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.

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

Most negative ΔG

Reaction - Table

File Units Output Figure Help

T(C) P(bar) Energy(J) Quantity(mol) Vol(litre)

Reaction 1

Isothermal Standard State Reaction: Delta G° = Delta H° - T.Delta S° = - RT.ln(Keq) where (T/K)

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(litre)	Delta S°(J/K)	Delta Cp(J/K)	Keq	T
25.00	-698504.2	-674681.9	0.0000E+00	-79.900	-6.5179E+01	1.5794E+118	

$\Delta G_1 \approx$ -675 kJ

Reaction 2

Isothermal Standard State Reaction: Delta G° = Delta H° - T.Delta S° = - RT.ln(Keq) where (T/K)

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(litre)	Delta S°(J/K)	Delta Cp(J/K)	Keq	T
25.00	-690602.8	-663803.1	0.0000E+00	-89.887	-6.6455E+01	1.9616E+116	

$\Delta G_2 \approx$ -664 kJ

Reaction 3

Isothermal Standard State Reaction: Delta G° = Delta H° - T.Delta S° = - RT.ln(Keq) where (T/K)

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(litre)	Delta S°(J/K)	Delta Cp(J/K)	Keq	T
25.00	-649992.0	-626475.3	0.0000E+00	-78.875	-7.3197E+01	5.6637E+109	

$\Delta G_3 \approx$ -626 kJ

Reaction 4

Isothermal Standard State Reaction: Delta G° = Delta H° - T.Delta S° = - RT.ln(Keq) where (T/K)

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,s) + 0.333 MgO (T,s) + Ar (T,g)

T(C)	Delta H°(J)	Delta G°(J)	Delta Vol(litre)	Delta S°(J/K)	Delta Cp(J/K)	Keq	T
25.00	-691650.0	-666664.0	0.0000E+00	-83.804	-6.5732E+01	6.2203E+116	

$\Delta G_4 \approx$ -667 kJ

Gibbs Energy Minimization

$$G = \sum_{\substack{ideal\\gas}} n_i (g_i^o + RT \ln P_i)$$

$$+ \sum_{\substack{pure\\condensed\\phases}} n_i g_i^o$$

$$+ \sum_{solution-1} n_i (g_i^o + RT \ln X_i + RT \ln \gamma_i)$$

$$+ \sum_{solution-2} n_i (g_i^o + RT \ln X_i + RT \ln \gamma_i)$$

$$+ \cdots$$

$$+ \cdots$$

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

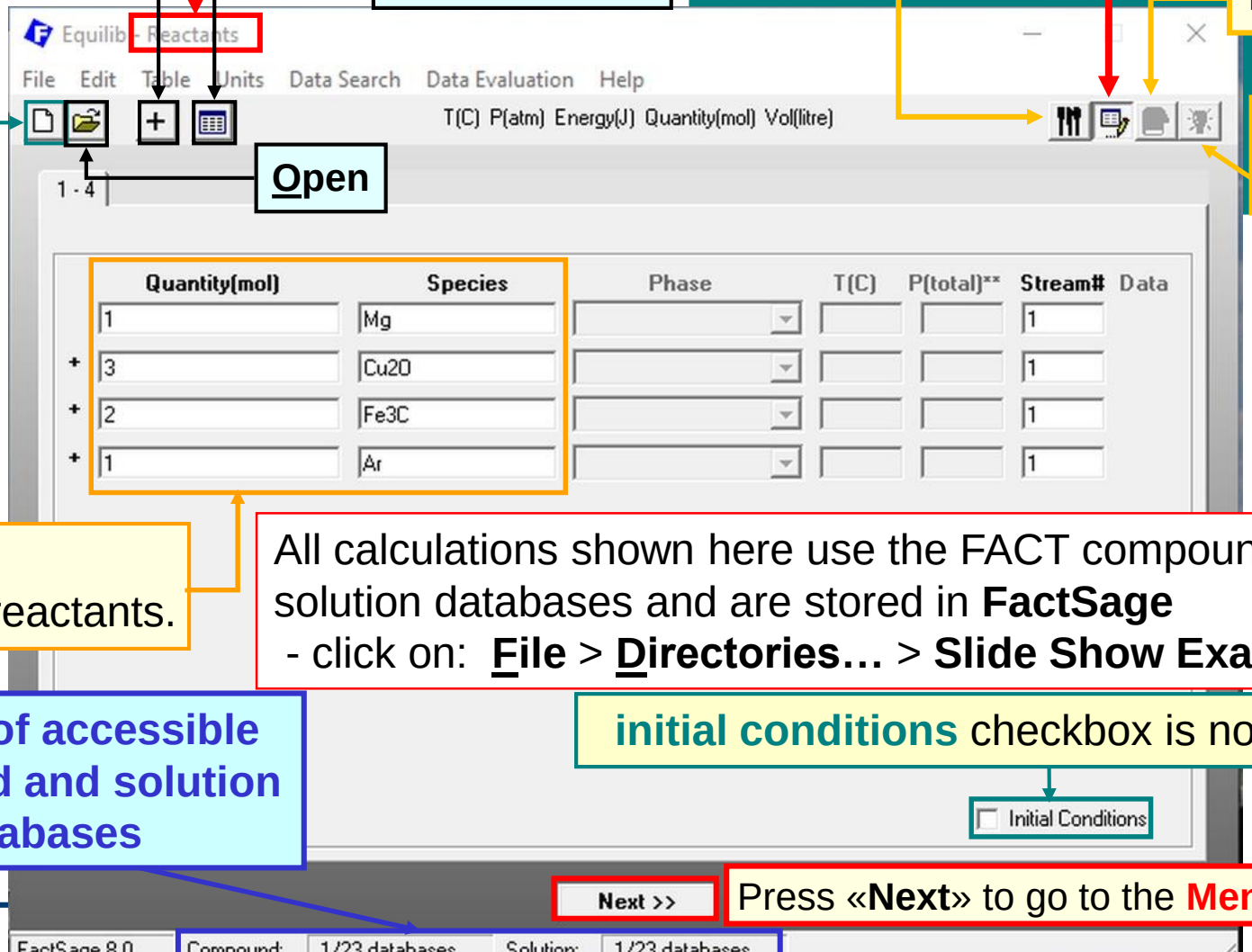
***Equilib* has 4 windows:**

Reactants window

Menu window

List window

Results window



Open

1st entry: Click on New Reaction

2nd entry: Define the reactants.

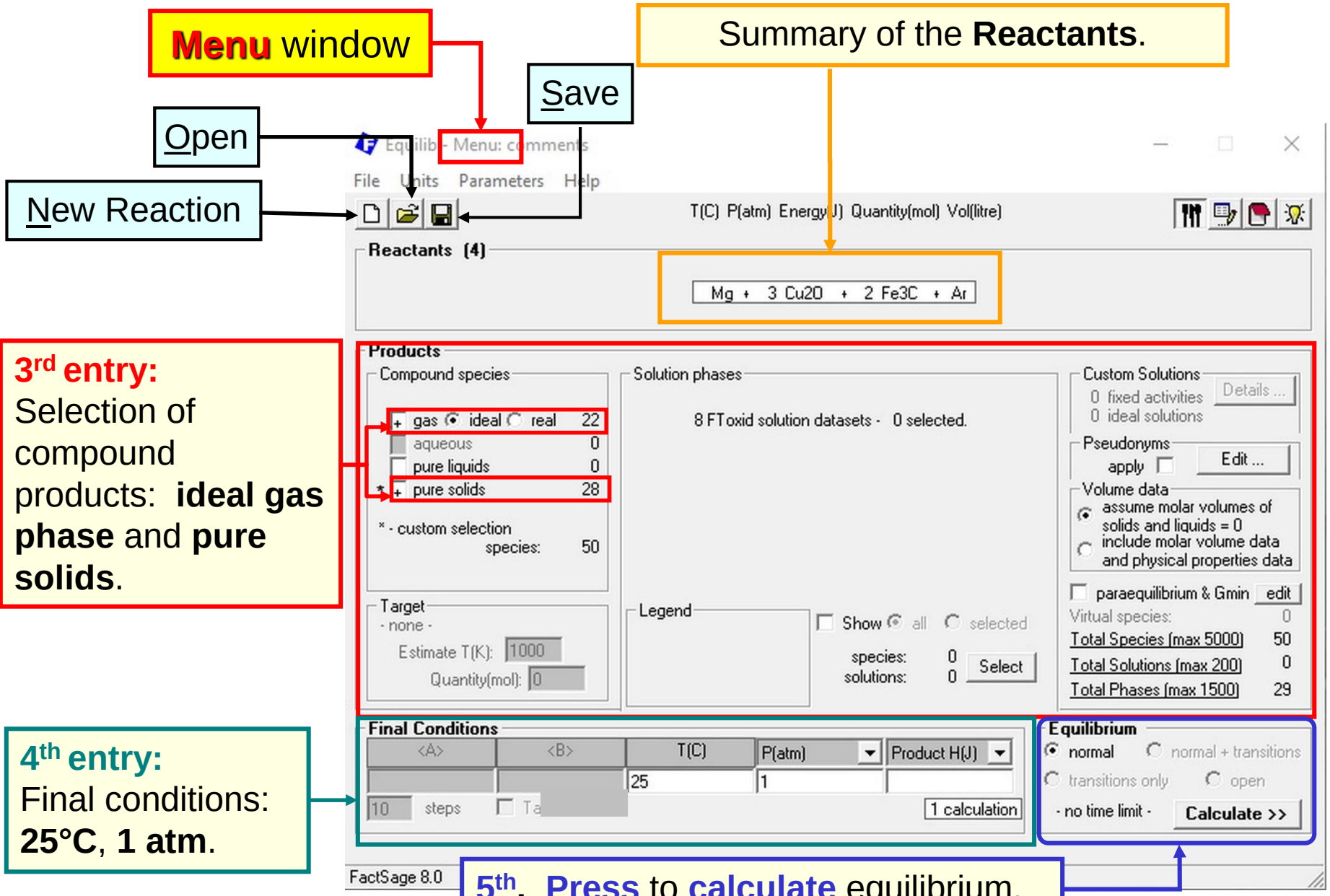
All calculations shown here use the FACT compound and solution databases and are stored in **FactSage**
- click on: **File** > **Directories…** > **Slide Show Examples** …

Number of accessible 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

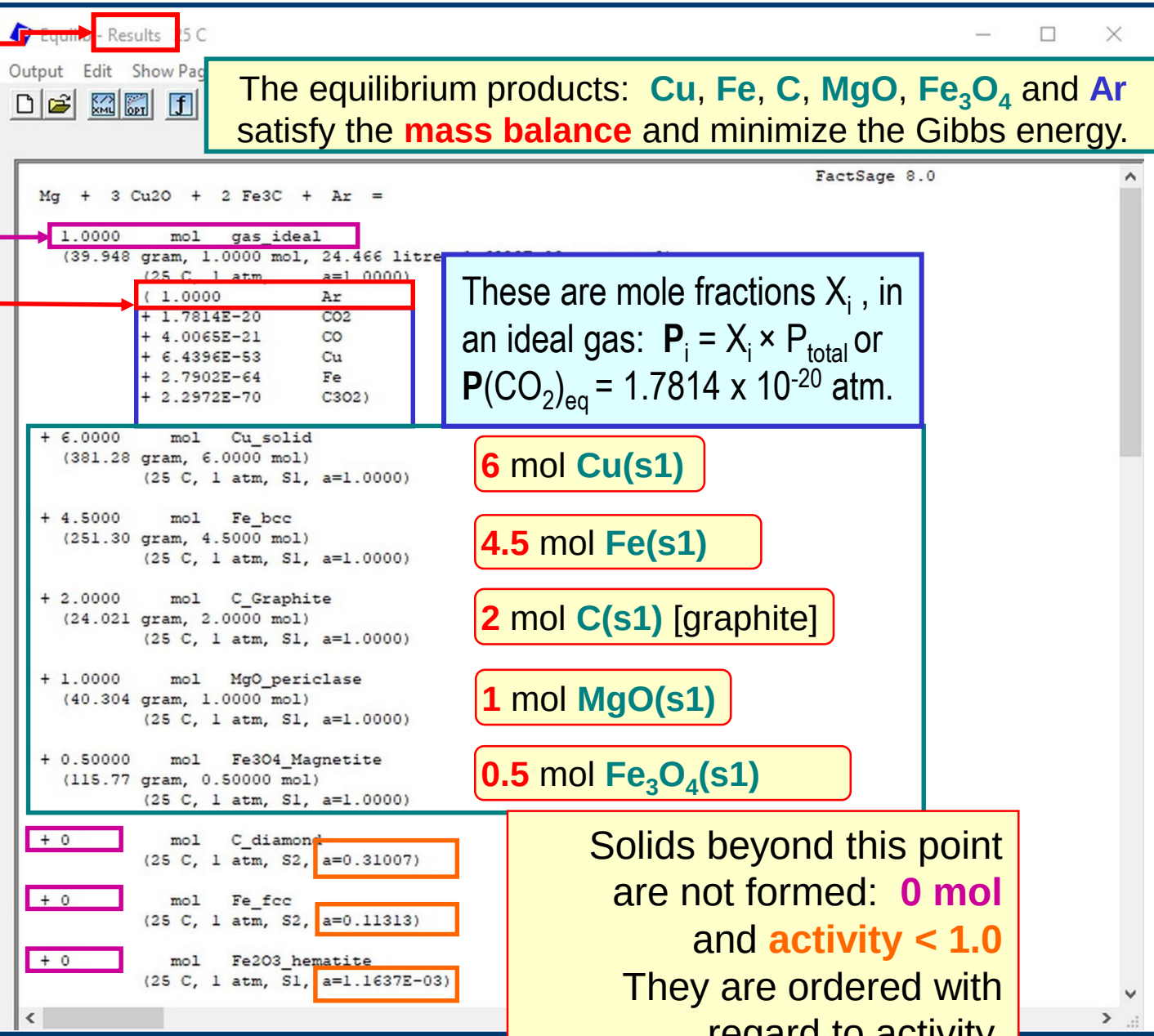


Results window – *FACT* format output.

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**.



These are mole fractions X_i , in an ideal gas: $P_i = X_i \times P_{total}$ or $P(CO_2)_{eq} = 1.7814 \times 10^{-20}$ atm.

6 mol **Cu(s1)**

4.5 mol **Fe(s1)**

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

1 mol **MgO(s1)**

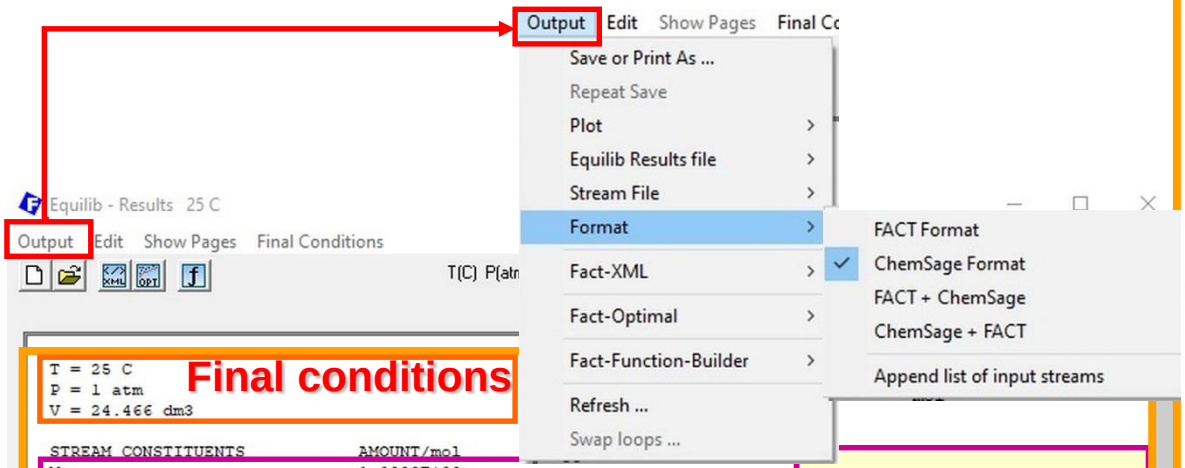
0.5 mol Fe_3O_4**(s1)**

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.

Results window – ***ChemSage*** format output

Menu bar: Output > **Format** > ***ChemSage* Format**



Equilib - Results 25 C

Output Edit Show Pages Final Conditions

Final conditions

```
T = 25 C
P = 1 atm
V = 24.466 dm3

 STREAM CONSTITUENTS          AMOUNT/mol
 Mg                           1.0000E+00
 Cu2O                         3.0000E+00
 Fe3C                         2.0000E+00
 Ar                           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
    System component          Amount/mol     Amount/gram    Mole fraction
    Cu                        6.4396E-53     4.0921E-51     6.4396E-53
    Fe                        2.7902E-64     1.5582E-62     2.7902E-64
    Ar                        1.0000         39.948         1.0000
    O                         3.9635E-20     6.3413E-19     3.9635E-20
    C                         2.1821E-20     2.6208E-19     2.1821E-20
                                 mol                          ACTIVITY
 Cu_solid(s)                  6.0000E+00                     1.0000E+00
 Fe_bcc(s)                    4.5000E+00                     1.0000E+00
 C_Graphite(s)                2.0000E+00                     1.0000E+00
 MgO_periclase(s)             1.0000E+00                     1.0000E+00
 Fe3O4_Magnetite(s)           5.0000E-01                     1.0000E+00
 C_diamond(s2)                0.0000E+00                     3.1007E-01
 Fe_fcc(s2)                   0.0000E+00                     1.1313E-01
 Fe2O3_hematite(s)            0.0000E+00                     1.1637E-03
 Fe3C_CEMENTITE(s)            0.0000E+00                     2.0900E-04
```

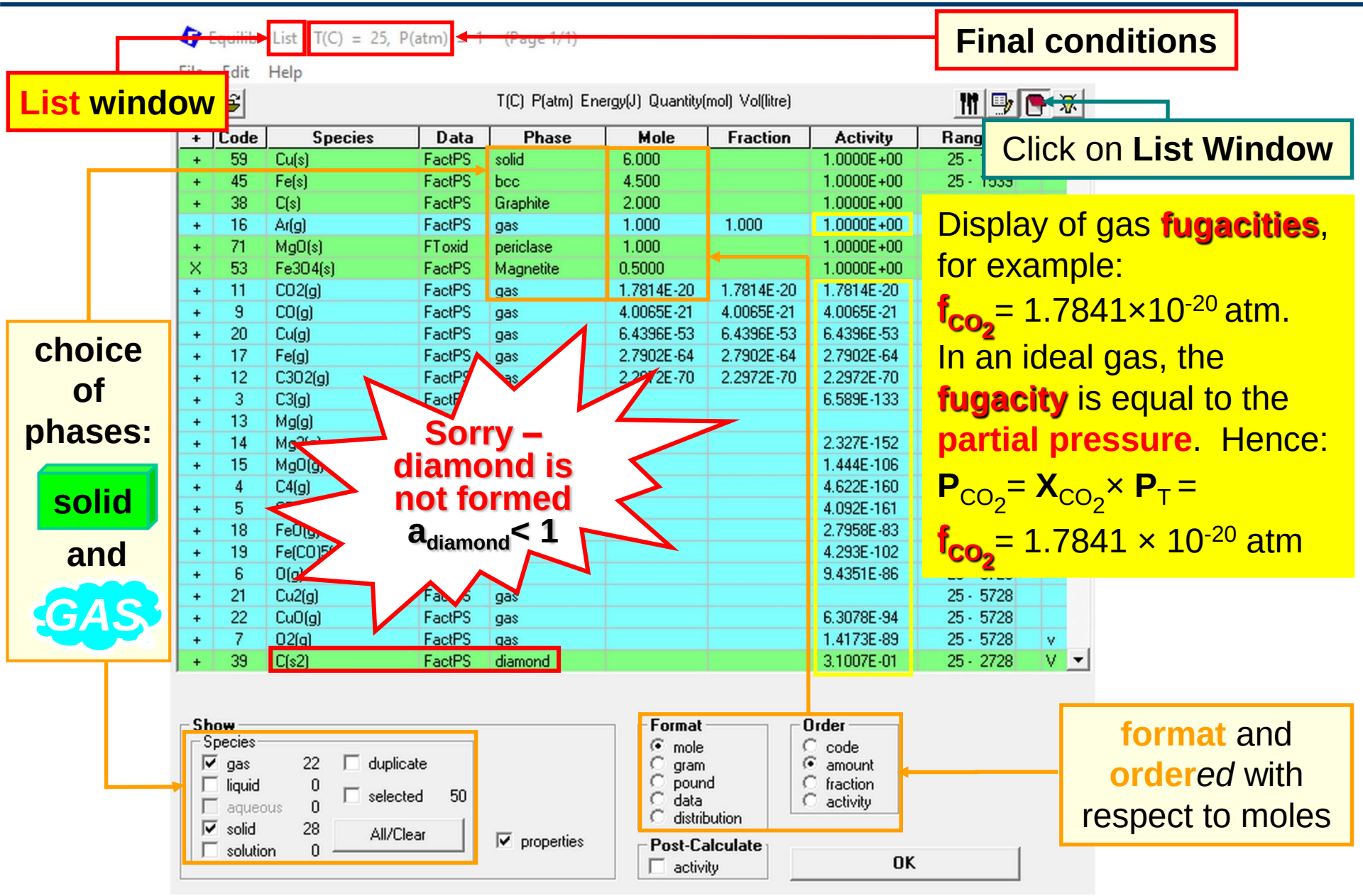
Amount of reactants

Product gases: gas *fugacities* are calculated

Product: stable pure stoichiometric solids

```
T = 25 C
P = 1 atm
V = 24.466 dm3

STREAM CONSTITUENTS          AMOUNT/mol
Mg                           1.0000E+00
Cu2O                         3.0000E+00
Fe3C                         2.0000E+00
Ar                           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
   System component          Amount/mol     Amount/gram    Mole fraction  Mass fraction
   Cu                        6.4396E-53     4.0921E-51     6.4396E-53     1.0244E-52
   Fe                        2.7902E-64     1.5582E-62     2.7902E-64     3.9005E-64
   Ar                        1.0000         39.948         1.0000         1.0000
   O                         3.9635E-20     6.3413E-19     3.9635E-20     1.5874E-20
   C                         2.1821E-20     2.6208E-19     2.1821E-20     6.5606E-21
                                mol                          ACTIVITY
Cu_solid(s)                  6.0000E+00                     1.0000E+00
Fe_bcc(s)                    4.5000E+00                     1.0000E+00
C_Graphite(s)                2.0000E+00                     1.0000E+00
MgO_periclase(s)             1.0000E+00                     1.0000E+00
Fe3O4_Magnetite(s)           5.0000E-01                     1.0000E+00
C_diamond(s2)                0.0000E+00                     3.1007E-01
Fe_fcc(s2)                   0.0000E+00                     1.1313E-01
Fe2O3_hematite(s)            0.0000E+00                     1.1637E-03
Fe3C_CEMENTITE(s)            0.0000E+00                     2.0900E-04
Fe3C_KSI_CARBIDE(s2)         0.0000E+00                     1.2625E-07
CuFeO2_solid(s)              0.0000E+00                     6.1975E-09
CuFeO2_solid(s2)             0.0000E+00                     5.5491E-09
MgCO3_magnesite_CaCO3(s)     0.0000E+00                     3.5860E-09
FeCO3_Siderite(s)            0.0000E+00                     1.8979E-13
Fe2O3_High-Pressure-(s2)     0.0000E+00                     6.0428E-17
(Cu2O)(Fe2O3)_Solid-A(s)     0.0000E+00                     3.8423E-17
(Cu2O)(Fe2O3)_Solid-(s2)     0.0000E+00                     3.0811E-17
Fe2O3_High-Pressure-(s3)     0.0000E+00                     7.9278E-18
Cu2O_solid(s)                0.0000E+00                     3.0689E-19
CuO_Tenorite(s)              0.0000E+00                     1.1332E-22
(CuO)(Fe2O3)_solid(s)        0.0000E+00                     3.5207E-27
(CuO)(Fe2O3)_solid(s2)       0.0000E+00                     2.9715E-27
(CuO)(Fe2O3)_solid(s3)       0.0000E+00                     2.9640E-27
CuCO3_solid(s)               0.0000E+00                     4.7043E-43
Cu2Mg_laves_C14(s)           0.0000E+00                     2.3485E-55
Mg_solid(s)                  0.0000E+00                     5.0150E-56
MgC2_solid(s)                0.0000E+00                     6.9530E-71
*****************************************************************
     Cp             H              S              G              V
    J.K-1           J            J.K-1            J            dm3
*****************************************************************************
 4.09293E+02  -1.16020E+06   5.87967E+02  -1.33550E+06   2.44656E+01

                              Cp             H              S              G
                             J.K-1           J            J.K-1            J
gas_ideal                 2.07860E+01 -1.10720E-14   1.54736E+02 -4.61344E+04
C_Graphite(s)             1.70440E+01  0.00000E+00   1.14800E+01 -3.42276E+03
Fe_bcc(s)                 1.11801E+02 -1.42083E-01   1.22759E+02 -3.66006E+04
Fe3O4_Magnetite(s)        7.57824E+01 -5.58701E+05   7.30571E+01 -5.80483E+05
Cu_solid(s)               1.46692E+02  0.00000E+00   1.98984E+02 -5.93271E+04
MgO_periclase(s)          3.71885E+01 -6.01500E+05   2.69514E+01 -6.09536E+05
```

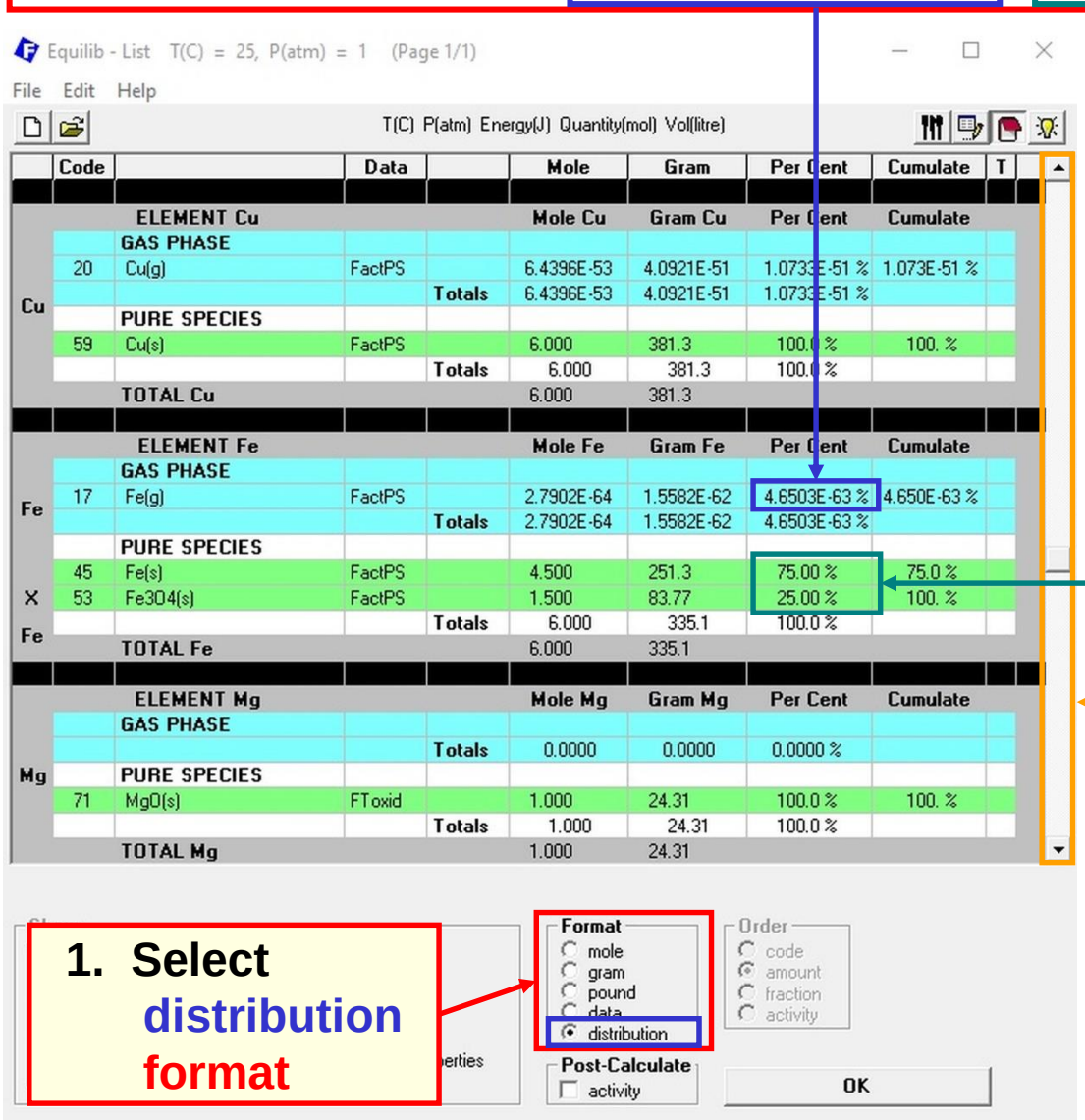
List window – manipulating the results



+	Code	Species	Data	Phase	Mole	Fraction	Activity	Rang
+	59	Cu(s)	FactPS	solid	6.000		1.0000E+00	25 -
+	45	Fe(s)	FactPS	bcc	4.500		1.0000E+00	25 -
+	38	C(s)	FactPS	Graphite	2.000		1.0000E+00	
+	16	Ar(g)	FactPS	gas	1.000	1.000	1.0000E+00	
+	71	MgO(s)	FToxid	periclase	1.000		1.0000E+00	
X	53	Fe3O4(s)	FactPS	Magnetite	0.5000		1.0000E+00	
+	11	CO2(g)	FactPS	gas	1.7814E-20	1.7814E-20	1.7814E-20	
+	9	CO(g)	FactPS	gas	4.0065E-21	4.0065E-21	4.0065E-21	
+	20	Cu(g)	FactPS	gas	6.4396E-53	6.4396E-53	6.4396E-53	
+	17	Fe(g)	FactPS	gas	2.7902E-64	2.7902E-64	2.7902E-64	
+	12	C3O2(g)	FactPS	gas	2.2972E-70	2.2972E-70	2.2972E-70	
+	3	C3(g)	FactPS				6.589E-133	
+	13	Mg(g)						
+	14	Mg2(g)					2.327E-152	
+	15	MgO(g)					1.444E-106	
+	4	C4(g)					4.622E-160	
+	5						4.092E-161	
+	18	FeO(g)					2.7958E-83	
+	19	Fe(CO)5					4.293E-102	
+	6	O(g)					9.4351E-86	
+	21	Cu2(g)	FactPS	gas				25 - 5728
+	22	CuO(g)	FactPS	gas			6.3078E-94	25 - 5728
+	7	O2(g)	FactPS	gas			1.4173E-89	25 - 5728
+	39	C(s2)	FactPS	diamond			3.1007E-01	25 - 2728

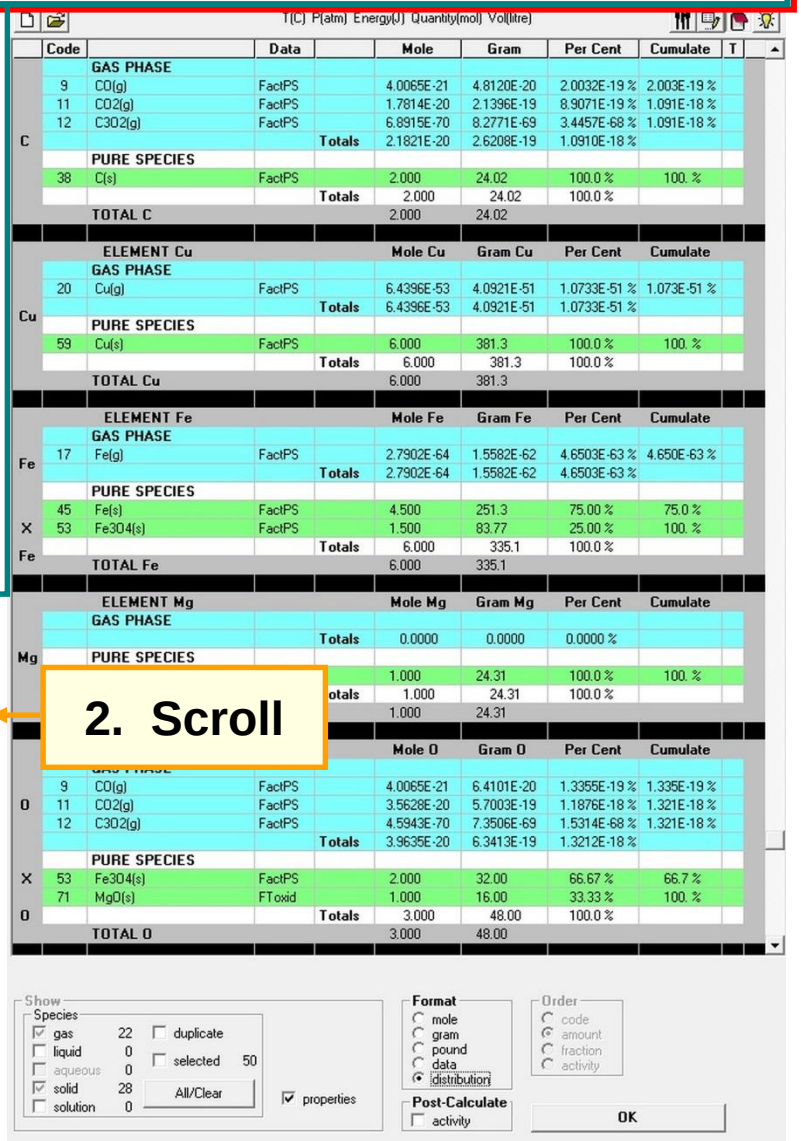
List window – distribution format

For example, Fe is distributed in: a gas phase: 0% as Fe(g) | 2 solid phases: 75% as Fe and 25% as Fe_2O_3(s)



1. Select distribution format

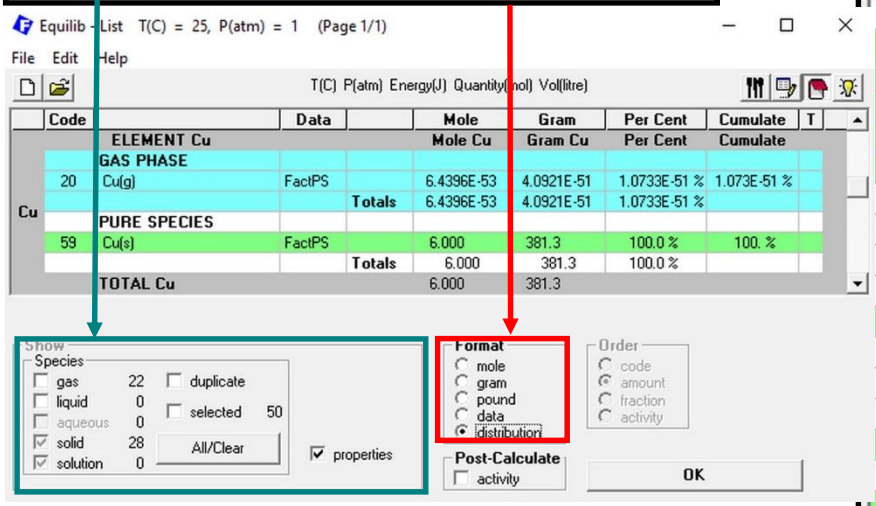
2. Scroll



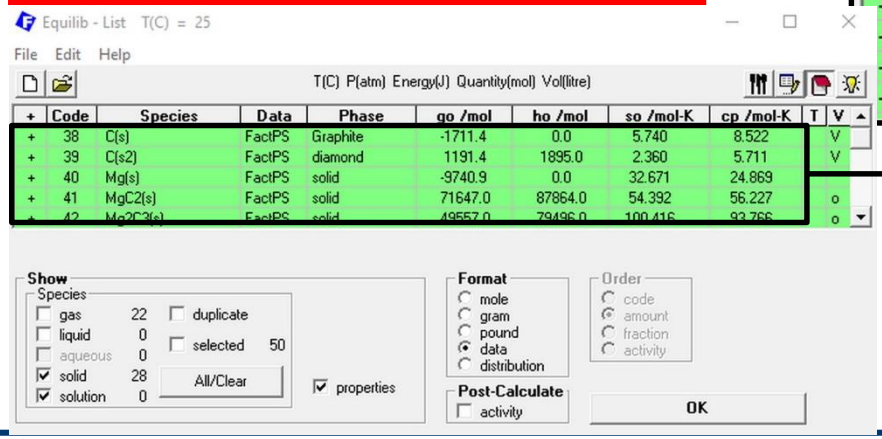
List window – thermodynamic **data** format

Selection:

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



3. To obtain the thermodynamic data format



+	38	C(s)	FactPS	Graphite	-1711.4	0.0	5.740	8.522
+	39	C(s2)	FactPS	diamond	1191.4	1895.0	2.360	5.711
+	40	Mg(s)	FactPS	solid	-9740.9	0.0	32.671	24.869
+	41	MgC2(s)	FactPS	solid	71647.0	87864.0	54.392	56.227
+	42	Mg2C3(s)	FactPS	solid	49557.0	79496.0	100.416	93.766
X	43	MgO(s)	FactPS	Periclase	-609535.6	-601500.0	26.951	37.189
+	44	MgCO3(s)	FactPS	magnesite_CaCO	-1131323.4	-1111689.0	65.854	76.208
+	45	Fe(s)	FactPS	bcc	-8133.5	0.0	27.280	24.845
+	46	Fe(s2)	FactPS	fcc	-2731.2	7972.9	35.902	25.198
+	47	Fe3C(s)	FactPS	CEMENTITE	-5107.0	25211.9	101.690	120.600
+	48	Fe3C(s2)	FactPS	KSI_CARBIDE	13266.7	41988.3	96.333	81.819
X	49	FeO(s)	FactPS	Wustite	-283570.9	-265832.2	59.496	49.526
X	50	Fe2O3(s)	FactPS	hematite	-851943.3	-825787.0	87.729	105.483
X	51	Fe2O3(s2)	FactPS	High-Pressure-H	-776114.1	-750044.8	87.437	103.980
X	52	Fe2O3(s3)	FactPS	High-Pressure-H	-771079.2	-742057.5	97.339	103.955
X	53	Fe3O4(s)	FactPS	Magnetite	-1160966.5	-1117402.6	146.114	151.565
X	54	Fe3O4(s2)	FactPS	Magnetite	-1152285.9	-1102701.6	166.307	151.514
X	55	Fe3O4(s3)	FactPS	High-Pressure-m	-1000173.5	-947855.9	175.474	151.565
X	56	Fe3O4(s4)	FactPS	High-Pressure-m	-991491.4	-933153.3	195.667	151.514
+	57	FeCO3(s)	FactPS	Siderite	-789653.3	-761180.0	95.500	82.274
X	58	(MgO)(Fe2O3)(s)	FactPS	solid	-1465768.0	-1428857.0	123.800	143.755
+	59	Cu(s)	FactPS	solid	-9887.8	0.0	33.164	24.449
X	60	CuO(s)	FactPS	Tenorite	-168031.2	-155192.1	43.063	42.325
X	61							
+	62							
+	63							
+	64							
+	65							
+	66							
+	67							

«Absolute» values of Gibbs energy G°.

$\Delta G°$ for the reaction:

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

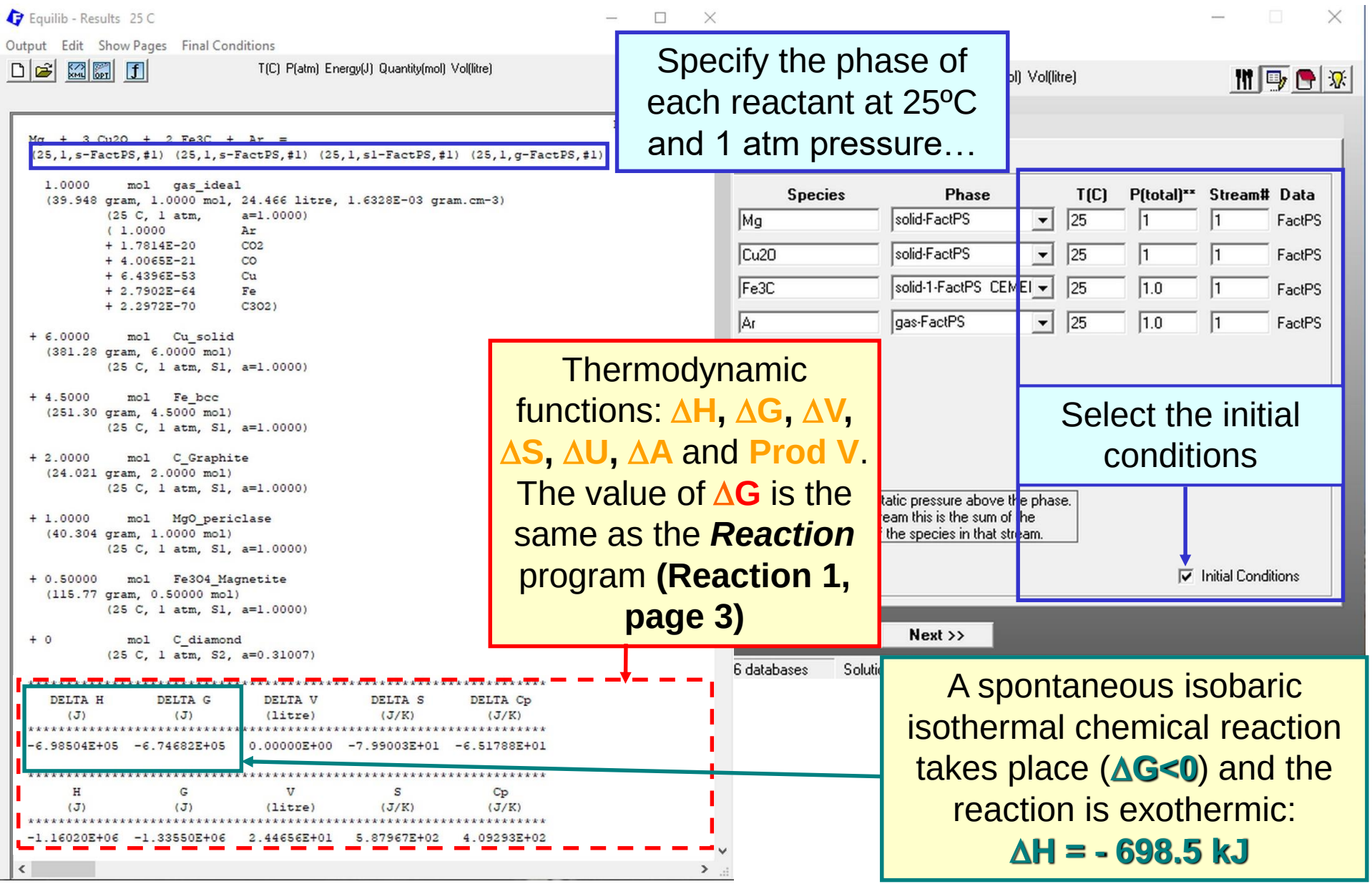
is given by:

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

$$= -5107.0 - [\,3(-8133.5) + (-1711.4)\,]$$

$$= 21604.9\ J/mol$$

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



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

Select the initial conditions

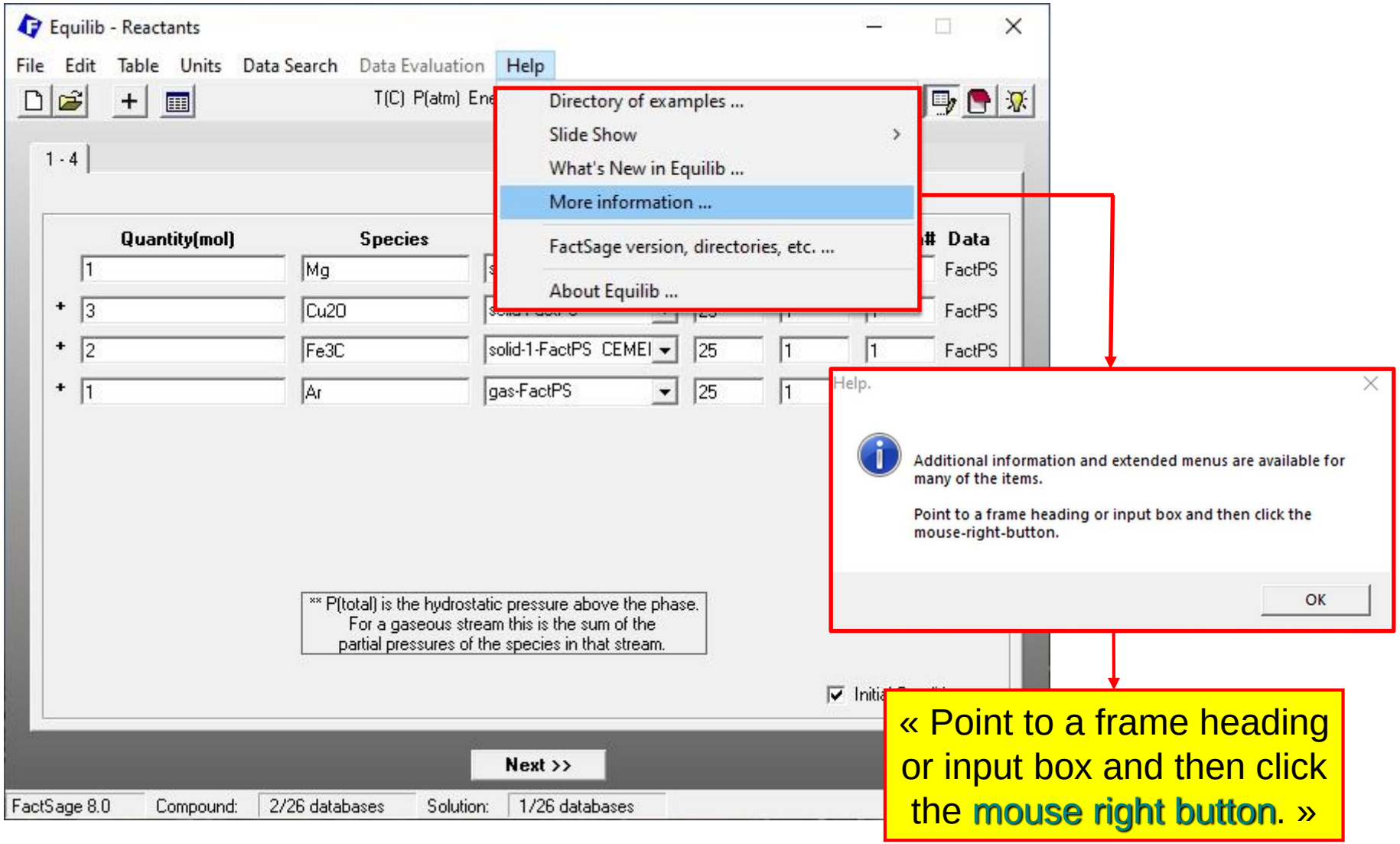
Thermodynamic functions: **ΔH**, **ΔG**, **ΔV**, **ΔS**, **ΔU**, **ΔA** and **Prod V**. The value of **ΔG** is the same as the ***Reaction*** program **(Reaction 1, page 3)**

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

ΔH = - 698.5 kJ

Reactants window – Help > More information...

Menu bar: Help > **More information...**

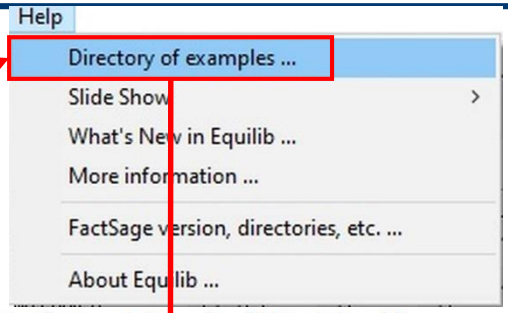


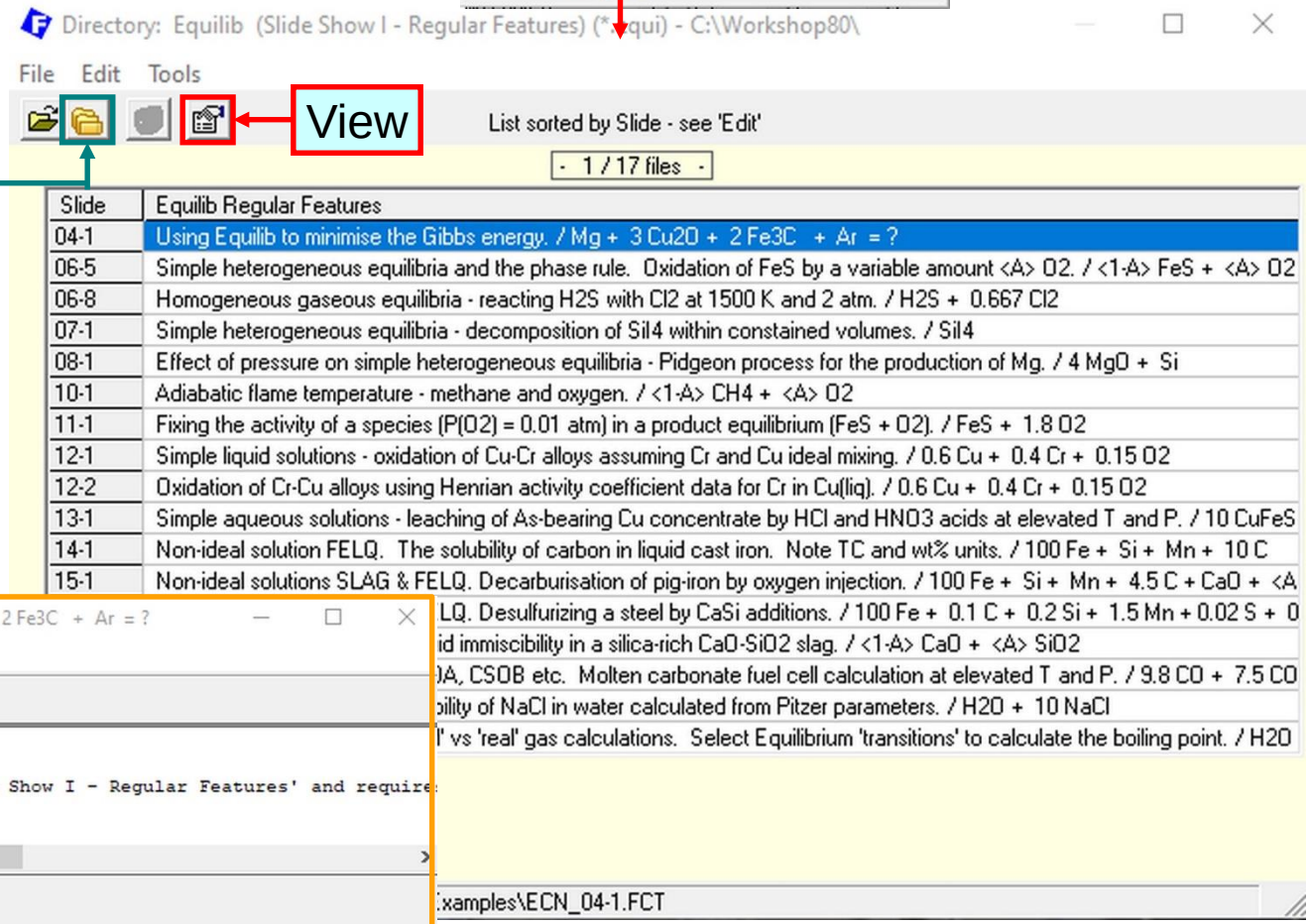
« Point to a frame heading or input box and then click the **mouse right button**. »

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

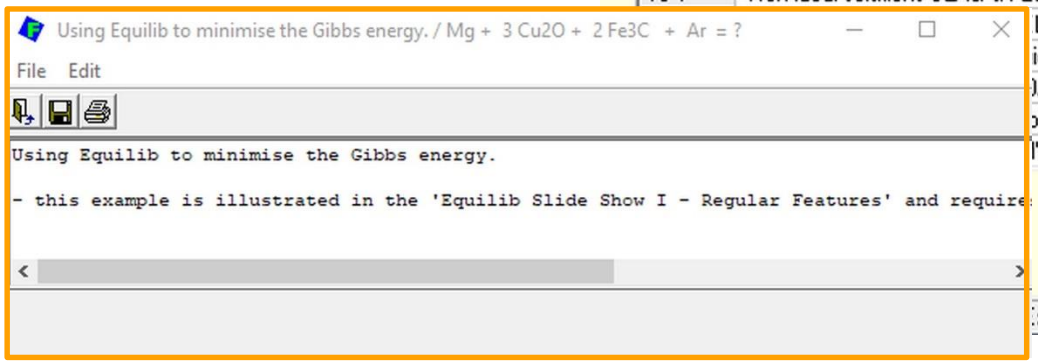
Reactants or Menu window menu bar:
Help > **Directory of examples...**

If you want to Change Directory then go to **File > Directory >** [Select a directory] or press on



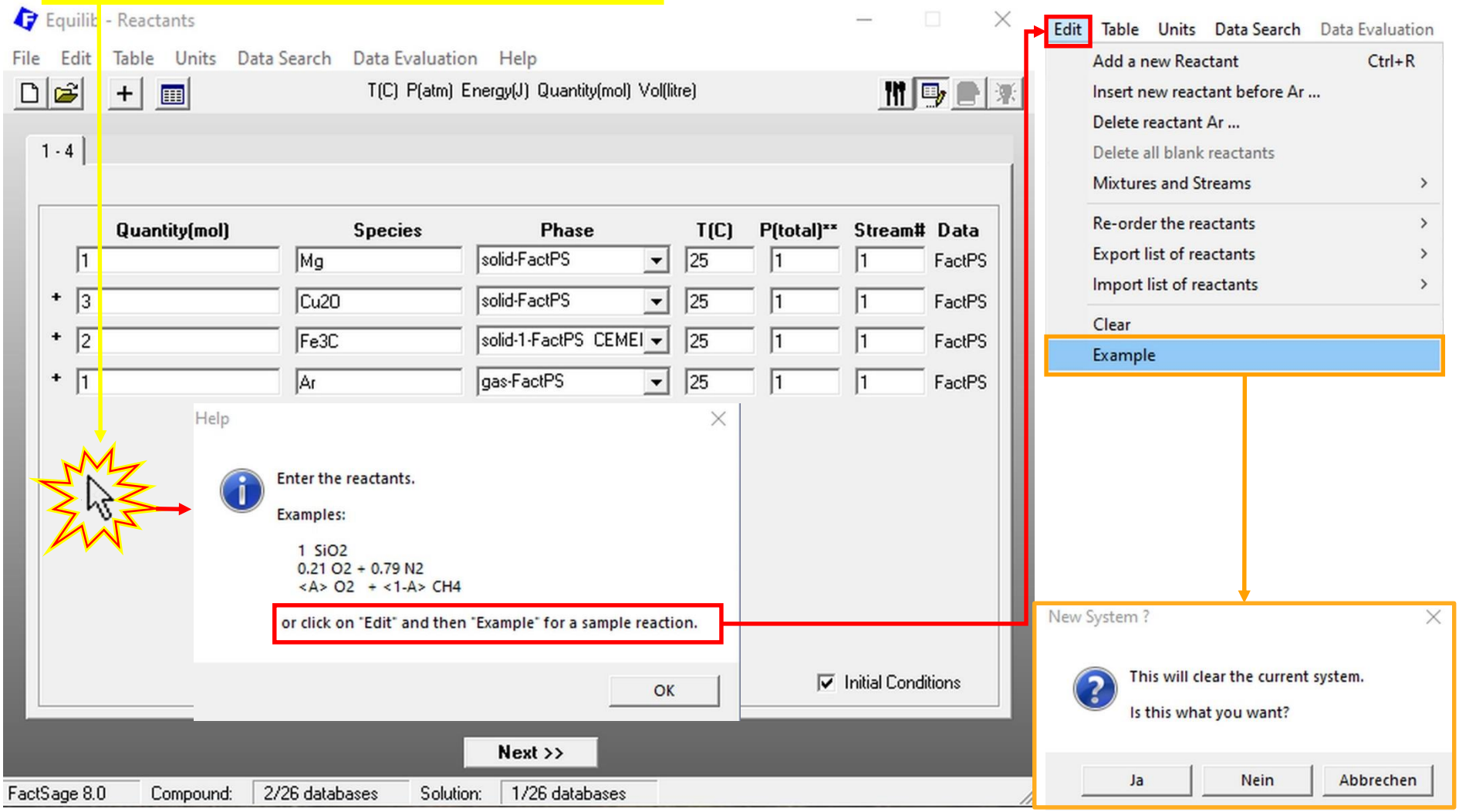


Short description of the example



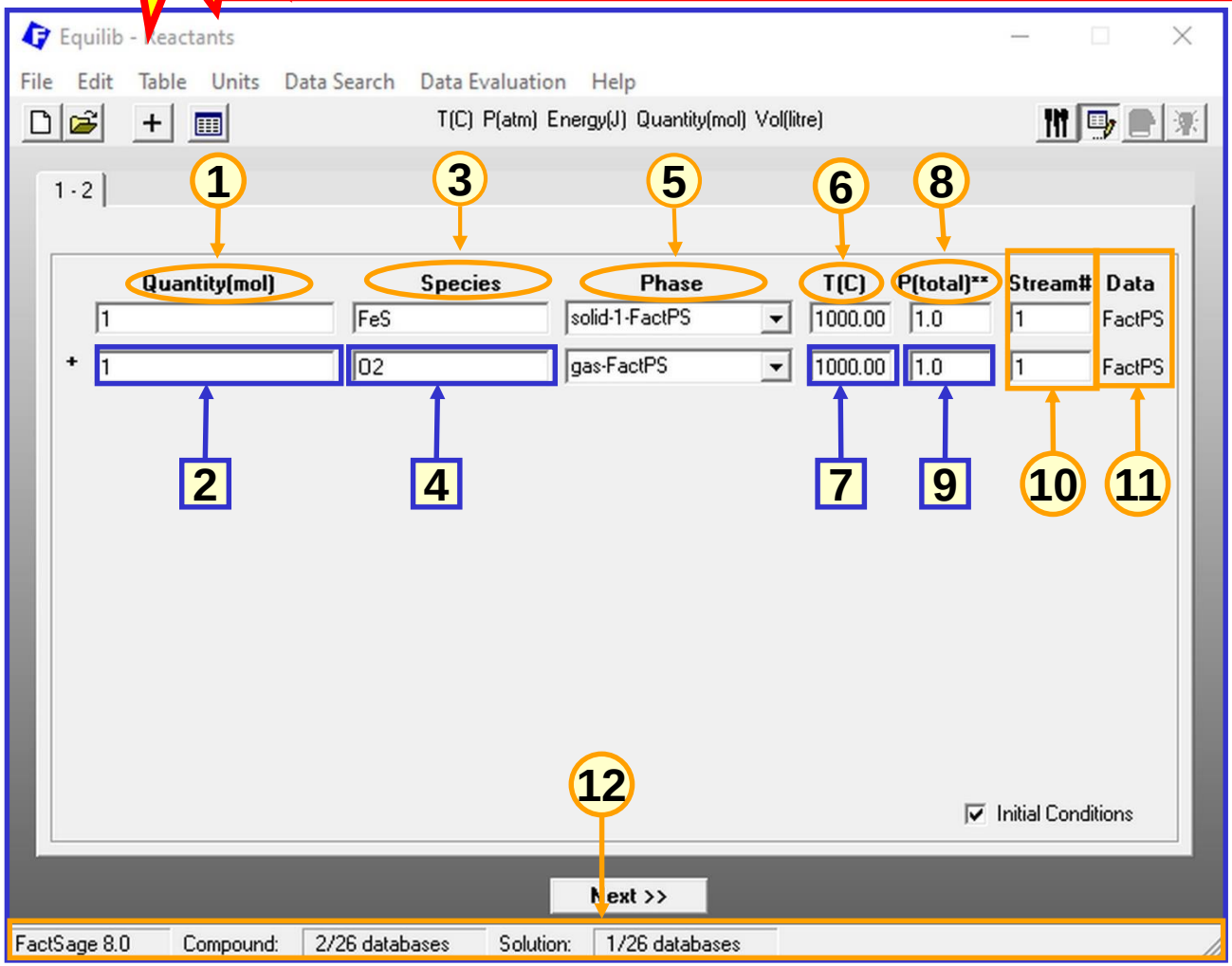
The mouse right button - Reactants

Click with the mouse right button



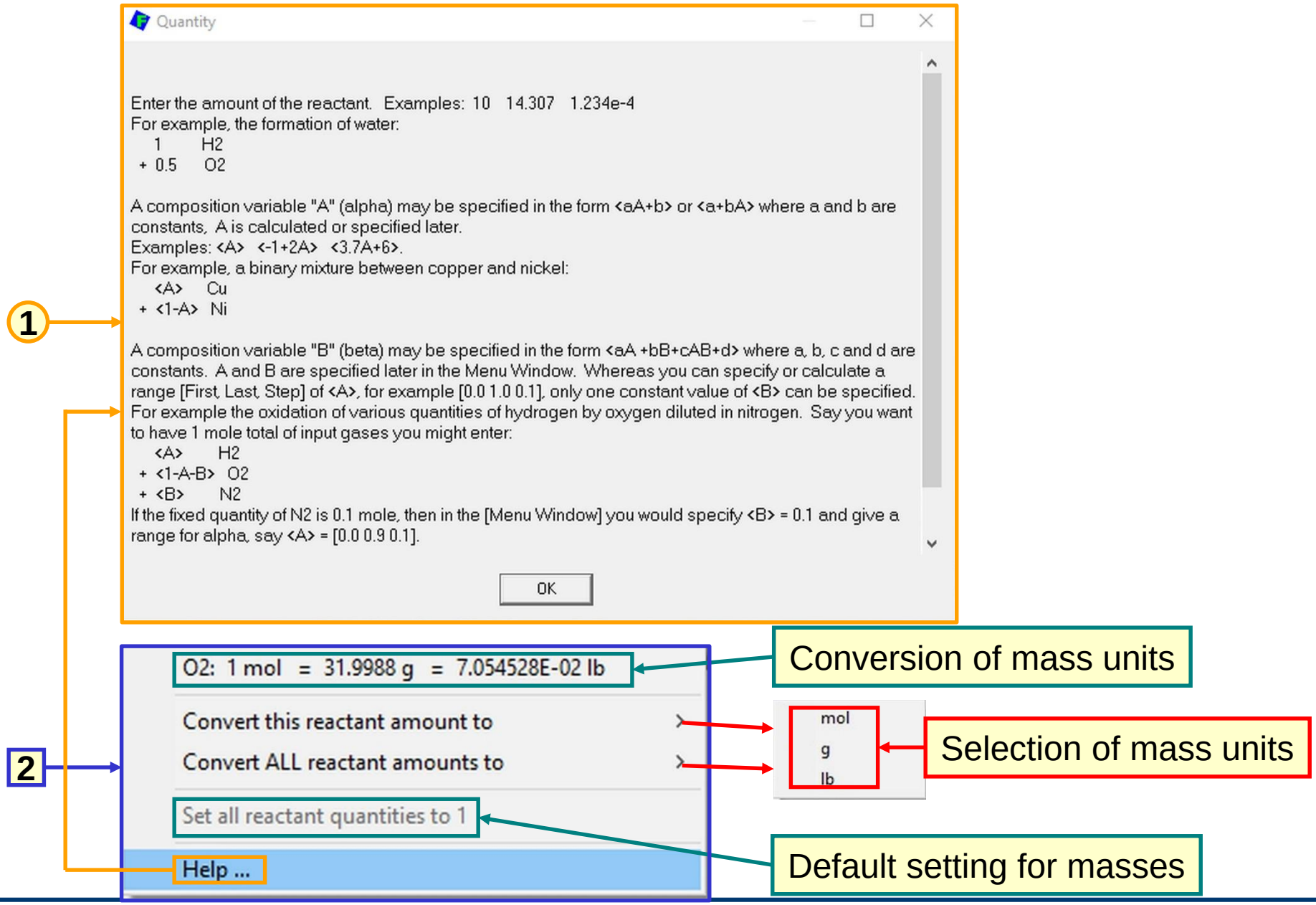
Help: – the **mouse right button**

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
```

Quantity:

```
1 gram    =  0.00220462262 lb
1 lb      =  453.59237 gram =  0.45359237 kg
1 kg      =  2.20462262 lb  =  1000 gram
1 tonne   =  2204.62262 lb  =  1000 kg
```

Pressure:

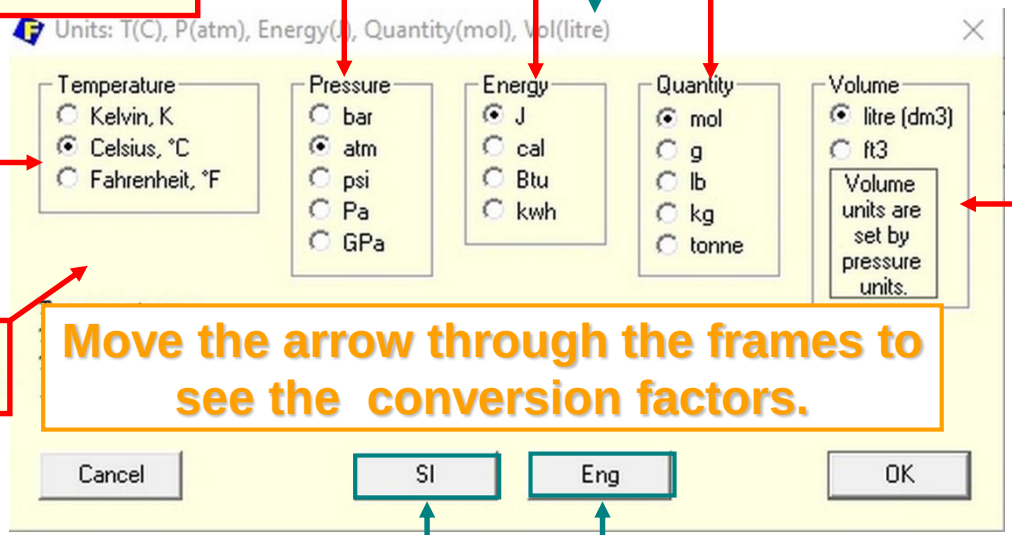
```
1 bar           = 100000 Pa    = 1/1.01325 atm     = 1/0.06894757 psi
0.00001 bar     = 1 Pa         = 1/101325 atm      = 1/6894.757   psi
1.01325 bar     = 101325 Pa    = 1 atm       = 1.01325/0.06894745 psi
0.06894757 bar  = 6894.757 Pa  = 0.06894757/1.01325 atm      = 1 psi
```

Volume:

```
1 litre (or 1 dm3)   = 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 = 1.98722...    cal/mol-K
  = 22.4141/273.15 = 0.0820578...  l-atm/mol-K
```

```
SI units:

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

```
English units:

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

Homogeneous Gaseous Equilibria

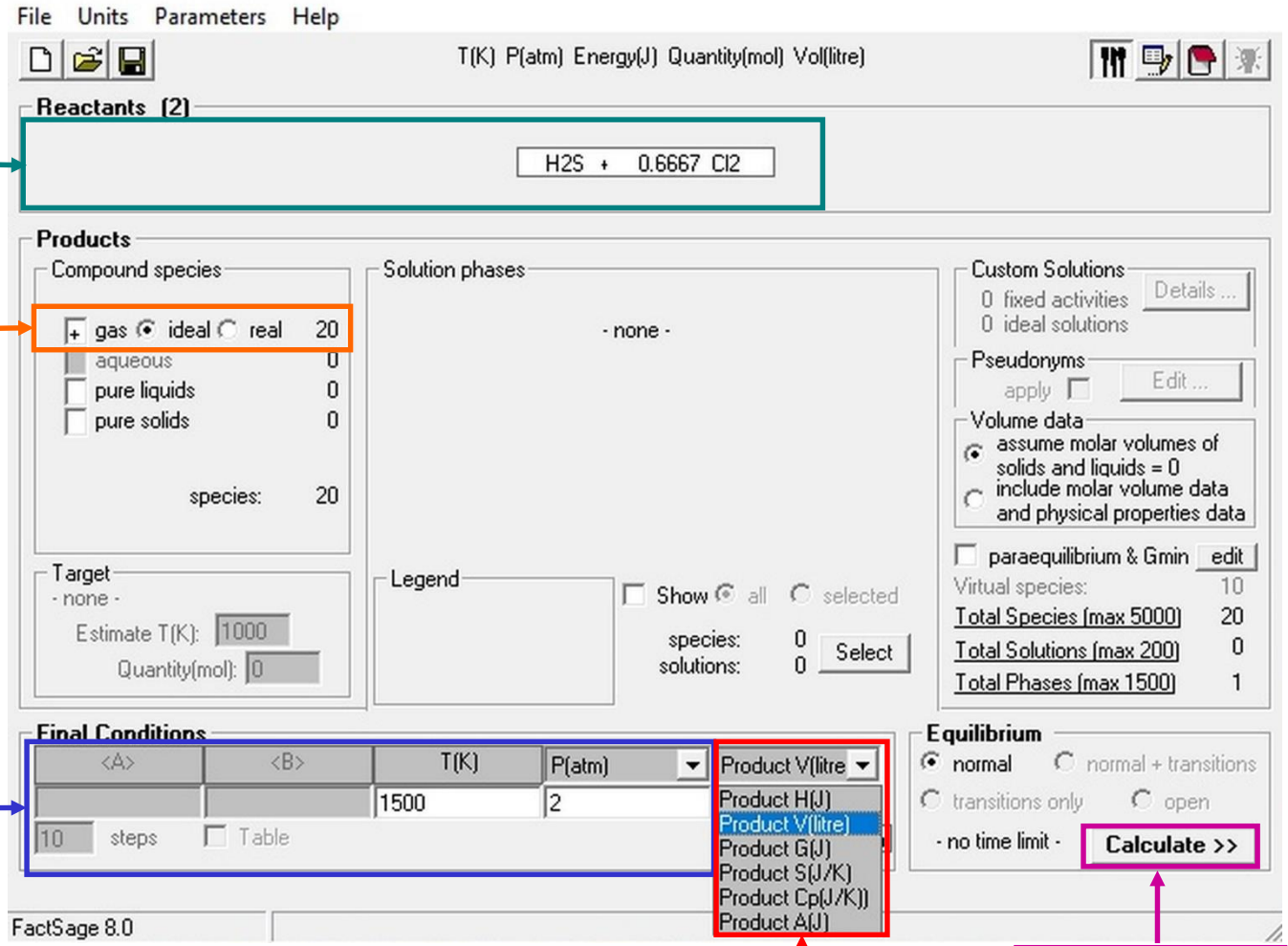
Reacting H_2S with Cl_2

Products selection: ideal gas solution phase

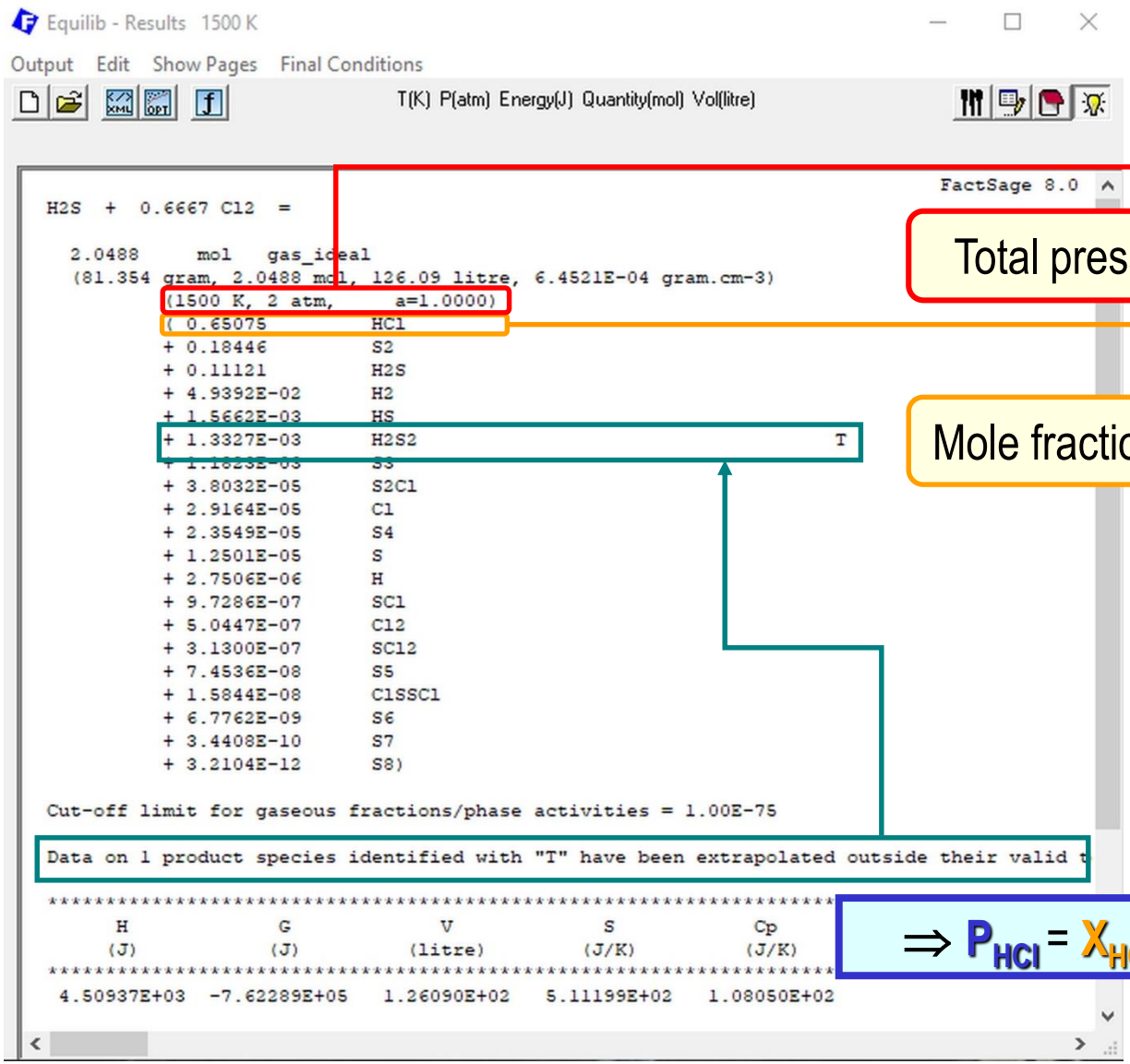
Product T= 1500 K and P=2 atm

Drop-down menu for extensive property

Press «Calculate»



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

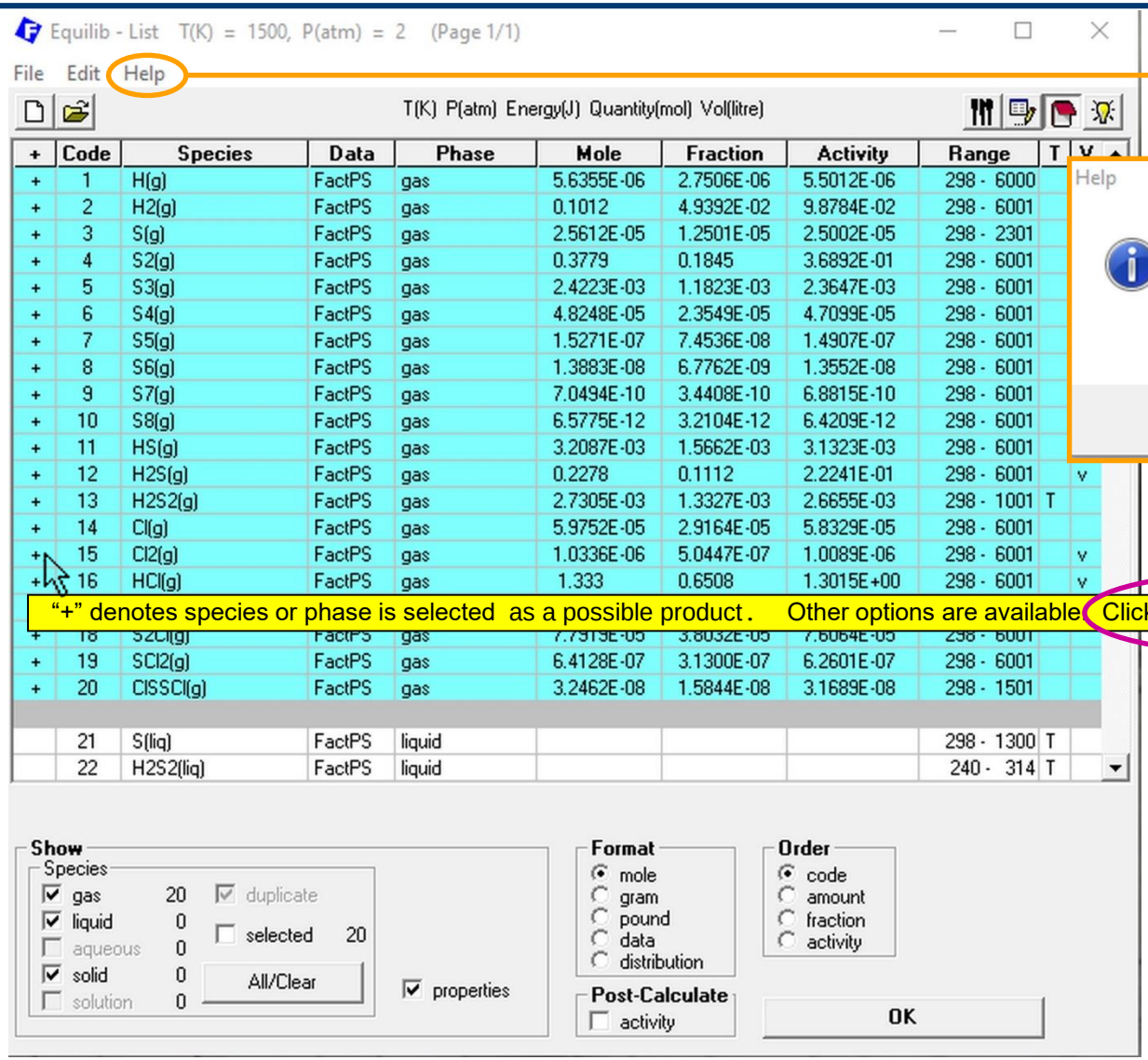


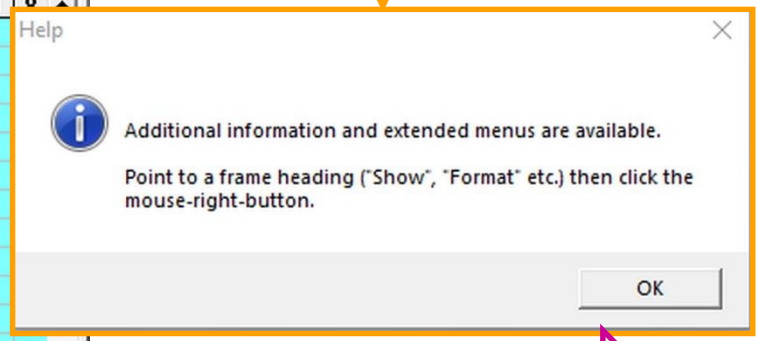
Total pressure P_{total} = 2.0 atm

Mole fraction X_{HCl} = 0.65075

$\Rightarrow P_{HCl} = X_{HCl} \times P_{total}$ = 1.3015 atm

List window – Help >

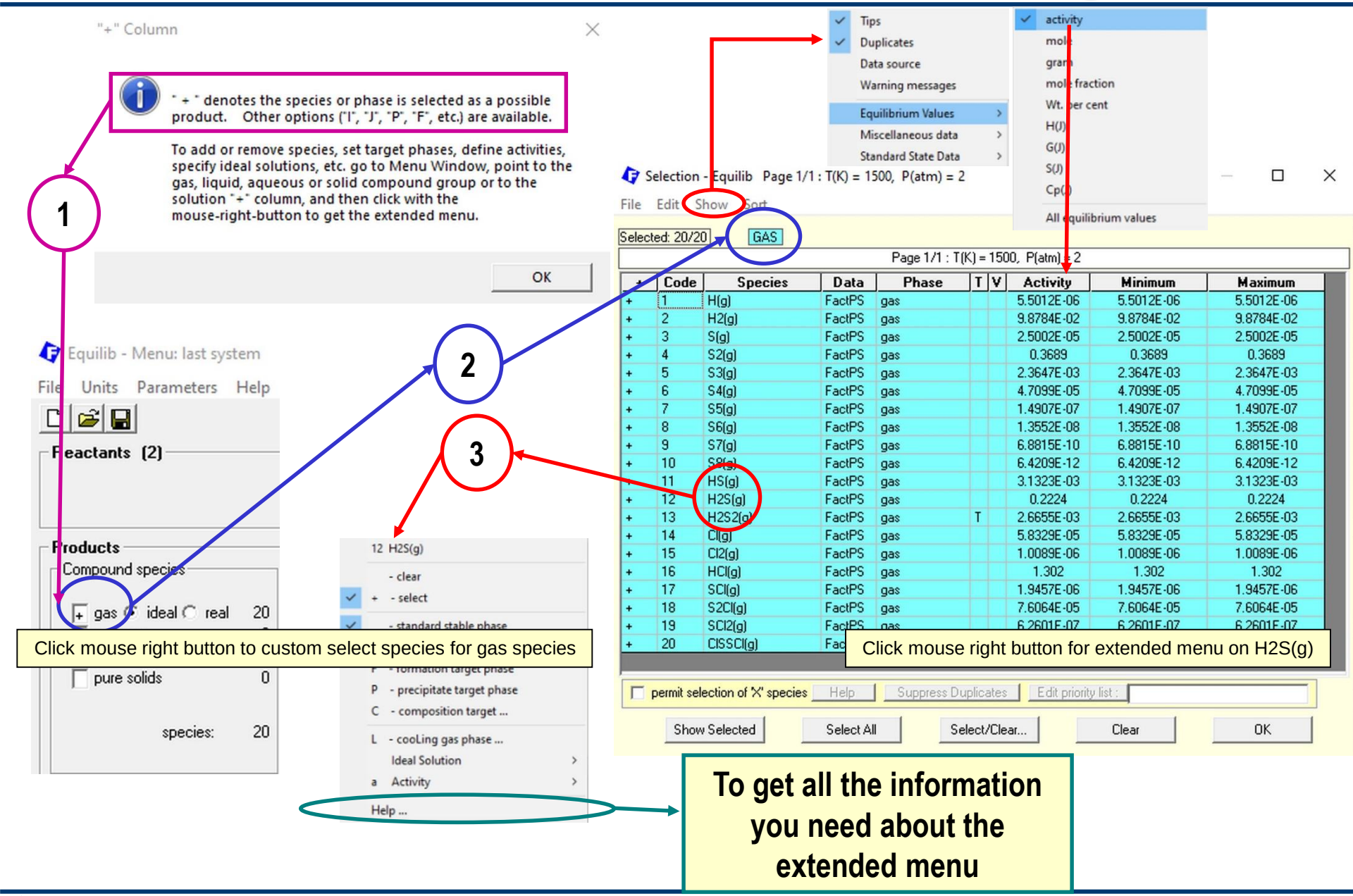




…and go to the next slide

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

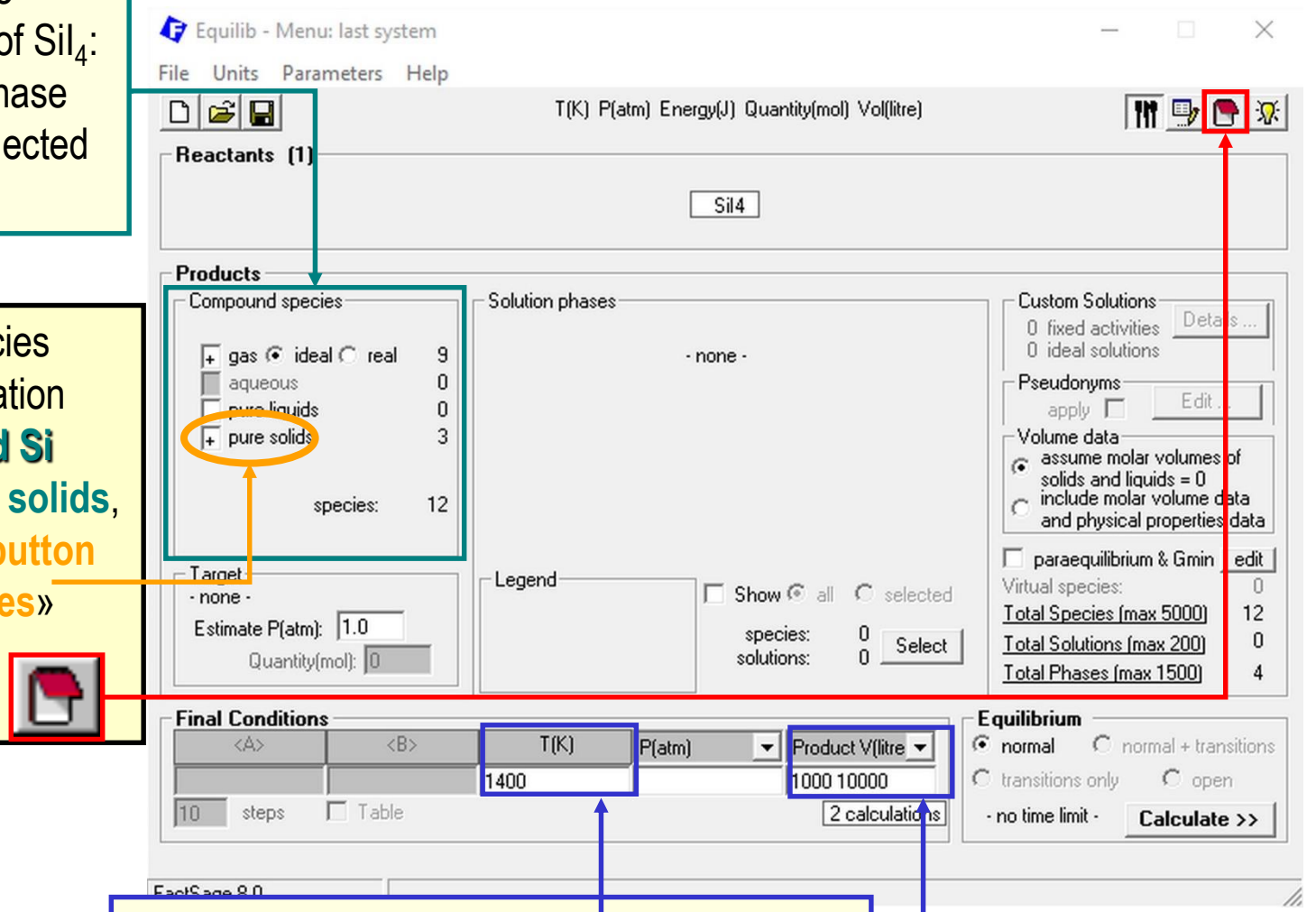
Help – Another example of the use of the **mouse right button**



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**.

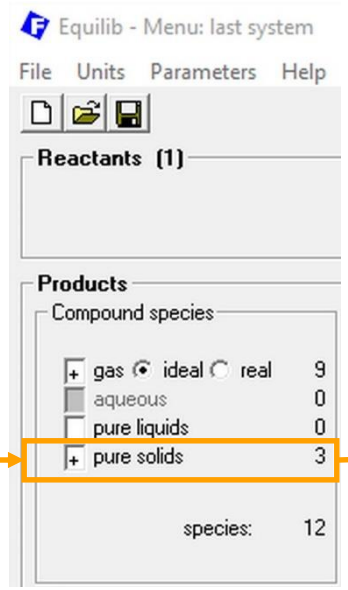
To view a list of the species selected before computation and specify a **pure solid Si** phase instead of **3 pure solids**, **click the mouse right button** at a «**Compound species**» **input box** or press the «**List Window**» **button**

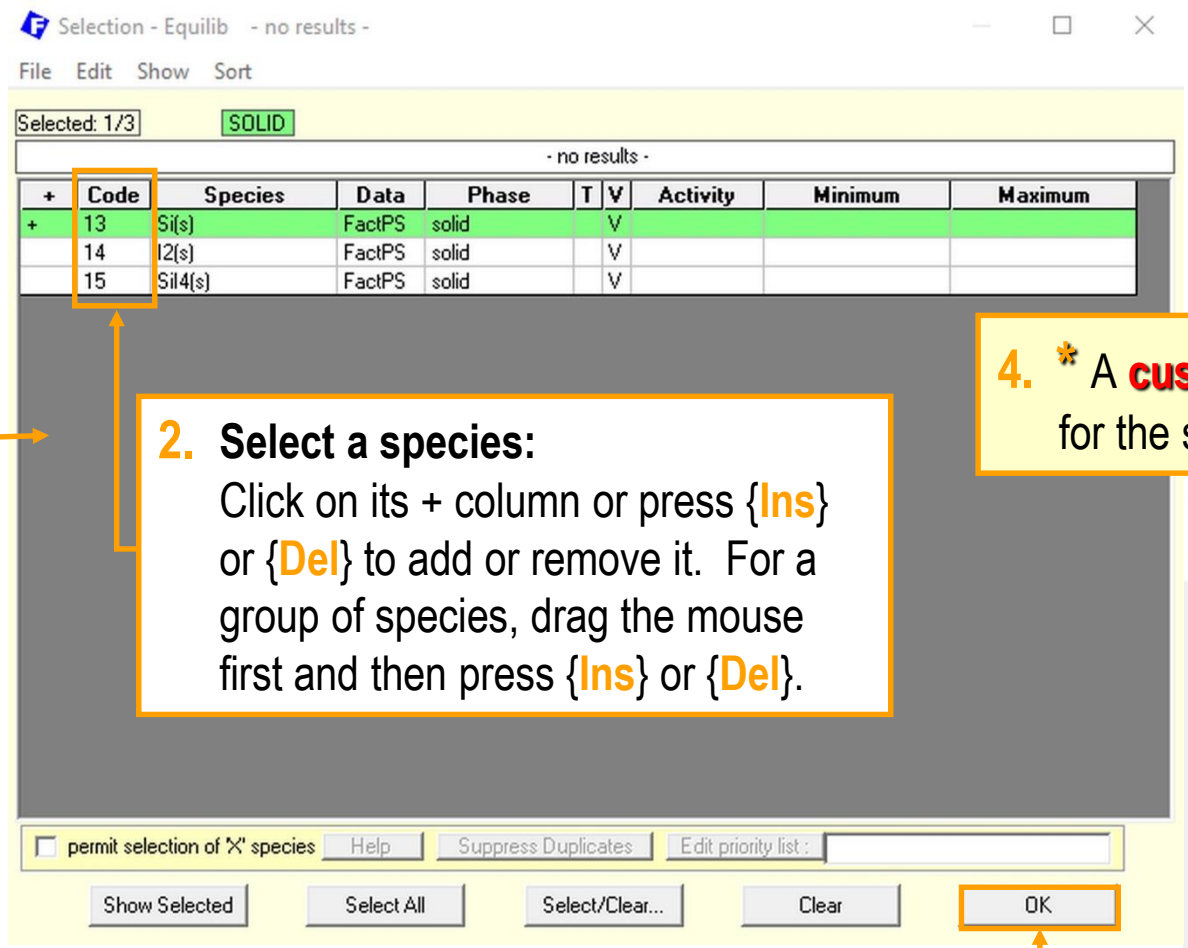


Computations are at **1400 K** for two fixed volumes: **1000** and **10000** **litres**.

Custom selection of product species: a short-cut

1. Click with mouse right button.

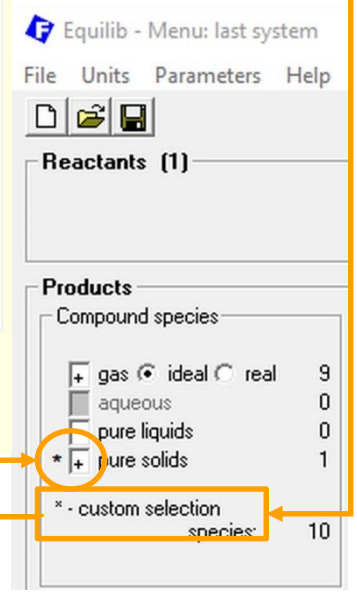




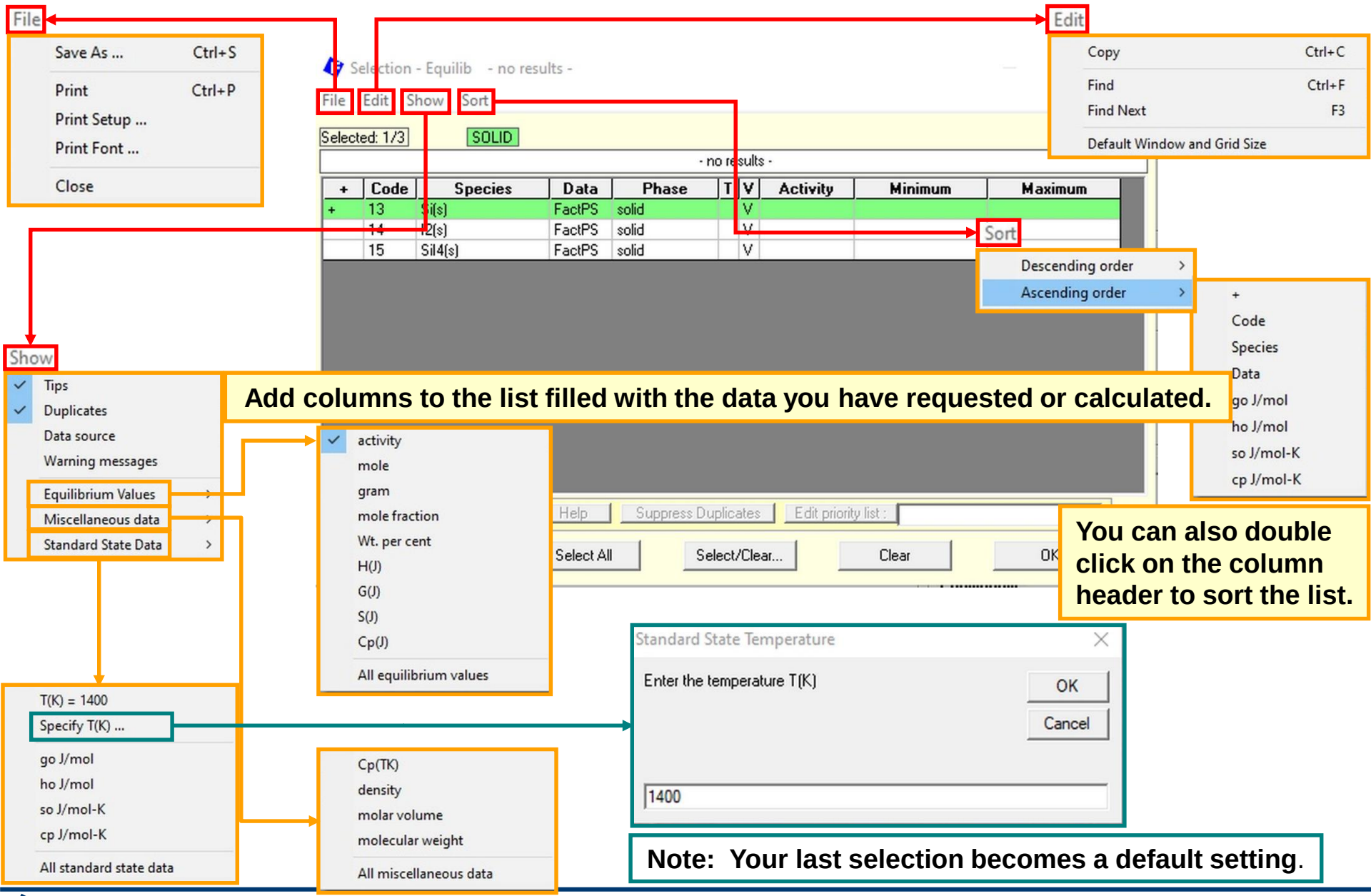
2. **Select a species:**
Click on its + column or press {Ins} or {Del} to add or remove it. For a group of species, drag the mouse first and then press {Ins} or {Del}.

3. Press «OK»

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

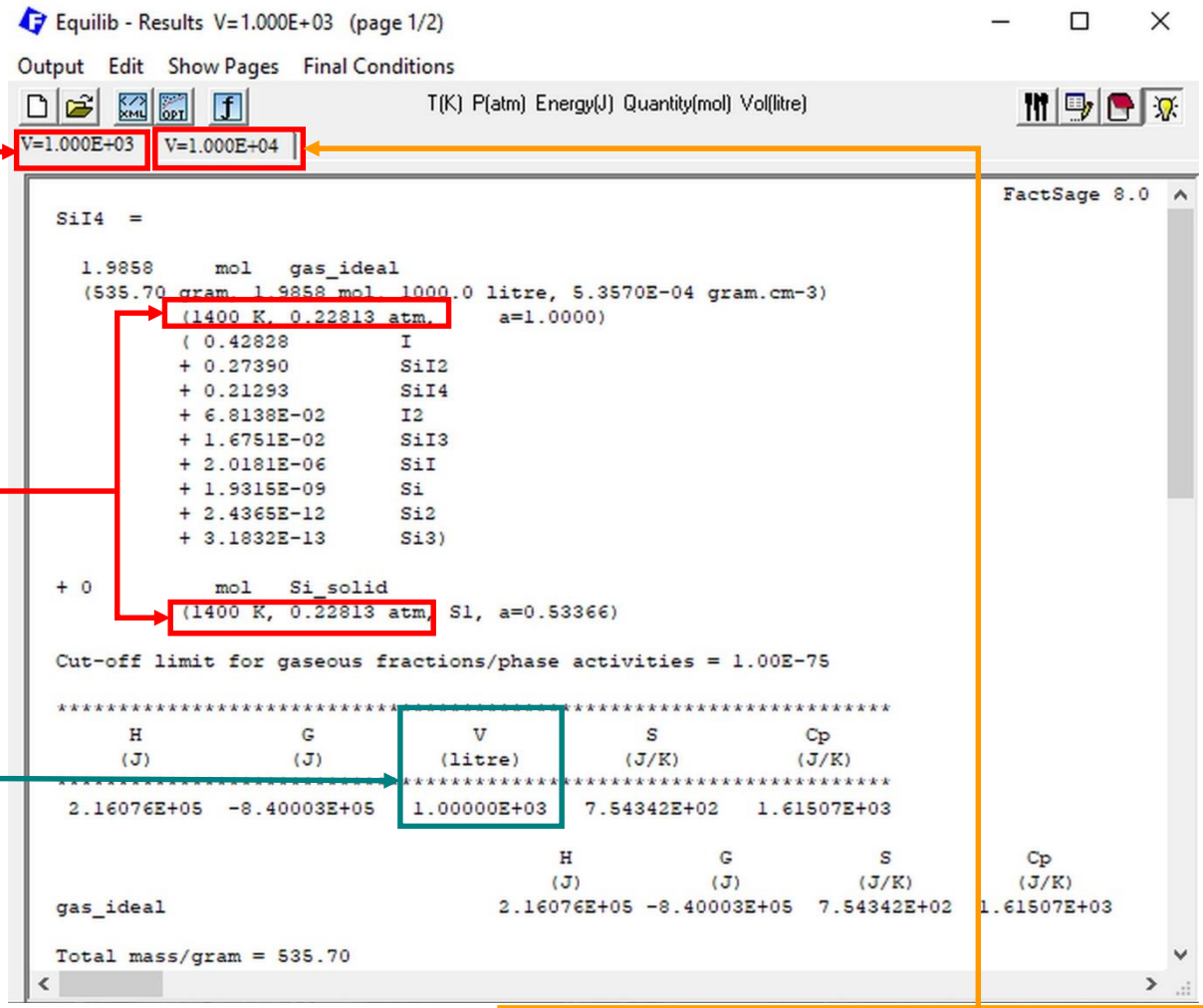


The **Selection** Window



Results window – 1400 K, 1000 L for SiI_4

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



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

Equilib - Results V=1.000E+03 (page 1/2)

Output Edit Show Pages Final Conditions

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

V=1.000E+03 | V=1.000E+04

```
SiI4  =

  1.9858      mol    gas_ideal
 (535.70 gram, 1.9858 mol, 1000.0 litre, 5.3570E-04 gram.cm-3
         1400 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
        + 2.4365E-12       Si2
        + 3.1832E-13       Si3)

+ 0           mol    Si_solid
          (1400 K, 0.22813 atm, Si  a=0.53366)

Cut-off limit for gaseous fractions/phase activities = 1.00E-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

                                    H             G             S             Cp
                                   (J)           (J)         (J/K)         (J/K)
gas_ideal                   2.16076E+05  -8.40003E+05   7.54342E+02   1.61507E+03

Total mass/gram = 535.70
```

Equilib - Results V=1.000E+04 (page 2/2)

Output Edit Show Pages Final Conditions

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

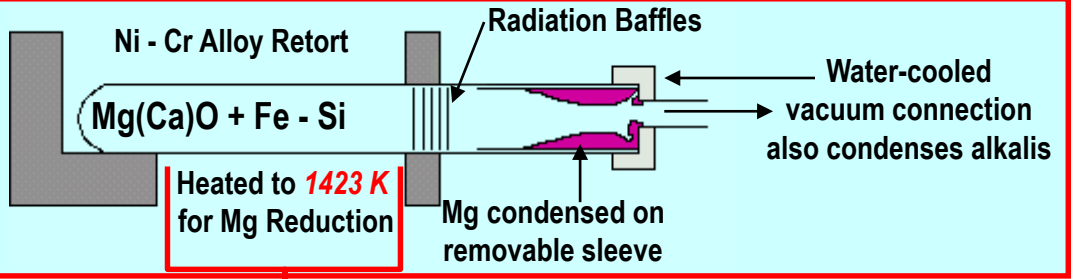
V=1.000E+03 - V=1.000E+04 -

```
                                                          FactSage 8.0
SiI4  =

  3.0718      mol    gas_ideal
 (528.66 gram, 3.0718 mol, 10000. litre, 5.2866E-05 gram.cm-3)
         (1400 K, 3.5289E-02 atm,      a=1.0000)
        ( 0.72584          I
        + 0.22804          SiI2
        + 3.0274E-02       I2
        + 1.2185E-02       SiI4
        + 3.6562E-03       SiI3
        + 6.4089E-06       SiI
        + 2.3398E-08       Si
        + 5.5307E-11       Si2
        + 1.3540E-11       Si3)

+ 0.25083     mol    Si_solid
  (7.0448 gram, 0.25083 mol)
         (1400 K, 3.5289E-02 atm, Si  a=1.0000)

Cut-off limit for gaseous fractions/phase activities = 1.00E-75

*****************************************************************************
      H             G             V             S             Cp
     (J)           (J)         (litre)       (J/K)         (J/K)
*****************************************************************************
 4.16538E+05  -8.95028E+05   1.00000E+04   9.36833E+02   1.95575E+02
```

V = **10000 L**
T = **1400 K**, P = 0.03529 atm
0.25083 mol Si(s) formed
activity = 1

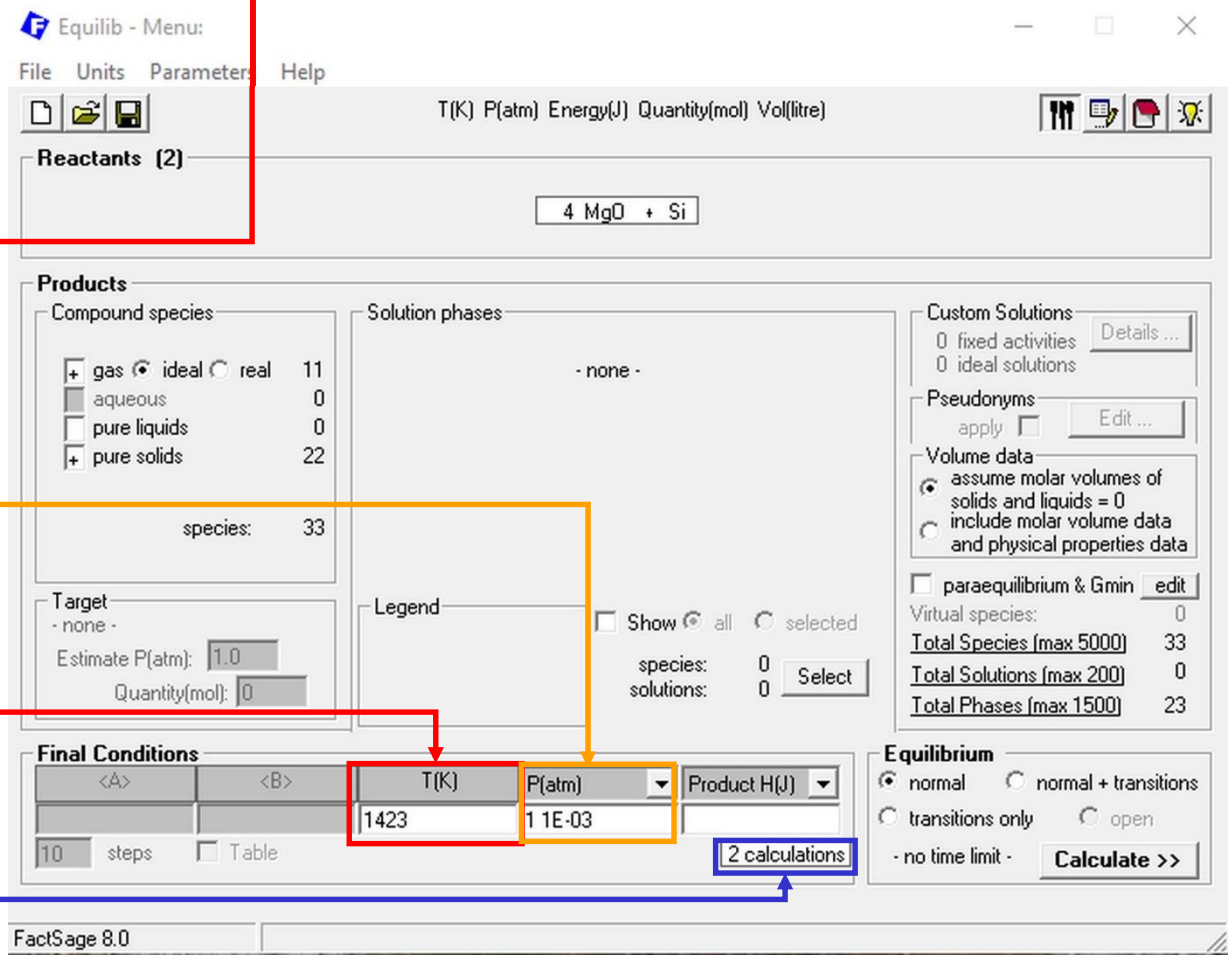
Effect of Pressure on Simple Heterogeneous Equilibria:

Pidgeon Process
for the Production of
Magnesium:
Apparatus Schema



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

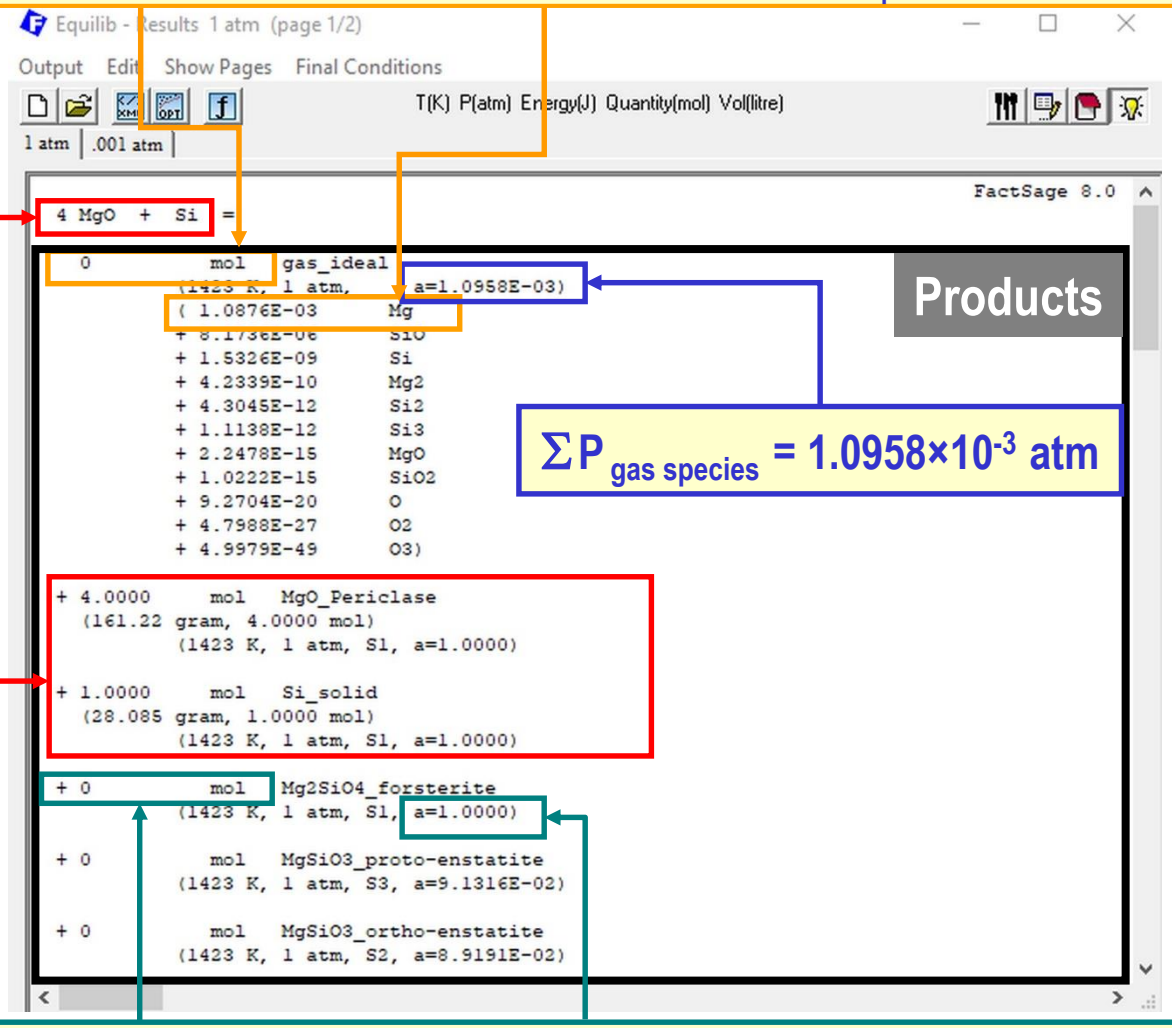
Final Conditions:
two different pressures
and
one temperature
result in
2 calculations



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



$\Sigma P_{gas\ species}$ = 1.0958×10^{-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}= 0.99254 and P_{total}= 0.001 atm, hence $P_{Mg_{eq}}$= 9.93×10^{-4} atm

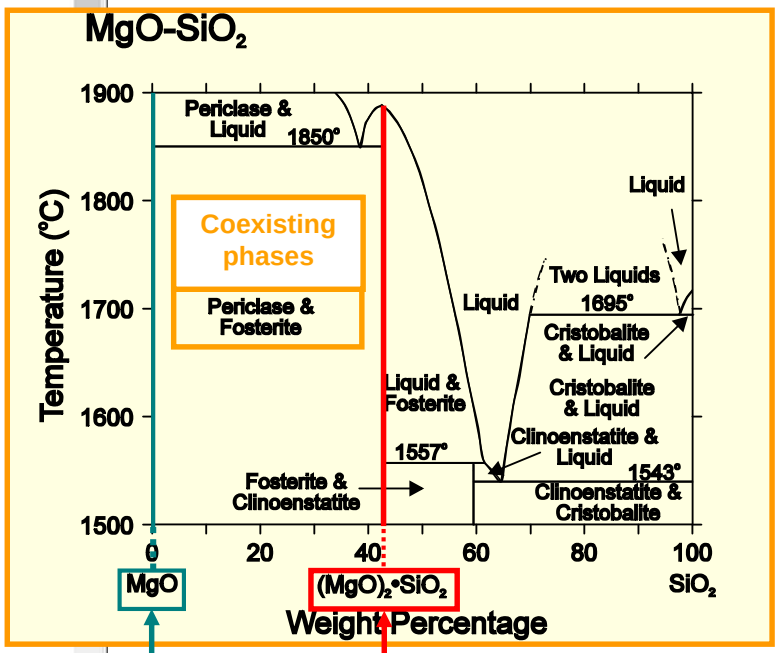
Equilib - Results .001 atm (page 2/2)

Output Edit Show Pages Final Conditio

1 atm - .001 atm -

```
                                                        FactSage 8.0
4 MgO  +  Si  =

  2.0000     mol   gas_ideal
  (48.905 gram, 2.0000 mol, 2.3354E+05 litre, 2.0941E-07 gram.cm-3)
          (1423 K, 1.0000E-03 atm,      a=1.0000)
          (  0.99254          Mg
          + 7.4591E-03        SiO
          + 1.2763E-06        Si
          + 3.5261E-07        Mg2
          + 2.9855E-09        Si2
          + 6.4339E-10        Si3
          + 2.2478E-12        MgO
          + 1.0222E-12        SiO2
          + 1.0158E-16        O
          + 5.7622E-24        O2
          + 6.5760E-46        O3)

+ 0.98508     mol   Mg2SiO4_forsterite
  (138.59 gram, 0.98508 mol)
          (1423 K, 1.0000E-03 atm, S1, a=1.0000)

+ 4.4765E-02 mol   MgO_Periclase
  (1.8042 gram, 4.4765E-02 mol)
          (1423 K, 1.0000E-03 atm, S1, a=1.0000)

+ 0           mol   Si_solid
          (1423 K, 1.0000E-03 atm, S1, a=0.83282)

+ 0           mol   MgSiO3_proto-enstatite
          23 K, 1.0000E-03 atm, S3, a=9.1316E-02)
```

Gas phase: numbers are mole fractions



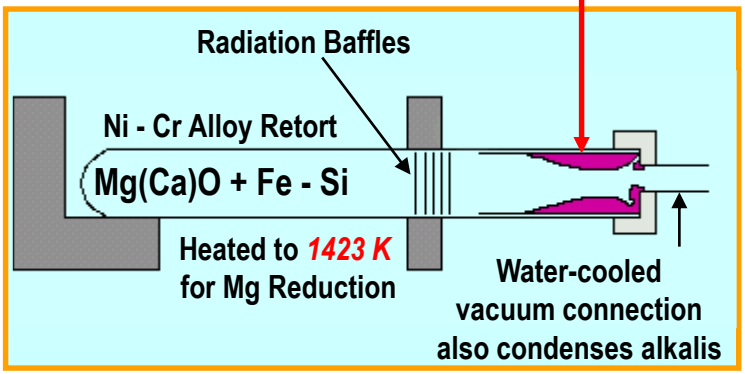
Compare the formation of the gas phase here at 10^{-3} atm with the previous page where pressure is 1 atm.

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



Equilib - List T(K) = 1423, P(atm) = 1.0000E-03 (Page 2/2)

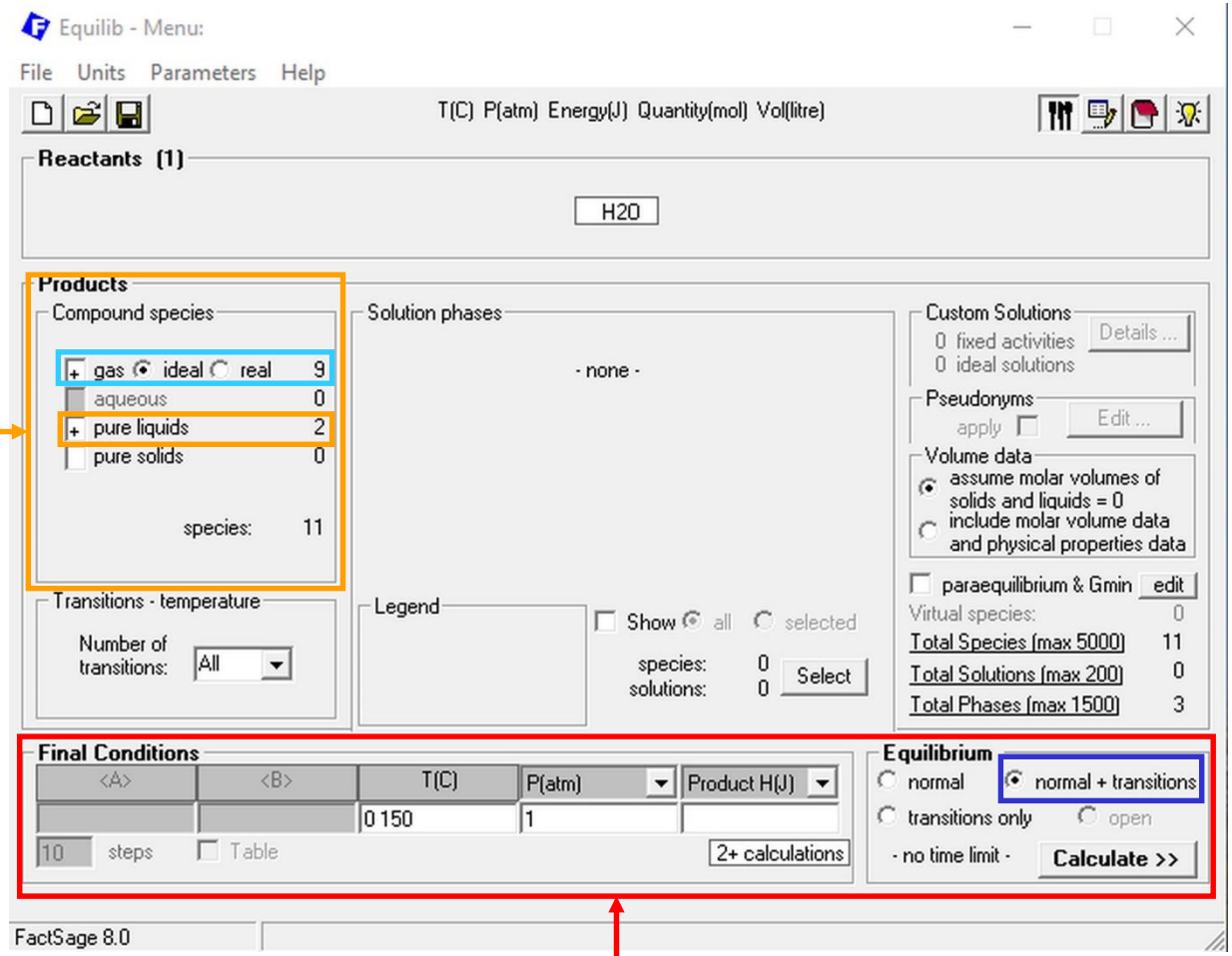
File Edit Help

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

	Code		Data		Mole	Gram	Per Cent	Cumulate	T
		ELEMENT Mg			Mole Mg	Gram Mg	Per Cent	Cumulate	
		GAS PHASE							
	4	Mg(g)	FactPS		1.985	48.25	49.63 %	49.6 %	
	5	Mg2(g)	FactPS		1.4104E-06	3.4280E-05	3.5261E-05 %	49.6 %	
	6	MgO(g)	FactPS		4.4955E-12	1.0926E-10	1.1239E-10 %	49.6 %	
Mg				Totals	1.985	48.25	49.63 %		
		PURE SPECIES							
	17	MgO(s)	FactPS		4.4765E-02	1.088	1.119 %	50.7 %	
	35	Mg2SiO4(s)	FactPS		1.970	47.88	49.25 %	100. %	
				Totals	2.015	48.97	50.37 %		
		TOTAL Mg			4.000	97.22			
		ELEMENT O			Mole O	Gram O	Per Cent	Cumulate	
		GAS PHASE							
	1	O(g)	FactPS		2.0317E-16	3.2506E-15	5.0792E-15 %	5.079E-15 %	
	2	O2(g)	FactPS		2.3049E-23	3.6876E-22	5.7622E-22 %	5.079E-15 %	
	3	O3(g)	FactPS		3.9456E-45	6.3127E-44	9.8640E-44 %	5.079E-15 %	
	6	MgO(g)	FactPS		4.4955E-12	7.1926E-11	1.1239E-10 %	1.124E-10 %	
	10	SiO(g)	FactPS		1.4918E-02	0.2387	0.3730 %	0.373 %	
O	11	SiO2(g)	FactPS		4.0888E-12	6.5418E-11	1.0222E-10 %	0.373 %	
				Totals	1.4918E-02	0.2387	0.3730 %		
		PURE SPECIES							
	17	MgO(s)	FactPS		4.4765E-02	0.7162	1.119 %	1.49 %	
	35	Mg2SiO4(s)	FactPS		3.940	63.04	98.51 %	100. %	
				Totals	3.985	63.76	99.63 %		
		TOTAL O			4.000	64.00			
		ELEMENT Si			Mole Si	Gram Si	Per Cent	Cumulate	
		GAS PHASE							
	7	Si(g)	FactPS		2.5527E-06	7.1693E-05	2.5527E-04 %	2.553E-04 %	
	8	Si2(g)	FactPS		1.1942E-08	3.3540E-07	1.1942E-06 %	2.565E-04 %	
	9	Si3(g)	FactPS		3.8603E-09	1.0842E-07	3.8603E-07 %	2.568E-04 %	
	10	SiO(g)	FactPS		1.4918E-02	0.4190	1.492 %	1.49 %	
Si	11	SiO2(g)	FactPS		2.0444E-12	5.7417E-11	2.0444E-10 %	1.49 %	
				Totals	1.4921E-02	0.4191	1.492 %		
		PURE SPECIES							
	35	Mg2SiO4(s)	FactPS		0.9851	27.67	98.51 %	100. %	
				Totals	0.9851	27.67	98.51 %		
		TOTAL Si			1.000	28.09			

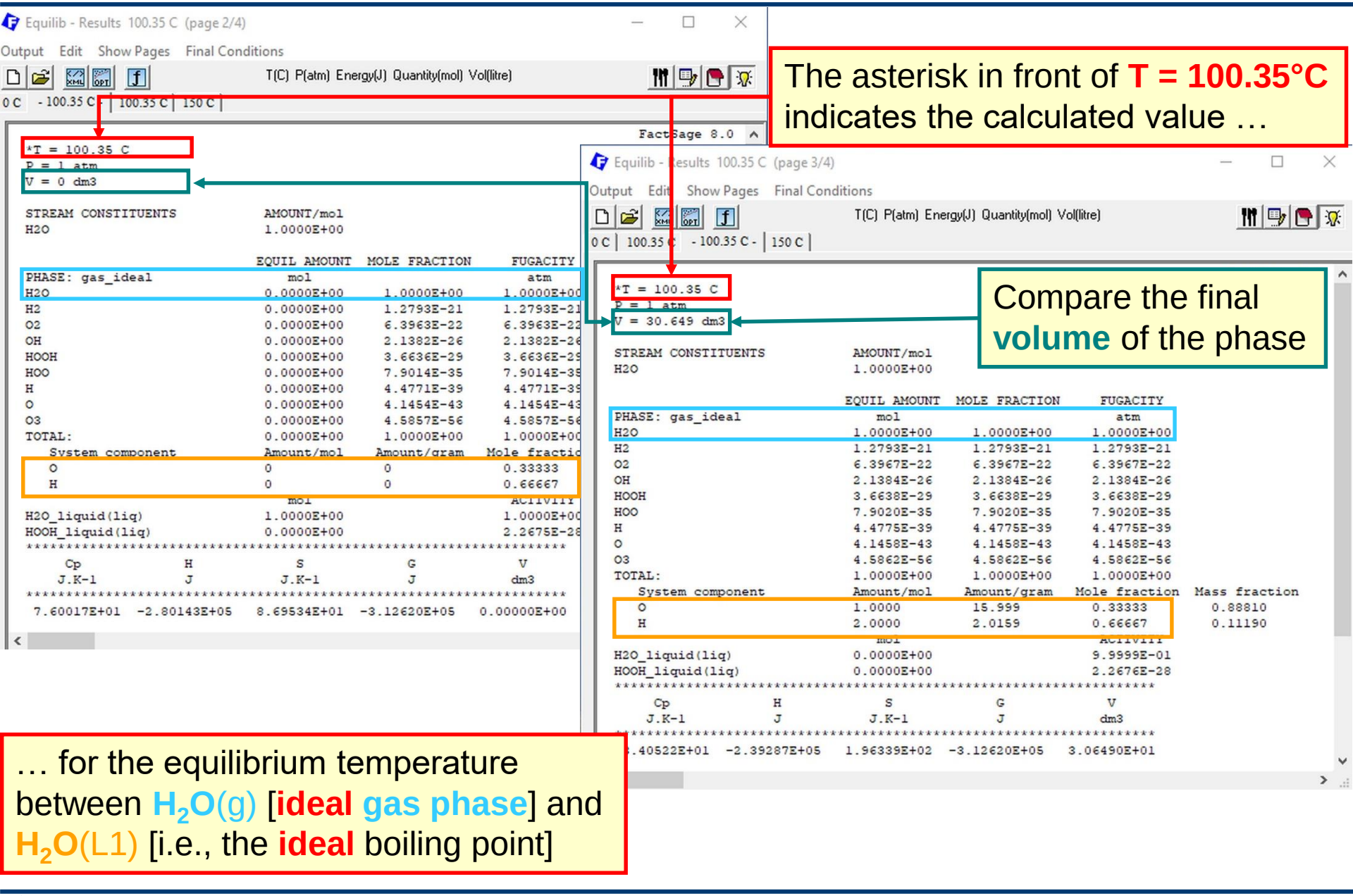
Boiling Point of Water: Ideal Gas Calculation Settings

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

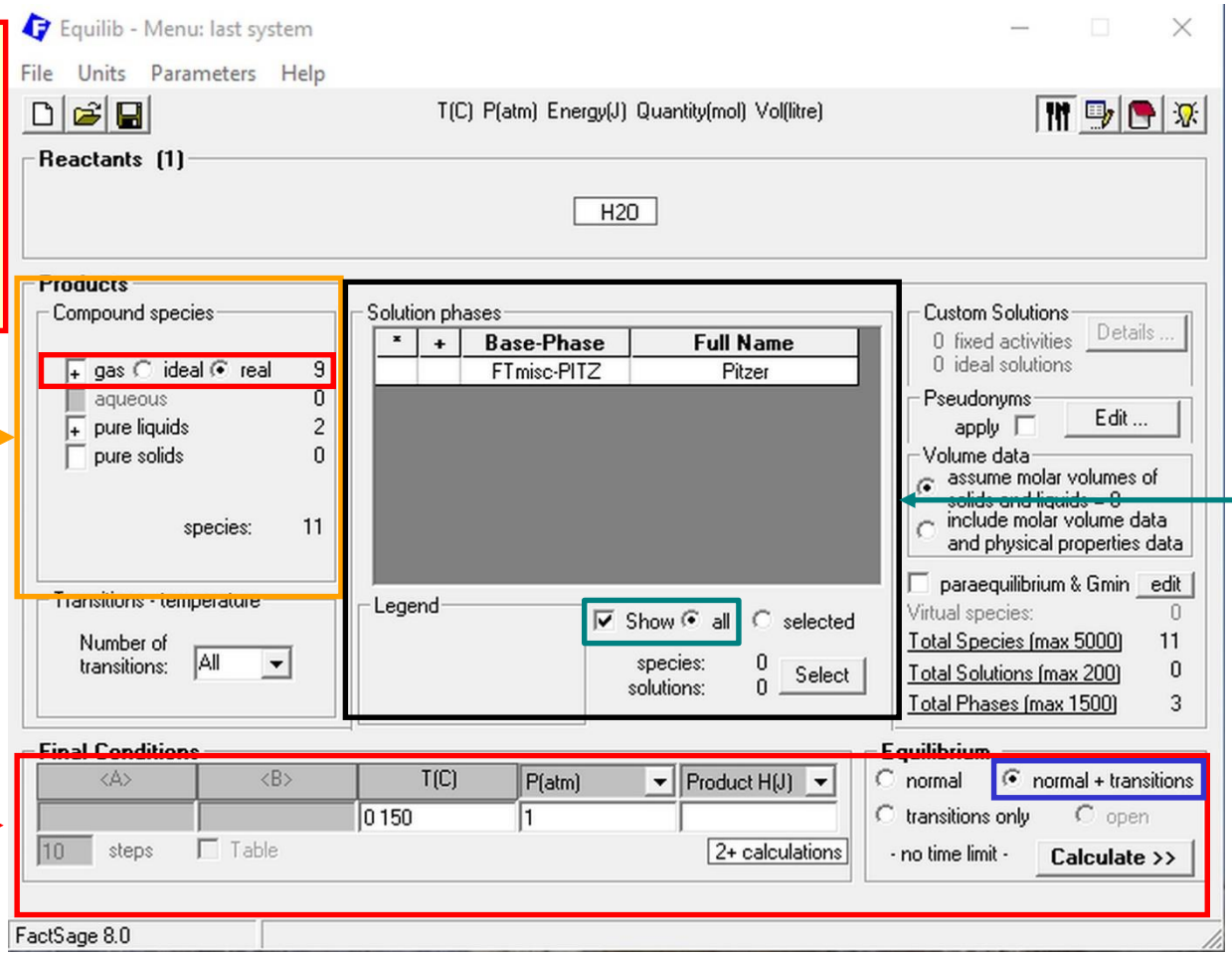
Boiling Point of Water: Ideal Gas Calculation; Results: T_b(water) = 100.35°C



Boiling Point of Water: Real Gas Calculation Settings

For **real gas** equations see **ViewData** slide show, slide **7.2** or **Compound** slide show, slide **8.3**

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]

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

Equilib - Results 100 C (page 2/4)

Output Edit Show Pages Final Conditions

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

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

```
*T = 100.00 C
P = 1 atm
V = 0 dm3

STREAM CONSTITUENTS          AMOUNT/mol
H2O                          1.0000E+00

                          EQUIL AMOUNT   MOLE FRACTION     FUGACITY
PHASE: gas_real               mol                           atm
H2O                  V    0.0000E+00     1.0000E+00      9.8754E-(
H2                   V    0.0000E+00     1.1937E-21      1.2087E-
O2                   V    0.0000E+00     5.9683E-22      6.0207E-
OH                   V    0.0000E+00     2.0176E-26      1.9925E-
HOOH                 V    0.0000E+00     3.4412E-29      3.3983E-
HOO                  V    0.0000E+00     7.3173E-35      7.2261E-
H                    V    0.0000E+00     4.1210E-39      4.0696E-
O                    V    0.0000E+00     3.7721E-43      3.7251E-
O3                   V    0.0000E+00     3.9962E-56      4.0086E-
TOTAL:                    0.0000E+00     1.0000E+00      1.0000E+(
   System component       Amount/mol     Amount/gram     Mole fract
   O                      0              0               0.33333
   H                      0              0               0.66667
                             mol                          ACTIVIT
H2O_liquid(liq)           1.0000E+00                      1.0000E+(
HOOH_liquid(liq)          0.0000E+00                      2.1346E-
*************************************************************************
     Cp             H              S              G              V
   J.K-1            J            J.K-1            J            dm3
*************************************************************************
 7.59935E+01  -2.80170E+05   8.68810E+01  -3.12589E+05   0.00000E+00
```

Equilib - Results 100 C (page 3/4)

Output Edit Show Pages Final Conditions

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

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

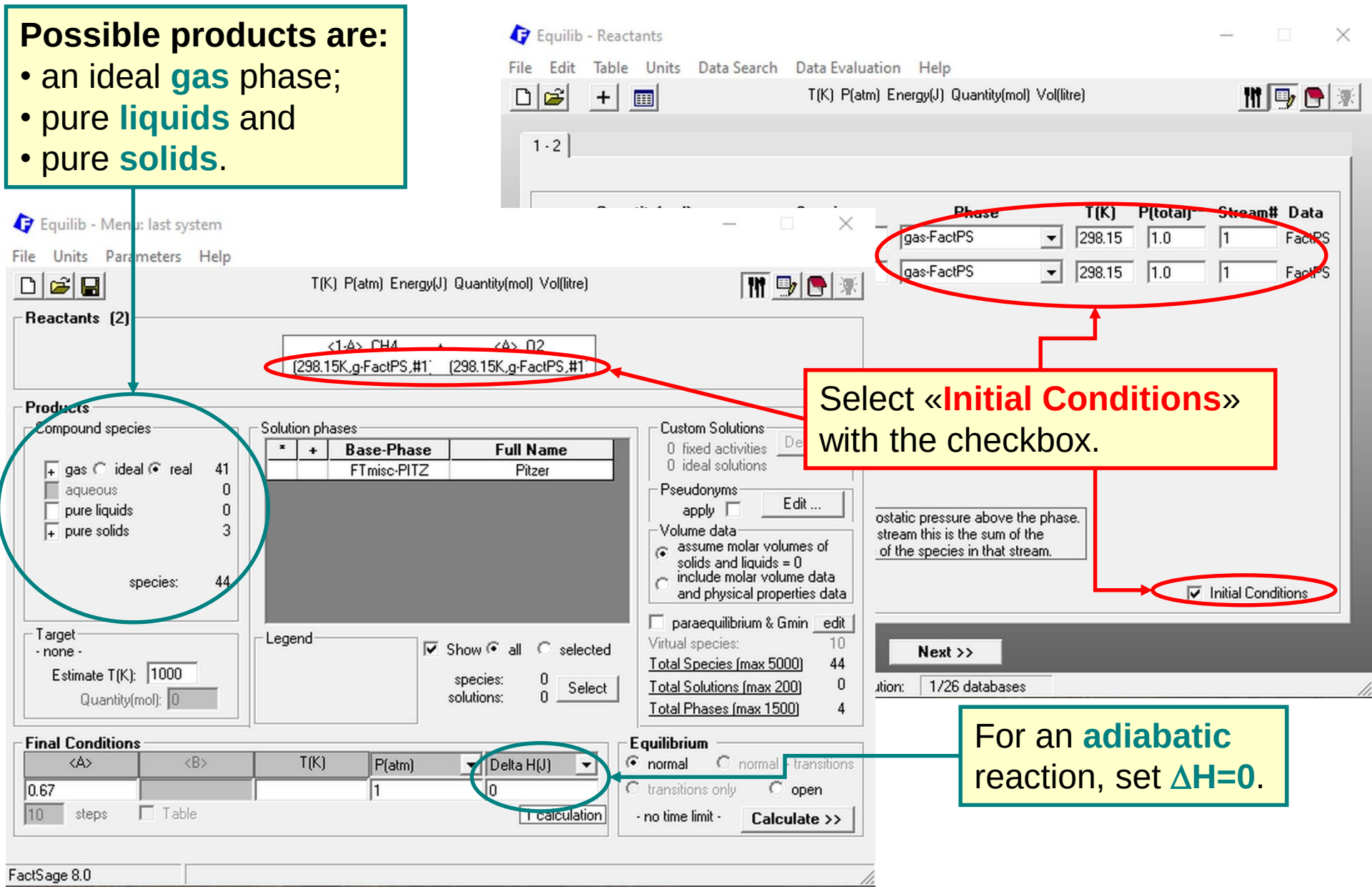
```
*T = 100.00 C
P = 1 atm
V = 30.236 dm3

STREAM CONSTITUENTS          AMOUNT/mol
H2O                          1.0000E+00

                          EQUIL AMOUNT   MOLE FRACTION     FUGACITY
PHASE: gas_real               mol                           atm
H2O                  V    1.0000E+00     1.0000E+00      9.8754E-01
H2                   V    1.1937E-21     1.1937E-21      1.2088E-21
O2                   V    5.9687E-22     5.9687E-22      6.0210E-22
OH                   V    2.0178E-26     2.0178E-26      1.9926E-26
HOOH                 V    3.4414E-29     3.4414E-29      3.3985E-29
HOO                  V    7.3179E-35     7.3179E-35      7.2267E-35
H                    V    4.1214E-39     4.1214E-39      4.0700E-39
O                    V    3.7725E-43     3.7725E-43      3.7255E-43
O3                   V    3.9967E-56     3.9967E-56      4.0091E-56
TOTAL:                    1.0000E+00     1.0000E+00      1.0000E+00
   System component       Amount/mol     Amount/gram     Mole fractior   Mass fraction
   O                      1.0000         15.999          0.33333         0.88810
   H                      2.0000         2.0159          0.66667         0.11190
                             mol                          ACTIVITY
H2O_liquid(liq)           0.0000E+00                      9.9999E-01
HOOH_liquid(liq)          0.0000E+00                      2.1347E-28
*************************************************************************
     Cp             H              S              G              V
   J.K-1            J            J.K-1            J            dm3
*************************************************************************
 3.61170E+01  -2.39471E+05   1.95950E+02  -3.12589E+05   3.02358E+01
```

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, $\Delta H=0$

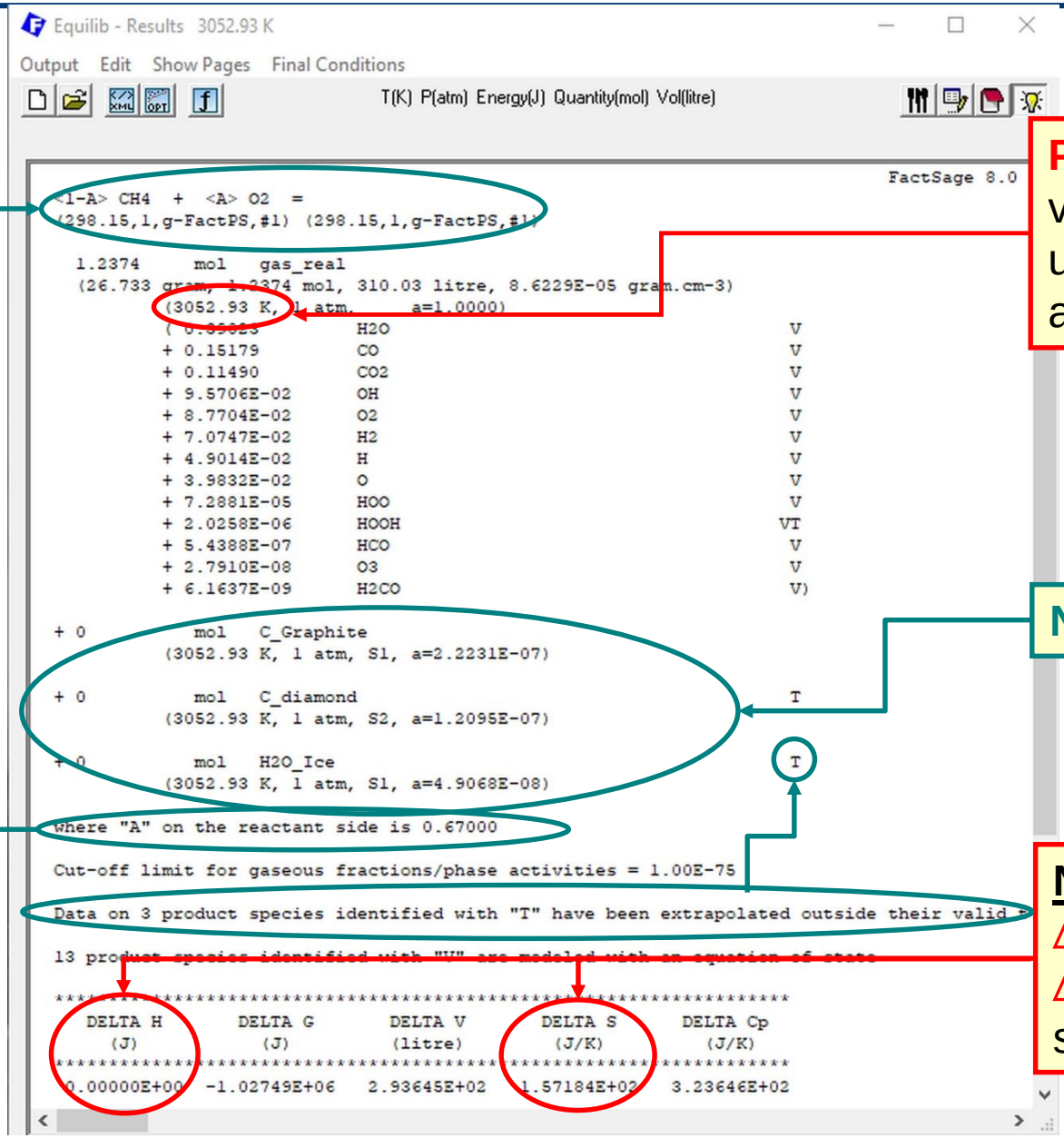
Possible products are:
- an ideal **gas** phase;
- pure **liquids** and
- pure **solids**.



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



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

No condensed phases

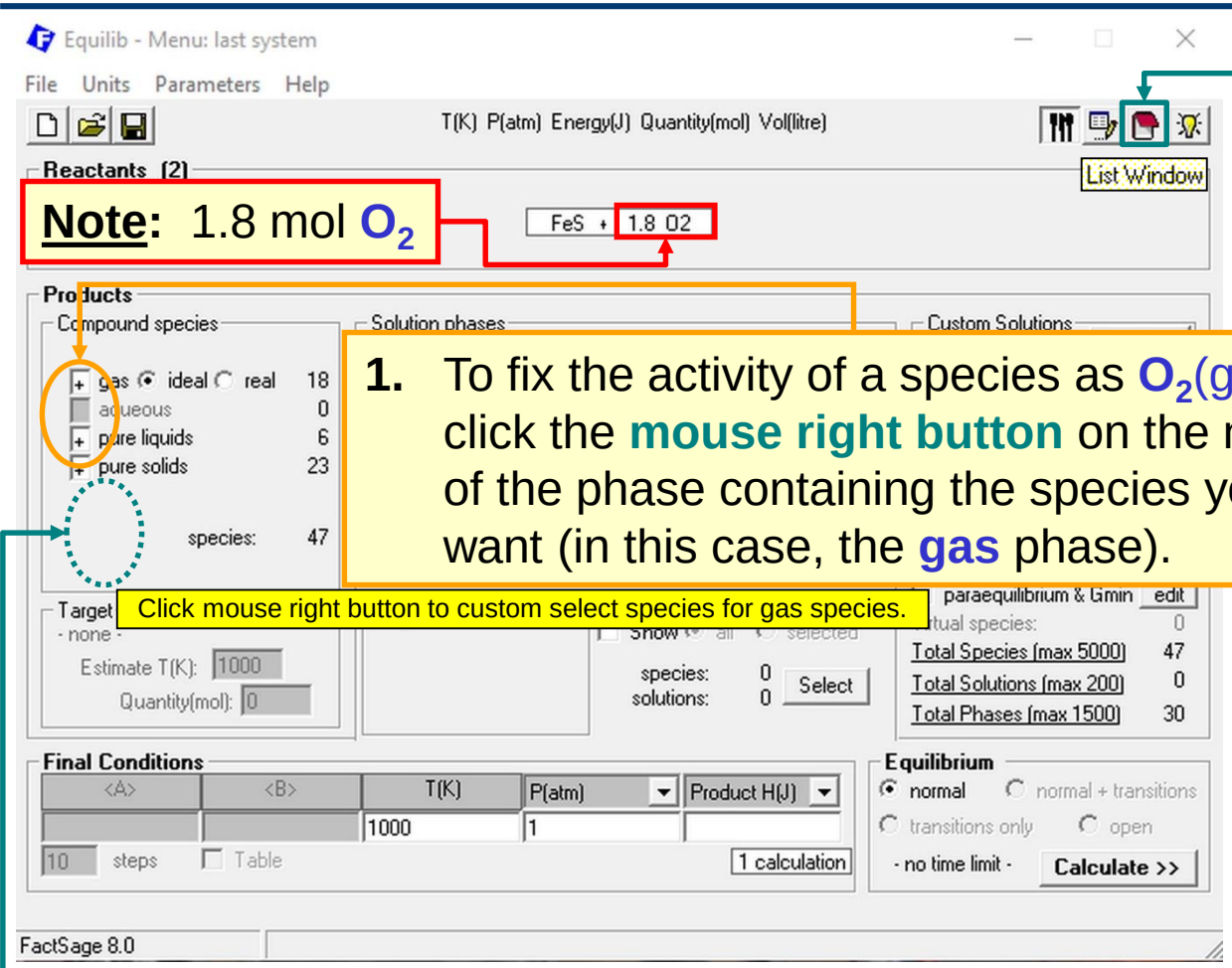
Note:
ΔH=0;
ΔS is a maximum for specified input conditions

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

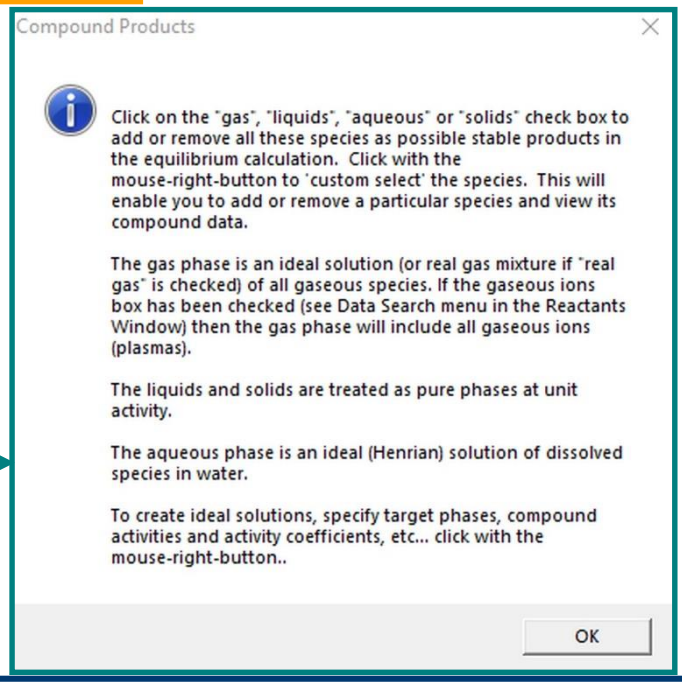


Note: 1.8 mol O_2

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).

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

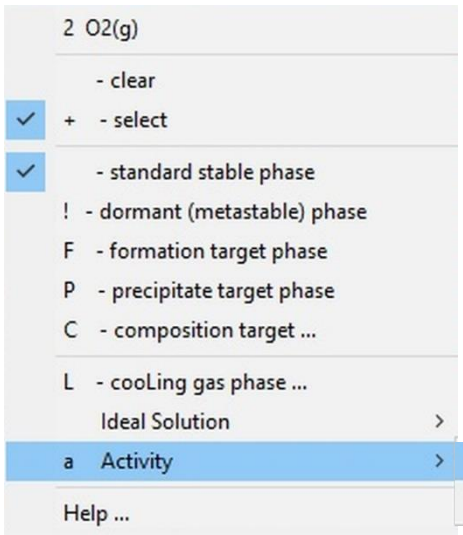


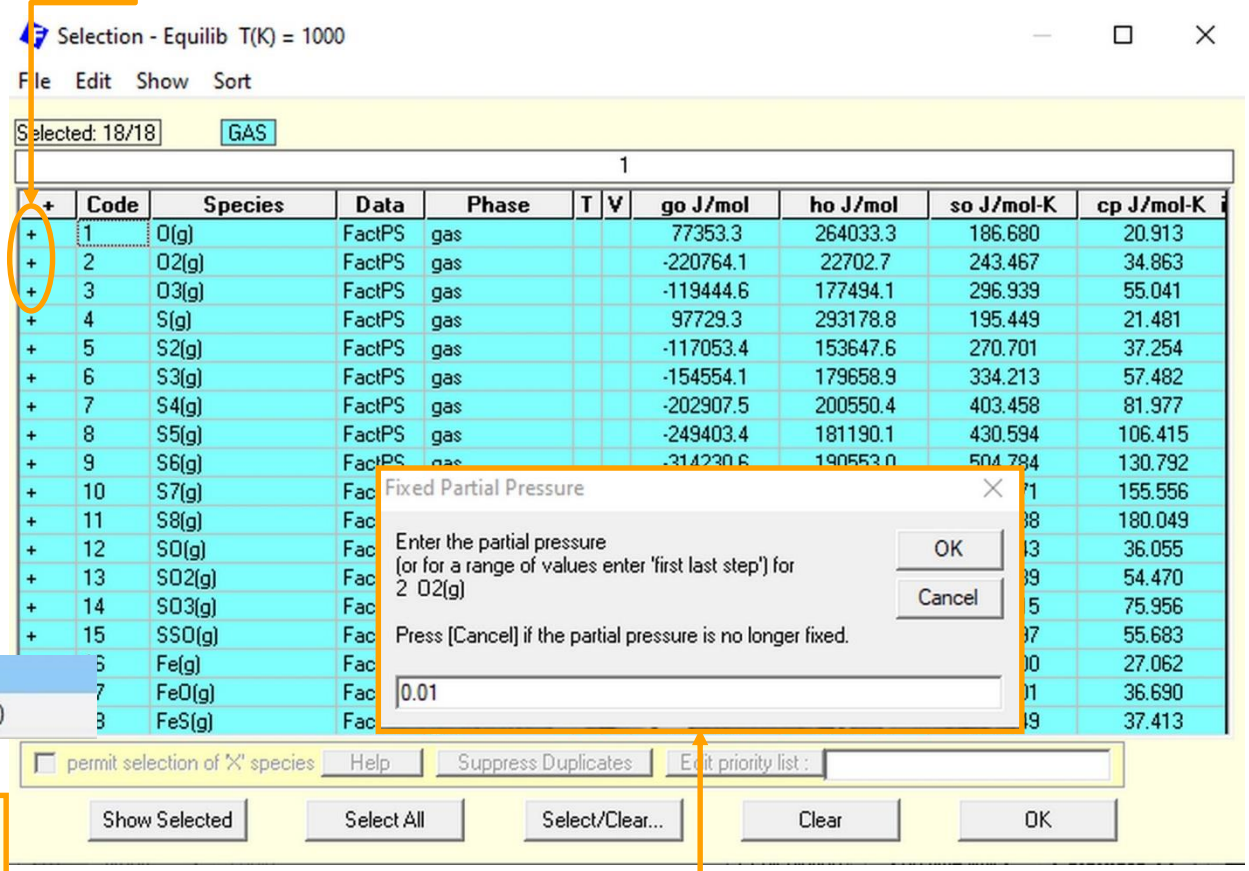
A right click in the «**compound species**» frame will provide you some information

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**

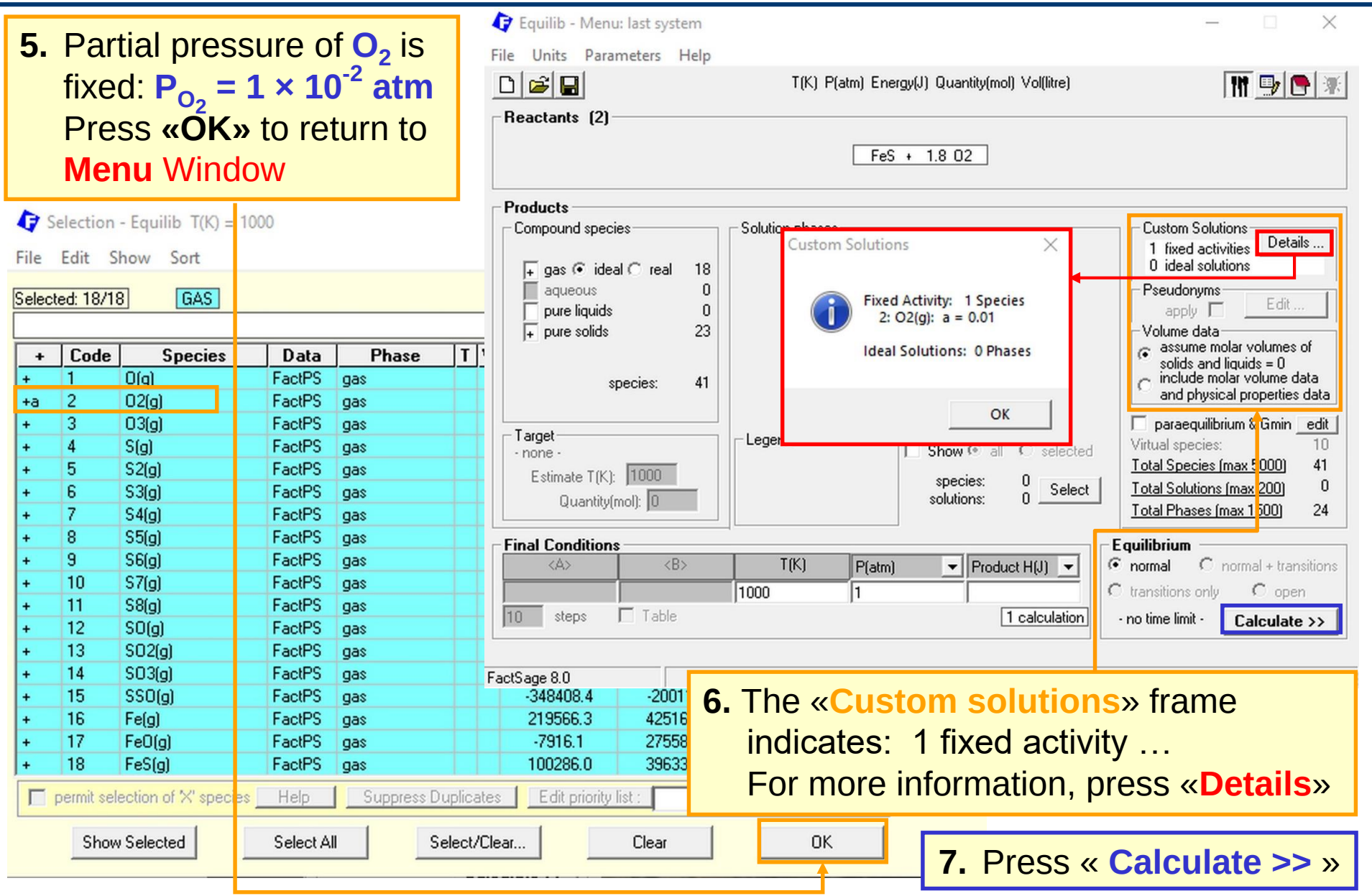




4. Fix the activity (or partial pressure) of the species; Press «**OK**».

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

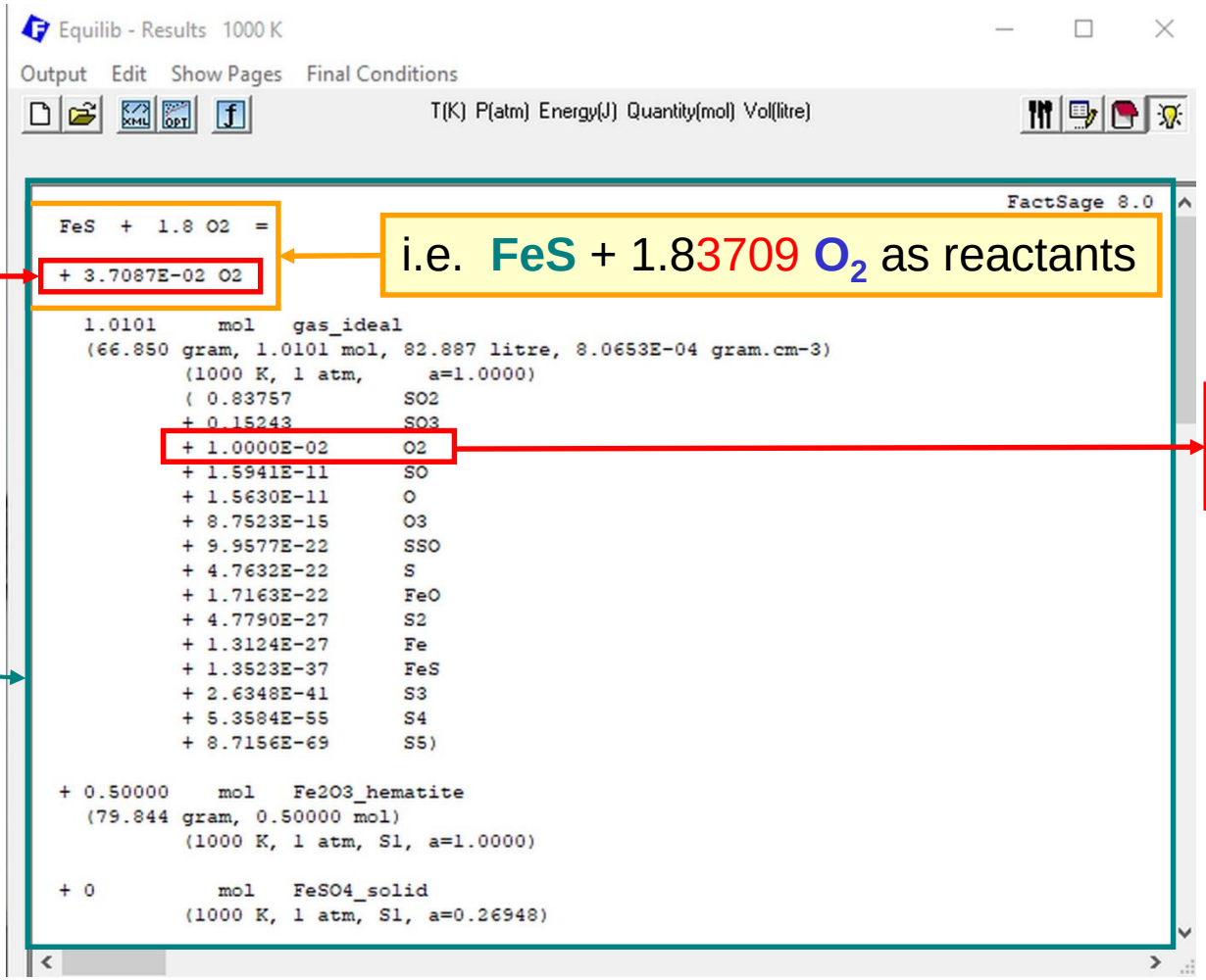


6. The «**Custom solutions**» frame indicates: 1 fixed activity …
For more information, press «**Details**»

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



i.e. **FeS** + 1.83709 O_2 as reactants

Products

P_{O_2} = **0.01** atm

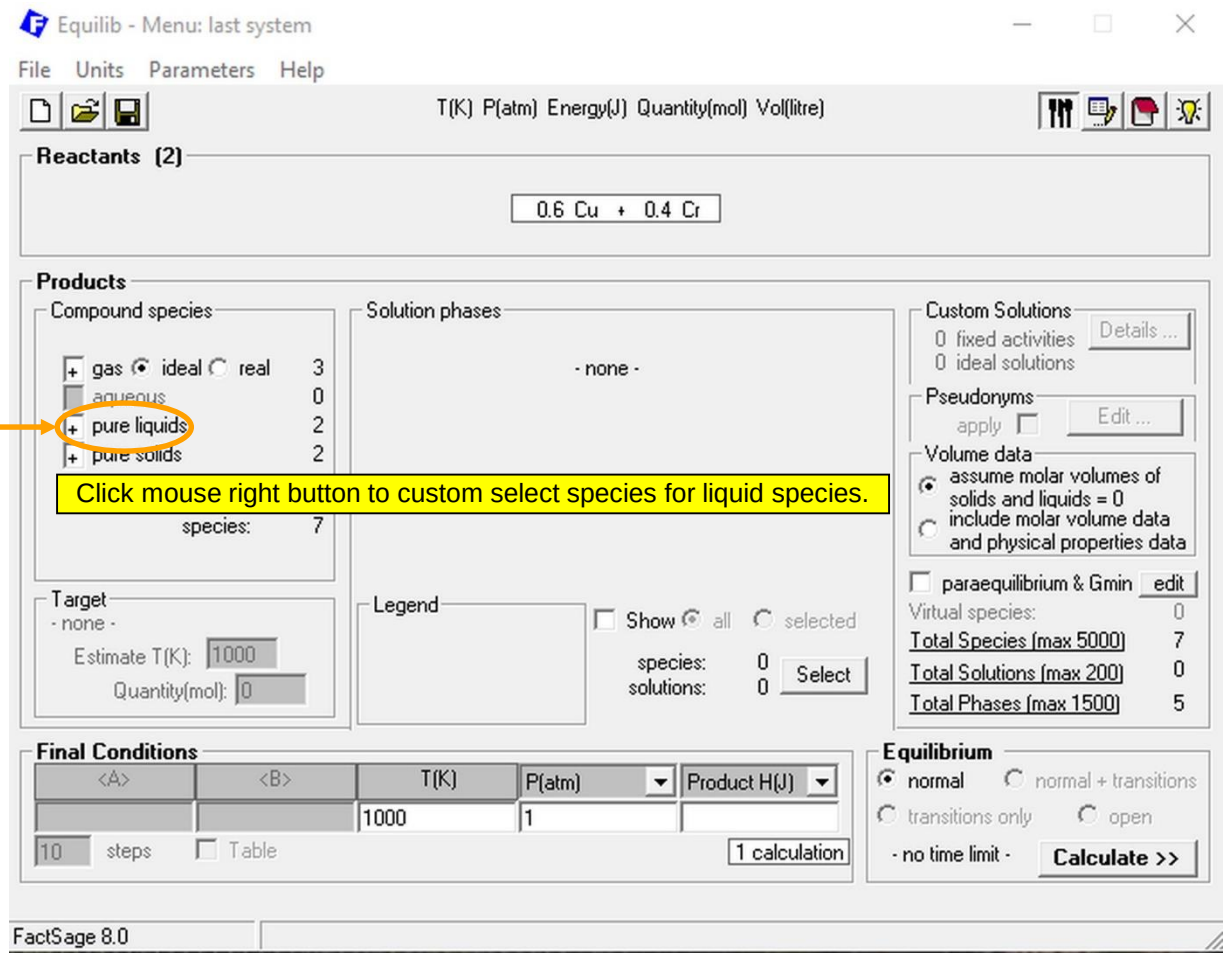
Assembling an **ideal liquid** and adding **activity coefficients**

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.

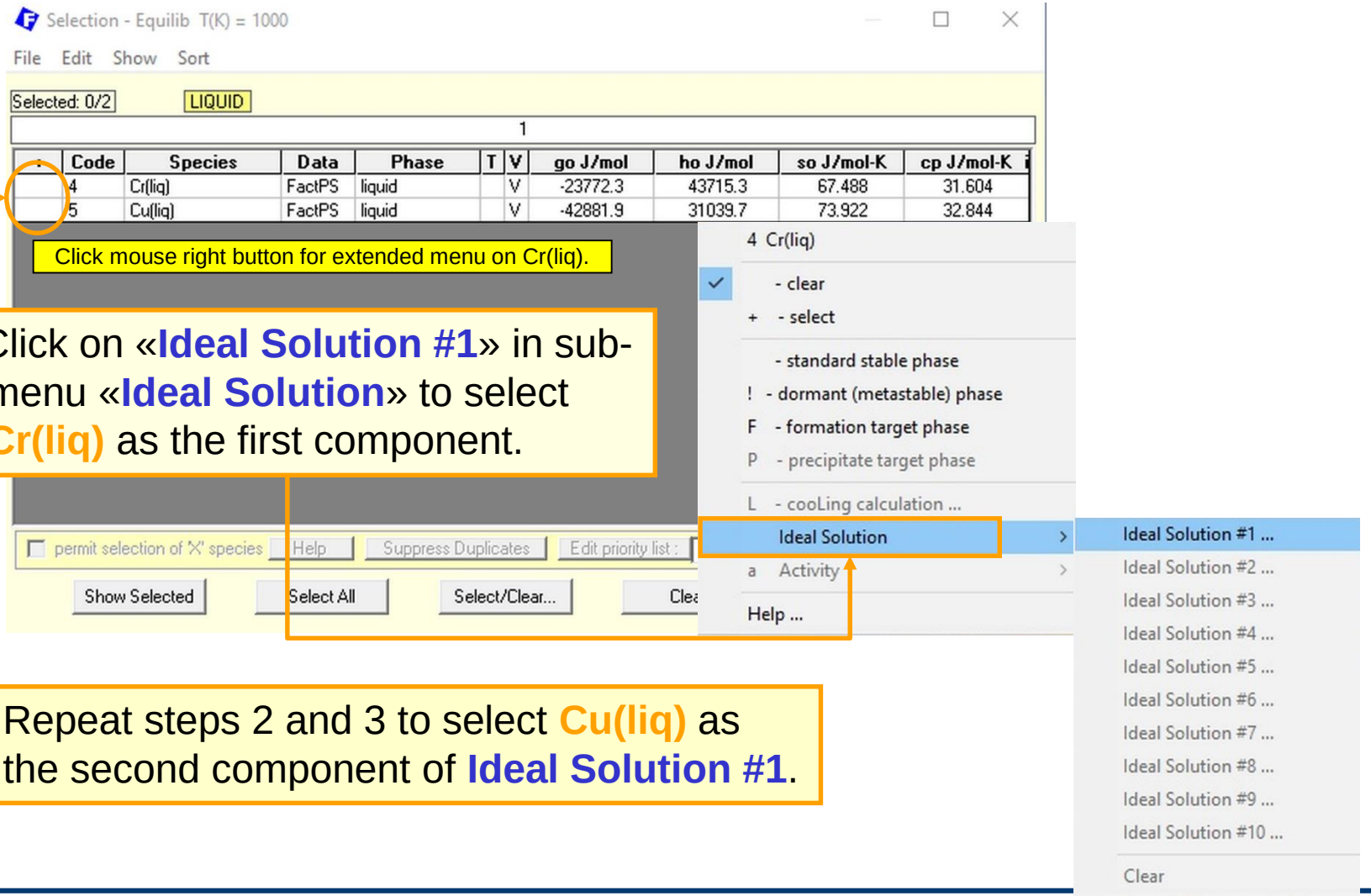
Setting up of an ideal liquid solution of Cu and Cr

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**).



Setting up of an ideal liquid solution of Cu and Cr

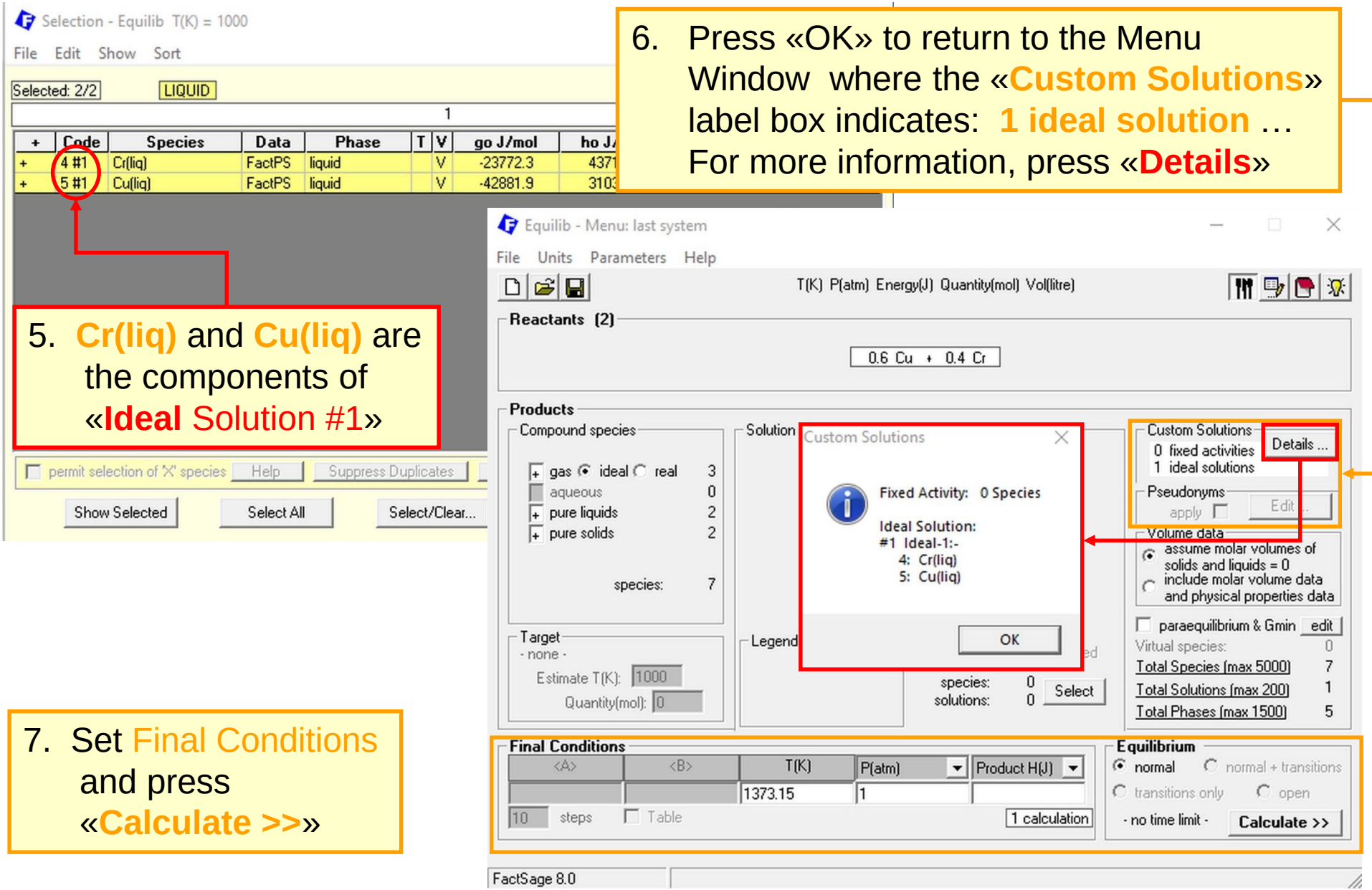
2. Click the **mouse right button** in the first column (+) of the line containing **Cr(liq)** species – **an extended menu appears**.



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



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

ChemSage format

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

Equilib - Results 1373.15 K

Output Edit Show Pages Final Conditions

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

```
                                                                    FactSage 8.0
 T = 1373.15 K
 P = 1 atm
 V = 0 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(liq)          +    4.0000E-01     4.0000E-01     4.0000E-01
 Cu_liquid(liq)          +    6.0000E-01     6.0000E-01     6.0000E-01
 TOTAL:                       1.0000E+00     1.0000E+00     1.0000E+00
    System component          Amount/mol     Amount/gram    Mole fraction  Mass fraction
    Cu                        0.60000        38.128         0.60000        0.64704
    Cr                        0.40000        20.798         0.40000        0.35296
                                 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              H              S              G              V
    J.K-1             J            J.K-1            J             dm3
 ************************************************************************
  3.47467E+01   4.86096E+04   8.75461E+01  -7.16043E+04   0.00000E+00
```

```
 0.6 Cu  +  0.4 Cr  =

   0          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          Amount/mol     Amount/gram    Mole fraction  Mass fractio
             Cu                        0.60000        38.128         0.60000        0.64704
             Cr                        0.40000        20.798         0.40000        0.35296

 + 0          mol   Cr_solid
             (1373.15 K, 1 atm, S1, a=0.85555)

 + 0          mol   Cu_liquid
             (1373.15 K, 1 atm, L1, a=0.60000)
```

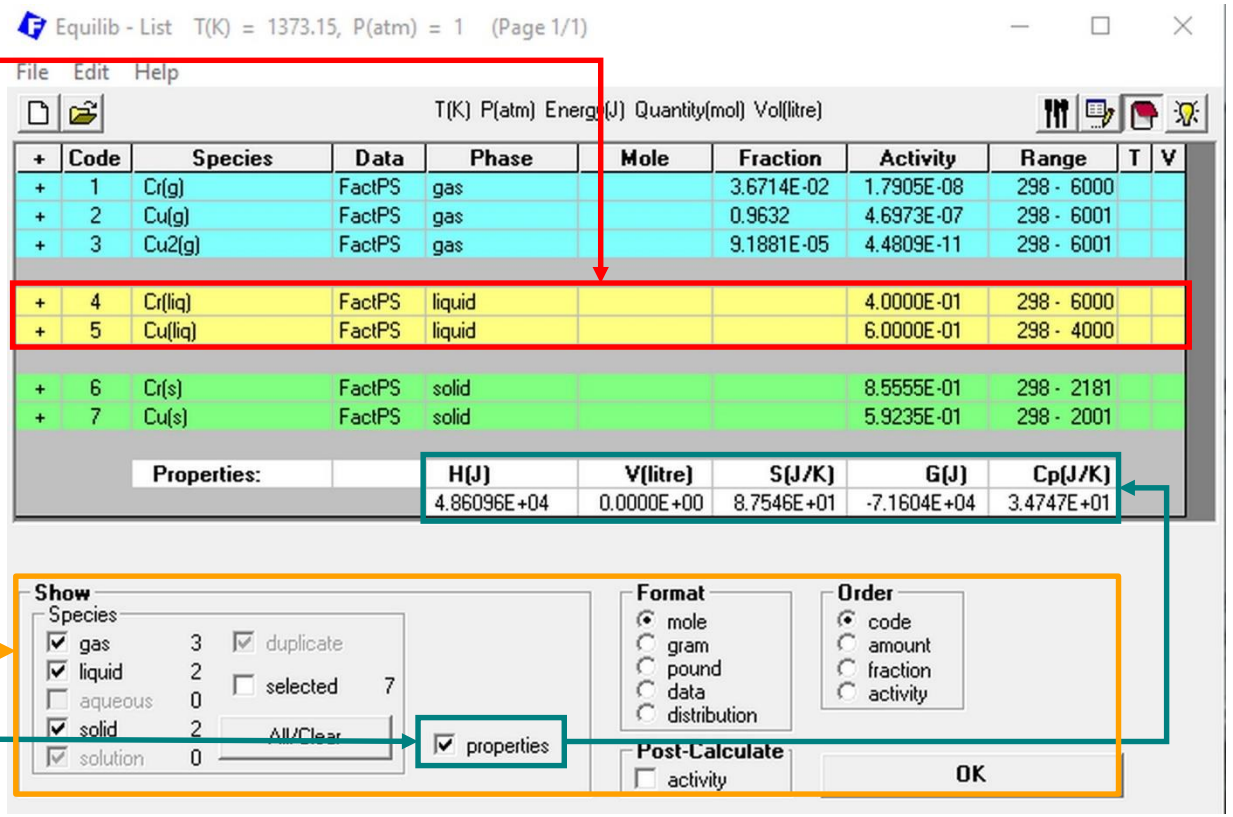
FACT format

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

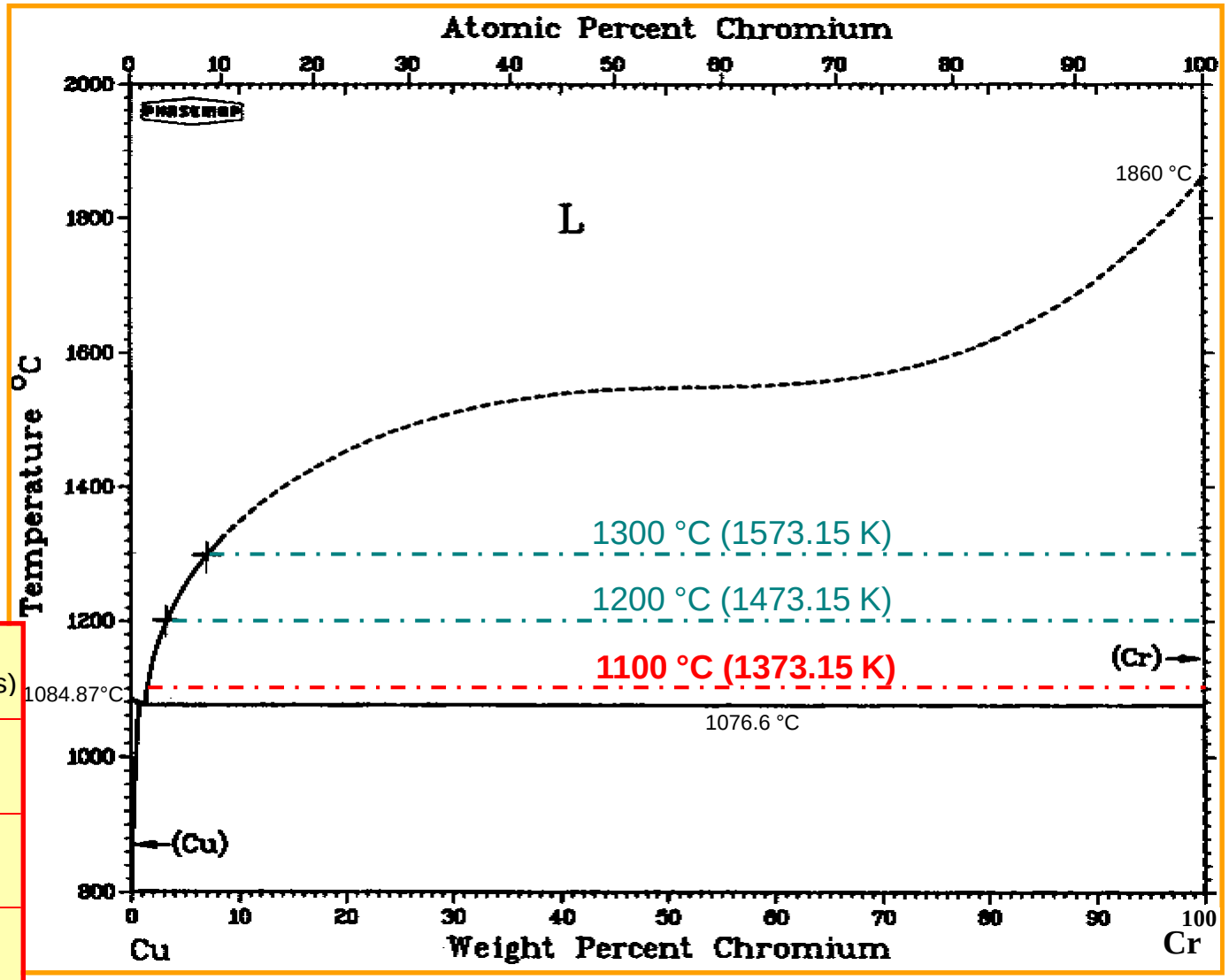


According to the phase diagram (next page):
$X_{Cr(liq)}$ = **0.01837** at **1373.15 K** (1100°C).
Hence, the assumption of an ideal solution is **not very good** in this example.

Tie-lines in the Cu-Cr phase diagram

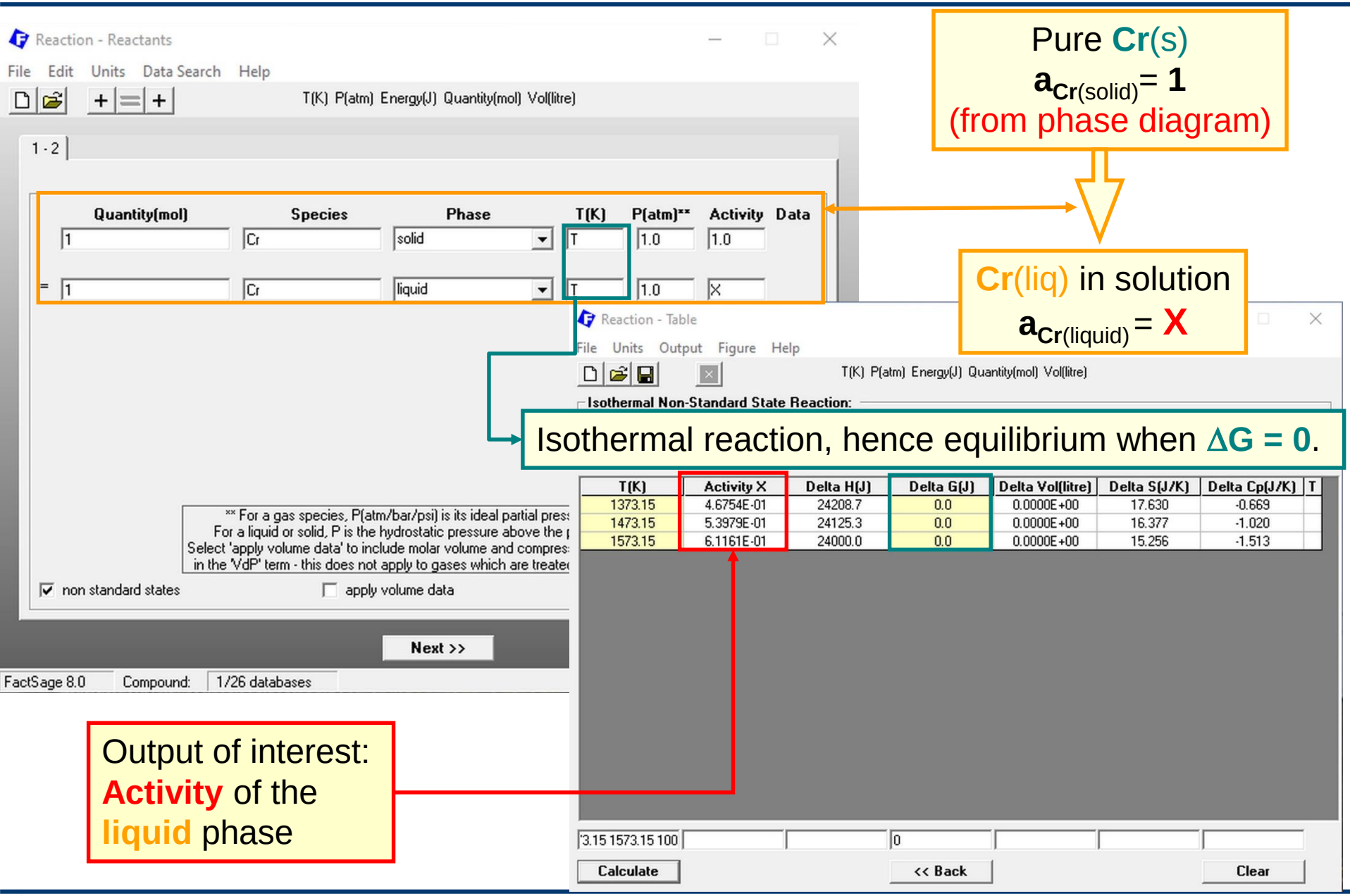
T (°C)	Cr(liq) (wt %)	Cr(s) (wt %)
1100	**1.508**	**100**
1200	3.456	100
1300	7.155	100

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 **ΔG = 0**.

Output of interest:
Activity of the
liquid phase

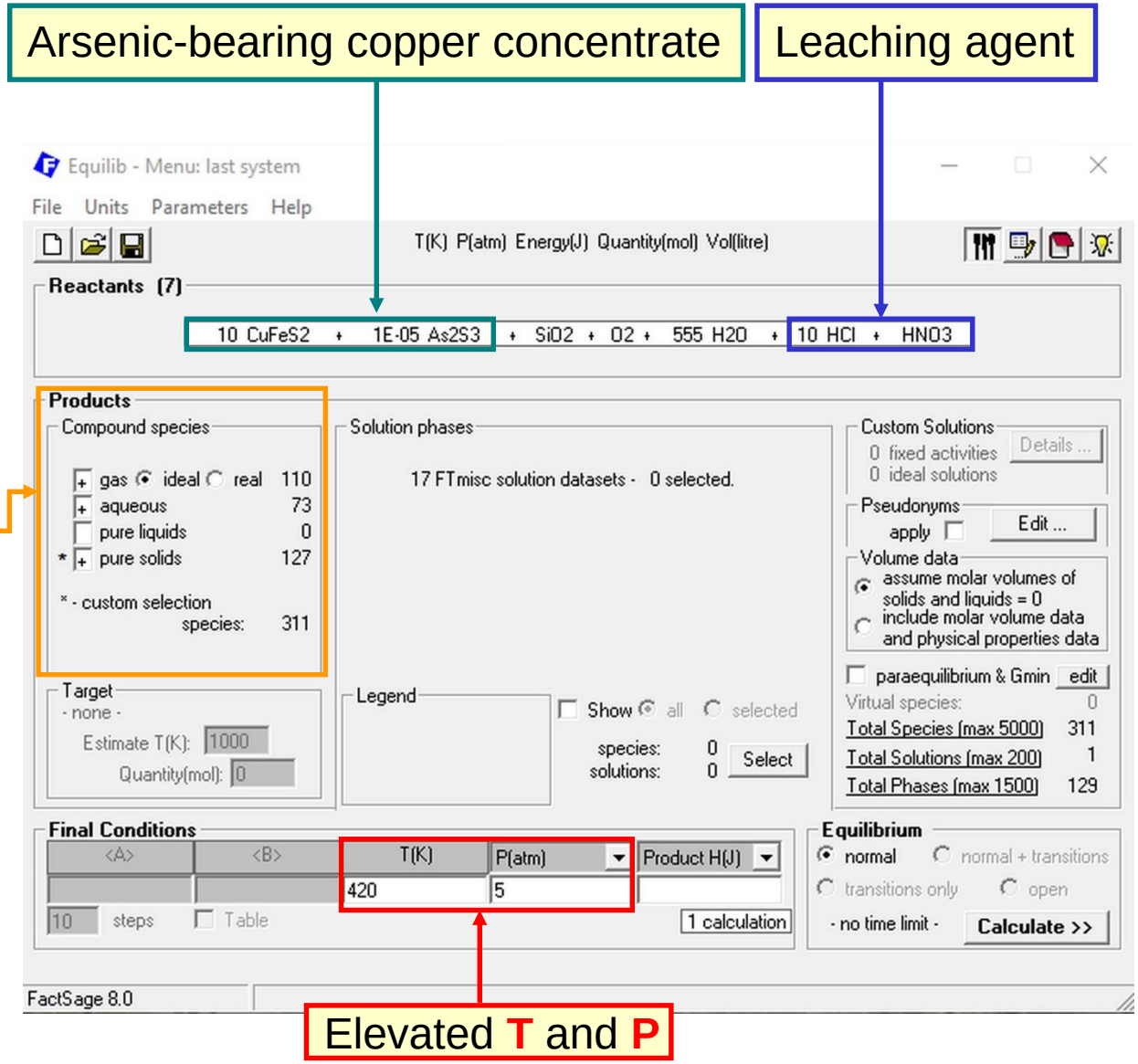
Standard equilibrium with **ideal aqueous solution**

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.

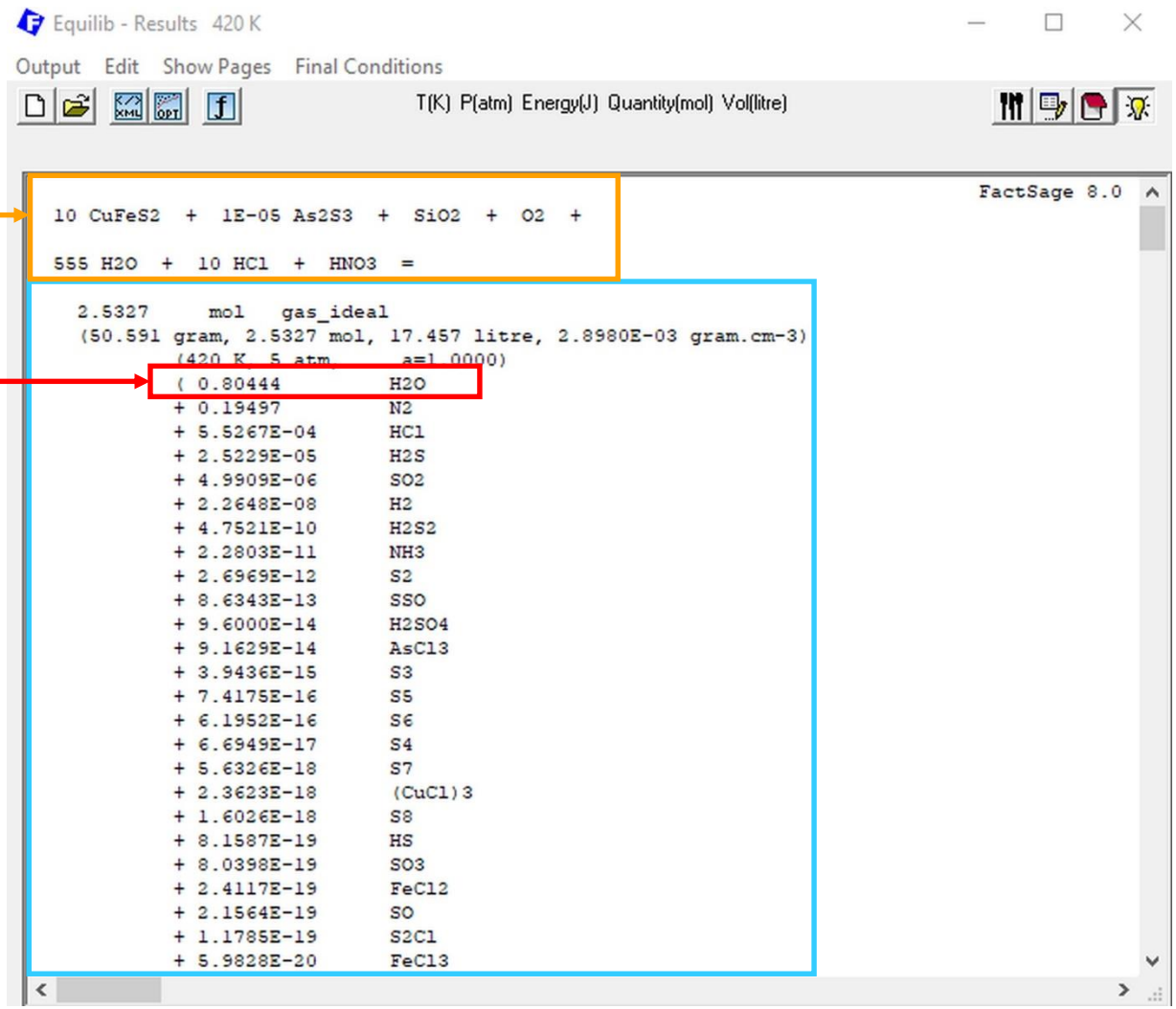
- Two **ideal solutions**: **gas** and **aqueous**;
- and **pure solids**.



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

The **ideal gas phase** species

The **reactants**



$X_{H_2O} = 0.80444$

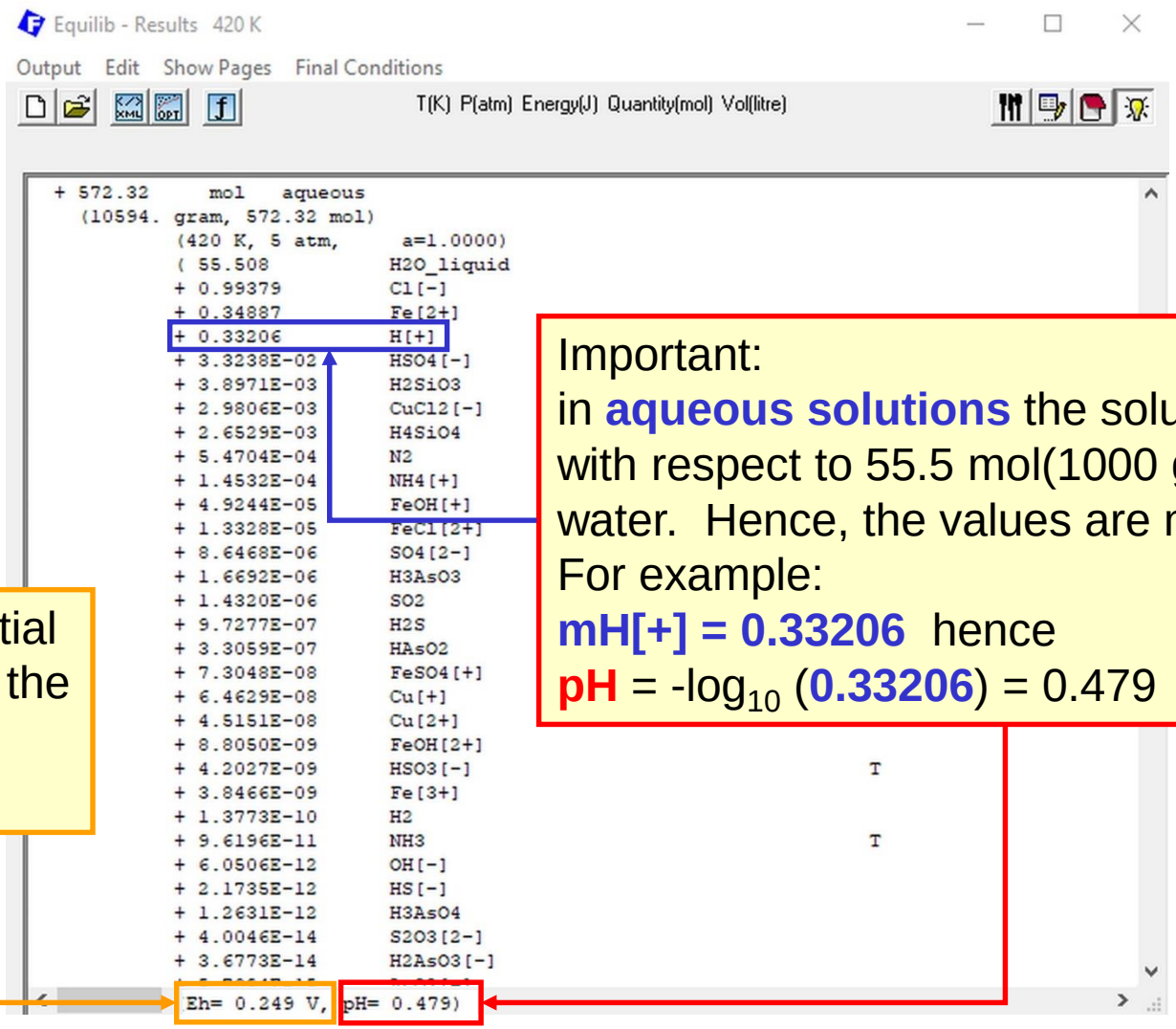
$P_{total} = 5.0$ atm

$P_{H_2O} = X_{H_2O} \times P_{total}$

$= 4.0222$ atm

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

The **aqueous phase** species

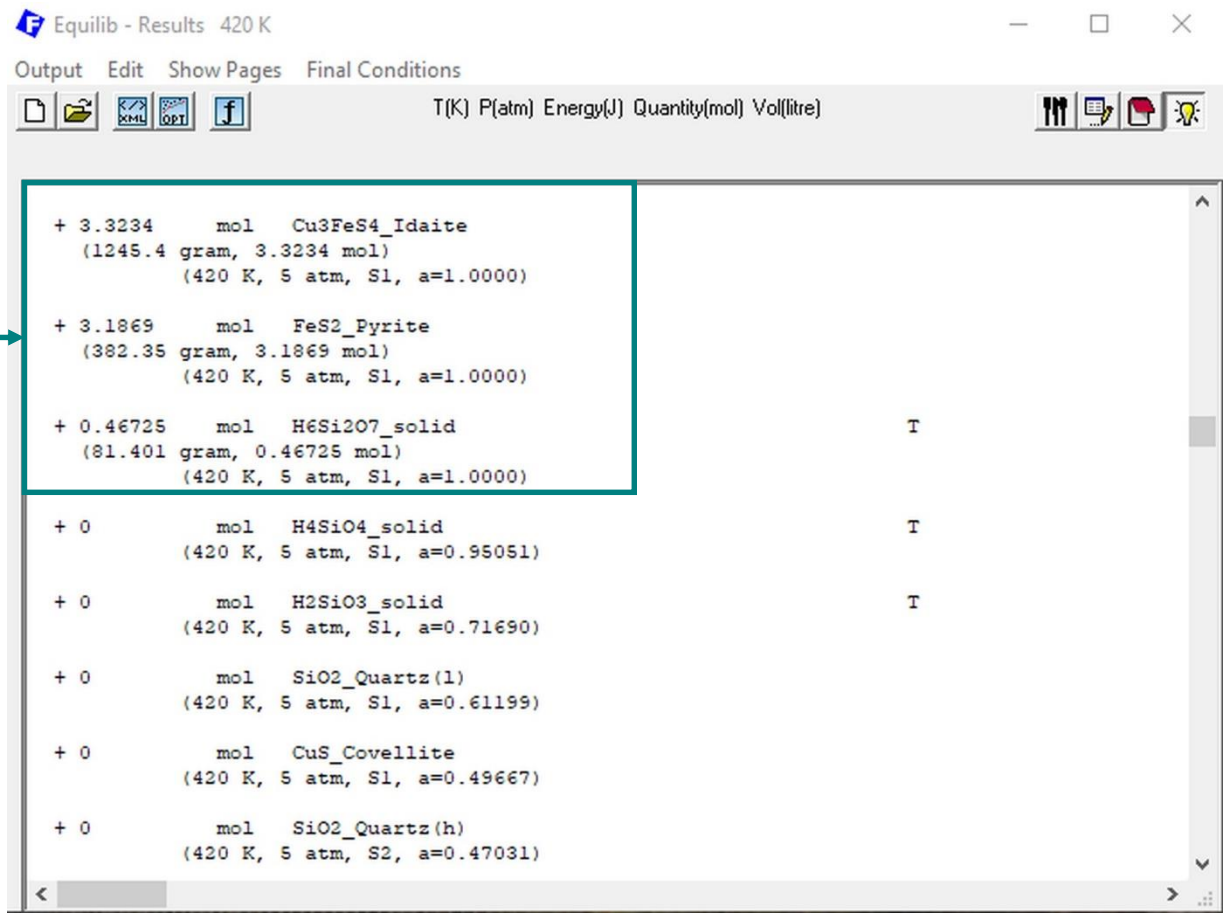


Important:
in **aqueous solutions** the solutes are given with respect to 55.5 mol(1000 g or 1L) of water. Hence, the values are molalities.
For example:
mH[+] = 0.33206 hence
pH = $-\log_{10}$ (**0.33206**) = 0.479

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.

Standard equilibrium with **dilute solution phase**

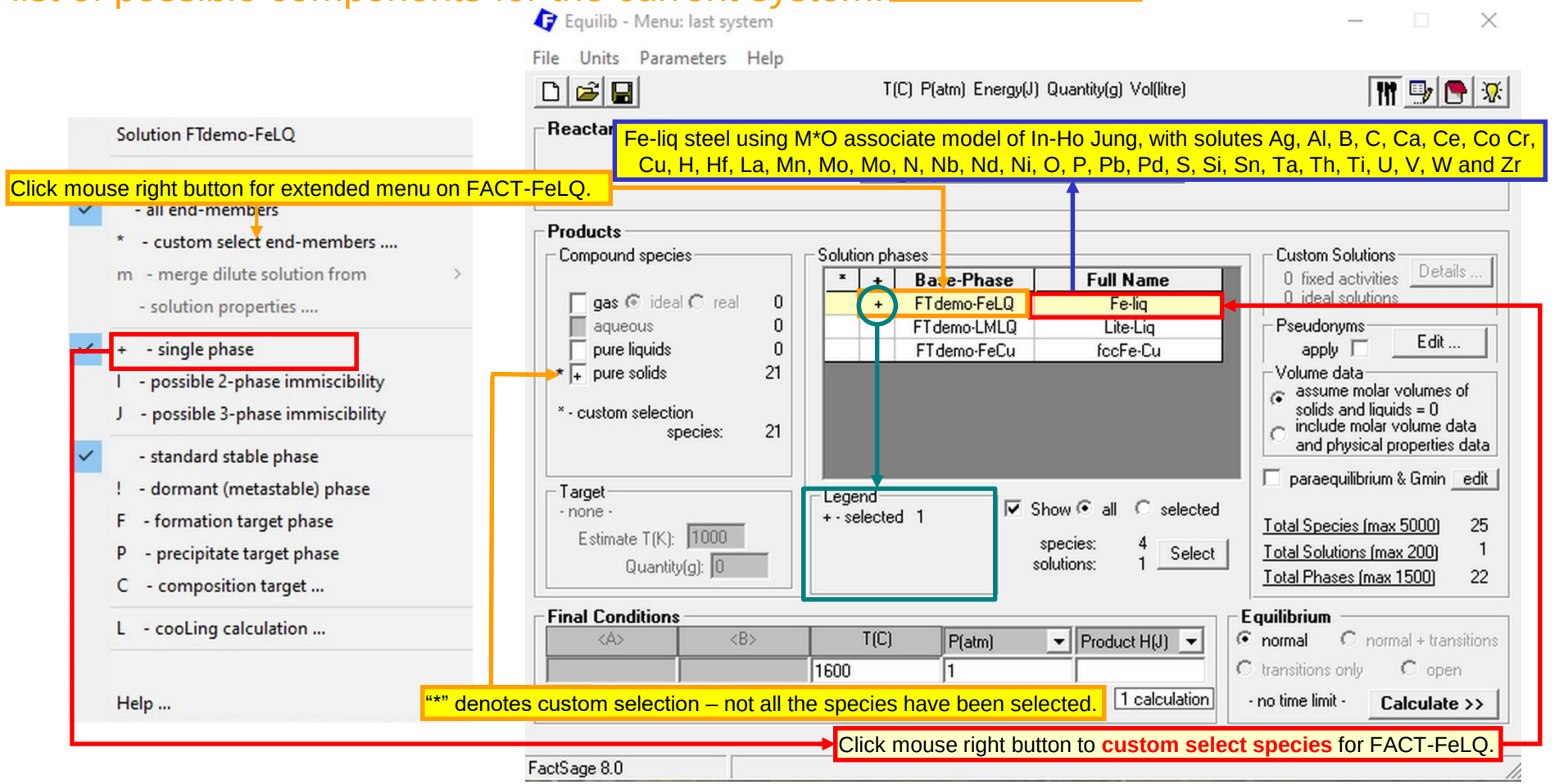
The following two slides show the use of a **dilute metallic liquid** phase from the ***FTdemo*** database, here Fe-liq, in the ***Equilib*** module.

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

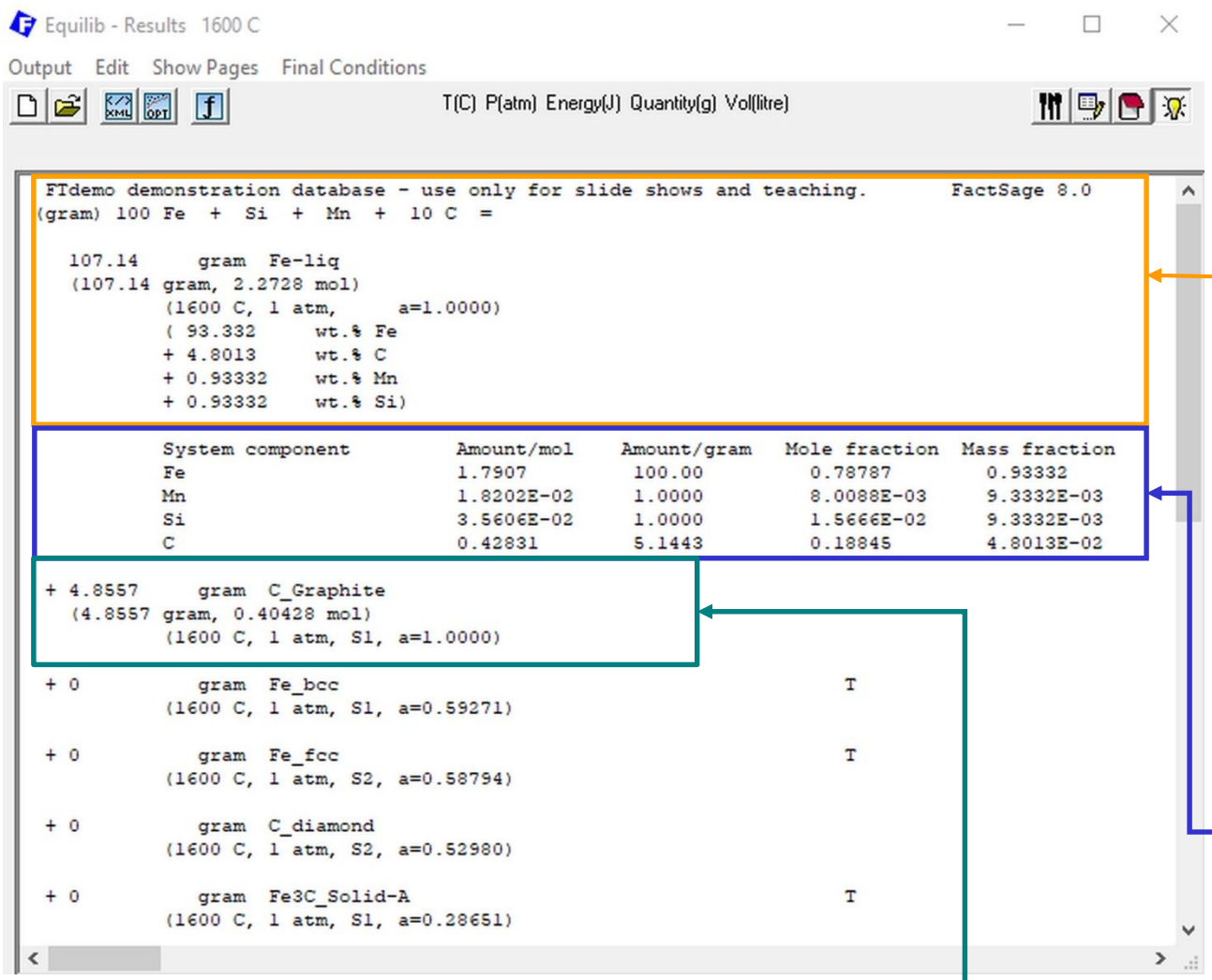
full title name: FACT Solution Phase FeLQ

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**



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

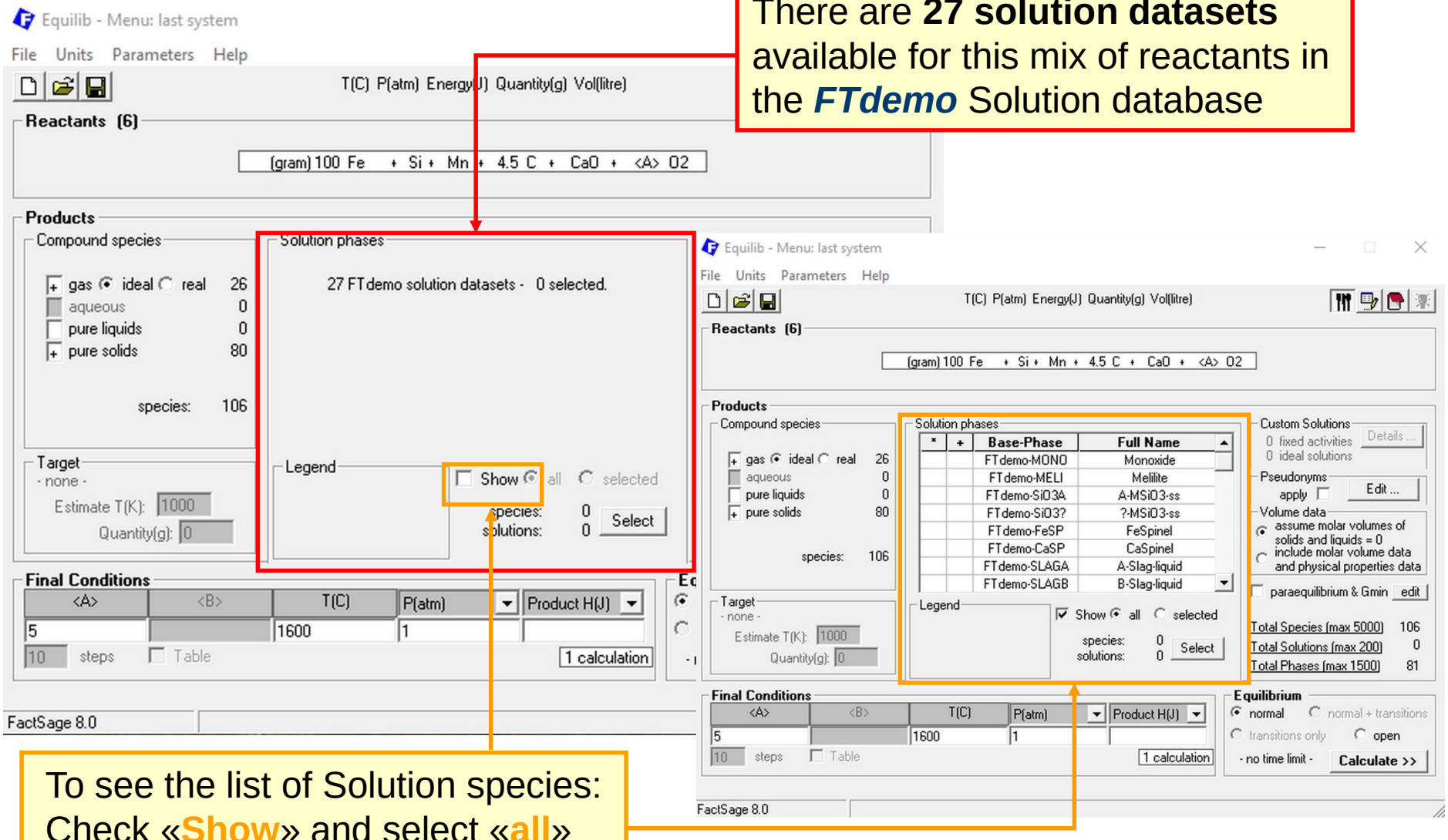
The following six slides are devoted to a special case in the ***FTdemo*** database: The use of a slag phase when several options concerning the composition of the slag (SlagA, SlagB, Slag?) are available.

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 **27 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 phases

*	+	Base-Phase	Full Name
		FTdemo-MONO	Monoxide
		FTdemo-MELI	Melilite
		FTdemo-SiO3A	A-MSiO3-ss
		FTdemo-SiO3?	?-MSiO3-ss
		FTdemo-FeSP	FeSpinel
		FTdemo-CaSP	CaSpinel
		FTdemo-SLAGA	A-Slag-liquid
		FTdemo-SLAGB	B-Slag-liquid

Legend

*	+	Base-Phase	Full Name
		FTdemo-MONO	Monoxide
		FTdemo-MELI	Melilite
		FTdemo-SiO3A	A-MSiO3-ss
		FTdemo-SiO3?	?-MSiO3-ss
		FTdemo-FeSP	FeSpinel
		FTdemo-CaSP	CaSpinel
		FTdemo-SLAGA	A-Slag-liquid
		FTdemo-SLAGB	B-Slag-liquid
		FTdemo-SLAG?	?-Slag-liquid
		FTdemo-SPIN	Spinel
		FTdemo-oPyr	Orthopyroxene
		FTdemo-cPyr	Clinopyroxene
		FTdemo-pPyr	Protopyroxene
		FTdemo-WOLL	Wollastonite,
		FTdemo-Oli1	Olivine1
		FTdemo-MeO	Monoxide
		FTdemo-"C2S	a'Ca2SiO4
		FTdemo-aC2S	a-Ca2SiO4
		FTdemo-WilF	Willemite
		FTdemo-Oli2	Olivine2
		FTdemo-CORU	M2O3(Corundum)
		FTdemo-MelA	Melilite
		FTdemo-LCSO	liq-K,Ca/CO3,SO4
		FTdemo-FeLQ	Fe-liq
		FTdemo-CuLQ	Cu-liq
		FTdemo-LMLQ	Lite-Liq
		FTdemo-FeCu	fccFe-Cu

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

Solution Phase FTdemo-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

The components in FTdemo-SLAG? for the current calculation are:
FeO, MnO, SiO2, CaO, Fe2O3, CaCO3

Warning! "?" denotes that the properties of solutions containing all of these components together have not been thoroughly evaluated. It is recommended that you select an approved (i.e. evaluated) sub-system (A, B, C, ...). If you select this (?) solution, then unsatisfactory estimates of the properties may result.

IMPORTANT MESSAGE! - The solution phase SLAG? has unique properties that make the selection of components very important. If components are not selected correctly then totally incorrect calculations or a crash may result. This may happen when you select all the components in the list of components for the present calculation.

If you insist on using SLAG? you must:

(1) ensure that all combinations of cations and anions for non-oxide components are in the component list. This may entail right-clicking on SLAG? and then de-selecting certain components.
For example, MgS, CaS and CaCO3 are all components of 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 SLAG? but MgCO3 will not. Hence, to respect this rule you must right-click on SLAG? and remove either CaCO3 or MgS.

(2) never de-select an oxide component (ex. CaO) without also de-selecting all corresponding non-oxide components (CaS, CaSO4, ...)

Solution Phase FTdemo-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

FTdemo-SLAGA sub-system

The components in FTdemo-SLAGA for the current calculation are:
FeO, MnO, SiO2, CaO, Fe2O3

Solution Phase FTdemo-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

FTdemo-SLAGB sub-system

The components in FTdemo-SLAGB for the current calculation are:
SiO2, CaO, CaCO3

Solution Phase FTdemo-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

The components in FTdemo-FeLQ for the current calculation are:
Fe, C, Ca, Mn, O, Si, CaO, SiO, MnO

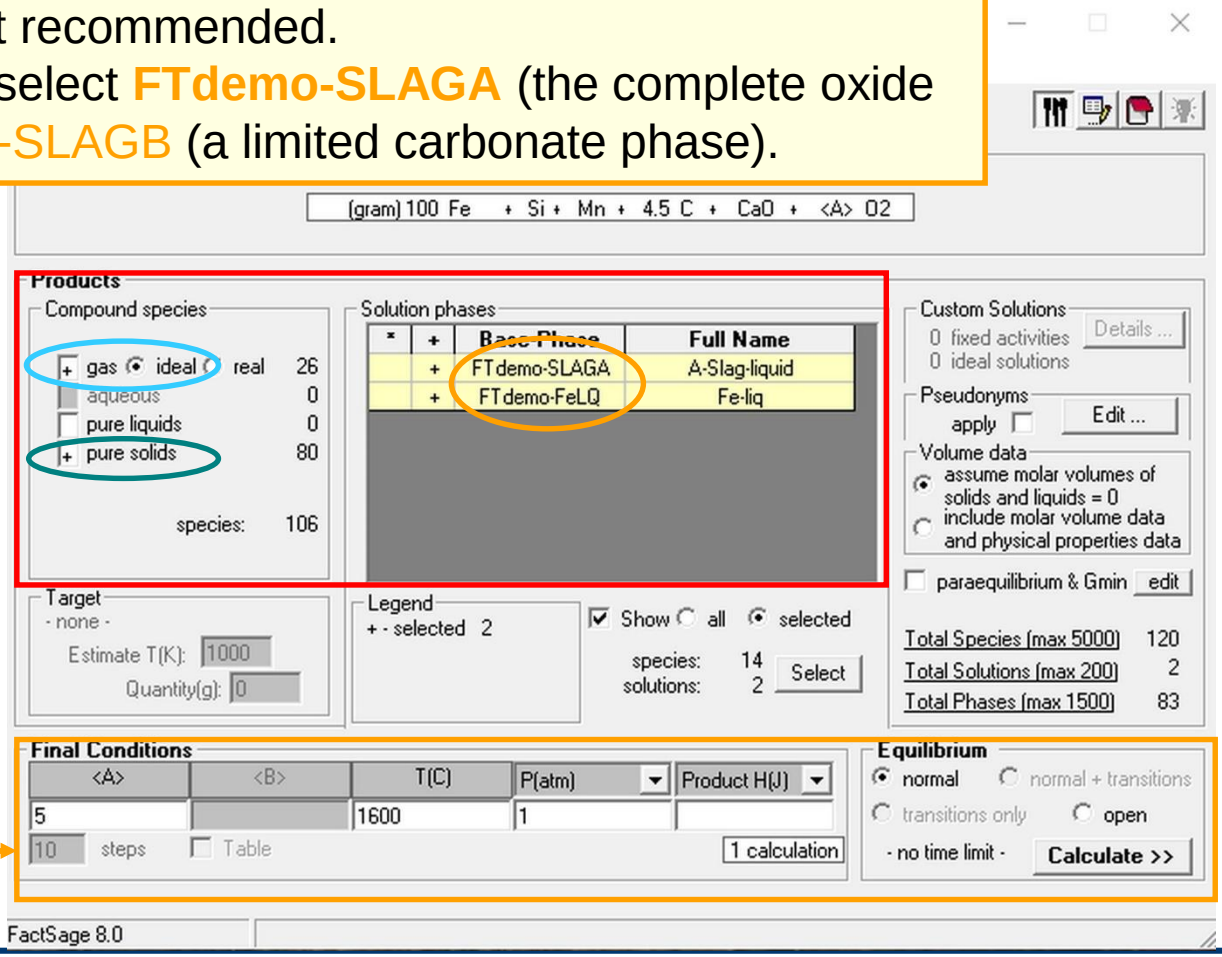
You can select only one phase in a list of phases with 5-character names differing only by their last character. Here, **SLAGA**, **SLAGB** and **SLAG?** are mutually exclusive.

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

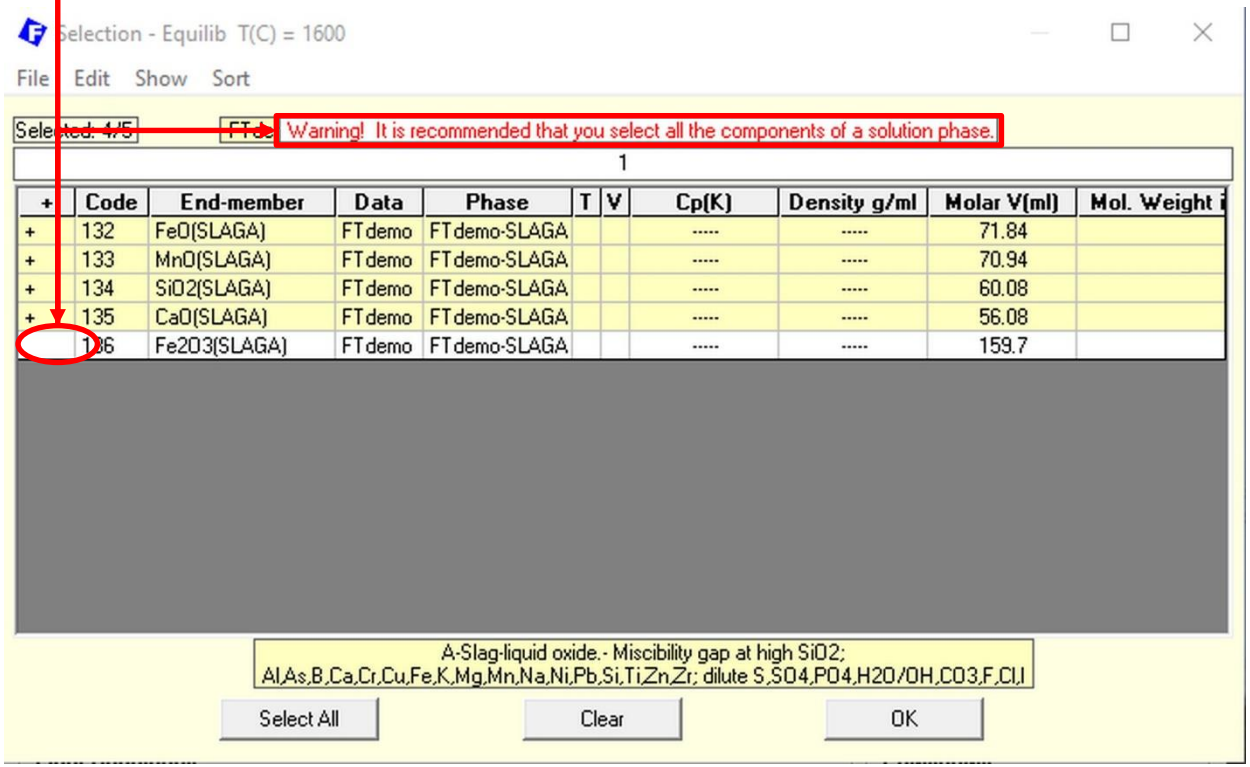
There are 3 subsets of the solution phase **FTdemo-SLAG**: **FTdemo-SLAG?**; **FTdemo-SLAGA**; **FTdemo-SLAGB**. Only one can be selected. The reason why there are solution subsets is because not all the binary, ternary systems, etc…, in the complete solution have been optimized yet. «**?**» indicates 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 >>**



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



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

Reactants, <A>= 5

Almost 100 % **CO**(g)

- 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**.

CaO addition promotes **slag** formation.

No **solid** phases

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

(gram) CaO  +  <A> O2  =

   0.28749     mol    gas_ideal
   (8.0621 gram, 0.28749 mol, 44.189 litre, 1.8245E-04 gram.cm-3)
          (1600 C, 1 atm,       a=1.0000)
          ( 0.99829          CO
          + 1.0682E-03       CO2
          + 4.3786E-04       Mn
          + 1.2863E-04       SiO
          + 7.6075E-05       Fe
          + 1.0101E-07       Ca
          + 4.5820E-09       FeO
          + 2.5893E-10       Si
          + 1.0454E-10       O
          + 2.2744E-11       C2O
          + 8.8678E-12       C3O2
          + 5.9593E-12       CaO

+ 102.68      gram  Fe-liq
  (102.68 gram, 1.9193 mol)
          (1600 C, 1 atm,       a=1.0000)
          ( 97.387      wt.% Fe
          + 1.0219      wt.% C
          + 6.4832E-09  wt.% Ca
          + 0.94518     wt.% Mn
          + 3.5854E-03  wt.% O
          + 0.64241     wt.% Si
          + 5.9576E-05  wt.% CaO
          + 2.5772E-05  wt.% SiO
          + 1.9970E-04  wt.% MnO)

+ 1.7589      gram  Slag-liquid
  (1.7589 gram, 3.0378E-02 mol)
          (1600 C, 1 atm,       a=1.0000)
          ( 0.23223     wt.% FeO
          + 1.6466      wt.% MnO
          + 41.271      wt.% SiO2
          + 56.850      wt.% CaO
          + 1.6016E-04  wt.% Fe2O3)

+ 0           gram  Ca2SiO4_alpha
          (1600 C, 1 atm, S3, a=0.92748)

+ 0           gram  Fe_bcc                                    T
          (1600 C, 1 atm, S1, a=0.88829)

+ 0           gram  Fe_fcc                                    T
          (1600 C, 1 atm, S2, a=0.88115)
```

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

FTdemo demonstration database - use only for slide shows and teaching. FactSage 8.0
T = 1600 C
P = 1 atm
V = 44.189 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

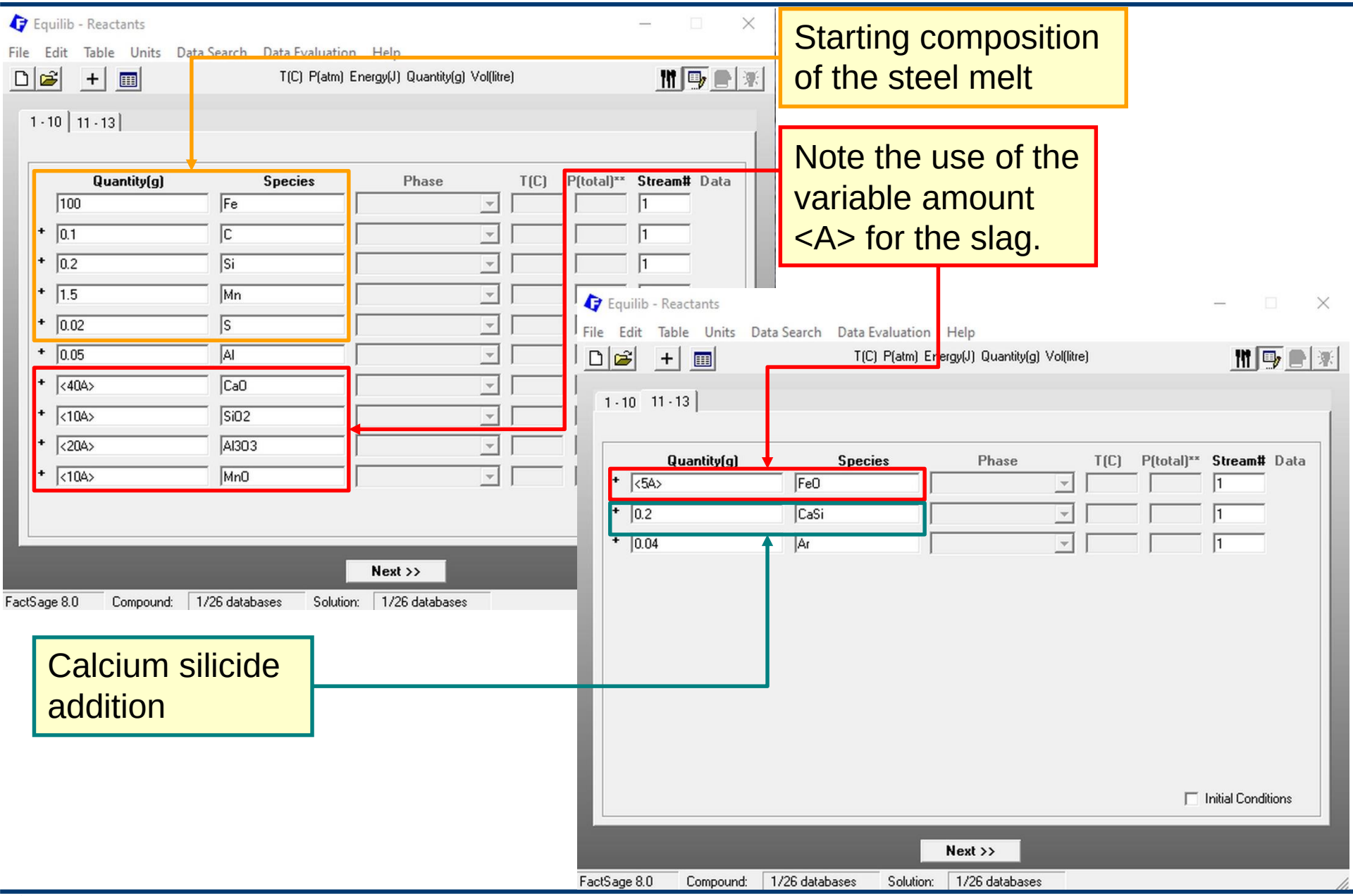
PHASE: gas_ideal	EQUIL AMOUNT mol	MOLE FRACTION	FUGACITY atm
CO	2.8700E-01	9.9829E-01	9.9829E-01
CO2	3.0710E-04	1.0682E-03	1.0682E-03
Mn	1.2588E-04	4.3786E-04	4.3786E-04
SiO	3.6979E-05	1.2863E-04	1.2863E-04
Fe	2.1871E-05	7.6075E-05	7.6075E-05
Ca	2.9040E-08	1.0101E-07	1.0101E-07
FeO	1.3173E-09	4.5820E-09	4.5820E-09
Si	7.4441E-11	2.5893E-10	2.5893E-10
O	3.0054E-11	1.0454E-10	1.0454E-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		1.0493E+00	1.0219E-02	4.7428E-02
Ca		6.6569E-09	6.4832E-11	1.0101E-07
Mn		9.7050E-01	9.4518E-03	8.2970E-03
O		3.6815E-03	3.5854E-05	4.4135E-07
Si		6.5962E-01	6.4241E-03	2.9403E-05
CaO		6.1172E-05	5.9576E-07	5.5785E-07
SiO		2.6462E-05	2.5772E-07	3.0697E-07
MnO		2.0505E-04	1.9970E-06	1.4782E-06
TOTAL:		1.0268E+02	1.0000E+00	1.0000E+00
PHASE: Slag-liquid		gram	MASS FRACTION	ACTIVITY
FeO		4.0846E-03	2.3223E-03	5.4909E-03
MnO		2.8962E-02	1.6466E-02	1.4300E-02
SiO2		7.2592E-01	4.1271E-01	6.5155E-02
CaO		9.9994E-01	5.6850E-01	5.7078E-03
Fe2O3		2.8171E-06	1.6016E-06	3.4982E-10
TOTAL:		1.7589E+00	1.0000E+00	1.0000E+00
Ca2SiO4_alpha(s3)		0.0000E+00		9.2748E-01
Fe_bcc(s)	T	0.0000E+00		8.8829E-01
Fe_fcc(s2)	T	0.0000E+00		8.8115E-01

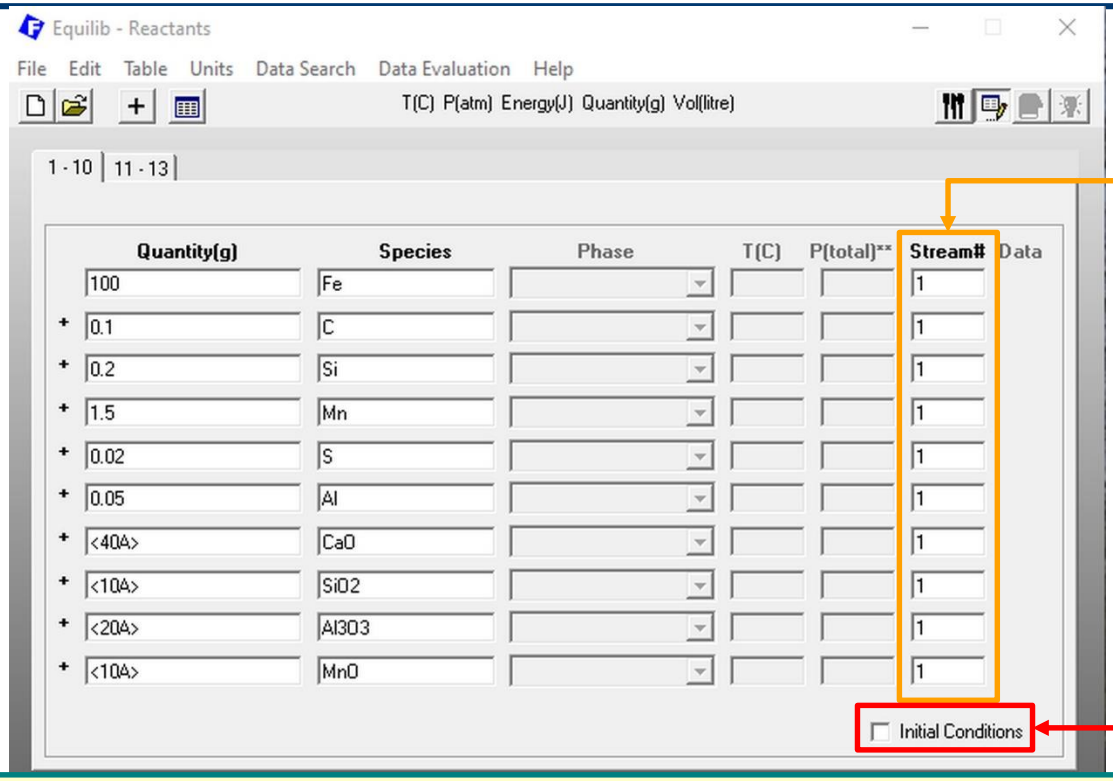
A standard case with slag-metal input plus additives

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.



«initial conditions» Default Values and Stream Features



Stream# boxes

«initial conditions» check box

«**Initial Conditions**»:

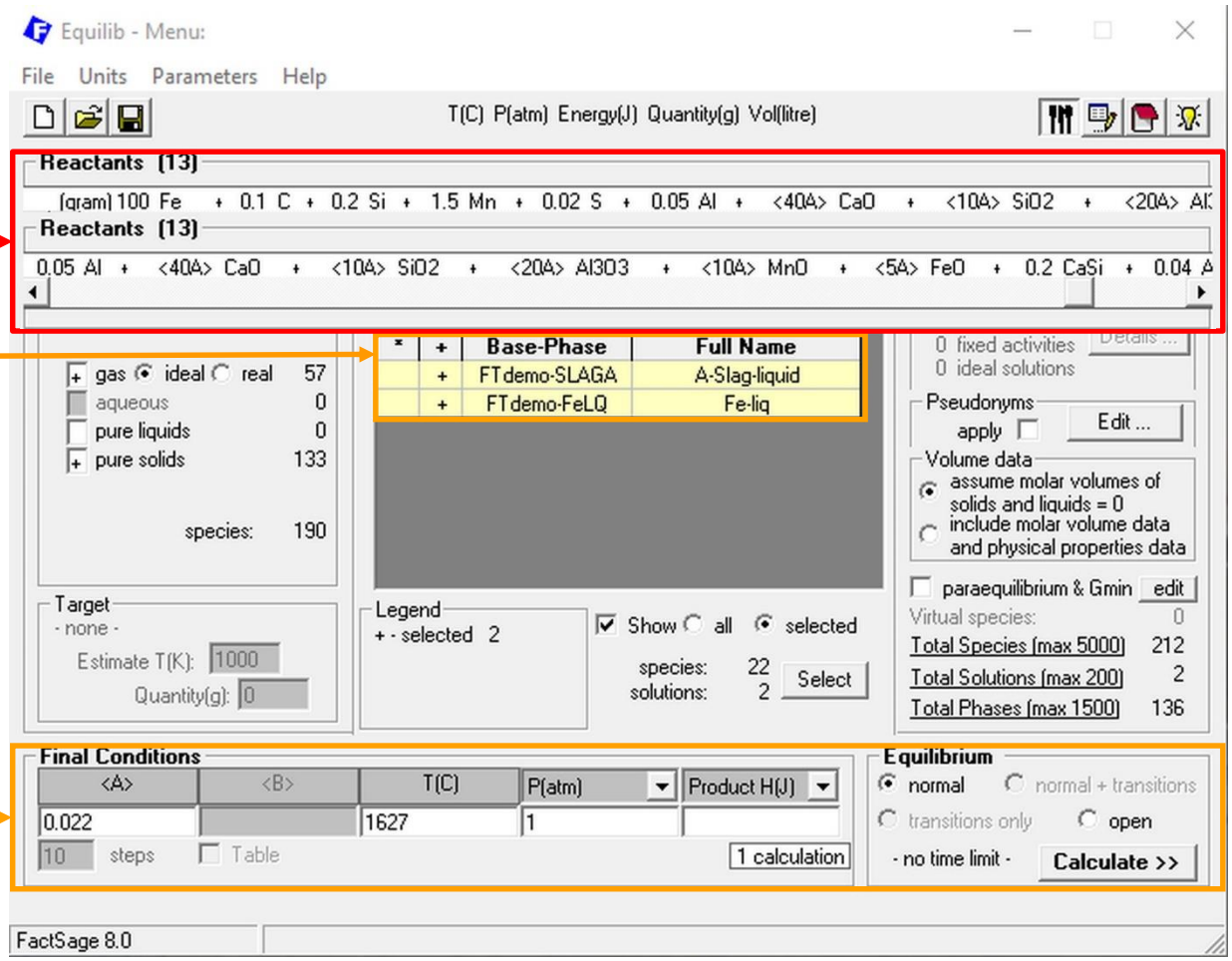
- Specifying initial conditions is only useful if you want to calculate or constrain changes in the extensive properties (ΔV, ΔH, etc…). You have to select, for each reactant species, the phase, the temperature, the total pressure and the stream number.
- All reactants in a given **stream** are grouped 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.

Summary of the **Reactants** window

Solution species selected

Final conditions:
- <A> = 0.022
- T = 1627°C
- P = 1 atm

and **Calculate >>**



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

Gas phase, mainly Ar

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

No solid phases formed

```
FTdemo demonstration database - use only for slide shows and teaching.      FactSage 8.0
(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> Al3O3  +  <10A> MnO  +  <5A> FeO  +  0.2 CaSi  +

(gram) 0.04 Ar  =

   1.0055E-03 mol   gas_ideal
   (4.0151E-02 gram, 1.0055E-03 mol, 0.15678 litre, 2.5610E-04 gram.cm-3)
            (1627 C, 1 atm,      a=1.0000)
            ( 0.99583          Ar
            + 2.8765E-03       CO
            + 1.0706E-03       Mn
            + 1.1342E-04       Fe
            + 1.0796E-04       Ca)

+ 102.23      gram  Fe-liq
   (102.23 gram, 1.8441 mol)
            (1627 C, 1 atm,      a=1.0000)
            ( 97.905      wt.% Fe
            + 3.2117E-02 wt.% Al
            + 9.7788E-02 wt.% C
            + 3.5907E-06 wt.% Ca
            + 1.6336      wt.% Mn
            + 7.6196E-05 wt.% O
            + 3.8365E-04 wt.% S
            + 0.32815     wt.% Si
            + 2.6485E-03 wt.% CaO
            + 1.2767E-04 wt.% AlO
            + 4.2978E-07 wt.% SiO
            + 1.8944E-05 wt.% MnO
            + 1.3383E-05 wt.% Al2O)

+ 1.7129      gram  Slag-liquid
   (1.7129 gram, 2.5794E-02 mol)
            (1627 C, 1 atm,      a=1.0000)
            ( 8.7518E-03 wt.% FeO
            + 2.5826E-02 wt.% MnO
            + 6.2180      wt.% SiO2
            + 58.820      wt.% CaO
            + 32.352      wt.% Al2O3
            + 2.5743      wt.% CaS
            + 3.6431E-04 wt.% FeS
            + 1.0776E-03 wt.% MnS
            + 2.1209E-05 wt.% Fe2O3)

+ 0           gram  CaO_lime
            (1627 C, 1 atm, S1, a=0.98782)

+ 0           gram  Fe_bcc                                              T
            (1627 C, 1 atm, S1, a=0.93045)

+ 0           gram  Fe_fcc                                              T
            (1627 C, 1 atm, S2, a=0.92198)
```

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

1

Final Conditions

STREAM CONSTITUENTS or **AMOUNT** of reactants

FTdemo demonstration data

T = 1627 C
P = 1 atm
V = 0.15678 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	8.8000E-01
SiO2	2.2000E-01
Al3O3	4.4000E-01
MnO	2.2000E-01
FeO	1.1000E-01
CaSi	2.0000E-01
Ar	4.0000E-02

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

PHASE: gas_ideal	EQUIL AMOUNT mol	MOLE FRACTION	FUGACITY atm
Ar	1.0013E-03	9.9583E-01	9.9583E-01
CO	2.8923E-06	2.8765E-03	2.8765E-03
Mn	1.0765E-06	1.0706E-03	1.0706E-03
Fe	1.1405E-07	1.1342E-04	1.1342E-04
Ca	1.0856E-07	1.0796E-04	1.0796E-04
TOTAL:	1.0055E-03	1.0000E+00	1.0000E+00

PHASE: Fe-liq	gram	MASS FRACTION	ACTIVITY
Fe	1.0009E+02	9.7905E-01	9.7128E-01
Al	3.2832E-02	3.2117E-04	4.3026E-05
C	9.9965E-02	9.7788E-04	2.6150E-03
Ca	3.6706E-06	3.5907E-08	1.0796E-04
Mn	1.6700E+00	1.6336E-02	1.6336E-02
O	7.7893E-05	7.6196E-07	2.5677E-08
S	3.9220E-04	3.8365E-06	1.2671E-06
Si	3.3546E-01	3.2815E-03	1.1275E-05
CaO	2.7075E-03	2.6485E-05	2.6166E-05
AlO	1.3051E-04	1.2767E-06	1.6456E-06
SiO	4.3935E-07	4.2978E-09	5.4010E-09
MnO	1.9366E-05	1.8944E-07	1.4795E-07
Al2O	1.3681E-05	1.3383E-07	1.0598E-07
TOTAL:	1.0223E+02	1.0000E+00	1.0000E+00

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

2

PHASE: Slag-liquid	gram	MASS FRACTION	ACTIVITY
FeO	1.4991E-04	8.7518E-05	2.7158E-04
MnO	4.4238E-04	2.5826E-04	1.1906E-03
SiO2	1.0651E-01	6.2180E-02	3.6030E-05
CaO	1.0075E+00	5.8820E-01	1.8572E-01
Al2O3	5.5416E-01	3.2352E-01	1.6244E-03
CaS	4.4095E-02	2.5743E-02	1.7361E-01
FeS	6.2403E-06	3.6431E-06	3.5674E-05
MnS	1.8458E-05	1.0776E-05	3.2755E-04
Fe2O3	3.6330E-07	2.1209E-07	3.8707E-14
TOTAL:	1.7129E+00	1.0000E+00	1.0000E+00

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

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

3

Equilibrium thermodynamic values

Solid phases

		gram	ACTIVITY
CaO_lime(s)		0.0000E+00	9.8782E-01
Fe_bcc(s)	T	0.0000E+00	9.3045E-01
Fe_fcc(s2)	T	0.0000E+00	9.2198E-01
Ca3Al2O6_solid(s)	T	0.0000E+00	5.8877E-01
Ca3SiO5_Hatrurite(s)		0.0000E+00	4.2747E-01
Ca2SiO4_alpha(s3)		0.0000E+00	4.2644E-01
Ca2SiO4_alpha-prime(s2)		0.0000E+00	3.9330E-01
CaS_solid(s)		0.0000E+00	2.4868E-01
CaAl2O4_solid(s)	T	0.0000E+00	2.0566E-01
Ca2SiO4_gamma(olivine(s)	T	0.0000E+00	8.5467E-02
Ca2Al2SiO7_Gehlenite(s)		0.0000E+00	2.2531E-02
Mn_Solid_Delta(s4)		0.0000E+00	1.3704E-02
Mn_Solid_Gamma(s3)	T	0.0000E+00	1.3121E-02
Mn_Solid_Beta(s2)	T	0.0000E+00	1.2481E-02
Mn_Solid_Alpha(s)	T	0.0000E+00	1.0833E-02
CaSiO3_Pseudowollast(s2)	T	0.0000E+00	9.7943E-03
CaSiO3_Wollastonite(s)	T	0.0000E+00	8.2208E-03
Al2O3_corundum(alpha(s4)		0.0000E+00	6.3333E-03
FeSi_solid(s)	T	0.0000E+00	5.6290E-03
Al2O3_delta(s2)		0.0000E+00	5.1320E-03
Al2O3_kappa(s3)		0.0000E+00	
CaAl4O7_solid(s)		0.0000E+00	
Al2O3_gamma(s)		0.0000E+00	
Ca3Si2O7_Rankinite(s)		0.0000E+00	
Fe3C_Solid-A(s)	!T	0.0000E+00	
C_Graphite(s)		0.0000E+00	
Fe3C_Solid-B(s2)	T	0.0000E+00	2.5519E-03
MnO_solid(s)		0.0000E+00	1.6895E-03
C_diamond(s2)		0.0000E+00	1.3821E-03
MnS_Alabandite(s)	T	0.0000E+00	2.9935E-04
FeO_Wustite(s)		0.0000E+00	1.9971E-04

No solid phases formed

Cp	H	S	G	V
J.K-1	J	J.K-1	J	dm3
8.73176E+01	1.20374E+05	1.95010E+02	-2.50174E+05	1.56779E-01

A standard case with **aqueous solutions**

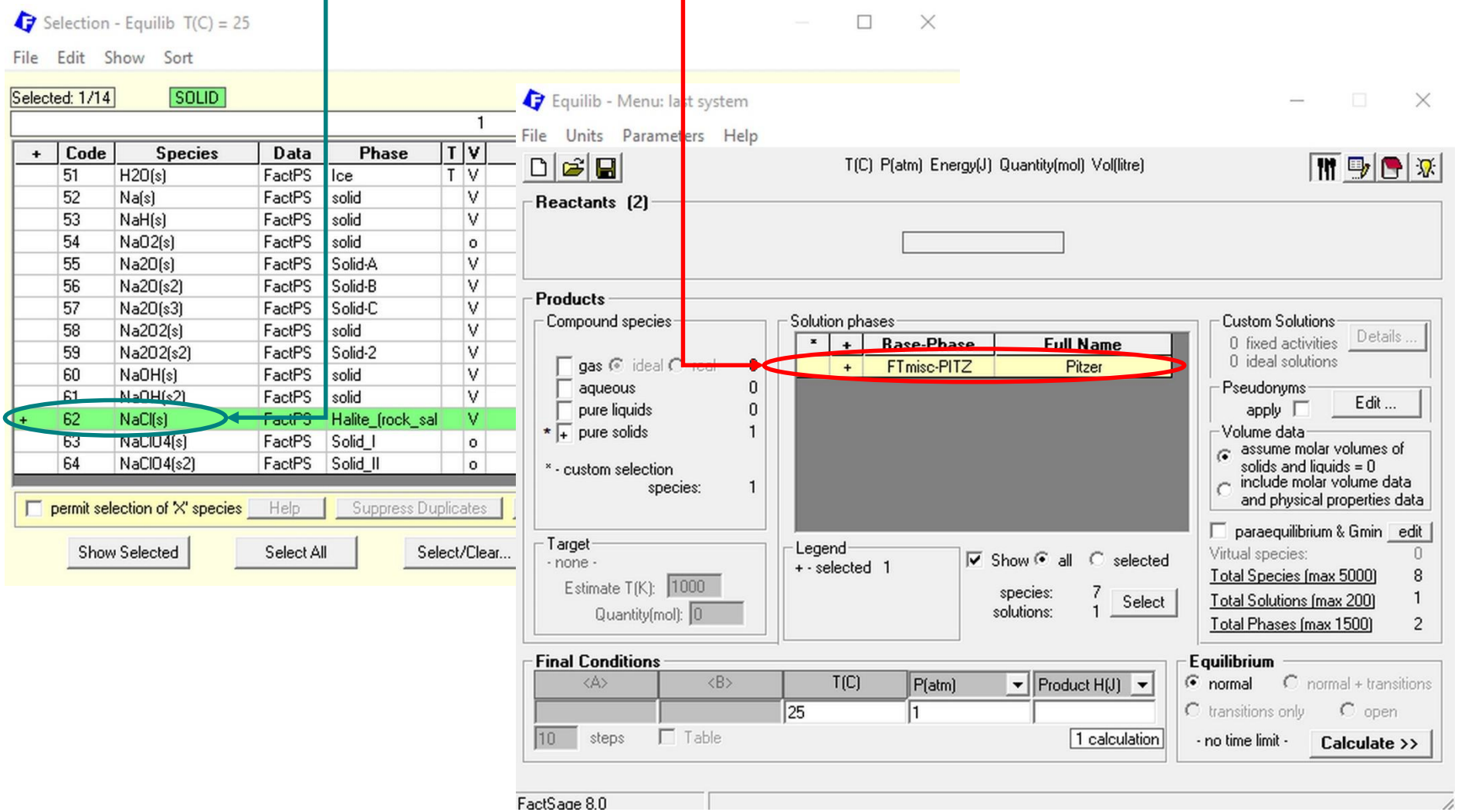
The following slides show how ***Equilib*** is used for calculations of equilibria in which a non-ideal aqueous phase is involved.

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)

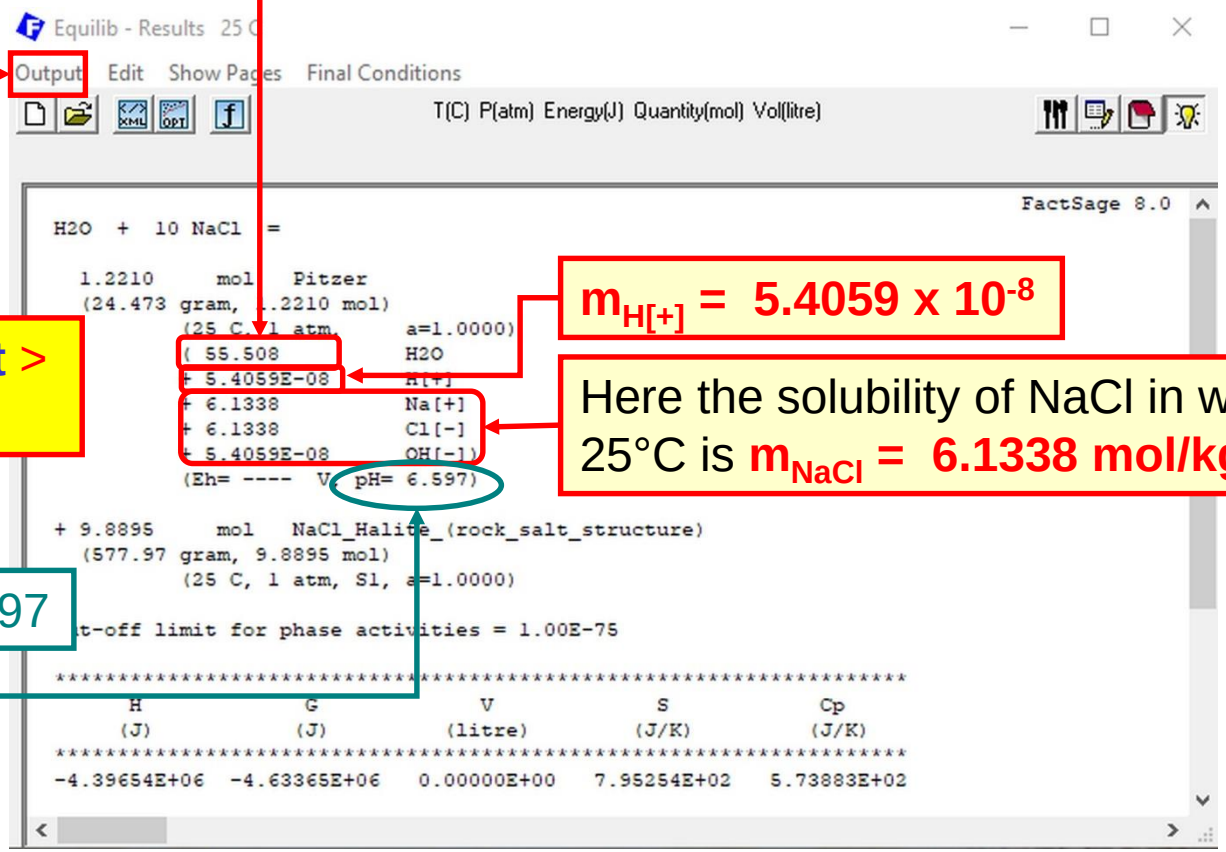
Mixing **10 mol** of **NaCl** and **1 mol** of **water** at **25°C** and **1 atm** creates **brine** saturated in **NaCl**.



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**.

Output > Format > *FACT* Format

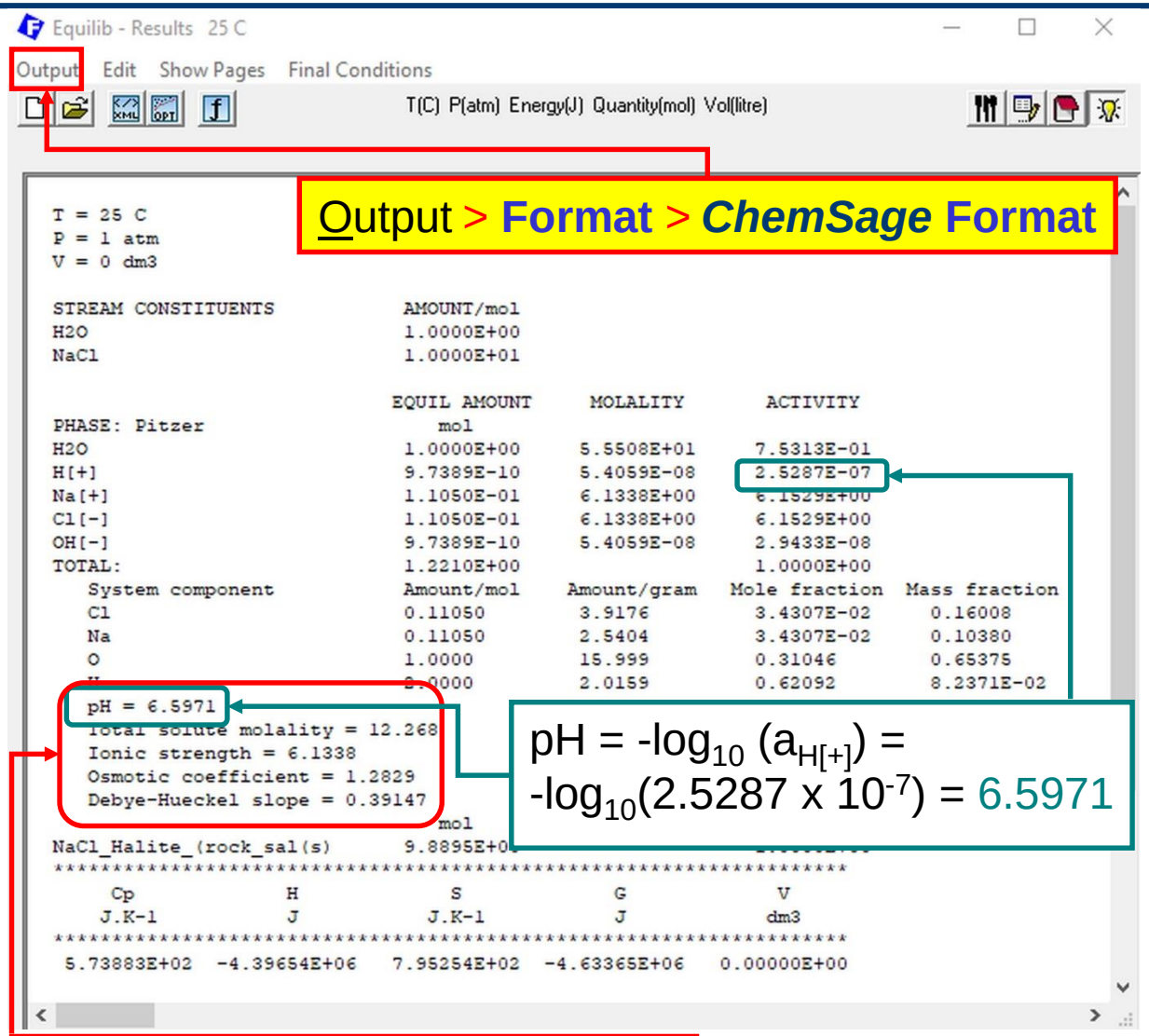


$m_{H[+]} = 5.4059 \times 10^{-8}$

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

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

Solubility of NaCl in water – *ChemSage* format output



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

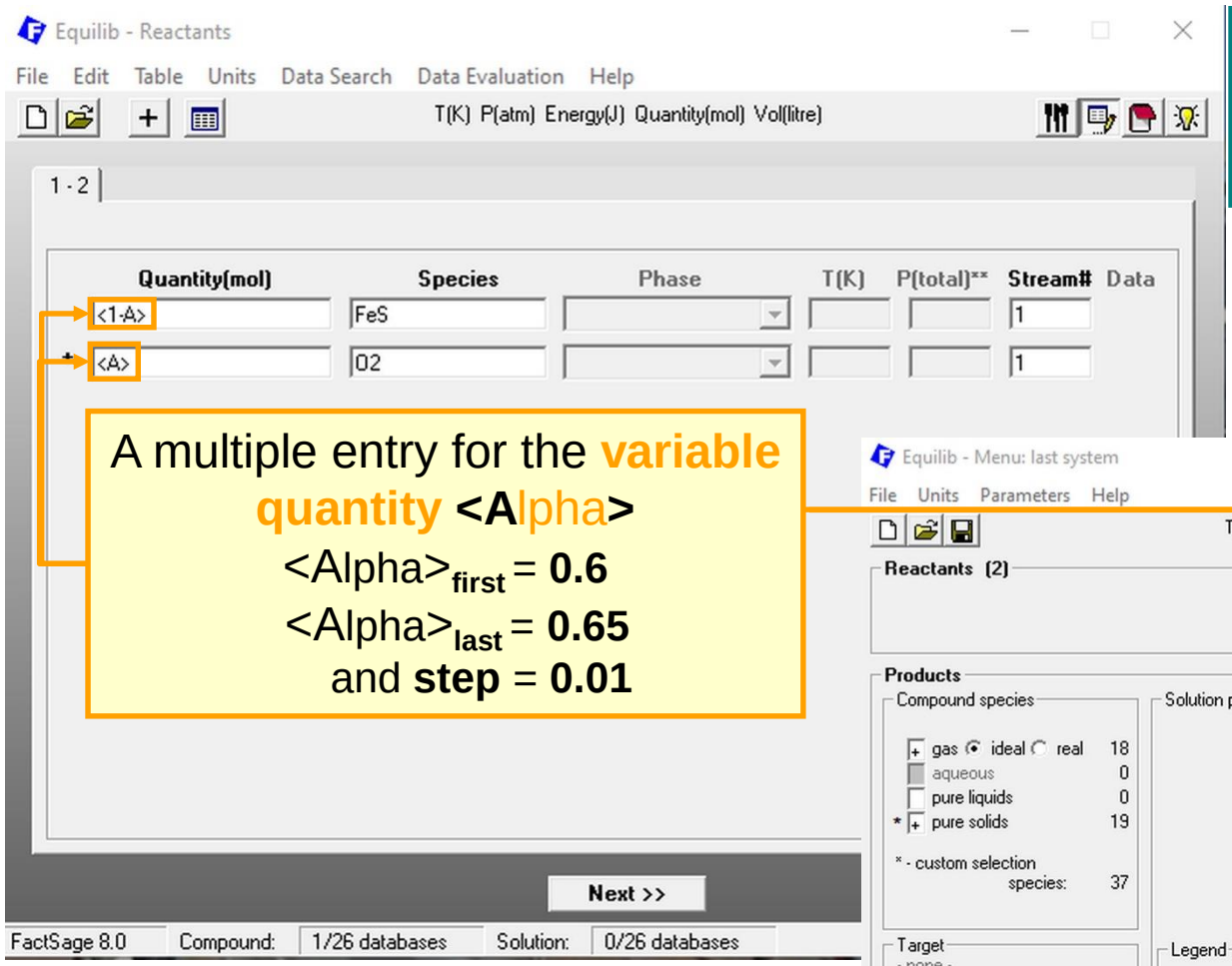
A multiple entry for the **variable quantity <A**lpha**>**

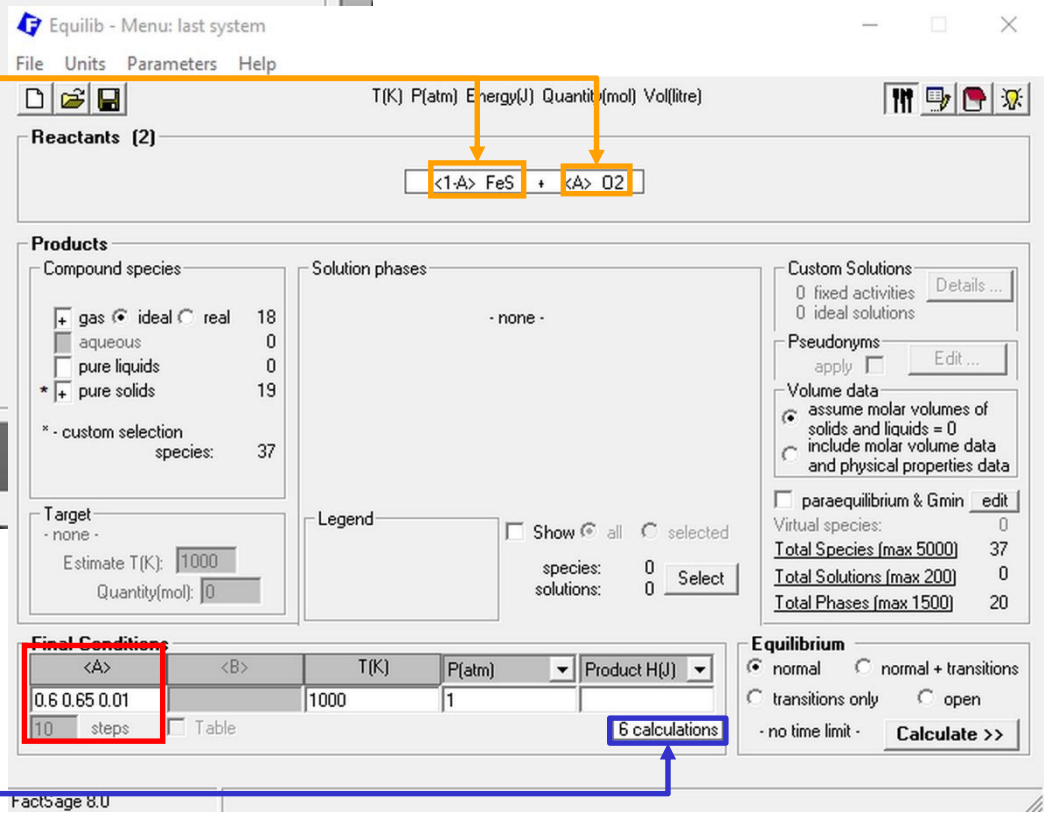
$<Alpha>_{first} = 0.6$

$<Alpha>_{last} = 0.65$

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

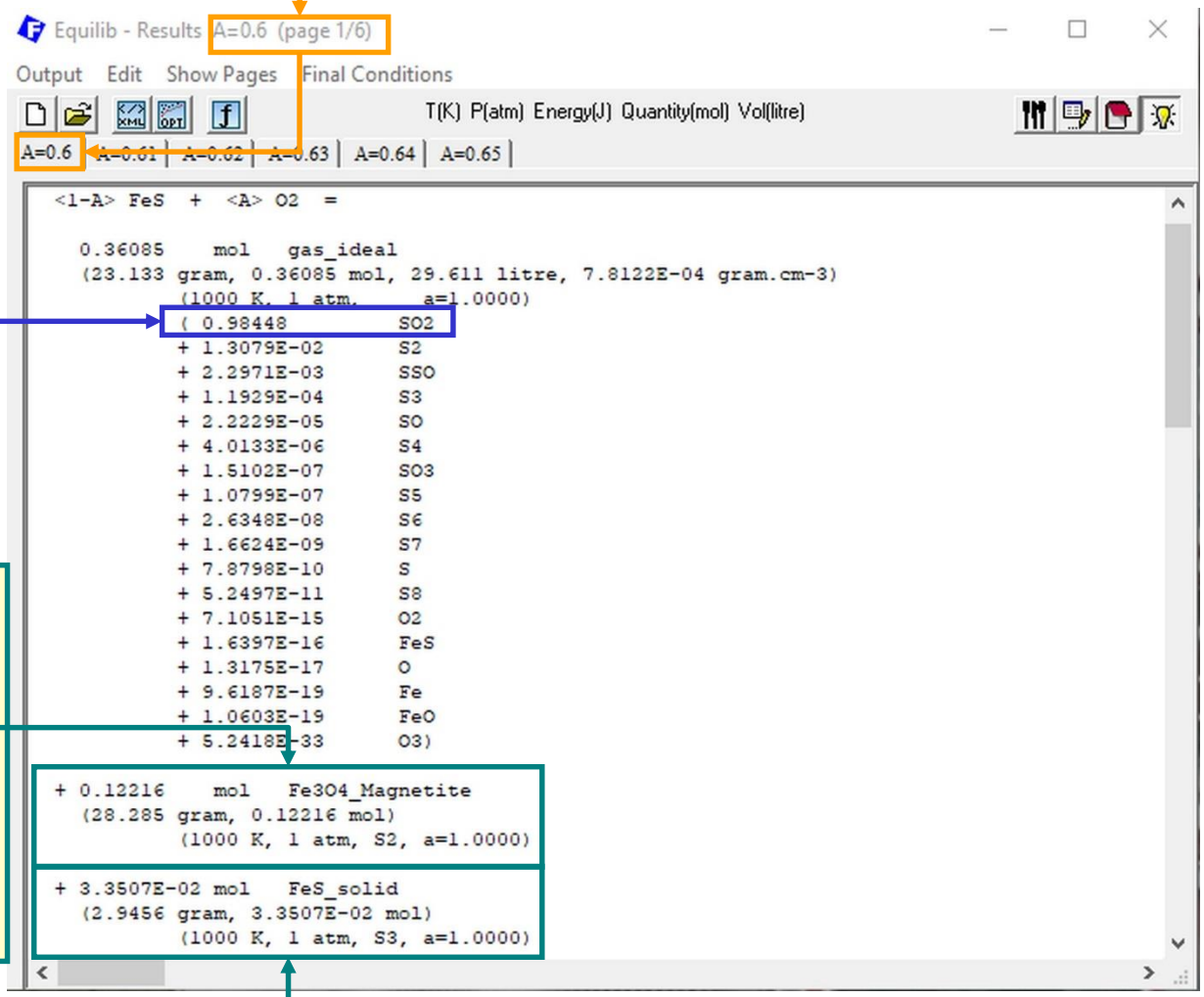
6 **calculations** will be performed for **<A>** from 0.60 to 0.65 in increments of 0.01 (0.60, 0.61, 0.62, … , 0.65).





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

T=1000 K, <A> = 0.60 mol



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)

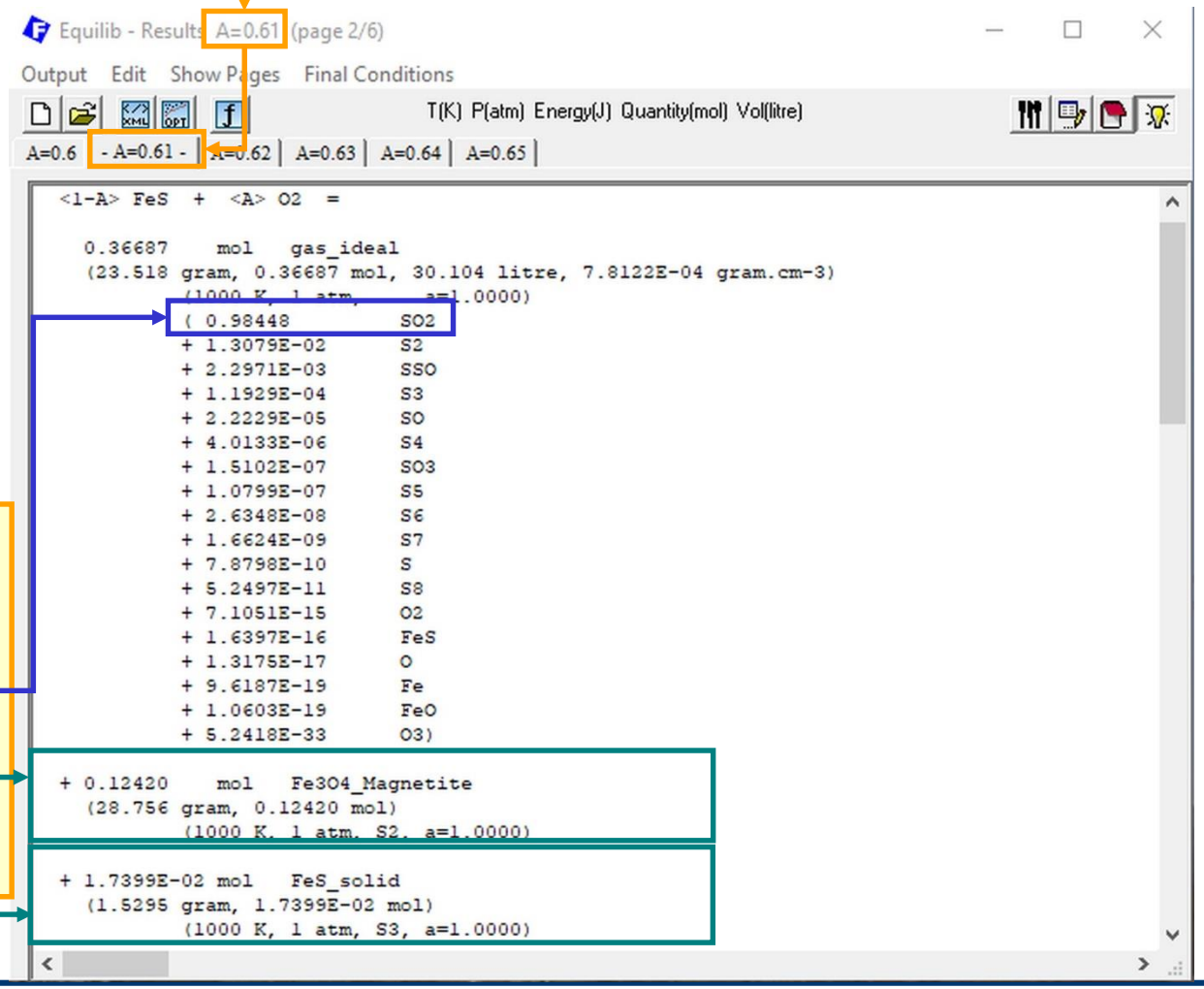
Note:
Same phases and gas partial pressure as for <A> = 0.60 mol but different amounts.
This is explained by the

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



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:

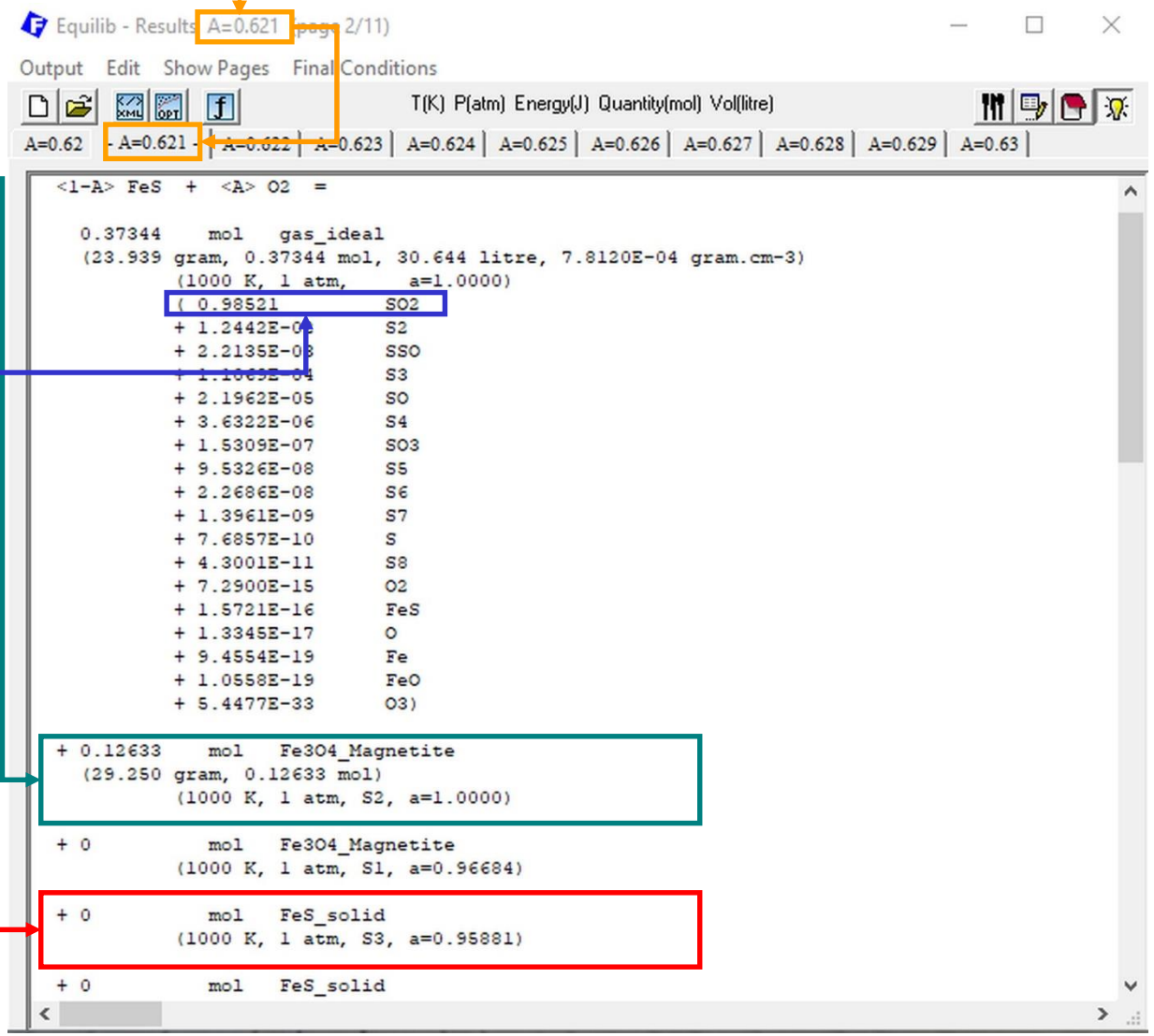
All FeS(s3) is oxidized

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.



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

T=1000 K, <A> = 0.65 mol

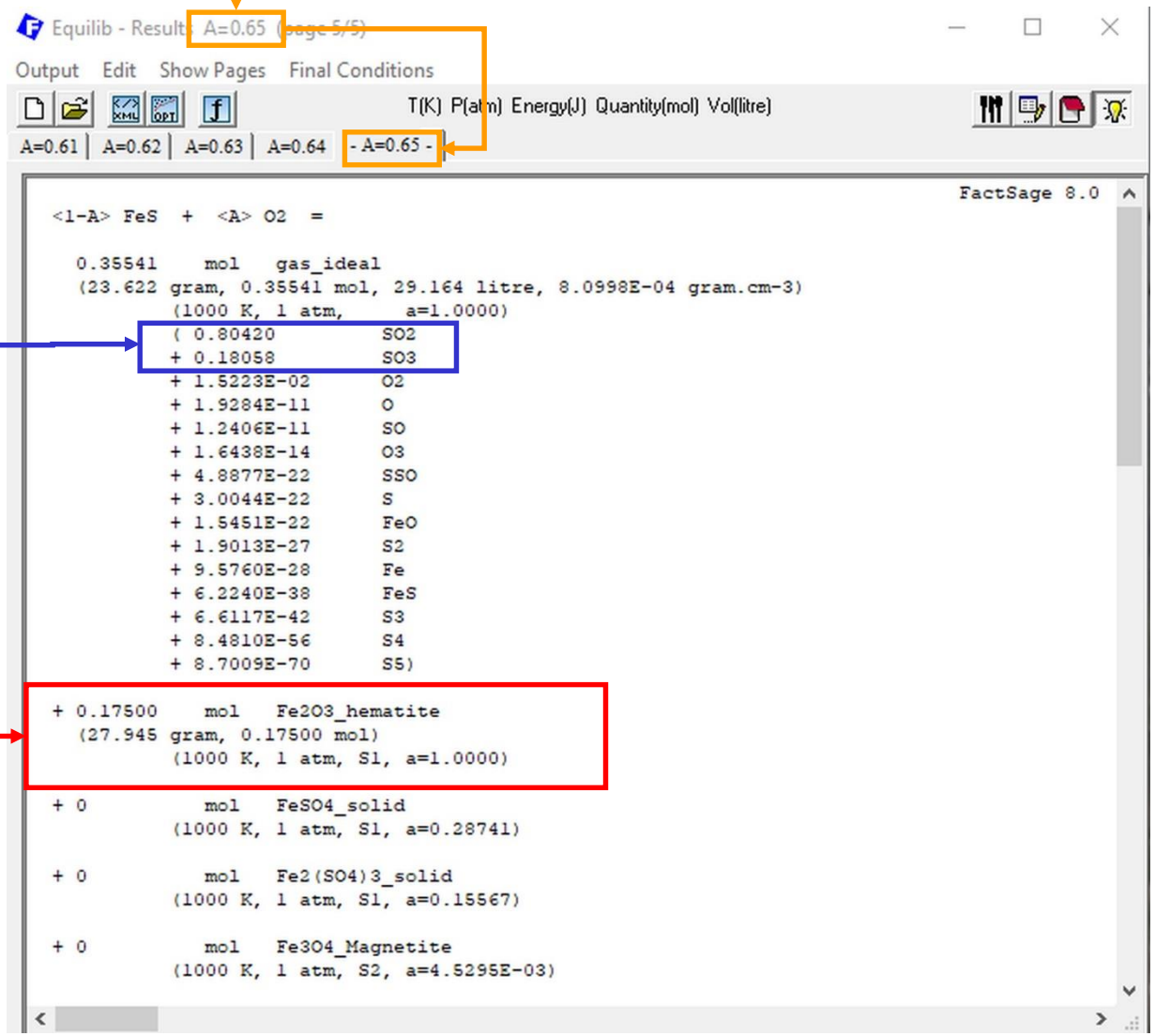
Products:

- 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.



Compound species selection

Since **FactSage 6.4** there is a new default exclusion of species from compound species selection

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.

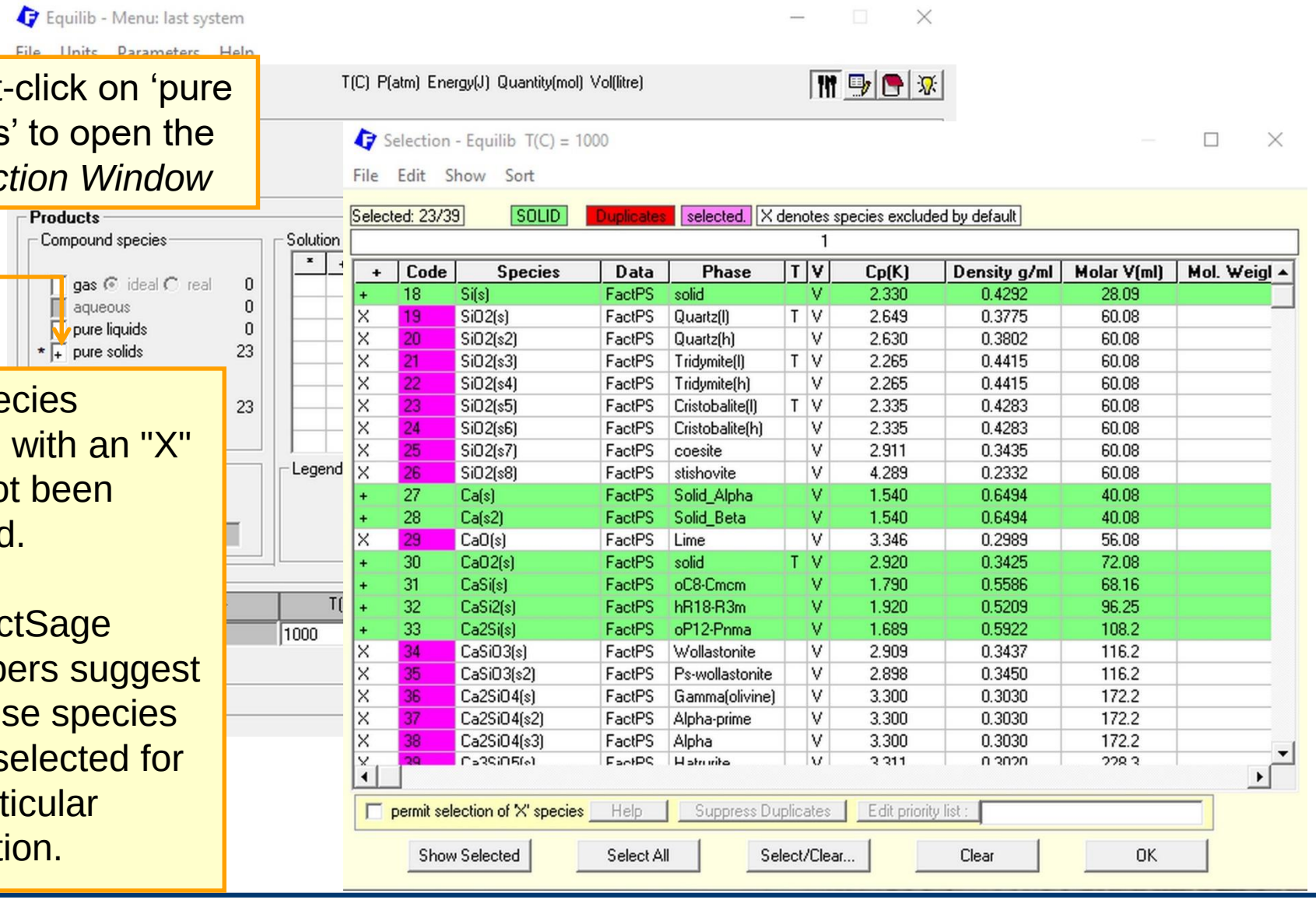
If you wish to select species marked with an "X" you must first click on 'permit selection of "X" species'. This will then override the default setting and permit you to select species. This will also activate the 'suppress duplicates' button and enable you to define a database priority list.

IMPORTANT : 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

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

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

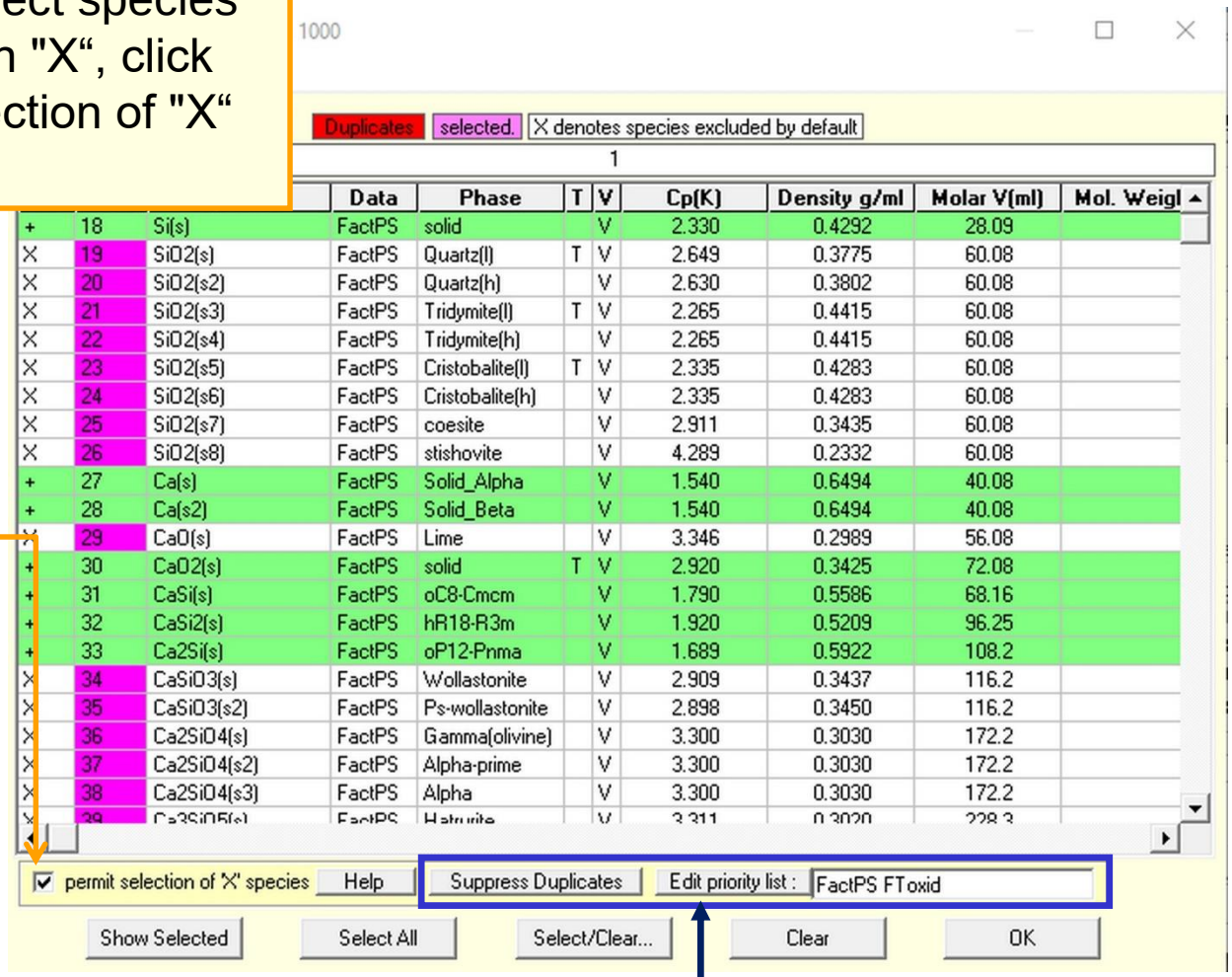


The species marked with an "X" have not been selected.

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

Compound species selection

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



			Data	Phase	T	V	Cp(K)	Density g/ml	Molar V(ml)	Mol. Weigl
+	18	Si(s)	FactPS	solid		V	2.330	0.4292	28.09	
X	19	SiO2(s)	FactPS	Quartz(l)	T	V	2.649	0.3775	60.08	
X	20	SiO2(s2)	FactPS	Quartz(h)		V	2.630	0.3802	60.08	
X	21	SiO2(s3)	FactPS	Tridymite(l)	T	V	2.265	0.4415	60.08	
X	22	SiO2(s4)	FactPS	Tridymite(h)		V	2.265	0.4415	60.08	
X	23	SiO2(s5)	FactPS	Cristobalite(l)	T	V	2.335	0.4283	60.08	
X	24	SiO2(s6)	FactPS	Cristobalite(h)		V	2.335	0.4283	60.08	
X	25	SiO2(s7)	FactPS	coesite		V	2.911	0.3435	60.08	
X	26	SiO2(s8)	FactPS	stishovite		V	4.289	0.2332	60.08	
+	27	Ca(s)	FactPS	Solid_Alpha		V	1.540	0.6494	40.08	
+	28	Ca(s2)	FactPS	Solid_Beta		V	1.540	0.6494	40.08	
X	29	CaO(s)	FactPS	Lime		V	3.346	0.2989	56.08	
+	30	CaO2(s)	FactPS	solid	T	V	2.920	0.3425	72.08	
+	31	CaSi(s)	FactPS	oC8-Cmcm		V	1.790	0.5586	68.16	
+	32	CaSi2(s)	FactPS	hR18-R3m		V	1.920	0.5209	96.25	
+	33	Ca2Si(s)	FactPS	oP12-Pnma		V	1.689	0.5922	108.2	
X	34	CaSiO3(s)	FactPS	Wollastonite		V	2.909	0.3437	116.2	
X	35	CaSiO3(s2)	FactPS	Ps-wollastonite		V	2.898	0.3450	116.2	
X	36	Ca2SiO4(s)	FactPS	Gamma(olivine)		V	3.300	0.3030	172.2	
X	37	Ca2SiO4(s2)	FactPS	Alpha-prime		V	3.300	0.3030	172.2	
X	38	Ca2SiO4(s3)	FactPS	Alpha		V	3.300	0.3030	172.2	

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