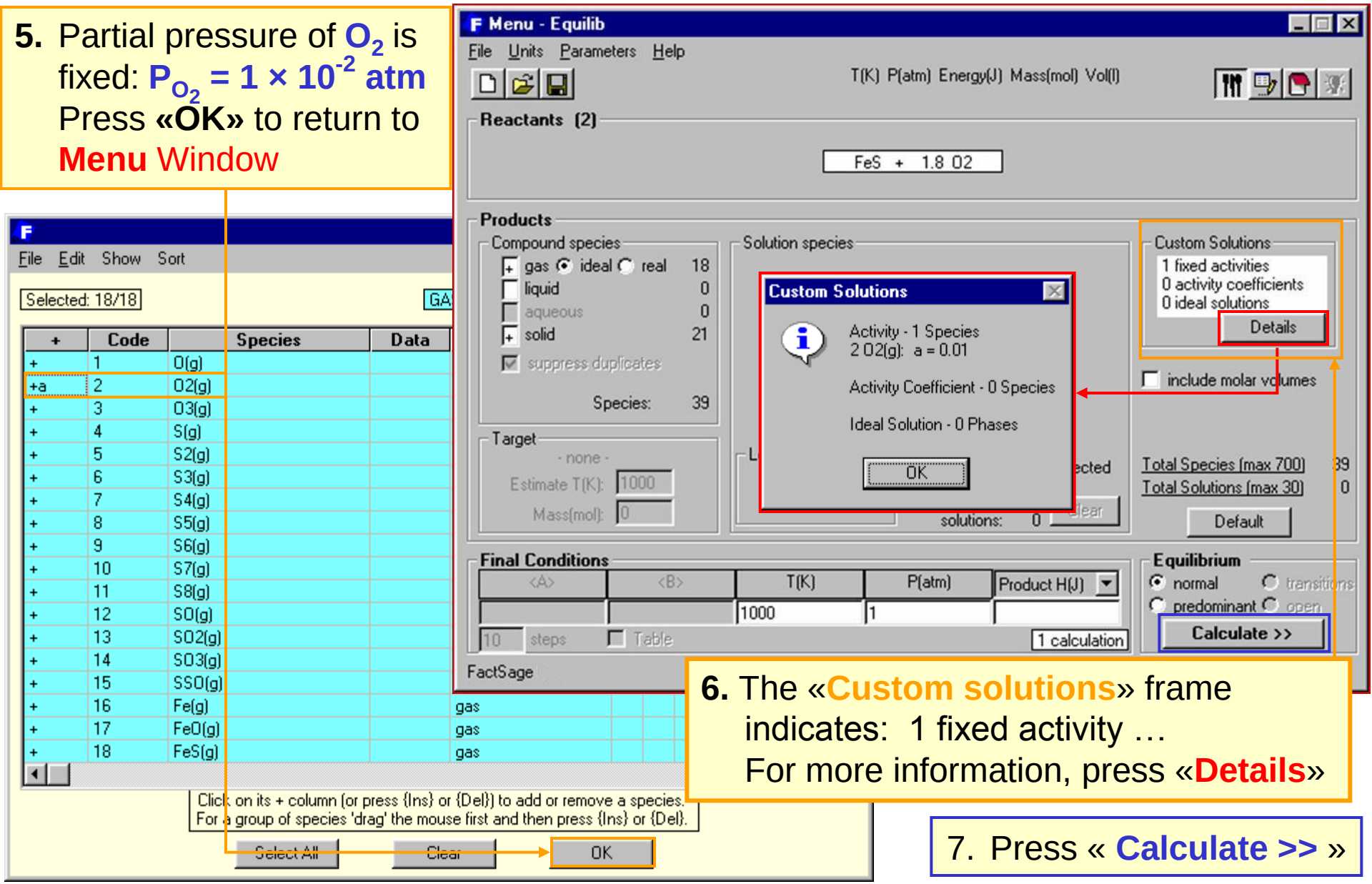
3. Select «**activity**» in the sub-menu «a **Activity**» to open a **dialog box**

4. Fix the activity (or partial pressure) of the species; Press «**OK**».



Activity of O_2(g) in the product equilibrium FeS and O_2: Custom activity details

5. Partial pressure of O_2 is fixed: $P_{O_2} = 1 \times 10^{-2}$ atm
Press **«OK»** to return to **Menu** Window



6. The «**Custom solutions**» frame indicates: 1 fixed activity …
For more information, press «**Details**»

7. Press « **Calculate >>** »

Activity of a Species O_2(g) in the Product Equilibrium FeS and O_2 : Results window

0.03709 mol O_2 must be added to the reactants in order to have the **final equilibrium partial pressure** for O_2

F Results - Equilib 1000 K

Output Edit Show Pages

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

```
  FeS +  1.8 O2 =

+ 3.7087E-02 O2
```

i.e. FeS + 1.83709 O_2 as reactants

```
  1.0101      mol    gas_ideal
  (66.851 gram, 1.0101 mol, 82.887 litre, 8.0654E-04 g/ml)
          (1000.00 K, 1 atm,      a=1.0000)
          ( 0.83757          SO2
          + 0.15243          SO3
          + 1.0000E-02       O2
          + 1.5941E-11       SO
          + 1.5630E-11       O
          + 8.7523E-15       O3
          + 9.9577E-22       SSO
          + 4.8238E-22       S
          + 1.7163E-22       FeO
          + 4.7790E-27       S2
          + 1.3124E-27       Fe
          + 1.3523E-37       FeS
          + 2.6348E-41       S3
          + 5.3584E-55       S4
          + 8.7156E-69       S5)

+ 0.50000     mol    Fe2O3_hematite
  (79.846 gram, 0.50000 mol)
          (1000.00 K, 1 atm, S1, a=1.0000)

+ 0.00000     mol    FeSO4_solid
          (1000.00 K, 1 atm, S1, a=0.26948)
```

P_{O_2} = **0.01** atm

Products

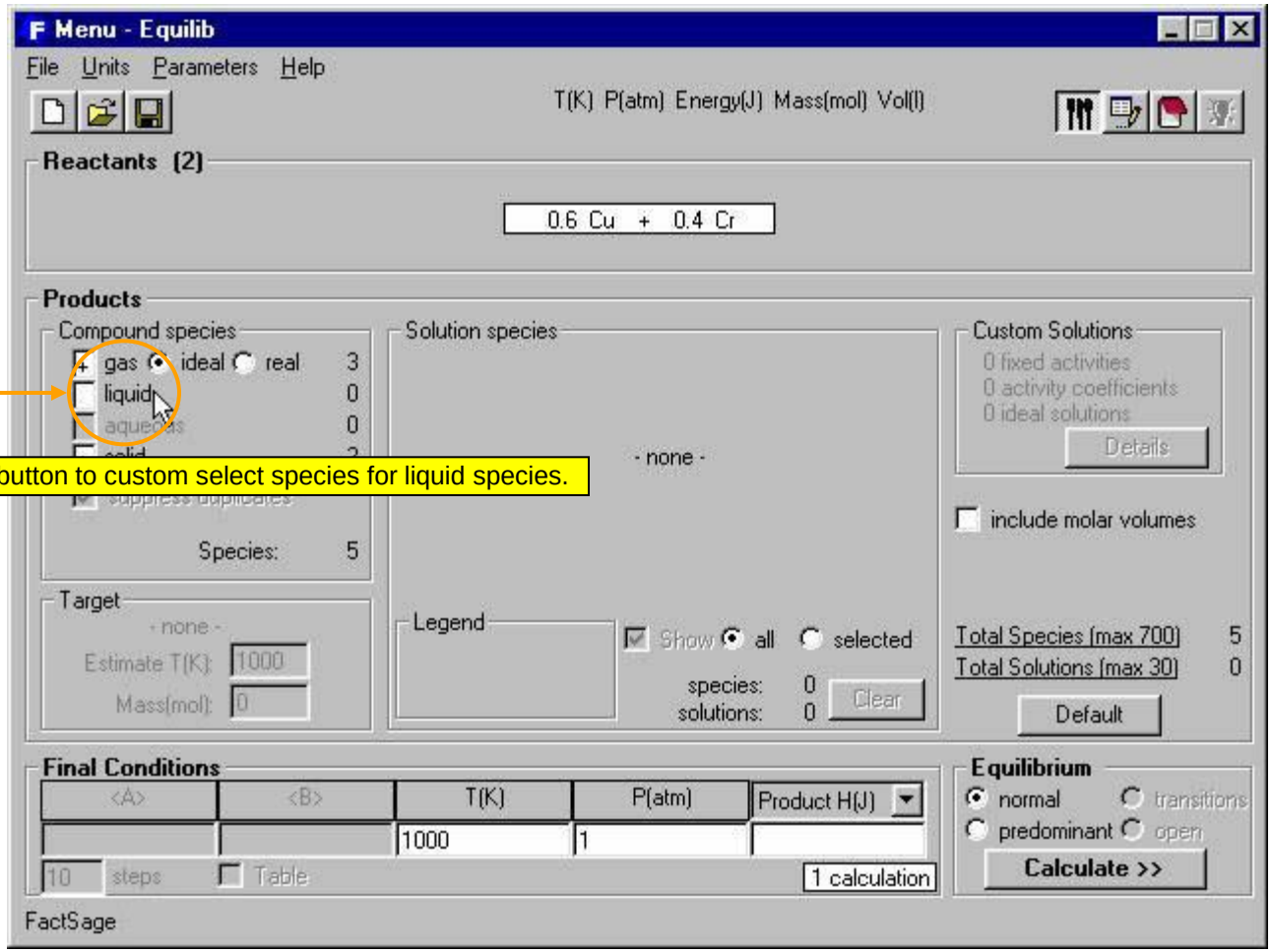
Assembling an **ideal liquid** and adding **activity coefficients**

In the following 16 slides is shown how in the ***Equilib*** module two pure liquid components are used to describe a custom defined liquid solution.

First ideal mixing is assumed, then a comparison with the known phase diagram is used to derive activity coefficients via the Reaction module. Finally the activity coefficients are applied in complex equilibrium calculations using the ***Equilib*** module.

Setting up of an ideal liquid solution of Cu and Cr

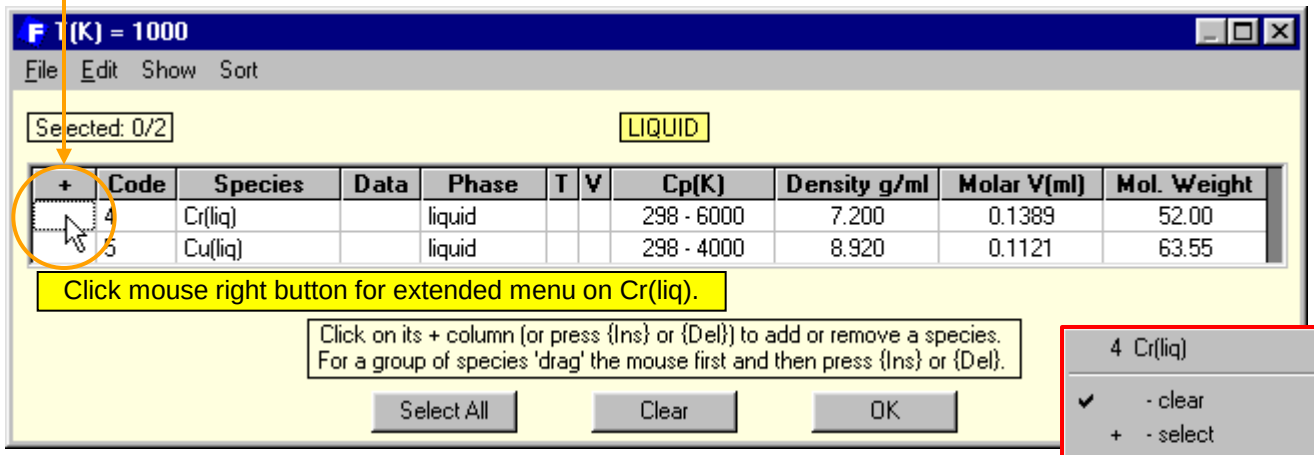
1. In order to define the components of an ideal liquid solution, click the **mouse right button** on the name of the phase containing the species you want (in this case, **liquid**).

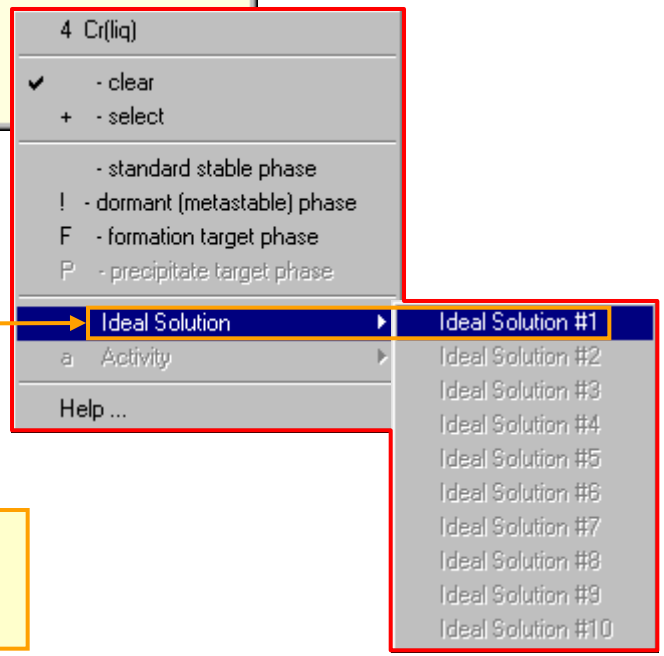


Click mouse right button to custom select species for liquid species.

Setting up of an ideal liquid solution of Cu and Cr

2. Click the **mouse right button** in the first column (+) of the line containing **Cr(liq)** species – **an extended menu appears**.

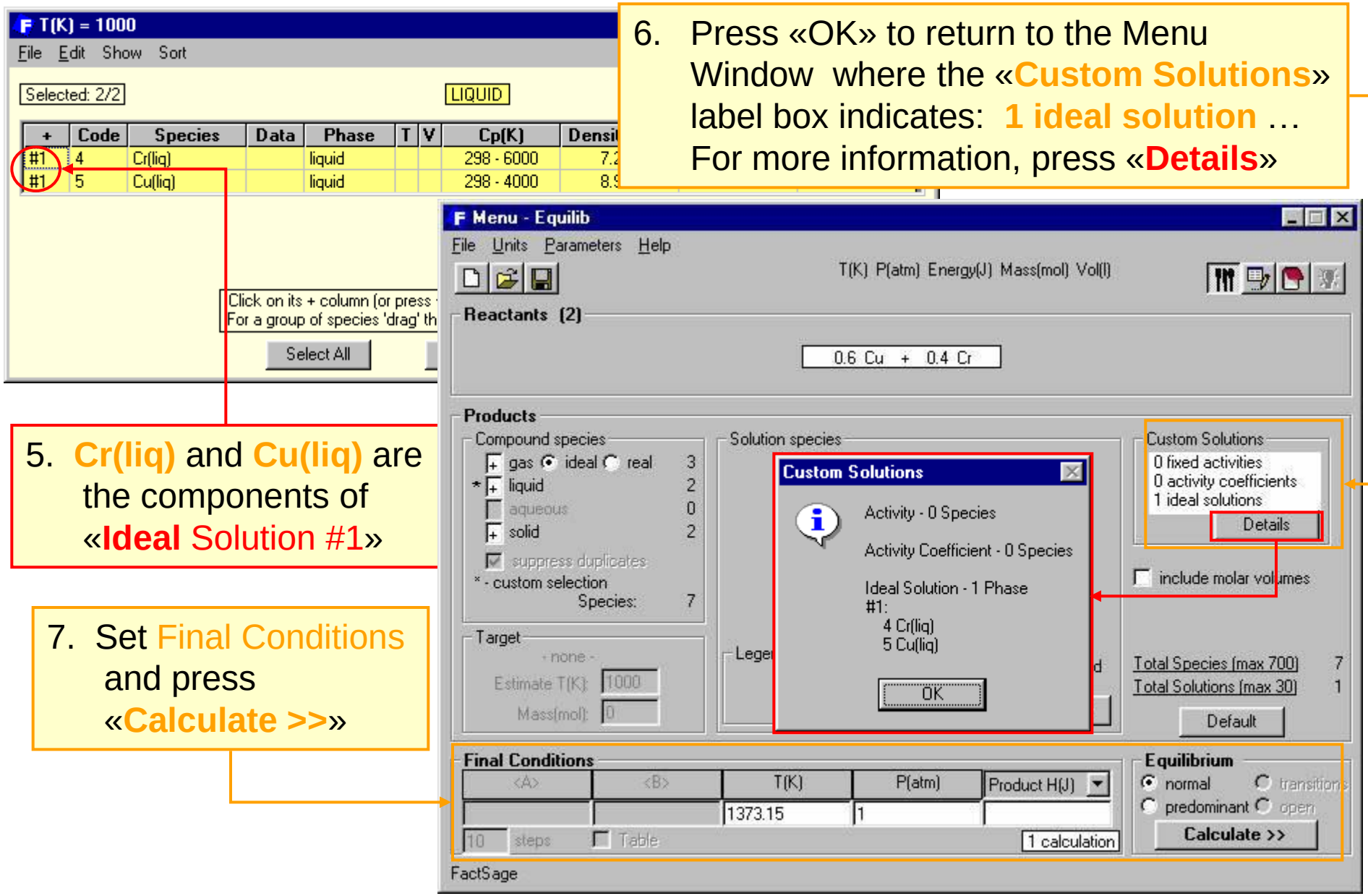




3. Click on «**Ideal Solution #1**» in sub-menu «**Ideal Solution**» to select **Cr(liq)** as the first component.

4. Repeat steps 2 and 3 to select **Cu(liq)** as the second component of **Ideal Solution #1**.

Liquid Cu-Cr alloy assuming ideal mixing of Cu and Cr



6. Press «OK» to return to the Menu Window where the «**Custom Solutions**» label box indicates: **1 ideal solution** … For more information, press «**Details**»

5. **Cr(liq)** and **Cu(liq)** are the components of «**Ideal** Solution #1»

7. Set Final Conditions and press «**Calculate >>**»

Results window – assumption of Cr(liq) - Cu(liq) ideal mixing.

ChemSage format

```
T = 1373.15 K
P = 1.00000E+00 atm
V = 0.00000E+00 dm3

STREAM CONSTITUENTS          AMOUNT/mol
Cu                           6.0000E-01
Cr                           4.0000E-01

                            EQUIL AMOUNT  MOLE FRACTION     FUGACITY
PHASE: gas_ideal               mol                            atm
Cu                           0.0000E+00     9.6319E-01     4.6973E-07
Cr                           0.0000E+00     3.6714E-02     1.7905E-08
Cu2                          0.0000E+00     9.1881E-05     4.4809E-11
TOTAL:                       0.0000E+00     1.0000E+00     4.8768E-07
PHASE: Ideal-1                 mol        MOLE FRACTION     ACTIVITY
Cr_liquid                    4.0000E-01     4.0000E-01     4.0000E-01
Cu_liquid                    6.0000E-01     6.0000E-01     6.0000E-01
TOTAL:                       1.0000E+00     1.0000E+00     1.0000E+00
                               mol                          ACTIVITY
Cr_solid(s)                  0.0000E+00                    8.5555E-01
Cu_liquid(liq)               0.0000E+00                    6.0000E-01
Cu_solid(s)                  0.0000E+00                    5.9235E-01
Cr_liquid(liq)               0.0000E+00                    4.0000E-01
*********************************************************************
  Cp_EQUIL       H_EQUIL        S_EQUIL        G_EQUIL        V_EQUIL
   J.K-1            J             J.K-1            J             dm3
*********************************************************************
 3.47467E+01   4.86096E+04   8.75461E+01  -7.16043E+04   0.00000E+00
```

Ideal solution phase:
liquid#1
Numbers are mole fractions
$X_{Cr(liq)} = 0.4$
$X_{Cu(liq)} = 0.6$

```
 0.6 Cu +  0.4 Cr =

 0.00000    mol   gas_ideal
          (1373.15 K, 1 atm,      a=4.8768E-07)
          ( 4.6973E-07       Cu
          + 1.7905E-08       Cr
          + 4.4809E-11       Cu2)

+ 1.0000     mol   Ideal-1
  (58.926 gram, 1.0000 mol)
          (1373.15 K, 1 atm,      a=1.0000)
          ( 0.40000          Cr_liquid
          + 0.60000          Cu_liquid)

          System component       Mole fraction  Mass fraction
          Cu                       0.60000        0.64704
          Cr                       0.40000        0.35296

+ 0.00000    mol   Cr_solid
          (1373.15 K, 1 atm, S1, a=0.85555)

+ 0.00000    mol   Cu_solid
          (1373.15 K, 1 atm, S1, a=0.59235)
```

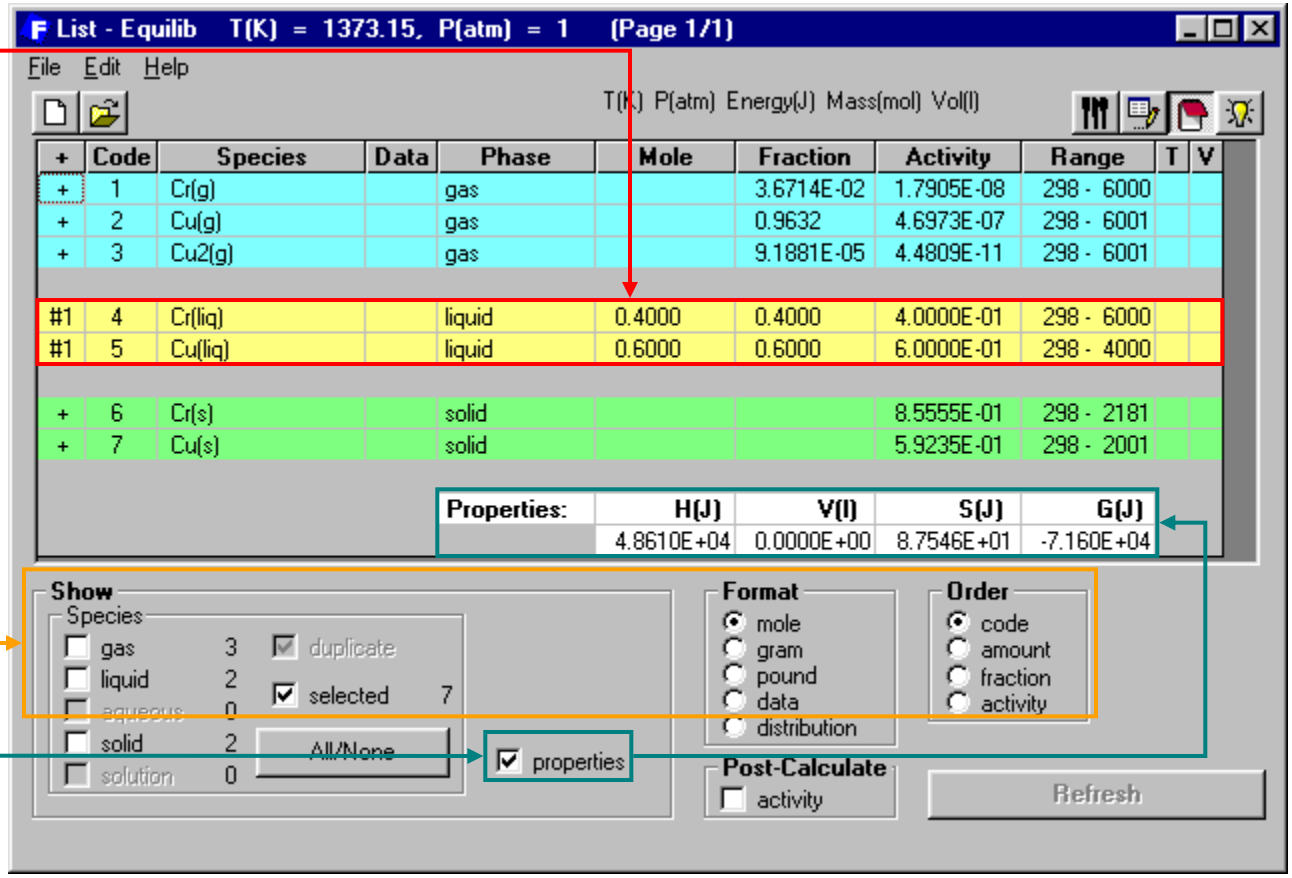
FACT format

List window – assumption of Cr(liq) - Cu(liq) ideal mixing

Ideal **solution**, hence
$X_{Cu(liq)} = a_{Cu(liq)} = 0.6$
$X_{Cr(liq)} = a_{Cr(liq)} = 0.4$

List Window
- check **Show**, Species «selected»;
- select: **Format** «mole» and **Order** «code».

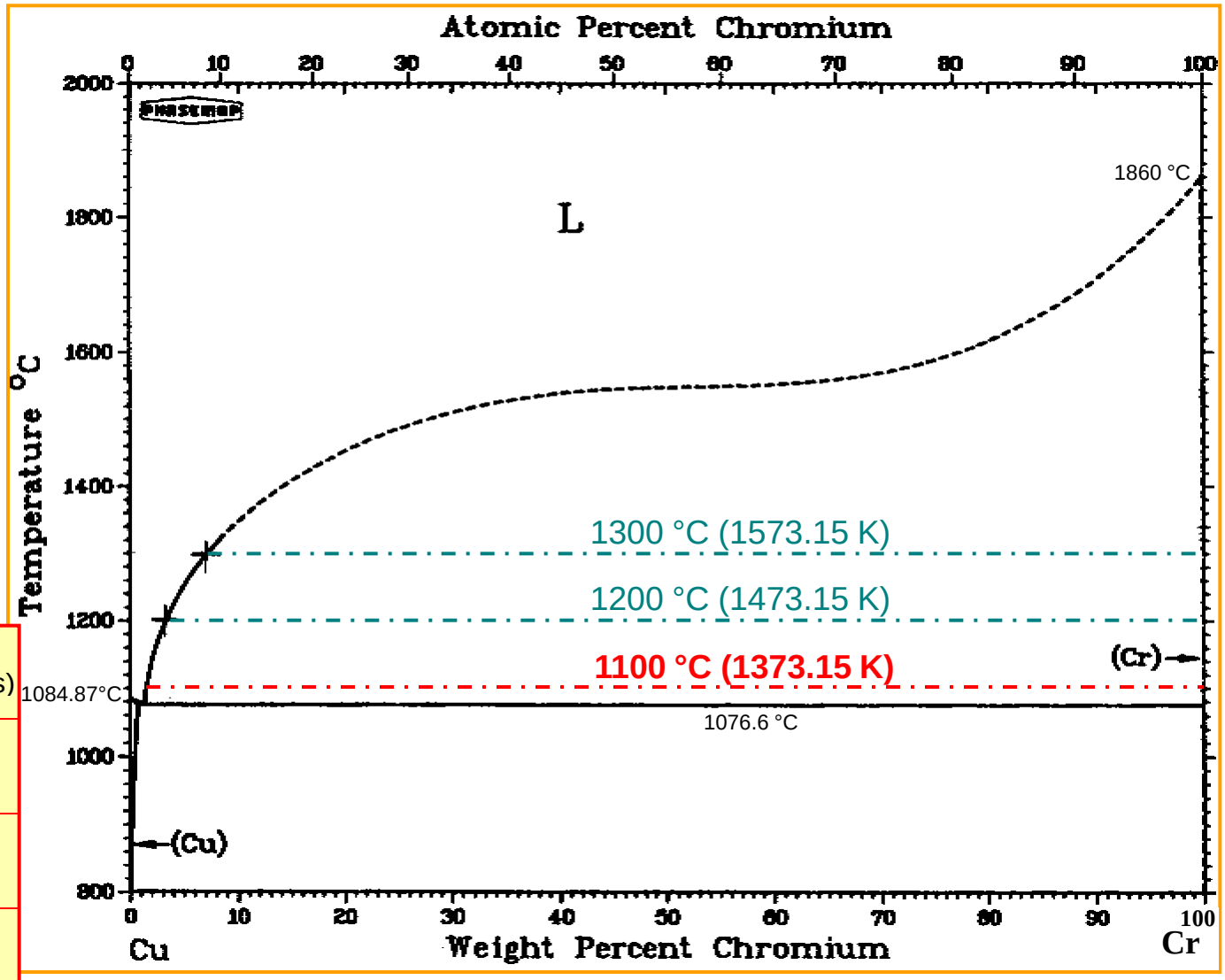
Option **Show** «properties» checked



According to the phase diagram (next page):
$X_{Cr(liq)}$ = **0.01837** at **1373.15 K** (1100°C).
Hence, the assumption of an ideal solution is **not very good** in this example.

Tie-lines in the Cu-Cr phase diagram

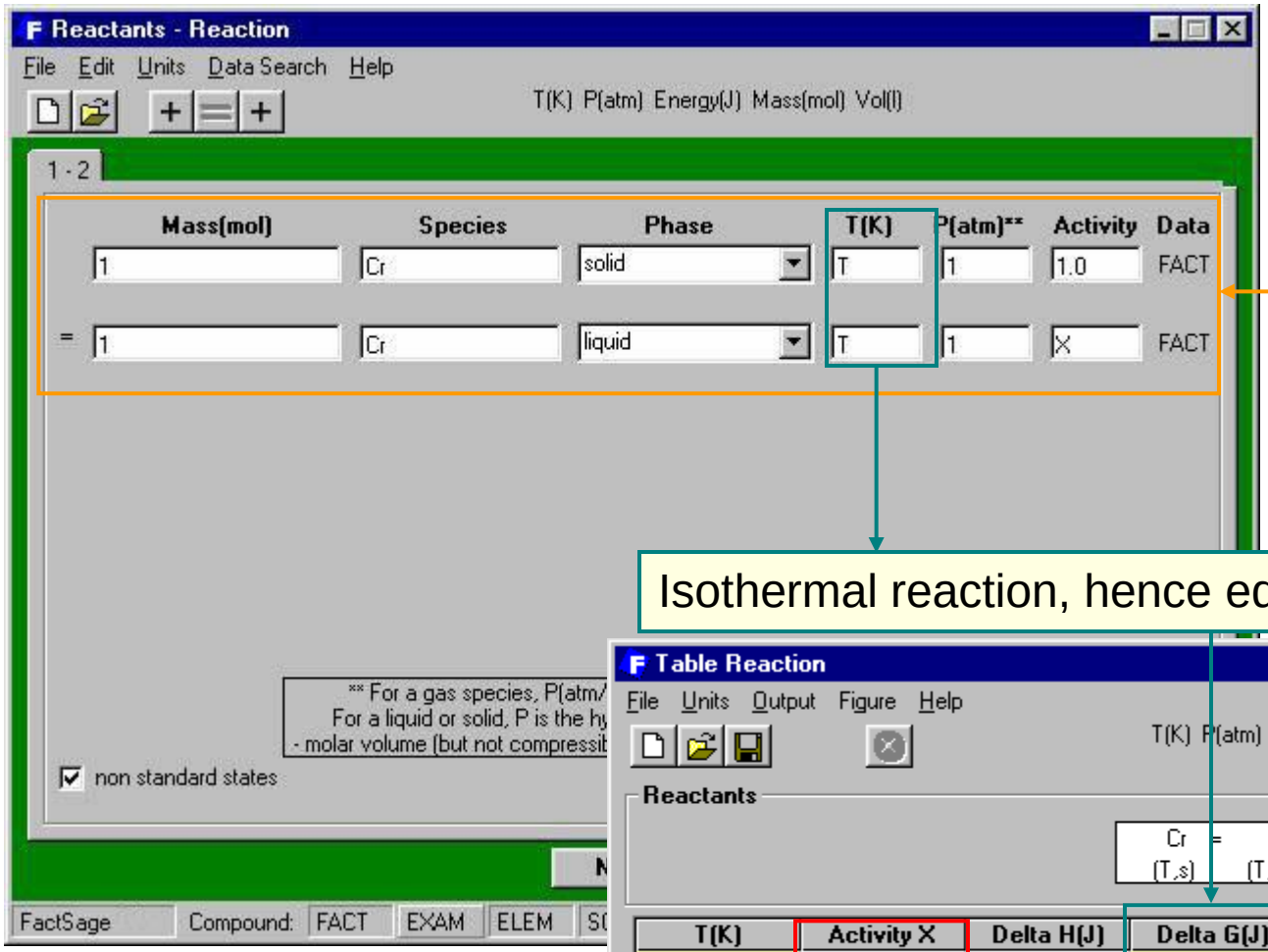
T (°C)	Cr(liq) (wt %)	Cr(s) (wt %)
1100	**1.508**	**100**
1200	3.456	100
1300	7.155	100



T (K)	$X_{Cr(liq)}$	$X_{Cr(s)}$
1373.15	**0.01837**	**1.0**
1473.15	0.04193	1.0
1573.15	0.08608	1.0

(**ref.** D.J. Chakrabarti and D.E. Laughlin, Bull. Alloy Phase Diagrams, p. 100, 1984)

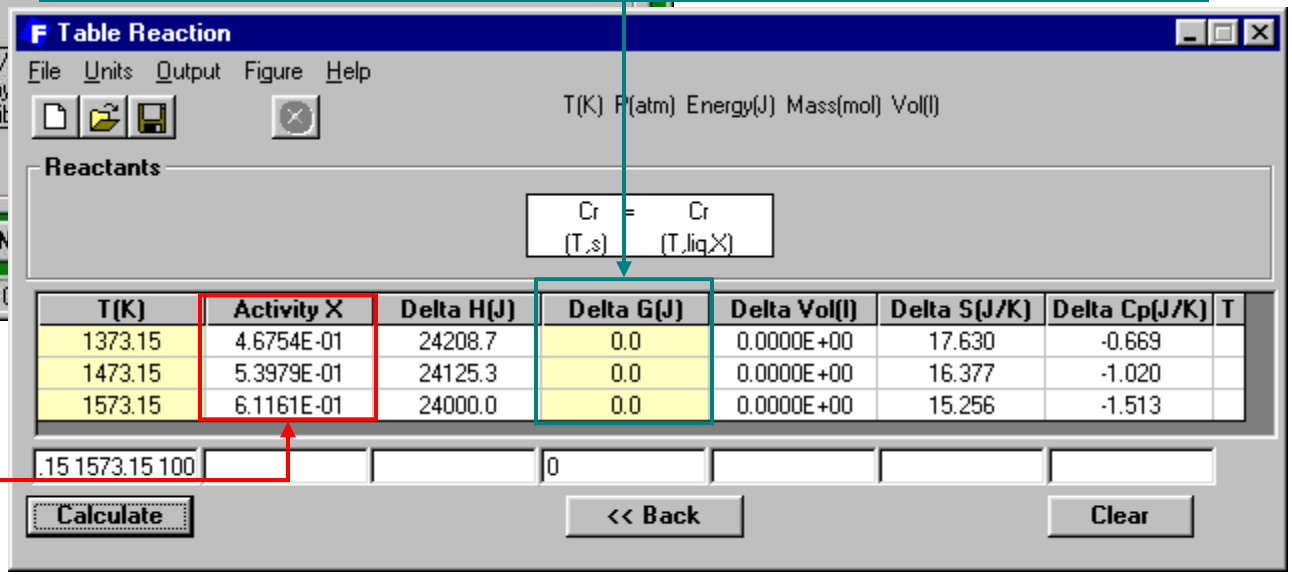
Input to program *Reaction* to calculate activity of Cr liquid in equilibrium with solid Cr



Pure Cr(s)
$a_{Cr(solid)} = 1$
(from phase diagram)

Cr(liq) in solution
$a_{Cr(liquid)} = X$

Isothermal reaction, hence equilibrium when $\Delta G = 0$.



Output of interest:
Activity of the
liquid phase

Estimation of the Henrian activity coefficient of Cr(liq) in Cu(liq)

For dilute solutions we can express the activity $a_{Cr(liq)}$ as a function of the molar fraction $X_{Cr(liq)}$, by applying Henry's law:

$$a_{Cr(liq)} = \gamma^{\circ}_{Cr(liq)} X_{Cr(liq)}$$

where $\gamma^{\circ}_{Cr(liq)}$ is the temperature dependant Henrian activity coefficient.

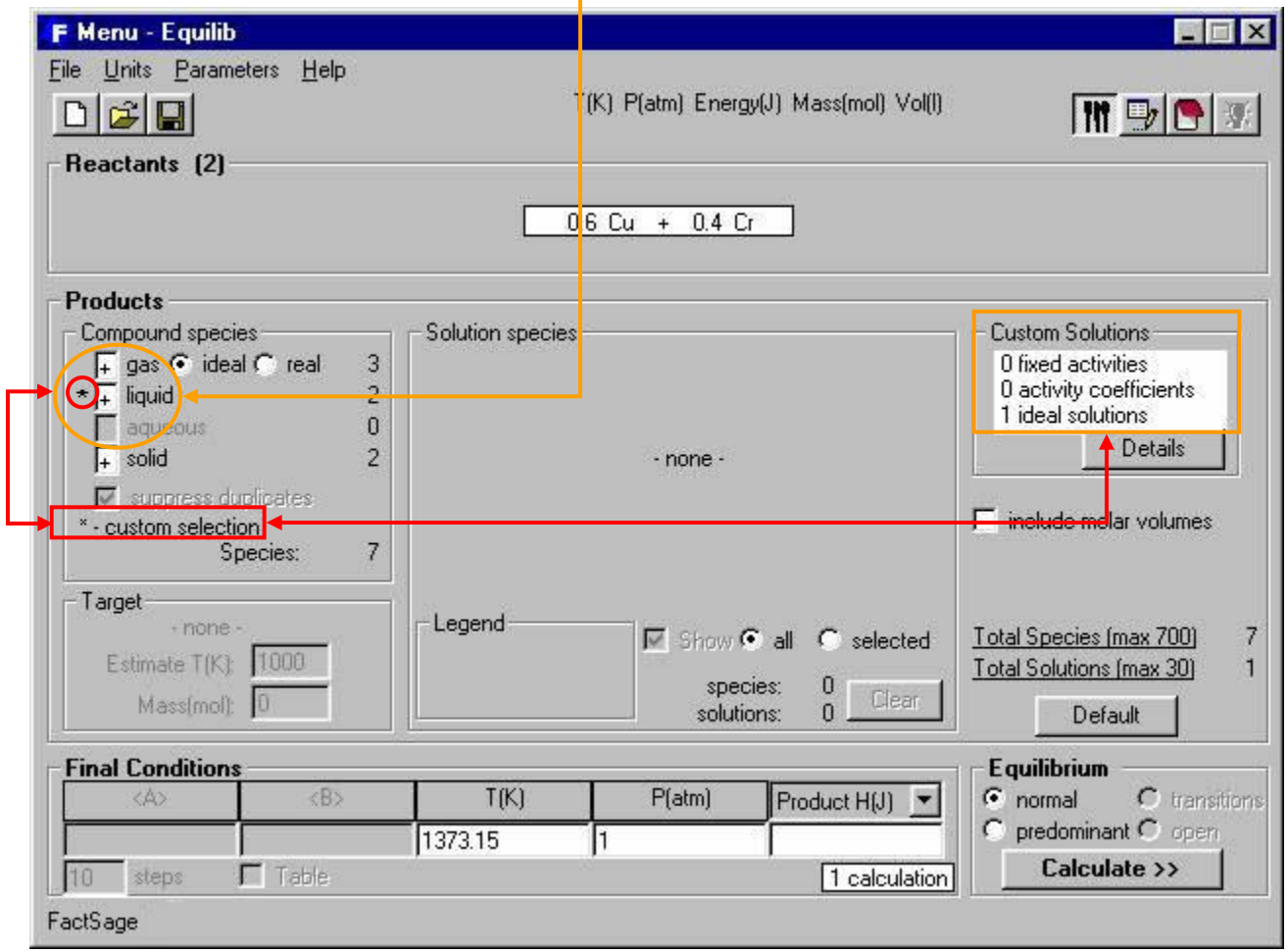
T (K)	$X_{Cr(liq)}$	$a_{Cr(liq)}$	$T^{-1}(10^{-4}\ K^{-1})$	$\gamma^{\circ}_{Cr(liq)}$	$Log_{10}[\gamma^{\circ}_{Cr(liq)}]$
1373.15	0.01837	0.46754	7.2825	25.4513	1.4057
1473.15	0.04193	0.53979	6.7882	12.8736	1.1097
1573.15	0.08608	0.61161	6.3567	7.1051	0.85157

The solution is **fairly** dilute, hence Henry's law is **fairly** applicable.

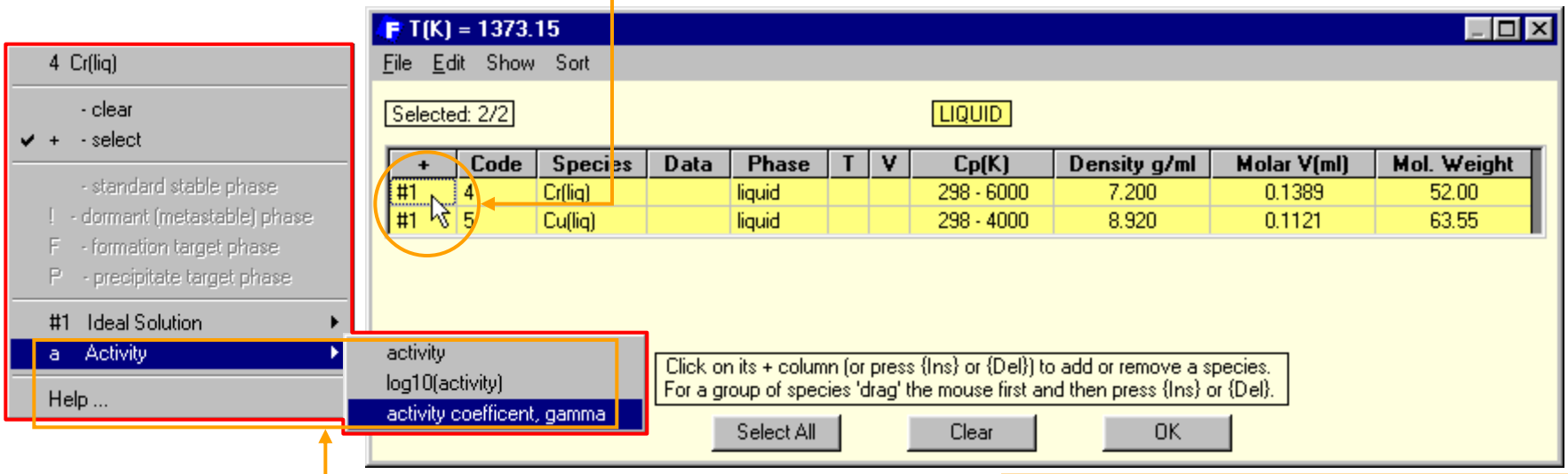
We find that: $\log_{10}\left[\gamma^{\circ}_{Cr(liq)}\right](T^{-1}) = 5983.29\ T^{-1} - 2.9522$

Modifying the **Custom Solution Selection**

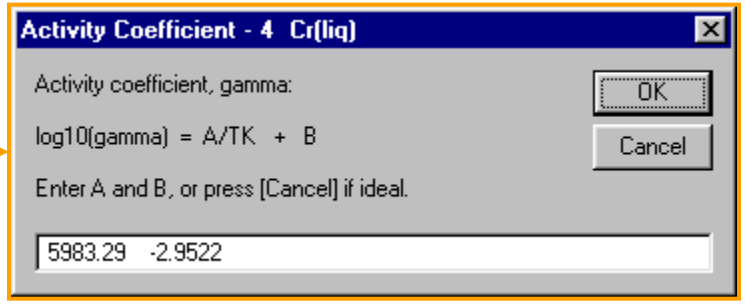
1. A custom solution selection of the liquid phase species exists. In order to modify it, click the **mouse right button** on **liquid** phase.



2. Click the **mouse right button** in the first column (+) of the line containing **Cr**(liq) species and an extended menu appears.



3. Click on «**activity coefficient gamma**» in «**a Activity**» sub-menu to open the **dialog box** for **Cr**(liq).



4. Enter the values A and B of the activity coefficient $\gamma^{o}_{Cr(liq)}$ in the expression:

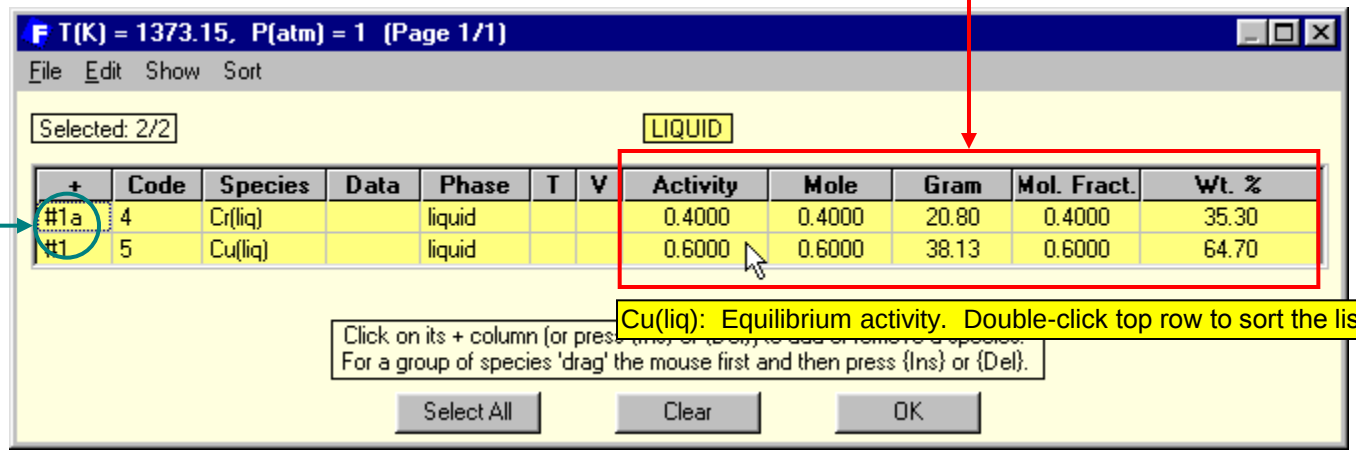
$\log_{10} [\gamma^{o}] = A / T(K) + B$ (Note: **T** is in Kelvin)

From the previous page, we have: $\log_{10} [\gamma^{o}_{Cr(liq)}] (T^{-1}) = 5983.29\ T^{-1} - 2.9522$

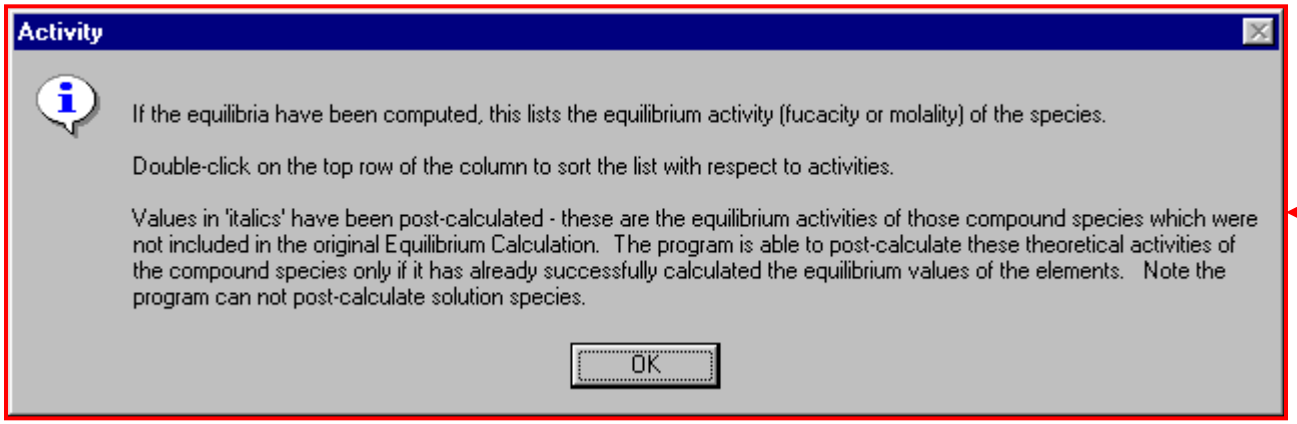
View of the Selection Window and use of the Show feature

The symbol «a» indicates that an activity coefficient (γ or $\log_{10}\gamma$) has been specified for Cr(liq) in the ideal solution #1.

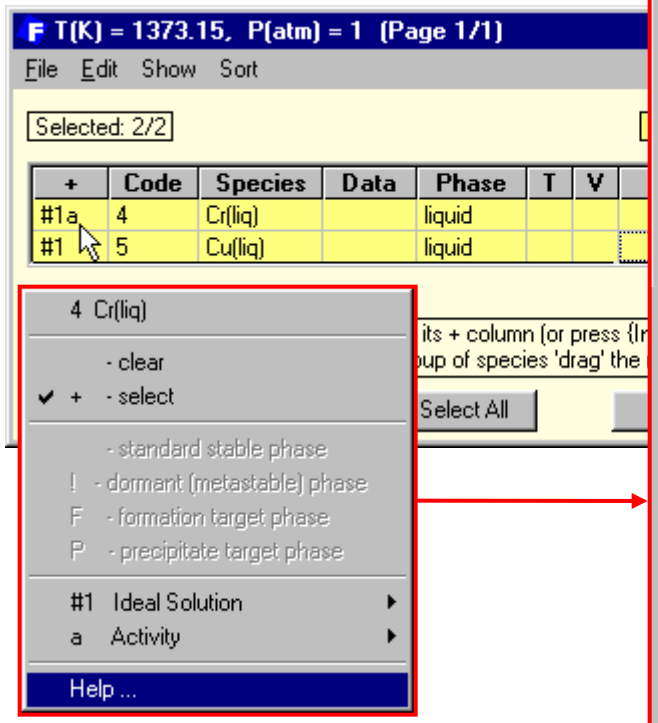
This view of the table with the **activity**, **mole**, **gram** and **molar fraction** and **weight percent** was obtained by selecting: **Show > Equilibrium values > All Equilibrium values** from the menu bar.

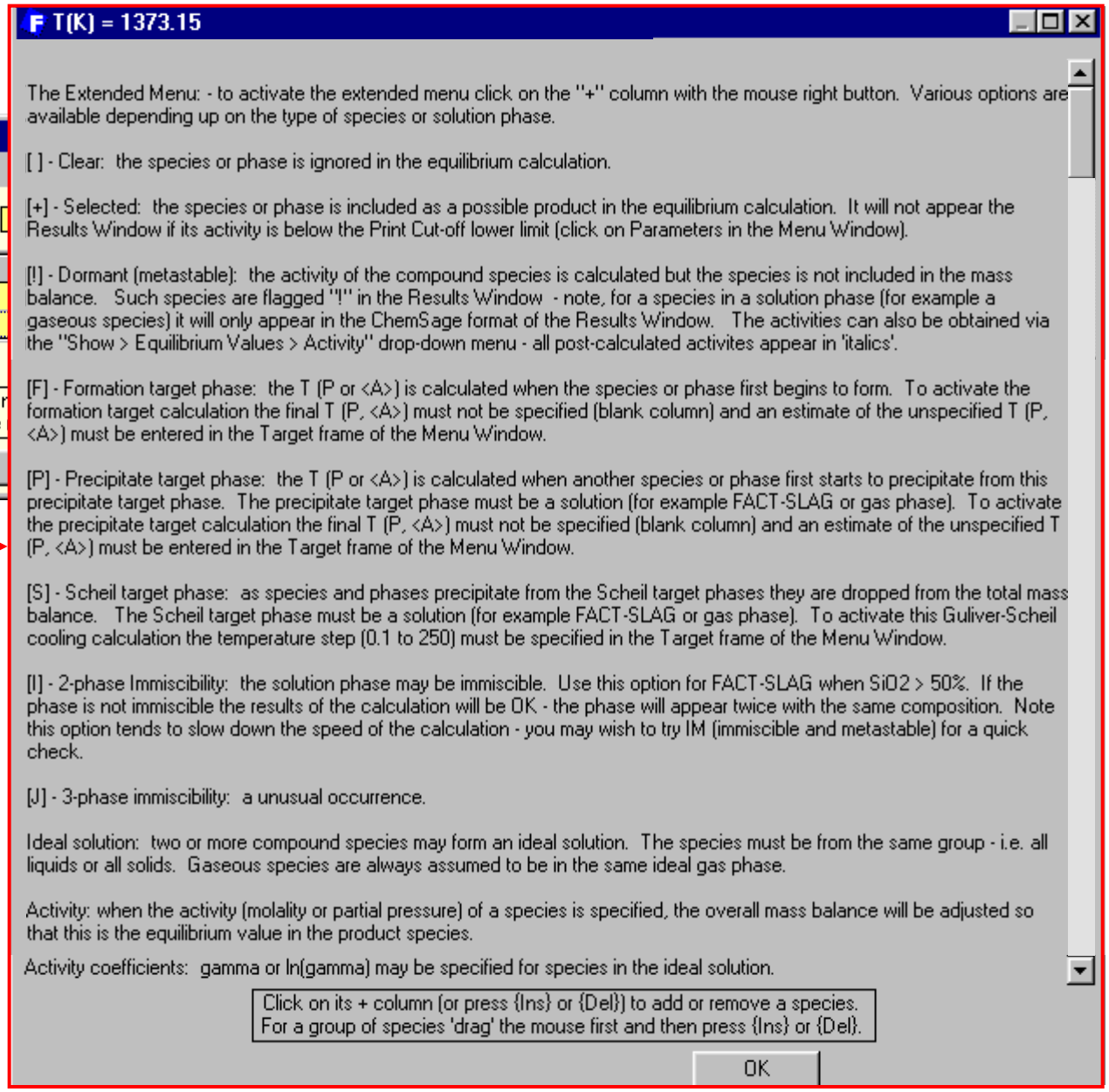


Cu(liq): Equilibrium activity. Double-click top row to sort the list. Click mouse right button for more…



View of the Selection Window Help (detailed information)

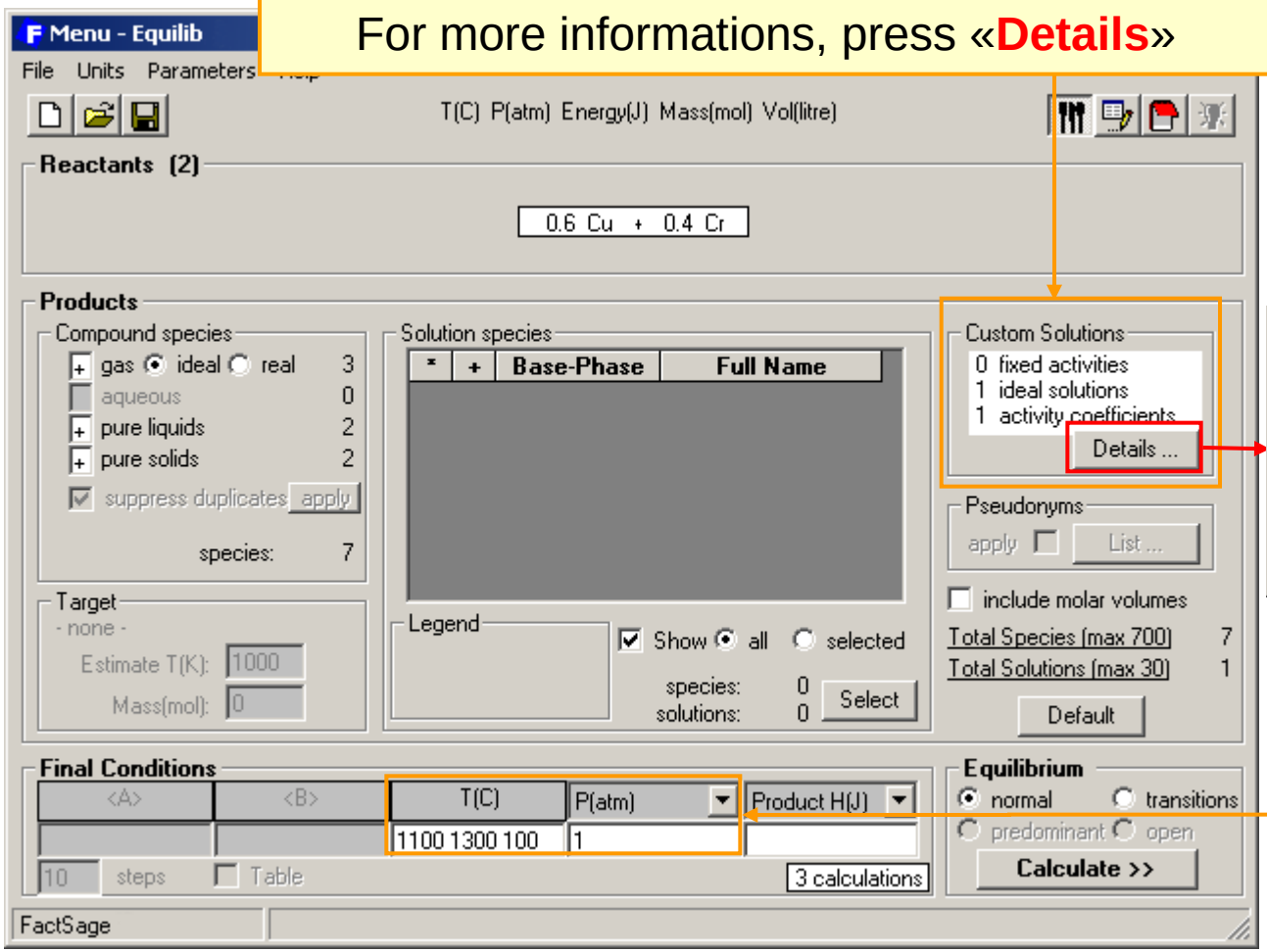


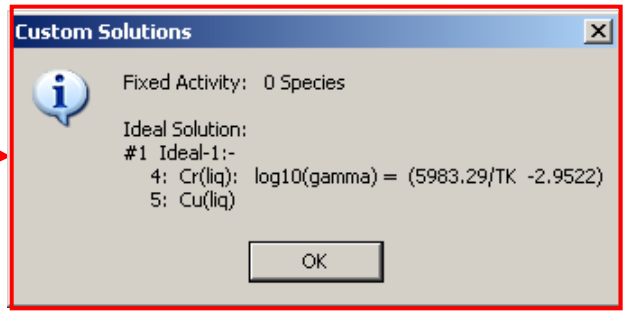


Setting the **Final Conditions** for the **Cr-Cu** Calculation

5. Return to Menu Window
   The «**Custom Solutions**» label box indicates:
   - 1 activity coefficient
   - 1 ideal solution

   For more informations, press «**Details**»





6. Set **Final Conditions** and **press «Calculate>>»**

Results for oxidation of Cu-Cr alloy at 1100 °C.

Liquid alloy coexists with solid **Cr** – the composition agrees with the phase diagram.

0 mol i.e. no gas phase. However, these mole fractions give equilibrium partial pressures. For example: P_{cu} = **0.76848 × 10^{-6} atm**.

Flag to a **custom solution**

$X_{Cr(l)}$ = **0.01839** same value as phase diagram

Pure solid **Cr**

Results - Equilib 1100 C (page 1/3)

Output Edit Show Pages

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

1100 C | 1200 C | 1300 C

```
 0.6 Cu +  0.4 Cr =

  0.00000     mol    gas_ideal
            (1100.00 C, 1 atm,      a=7.8953E-07)
            ( 7.6848E-07       Cu
            + 2.0928E-08       Cr
            + 1.1993E-10       Cu2)

+ 0.61124     mol    Ideal-l
  (38.712 gram, 0.61124 mol)
            (1100.00 C, 1 atm,      a=1.0000)
            ( 1.8394E-02       Cr_liquid
            + 0.98161          Cu_liquid)

+ 0.38876     mol    Cr_solid
  (20.214 gram, 0.38876 mol)
            (1100.00 C, 1 atm, S1, a=1.0000)

+ 0.00000     mol    Cu_liquid
            (1100.00 C, 1 atm, L1, a=0.98161)

*****************************************************************
      H            G            V            S            Cp
     (J)          (J)        (litre)      (J/K)        (J/K)
*****************************************************************
 4.04862E+04 -6.75197E+04  0.00000E+00  7.86555E+01  4.90735E+01
```

#

More Results for Cu - Cr Alloy – T = 1200 °C and 1300 °C

1200 °C

$X_{Cr(l)}$ = **0.041963**, same value as phase diagram.

Pure solid **Cr**

1300 °C

$X_{Cr(l)}$ = **0.086158**, same value as phase diagram.

Pure solid **Cr**

Results - Equilib 1200 C (page 2/3)

Output Edit Show Pages

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

1100 C | - 1200 C - | 1300 C

```
 0.6 Cu +  0.4 Cr =

  0.00000    mol   gas_ideal
            (1200.00 C, 1 atm,      a=5.1306E-06)
            ( 4.9114E-06      Cu
            + 2.1767E-07      Cr
            + 1.5449E-09      Cu2)

+ 0.62628    mol   Ideal-1
  (39.494 gram, 0.62628 mol)
            (1200.00 C, 1 atm,      a=1.0000)
            ( 4.1963E-02      Cr_liquid                    #
            + 0.95804         Cu_liquid)

+ 0.37372    mol   Cr_solid
  (19.432 gram, 0.37372 mol)
            (1200.00 C, 1 atm, S1, a=1.0000)

+ 0.00000    mol   Cu_solid
            (1200.00 C, 1 atm, S1, a=0.87519)
```

Results - Equilib 1300 C (page 3/3)

Output Edit Show Pages

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

1100 C | 1200 C | - 1300 C -

```
 0.6 Cu +  0.4 Cr =

  0.00000    mol   gas_ideal
            (1300.00 C, 1 atm,      a=2.5694E-05)
            ( 2.4008E-05      Cu
            + 1.6726E-06      Cr
            + 1.3459E-08      Cu2)

+ 0.65657    mol   Ideal-1
  (41.069 gram, 0.65657 mol)
            (1300.00 C, 1 atm,      a=1.0000)
            ( 8.6158E-02      Cr_liquid                    #
            + 0.91384         Cu_liquid)

+ 0.34343    mol   Cr_solid
  (17.857 gram, 0.34343 mol)
            (1300.00 C, 1 atm, S1, a=1.0000)

+ 0.00000    mol   Cu_solid
            (1300.00 C, 1 atm, S1, a=0.78134)
```

List Window – a Summary of Activities of Cr and Cu in Liquid Alloy

1373.15 K

List - Equilib T(K) = 1373.15, P(atm) = 1 (Page 1/3)

File Edit Help

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

+	Code	Species	Data	Phase	Mole	Fraction	Activity	Range	T	V
#1a	4	Cr(liq)		liquid	**1.1243E-02**	1.8394E-02	1.8394E-02	298 - 6000		
#1	5	Cu(liq)		liquid	0.6000	0.9816	9.8161E-01	298 - 4000		
+	6	Cr(s)		solid	0.3888		1.0000E+00	298 - 2181		
+	7	Cu(s)		solid			9.6909E-01	298 - 2001		

Properties:	H(J)	V(l)	S(J)	G(J)
	4.0486E+04	0.0000E+00	7.8656E+01	-6.752E+04

Show – Species: gas 3, liquid 2, aqueous 0, solid 2, solution 0; duplicate

Format: mole, gram, pound

Order: code, amount, fraction

Page: 1 of

1473.15 K

List - Equilib T(K) = 1473.15, P(atm) = 1 (Page 2/3)

File Edit Help

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

+	Code	Species	Data	Phase	Mole	Fraction	Activity	Range	T	V
#1a	4	Cr(liq)		liquid	**2.6281E-02**	4.1963E-02	4.1963E-02	298 - 6000		
#1	5	Cu(liq)		liquid	0.6000	0.9580	9.5804E-01	298 - 4000		
+	6	Cr(s)		solid	0.3737		1.0000E+00	298 - 2181		
+	7	Cu(s)		solid			8.7519E-01	298 - 2001		

1573.15 K

List - Equilib T(K) = 1573.15, P(atm) = 1 (Page 3/3)

File Edit Help

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

+	Code	Species	Data	Phase	Mole	Fraction	Activity	Range	T	V
#1a	4	Cr(liq)		liquid	**5.6568E-02**	8.6158E-02	8.6158E-02	298 - 6000		
#1	5	Cu(liq)		liquid	0.6000	0.9138	9.1384E-01	298 - 4000		
+	6	Cr(s)		solid	0.3434		1.0000E+00	298 - 2181		
+	7	Cu(s)		solid			7.8134E-01	298 - 2001		

Compare Cr concentration in liquid alloy with **liquidus** in the binary phase diagram **Cu - Cr** (see earlier slide 12.6).

Standard equilibrium with **ideal aqueous solution**

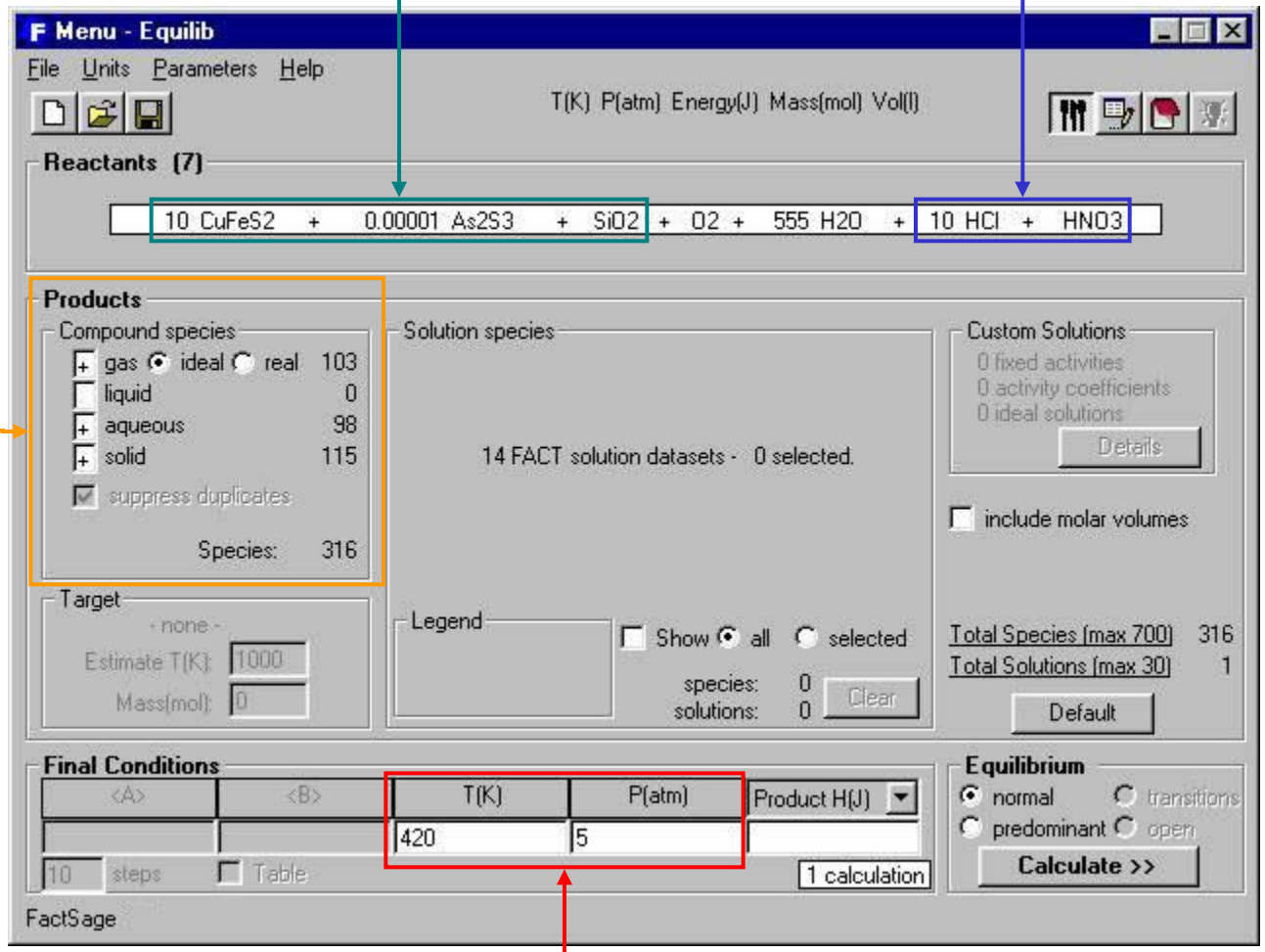
In the following four slides is shown how use is made of the ideal aqueous solution data for elevated temperatures and pressures.

The leaching of an arsenic-bearing copper concentrate is used as an example.

Leaching of an **arsenic-bearing copper concentrate**.

Arsenic-bearing copper concentrate

Leaching agent



- Two **ideal solutions**: **gas** and **aqueous**;
- and **pure solids**.

Elevated **T** and **P**

Results Window ***FACT*** output for the leaching of an **copper concentrate**

The **ideal gas phase** species

The **reactants**

X_{H_2O} = 0.80267

P_{total}= 5.0 atm

P_{H_2O}=X_{H_2O}×P_{total}

= 4.01335 atm

Results - Equilib 420 K

Output Edit Show Pages

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

```
10 CuFeS2 +  0.00001 As2S3 +  SiO2 +  O2 +

555 H2O +  10 HCl +  HNO3 =

 2.5127      mol    gas_ideal
 (50.243 gram, 2.5127 mol, 17.319 litre, 2.9010E-03 g/ml)
         (420.00 K, 5.0000 atm,      a=1.0000)
         ( 0.80267          H2O
         + 0.19645          N2
         + 8.3323E-04       HCl
         + 3.6799E-05       H2S
         + 1.1202E-05       SO2
         + 1.9588E-08       H2
         + 1.1690E-09       H2S2
         + 1.8411E-11       NH3
         + 7.6705E-12       S2
         + 2.8331E-12       SSO
         + 1.9110E-12       AsCl3
         + 2.4814E-13       O2S(OH)2
         + 1.8916E-14       S3
         + 1.4254E-14       S6
         + 1.0119E-14       S5
         + 5.4158E-16       S4
         + 2.1855E-16       S7
         + 1.0487E-16       S8
         + 2.0818E-18       SO3
         + 1.2796E-18       HS
         + 1.2002E-18       (CuCl)3
         + 5.4338E-19       S2Cl
         + 4.1955E-19       SO
         + 1.9349E-19       FeCl2
         + 7.7813E-20       FeCl3
```

Results Window ***FACT*** output for the leaching of an **copper concentrate**

The **aqueous phase** species

Results - Equilib 420 K

Output Edit Show Pages

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

```
+ 572.59      mol    aqueous
  (10562. gram, 572.59 mol)
          (420.00 K, 5.0000 atm,      a=1.0000)
          ( 55.508          H2O_liquid
          + 0.99659         Cl[-]
          + 0.49922         H[+]
          + 0.27833         Fe[2+]
          + 5.7123E-02      HSO4[-]
          + 3.9014E-03      H2SiO3
          + 2.6500E-03      H4SiO4
          + 2.3850E-03      CuCl2[-]
          + 5.5119E-04      N2
          + 1.7640E-04      NH4[+]
          + 2.6074E-05      FeOH[+]
          + 1.7237E-05      FeCl[2+]
          + 9.8844E-06      SO4[2-]
          + 3.2141E-06      SO2
          + 2.0032E-06      HAsO2
          + 1.4189E-06      H2S
          + 1.0769E-07      FeSO4[+]
          + 5.8077E-08      Cu[2+]
          + 5.1425E-08      Cu[+]
          + 7.5367E-09      FeOH[2+]
          + 6.2607E-09      HSO3[-]                                T
          + 4.9609E-09      Fe[3+]
          + 1.1912E-10      H2
          + 7.7669E-11      NH3                                    T
          + 8.8103E-12      H3AsO4
          + 4.0157E-12      OH[-]
          + 2.1088E-12      HS[-]
          + 1.4788E-13      H2AsO3[-]
          + 6.6921E-14      S2O3[2-]
          + 2.3011E-14      AsO2[-]
          + 1.8380E-14      H2AsO4[-]
          + 2.7937E-15      Cu(NH3)[2+]
          + 1.9635E-17      SO3[2-]                                T
          + 1.8821E-17      Fe2(OH)2[4+]
          + 4.4156E-18      S4O6[2-]
          (Eh= 0.267 V, pH= 0.302)
```

Important:
in **aqueous solutions** the solutes are given with respect to 55.5 mol(1000 g or 1L) of water. Hence, the values are molalities.
For example:
mH[+] = 0.49922 hence
pH = $-\log_{10}$ (**0.49922**) = **0.302**

Note the potential with respect to the standard **H_2(g)** electrode.

Results Window *FACT* output for the leaching of an copper concentrate

The **solid phase** species

Three **pure solids** at equilibrium with the **aqueous** and **gas** solutions.

Results - Equilib 420 K

Output Edit Show Pages

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

```
+ 7.2207      mol    FeS2_pyrite
  (866.33 gram, 7.2207 mol)
          (420.00 K, 5.0000 atm, S1, a=1.0000)

+ 4.9881      mol    Cu2S_solid-b
  (793.89 gram, 4.9881 mol)
          (420.00 K, 5.0000 atm, S2, a=1.0000)

+ 0.46729     mol    H6Si2O7_solid                                    T
  (81.410 gram, 0.46729 mol)
          (420.00 K, 5.0000 atm, S1, a=1.0000)

+ 0.00000     mol    H4SiO4_solid                                     T
          (420.00 K, 5.0000 atm, S1, a=0.94946)

+ 0.00000     mol    Cu2S_solid-c
          (420.00 K, 5.0000 atm, S3, a=0.92489)

+ 0.00000     mol    Cu2S_chalcocite
          (420.00 K, 5.0000 atm, S1, a=0.87898)

+ 0.00000     mol    H2SiO3_solid                                     T
          (420.00 K, 5.0000 atm, S1, a=0.71769)

+ 0.00000     mol    SiO2_quartz(l)
          (420.00 K, 5.0000 atm, S1, a=0.61402)

+ 0.00000     mol    FeAsS_solid                                      T
          (420.00 K, 5.0000 atm, S1, a=1.1800E-20)

The cutoff concentration has been specified to 1.0000E-75

Data on 32 product species identified with "T" have been extrapolated

*****************************************************************
      H            G            V            S            Cp
     (J)          (J)        (litre)      (J/K)        (J/K)
*****************************************************************
-1.59216E+08 -1.82429E+08  1.73194E+01  5.52696E+04  5.38310E+04
```

Standard equilibrium with **dilute solution phase**

The following two slides show the use of a **dilute metallic liquid** phase from the ***FTdemo*** database, here Fe-liq, in the ***Equilib*** module.

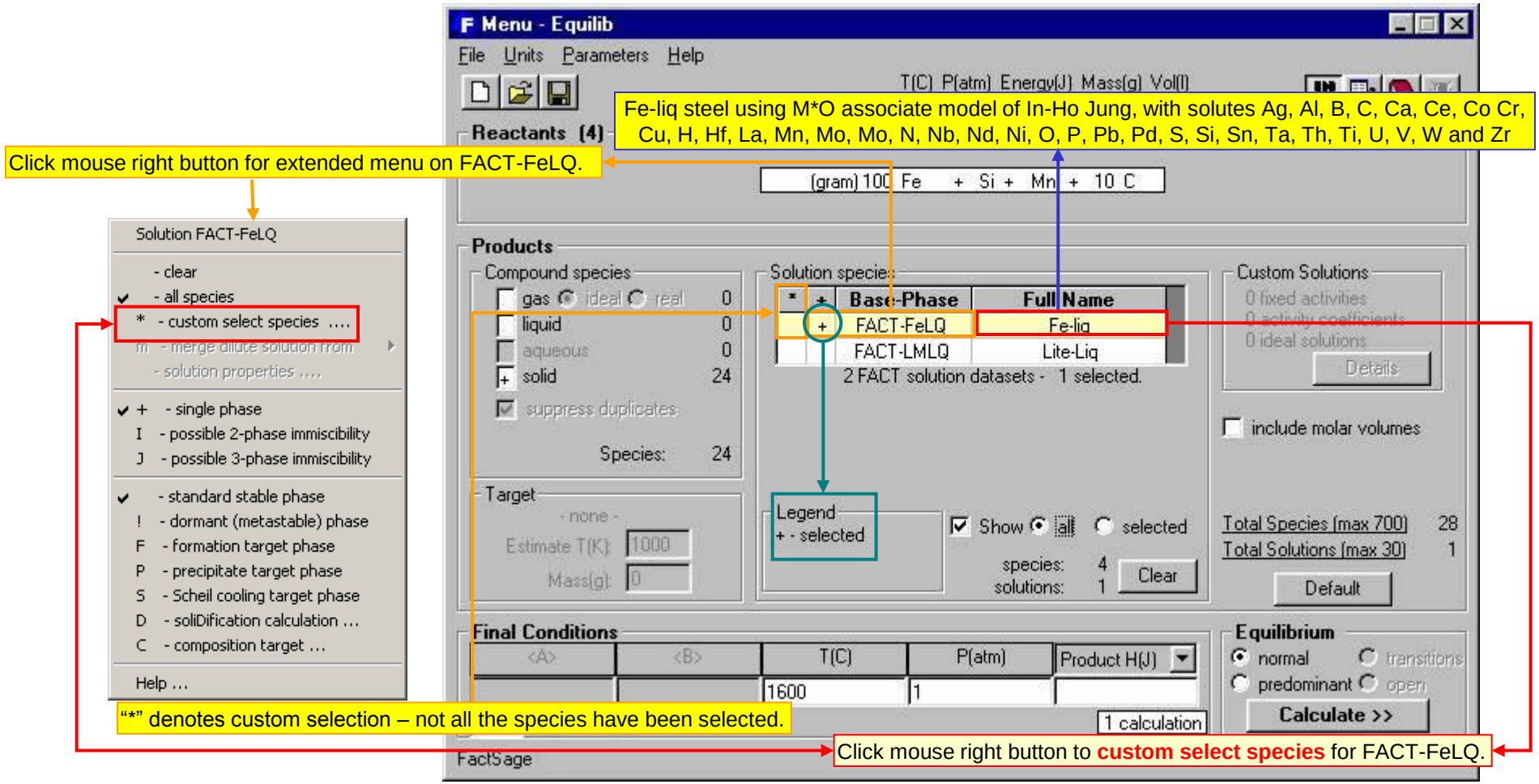
Selection of *FTdemo* Non-Ideal Solutions: FTdemo-FeLQ. The Menu Window Interface.

A click in the «**Fe-liq**» cell gives (note that all this info appears in the «**Custom Select Species**» window):

full title name: FACT Solution Phase FeLQ

short description of the complete solution phase: Fe-liq steel using M*O associate model of In-Ho Jung, with solutes Ag,Al,B,C,Ca, Ce,Co,Cr,Cu,H,Hf,La,Mn,Mo,N,Nb,Nd,Ni,O,P,Pb,Pd,S,Si,Sn,Ta,Th,Ti,U,V,W and Zr

list of possible components for the current system: 44 Fe, 45 C, 46 Mn, 47 Si



Results Window *FACT* format output –solubility of **C** in liquid cast iron

F Results - Equilib 1600 C

Output Edit Show Pages

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

```
(gram) 100 Fe +  Si +  Mn +  10 C =

 107.14      gram  Fe-liq
 (107.14 gram, 2.2727 mol)
         (1600.00 C, 1 atm,      a=1.0000)
         ( 93.332      wt.% Fe
         + 4.8012      wt.% C
         + 0.93332     wt.% Mn
         + 0.93332     wt.% Si)

         System component        Mole fraction  Mass fraction
         Fe                        0.78787        0.93332
         Mn                        8.0091E-03     9.3332E-03
         Si                        1.5667E-02     9.3332E-03
         C                         0.18845        4.8012E-02

+ 4.8558      gram  C_graphite
  (4.8558 gram, 0.40428 mol)
         (1600.00 C, 1 atm, S1, a=1.0000)

+ 0.00000     gram  Fe_bcc                                      T
         (1600.00 C, 1 atm, S1, a=0.59271)

+ 0.00000     gram  Fe_fcc                                      T
         (1600.00 C, 1 atm, S2, a=0.58794)

+ 0.00000     gram  C_diamond
         (1600.00 C, 1 atm, S2, a=0.52980)

+ 0.00000     gram  Fe3C_solid-a                                X
         (1600.00 C, 1 atm, S1, a=0.28650)

*****************************************************************
      H            G            V            S            Cp
     (J)          (J)        (litre)      (J/K)        (J/K)
*****************************************************************
 1.78129E+05 -2.64690E+05  0.00000E+00  2.36404E+02  1.22050E+02
```

Compositions in the **liquid solution** phase **Fe-liq** are given in weight percent (wt. %).

The amount of:

- **Fe** is 100.00 g = 93.332 % × 107.14 g
- **Mn** is 1.00 g = 0.93332 % × 107.14 g
- **Si** is 1.00 g = 0.93332 % × 107.14 g
- **C** is 5.1440 g = 4.8011 % × 107.14 g

Compositions of the solution in **mole** and **mass** fraction

Graphite saturation

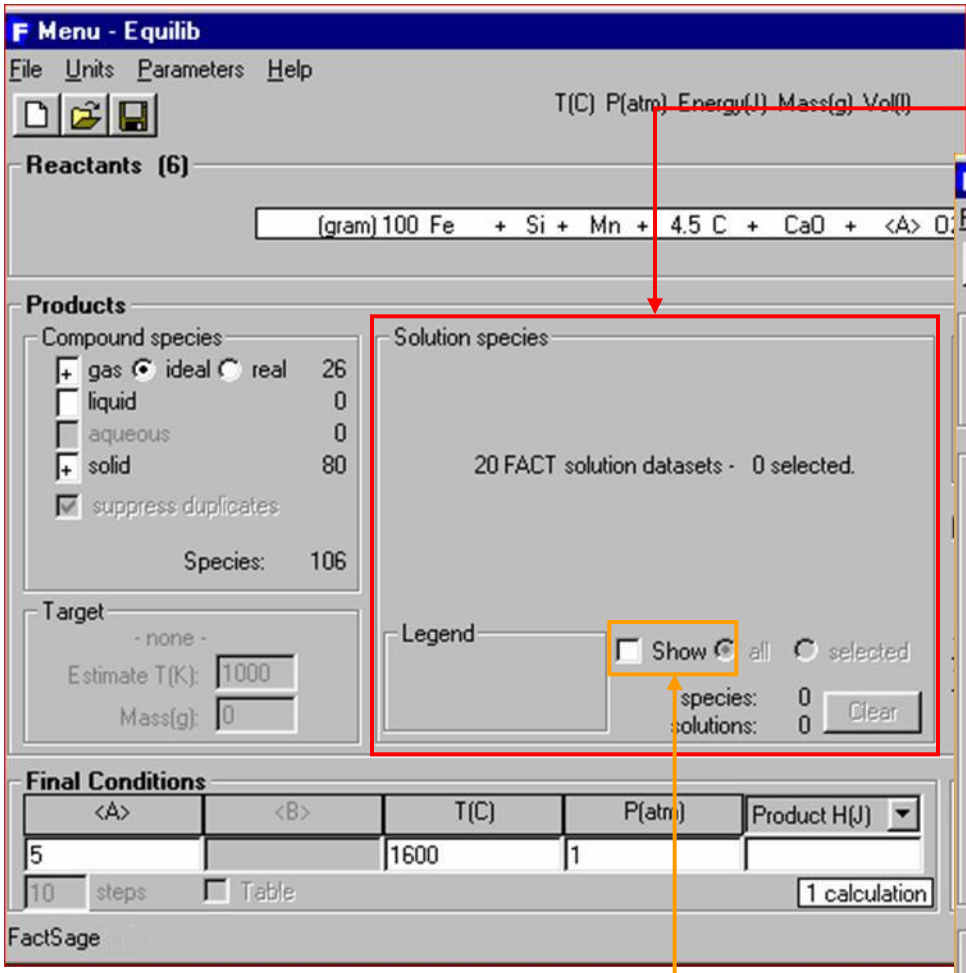
Adding a slag to the Fe-Mn-Si-C system

The following six slides are devoted to a special case in the ***FTdemo*** database: The use of a slag phase when several options concerning the composition of the slag (SlagA, SlagB, Slag?) are available.

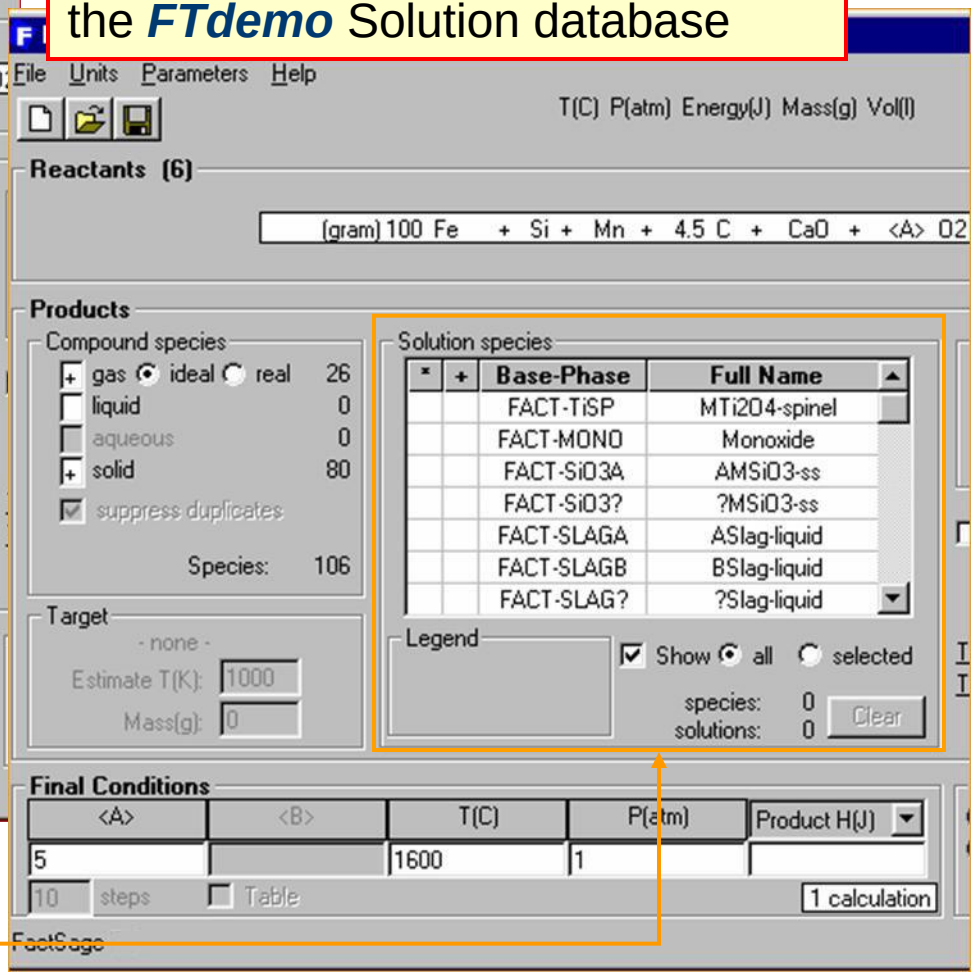
Here the ***FTdemo*** database (called **FACT** in some of the slides) is used for purposes of teaching. Since the results can be imprecise and even totally wrong you must **never** publish results that employ ***FTdemo*** data.

For research and publications use the protected public databases that are regularly updated: **FactPS**, **FToxid** etc.

FTdemo Non-Ideal Solutions: Listing the available solution datasets.



There are **20 solution datasets** available for this mix of reactants in the ***FTdemo*** Solution database



To see the list of Solution species:
Check «**Show**» and select «**all**»
Then scroll through the list.

More information about the available slag and liquid iron solution phases.

Solution species

*	+	Base-Phase	Full Name
		FACT-TiSP	MTi2O4-spinel
		FACT-MONO	Monoxide
		FACT-SiO3A	AMSiO3-ss
		FACT-SiO3?	?MSiO3-ss
		FACT-SLAGA	ASlag-liquid
		FACT-SLAGB	BSlag-liquid
		FACT-SLAG?	?Slag-liquid

Legend

☑ Show ◉ all ○ selected

species: 0
solutions: 0

Clear

*	+	Base-Phase	Full Name
		FACT-TiSP	MTi2O4-spinel
		FACT-MONO	Monoxide
		FACT-SiO3A	AMSiO3-ss
		FACT-SiO3?	?MSiO3-ss
		FACT-SLAGA	ASlag-liquid
		FACT-SLAGB	BSlag-liquid
		FACT-SLAG?	?Slag-liquid
		FACT-SPIN	Spinel
		FACT-oPyr	Orthopyroxene
		FACT-cPyr	Clinopyroxene
		FACT-pPyr	Protopyroxene
		FACT-WOLL	Wollastonite,
		FACT-Oli1	Olivine1
		FACT-MeO	Monoxide
		FACT-"C2S	a'Ca2SiO4
		FACT-Oli2	Olivine2
		FACT-Mel	Melilite
		FACT-FeLQ	Fe-liq
		FACT-CuLQ	Cu-liq
		FACT-LMLQ	Lite-Liq

Possible «**solutions**» for the calculation.

FACT Solution Phase SLAG?

?Slag-liquid oxide.- Miscibility gap at high SiO2;
Al,As,B,Ca,Cr,Cu,Fe,K,Mg,Mn,Na,Ni,Pb,Si,Ti,Zn,Zr; dilute S,SO4,PO4,H2O/OH,CO3,F,Cl,I

141 FeO, 142 MnO, 143 SiO2, 144 CaO, 145 Fe2O3, 146 CaCO3

IMPORTANT MESSAGE! - The solution phase FACT-SLAG? has unique properties which make the selection of species very important. If species are not selected correctly then unsatisfactory or totally incorrect results may result - the program may even crash! This often happens when you select all the species. (Selecting all the species in other ?-type solution phases may be acceptable.)

If you insist on using FACT-SLAG? you must:

(1) never select a non-oxide component (e.g. CaS) without also selecting the corresponding oxide (e.g. CaO);
(2) ensure that all combinations of cations and anions are selected for non-oxide components. This may entail removing certain components from the species selection.

For example, MgS, CaS and CaCO3 are all components of FACT-SLAG? but MgCO3 is not. If your reactants include Mg, Ca, S, C and O, then MgS, CaS and CaCO3 will appear in the list of components of FACT-SLAG? but MgCO3 will not. Hence, to respect this rule You must remove either CaCO3 or MgS from your selected components of FACT-SLAG?See the Equilib manual for more information

FACT Solution Phase SLAGA

ASlag-liquid oxide.- Miscibility gap at high SiO2;
Al,As,B,Ca,Cr,Cu,Fe,K,Mg,Mn,Na,Ni,Pb,Si,Ti,Zn,Zr; dilute S,SO4,PO4,H2O/OH,CO3,F,Cl,I

133 FeO, 134 MnO, 135 SiO2, 136 CaO, 137 Fe2O3

FACT Solution Phase SLAGB

BSlag-liquid oxide.- Miscibility gap at high SiO2;
Al,As,B,Ca,Cr,Cu,Fe,K,Mg,Mn,Na,Ni,Pb,Si,Ti,Zn,Zr; dilute S,SO4,PO4,H2O/OH,CO3,F,Cl,I

138 SiO2, 139 CaO, 140 CaCO3

FACT Solution Phase FeLQ

Fe-liq steel using M*O associate model of In-Ho Jung, with solutes Ag,Al,B,C,Ca, Ce,Co,Cr,Cu,H,Hf,La,Mn,Mo,N,Nb,Nd,Ni,O,P,Pb,Pd,S,Si,Sn,Ta,Th,Ti,U,V,W and Zr

177 Fe, 178 C, 179 Ca, 180 Mn, 181 O, 182 Si, 183 CaO,
184 SiO, 185 MnO

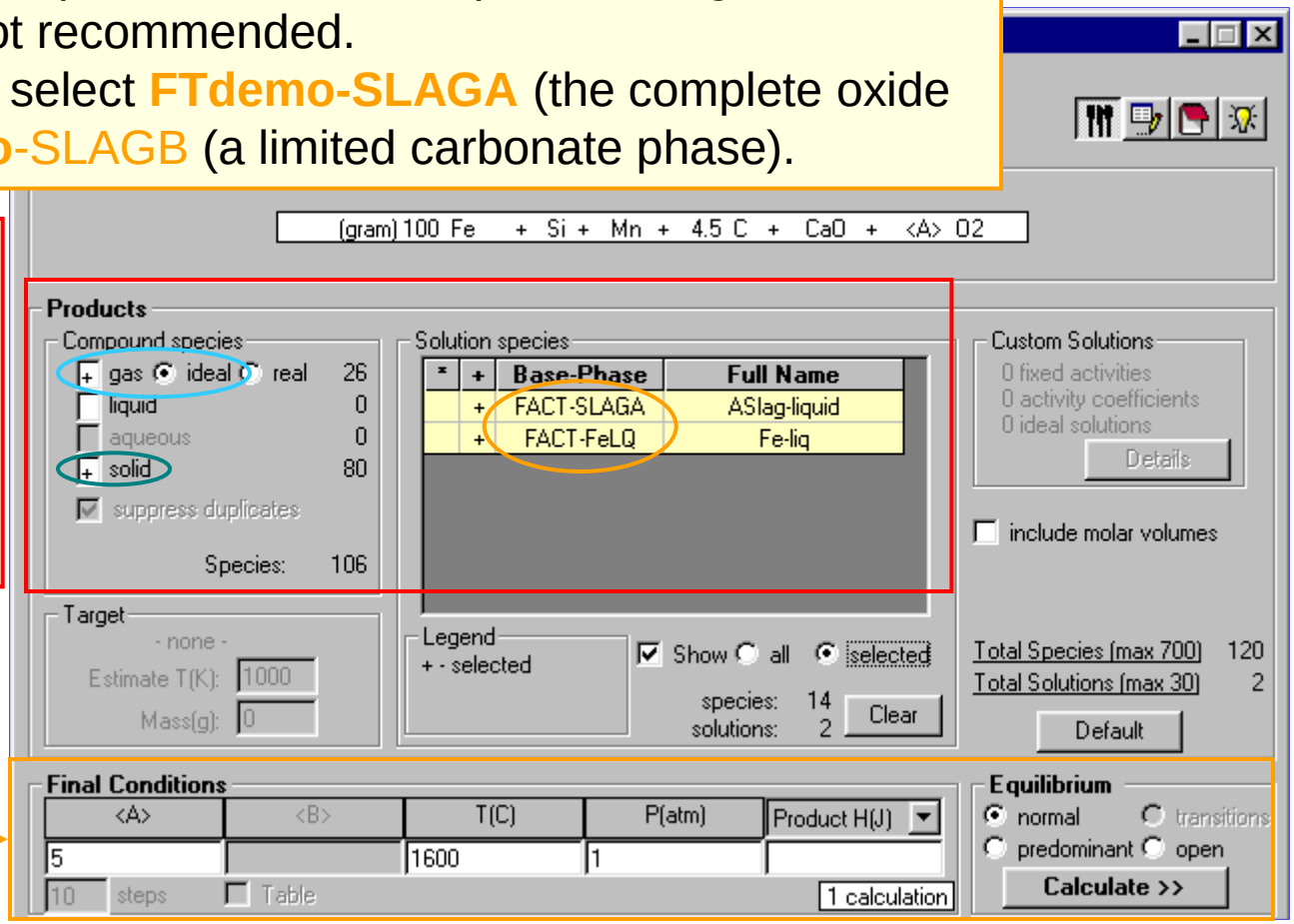
You can select only one phase in a list of phases with 5-character names differing only by their last character. Here, **SLAGA**, **SLAGB** and **SLAG?** are mutually exclusive.

Selection of the solution phases for the decarburisation of pig iron by oxygen injection

There are 3 subsets of the solution phase **FTdemo-SLAG**: **FTdemo-SLAG?**; **FTdemo-SLAGA**; **FTdemo-SLAGB**. Only one can be selected. The reason why there are solution subsets is because not all the binary, ternary systems, etc…, in the complete solution have been optimized yet. «**?**» indicates that not all the species have been optimized together and a selection of this phase is not recommended.
In the present example, we select **FTdemo-SLAGA** (the complete oxide phase) rather than **FTdemo-SLAGB** (a limited carbonate phase).

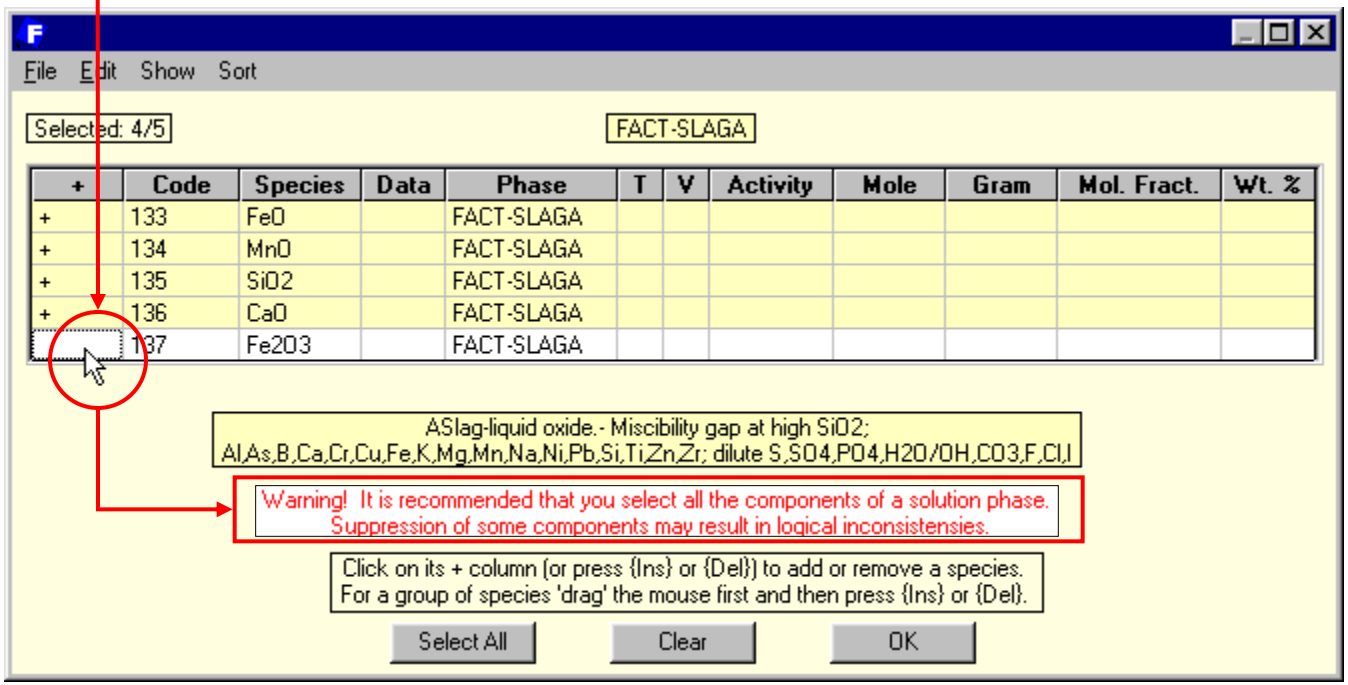
Selection of 2 liquid solution phases: **FTdemo-SLAGA**, **FTdemo-FeLQ**; and 2 phases: **ideal gas** and **pure solids**.

Enter the **Final Conditions** and **Calculate >>**



FACT Non-Ideal Solutions: **warning** about the **modification** of a **solution phase**.

You can examine or **modify** a **solution phase** but …



Decarburisation of pig-iron by oxygen injection (**Results** window, ***FACT*** format)

Reactants, <A>= 5

```
(gram) 100 Fe +  Si +  Mn +  4.5 C +

(gram) CaO +  <A> O2 =
```

Almost 100 % **CO**(g)

```
  0.28749    mol    gas_ideal
  (8.0622 gram, 0.28749 mol, 44.189 litre, 1.8245E-04 g/ml)
          (1600.00 C, 1 atm,      a=1.0000)
          ( 0.99829          CO
          + 1.0683E-03       CO2
          + 4.3787E-04       Mn
          + 1.2864E-04       SiO
          + 7.6075E-05       Fe
          + 1.0099E-07       Ca
          + 4.5825E-09       FeO
          + 2.5893E-10       Si
          + 1.0455E-10       O
          + 2.2742E-11       C2O
          + 8.8670E-12       C3O2
          + 5.9586E-12       CaO
```

- Less **C** in liquid steel because **C** has mostly gone into the **gas phase**.
- Less **Si** in liquid steel because of its oxidation into the **slag**.

```
+ 102.68     gram  Fe-liq
  (102.68 gram, 1.9193 mol)
          (1600.00 C, 1 atm,      a=1.0000)
          ( 97.387      wt.% Fe
          + 1.0218      wt.% C
          + 6.4813E-09 wt.% Ca
          + 0.94517     wt.% Mn
          + 3.5854E-03 wt.% O
          + 0.64240     wt.% Si
          + 5.9566E-05 wt.% CaO
          + 2.5773E-05 wt.% SiO
          + 1.9972E-04 wt.% MnO)
```

CaO addition promotes **slag** formation.

```
+ 1.7589     gram  ASlag-liquid
  (1.7589 gram, 3.0379E-02 mol)
          (1600.00 C, 1 atm,      a=1.0000)
          ( 0.23228     wt.% FeO
          + 1.6469      wt.% MnO
          + 41.272      wt.% SiO2
          + 56.849      wt.% CaO
          + 1.6020E-04 wt.% Fe2O3)
```

No **solid** phases

```
+ 0.00000    gram  Ca2SiO4_alpha
          (1600.00 C, 1 atm, S3, a=0.92741)

+ 0.00000    gram  Fe_bcc                                    T
          (1600.00 C, 1 atm, S1, a=0.88829)

+ 0.00000    gram  Fe_fcc                                    T
          (1600.00 C, 1 atm, S2, a=0.88115)
```

Decarburisation of pig-iron by oxygen injection (**Results** window, ***ChemSage*** format)

```
T = 1600.00 C
P = 1.00000E+00 atm
V = 4.41890E+01 dm3

STREAM CONSTITUENTS        AMOUNT/gram
Fe                          1.0000E+02
Si                          1.0000E+00
Mn                          1.0000E+00
C                           4.5000E+00
CaO                         1.0000E+00
O2                          5.0000E+00

                           EQUIL AMOUNT  MOLE FRACTION     FUGACITY
PHASE: gas_ideal               mol                          atm
CO                          2.8700E-01     9.9829E-01    9.9829E-01
CO2                         3.0713E-04     1.0683E-03    1.0683E-03
Mn                          1.2588E-04     4.3787E-04    4.3787E-04
SiO                         3.6983E-05     1.2864E-04    1.2864E-04
Fe                          2.1871E-05     7.6075E-05    7.6075E-05
Ca                          2.9034E-08     1.0099E-07    1.0099E-07
FeO                         1.3174E-09     4.5825E-09    4.5825E-09
Si                          7.4440E-11     2.5893E-10    2.5893E-10
O                           3.0057E-11     1.0455E-10    1.0455E-10
TOTAL:                      2.8749E-01     1.0000E+00    1.0000E+00
```

```
PHASE: Fe-liq                   gram       MASS FRACTION     ACTIVITY
Fe                          9.9996E+01     9.7387E-01     9.1571E-01
C                           1.0492E+00     1.0218E-02     4.7424E-02
Ca                          6.6550E-09     6.4813E-11     1.0099E-07
Mn                          9.7049E-01     9.4517E-03     8.2974E-03
O                           3.6815E-03     3.5854E-05     4.4139E-07
Si                          6.5961E-01     6.4240E-03     2.9403E-05
CaO                         6.1162E-05     5.9566E-07     5.5779E-07
SiO                         2.6463E-05     2.5773E-07     3.0699E-07
MnO                         2.0507E-04     1.9972E-06     1.4784E-06
TOTAL:                      1.0268E+02     1.0000E+00     1.0000E+00
PHASE: ASlag-liquid             gram       MASS FRACTION     ACTIVITY
FeO                         4.0857E-03     2.3228E-03     5.4914E-03
MnO                         2.8968E-02     1.6469E-02     1.4302E-02
SiO2                        7.2595E-01     4.1272E-01     6.5166E-02
CaO                         9.9994E-01     5.6849E-01     5.7071E-03
Fe2O3                       2.8177E-06     1.6020E-06     3.4992E-10
TOTAL:                      1.7589E+00     1.0000E+00     1.0000E+00
                                gram                         ACTIVITY
Ca2SiO4_alpha(s3)           0.0000E+00                     9.2741E-01
Fe_bcc(s)                 T 0.0000E+00                     8.8829E-01
Fe_fcc(s2)                T 0.0000E+00                     8.8115E-01
```

A standard case with slag-metal input plus additives

The following six slides show how the ***Equilib*** module is applied to a steel metallurgical question involving a liquid Fe-based solution, a slag phase, a gas phase based on argon and the addition of CaSi to treat the sulfur content of the Fe-liquid phase.

Desulfurizing a steel by CaSi addition. Reactants entry.

Starting composition of the steel melt

Note the use of the variable amount <A> for the slag.

Calcium silicide addition

Reactants - Equilib

File Edit Table Units Data Search Help

T(C) P(atm) Energy(J) Mass(g) Vol(l)

1 - 10 | 11 - 13

Mass(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
100	Fe	solid-1 bcc	1000	1.0	1	FACT
0.1	C	solid-1 graphite	1000	1.0	1	FACT
0.2	Si	solid	1000	1.0	1	FACT
1.5	Mn	solid-1	1000	1.0	1	FACT
0.02	S	solid-1 orthorhombic	1000	1.0	1	FACT
0.05	Al	solid	1000	1.0	1	FACT
<40A>	CaO	solid lime	1000	1.0	1	FACT
<10A>	SiO2	solid-1 quartz(l)	1000	1.0	1	FACT
<20A>	Al2O3	solid-1 gamma	1000	1.0	1	FACT
<10A>	MnO	solid	1000	1.0	1	FACT

initial conditions

Next >>

FactSage 5.0 Compound: 1/6 database(s) Solution: 1/5 database(s)

1 - 10 | 11 - 13

Mass(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
<5A>	FeO	solid wustite	1000	1.0	1	FACT
0.2	CaSi	solid	1000	1.0	1	FACT
0.04	Ar	gas	1000	1.0	1	FACT

«initial conditions» Default Values and Stream Features

1 - 10 | 11 - 13

	Mass(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
	100	Fe	solid-1 bcc	1000	1.0	1	FACT
+	0.1	C	solid-1 graphite	1000	1.0	1	FACT
+	0.2	Si	solid	1000	1.0	1	FACT
+	1.5	Mn	solid-1	1000	1.0	1	FACT
+	0.02	S	solid-1 orthorhombic	1000	1.0	1	FACT
+	0.05	Al	solid	1000	1.0	1	FACT
+	<40A>	CaO	solid lime	1000	1.0	1	FACT
+	<10A>	SiO2	solid-1 quartz(l)	1000	1.0	1	FACT
+	<20A>	Al2O3	solid-1 gamma	1000	1.0	1	FACT
+	<10A>	MnO	solid	1000	1.0	1	FACT

☐ initial conditions

Stream# boxes

«**initial conditions**» check box

These are the defaults values for the reactant species when the «**initial conditions**» box has been checked.

- Specifying initial conditions is only useful if you want to calculate or constrain changes in the extensive properties (ΔV, ΔH, etc…). You have to select, for each reactant species, the phase, the temperature, the total pressure and the stream number.
- All reactants in a given **stream** are grouped together, they have the same temperature and total pressure. If you change the temperature (or pressure) of any one member of the stream, then the temperature (or pressure) of all the other members of the stream will be changed to the same common value.

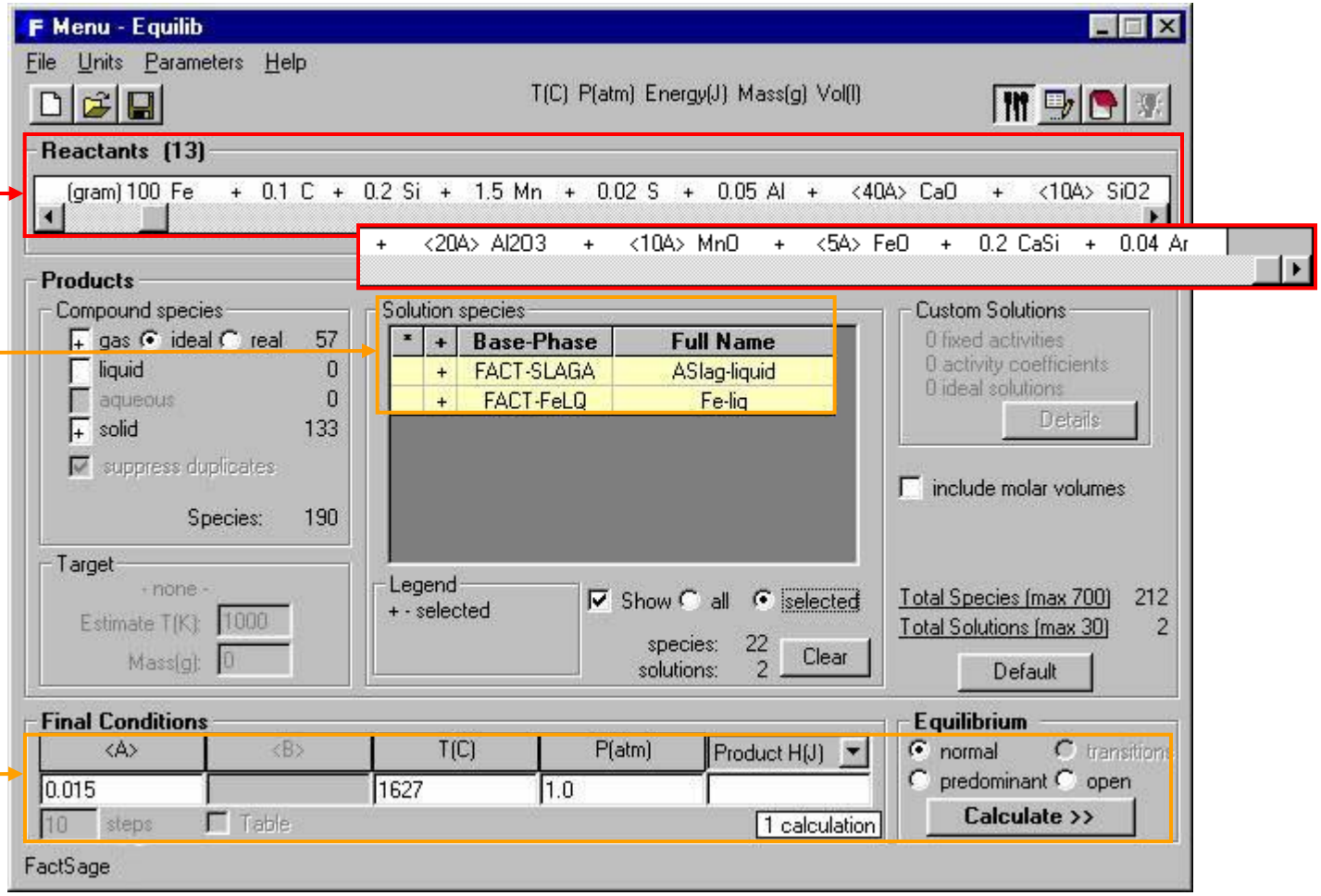
Desulfurizing a steel by CaSi addition, selection of solution phases and final conditions

Summary of the **Reactants** window

Solution species selected

Final conditions:
- <A> = 0.015
- T = 1627°C
- P = 1 atm

and **Calculate >>**



Desulfurizing a Steel by CaSi Addition. *FACT* Format Results.

```
(gram) 100 Fe +  0.1 C +  0.2 Si +  1.5 Mn +

(gram) 0.02 S +  0.05 Al +  <40A> CaO +  <10A> SiO2 +

(gram) <20A> Al2O3 +  <10A> MnO +  <5A> FeO +  0.2 CaSi +

(gram) 0.04 Ar =

  1.0069E-03 mol   gas_ideal
  (4.0188E-02 gram, 1.0069E-03 mol, 0.15699 litre, 2.5599E-04 g/ml)
          (1627.00 C, 1 atm,     a=1.0000)
          ( 0.99448          Ar
          + 4.3098E-03       CO
          + 1.0377E-03       Mn
          + 1.1361E-04       Fe)

+ 102.09     gram  Fe-liq
  (102.09 gram, 1.8407 mol)
          (1627.00 C, 1 atm,     a=1.0000)
          ( 98.008     wt.% Fe
          + 2.0738E-02 wt.% Al
          + 9.7900E-02 wt.% C
          + 1.5825     wt.% Mn
          + 1.1478E-04 wt.% O
          + 9.2123E-04 wt.% S
          + 0.28770    wt.% Si
          + 2.1753E-03 wt.% CaO
          + 1.2349E-04 wt.% AlO)

+ 1.2528     gram  ASlag-liquid
  (1.2528 gram, 1.9174E-02 mol)
          (1627.00 C, 1 atm,     a=1.0000)
          ( 1.5496E-02 wt.% FeO
          + 4.7420E-02 wt.% MnO
          + 10.041     wt.% SiO2
          + 58.191     wt.% CaO
          + 28.282     wt.% Al2O3
          + 3.4200     wt.% CaS
          + 8.6622E-04 wt.% FeS
          + 2.6569E-03 wt.% MnS)

+ 0.00000    gram  Fe_bcc                                          T
          (1627.00 C, 1 atm, S1, a=0.93200)

+ 0.00000    gram  Fe_fcc                                          T
          (1627.00 C, 1 atm, S2, a=0.92352)
```

Gas phase, mainly **Ar**

Two liquid solutions:
- **liquid steel**
- slag containing **sulfur**

No **solid** phases (activity<1)

Desulfurizing a Steel by CaSi Addition. *ChemSage* Format Results (4 parts)

1

2

Final Conditions

```
T = 1627.00 C
P = 1.00000E+00 atm
V = 1.56992E-01 dm3
```

STREAM CONSTITUENTS	AMOUNT/gram
Fe	1.0000E+02
C	1.0000E-01
Si	2.0000E-01
Mn	1.5000E+00
S	2.0000E-02
Al	5.0000E-02
CaO	6.0000E-01
SiO2	1.5000E-01
Al2O3	3.0000E-01
MnO	1.5000E-01
FeO	7.5000E-02
CaSi	2.0000E-01
Ar	4.0000E-02

STREAM CONSTITUENTS or **AMOUNT** of reactants

PHASE: ASlag-liquid	gram	MASS FRACTION	ACTIVITY
FeO	1.9414E-04	1.5496E-04	4.0994E-04
MnO	5.9407E-04	4.7420E-04	1.7391E-03
SiO2	1.2579E-01	1.0041E-01	7.0978E-05
CaO	7.2901E-01	5.8191E-01	1.5263E-01
Al2O3	3.5431E-01	2.8282E-01	2.2932E-03
CaS	4.2845E-02	3.4200E-02	2.2633E-01
FeS	1.0852E-05	8.6622E-06	8.5416E-05
MnS	3.3285E-05	2.6569E-05	7.5892E-04
Fe2O3	4.2893E-07	3.4238E-07	1.3290E-13
TOTAL:	1.2528E+00	1.0000E+00	1.0000E+00

Product solution slag (**SLAGA** or **Aslag-liquid**) phase

PHASE: gas_ideal	EQUIL AMOUNT mol	MOLE FRACTION	FUGACITY atm
Ar	1.0013E-03	9.9448E-01	9.9448E-01
CO	4.3393E-06	4.3098E-03	4.3098E-03
Mn	1.0449E-06	1.0377E-03	1.0377E-03
Fe	1.1439E-07	1.1361E-04	1.1361E-04
TOTAL:	1.0069E-03	1.0000E+00	1.0000E+00

Product **gas** phase, mainly **Ar**

PHASE: Fe-liq	gram	MASS FRACTION	ACTIVITY
Fe	1.0006E+02	9.8008E-01	9.7290E-01
Al	2.1172E-02	2.0738E-04	2.7635E-05
C	9.9948E-02	9.7900E-04	2.5999E-03
Ca	1.9756E-06	1.9351E-08	5.8880E-05
Mn	1.6156E+00	1.5825E-02	1.5835E-02
O	1.1718E-04	1.1478E-06	3.8695E-08
S	9.4050E-04	9.2123E-06	3.0289E-06
Si	2.9372E-01	2.8770E-03	9.7811E-06
CaO	2.2208E-03	2.1753E-05	2.1505E-05
AlO	1.2607E-04	1.2349E-06	1.5928E-06
SiO	5.7320E-07	5.6145E-09	7.0605E-09
MnO	2.8232E-05	2.7653E-07	2.1611E-07
Al2O	8.4883E-06	8.3143E-08	6.5883E-08
TOTAL:	1.0209E+02	1.0000E+00	1.0000E+00

Product solution steel (**FELQ** or **Fe-liq**) phase

Desulfurizing a Steel by CaSi Addition. *ChemSage* Format Results (4 parts)

3

Fe_bcc(s)	T	0.0000E+00	9.3200E-01
Fe_fcc(s2)	T	0.0000E+00	9.2352E-01
CaO_lime(s)		0.0000E+00	8.1184E-01
Ca2SiO4_alpha(s3)		0.0000E+00	5.6742E-01
Ca2SiO4_alpha-prime(s2)		0.0000E+00	5.2332E-01
Ca3SiO5_hatrurite(s)		0.0000E+00	4.6746E-01
Ca3Al2O6_solid(s)	T	0.0000E+00	4.6140E-01
CaS_solid(s)		0.0000E+00	3.2418E-01
CaAl2O4_solid(s)	T	0.0000E+00	2.3861E-01
Ca2SiO4_gamma(olivine(s)	T	0.0000E+00	1.1372E-01
Ca2Al2SiO7_gehlenite(s)		0.0000E+00	4.2324E-02
CaSiO3_pseudowollast(s2)	T	0.0000E+00	1.5857E-02
CaSiO3_wollastonite(s)	T	0.0000E+00	1.3310E-02
Mn_solid_delta(s4)		0.0000E+00	1.3283E-02
Mn_solid_gamma(s3)	T	0.0000E+00	1.2718E-02
Mn_solid_beta(s2)	T	0.0000E+00	1.2098E-02
Mn_solid_alpha(s)	T	0.0000E+00	1.0501E-02
Al2O3_corundum(alpha(s4)		0.0000E+00	8.9409E-03
Ca3Si2O7_rankinite(s)		0.0000E+00	8.1167E-03
CaAl4O7_solid(s)		0.0000E+00	7.4420E-03
Al2O3_delta(s2)		0.0000E+00	7.2450E-03
Al2O3_kappa(s3)		0.0000E+00	7.1040E-03
Al2O3_gamma(s)		0.0000E+00	6.0336E-03
FeSi_solid(s)	T	0.0000E+00	4.8912E-03
Fe3C_solid-a(s)	!T	0.0000E+00	2.8713E-03
C_graphite(s)		0.0000E+00	2.5912E-03
Fe3C_solid-b(s2)	T	0.0000E+00	2.5499E-03
MnO_solid(s)		0.0000E+00	2.4679E-03
C_diamond(s2)		0.0000E+00	1.3741E-03
MnS_alabandite(s)	T	0.0000E+00	6.9359E-04
FeO_wustite(s)		0.0000E+00	3.0146E-04
CaAl2SiO6_ca-tscherma(s)		0.0000E+00	2.9535E-04
Al2MnO4_galaxite(spin(s)		0.0000E+00	1.3348E-04
Fe3Si_solid(s)	T	0.0000E+00	1.1037E-04

No pure **solid** phases

Cp_EQUIL	H_EQUIL	S_EQUIL	G_EQUIL	V_EQUIL
J.K-1	J	J.K-1	J	dm3
8.64294E+01	1.25535E+05	1.93301E+02	-2.41766E+05	1.56992E-01

Equilibrium thermodynamic values

4

Mass fraction of system components:

	gas_ideal	ASlag-liquid	Fe-liq
Fe	1.5897E-04	1.2620E-04	0.98008
Mn	1.4284E-03	3.8403E-04	1.5825E-02
Ca	5.9126E-05	0.43488	1.5566E-05
Ar	0.99533	0.00000	0.00000
S	3.8076E-08	1.5214E-02	9.2123E-06
Si	2.2998E-06	4.6935E-02	2.8770E-03
Al	4.3642E-08	0.14968	2.0822E-04
O	1.7291E-03	0.35278	7.8972E-06
C	1.2970E-03	0.00000	9.7900E-04

Mass fractions of system components

A standard case with **aqueous solutions**

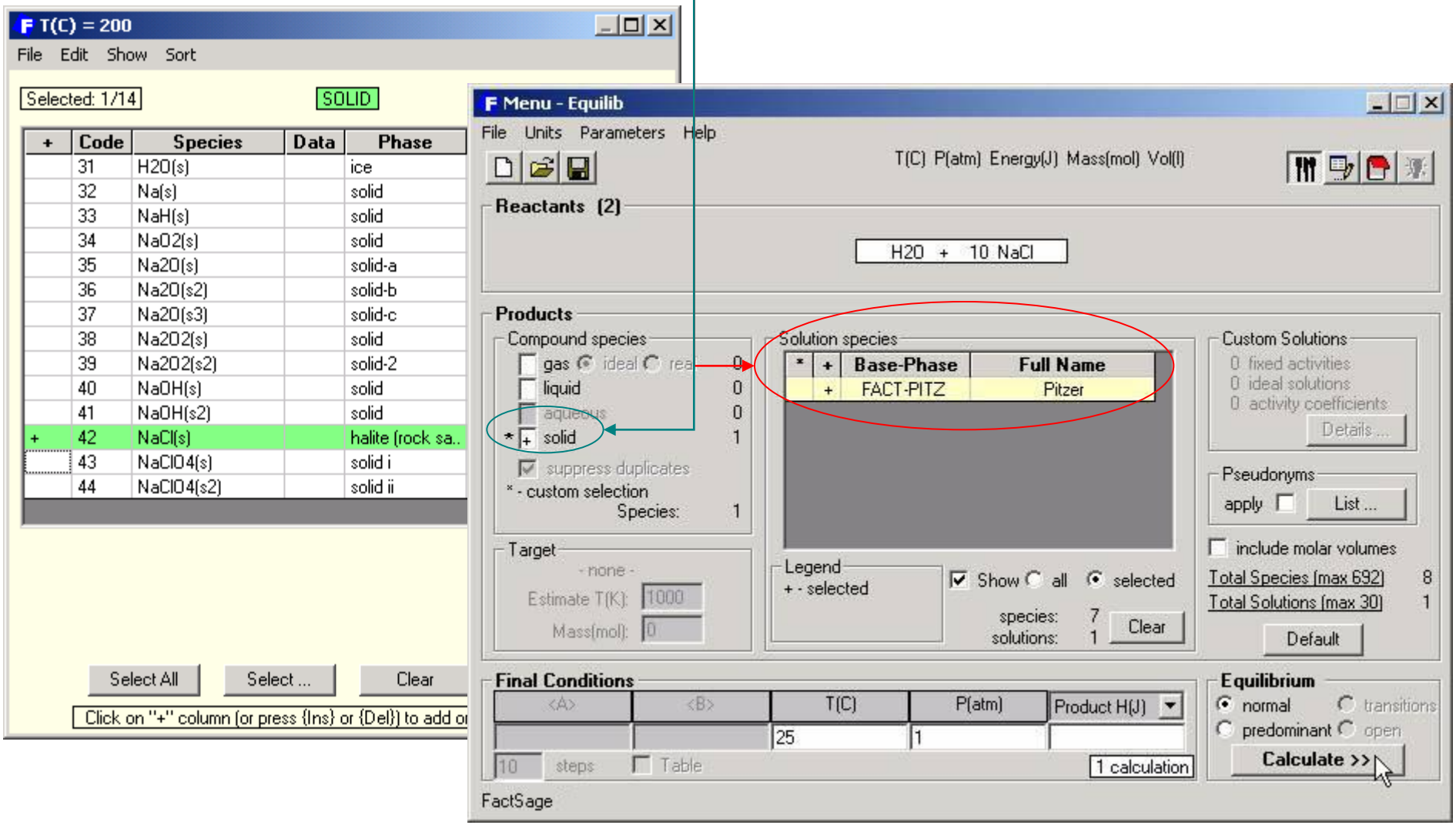
The following slides show how ***Equilib*** is used for calculations of equilibria in which a non-ideal aqueous phase is involved.

The aqueous phase is described by the Pitzer model which permits high concentrations of dissolved aqueous species to be treated.

In addition to listing the calculated aqueous concentrations, the results include the aqueous properties pH, Eh/V, Total solute molality, Ionic strength, Osmotic coefficient and Debye-Hueckel slope.

Non-Ideal Aqueous Solutions: FACT-PITZ (Pitzer)

Mixing **10 mol** of **NaCl** and **1 mol** of **water** at **25°C** and **1 atm** creates **brine** saturated in **NaCl**.



Solubility of NaCl in water – *FACT* format output

Aqueous phase results with respect to **55.508 mol H_2O** (i.e. **1 Kg H_2O**) hence in **molalities**.

F Results - Equilib 25 C

Output Edit Show Pages

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

```
H20 +  10 NaCl =

 1.2210      mol    Pitzer
 (24.473 gram, 1.2210 mol)
          (25.00 C, 1 atm,      a=1.0000)
          ( 55.508              H20
          + 5.4059E-08          H[+]
          + 6.1338              Na[+]
          + 6.1338              Cl[-]
          + 5.4059E-08          OH[-])
          (Eh=-1.355 V, pH= 6.597)

            + 9.8895      mol    NaCl_halite_(rock_salt_structure)
            (577.97 gram, 9.8895 mol)
            (25.00 C, 1 atm, S1, a=1.0000)

*****************************************************************
      H            G            V            S            Cp
     (J)          (J)        (litre)      (J/K)        (J/K)
*****************************************************************
-4.39654E+06 -4.63365E+06  0.00000E+00  7.95254E+02  5.73883E+02
```

$m_{H[+]}$ = **5.4059 x 10^{-8}**

Here the solubility of NaCl in water at 25°C is **m_{NaCl} = 6.1338 mol/kg H_2O**

Output > Format > *FACT* Format

$-\log_{10}$ (aH[+]) = 6.597

Solubility of NaCl in water – *ChemSage* format output

Results - Equilib 25 C

Output Edit Show Pages

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

Output > Format > *ChemSage* Format

```
T = 25.00 C
P = 1.00000E+00 atm
V = 0.00000E+00 dm3

STREAM CONSTITUENTS          AMOUNT/mol
H2O                          1.0000E+00
NaCl                         1.0000E+01

                            EQUIL AMOUNT     MOLALITY       ACTIVITY
PHASE: Pitzer                  mol
H2O                          1.0000E+00     5.5508E+01     7.5313E-01
H[+]                         9.7389E-10     5.4059E-08     2.5287E-07
Na[+]                        1.1050E-01     6.1338E+00     6.1529E+00
Cl[-]                        1.1050E-01     6.1338E+00     6.1529E+00
ClO4[-]                      NOT CALCD.     NOT CALCD.    <1.0000E-75
ClO3[-]                      NOT CALCD.     NOT CALCD.    <1.0000E-75
OH[-]                        9.7389E-10     5.4059E-08     2.9433E-08
TOTAL:                       1.2210E+00                    1.0000E+00
                               mol                          ACTIVITY
NaCl_halite_(rock_sal(s)     9.8895E+00                    1.0000E+00
NaH_solid(s)                 0.0000E+00                    1.0000E+00
H2O_ice(s)                 T 0.0000E+00                    5.9288E-01
NaOH_solid(s)                0.0000E+00                    2.3666E-14
NaOH_solid(s2)               0.0000E+00                    6.9593E-15
Na_solid(s)                  0.0000E+00                    6.5865E-23
Na2O_solid-a(s)              0.0000E+00                    5.9750E-53
Na2O_solid-b(s2)             0.0000E+00                    3.6158E-53
Na2O_solid-c(s3)             0.0000E+00                    9.3376E-55
*********************************************************************
  Cp_EQUIL       H_EQUIL        S_EQUIL        G_EQUIL        V_EQUIL
    J.K-1           J             J.K-1           J             dm3
*********************************************************************
 5.73883E+02  -4.39654E+06   7.95254E+02  -4.63365E+06   0.00000E+00

Properties for Pitzer:
pH = 6.5971
Eh/V = -1.3548
Total solute molality = 12.268
Ionic strength = 6.1338
Osmotic coefficient = 1.2829
Debye-Hueckel slope = 0.39160
```

$pH = -\log_{10}(aH[+]) = -\log_{10}(2.5287 \times 10^{-7}) = 6.5971$

Summary of aqueous properties

Heterogeneous equilibria and the **phase rule**

The following five slides show how the heterogeneous phase equilibria calculated using ***Equilib*** are subject to the Phase Rule.

For a series of calculations with fixed temperature and pressure and variable composition it is shown how many degrees of freedom are left for the various equilibrium states calculated.

Simple Heterogeneous Equilibria and the **Phase Rule**:

Oxidation of iron sulfide by a variable amount (**<A>**) of oxygen

F Reactants - Equilib

File Edit Table Units Data Search Help

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

1 - 2

Mass(mol)	Species	Phase	T(K)	P(total)**	Stream#	Data
<1-A>	FeS	solid-1	1000	1.0	1	FACT
<A>	O2	gas	1000			

A multiple entry for the **variable quantity <Alpha>**

$<Alpha>_{first}$ = **0.6**

$<Alpha>_{last}$ = **0.65**

and **step** = **0.01**

** P(total) is the hydrostatic pressure above the phase. For a gaseous stream this is the sum of the partial pressures of the species in that stream.

Next >>

FactSage Compound: 1/6 database(s) Solution: 1/5 database(s)

F Menu - Equilib

File Units Parameters Help

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

Reactants (2)

<1-A> FeS (1000K,s1,#1) + <A> O2 (1000K,g,#1)

Products

Compound species

gas ideal real 18

liquid 0

aqueous 0

solid 21

suppress duplicates

Species: 39

Solution species

8 FACT solution datasets - 0 selected.

Target

- none -

Estimate T(K): 1000

Mass(mol): 0

Legend

Show all selected

species: 0

solutions: 0

Clear

Final Conditions

<A>	<B>	T(K)	P(atm)	Delta H(J)
0.6 0.65 0.01		1000	1	

10 steps Table 6 calculations

6 **calculations** will be performed for **<A>** from 0.60 to 0.65 in increments of 0.01 (0.60, 0.61, 0.62, … , 0.65).

FeS Oxidation and Results when <A> = 0.60 mol (*FACT* Format)

T=1000 K, **<A> = 0.60 mol**

Results - Equilib A=0.6 (page 1/6)

Output Edit Show Pages

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

A=0.6 | A=0.61 | A=0.62 | A=0.63 | A=0.64 | A=0.65

```
<1-A> FeS +  <A> O2 =
(1000,l,sl,#1) (1000,l,g,#1)

 0.36178    mol    gas_ideal
 (23.205 gram, 0.36178 mol, 29.687 litre, 7.8167E-04 g/ml)
         (1000.00 K, 1 atm,      a=1.0000)
         ( 0.96869          SO2
         + 2.6993E-02       S2
         + 3.9234E-03       SSO
         + 3.5368E-04       S3
         + 2.6429E-05       SO
         + 1.7094E-05       S4
         + 6.6079E-07       S5
         + 2.3162E-07       S6
         + 1.2298E-07       SO3
         + 2.0994E-08       S7
         + 1.1464E-09       S
         + 9.5243E-10       S8
         + 4.8664E-15       O2
         + 3.0316E-16       FeS
         + 1.0904E-17       O
         + 1.2379E-18       Fe
         + 1.1294E-19       FeO
         + 2.9713E-33       O3)

+ 0.12442    mol    Fe3O4_magnetite
  (28.807 gram, 0.12442 mol)
         (1000.00 K, 1 atm, S2, a=1.0000)

+ 2.6755E-02 mol    FeS_solid
  (2.3521 gram, 2.6755E-02 mol)
         (1000.00 K, 1 atm, S3, a=1.0000)
```

Products:

- ideal gas phase solution: mainly **SO_2**
- 1st solid phase: **Fe_3O_4(s2)**
- 2nd solid phase: **FeS (s3)**

FeS Oxidation and Results when <A> = 0.61 mol (*FACT* Format)

Note:
Same phases and gas partial pressure as for <A> = 0.60 mol but different amounts.
This is explained by the

Phase Rule:

$$F=C-P+2$$

where C=3 and P=3, hence F=2 (T and P).
At 1000 K and 1 atm, the system is invariant.

T=1000 K, <A> = 0.61 mol

Results - Equilib A=0.61 (page 2/6)

Output Edit Show Pages

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

A=0.6 | - A=0.61 - | A=0.62 | A=0.63 | A=0.64 | A=0.65

```
<1-A> FeS +  <A> O2 =
(1000,1,sl,#1) (1000,1,g,#1)

 0.36781    mol    gas_ideal
 (23.592 gram, 0.36781 mol, 30.182 litre, 7.8167E-04 g/ml)
         (1000.00 K, 1 atm,      a=1.0000)
         ( 0.96869          SO2
         + 2.6993E-02       S2
         + 3.9234E-03       SSO
         + 3.5368E-04       S3
         + 2.6429E-05       SO
         + 1.7094E-05       S4
         + 6.6079E-07       S5
         + 2.3162E-07       S6
         + 1.2298E-07       SO3
         + 2.0994E-08       S7
         + 1.1464E-09       S
         + 9.5243E-10       S8
         + 4.8664E-15       O2
         + 3.0316E-16       FeS
         + 1.0904E-17       O
         + 1.2379E-18       Fe
         + 1.1294E-19       FeO
         + 2.9713E-33       O3)

+ 0.12649    mol    Fe3O4_magnetite
  (29.287 gram, 0.12649 mol)
         (1000.00 K, 1 atm, S2, a=1.0000)

+ 1.0534E-02 mol    FeS_solid
  (0.92608 gram, 1.0534E-02 mol)
         (1000.00 K, 1 atm, S3, a=1.0000)
```

Products:

- ideal gas phase solution: mainly SO_2
- 1st solid phase: Fe_3O_4(s2)
- 2nd solid phase: FeS (s3)

FeS Oxidation and Results when <A> = 0.62 mol (*FACT* Format)

T=1000 K, <A> = 0.62 mol

Products:

- ideal gas phase solution: mainly SO_2
- a solid phase: Fe_3O_4(s2)

Note:

All FeS(s3) is oxidized

Now only 2 phases (P = 2) exist.

From **Phase Rule**:

F = 3

and gas phase composition varies in equilibrium with **Fe_3O_4 (s2)**, the system is univariant.

Results - Equilib A=0.62 (page 3/6)

Output Edit Show Pages

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

A=0.6 | A=0.61 | - A=0.62 - | A=0.63 | A=0.64 | A=0.65

```
<1-A> FeS +  <A> O2 =
(1000,1,s1,#1) (1000,1,g,#1)

 0.37306    mol    gas_ideal
 (23.918 gram, 0.37306 mol, 30.612 litre, 7.8132E-04 g/ml)
         (1000.00 K, 1 atm,      a=1.0000)
         ( 0.98154          SO2
         + 1.5650E-02       S2
         + 2.6241E-03       SSO
         + 1.5614E-04       S3
         + 2.3215E-05       SO
         + 5.7464E-06       S4
         + 1.6914E-07       S5
         + 1.4375E-07       SO3
         + 4.5144E-08       S6
         + 3.1157E-09       S7
         + 8.7293E-10       S
         + 1.0763E-10       S8
         + 6.4759E-15       O2
         + 1.9080E-16       FeS
         + 1.2578E-17       O
         + 1.0232E-18       Fe
         + 1.0768E-19       FeO
         + 4.5611E-33       O3)

+ 0.12667    mol    Fe3O4_magnetite
  (29.328 gram, 0.12667 mol)
         (1000.00 K, 1 atm, S2, a=1.0000)

+ 0.00000    mol    Fe3O4_magnetite
         (1000.00 K, 1 atm, S1, a=0.96684)

+ 0.00000    mol    FeS_solid
         (1000.00 K, 1 atm, S3, a=0.62938)
```

FeS Oxidation and Results when <A> = 0.65 mol (*FACT* Format)

T=1000 K, <A> = 0.65 mol

Products:

- ideal gas phase solution: mainly a mixture of SO_2 and SO_3

Note:

Oxidation is complete.

Fe_2O_3(S1) is the stable product.

Results - Equilib A=0.65 (page 6/6)

Output Edit Show Pages

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

A=0.6 | A=0.61 | A=0.62 | A=0.63 | A=0.64 | - A=0.65 -

```
<1-A> FeS +  <A> O2 =
(1000,1,s1,#1) (1000,1,g,#1)

 0.35541    mol    gas_ideal
 (23.623 gram, 0.35541 mol, 29.164 litre, 8.0999E-04 g/ml)
         (1000.00 K, 1 atm,      a=1.0000)
         ( 0.80420          SO2
         + 0.18058          SO3
         + 1.5223E-02       O2
         + 1.9284E-11       O
         + 1.2406E-11       SO
         + 1.6438E-14       O3
         + 4.8877E-22       SSO
         + 3.0426E-22       S
         + 1.5451E-22       FeO
         + 1.9013E-27       S2
         + 9.5760E-28       Fe
         + 6.2240E-38       FeS
         + 6.6117E-42       S3
         + 8.4810E-56       S4
         + 8.7009E-70       S5)

+ 0.17500    mol    Fe2O3_hematite
  (27.946 gram, 0.17500 mol)
         (1000.00 K, 1 atm, S1, a=1.0000)

+ 0.00000    mol    FeSO4_solid
         (1000.00 K, 1 atm, S1, a=0.28741)

+ 0.00000    mol    Fe2(SO4)3_solid
         (1000.00 K, 1 atm, S1, a=0.15567)

+ 0.00000    mol    Fe3O4_magnetite
         (1000.00 K, 1 atm, S2, a=4.5295E-03)
```

Compound species selection - *FactSage 6.4*

In **FactSage 6.4** there is a new <u>default exclusion of species from compound species selection</u>

When two or more databases are connected, the same species may appear in more than one database. In such cases, a species should generally only be selected from one database. Otherwise conflicts will probably occur. In order to assist users in deciding which species to exclude, the FactSage developers have assigned priorities. When you initially click on "pure solids", "pure liquids", or "gas" you may now see that several species marked with an "X" have not been selected. That is, they have been excluded by default because of probable conflicts between databases. The FactSage developers suggest that these species not be selected for this particular calculation.

If you wish to select species marked with an "X" you must first click on 'permit selection of "X" species'. This will then override the default setting and permit you to select species as in FactSage 6.3. This will also activate the 'suppress duplicates' button and enable you to define a database priority list as in FactSage 6.3.

<u>IMPORTANT</u> : For many calculations, it may frequently be advisable or necessary to de-select other species in addition to those marked with an "X."

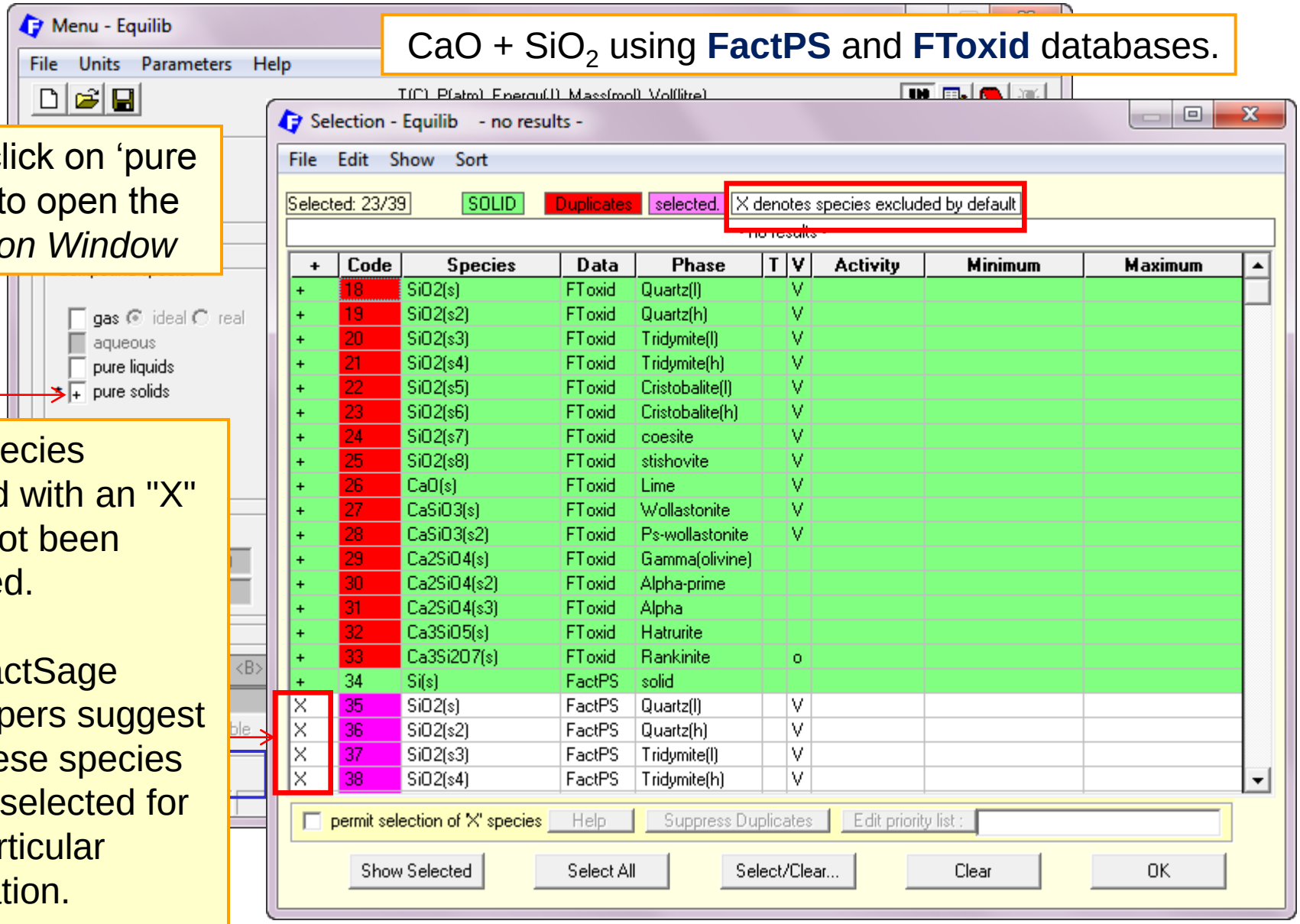
Compound species selection - *FactSage 6.4*

CaO + SiO_2 using **FactPS** and **FToxid** databases.

Right-click on 'pure solids' to open the *Selection Window*

The species marked with an "X" have not been selected.

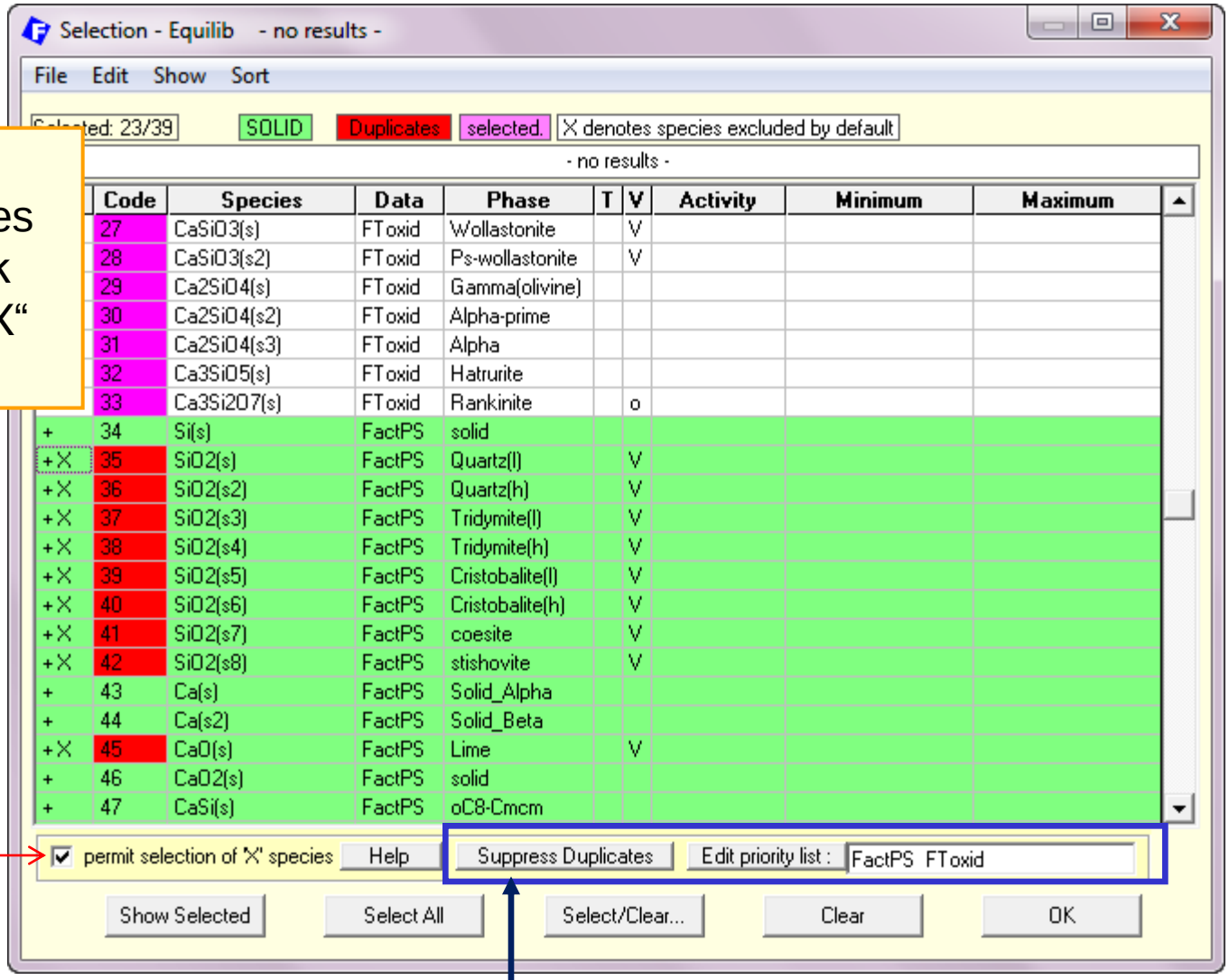
The FactSage developers suggest that these species not be selected for this particular calculation.



+	Code	Species	Data	Phase	T	V	Activity	Minimum	Maximum
+	18	SiO2(s)	FToxid	Quartz(l)		V			
+	19	SiO2(s2)	FToxid	Quartz(h)		V			
+	20	SiO2(s3)	FToxid	Tridymite(l)		V			
+	21	SiO2(s4)	FToxid	Tridymite(h)		V			
+	22	SiO2(s5)	FToxid	Cristobalite(l)		V			
+	23	SiO2(s6)	FToxid	Cristobalite(h)		V			
+	24	SiO2(s7)	FToxid	coesite		V			
+	25	SiO2(s8)	FToxid	stishovite		V			
+	26	CaO(s)	FToxid	Lime		V			
+	27	CaSiO3(s)	FToxid	Wollastonite		V			
+	28	CaSiO3(s2)	FToxid	Ps-wollastonite		V			
+	29	Ca2SiO4(s)	FToxid	Gamma(olivine)					
+	30	Ca2SiO4(s2)	FToxid	Alpha-prime					
+	31	Ca2SiO4(s3)	FToxid	Alpha					
+	32	Ca3SiO5(s)	FToxid	Hatrurite					
+	33	Ca3Si2O7(s)	FToxid	Rankinite		o			
+	34	Si(s)	FactPS	solid					
X	35	SiO2(s)	FactPS	Quartz(l)		V			
X	36	SiO2(s2)	FactPS	Quartz(h)		V			
X	37	SiO2(s3)	FactPS	Tridymite(l)		V			
X	38	SiO2(s4)	FactPS	Tridymite(h)		V			

Compound species selection - *FactSage 6.4*

To override the default setting and select species marked with an "X“, click on 'permit selection of "X“ species'.



	Code	Species	Data	Phase	T	V	Activity	Minimum	Maximum
	27	CaSiO3(s)	FToxid	Wollastonite		V			
	28	CaSiO3(s2)	FToxid	Ps-wollastonite		V			
	29	Ca2SiO4(s)	FToxid	Gamma(olivine)					
	30	Ca2SiO4(s2)	FToxid	Alpha-prime					
	31	Ca2SiO4(s3)	FToxid	Alpha					
	32	Ca3SiO5(s)	FToxid	Hatrurite					
	33	Ca3Si2O7(s)	FToxid	Rankinite		o			
+	34	Si(s)	FactPS	solid					
+X	35	SiO2(s)	FactPS	Quartz(l)		V			
+X	36	SiO2(s2)	FactPS	Quartz(h)		V			
+X	37	SiO2(s3)	FactPS	Tridymite(l)		V			
+X	38	SiO2(s4)	FactPS	Tridymite(h)		V			
+X	39	SiO2(s5)	FactPS	Cristobalite(l)		V			
+X	40	SiO2(s6)	FactPS	Cristobalite(h)		V			
+X	41	SiO2(s7)	FactPS	coesite		V			
+X	42	SiO2(s8)	FactPS	stishovite		V			
+	43	Ca(s)	FactPS	Solid_Alpha					
+	44	Ca(s2)	FactPS	Solid_Beta					
+X	45	CaO(s)	FactPS	Lime		V			
+	46	CaO2(s)	FactPS	solid					
+	47	CaSi(s)	FactPS	oC8-Cmcm					

You can then also set a database priority list and ‘Suppress Duplicates’.