# Advanced features of *Equilib*

The ***Equilib*** module has many advanced features which are described here.

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**(continued)**

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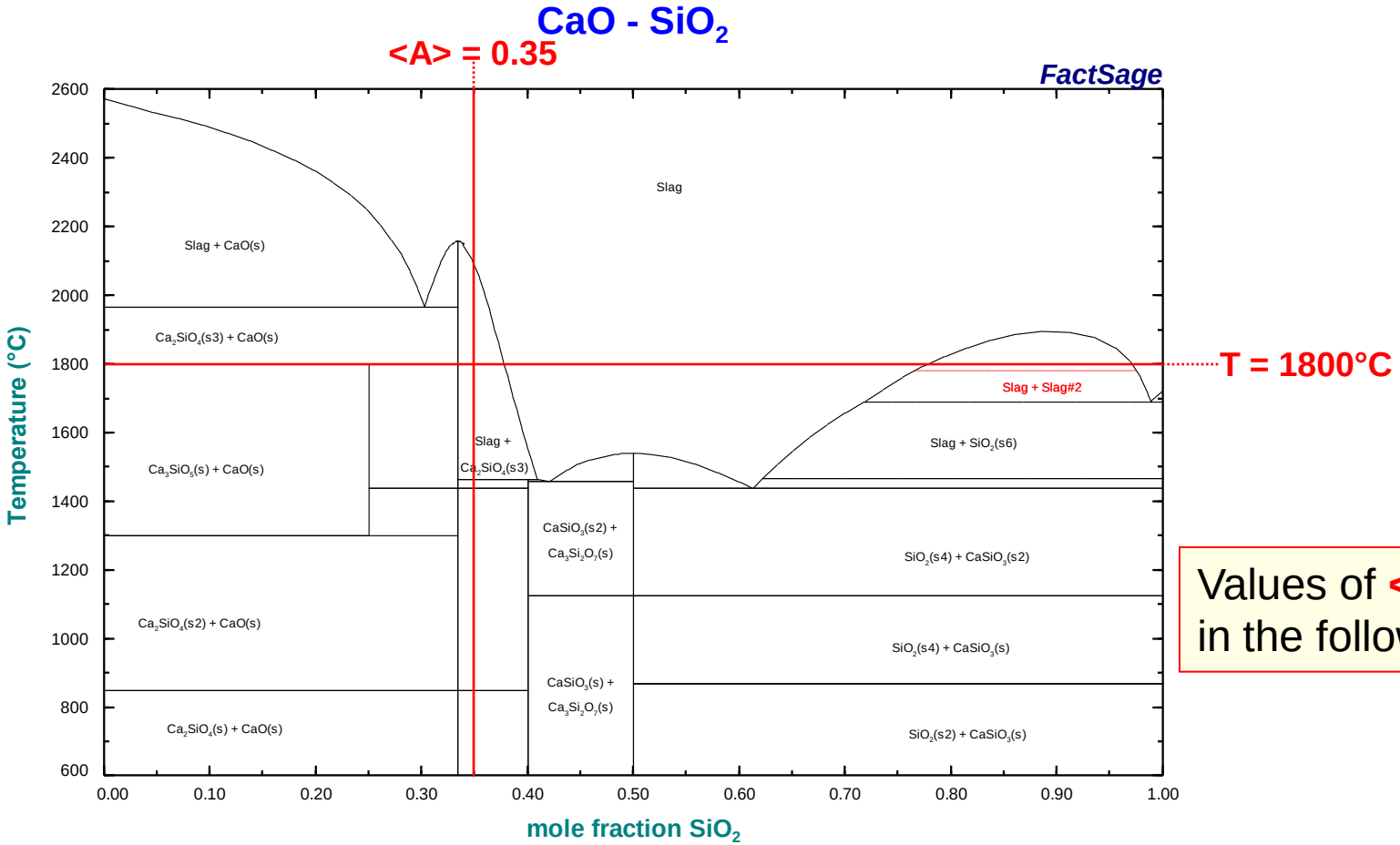
# Target phase options

A species or solution phase may be declared as a Target phase. There are several types of target phases:

1. **[F] - Formation target phase:** the T (P or <A>) is calculated when the species or phase first begins to form. The final T (P, <A>) must not be specified (blank column) and an estimate of the unspecified T (P, <A>) must be entered.
2. **[P] - Precipitate target phase:** the T (P or <A>) is calculated when another species or phase first starts to precipitate from this phase.
   The precipitate target phase must be a solution (for example FACT-SLAG or gas phase). The final T (P, <A>) must not be specified (blank column) and an estimate of the unspecified T (P, <A>) must be entered.
3. **[C] - Composition target phase:** the <A> is calculated for a given solution composition. The final T and P must also be specified and final <A> must not be specified (blank column) .

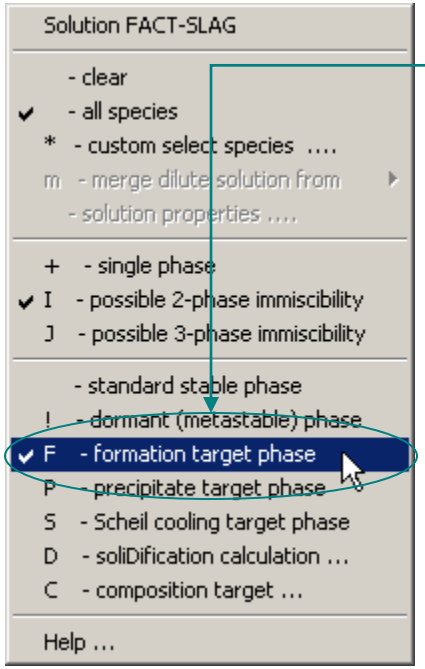
# Formation target phase

The program calculates when this phase first forms (activity = 1, and generally zero mass). One of T, P or alpha must not be specified (i.e. blank) so that ***Equilib*** can calculate the limiting T (P or alpha) when the **formation target** phase first forms. The formation target phase may be a compound species (for example a pure solid or liquid) or a solution phase (gas phase or real solution such as FACT-SLAG).



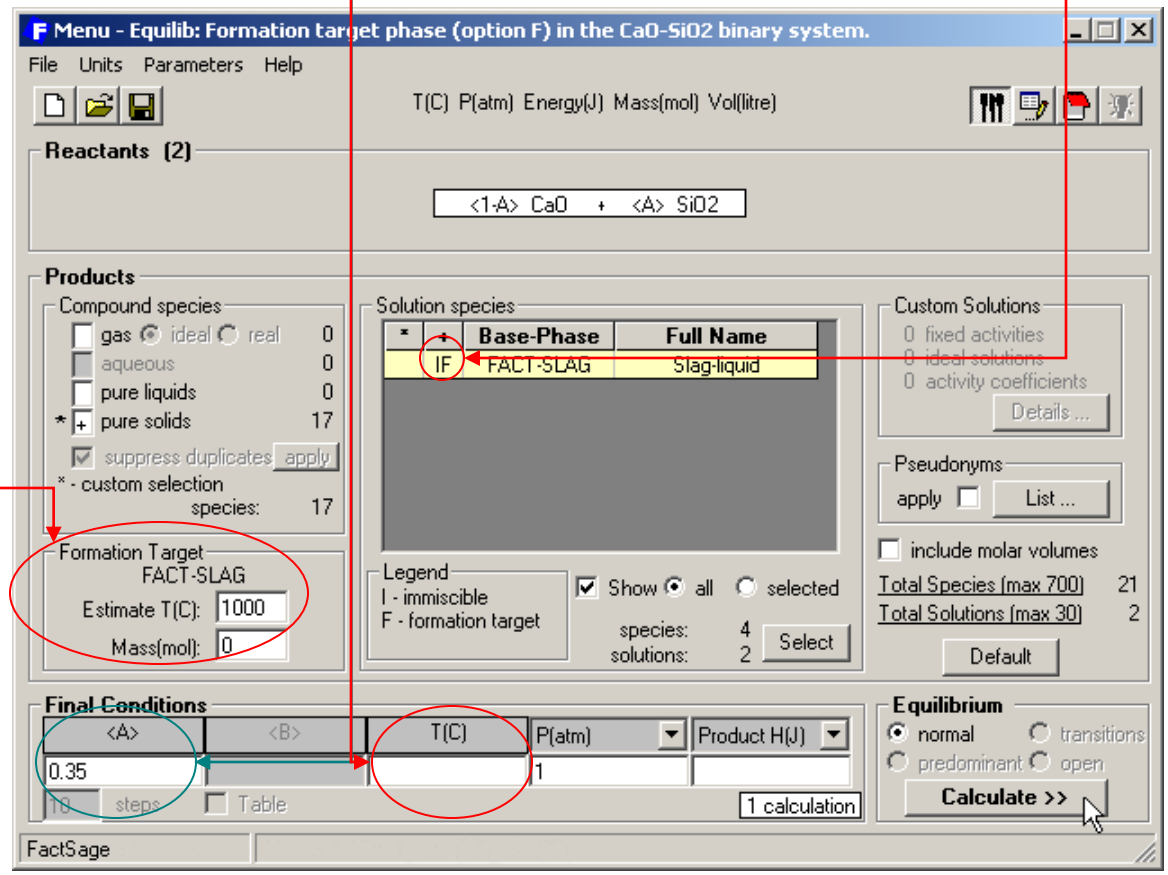

Values of **<A>** and **T** used in the following example.

# Setting a **FACT-SLAG** **formation target** at a given composition




**1°** **Right-click** on the + column to open the **FACT-SLAG** extended menu and **select F - formation target phase**.

**2°** **Enter** a value of <A> (**0.35**) and leave a **blank** for the value of T(C) in the input boxes of the **Final Conditions** frame. This activates the **Formation Target** frame.




**3°** The **Formation Target** frame is **enabled**. **Enter** an estimate for the value of T(C). Here T(C)= **1000°C**.

The program will calculate that temperature when FACT-SLAG first starts to form (**0 mole**).

# Calculation of the **FACT-SLAG** formation target at a given composition

Results - Equilib 1464.19 C

Output Edit Show Pages

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

```
 <1-A> CaO +  <A> SiO2 =

  0.00000    mol   Slag-liquid#1
          (1464.19 C, 1 atm,     a=1.0000)
          ( 0.40851         SiO2
          + 0.59149         CaO)

          System component       Mole fraction  Mass fraction
          Ca                       0.24558        0.41074
          Si                       0.16961        0.19879
          O                        0.58481        0.39046

+ 0.00000    mol   Slag-liquid#2
          (1464.19 C, 1 atm,     a=1.0000)
          ( 0.40851         SiO2
          + 0.59149         CaO)

+ 0.25000    mol   Ca2SiO4_alpha
  (43.060 gram, 0.25000 mol)
          (1464.19 C, 1 atm, S3, a=1.0000)

+ 5.0000E-02 mol   Ca3Si2O7_rankinite
  (14.420 gram, 5.0000E-02 mol)
          (1464.19 C, 1 atm, S1, a=1.0000)

+ 0.00000    mol   Ca2SiO4_alpha-prime
          (1464.19 C, 1 atm, S2, a=0.98736)

where "A" on the reactant side is 0.35000

The cutoff concentration has been specified to 1.0000E-75

Data on 4 product species identified with "T" have been extrapolated

*****************************************************************
      H            G            V            S            Cp
     (J)          (J)        (litre)      (J/K)        (J/K)
*****************************************************************
-6.82202E+05 -9.34539E+05  0.00000E+00  1.45244E+02  6.44500E+01
```

Note:
activity = 1.0
number of moles = 0
for the slag phase (liquid)
i.e. FACT-SLAG is just **beginning to form**.

Compositions and quantities of the solid oxides in equilibrium with FACT-SLAG.

Value of <A>, $X_{SiO_2}$ **= 0.35**

# Formation Target phase: specifying the target phase mass

In the **Menu-Equilib** window **Formation Target** frame, the target phase mass is set to **0.5 mole**.

Formation Target
FACT-SLAG
Estimate T(C): 1000
Mass(mol): 0.5

Note: The slag-liquid composition is now: $X_{SiO_2}$ = **0.36667**

Results - Equilib 1922.8 C

Output Edit Show Pages

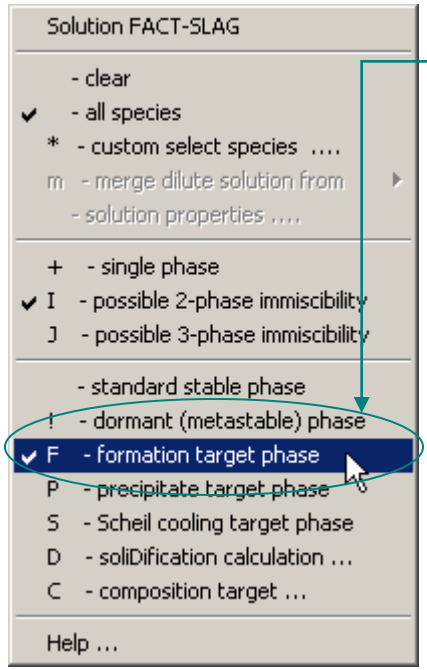
T(C) P(atm) Energy(J) Mass(mol) Vol(litre)

```
 <1-A> CaO +  <A> SiO2 =

  0.50000     mol   Slag-liquid#1
  (28.773 gram, 0.50000 mol)
          (1922.80 C, 1 atm,      a=1.0000)
          ( 0.36667          SiO2
          + 0.63333          CaO)

+ 0.00000     mol   Slag-liquid#2
          (1922.80 C, 1 atm,      a=1.0000)
          ( 0.36667          SiO2
          + 0.63333          CaO)

+ 0.16667     mol   Ca2SiO4_alpha
  (28.707 gram, 0.16667 mol)
          (1922.80 C, 1 atm, S3, a=1.0000)

+ 0.00000     mol   Ca2SiO4_alpha-prime
          (1922.80 C, 1 atm, S2, a=0.83616)

where "A" on the reactant side is 0.35000

The cutoff concentration has been specified to 1.0000E-75

Data on 6 product species identified with "T" have been extrapolated

*****************************************************************
      H            G            V            S            Cp
     (J)          (J)        (litre)      (J/K)        (J/K)
*****************************************************************
-6.45531E+05 -1.00625E+06  0.00000E+00  1.64265E+02  7.66105E+01
```

and the temperature has increased to: **T = 1922.80°C**

Value of <A>, $X_{SiO_2}$ = **0.35**

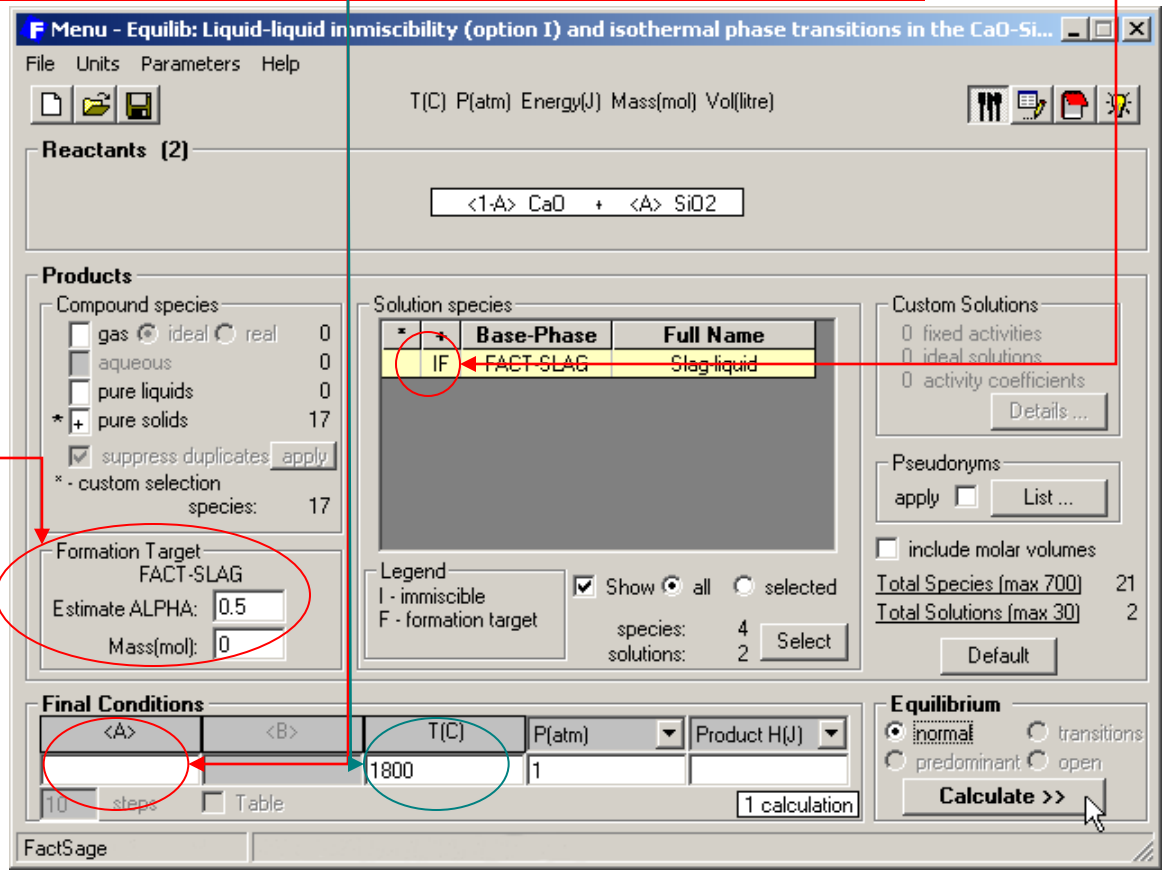
# Setting a **FACT-SLAG** **formation target** at a given temperature




**1°** **Right-click** on the + column to open the **FACT-SLAG** extended menu and **select** **F –formation target phase**.

**2°** **Enter** a value of T (**1800 °C**) and leave a **blank** for the value of <A> in the input boxes of the **Final Conditions** frame.

**3°** The **Formation Target** frame is **enabled**. **Enter** an estimate of the value of <A>. Here <A> = **0.5**.




The program will calculate that composition when FACT-SLAG first starts to form (**0 mole**).

# Calculation of the **FACT-SLAG** **formation** **target** at a given temperature (1800°C)

Results - Equilib 1800 C, A=0.3333

Output Edit Show Pages

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

```
 <1-A> CaO +  <A> SiO2 =

  0.00000    mol   Slag-liquid#1
          (1800.00 C, 1 atm,     a=1.0000)
          ( 0.34683         SiO2
          + 0.65317         CaO)

+ 0.00000    mol   Slag-liquid#2
          (1800.00 C, 1 atm,     a=1.0000)
          ( 0.34683         SiO2
          + 0.65317         CaO)

+ 0.33333    mol   Ca2SiO4_alpha
  (57.413 gram, 0.33333 mol)
          (1800.00 C, 1 atm, S3, a=1.0000)

+ 0.00000    mol   CaO_lime
          (1800.00 C, 1 atm, S1, a=1.0000)

+ 0.00000    mol   CaSiO3_pseudowollastonite                    T
          (1800.00 C, 1 atm, S2, a=1.0000)

+ 0.00000    mol   Ca2SiO4_alpha-prime
          (1800.00 C, 1 atm, S2, a=0.86793)

+ 0.00000    mol   SiO2_tridymite(l)                            T
          (1800.00 C, 1 atm, S3, a=6.0700E-07)

where "A" on the reactant side is 0.33333

The cutoff concentration has been specified to 1.0000E-75

Data on 6 product species identified with "T" have been extrapolated

*****************************************************************
      H            G            V            S            Cp
     (J)          (J)        (litre)      (J/K)        (J/K)
*****************************************************************
-6.53962E+05 -9.80938E+05  0.00000E+00  1.57719E+02  6.41837E+01
```

Note:
activity = 1.0
number of moles = 0
for the slag phase (liquid)
i.e. FACT-SLAG is just **beginning to form**.

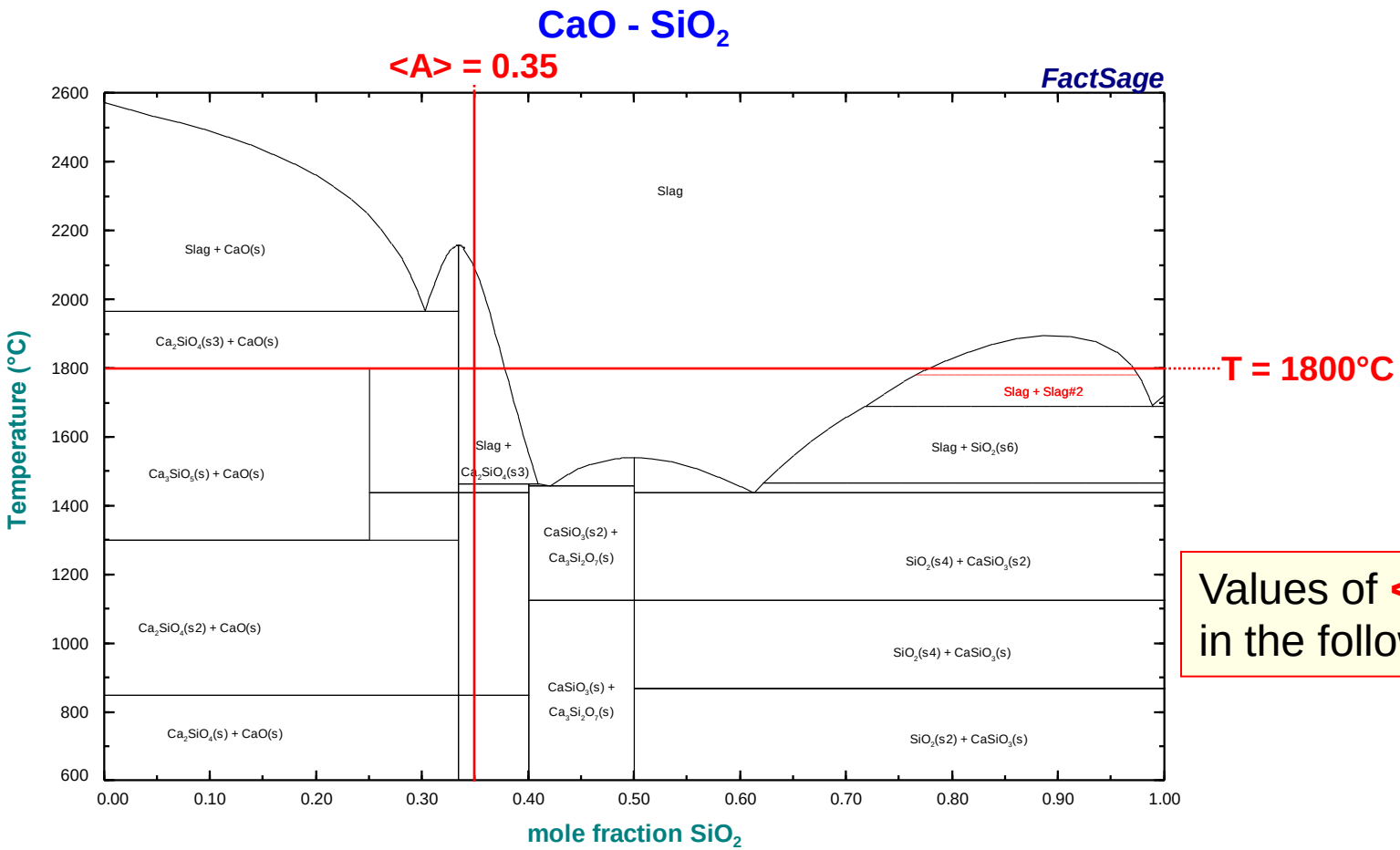
Compositions and quantities of the solid phases in equilibrium (activity =1) with FACT-SLAG.

Calculated value of **<A> = 0.3333**

# Precipitate target

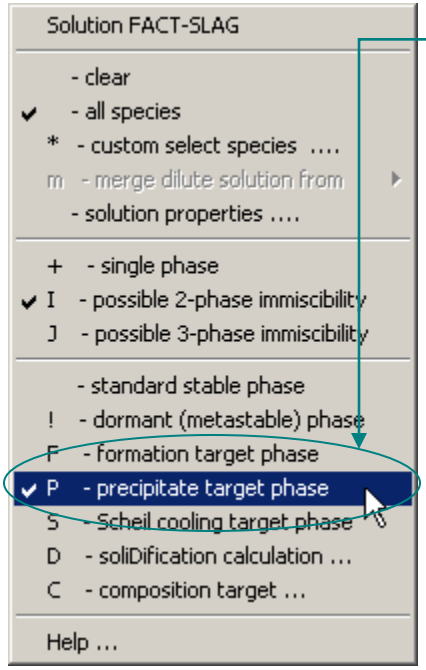
The program calculates when a second phase first starts to precipitate (activity = 1, zero mass) from this target solution phase (activity = 1, 100% mass). One of T, P or alpha must not be specified (i.e. blank) so that ***Equilib*** can calculate the limiting T (P or alpha) when the second phase precipitates.

The precipitate target phase must be a solution phase for example gas or FACT-SLAG.



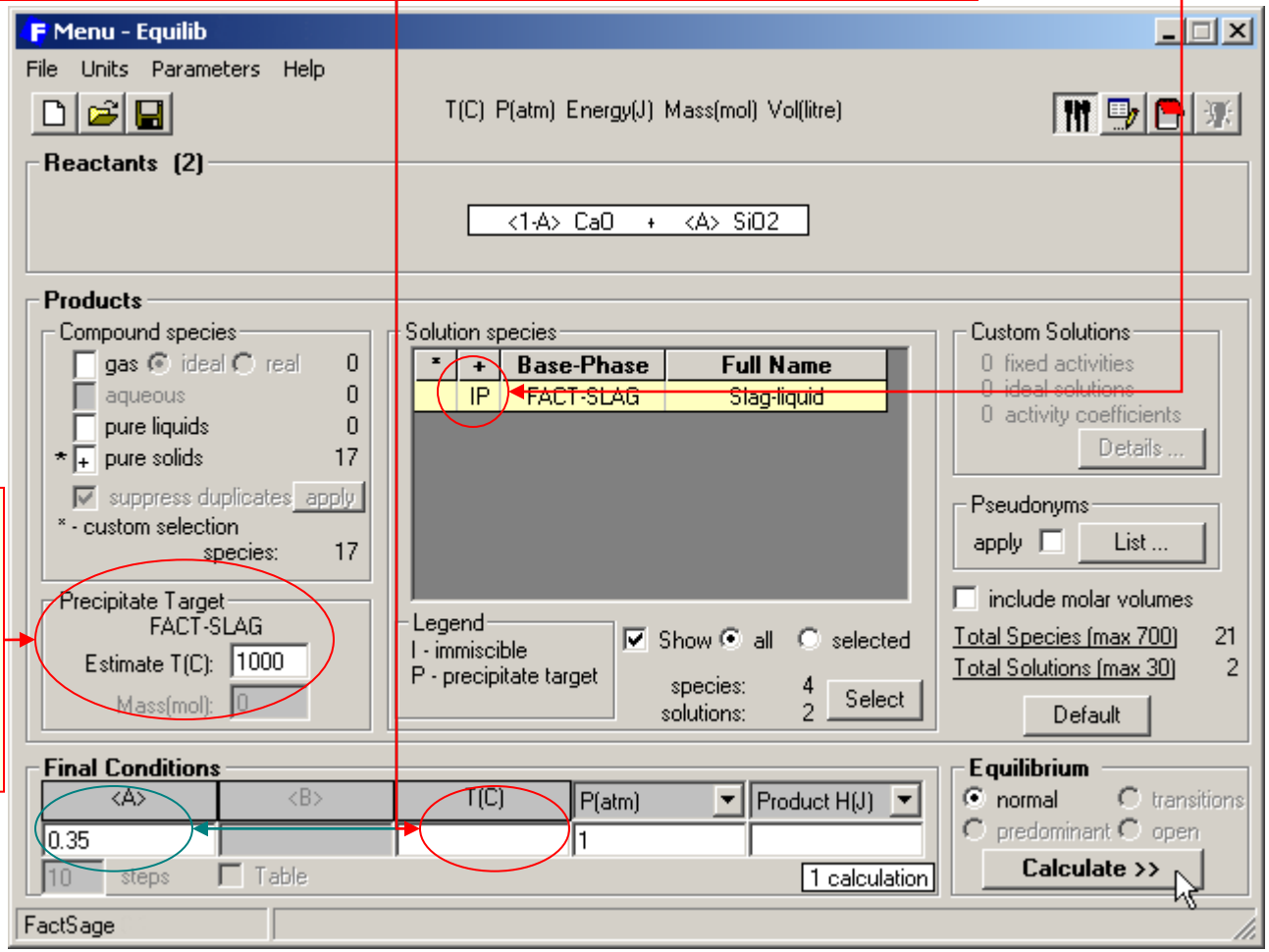

Values of **<A>** and **T** used in the following example.

# Setting a **FACT-SLAG precipitate target** at a given composition




1° **Right-click** on the + column to open the **FACT-SLAG** extended menu and **select P –precipitate target phase**.

2° **Enter** a value of <A> (**0.35**) and leave T(C) **blank**.




3° The **Precipitate Target** frame is **enabled**. **Enter** an estimate of the value of T(C).
Here T(C)= **1000°C**.

# Calculation of the **FACT-SLAG precipitate target** at a given composition

Results - Equilib 2085.37 C

Output Edit Show Pages

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

```
 <1-A> CaO +  <A> SiO2 =

  1.0000     mol   Slag-liquid#1
  (57.480 gram, 1.0000 mol)
          (2085.37 C, 1 atm,      a=1.0000)
          ( 0.35000          SiO2
          + 0.65000          CaO)

+ 0.00000    mol   Slag-liquid#2
          (2085.37 C, 1 atm,      a=1.0000)
          ( 0.35000          SiO2
          + 0.65000          CaO)

+ 0.00000    mol   Ca2SiO4_alpha
          (2085.37 C, 1 atm, S3, a=1.0000)

+ 0.00000    mol   Ca2SiO4_alpha-prime
          (2085.37 C, 1 atm, S2, a=0.80064)

+ 0.00000    mol   CaSiO3_pseudowollastonite                    T
          (2085.37 C, 1 atm, S2, a=0.17022)

+ 0.00000    mol   SiO2_cristobalite(l)                         T
          (2085.37 C, 1 atm, S5, a=2.6429E-05)

+ 0.00000    mol   SiO2_tridymite(l)                            T
          (2085.37 C, 1 atm, S3, a=4.7013E-06)

where "A" on the reactant side is 0.35000

The cutoff concentration has been specified to 1.0000E-75

Data on 6 product species identified with "T" have been extrapolated

*****************************************************************
      H            G            V            S            Cp
     (J)          (J)        (litre)      (J/K)        (J/K)
*****************************************************************
-6.30362E+05 -1.03345E+06  0.00000E+00  1.70907E+02  6.93966E+01
```

Equilibrium at **2085.37 °C**

Note:
activity = **1.0**
number of moles =**1** (100%)
for the first phase:
the slag phase (liquid).

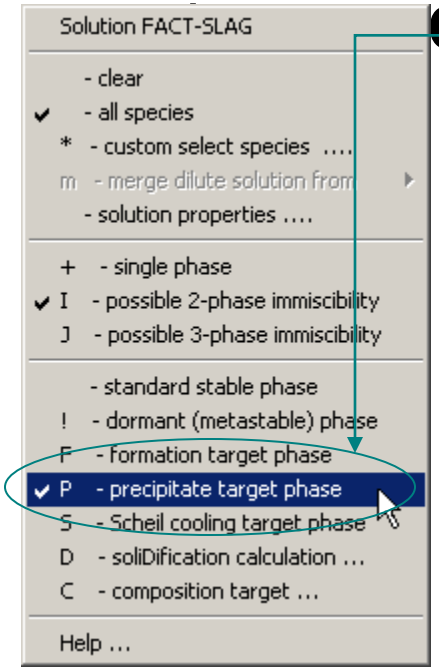
First precipitate to deposit from the slag phase
activity = **1.0**
number of moles = **0**.

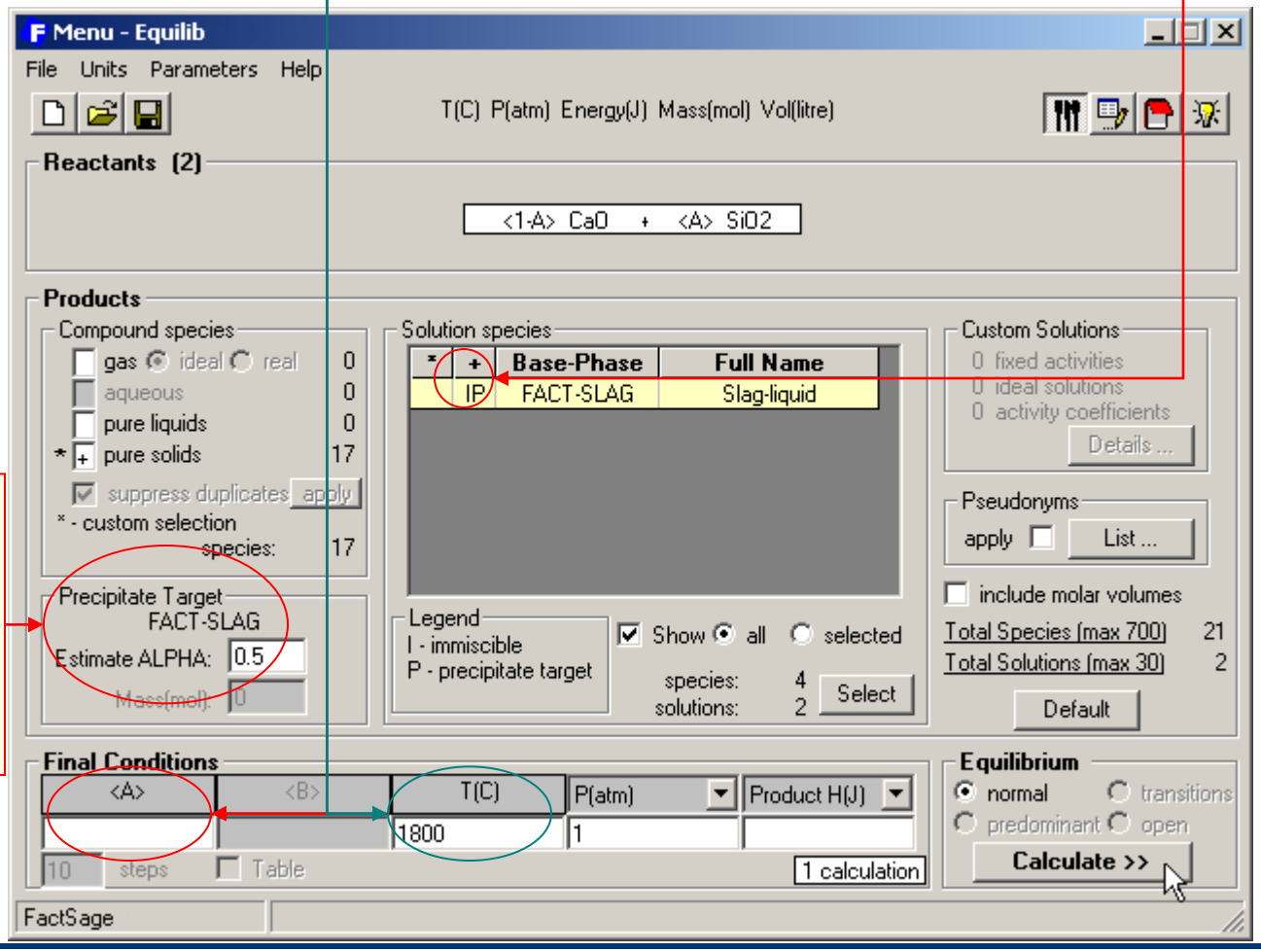
Value of <A>, $X_{SiO_2}$ **= 0.35**

C ... ture

1° **Right-click** on the + column to open the **FACT-SLAG** extended menu and **select P –precipitate target phase**.

2° **Enter** a value of T (**1800°C**) and **leave <A> blank**.




3° The **Precipitate Target** frame is **enabled**. **Enter** an estimate of the value of **<A>**. Here **<A>** = **0.5**.

# Calculation of a **FACT-SLAG** precipitate target at a given temperature

Results - Equilib 1800 C, A=0.3777

Output Edit Show Pages

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

```
 <1-A> CaO +  <A> SiO2 =

 1.0000      mol    Slag-liquid#1
 (57.591 gram, 1.0000 mol)
          (1800.00 C, 1 atm,      a=1.0000)
          ( 0.37767          SiO2
          + 0.62233          CaO)

+ 0.00000     mol    Slag-liquid#2
          (1800.00 C, 1 atm,      a=1.0000)
          ( 0.37767          SiO2
          + 0.62233          CaO)

+ 0.00000     mol    Ca2SiO4_alpha
          (1800.00 C, 1 atm, S3, a=1.0000)

+ 0.00000     mol    Ca2SiO4_alpha-prime
          (1800.00 C, 1 atm, S2, a=0.86793)

+ 0.00000     mol    SiO2_cristobalite(l)                          T
          (1800.00 C, 1 atm, S5, a=2.0833E-04)

+ 0.00000     mol    SiO2_tridymite(l)                             T
          (1800.00 C, 1 atm, S3, a=3.9282E-05)

where "A" on the reactant side is 0.37767

The cutoff concentration has been specified to 1.0000E-75

Data on 6 product species identified with "T" have been extrapolated

*****************************************************************
      H            G            V            S            Cp
     (J)          (J)        (litre)      (J/K)        (J/K)
*****************************************************************
-6.55427E+05 -9.95296E+05  0.00000E+00  1.63939E+02  6.74833E+01
```

Note:
activity = **1.0**
number of moles =**1** (100%)
for the first phase:
the slag phase (liquid).

First precipitate to deposit from the slag phase
activity = **1.0**
number of moles = **0**.

Calculated value of **<A>**, **$X_{SiO_2}$ = 0.3767**.

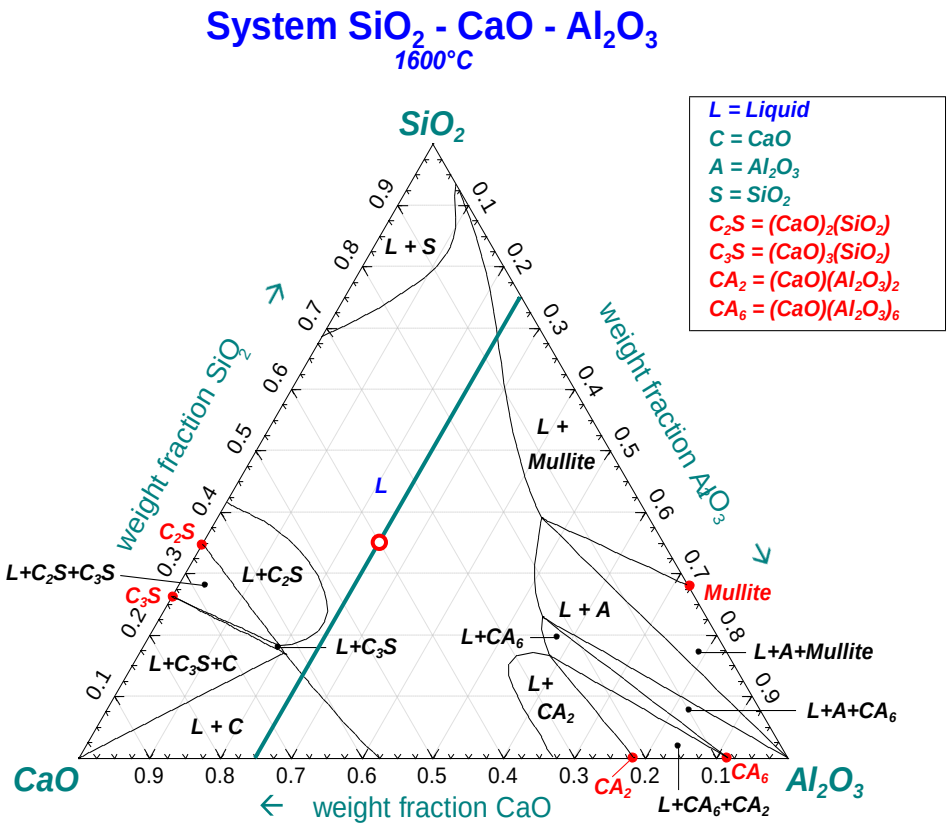
# Precipitate target phase calculation for a more complex system

This is an example of a Slag-liquid precipitate target phase calculation in the **$CaO$-$SiO_2$-$Al_2O_3$** ternary system.

In a precipitate target phase calculation, the temperature (or composition) is calculated when a second phase first starts to form (activity = 1, and zero mole) from the «**precipitate target phase**». The «**precipitate target phase**» must be a solution for example, gas, FACT-SLAG, etc. (this differs from the «**formation target phase**» that can be any type of phase).

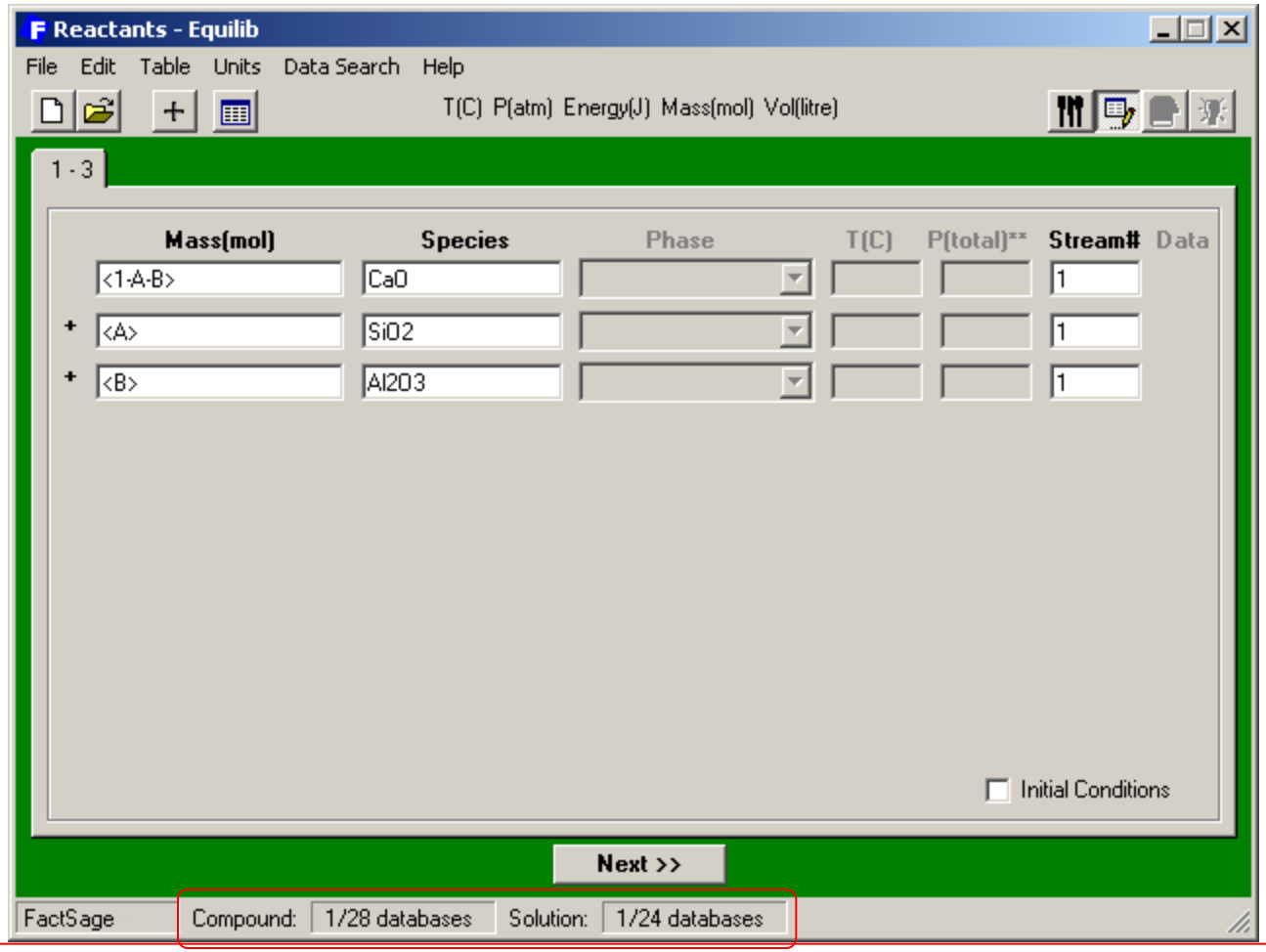
In this example that temperature is calculated when the first solid precipitate starts to deposit when Slag-liquid (FACT-SLAG) is cooled. Such a calculation is extremely important for example in the pyrometallurgy and glass industries. In principle one could select the equilibrium «**transitions**» option and execute a normal calculation, but this may lead to lot of unwanted output, especially if the system is complex.

**Red** rimmed dot: for the 1st example
**Teal** line for <B> = 25% (2nd example)



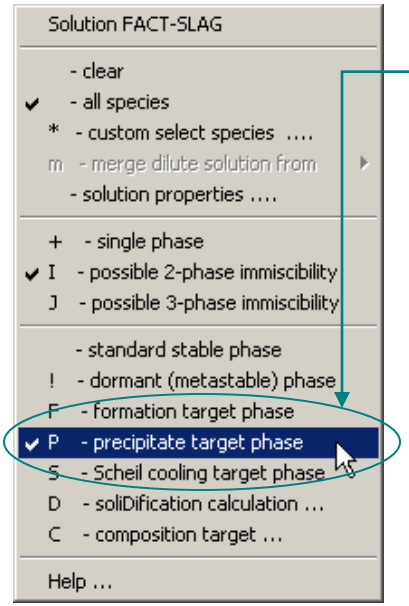
# Setting a ternary system in the *Equilib* Reactants Window

In the **Reactants Window** the reactants are **<1-A-B> CaO** + **<A> $SiO_2$** + **<B> $Al_2O_3$**.
This defines a **CaO-$SiO_2$-$Al_2O_3$** ternary system if **<A> + <B>** is in the range **0** to **1**.
The use of unit mass (g or lb) will give the compositions in weight %.




**All data** taken from the ***FACT*** **compound** and **solution databases**.

# Setting the FACT-SLAG **precipitate target** at a given composition

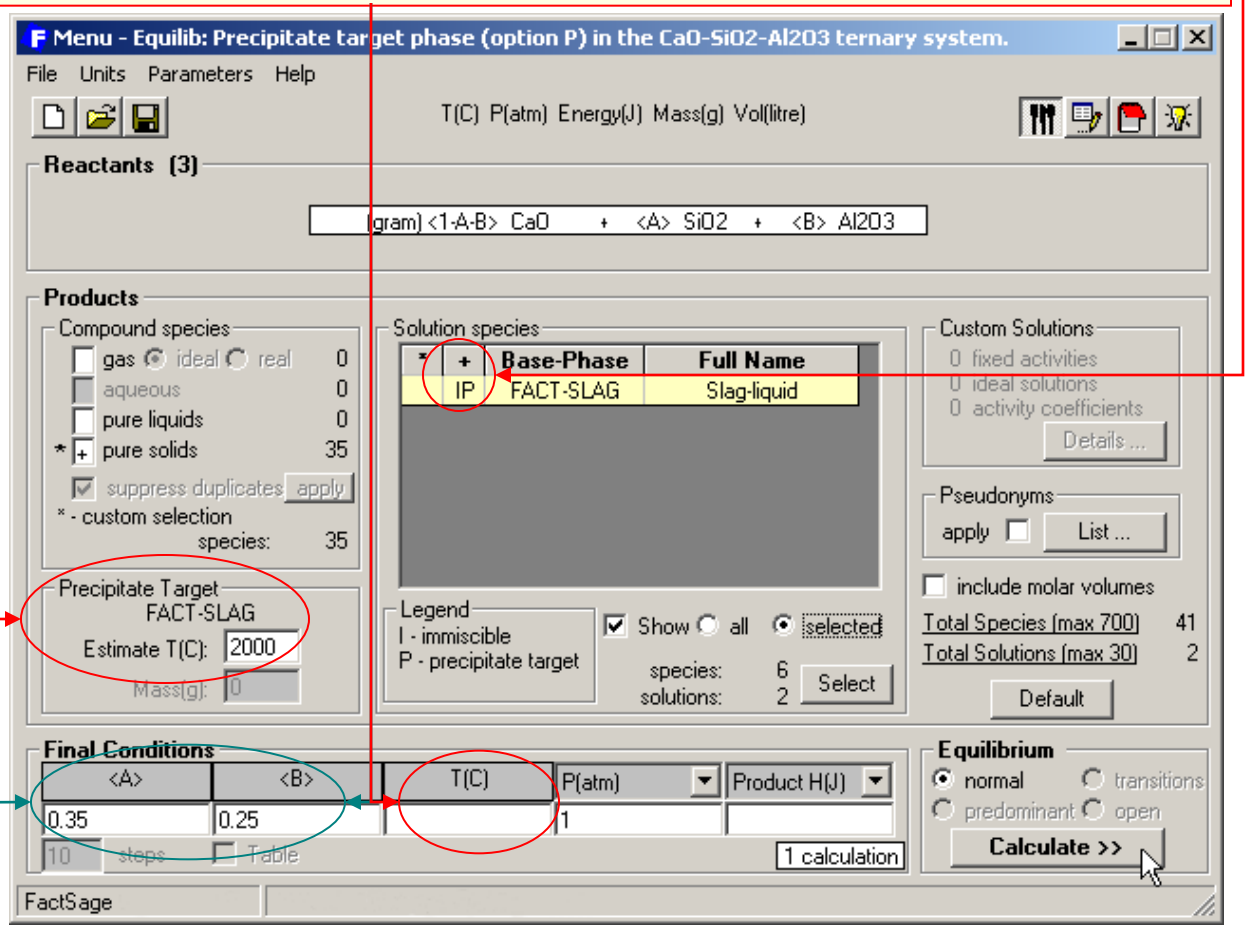



**1°** **Right-click** on the + column to open the **FACT-SLAG** extended menu and **select P –precipitate target phase**.

**2°** **Enter** values for <A> (**0.35**) and <B> (**0.25**) (i.e. %wt CaO = **40%**, %wt $SiO_2$ = **35%**, %wt $Al_2O_3$ = **25%**) and leave **T(C) blank**.

**3°** The **Precipitate Target** frame is **enabled**. **Enter** an estimate of the value of T(C). Here T(C) = **2000°C**.

**<A>** is a **variable**, **<B>** is a **constant** (here, 25 wt.%) that **must** be defined.



# Precipitate target Results

***Equilib*** reports the temperature (**1458.99 °C**) where the second phase (**$Ca_2Al_2SiO_7$(s1)**) starts to precipitate from the target phase (**Slag-liquid**).

Results - Equilib 1458.99 C

Output Edit Show Pages

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

```
(gram)  <1-A-(0.25)> CaO +  <A> SiO2 +  <(0.25)> Al2O3 =

    1.0000      gram  (   35.000      wt.% SiO2
                      +   40.000      wt.% CaO
                      +   25.000      wt.% Al2O3)
                         (1458.99 C, 1 atm, Slag-liquid#1)

+  0.00000      gram  (   35.000      wt.% SiO2
                      +   40.000      wt.% CaO
                      +   25.000      wt.% Al2O3)
                         (1458.99 C, 1 atm, Slag-liquid#2, a= 1.0000)

                    +  0.00000      gram Ca2Al2SiO7_gehlenite
                       (1458.99 C, 1 atm, S1, a= 1.0000)

                    +  0.00000      gram CaSiO3_pseudowollastoni
                       (1458.99 C, 1 atm, S2, a=0.44014)

 +...

                    +  0.00000      gram (Al2O3)(SiO2)2
                       (1458.99 C, 1 atm, S1, a=0.96234E-11)

where "A" on the reactant side is 0.3500

Data on 5 product species identified with "T" have been extrapolated

*****************************************************************
      H            G            V            S           Cp
     (J)          (J)          (1)         (J/K)       (J/K)
*****************************************************************
-1.24747E+04 -1.73319E+04  0.00000E+00  2.80414E+00  1.19458E+00
```

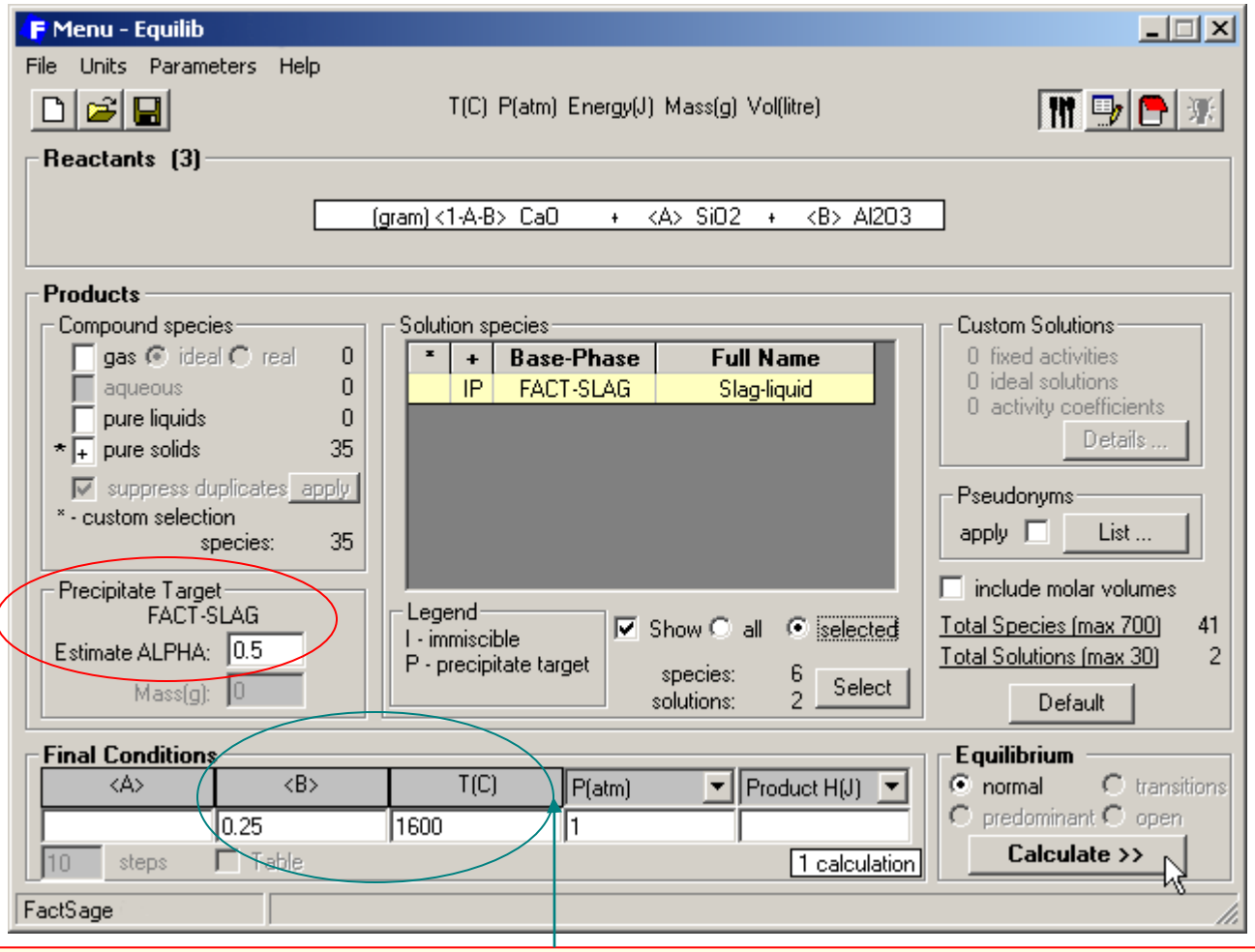
**Notes:** the composition of the first phase (Slag-liquid) is the same as the input values.
activity = **1.0**
number of grams = **1** (i.e. 100%)

First precipitate to deposit from the slag phase
activity = **1.0**
number of grams = **0**.

Value of **<A>**, **wt% $SiO_2$ = 35%**.

# Performing a **composition Precipitate Target** calculation

As in the previous example on **Formation Target** calculations, it is possible to perform a composition **Precipitate Target** calculation on **<A> (constant <B> remains unchanged)**.




For example, if in the **Menu Window** the composition **<A>** is now unspecified (**blank**), **<B>** is still **25%** and now the temperature is set to **1600°C**, an estimate of **<A>** is **50%**.

# Composition Precipitate Target calculation: Results

In the **Results** Window ***Equilib*** now reports the silica ($SiO_2$) composition (**<A> = 13.371 wt.%**) at **1600°C** where **CaO(s1)** first starts to precipitate (**activity = 1**, **0 gram**)

Results - Equilib 1600 C, A=0.1337

Output Edit Show Pages

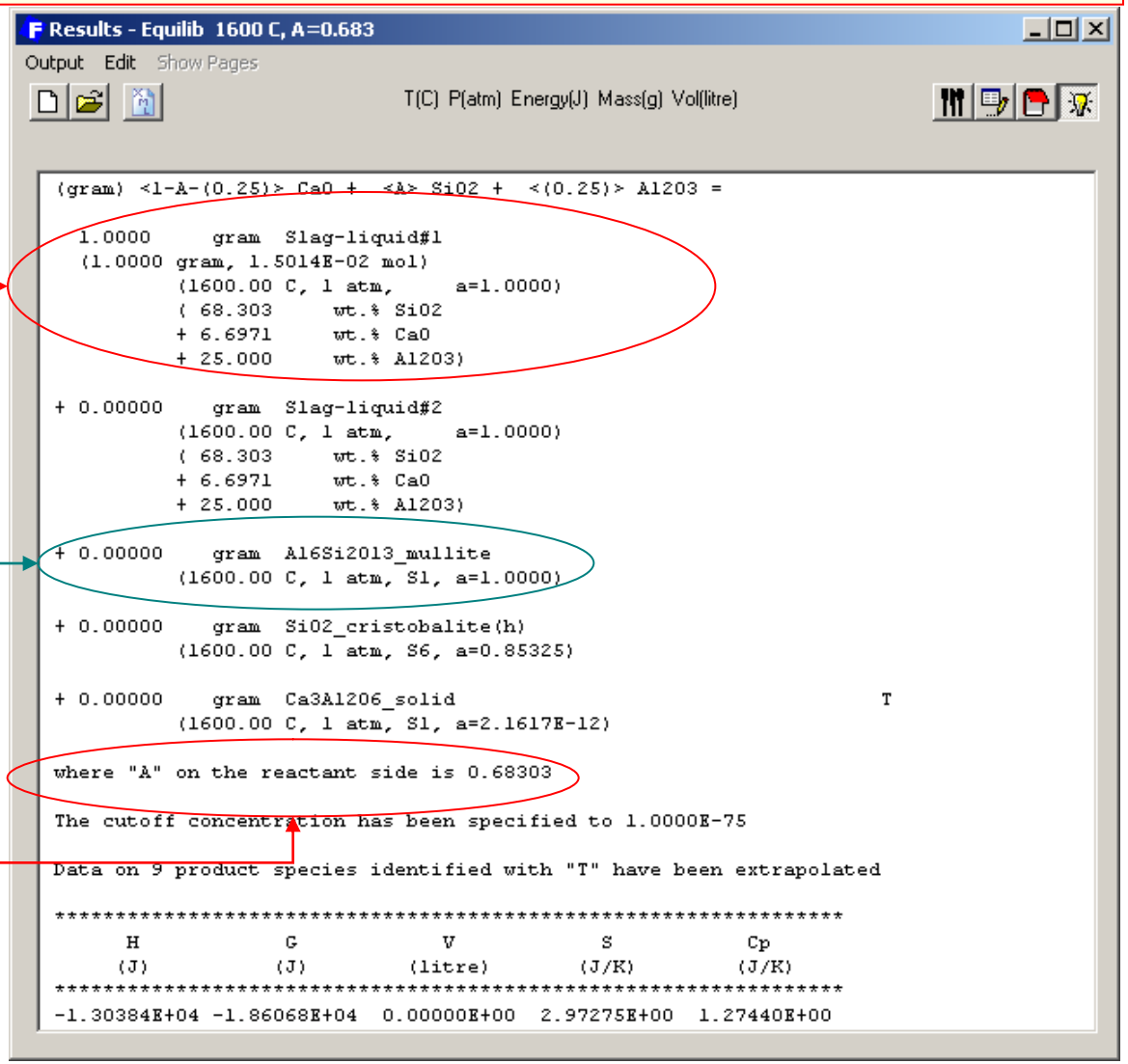
```
(gram) <1-A-(0.25)> CaO +  <A> SiO2 +  <(0.25)> Al2O3 =

  1.0000      gram  Slag-liquid#1
  (1.0000 gram, 1.5667E-02 mol)
          (1600.00 C, 1 atm,      a=1.0000)
          ( 13.371      wt.% SiO2
          + 61.629      wt.% CaO
          + 25.000      wt.% Al2O3)

+ 0.00000     gram  Slag-liquid#2
          (1600.00 C, 1 atm,      a=1.0000)
          ( 13.371      wt.% SiO2
          + 61.629      wt.% CaO
          + 25.000      wt.% Al2O3)

+ 0.00000     gram  CaO_lime
          (1600.00 C, 1 atm, S1, a=1.0000)

+ 0.00000     gram  Ca3SiO5_hatrurite
          (1600.00 C, 1 atm, S1, a=0.79106)


+ 0.00000     gram  (Al2O3)(SiO2)2_solid                          T
          (1600.00 C, 1 atm, S1, a=1.4858E-18)

where "A" on the reactant side is 0.13371

The cutoff concentration has been specified to 1.0000E-75

Data on 9 product species identified with "T" have been extrapolate

*****************************************************************
      H            G            V            S            Cp
     (J)          (J)        (litre)      (J/K)        (J/K)
*****************************************************************
-1.14071E+04 -1.66111E+04  0.00000E+00  2.77822E+00  1.24084E+00
```

In the ternary phase diagram at **1600°C** (see slide 4.0), there are **two liquidus lines** intersecting the composition line for which **<B> = 25wt.%**. One on the **CaO-rich side (calculated here)** and **one on the $SiO_2$-rich side**.

# Composition Precipitate Target calculation: setting another estimate

By setting (in the **Menu Window**) another estimate for ALPHA <A> on the **$SiO_2$-rich side**, one can calculate the other value of <A> for which a precipitate starts to form.

In the **Results Window** ***Equilib*** now reports the silica ($SiO_2$) composition (**<A> = 68.303 wt.%**) at **1600°C** where **mullite $Al_6Si_2O_{13}$(s1)** first starts to precipitate (**activity = 1, 0 gram**).

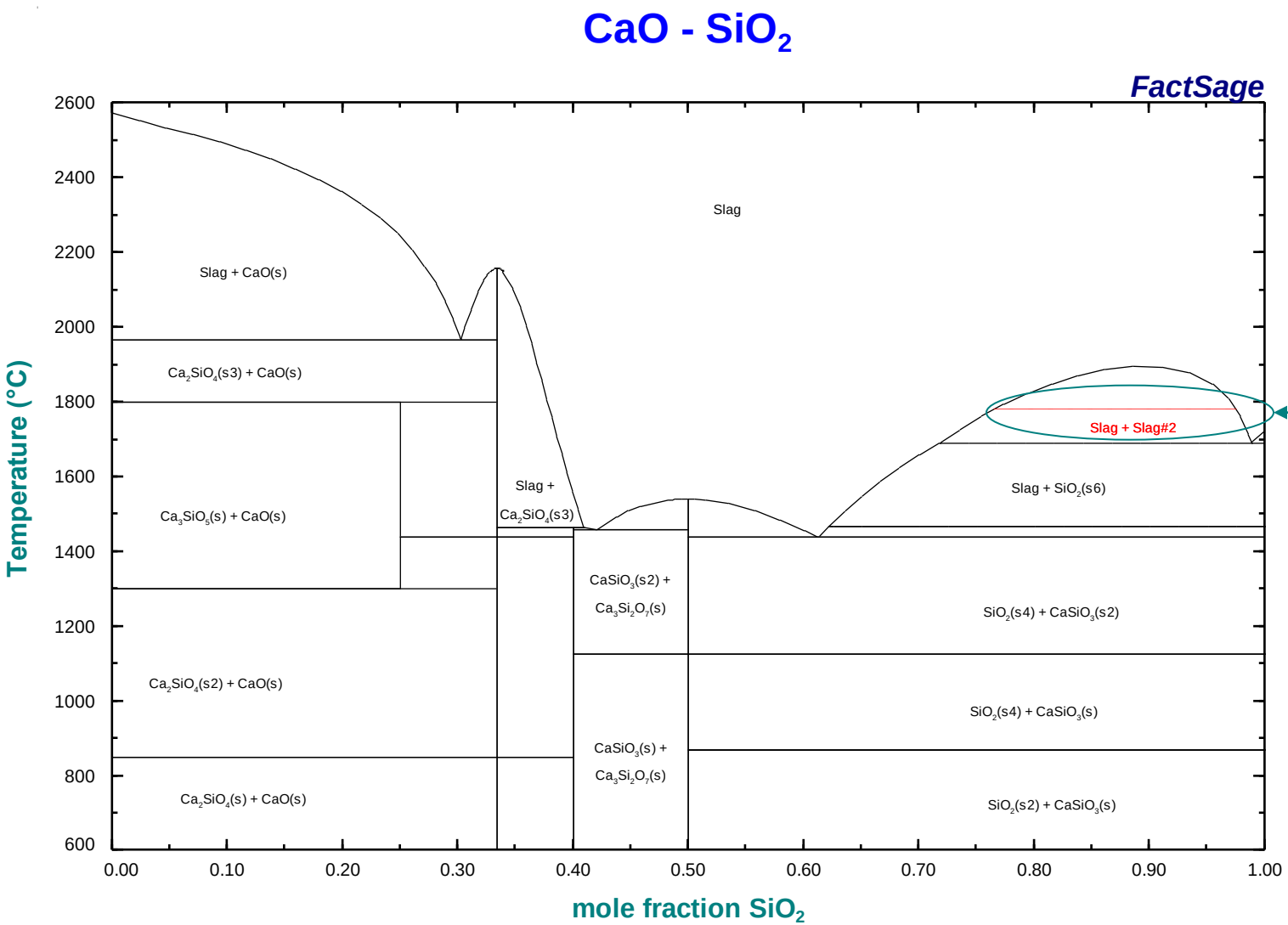


# Compostion target phase

TTD

# Transitions in the $CaO-SiO_2$ binary phase diagram

**Liquid phase immiscibility** – for example $X_{SiO_2}$= 0.7783 and 0.9707 at 1800°C.



# **Isothermal** phase transitions in the **$CaO$-$SiO_2$** binary system

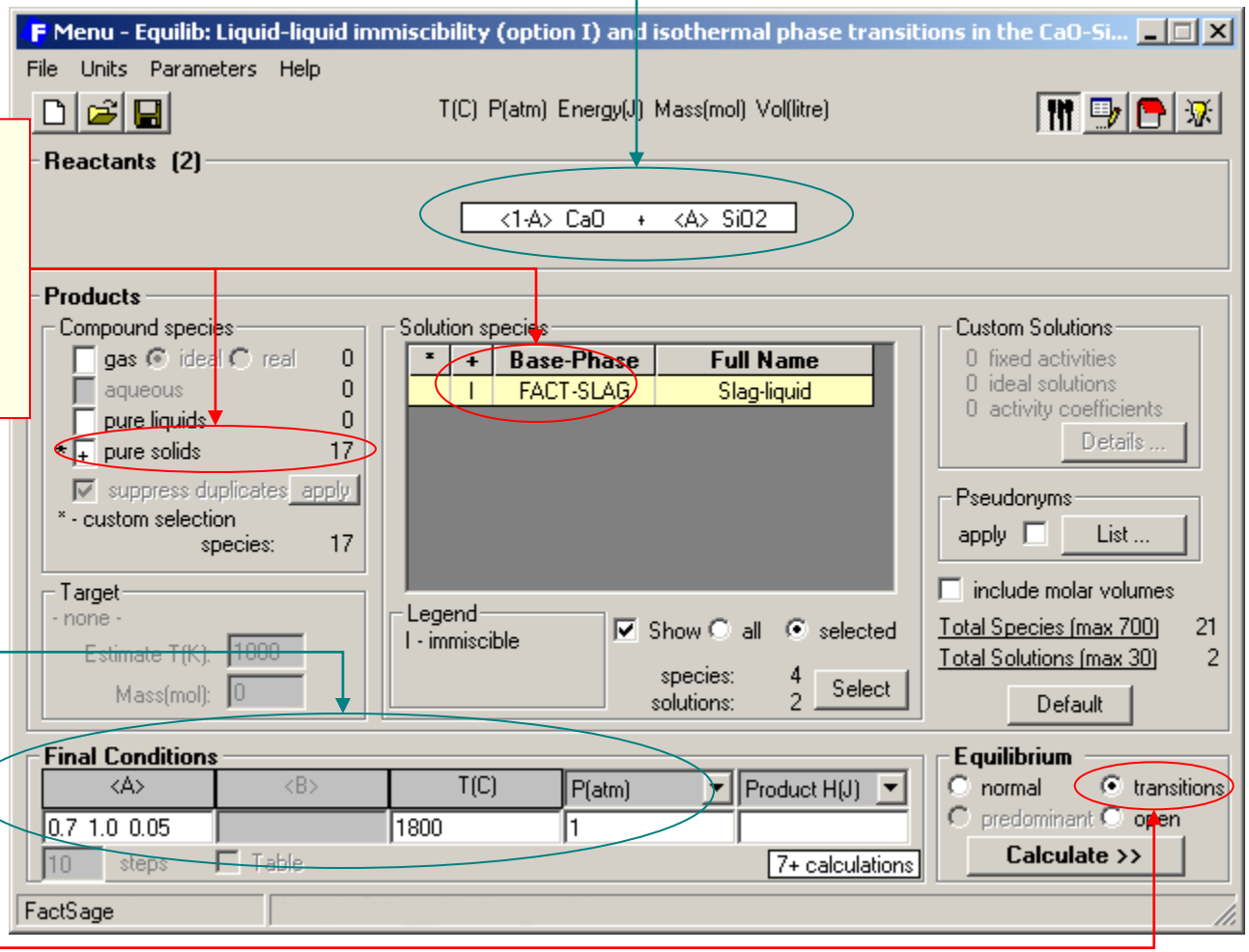
**1°** Binary system <1-A> CaO + <A> $SiO_2$.

**2°** Possible products:

- pure solid oxides
- liquid Slag (**FACT-SLAG**) with a **possible 2-phase immiscibility (I)**

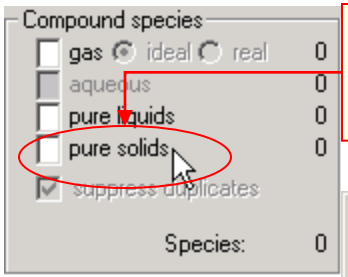
**3°** <A> = 0.7, 0.75, …, 1.0
T (°C) = 1800

**4°** Select **transitions**



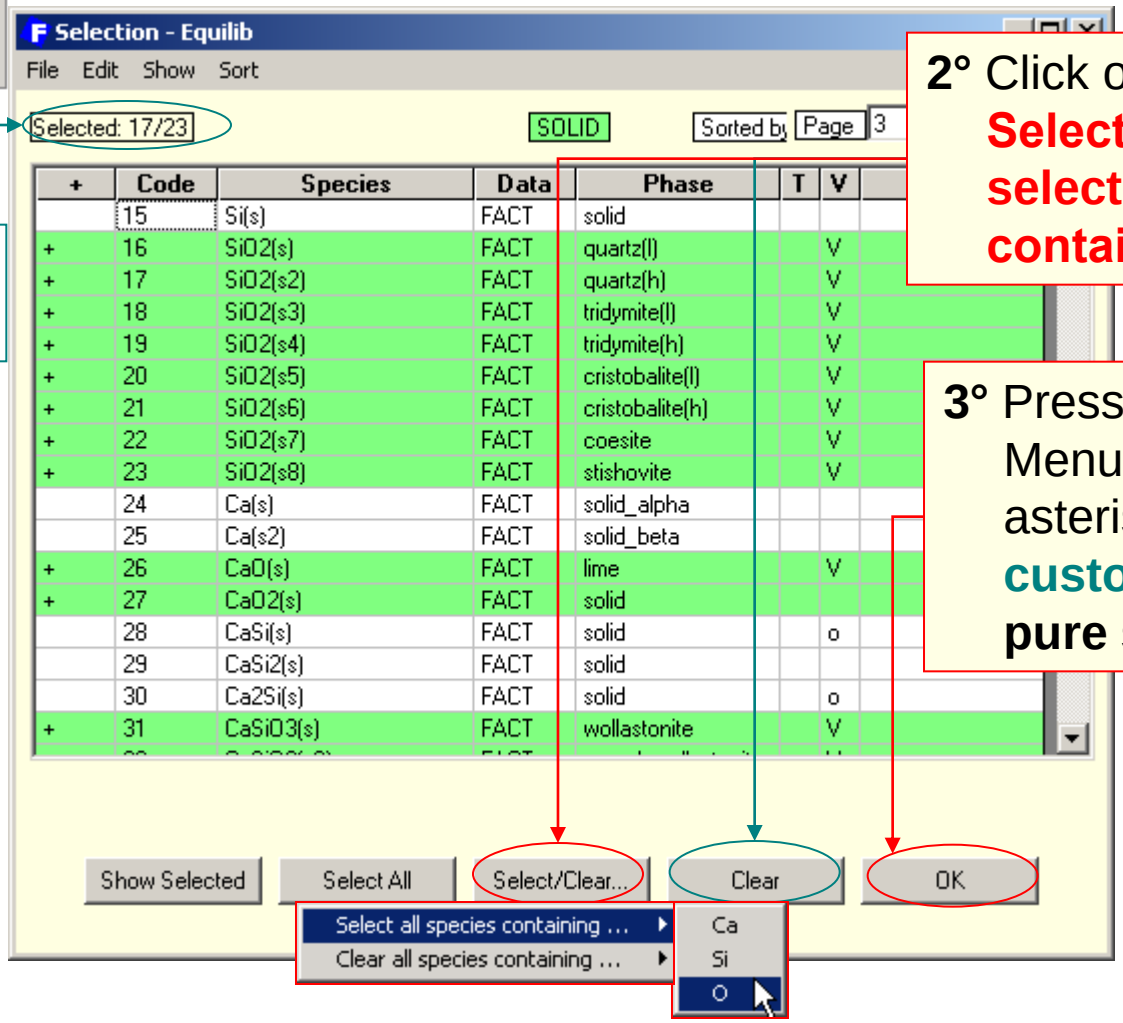

The program will calculate the equilibrium at **1800°C** for mole fractions of $SiO_2$ varying from **0.7** to **1** in increments of **0.05** and will search for all phase **transitions**.

# Step 2°: Products Selection – compound species




**1°** In the **Menu-Equilib** window **Compound species** frame, **right-click** on the **pure solids checkbox** to open the Species selection window.

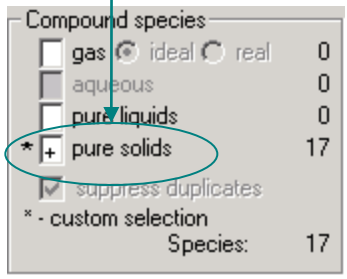
**17** pure solid oxides




| + | Code | Species | Data | Phase | T | V |
|---|---|---|---|---|---|---|
| | 15 | Si(s) | FACT | solid | | |
| + | 16 | SiO2(s) | FACT | quartz(l) | | V |
| + | 17 | SiO2(s2) | FACT | quartz(h) | | V |
| + | 18 | SiO2(s3) | FACT | tridymite(l) | | V |
| + | 19 | SiO2(s4) | FACT | tridymite(h) | | V |
| + | 20 | SiO2(s5) | FACT | cristobalite(l) | | V |
| + | 21 | SiO2(s6) | FACT | cristobalite(h) | | V |
| + | 22 | SiO2(s7) | FACT | coesite | | V |
| + | 23 | SiO2(s8) | FACT | stishovite | | V |
| | 24 | Ca(s) | FACT | solid_alpha | | |
| | 25 | Ca(s2) | FACT | solid_beta | | |
| + | 26 | CaO(s) | FACT | lime | | V |
| + | 27 | CaO2(s) | FACT | solid | | |
| | 28 | CaSi(s) | FACT | solid | | o |
| | 29 | CaSi2(s) | FACT | solid | | |
| | 30 | Ca2Si(s) | FACT | solid | | o |
| + | 31 | CaSiO3(s) | FACT | wollastonite | | V |

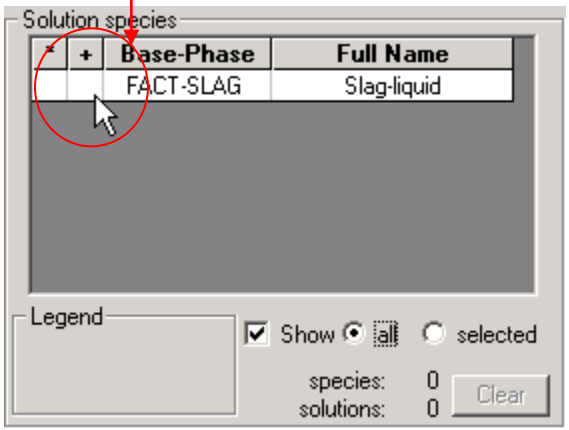
**2°** Click on **Clear**, then on **Select/Clear…** and then **select all (solid) species containing… O**xygen.

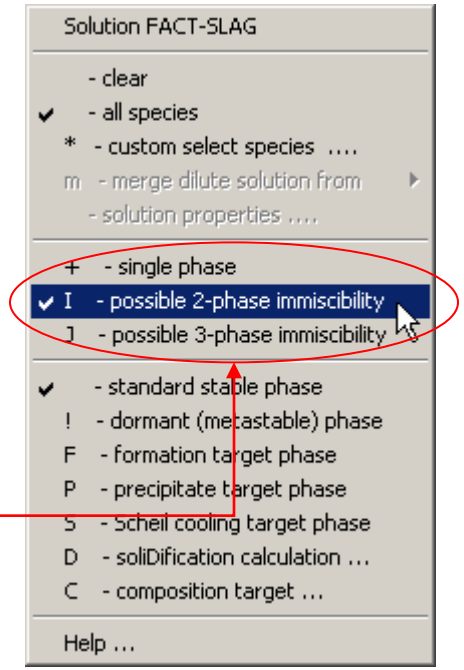
**3°** Press **OK** to return to the Menu-Equilib window. An asterisk (*) indicates **custom selection** for the **pure solids**.



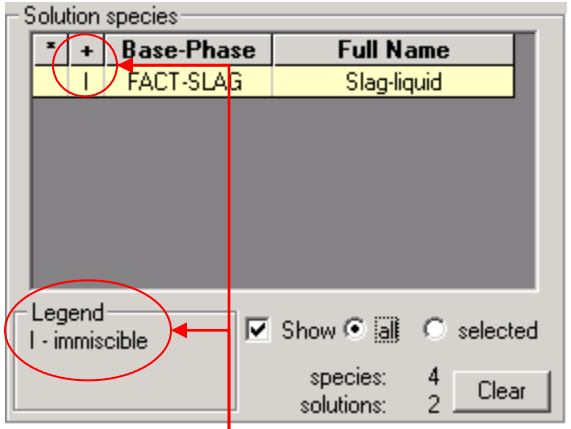
# Step 2°: Products Selection – solution species

**1°** In the **Menu-Equilib** window **Solution species** frame, **right-click** on the **+ column** to open the FACT-SLAG **extended menu**.




**2°** In the FACT-SLAG **extended menu**, **select** option **I**.




**3°** The **I** indicates a possible **2-phase immiscible** region.

- **[ I ] - 2-phase Immiscibility:** the solution phase may be immiscible. Use this option for FACT-SLAG when **$SiO_2$ > 50%** . If the phase is not immiscible the results of the calculation will be OK - the phase will appear twice with the same composition.
  **Note:** This option tends to slow down the speed of the calculation - you may wish to try **I!** (**immiscible** and **dormant**) to check if the phase is stable.

# **Compositions** at the two ends of the 1800°C tie-line

2-phase **transitions** – the **ends** of the **1800°C** tie-line.

F Results - Equilib A=0.7783 (page 3/9)

Output Edit Show Pages

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

A=0.7 | A=0.75 | - A=0.7783 - | A=0.8 | A=0.85 | A=0.9 | A=0.95 | A=0.9707 | A=1

```
<1-A> CaO + <A> SiO2 =

1.0000      mol    Slag-liquid#1
(59.196 gram, 1.0000 mol)
        (1800.00 C, 1 atm,      a=1.0000)
        ( 0.77829          SiO2
        + 0.22171          CaO)

+ 0.00000     mol    Slag-liquid#2
        (1800.00 C, 1 atm,      a=1.0000)
        ( 0.97074          SiO2
        + 2.9256E-02       CaO)

+ 0.00000     mol    SiO2_cristobalite(h)
        (1800.00 C, 1 atm, S6, a=0.95949)
```

F Results - Equilib A=0.9707 (page 8/9)

Output Edit Show Pages

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

A=0.7 | A=0.75 | A=0.7783 | A=0.8 | A=0.85 | A=0.9 | A=0.95 | - A=0.9707 - | A=1

```
<1-A> CaO + <A> SiO2 =

1.0000      mol    Slag-liquid#1
(59.967 gram, 1.0000 mol)
        (1800.00 C, 1 atm,      a=1.0000)
        ( 0.97074          SiO2
        + 2.9256E-02       CaO)

+ 0.00000     mol    Slag-liquid#2
        (1800.00 C, 1 atm,      a=1.0000)
        ( 0.77829          SiO2
        + 0.22171          CaO)

+ 0.00000     mol    SiO2_cristobalite(h)
        (1800.00 C, 1 atm, S6, a=0.95949)
```

i.e. ***Equilib*** reports two-phase stability within the composition range:

**$0.77829 < X_{SiO_2} < 0.97074$**

and one-phase stability outside this range.

# One-phase and two-phase stability at 1800°C

Results - Equilib A=0.85 (page 5/9)

Output Edit Show Pages

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

A=0.7 | A=0.75 | A=0.7783 | A=0.8 | - A=0.85 - | A=0.9 | A=0.95 | A=0.9707 | A=1

```
<1-A> CaO +  <A> SiO2 =

0.62739    mol   Slag-liquid#1
(37.139 gram, 0.62739 mol)
        (1800.00 C, 1 atm,      a=1.0000)
        ( 0.77829          SiO2
        + 0.22171          CaO)

+ 0.37261    mol   Slag-liquid#2
(22.344 gram, 0.37261 mol)
        (1800.00 C, 1 atm,      a=1.0000)
        ( 0.97074          SiO2
        + 2.9256E-02       CaO)

+ 0.00000    mol   SiO2_cristobalite(h)
        (1800.00 C, 1 atm, S6, a=0.95949)
```

Example of **two-phase** stability at $X_{SiO_2}$ = 0.85

Results - Equilib A=0.75 (page 2/9)

Output Edit Show Pages

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

A=0.7 | - A=0.75 - | A=0.7783 | A=0.8 | A=0.85 | A=0.9 | A=0.95 | A=0.9707 | A=1

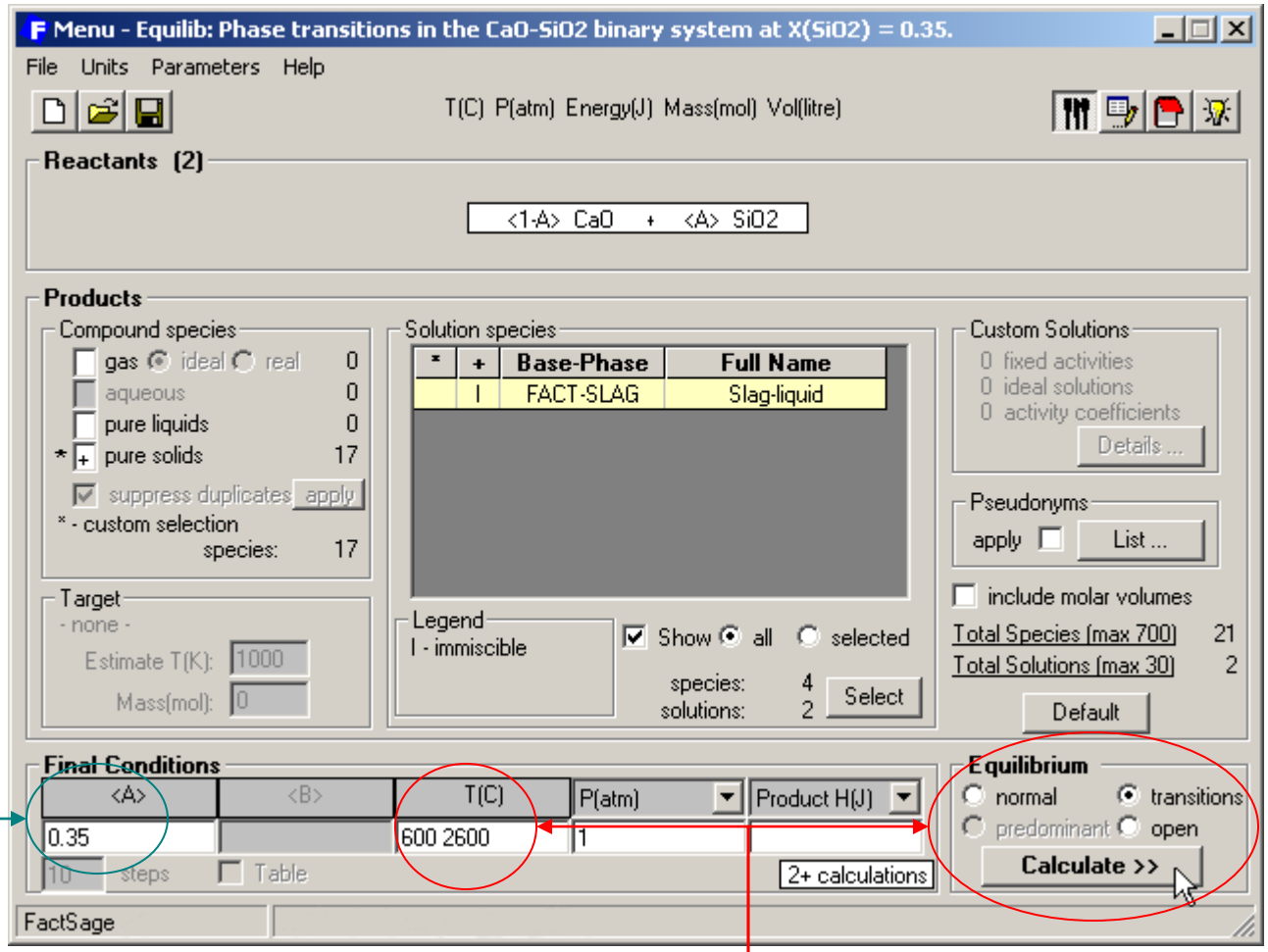
```
<1-A> CaO +  <A> SiO2 =

1.0000     mol   Slag-liquid#1
(59.083 gram, 1.0000 mol)
        (1800.00 C, 1 atm,      a=1.0000)
        ( 0.75000          SiO2
        + 0.25000          CaO)

+ 0.00000    mol   Slag-liquid#2
        (1800.00 C, 1 atm,      a=0.98105)
        ( 0.95531          SiO2
        + 4.4688E-02       CaO)

+ 0.00000    mol   SiO2_cristobalite(h)
        (1800.00 C, 1 atm, S6, a=0.93075)
```

Example of **one-phase** stability at $X_{SiO_2}$ = 0.75

**Slag-liquid#2** is close to forming – its activity is **0.98105**.

In such systems, if option «**I**» is not selected, the results may be in error even when the second liquid (Slag-liquid#2) is not stable (as in the above example).

# Constant composition in the $CaO-SiO_2$ binary system




$X_{SiO_2} = 0.35$

The program will calculate all phase transitions at $X_{SiO_2} = 0.35$ in the temperature range **600** to **2600°C**.

# Transition Temperatures for $X_{SiO_2}$ = 0.35 in $CaO\text{-}SiO_2$

In the **Results** Window, ***Equilib*** reports all phase transitions at **<A> = 0.35** within the temperature range 600 to 2600°C. **Most transitions report both compositions on each side of the tie-line.** Such information is important in complex systems.

**Transitions** at: **847.2°C**, **1436.85°C**, **1464.19°C**, **2085.37°C**.

Results - Equilib 1436.85 C (page 4/9)

Output Edit Show Pages

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

600 C | 847.19 C | 847.2 C | - 1436.85 C - | 1436.85 C | 1464.19 C | 1464.19 C | 2085.37 C | 2600 C

```
 <1-A> CaO +  <A> SiO2 =

  0.00000    mol   Slag-liquid#1
          (1436.85 C, 1 atm,     a=0.97437)
          ( 0.40247          SiO2
          + 0.59753          CaO)

+ 0.00000    mol   Slag-liquid#2
          (1436.85 C, 1 atm,     a=0.97437)
          ( 0.40247          SiO2
          + 0.59753          CaO)

+ 0.25000    mol   Ca2SiO4_alpha-prime
  (43.060 gram, 0.25000 mol)
          (1436.85 C, 1 atm, S2, a=1.0000)

+ 5.0000E-02 mol   Ca3Si2O7_rankinite
  (14.420 gram, 5.0000E-02 mol)
          (1436.85 C, 1 atm, S1, a=1.0000)

+ 0.00000    mol   Ca2SiO4_alpha
          (1436.85 C, 1 atm, S3, a=1.0000)

+ 0.00000    mol   CaSiO3_pseudowollastonite
          (1436.85 C, 1 atm, S2, a=0.88453)

where "A" on the reactant side is 0.35000

The cutoff concentration has been specified to 1.0000E-75

Data on 4 product species identified with "T" have been extrapolated

*****************************************************************
      H            G            V            S            Cp
     (J)          (J)        (litre)      (J/K)        (J/K)
*****************************************************************
-6.86837E+05 -9.30583E+05  0.00000E+00  1.42541E+02  6.76591E+01
```

**<A> = $X_{SiO_2}$ = 0.35**

Results - Equilib 1436.85 C (page 5/9)

Output Edit Show Pages

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

600 C | 847.19 C | 847.2 C | 1436.85 C | - 1436.85 C - | 1464.19 C | 1464.19 C | 2085.37 C | 2600 C

```
 <1-A> CaO +  <A> SiO2 =

  0.00000    mol   Slag-liquid#1
          (1436.85 C, 1 atm,     a=0.97437)
          ( 0.40247          SiO2
          + 0.59753          CaO)

+ 0.00000    mol   Slag-liquid#2
          (1436.85 C, 1 atm,     a=0.97437)
          ( 0.40247          SiO2
          + 0.59753          CaO)

+ 0.25000    mol   Ca2SiO4_alpha
  (43.060 gram, 0.25000 mol)
          (1436.85 C, 1 atm, S3, a=1.0000)

+ 5.0000E-02 mol   Ca3Si2O7_rankinite
  (14.420 gram, 5.0000E-02 mol)
          (1436.85 C, 1 atm, S1, a=1.0000)

+ 0.00000    mol   Ca2SiO4_alpha-prime
          (1436.85 C, 1 atm, S2, a=1.0000)

+ 0.00000    mol   CaSiO3_pseudowollastonite
          (1436.85 C, 1 atm, S2, a=0.88453)

where "A" on the reactant side is 0.35000

The cutoff concentration has been specified to 1.0000E-75

Data on 4 product species identified with "T" have been extrapolated

*****************************************************************
      H            G            V            S            Cp
     (J)          (J)        (litre)      (J/K)        (J/K)
*****************************************************************
-6.83963E+05 -9.30583E+05  0.00000E+00  1.44222E+02  6.43721E+01
```

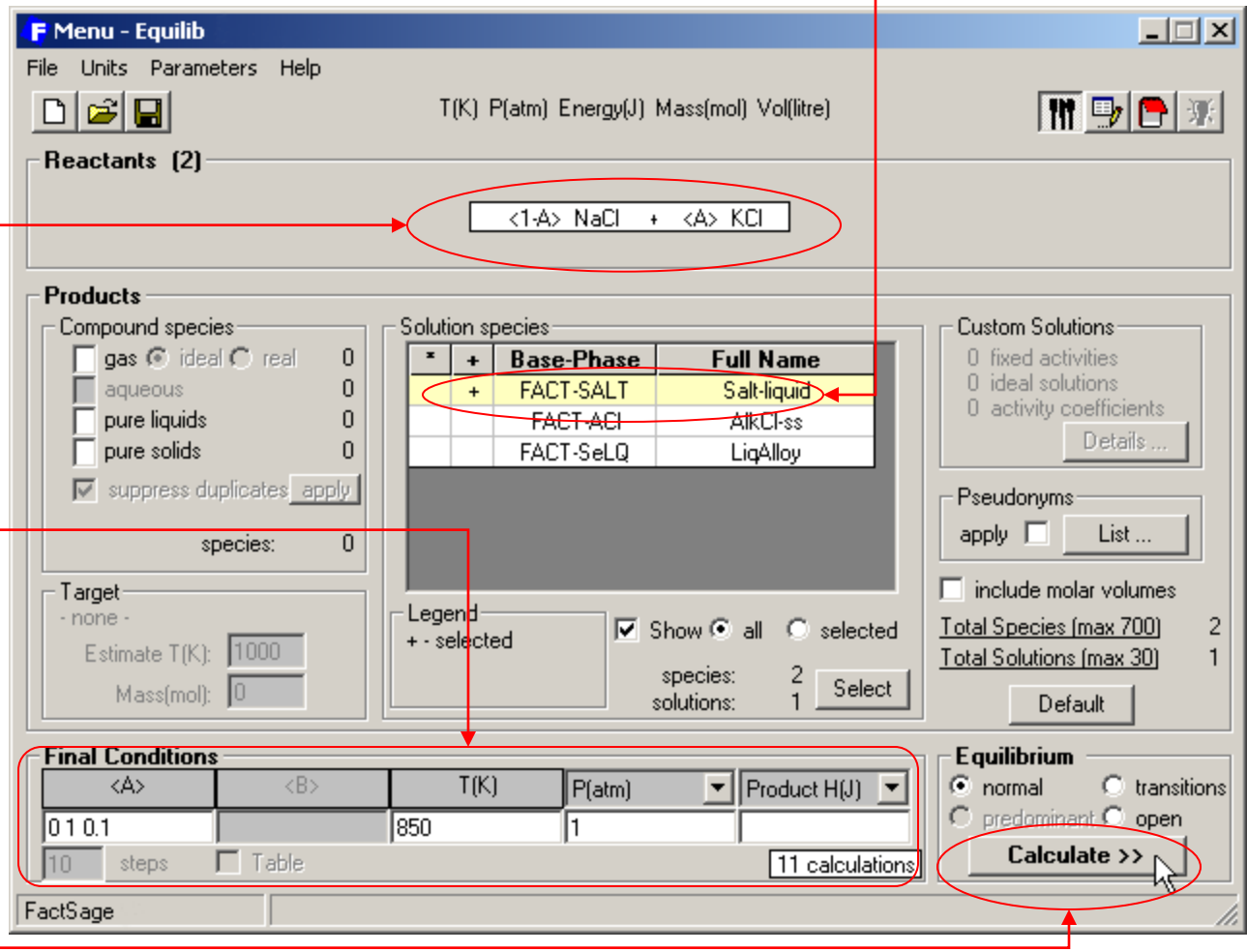
For example at **1436.85°C**:
**α'**-$Ca_2SiO_4$ to **α**-$Ca_2SiO_4$

# Solution Properties: FACT-Salt in the NaCl-KCl binary system

**1°** The reactants are <1-A> NaCl + <A> KCl – i.e. the NaCl-KCl binary system where <A> varies from 0 to 1.

**2°** The only possible product is the solution phase:

- Salt-liquid (**FACT-SALT**)



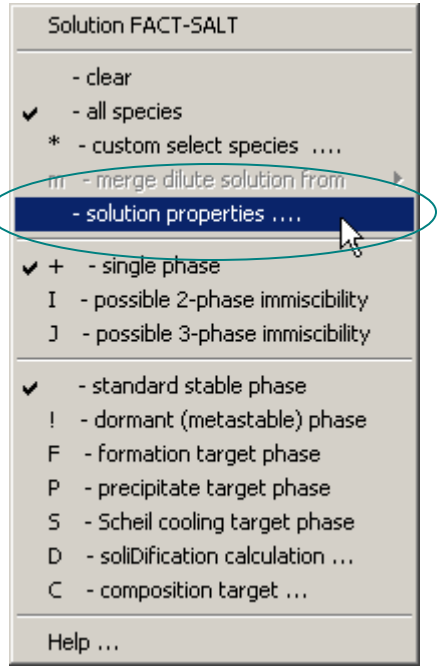

**3°** The final conditions

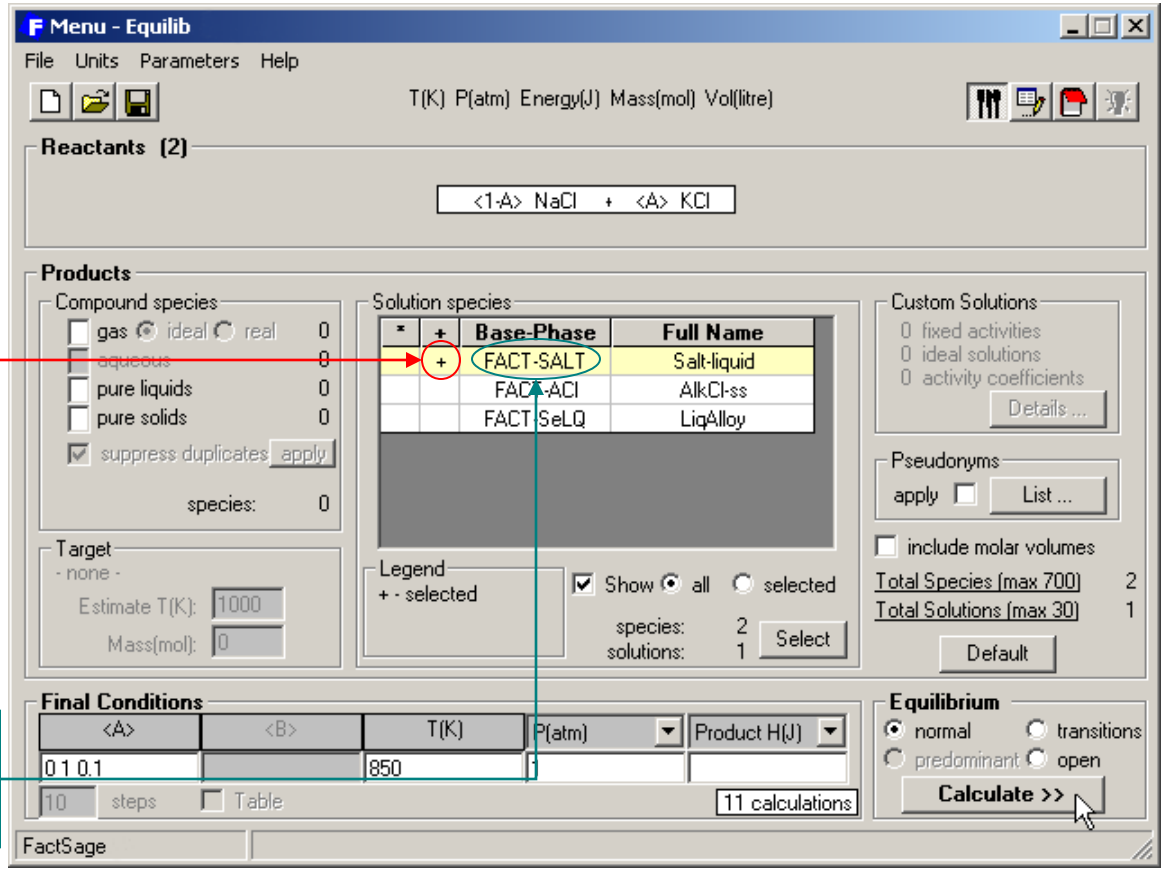
The program calculate the equilibrium in Salt-liquid at **850°C** for mole fractions of KCl varying from **0** to **1** in increments of **0.1**.

**4°** Calculate

# Solution Properties: opening the window

**1°** **Right-click** on the + column to open the **FACT-Salt** extended menu and **select** **solution properties…**




**1a°** …or point to FACT-SALT and **double-click**

This option lists the common partial and integral solution properties for the phase. The option is **only active** if the equilibrium has been calculated and the solution phase is stable.

# Solution Properties Window and menus

Open spreadsheet to view the selected **partial properties** of the selected phase: **FACT-SALT**

Output
- Open Spreadsheet
- Save Excel Spreadsheet ...
- Save Text Spreadsheet ...

Standard States
- Current Standard States ▸ NaCl, KCl
- Change Standard States ...

Species
- Select all
- Clear
- ✔ 19 NaCl
- ✔ 20 KCl

F Molar Partial Propeties FACT-SALT - Salt-liquid

Output | Species | Standard States

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

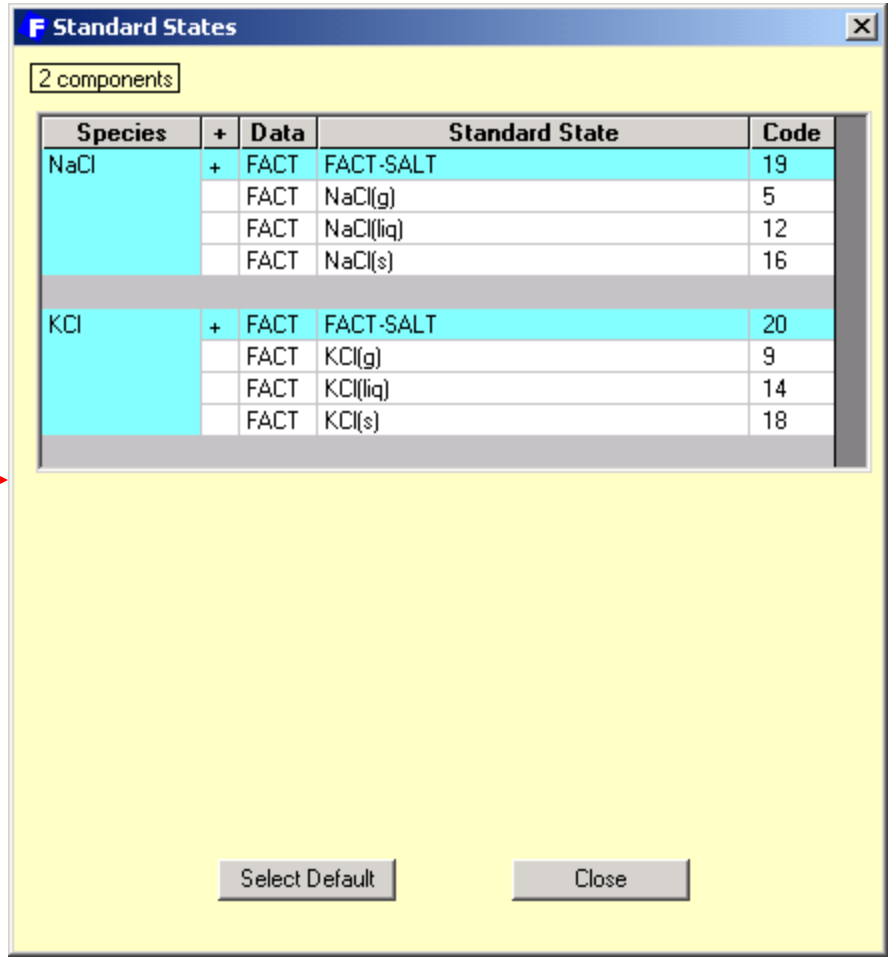
2/2 species | partial properties | integral properties | 17/17 properties

| + | Property | Description of Partial Property |
|---|---|---|
| + | a(i) | activity of species i |
| + | gamma(i) | activity coefficient of species i = a(i)/a_ideal(i) |
| + | Delta_g(i) | = g(i) - go(i) = RT ln a(i) |
| + | Delta_h(i) | = h(i) - ho(i) = h(excess)(i) |
| + | Delta_s(i) | = s(i) - so(i) |
| + | g(i) | = h(i) - T.s(i) |
| + | h(i) | absolute h of species i with respect to elements at 25 C |
| + | s(i) | absolute s of species i |
| + | go(i) | g of species i in standard state |
| + | ho(i) | h of species i in standard state |
| + | so(i) | s of species i in standard state |
| + | a_ideal(i) | ideal activity of species i = mole fraction X(i) |
| + | Delta_g_ideal(i) | = RT ln a_ideal(i) |
| + | Delta_s_ideal(i) | = -R ln a_ideal(i) |
| + | g_excess(i) | = Delta_g(i) - Delta_g_ideal(i) |
| + | s_excess(i) | = Delta_s(i) - Delta_s_ideal(i) |
| + | cp(i) | heat capacity of species i = d(h(i))/dT |

Select All | Clear | Close

# Solution Properties: Changing Standard States

In the **solution properties** window menu, **select Standard States > Change Standard States…** and **click** in the **+** column to **select** the new standard state.




| Species | + | Data | Standard State | Code |
|---|---|---|---|---|
| NaCl | + | FACT | FACT-SALT | 19 |
| | | FACT | NaCl(g) | 5 |
| | | FACT | NaCl(liq) | 12 |
| | | FACT | NaCl(s) | 16 |
| KCl | + | FACT | FACT-SALT | 20 |
| | | FACT | KCl(g) | 9 |
| | | FACT | KCl(liq) | 14 |
| | | FACT | KCl(s) | 18 |

# Solution Properties: Molar Partial Properties Spreadsheet

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

File
- Save As ▸
  - Text Spreadsheet ...
  - Excel Spreedsheet ...
- Print
- Print Setup ...
- Print Font ...
- Close

F Molar Partial Propeties FACT-SALT - Salt-liquid - Energy(J), (mol)

File Edit Swap rows and columns

| Component i | Page | <Alpha> | T(C) | P(atm) | X(NaCl) | X(KCl) | a(i) | gamma(i) | Delta_g(i) |
|---|---|---|---|---|---|---|---|---|---|
| NaCl_SALT | 1 | 0 | 850 | 1 | 1.0000 | 0.00000 | 1.0000 | 1.0000 | 0.00000 |
| | 2 | 0.1 | 850 | 1 | 0.90000 | 0.10000 | 0.89757 | 0.99730 | -1009.1 |
| | 3 | 0.2 | 850 | 1 | 0.80000 | 0.20000 | 0.79165 | 0.98956 | -2181.8 |
| | 4 | 0.3 | 850 | 1 | 0.70000 | 0.30000 | 0.68413 | 0.97733 | -3545.0 |
| | 5 | 0.4 | 850 | 1 | 0.60000 | 0.40000 | 0.57666 | 0.96110 | -5140.8 |
| | 6 | 0.5 | 850 | 1 | 0.50000 | 0.50000 | 0.47067 | 0.94133 | -7037.5 |
| | 7 | 0.6 | 850 | 1 | 0.40000 | 0.60000 | 0.36736 | 0.91839 | -9351.7 |
| | 8 | 0.7 | 850 | 1 | 0.30000 | 0.70000 | 0.26777 | 0.89257 | -12305. |
| | 9 | 0.8 | 850 | 1 | 0.20000 | 0.80000 | 0.17282 | 0.86408 | -16394. |
| | 10 | 0.9 | 850 | 1 | 0.10000 | 0.90000 | 8.33104E-02 | 0.83310 | -23208. |
| | 11 | 1 | 850 | 1 | 0.00000 | 1.0000 | 1.00000E-75 | <-not-calctd.-> | <-not-calctd.-> |
| Component i | Page | <Alpha> | T(C) | P(atm) | X(NaCl) | X(KCl) | a(i) | gamma(i) | Delta_g(i) |
| KCl_SALT | 1 | 0 | 850 | 1 | 1.0000 | 0.00000 | 1.00000E-75 | <-not-calctd.-> | <-not-calctd.-> |
| | 2 | 0.1 | 850 | 1 | 0.90000 | 0.10000 | 8.24309E-02 | 0.82431 | -23307. |
| | 3 | 0.2 | 850 | 1 | 0.80000 | 0.20000 | 0.17232 | 0.86162 | -16421. |
| | 4 | 0.3 | 850 | 1 | 0.70000 | 0.30000 | 0.26834 | 0.89445 | -12285. |
| | 5 | 0.4 | 850 | 1 | 0.60000 | 0.40000 | 0.36910 | 0.92274 | -9307.6 |
| | 6 | 0.5 | 850 | 1 | 0.50000 | 0.50000 | 0.47325 | 0.94651 | -6986.3 |
| | 7 | 0.6 | 850 | 1 | 0.40000 | 0.60000 | 0.57949 | 0.96582 | -5095.1 |
| | 8 | 0.7 | 850 | 1 | 0.30000 | 0.70000 | 0.68654 | 0.98078 | -3512.0 |
| | 9 | 0.8 | 850 | 1 | 0.20000 | 0.80000 | 0.79316 | 0.99145 | -2164.0 |
| | 10 | 0.9 | 850 | 1 | 0.10000 | 0.90000 | 0.89807 | 0.99786 | -1004.0 |
| | 11 | 1 | 850 | 1 | 0.00000 | 1.0000 | 1.0000 | 1.0000 | 0.00000 |

# Solution Properties: Molar Integral Properties Spreadsheet

Molar Integral Propeties FACT-SALT - Salt-liquid

Output Species Standard States

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

partial properties integral properties 11/11 properties

| + | Property | Description of Integral Property |
|---|---|---|
| + | g | =X1.g(1) + X2.g(2) + ... |
| + | h | =X1.h(1) + X2.h(2) + ... |
| + | s | =X1.s(1) + X2.s(2) + ... |
| + | Delta_g | =X1.(Delta_g(1)) + X2.(Delta_g(2)) + ... |
| + | Delta_h | =X1.(Delta_h(1)) + X2.(Delta_h(2)) + ... |
| + | Delta_s | =X1.(Delta_s(1)) + X2.(Delta_s(2)) + ... |
| + | g_excess | =X1.(g_excess(1)) + X2.(g_excess(2)) + ... |
| + | s_excess | =X1.(s_excess(1)) + X2.(s_excess(2)) + ... |
| + | Delta_g_ideal | =X1.(Delta_g_ideal(1)) + X2.(Delta_g_ideal(2)) + ... |
| + | Delta_s_ideal | =X1.(Delta_s_ideal(1)) + X2.(Delta_s_ideal(2)) + ... |
| + | cp | =X1.cp(1) + X2.cp(2) + ... |

Select All Clear

Output
Open Spreadsheet
Save Excel Spreadsheet ...
Save Text Spreadsheet ...

**Open spreadsheet** to view the selected **integral properties** of the selected phase: **FACT-SALT**

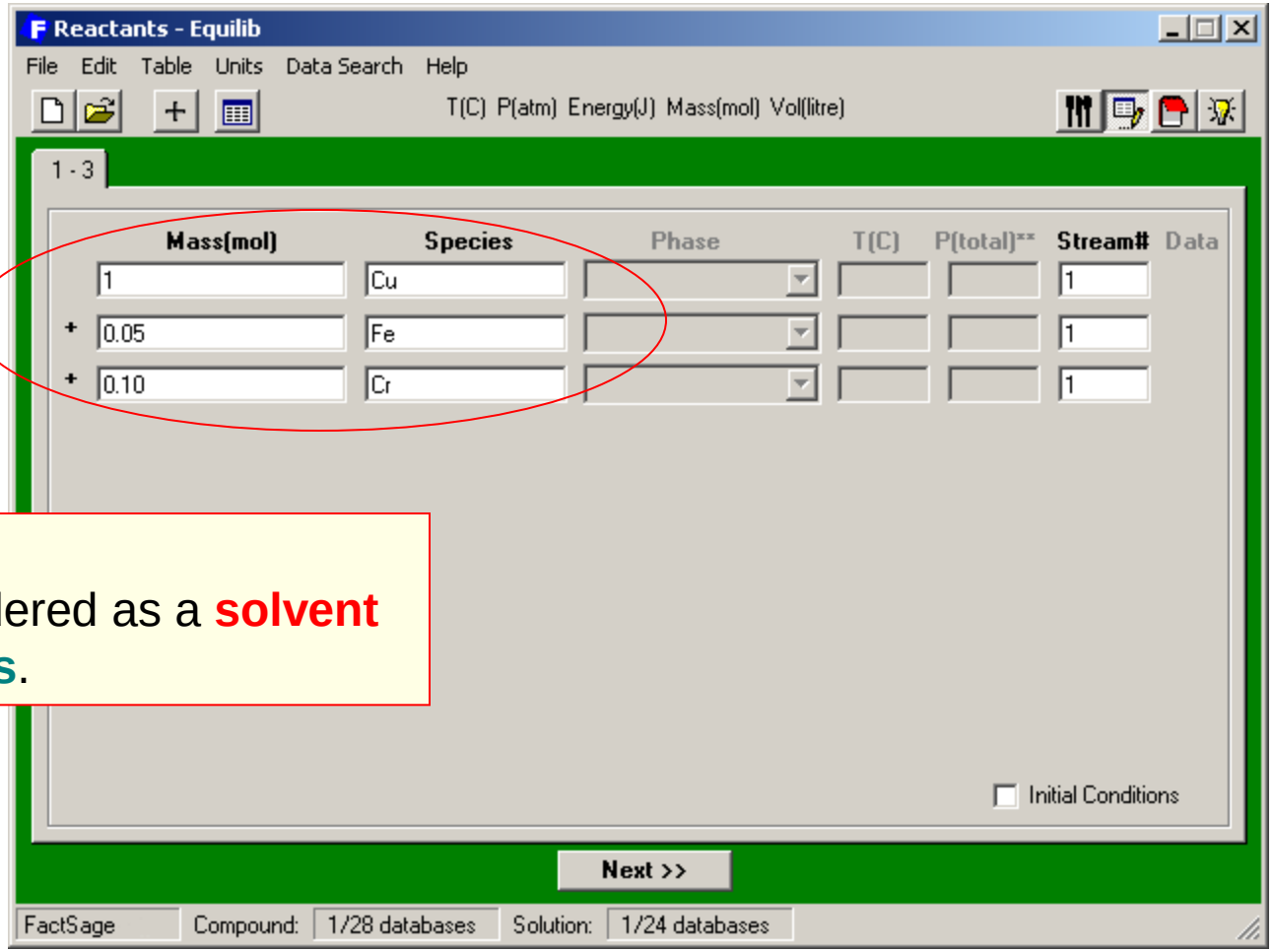
Molar Integral Propeties FACT-SALT - Salt-liquid - Energy(J), (mol)

File Edit Swap rows and columns

| Page | <Alpha> | T(C) | P(atm) | X(NaCl) | X(KCl) | g | h | s | Delta_g | Delta_h |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 850 | 1 | 1.0000 | 0.00000 | -5.29522E+05 | -3.35216E+05 | 173.00 | 0.00000 | -5.10481E-08 |
| 2 | 0.1 | 850 | 1 | 0.90000 | 0.10000 | -5.36600E+05 | -3.38009E+05 | 176.82 | -3238.9 | -203.82 |
| 3 | 0.2 | 850 | 1 | 0.80000 | 0.20000 | -5.42231E+05 | -3.40753E+05 | 179.39 | -5029.5 | -358.69 |
| 4 | 0.3 | 850 | 1 | 0.70000 | 0.30000 | -5.47208E+05 | -3.43450E+05 | 181.42 | -6166.9 | -465.99 |
| 5 | 0.4 | 850 | 1 | 0.60000 | 0.40000 | -5.51688E+05 | -3.46100E+05 | 183.05 | -6807.5 | -527.22 |
| 6 | 0.5 | 850 | 1 | 0.50000 | 0.50000 | -5.55731E+05 | -3.48706E+05 | 184.33 | -7011.9 | -543.84 |
| 7 | 0.6 | 850 | 1 | 0.40000 | 0.60000 | -5.59357E+05 | -3.51268E+05 | 185.27 | -6797.7 | -517.23 |
| 8 | 0.7 | 850 | 1 | 0.30000 | 0.70000 | -5.62548E+05 | -3.53789E+05 | 185.87 | -6149.8 | -448.58 |
| 9 | 0.8 | 850 | 1 | 0.20000 | 0.80000 | -5.65248E+05 | -3.56268E+05 | 186.07 | -5010.0 | -338.93 |
| 10 | 0.9 | 850 | 1 | 0.10000 | 0.90000 | -5.67302E+05 | -3.58708E+05 | 185.72 | -3224.3 | -189.16 |
| 11 | 1 | 850 | 1 | 0.00000 | 1.0000 | -5.67917E+05 | -3.61108E+05 | 184.13 | 0.00000 | -2.72004E-07 |

# Include dilute solution: Cr in Cu-Fe alloy

The **FACT-CuLQ solution** (Cu(liq) alloy) does not contain **Cr**. This example shows **how to create** a **dilute Henrian solution** of **Cr** and then **merge it** into the **FACT-CuLQ solution phase**.




**1 Cu + 0.05 Fe + 0.10 Cr**
that is, **Cu** may be considered as a **solvent** and **Fe** and **Cr** as **solutes**.

# Include dilute solution: Cr in Cu-Fe alloy – Possible products

Solution Phase FACT-CuLQ -
Cu-liq or speiss (presence of Cu not essential).
<50 mol% As, <15 mol% S, 300-1300 C; <10 mol% O (good around 1250 C).

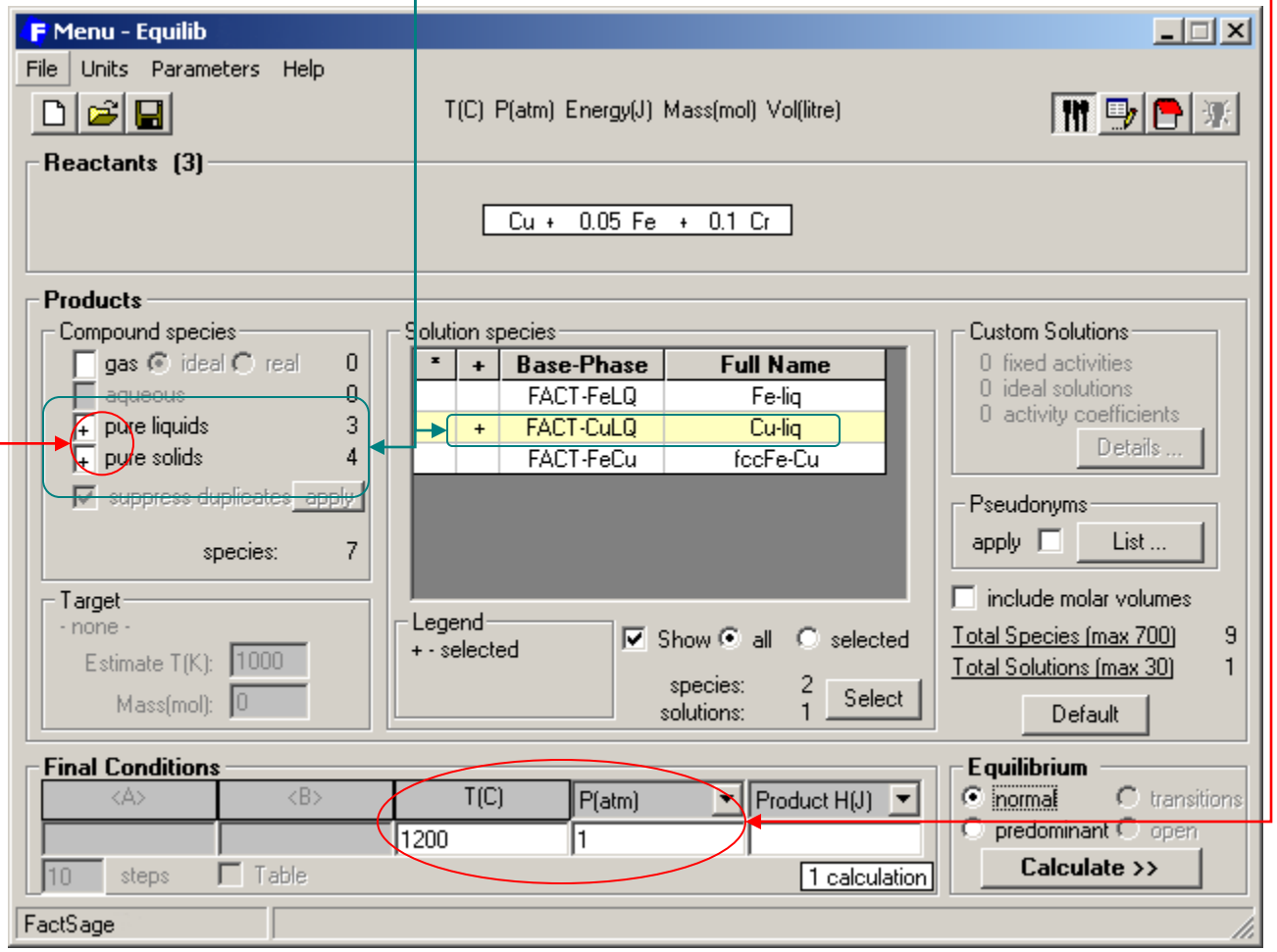
FACT-CuLQ:-
15 Cu, 16 Fe

**Possible products** at **1200°C** and **1 atm**:

- **Compound species: pure liquids, pure solids**
- **Solution species: FACT-CuLQ**

Short description of the **FACT-CuLQ Solution Phase**. It does not contain **Cr**.

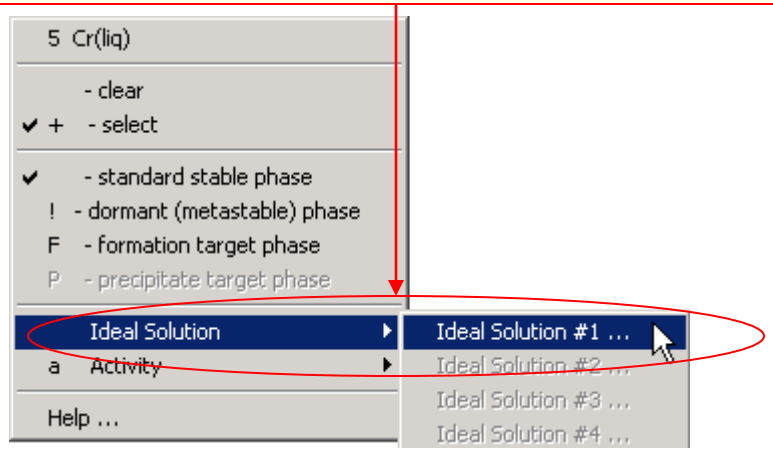
**Right-click** to **open** the **pure liquids Species Window**

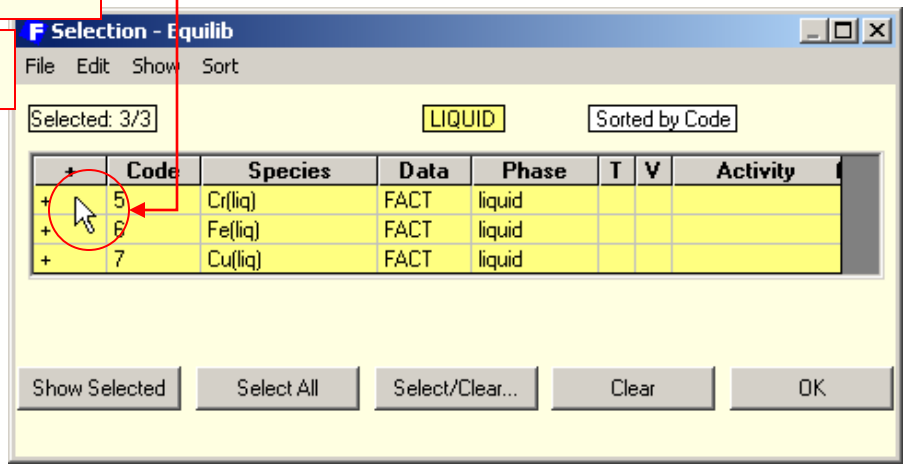


# Creating an ideal Henrian solution of Cr(liq)

1° **Right-click** to open the **Cr(liq)** extended menu

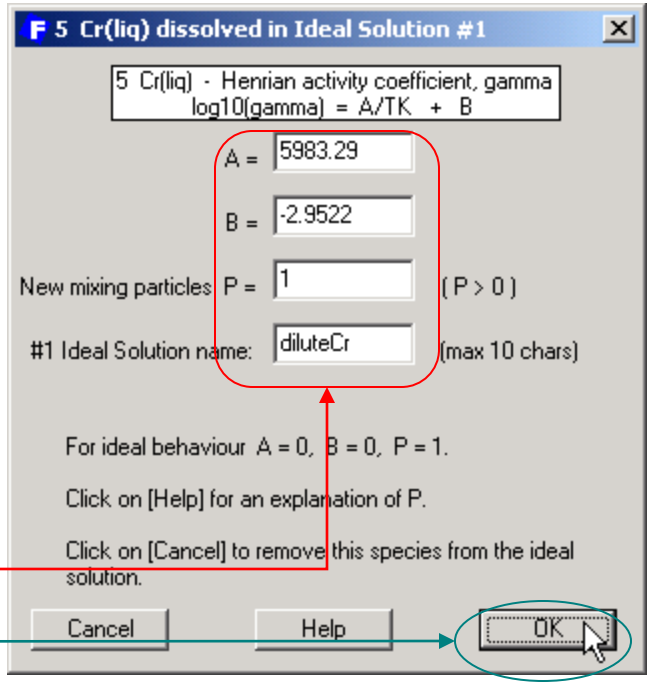
2° **Select** Ideal Solution > Ideal solution #1…




In an earlier example taken from the ***Equilib*** Slide Show – Regular Examples (slide 54), the **Henrian activity coefficient** of Cr(liq) in Cu(liq) was calculated from the binary Cu-Cr phase diagram and reported as:

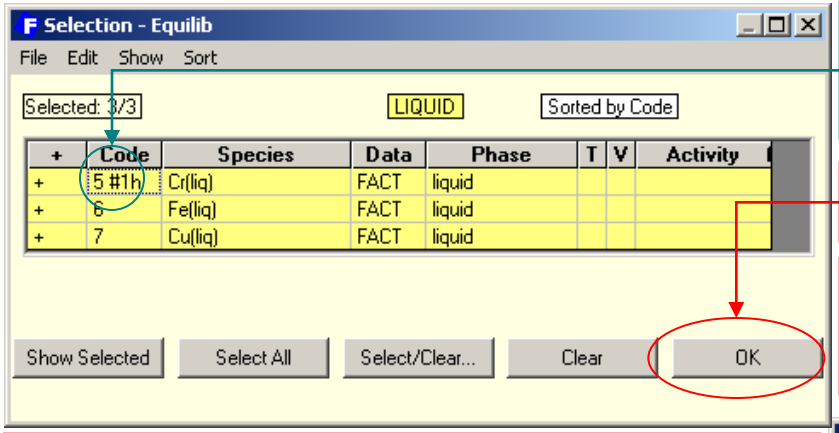
$$\log_{10}[\gamma_{Cr(liq)}] = 5983.29/T(K) - 2.9522 = A/TK + B$$




3° **Enter** the values of **A** and **B**.
**Specify New mixing particles P = 1** (this is the default setting), and **enter** the solution name **diluteCr**.

4° **Press OK**

# Merging the ideal solution diluteCr and FACT-CuLQ

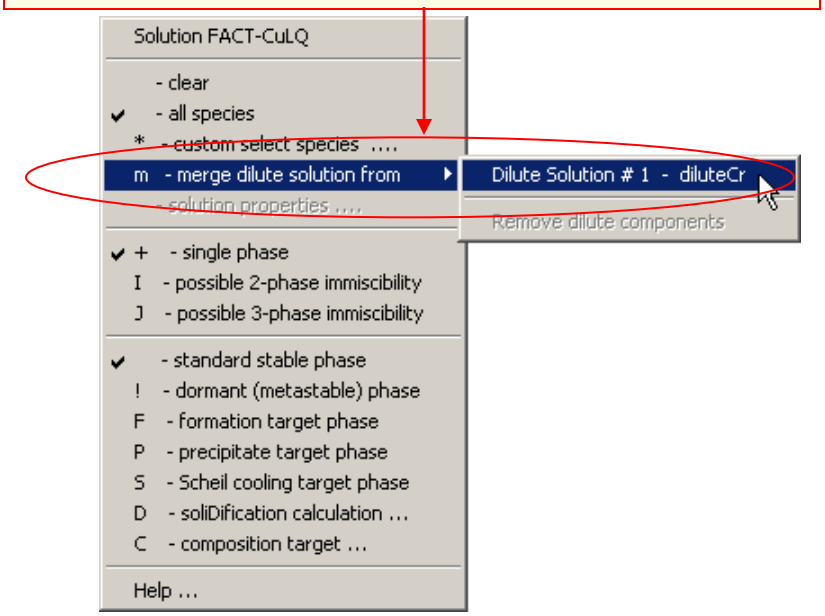


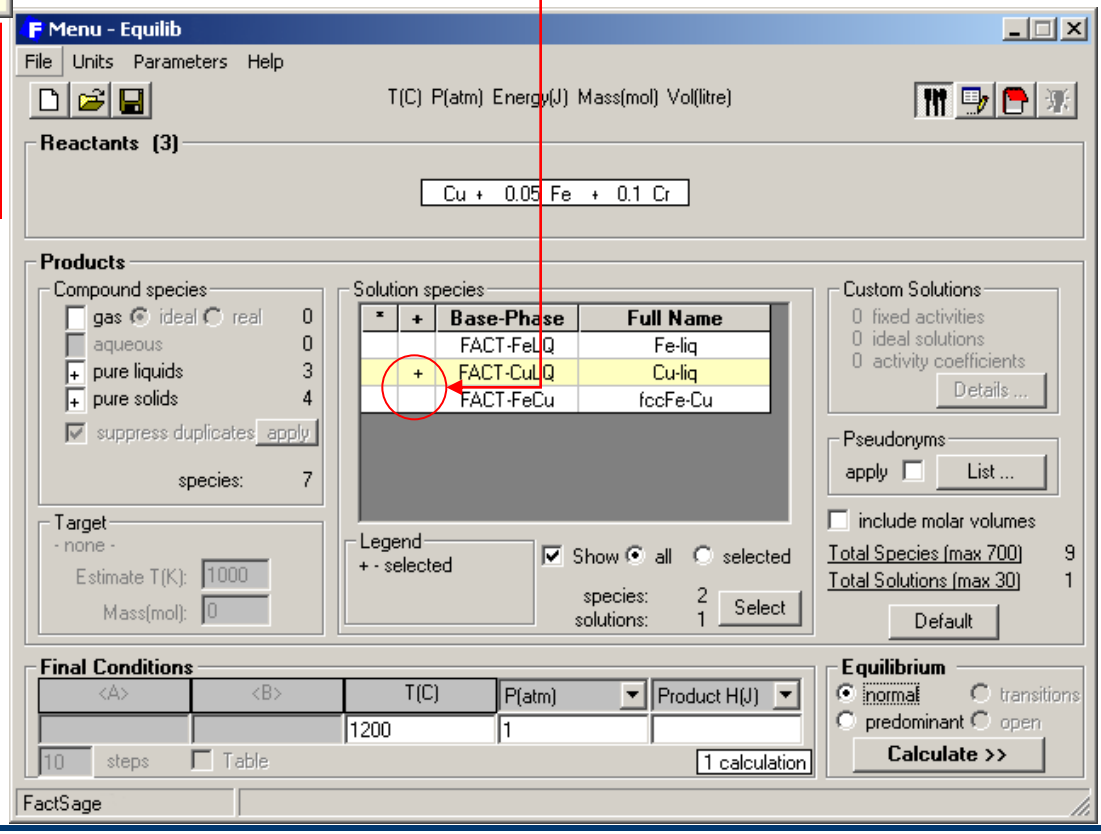

# denotes species also used in ideal solution **1** and **h** indicates an henrian activity coefficient

**5°** **Press OK** to return to the **Menu Window**

**6°** **Right-click** in the **+** column of **FACT-CuLQ** to open its extended menu.

**7° Select**
**m - merge dilute solution from**
**> Dilute Solution #1 - diluteCr**



# Calculation including a **dilute solution**: **Cr** in **Cu-Fe** alloy

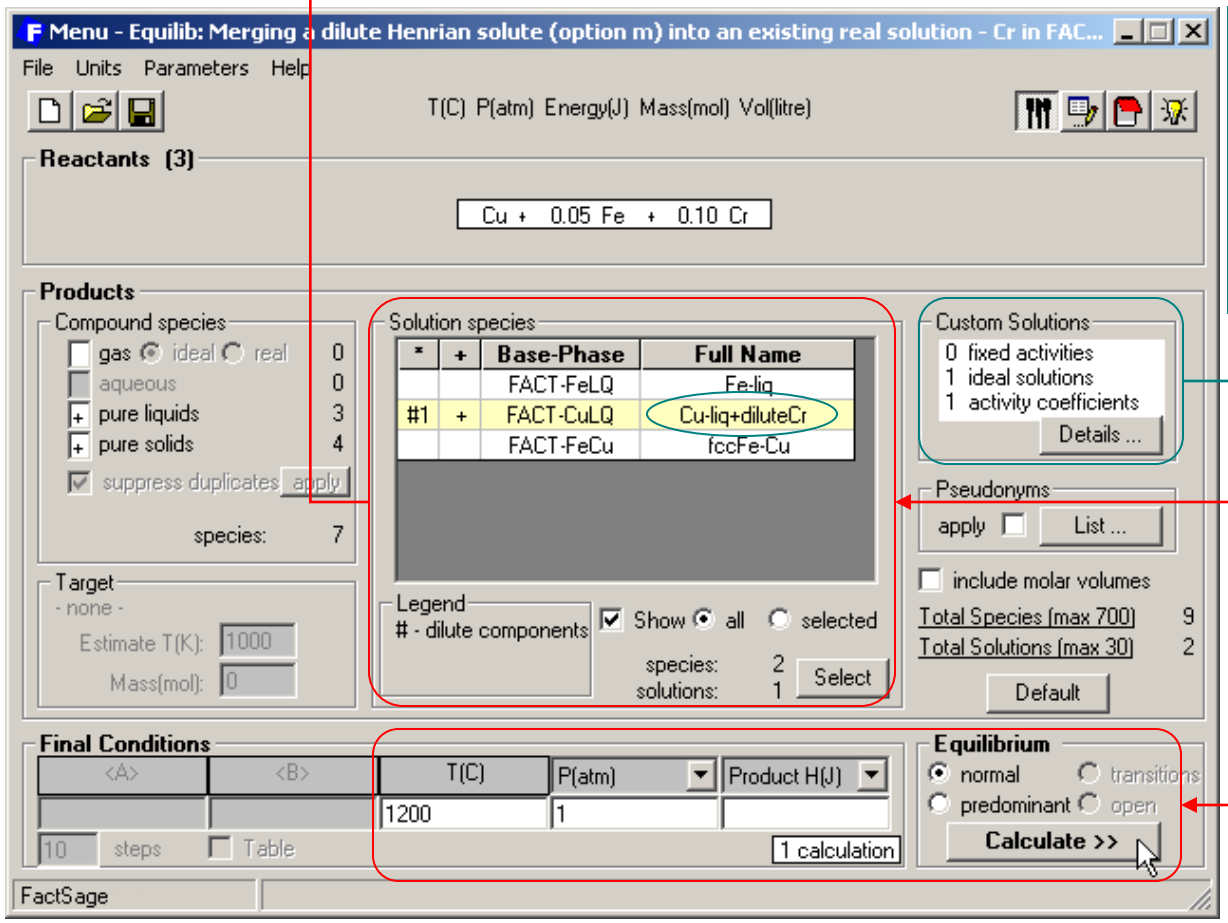
Solution Phase FACT-CuLQ -
Cu-liq or speiss (presence of Cu not essential).
<50 mol% As, <15 mol% S, 300-1300 C; <10 mol% O (good around 1250 C).

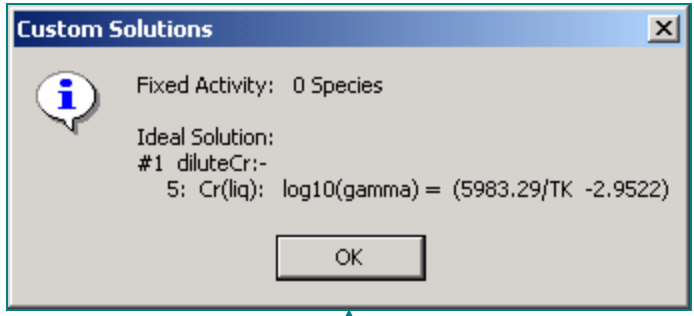
FACT-CuLQ:-
15 Cu, 16 Fe,
+
Ideal Solution #1 - diluteCr:-
5 Cr(liq)

Recalling that the **Henrian activity coefficient** of Cr(liq) in Cu(liq) is:

$\log_{10} [\gamma_{Cr(liq)}] = 5983.29/T(K) - 2.9522$

We have, at **1200°C** (1473.15 K), $\gamma_{Cr(liq)} = 12.86$




The dilute solute (**Cr**) is merged into the existing **FACT-CuLQ** solution.

Lets calculate the equilibrium and retrieve the calculated value of $\gamma_{Cr(liq)}$ at **1200°C**

# Cr in Cu-Fe alloy – Results

Results - Equilib 1200 C

Output Edit Show Page

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

```
 Cu +  0.05 Fe +  0.1 Cr =

  1.0960      mol    Cu-liq+diluteCr
  (68.730 gram, 1.0960 mol)
          (1200.00 C, 1 atm,      a=1.0000)
          ( 0.91242          Cu
          + 4.5621E-02       Fe
          + 4.1963E-02       Cr_liquid_diluteCr

+ 5.4009E-02 mol    Cr_solid
  (2.8083 gram, 5.4009E-02 mol)
          (1200.00 C, 1 atm, S1, a=1.0000)

+ 0.00000     mol    Cu_liquid
          (1200.00 C, 1 atm, L1, a=0.92180)

+ 0.00000     mol    Cu_solid
          (1200.00 C, 1 atm, S1, a=0.84209)

+ 0.00000     mol    Fe_fcc
          (1200.00 C, 1 atm, S2, a=0.75533)

+ 0.00000     mol    Fe_bcc
          (1200.00 C, 1 atm, S1, a=0.75115)

+ 0.00000     mol    Fe_liquid
          (1200.00 C, 1 atm, L1, a=0.61312)

+ 0.00000     mol    Cr_liquid
          (1200.00 C, 1 atm, L1, a=0.53979)

The cutoff concentration has been specified to 1.0000E-75

Data on 1 product species identified with "#" have been calculated with a
user-supplied activity-coefficient expression

*****************************************************************
      H            G            V            S            Cp
     (J)          (J)        (litre)      (J/K)        (J/K)
*****************************************************************
 6.13277E+04 -9.28131E+04  0.00000E+00  1.04633E+02  8.89343E+01
```

**T = 1200°C**

**$X_{Cr(liq)}$ = 0.041963**

**$a_{Cr(liq)}$ = 0.53979**

Hence, at 1200°C, the calculated activity coefficient is:

$$\gamma_{Cr(liq)} = \frac{a_{Cr(liq)}}{X_{Cr(liq)}} = \frac{0.53979}{0.041963} = 12.86$$

With the **m** option you can **merge** almost any type of dilute solute into an existing real solution.

# Include dilute solution: $Tl_2O$ and $HfO_2$ in FACT-Slag

The **FACT-SLAG** (Slag-liquid) solution does not contain the components **$Tl_2O$** and **$HfO_2$**. This example shows how to merge **$Tl_2O$** and **$HfO_2$** solutes into a **FACT-SLAG** containing $SiO_2$-CaO-$Al_2O_3$ taking into account the **«New mixing particles»** since **$HfO_2$** dissolves as **$Hf^{4+}$** and **2 $O^{2-}$**, and **$Tl_2O$** dissolves as **2 $Tl^{+}$** and **$O^{2-}$**.

We wish to create a liquid slag solution which is an equimolar mixture of $SiO_2$-CaO-$Al_2O_3$ containing small amounts of **$Tl_2O$** and **$HfO_2$**.

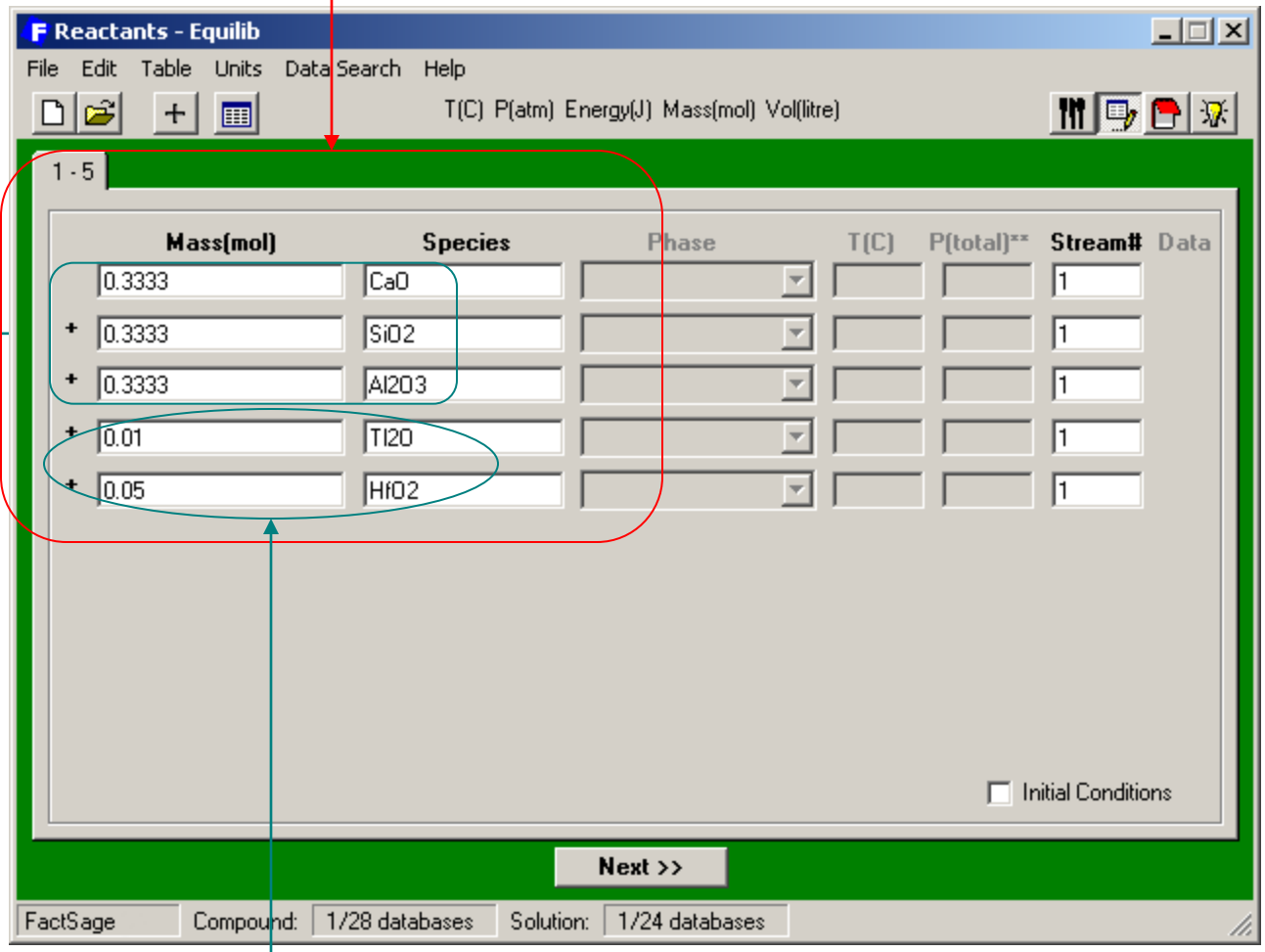
It is assumed that the activity coefficients (defined as $\gamma = a/X$ where a = activity and X = mole fraction) of the **dilute** constituents are independent of composition. That is, the dilute components obey **Henry's Law**. Also, for demonstration purposes let us assume that the activity coefficient of **$HfO_2$** at 1000°C in the equimolar mixture is approximately: $\gamma_{HfO_2}$ **= 9.0** with respect to its pure solid standard state.

Finally, suppose that there is no information on the activity coefficient of **$Tl_2O$** and so ideal solution behavior (**$\gamma = 1$**) is assumed for this component. In this case it is necessary to take into account the fact that a liquid slag is an ionic mixture and that **$Tl_2O$** dissociates in solution to form **two** independent **Tl** ions. That is, the formula «**$Tl_2O$**» really represents **two** moles of **Tl** ions dissolved in the slag. That is, it is actually the component **$TlO_{0.5}$** which follows **ideal solution behaviour**.

# $Tl_2O$ and $HfO_2$ in FACT-Slag – *Reactants*

The reactants are: 0.3333 CaO + 0.3333 $SiO_2$ + 0.3333 $Al_2O_3$ + 0.01 $Tl_2O$ + 0.05 $HfO_2$

The system is an equimolar mixture of CaO, $SiO_2$ and $Al_2O_3$…




…with $Tl_2O$ and $HfO_2$ added as **dilute components**.

# $Tl_2O$ and $HfO_2$ in FACT-Slag – Possible products

Solution Phase FACT-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

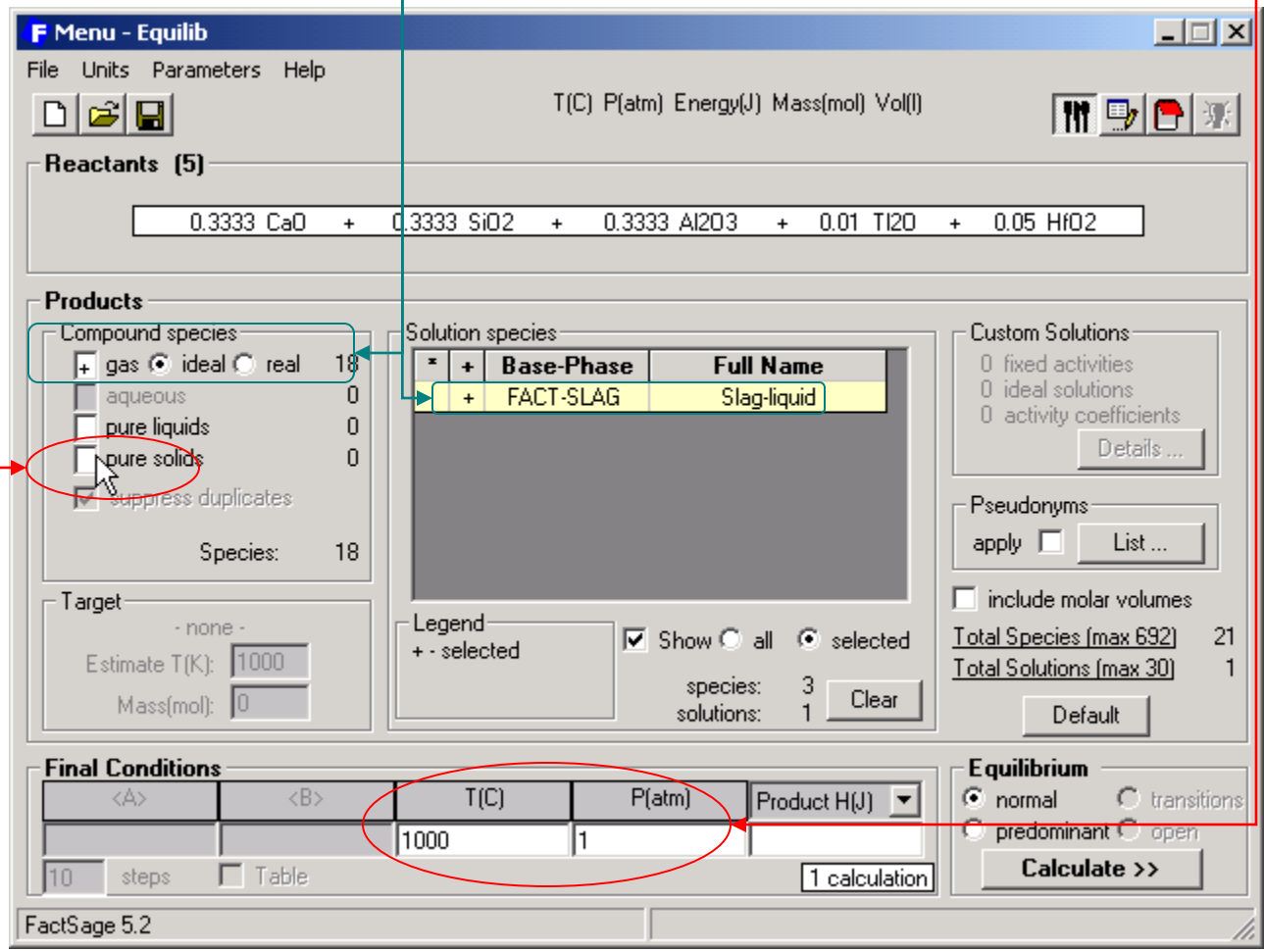
FACT-SLAG:-
90 SiO2, 91 CaO, 92 Al2O3

**Possible products** at **1000°C** and **1 atm**:

- **Solution species: FACT-SLAG**
- **Compound species: ideal gas**

Short description of the **FACT-Slag Solution Phase**. It does not contain **$Tl_2O$** nor **$HfO_2$** .

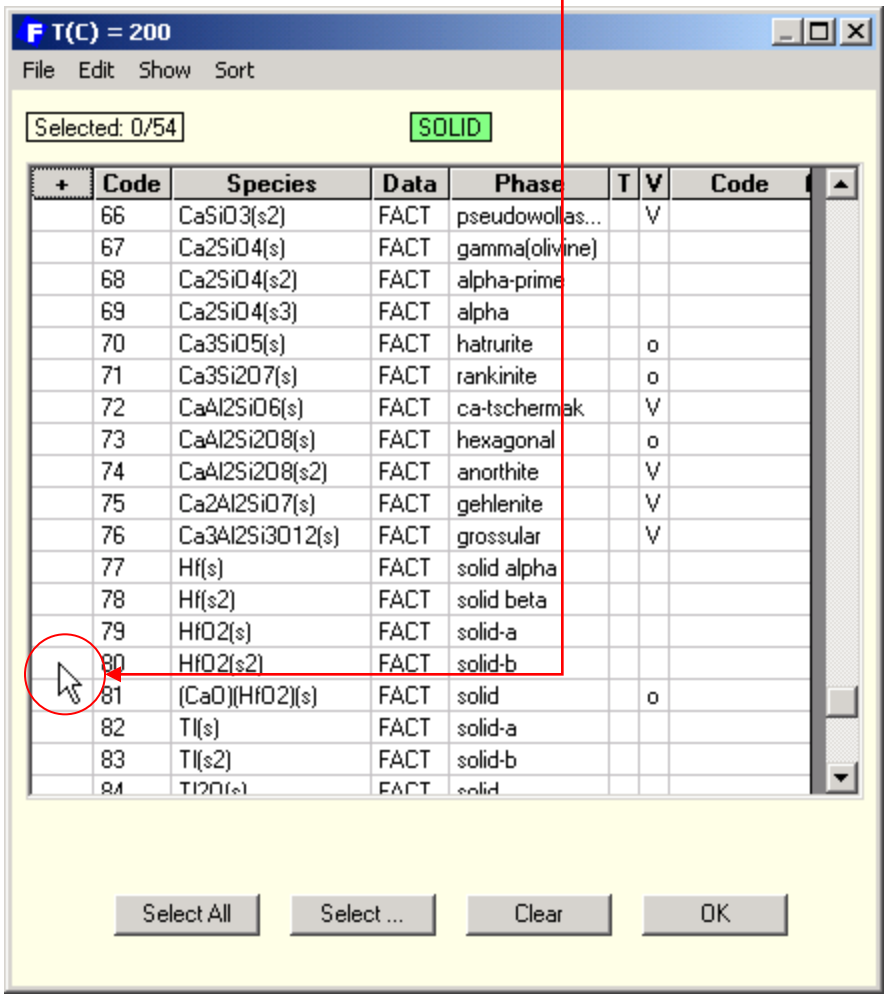
**Right-click** to **open** the **pure solids Species Window**



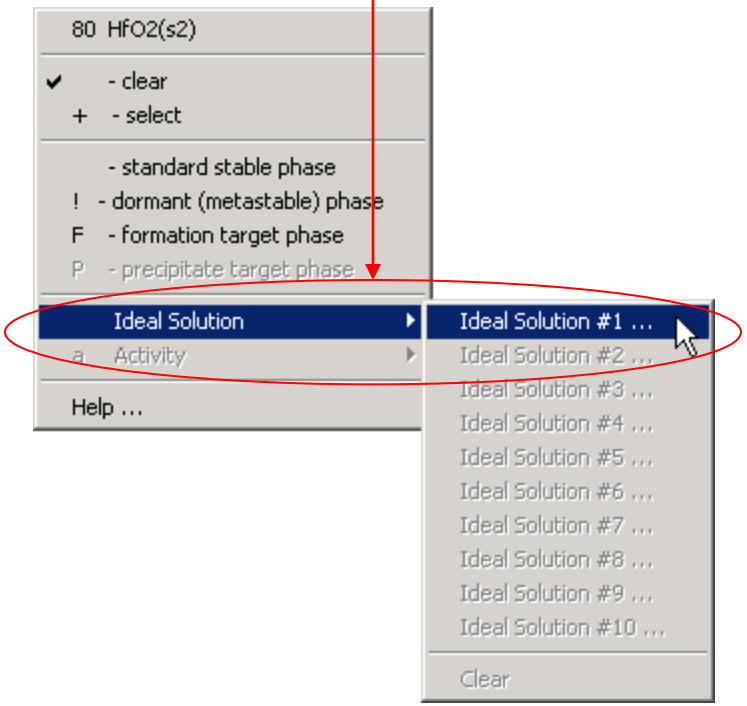
# Creating an ideal Henrian solution of $HfO_2(s)$

**1° Right-click** to open the $HfO_2$(s2) extended menu

**2° Select** Ideal Solution > Ideal solution #1…




| + | Code | Species | Data | Phase | T | V | Code |
|---|---|---|---|---|---|---|---|
| | 66 | CaSiO3(s2) | FACT | pseudowollas... | | V | |
| | 67 | Ca2SiO4(s) | FACT | gamma(olivine) | | | |
| | 68 | Ca2SiO4(s2) | FACT | alpha-prime | | | |
| | 69 | Ca2SiO4(s3) | FACT | alpha | | | |
| | 70 | Ca3SiO5(s) | FACT | hatrurite | | o | |
| | 71 | Ca3Si2O7(s) | FACT | rankinite | | o | |
| | 72 | CaAl2SiO6(s) | FACT | ca-tschermak | | V | |
| | 73 | CaAl2Si2O8(s) | FACT | hexagonal | | o | |
| | 74 | CaAl2Si2O8(s2) | FACT | anorthite | | V | |
| | 75 | Ca2Al2SiO7(s) | FACT | gehlenite | | V | |
| | 76 | Ca3Al2Si3O12(s) | FACT | grossular | | V | |
| | 77 | Hf(s) | FACT | solid alpha | | | |
| | 78 | Hf(s2) | FACT | solid beta | | | |
| | 79 | HfO2(s) | FACT | solid-a | | | |
| | 80 | HfO2(s2) | FACT | solid-b | | | |
| | 81 | (CaO)(HfO2)(s) | FACT | solid | | o | |
| | 82 | Tl(s) | FACT | solid-a | | | |
| | 83 | Tl(s2) | FACT | solid-b | | | |
| | 84 | Tl2O(s) | FACT | solid | | | |



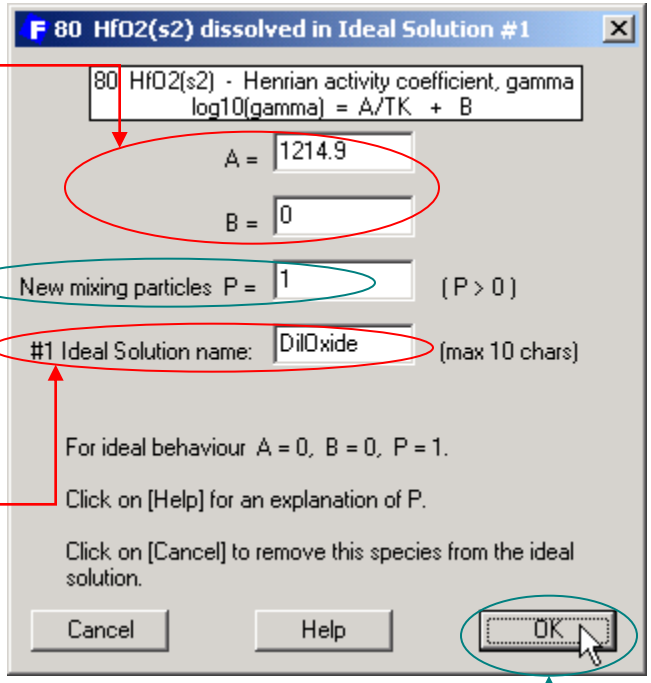
# Creating an ideal Henrian solution of $HfO_2(s)$ – setting $\gamma$

**3° Enter** $\log_{10}[\gamma_{HfO_2(s2)}] = 1214.9/T(K) + 0$
in order that $\gamma = 9.0$ when T = 1273.15K (1000°C).

**4° Specify New mixing particles P = 1**
(this is the default setting).

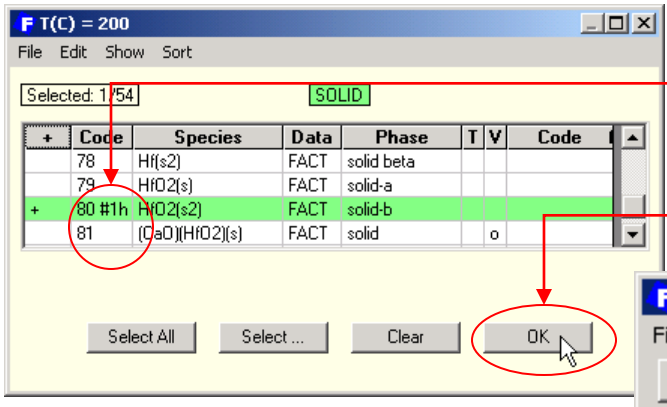
**5° Replace** the default solution name «**Ideal-1**» by a new name «**DilOxide**».

**6° Press OK** to return to the **Solid Species Window**.




Notes:
1. In general, if $\gamma$ is known at only one temperature, it is better to assume that RT log $\gamma$ = constant than to assume that log $\gamma$ = constant.
2. In this example note that $\gamma$ is the activity coefficient relative to SOLID $HfO_2(s2)$ as standard state.

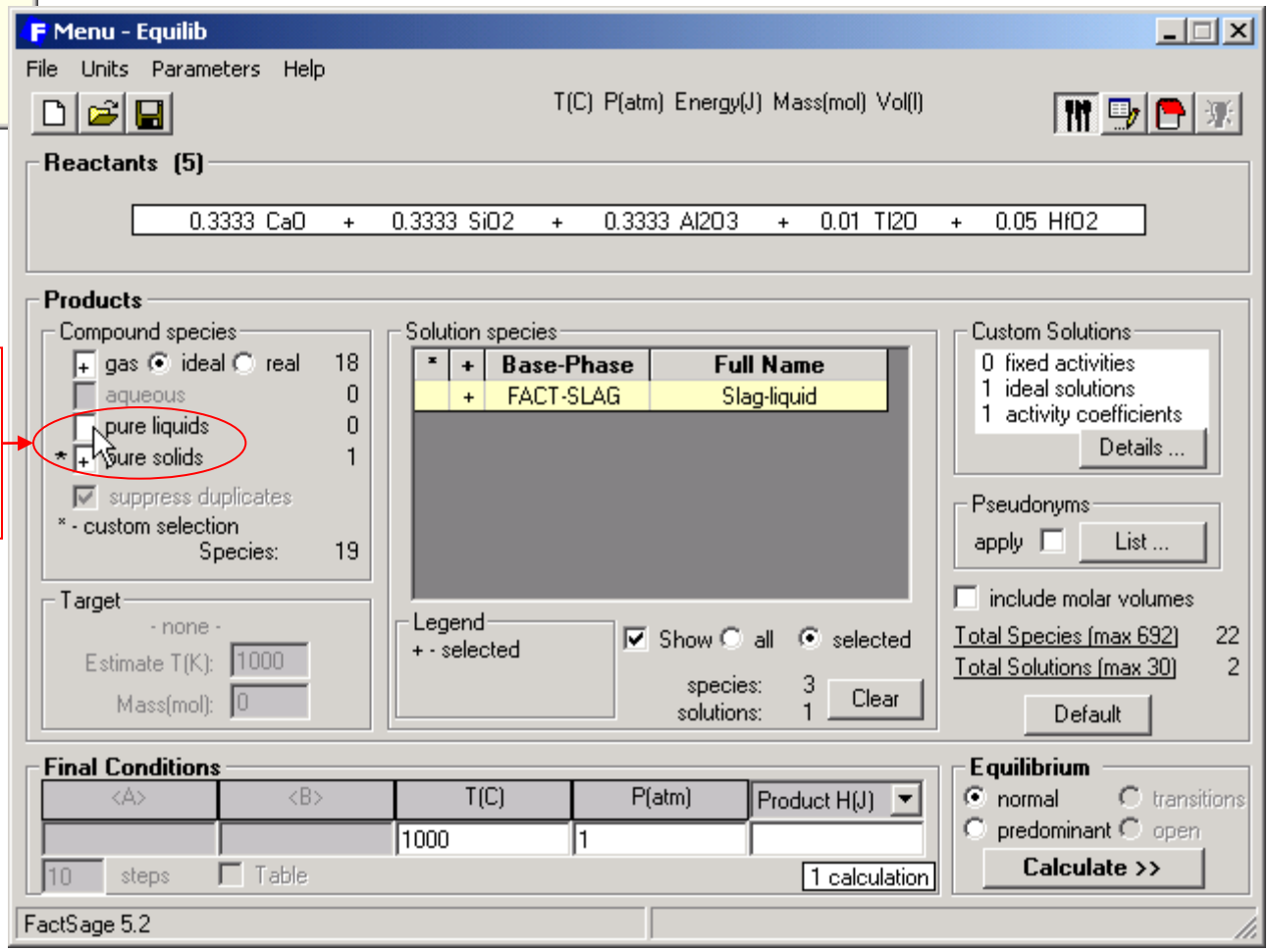
# Adding $Tl_2O(l)$ to the ideal solution




# denotes species also used in ideal solution **1** and **h** indicates an henrian activity coefficient

**7°** **Press OK** to return in the **Menu Window**

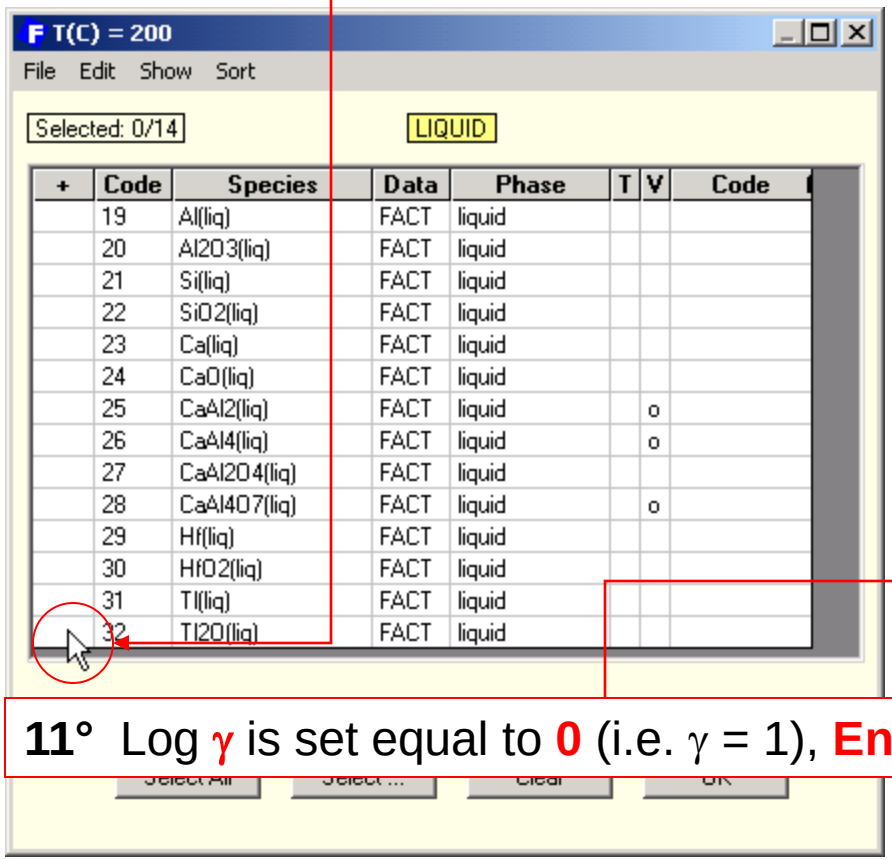
**8°** **Right-click** to **open** the **pure liquids Species Window**

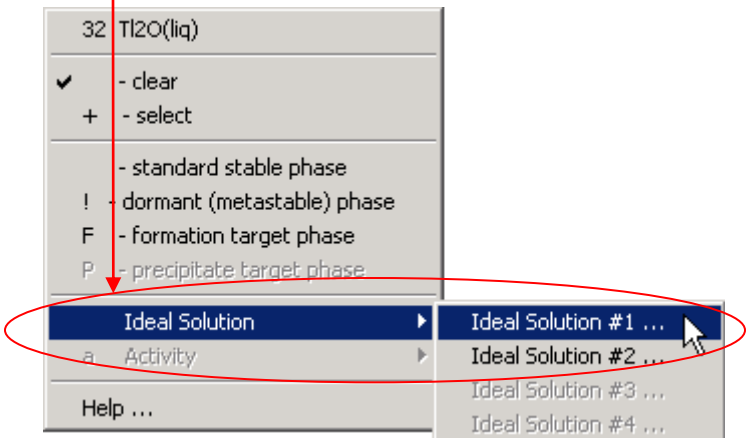


# Adding $Tl_2O(l)$ to the ideal solution – setting $\gamma$

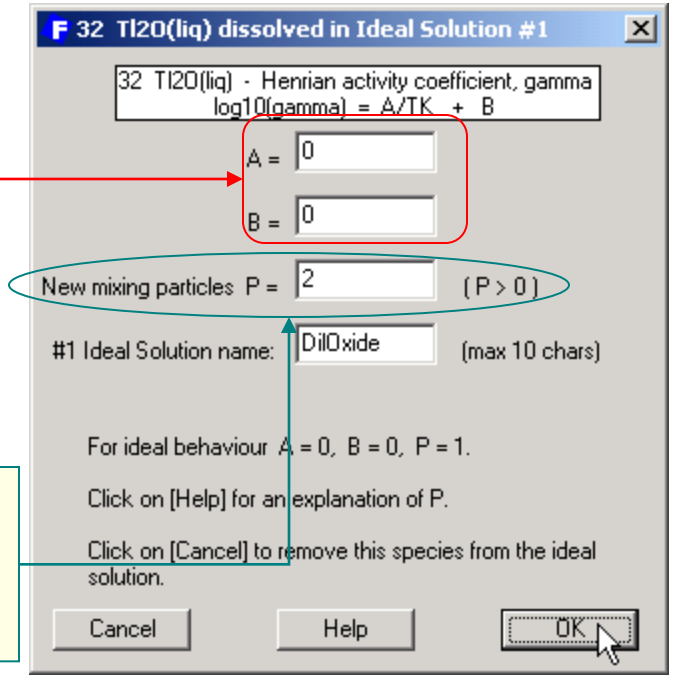
**9°** **Right-click** to open the **$Tl_2O$(liq)** extended menu

**10°** **Select** Ideal Solution > Ideal solution #1…




**11°** Log $\gamma$ is set equal to **0** (i.e. $\gamma = 1$), **Enter A = B = 0**




**12°** **Specify New mixing particles P = 2** to indicate that one mole of $Tl_2O$ **dissociates** into **2 independent particles** (**2[$Tl^+$]**) in the oxide solution.

# Henrian activity coefficient, $\gamma$ and new mixing particles, **P**

A **dilute solute** in an **ideal solution** may have a Henrian activity coefficient, $\gamma$, where:

$$\log_{10}\gamma = \mathbf{A}/TK + \mathbf{B}$$

You specify **A** and **B**, and the number of new mixing particles **P**.

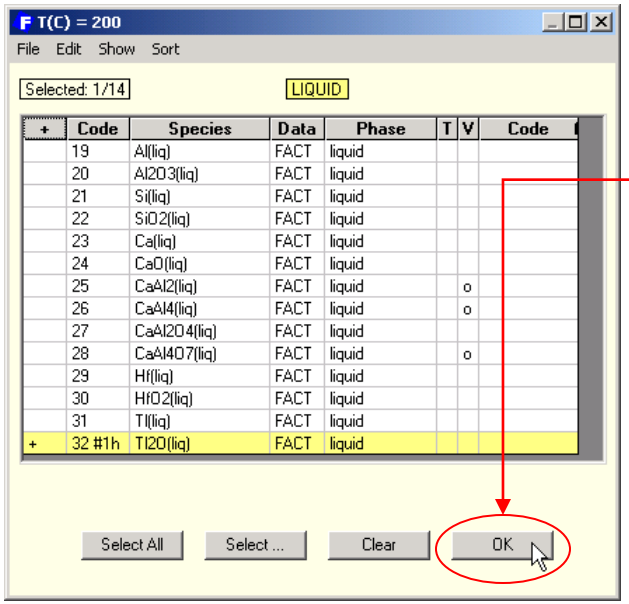
Examples:

1. Solute **Sn(s)** dissolving in **Pb(s)** :
   **P = 1** since **Sn** is a new particle.
2. Solute **NaF(liq)** dissolving in **LiCl(liq)** (i.e. **$Li^+$** and **$Cl^-$**):
   **P = 2** since **NaF** dissolves as new mixing particles **$Na^+$** and **$F^-$**.
3. Solute **NaCl(liq)** dissolving in **LiCl(liq)** (i.e. **$Li^+$** and **$Cl^-$**):
   **P = 1** since **NaCl** dissolves as **$Na^+$** and **$Cl^-$** but only **$Na^+$** is a new particle.
4. Solute **$S_2$(liq)** dissolving in **Fe(liq)** as **S**:
   **P = 2**.

In the present example **P = 2** because $Tl_2O$ dissociates in the slag as:

$$Tl_2O \rightarrow 2\,Tl^+ + O^{2-}$$

# Merging the ideal Henrian solution DilOxide and FACT-Slag

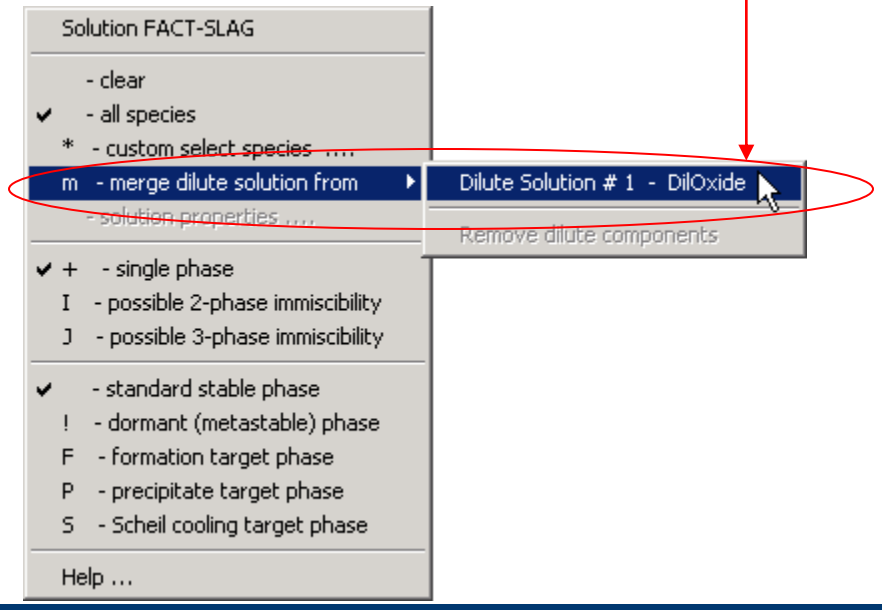


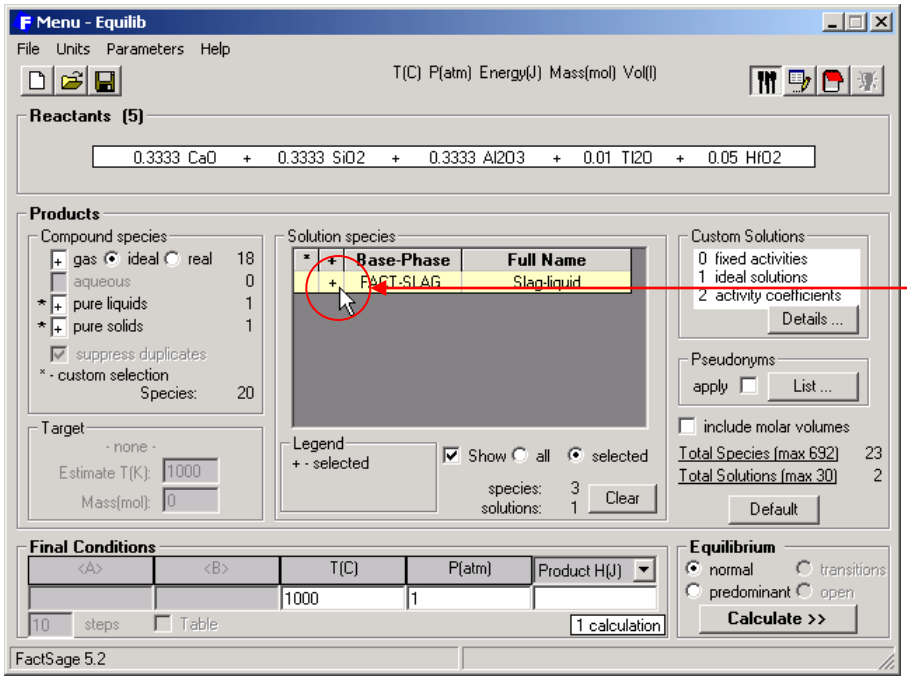

An **ideal Henrian solution** (**DilOxide**) of **$Tl_2O$** and **$HfO_2$** has now been **created**.

**13°** **Press OK** to return to the **Menu Window**

**14°** **Right-click** in the **+** column of **FACT-Slag** to open its extended menu.

**15°** **Select - merge dilute solution from > Dilute Solution #1 - DilOxide**

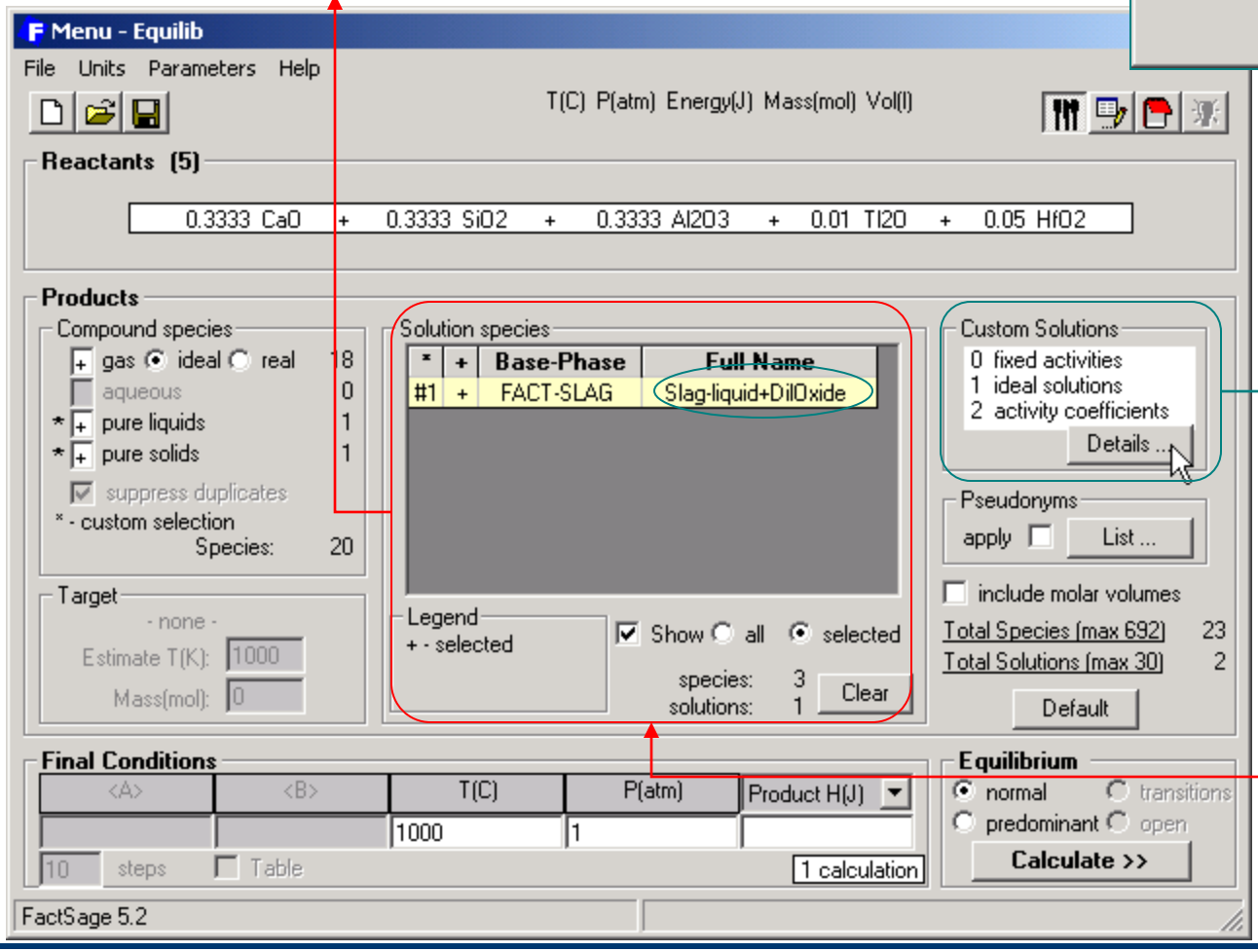


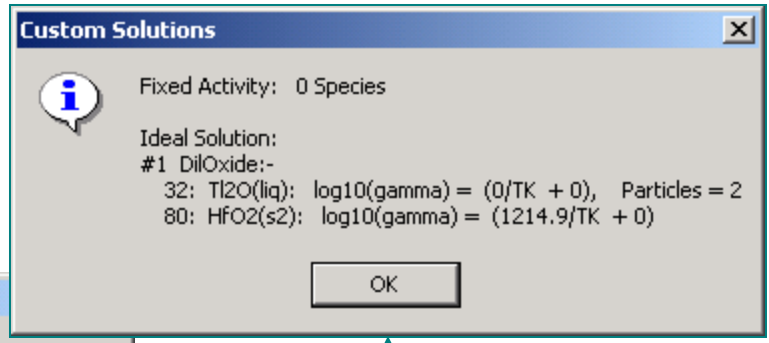



# Calculation including a **dilute solution**: $Tl_2O$ and $HfO_2$ in $CaO$-$SiO_2$-$Al_2O_3$ slag

Solution Phase FACT-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

FACT-SLAG:-
90 SiO2, 91 CaO, 92 Al2O3,
+
Ideal Solution #1 - DilOxide:-
32 Tl2O(liq), 80 HfO2(s2)




**Click** on **details** to display a **summary** of the **ideal solution data entry**.

The dilute solution (**DilOxide**) is merged into the existing **FACT-Slag** solution.

# $Tl_2O$ and $HfO_2$ in $CaO\text{-}SiO_2\text{-}Al_2O_3$ slag: Results (*FACT* format)

$$X_{HfO_2} = \frac{0.047174}{0.31446 + 0.31446 + (2 \times 0.31446) + (2 \times 0.0094349) + 0.047174} = 0.035632$$

```
F Results
Output  Edi

 0.3333 CaO +  0.3333 SiO2 +  0.3333 Al2O3 +  0.01 Tl2O +

 0.05 HfO2 =

   0.00000      mol   (  0.19880E-03       Tl)
                         (1000.00 C, 1 atm, gas_ideal, a=0.24851E-03)

+   1.0599      mol   (  0.31446           SiO2
                      +  0.31446           CaO
                      +  0.31446           Al2O3
                      +  0.94349E-02       Tl2O_DilOxide                T
                      +  0.47174E-01       HfO2(s2)_DilOxide          #)
                         (1000.00 C, 1 atm, Slag-liquid+DilOxide)

                      +  0.00000      mol  HfO2
                         (1000.00 C, 1 atm, S2, a=0.32070)

                      +  0.00000      mol  Tl2O                         T
                         (1000.00 C, 1 atm, L1, a=0.20315E-03)

The cutoff concentration has been specified to 1.000E-04

Data on 2 product species identified with "T" have been extrapolated

Data on 1 product species identified with "#" have been calculated with a
user-supplied activity-coefficient expression

*****************************************************************
      H            G            V            S           Cp
     (J)          (J)          (l)        (J/K)        (J/K)
*****************************************************************
-1.03501E+06 -1.28273E+06  0.00000E+00  1.94572E+02  9.71063E+01
```

…because $Tl_2O$ dissociates into **two** Tl ions and also $Al_2O_3$ dissociates into **two** Al ions: **$Al_2O_3$ ➔ 2 $Al^{3+}$ + 3 $O^{2-}$**

**Note:**
This information about $Al_2O_3$ is included in the FACT-SLAG database.

The calculated **activity** of $HfO_2$(s2) is:

$$a_{HfO_2} = \gamma_{HfO_2} X_{HfO_2} = (9.0)(0.035632)$$
$$= 0.32070$$

**Note:**
If we increase $\gamma_{HfO_2}$, the calculated activity would increase until solid $HfO_2$(s) would be calculated to precipitate when its activity = 1.0. If the solubility of $HfO_2$ were experimentally known for instance, then we could adjust $\gamma_{HfO_2}$ in this way in order to reproduce the measured solubility. That is, a measured solubility limit permits us to determine the value of the Henrian activity coefficient.

# $Tl_2O$ and $HfO_2$ in $CaO$-$SiO_2$-$Al_2O_3$ slag: Results (*ChemSage* format)

$$X_{TlO_{0.5}} = \frac{(2\times 0.0094349)}{0.31446+0.31446+(2\times 0.31446)+(2\times 0.0094349)+0.047174} = 0.014253$$

F Results

Output Ed

```
T = 1000.00 C
P = 1.00000E+00 atm
V = 0.00000E+00 dm3

STREAM CONSTITUENTS          AMOUNT/mol
CaO_lime(s)                  3.3330E-01
SiO2_quartz(l)(s)            3.3330E-01
Al2O3_gamma(s)               3.3330E-01
Tl2O(s)                      1.0000E-02
HfO2(s)                      5.0000E-02

                           EQUIL AMOUNT  MOLE FRACTION     FUGACITY
PHASE: gas_ideal               mol                          atm
Tl                           0.0000E+00    8.0000E-01    1.9880E-04
TOTAL:                       0.0000E+00    1.0000E+00    2.4851E-04
PHASE: Slag-liquid+DilOxide    mol        MOLE FRACTION    ACTIVITY
SiO2                         3.3330E-01    3.1446E-01    8.3320E-02
CaO                          3.3330E-01    3.1446E-01    9.5912E-05
Al2O3                        3.3330E-01    3.1446E-01    1.3193E-02
Tl2O_DilOxide              T 1.0000E-02    9.4349E-03    2.0315E-04
HfO2(s2)_DilOxide            5.0000E-02    4.7174E-02    3.2070E-01
TOTAL:                       1.0599E+00    1.0000E+00    1.0000E+00
                               mol                        ACTIVITY
HfO2(s2)                     0.0000E+00                  3.2070E-01
Tl2O(liq)                  T 0.0000E+00                  2.0315E-04
*******************************************************************
  Cp_EQUIL       H_EQUIL        S_EQUIL        G_EQUIL        V_EQUIL
   J.K-1           J             J.K-1           J             dm3
*******************************************************************
 9.71063E+01  -1.03501E+06   1.94572E+02  -1.28273E+06   0.00000E+00

Mole fraction of system components:
                gas_ideal     Slag-liquid
Tl               6.6667E-01    5.6931E-03
Hf               1.1605E-47    1.4233E-02
Ca               7.9696E-18    9.4876E-02
Si               2.0464E-15    9.4876E-02
Al               6.1172E-20    1.8975E-01
O                3.3333E-01    6.0057E-01

The cutoff limit for phase or gas constituent

Data on 2 constituents marked with 'T' are ext
temperature range
```

The calculated **activity** of $Tl_2O$(liq) is:

$$a_{Tl_2O} = \gamma_{Tl_2O} X_{Tl_2O} = \gamma_{Tl_2O}\left(X_{TlO_{0.5}}\right)^2$$

$$= (1.0)(0.014253)^2 = 2.0315\times 10^{-4}$$

**Note:**

The calculated vapor pressure of **Tl gas** is $1.988 \times 10^{-4}$ atm. If experimental vapor pressure data were available, then one could adjust $\gamma_{Tl_2O}$ in order to reproduce these data. That is, a measured vapor pressure permits one to determine the value of the Henrian activity coefficient.

# Limitations and restrictions of merging dilute solutes into solutions

1. Ions are not permitted as dilute species (ex: $Na^+$, $AlClO_3^-$ in 'diluteCr').
2. The resulting solution should be dilute in the solute(s) that are merged (ex: in the present case if the resulting solution phase is say >10% Cr then the validity of the results would be in question).
3. Try to avoid species that are already present in the existing database (ex: in the present case avoid adding dilute Fe(liq)).
4. You may create several different ideal Henrian solutions, each with one or more solutes, however:
   1. a given solute can only appear in one ideal solution (ex: in the present case Cr(liq) is a solute only in 'Ideal Solution #1 - diluteCr' ).
   2. each ideal Henrian solution can be merged only once into one real solution (ex: in the present case 'diluteCr' is merged into FACT-CuLQ and no other).
   3. each real solution can contain no more than one merged dilute solution (ex: in the present FACT-CuLQ contains only 'diluteCr').
5. Merging dilute solutions into complex solutions (ex: oxides into FACT-SLAG, salts into FACT-SALT) may require special consideration due to the number of "New mixing particles" (ex: please refer to the example on $Tl_2O$ and $HfO_2$ in FACT-SLAG).
6. Although the calculated solution phase composition is thermodynamically self-consistent, the results are an approximation only and only truly valid at infinite dilution.

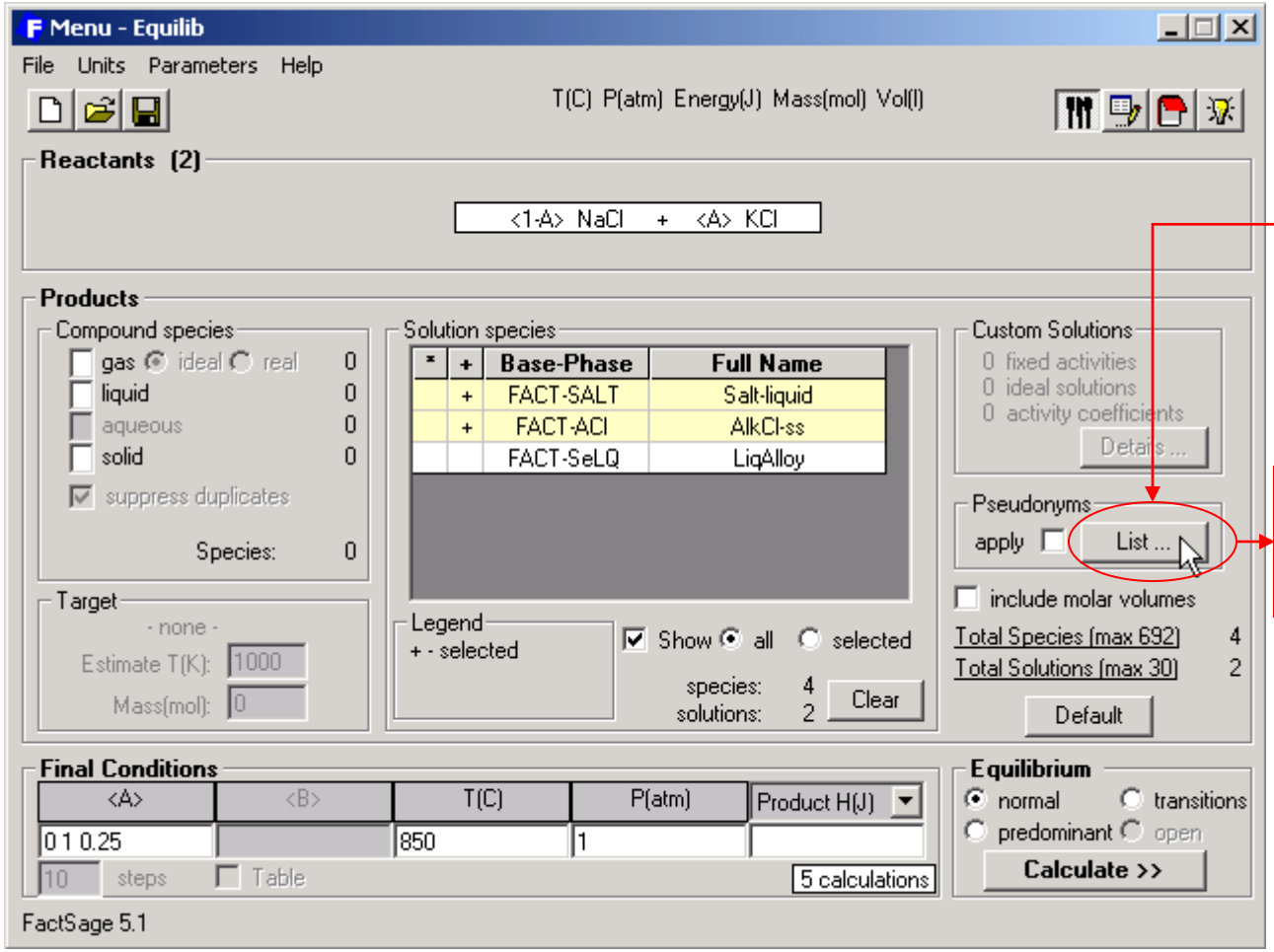
# Using Pseudonyms

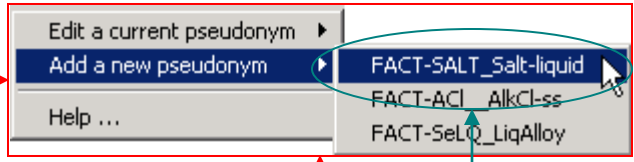
The following two slides show how a user defined list of phase names of solution phases (pseudonyms) can be applied in order to give output tables a user-specific appearance.

NOTE that this feature is also available in the ***Phase Diagram*** module where the user defined phase names are used for labelling the phase fields.

# Pseudonyms

This feature enables you to use your own description (that we call a '**pseudonym**') for a solution phase. For example, you could replace '?Slag-liquid' by say 'slag', or 'FCC-A1' by 'Fe(fcc)', etc.

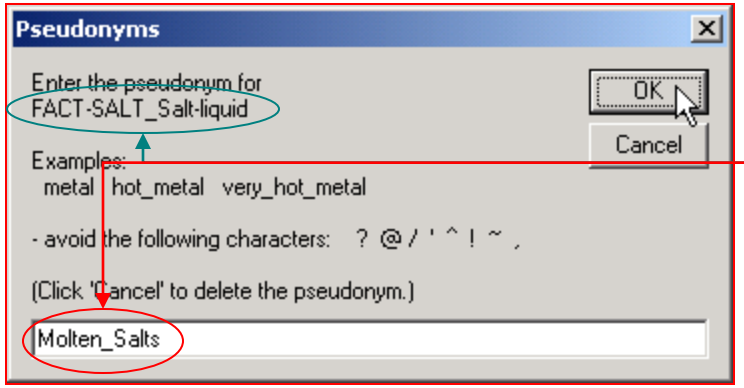



**1°** Click on the **List…** button to access the pseudonyms menu.

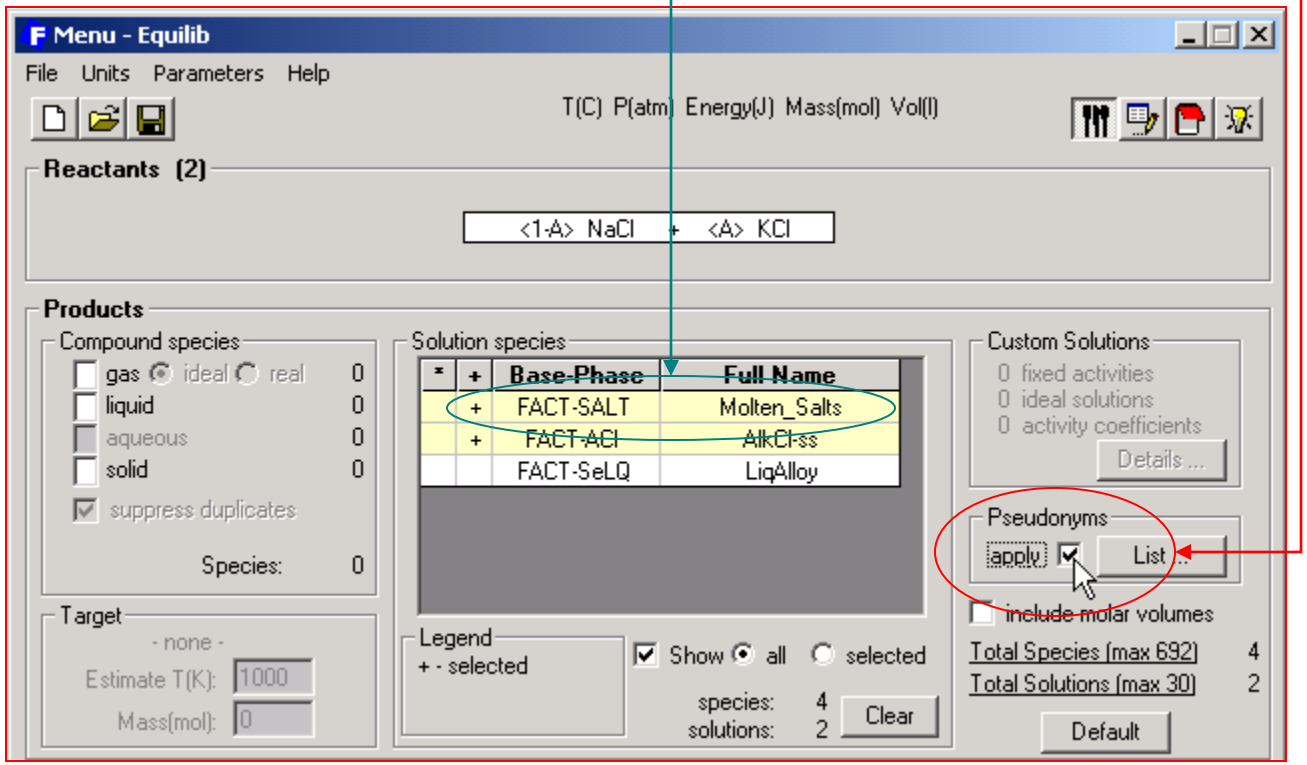
**2°** Select '**Edit…**' or '**Add…**' and then click on the **phase** to open the **Pseudonyms** dialog box.

# Pseudonyms




**3°** Enter a **pseudonym** for the **selected phase** and press **OK**.

If the '**apply**' box is checked the pseudonyms will appear in the **Equilib Results Window** and **Phase Diagram** plotted **Figure**.



# Including molar volume data

For some stoichiometric condensed substances, e.g. SiO2 or C, molar volume data are stored in the database which permit the influence of high pressure on the phase equilibria to be calculated.

The following two slides show how the use of molar volume data is controlled from the Equilib Menu screen.

NOTE that the use of molar volume data must be executed with great care in order to avoid erroneous results.

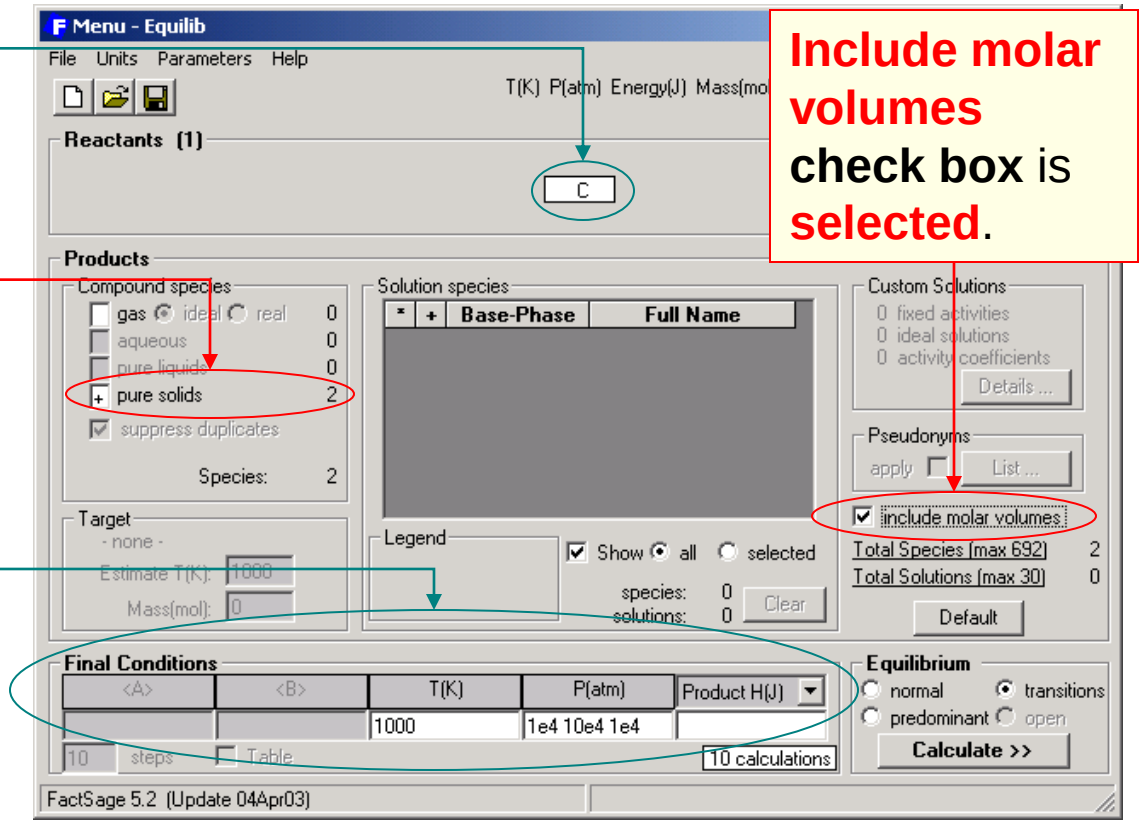
# Include molar volumes : graphite to diamond transition

Where available, **density** (i.e. molar volume) data for solids and liquids can be employed in ***Equilib*** (the "**VdP**" term) although their effect only becomes significant at high pressures. **Note** that (unlike ***Reaction***) compressibility and expansivity data are also employed in ***Equilib***.

**1°** Reactant: **C**

**2°** Possible products:
2 pure solids
- **Graphite**
- **Diamond**

**3°** T (K) = **1000 K**
P (atm) = **$1\times10^4$ atm**, **$2\times10^4$ atm**, …, **$1\times10^5$ atm**




**Include molar volumes check box** is **selected**.

The program will calculate the equilibrium at **1000K** for pressures varying from **$1\times10^4$ atm** to **$1\times10^5$ atm** in increments of **$1\times10^4$ atm** and will search for all phase **transitions**.

# Graphite to diamond transition: equilibrium calculation

**Note:** If molar volumes are **not** included then **no** transitions are found.

At **1000 K** and **31488 atm**, **graphite** and **diamond** are at equilibrium.

**Molar volume data** are **employed**

**The volume of diamond is smaller than graphite.**

Hence, at high pressures, the "**VdP**" term creates a **favorable negative contribution to the enthalpy change** associated with the **graphite** to **diamond** transition.

Results - Equilib 1000 K, 3.149E+04 atm (page 4/12)

Output Edit Show Pages

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

1000 K, 9.000E+04 atm | 1000 K, 1.000E+05 atm | 1000 K, 4.000E+04 atm | 1000 K, 5.000E+04 atm | 1000 K, 6.000E+04 atm | 1000 K, 7.000E+04 atm | 1000 K, 8.000E+04 atm | 1000 K, 1.000E+04 atm | 1000 K, 2.000E+04 atm | 1000 K, 3.000E+04 atm | 1000 K, 3.149E+04 atm | 1000 K, 3.149E+04 atm

```
C =

                    1.0000      mol  C_graphite                    V
                   (1000.00 K, 31488. atm, S1, a= 1.0000)

                +   0.00000     mol  C_diamond                     V
                   (1000.00 K, 31488. atm, S2, a= 1.0000)

*****************************************************************
      H            G            V            S            Cp
     (J)          (J)          (l)         (J/K)         (J/K)
*****************************************************************
 2.80832E+04  4.11377E+03  5.12697E-03  2.39695E+01  2.14886E+01


*****************************************

T = 1000.00 K
*P = 3.14879E+04 atm
V = 5.12697E-03 dm3

STREAM CONSTITUENTS          AMOUNT/mol
C_graphite(s)                1.0000E+00

                           EQUIL AMOUNT                  ACTIVITY
                              mol
C_graphite(s)              1.0000E+00                   1.0000E+00
C_diamond(s2)              0.0000E+00                   1.0000E+00
*****************************************************************
  Cp_EQUIL       H_EQUIL       S_EQUIL       G_EQUIL       V_EQUIL
    J.K-1           J            J.K-1          J            dm3
*****************************************************************
 2.14886E+01   2.80832E+04   2.39695E+01   4.11377E+03   5.12697E-03

System density/g.cm-3 =  2.34271
```

Results - Equilib 1000 K, 3.149E+04 atm (page 5/12)

Output Edit Show Pages

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

1000 K, 9.000E+04 atm | 1000 K, 1.000E+05 atm | 1000 K, 4.000E+04 atm | 1000 K, 5.000E+04 atm | 1000 K, 6.000E+04 atm | 1000 K, 7.000E+04 atm | 1000 K, 8.000E+04 atm | 1000 K, 1.000E+04 atm | 1000 K, 2.000E+04 atm | 1000 K, 3.000E+04 atm | 1000 K, 3.149E+04 atm | 1000 K, 3.149E+04 atm

```
C =

                    1.0000      mol  C_diamond                     V
                   (1000.00 K, 31488. atm, S2, a= 1.0000)

                +   0.00000     mol  C_graphite                    V
                   (1000.00 K, 31488. atm, S1, a=0.99999)

*****************************************************************
      H            G            V            S            Cp
     (J)          (J)          (l)         (J/K)         (J/K)
*****************************************************************
 2.39314E+04  4.11388E+03  3.42034E-03  1.98176E+01  2.09062E+01


*****************************************

T = 1000.00 K
*P = 3.14882E+04 atm
V = 3.42034E-03 dm3

STREAM CONSTITUENTS          AMOUNT/mol
C_graphite(s)                1.0000E+00

                           EQUIL AMOUNT                  ACTIVITY
                              mol
C_diamond(s2)              1.0000E+00                   1.0000E+00
C_graphite(s)              0.0000E+00                   9.9999E-01
*****************************************************************
  Cp_EQUIL       H_EQUIL       S_EQUIL       G_EQUIL       V_EQUIL
    J.K-1           J            J.K-1          J            dm3
*****************************************************************
 2.09062E+01   2.39314E+04   1.98176E+01   4.11388E+03   3.42034E-03

System density/g.cm-3 =  3.51163
```

# Open versus closed system calculations

Calculations with ***Equilib*** are usually Closed System calculations, i.e. calculations in which the amounts of all input substances are kept constant.

However, under certain conditions it is also possible to use ***Equilib*** for Open System calculations. In such cases it is assumed that all condensed substances/phases remain in the system while the gas phase is refresh in every calculational step.

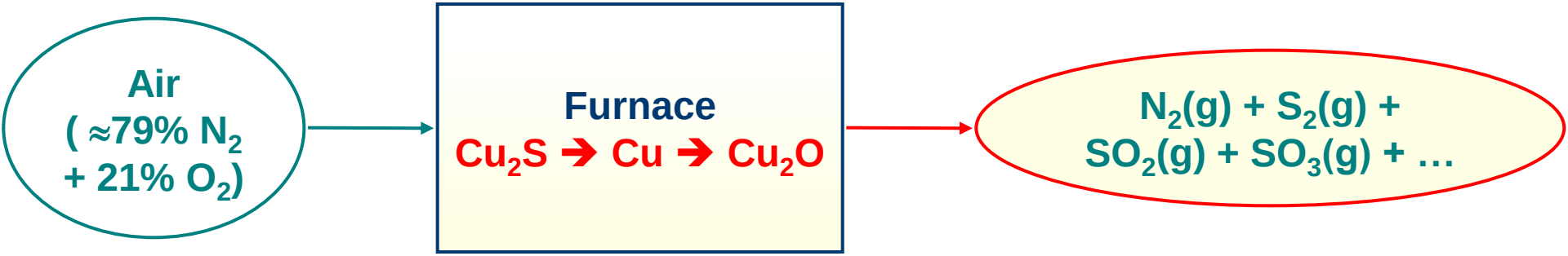
The following slide explains the general procedure in more detail. In sections 9.1 and 9.2 two example applications are shown.

# The *OPEN* Command

In many pyrometallurgical processes, for example copper converting (or steelmaking), the system is «**open**». **Gas**, typically in the form of **air** or **oxygen**, enters the **furnace**, **reacts** with the **system**, and then **leaves** the **reactor** as **$SO_2$(g)** and **$SO_3$(g)** (or as **CO(g)** and **$CO_2$(g)**). These product gaseous species, being removed from the system, change the overall mass balance. An **open** process, with the gaseous products being continuously removed from the calculation, can be simulated by the ***Equilibrium*** command ***OPEN***.

In the case of **$Cu_2S$** converting eventually all the sulfur leaves the system and then **$Cu_2O$** starts to form unless the converting is stopped.

The following figures demonstrate **$Cu_2S$** desulphurisation by air in an ***OPEN*** process.



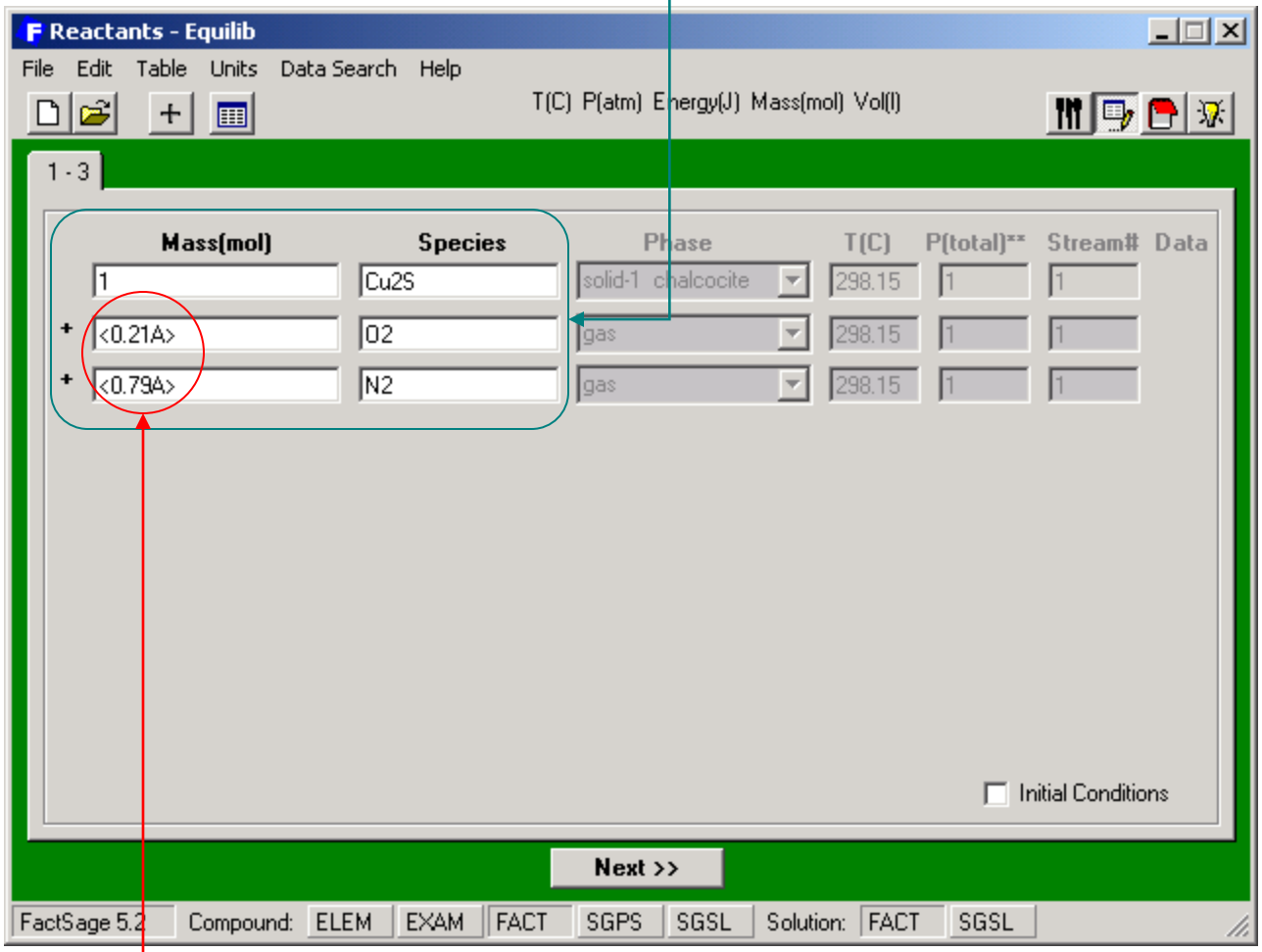
# Desulphuring of $Cu_2S$

The following six slides show how the Open command is applied for the stepped (open) desulphurisation of $Cu_2S$ with air.

Note how the variable Alpha is used to define the input amount of air (.21 $O_2$ and .79 $N_2$) for use with the Open command.

# Desulphurisation of $Cu_2S$ by air: setting the Reactants Window

The reactants are **one** mole of $Cu_2S$ with a **variable amount <A>** moles of **air**.

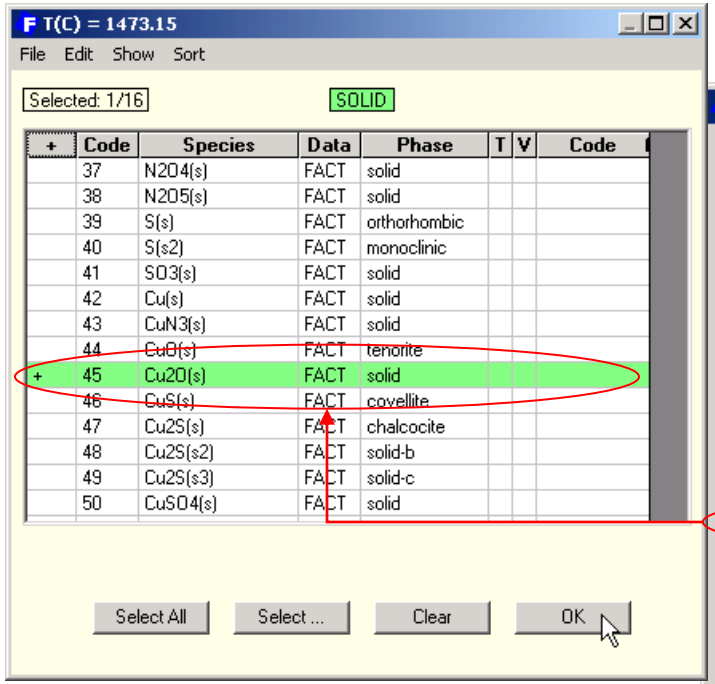


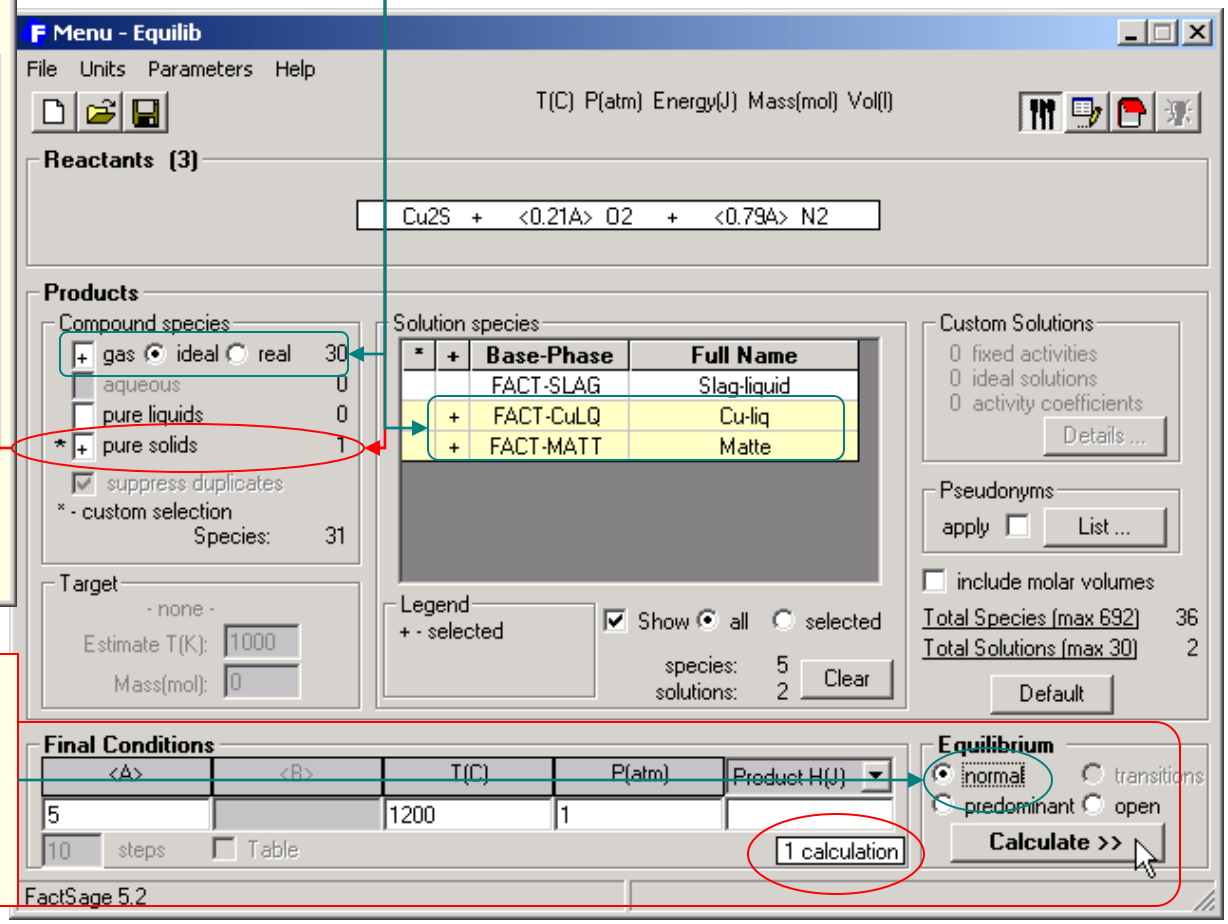

In an ***OPEN*** system, **<A>** moles of reactant are added at each step and then the gas species are removed after equilibration.

# Desulphurisation of $Cu_2S$ by air: setting the Menu Window

**Possible products:**

- **Solution species: FACT-CuLQ, FACT-MATT**
- **Compound species: ideal gas, $Cu_2O(s)$**




**Setting** the final conditions for a **normal** (i.e. **closed** system) equilibrium calculation at **1200°C** and **1 atm** for **<A> = 5**

# Desulphurisation: Closed system equilibrium calculation

Air
( ≈79% $N_2$ + 21% $O_2$)

$N_2(g) + S_2(g) + SO_2(g) + SO_3(g) + \ldots$

Furnace $Cu_2S \rightarrow Cu \rightarrow Cu_2O$

Results - Equilib 1200 C

Output Edit Show Pages

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

```
 Cu2S +  <0.21A> O2 +  <0.79A> N2 =

   4.9501      mol    (  0.79796          N2
                      +  0.20190          SO2)
                         (1200.00 C, 1 atm, gas_ideal)

+   2.0999      mol    (  0.95243          Cu
                      +  0.12303E-03      S
                      +  0.47443E-01      O)
                         (1200.00 C, 1 atm, Cu-liq)

+  0.00000      mol    (  0.18299          S                          C
                      +  0.81701          Cu)
                         (1200.00 C, 1 atm, Matte, a=0.64705E-01)

                      +  0.00000     mol  Cu2O
                         (1200.00 C, 1 atm, Sl, a=0.88881)

where "A" on the reactant side is  5.000

The cutoff concentration has been specified to 1.000E-04

Data on 1 solute identified with "C" have been extrapolated out of the
suggested composition range

*************************************************************
      H            G            V            S           Cp
     (J)          (J)          (l)         (J/K)       (J/K)
*************************************************************
 4.33759E+03 -2.18989E+06  5.98382E+02  1.48948E+03  2.59344E+02
```

$P_{SO_2}$ = **0.2019** atm in **4.9501** mol of gas

A = **5.0**, i.e. **5** moles of **air**

# Desulphurisation of $Cu_2S$ by air: Open calculation

**Setting** the final conditions for an **open** (i.e. **open** system) equilibrium calculation at **1200°C** and **1 atm** for **50** steps of incremental **<A> = 0.1**

**Air**
**( ≈79% $N_2$ + 21% $O_2$)**

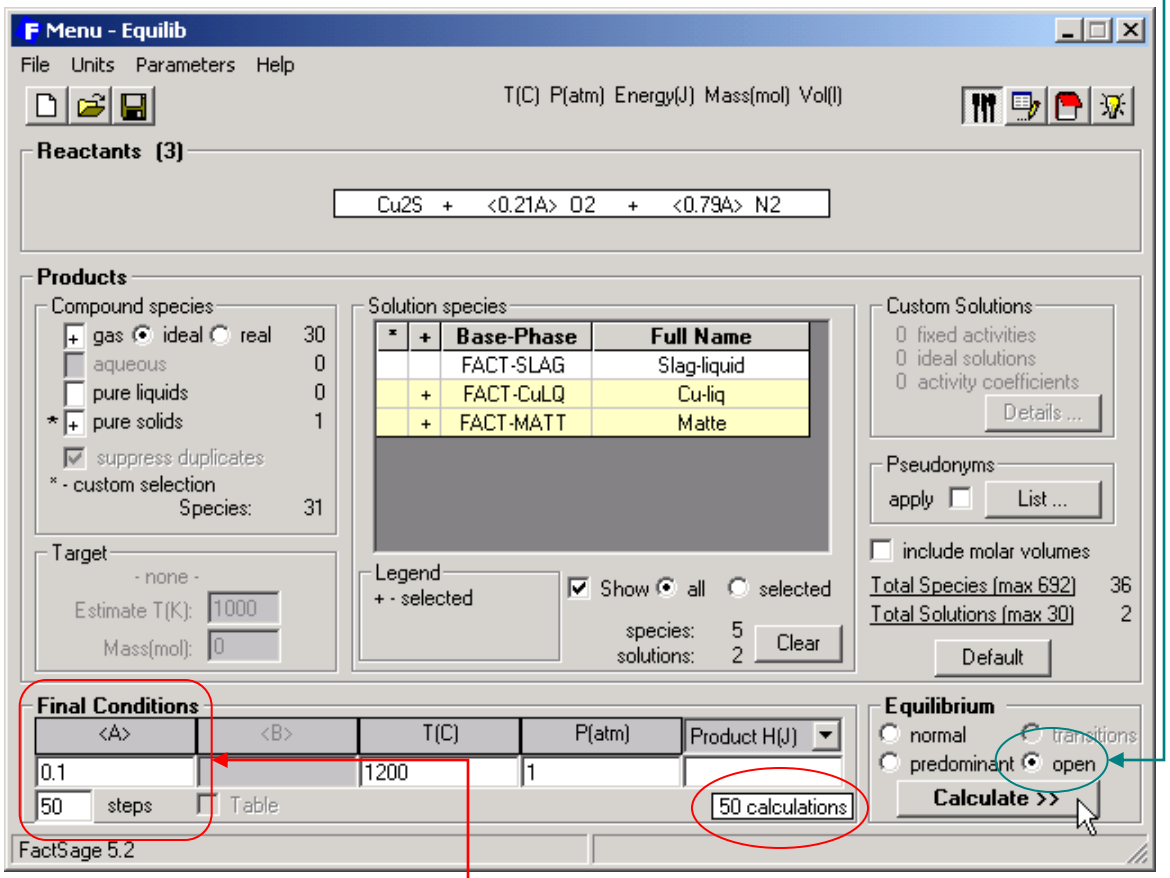
↓

**Furnace**
**$Cu_2S$ → Cu → $Cu_2O$**

↓

**$N_2(g)$ + $S_2(g)$ + $SO_2(g)$ + $SO_3(g)$ + …**

**1° Select open** in the **Equilibrium frame** to enable the **steps' Final Condition** input box




**2° Enter** the number of **steps** (here, **50**) and the amount **<A>** (here, **0.1** mole of air) of reactant added to the system at each step at the end of which the gas phase is removed.

# Desulphurisation: Open system equilibrium calculation

Air ( ≈79% $N_2$ + 21% $O_2$) → **Furnace** $Cu_2S$ ➔ Cu ➔ $Cu_2O$ → $N_2(g) + S_2(g) + SO_2(g) + SO_3(g) + \ldots$

Results - Equilib Step 50 (page 50/50)

Output Edit Show Pages

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

Step 38 | Step 39 | Step 40 | Step 41 | Step 42 | Step 43 | Step 44 | Step 45 | Step 46 | Step 47 | Step 48 | Step 49

Step 26 | Step 27 | Step 28 | Step 29 | Step 30 | Step 31 | Step 32 | Step 33 | Step 34 | Step 35 | Step 36 | Step 37

Step 50

```
 Cu2S +  <0.21A> O2 +  <0.79A> N2 =                    Total <A> =  5.0000

  0.79037E-01 mol   (  0.99952          N2
                    +  0.39905E-03      SO2
                    +  0.53085E-04      O2
                    +  0.20787E-04      NO
                    +  0.49238E-05      Cu
                    +  0.12596E-06      SO3
                    +  0.20251E-07      O
                    +  0.12280E-07      SO
                    +  0.76342E-08      CuO
                    +  0.18439E-08      NO2
                    +  0.15527E-08      Cu2
                    +  0.12770E-08      N2O)
                       (1200.00 C, 1 atm, gas_ideal)

+   2.1004      mol   (  0.95217          Cu
                    +  0.24057E-06      S
                    +  0.47829E-01      O)
                       (1200.00 C, 1 atm, Cu-liq)

+  0.00000      mol   (  0.18913          S                          C
                    +  0.81087          Cu)
                       (1200.00 C, 1 atm, Matte, a=0.67081E-02)

                    +  0.00000      mol  Cu2O
                       (1200.00 C, 1 atm, Sl, a=0.89444)
```

After 50 steps, A = **5.0**, i.e. **5** moles of **air** were added to 1 mole of **$Cu_2S$**

$P_{SO_2}$ = **$3.9905 \times 10^{-4}$** atm in **0.079037** mol of gas (mainly **$N_2$**)

**Note:**
The simulation is improved by specifying a smaller value of **<A>** (and a correspondingly larger number of steps).

# Deleading of a copper melt

Because of its relatively high partial pressure Pb can be removed from Cu-Pb melts by way of vacuum refining.

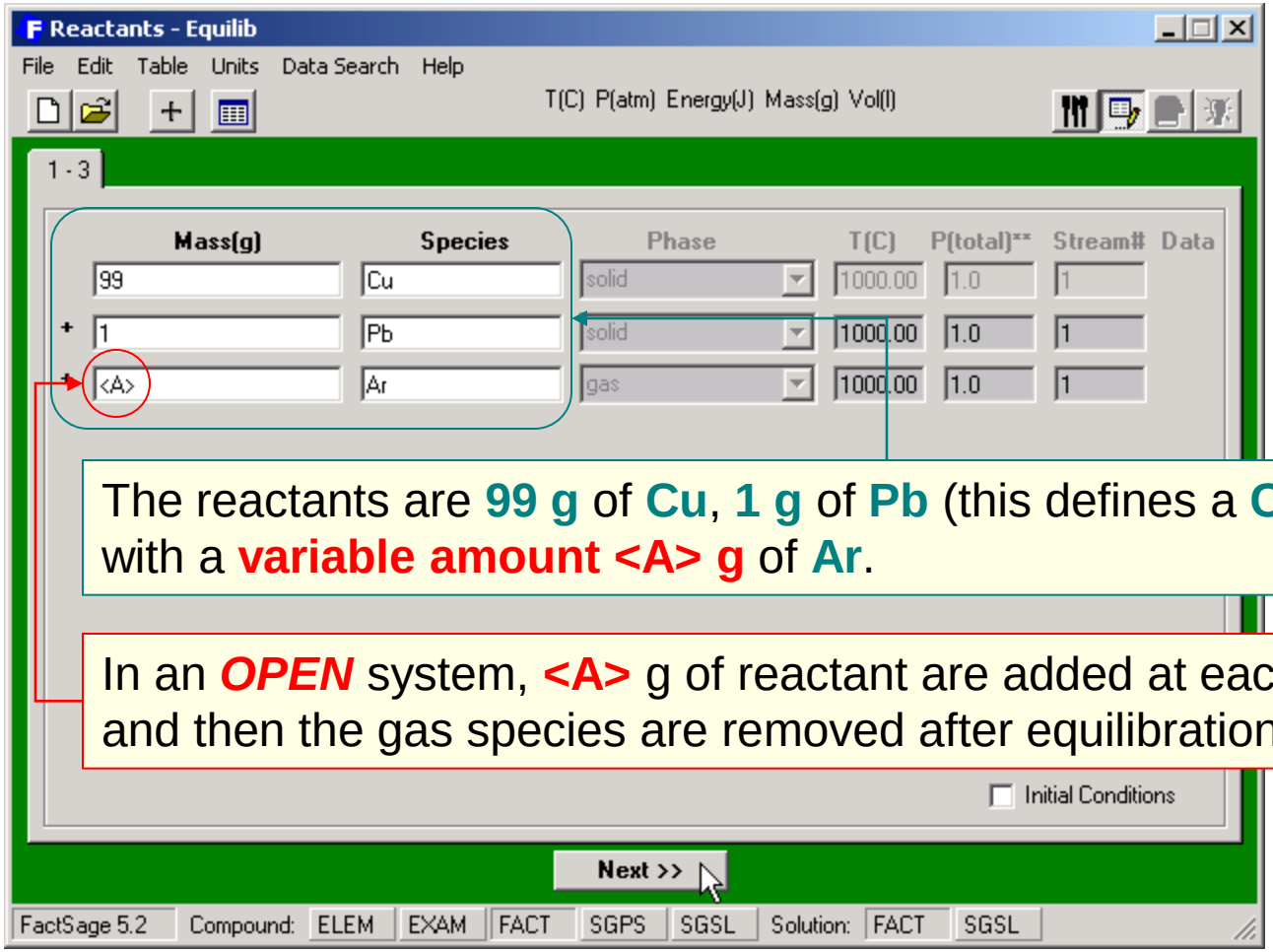
The following six slides show how the Open command can be employed to simulate the process.

Note that «Vacuum» is established by setting a low total pressure and adding a small amount of Argon into each calculational step. The amount of argon is needed to establish a certain volume into which the lead can evaporate in each step.

# Deleading of a Cu-1wt%Pb alloy by argon vacuum refining

The current example illustrates the concepts of **normal** (i.e. **closed** system) vs. **open** equilibrium calculations as applied to **argon** refining of a **Cu-1wt%Pb** alloy at reduced total pressures. It simulates deleading at 1200°C and 0.001 atm.

There are **no chemical reactions** involved in the process.




The reactants are **99 g** of **Cu**, **1 g** of **Pb** (this defines a **Cu-1 wt% Pb** alloy) with a **variable amount <A> g** of **Ar**.

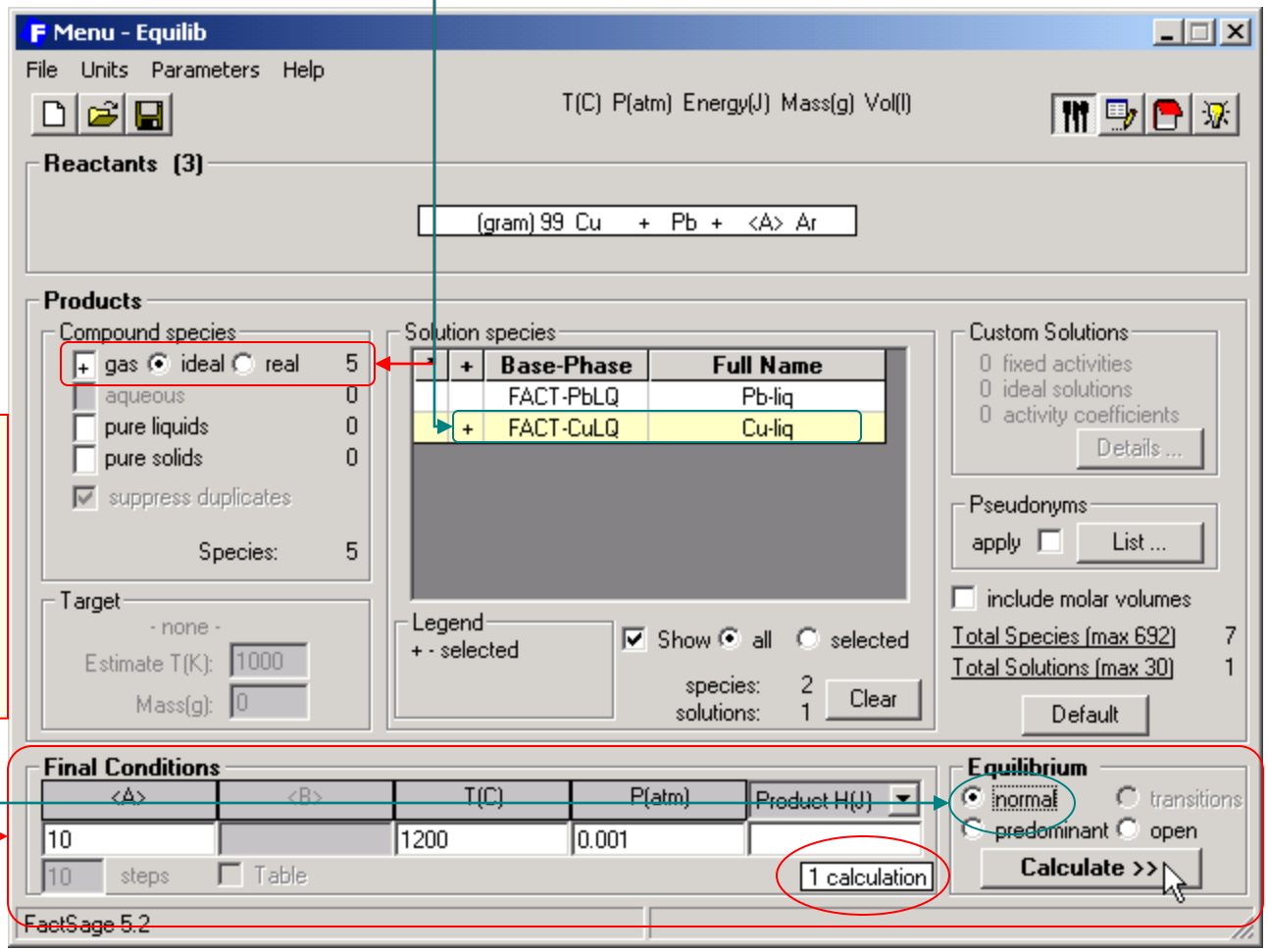
In an ***OPEN*** system, **<A>** g of reactant are added at each step and then the gas species are removed after equilibration.

# Deleading of a Cu-1wt%Pb alloy: setting the Menu Window

**Possible products:**

- **Solution species: FACT-CuLQ**
- **Compound species: ideal gas**

**Setting** the final conditions for a **normal** (i.e. **closed** system) equilibrium calculation at **1200°C** and **0.001 atm** for **<A> = 10**



# Deleading of a Cu-1wt%Pb alloy: Closed system equilibrium calculation

The **concentration** of **Pb** in **Cu(liq)** is **5.5876 × $10^{-2}$ wt.%**

in equilibrium with **30970 l** of **gas**, mainly **Ar**.

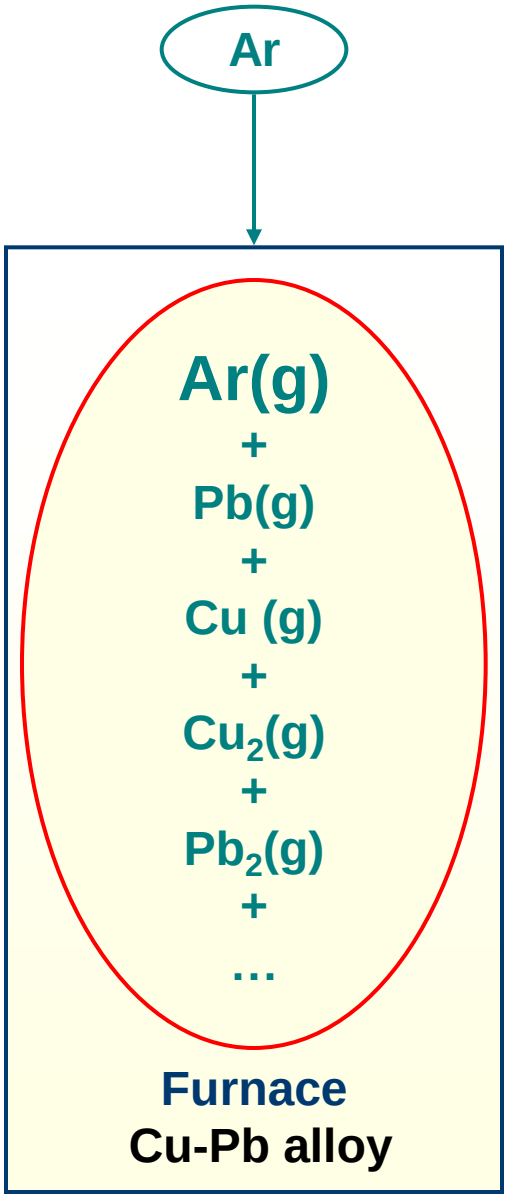
Results - Equilib 1200 C

Output Edit Show Pages

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

```
(gram)  99 Cu +  Pb +  <A> Ar =

   30970.      litre (   97.709      vol% Ar
                     +   1.7796      vol% Pb
                     +  0.51146      vol% Cu
                     +  0.16754E-03 vol% Cu2
                     +  0.59891E-06 vol% Pb2)
                        (1200.00 C,0.10000E-02 atm, gas_ideal)

+   98.972      gram (  0.55876E-01 wt.% Pb
                     +   99.944      wt.% Cu)
                        (1200.00 C,0.10000E-02 atm, Cu-liq)

where "A" on the reactant side is  10.00

*************************************************************
      H            G            V            S           Cp
     (J)          (J)          (l)        (J/K)       (J/K)
*************************************************************
 7.94952E+04 -2.11846E+05  3.09698E+04  1.97768E+02  5.41842E+01
```

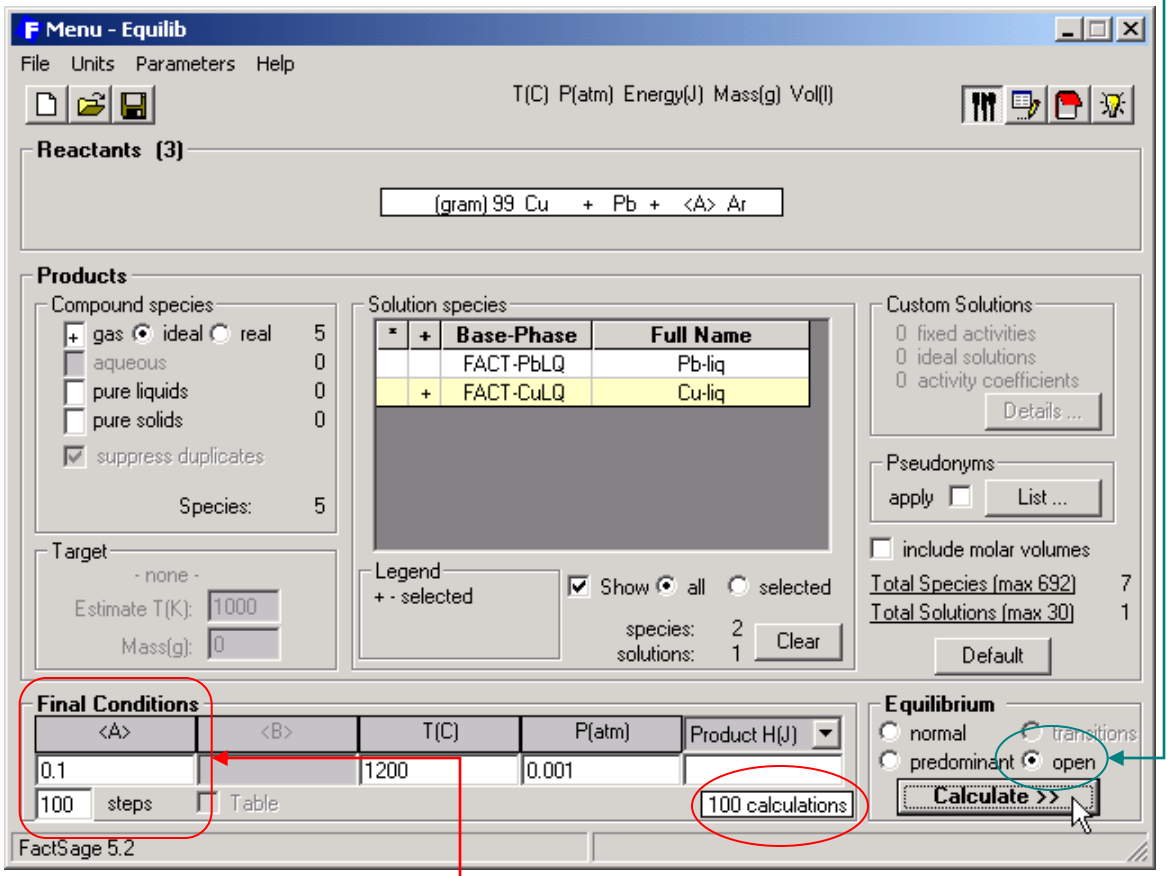
A = **10.0**, i.e. **10** g of **Ar** added to **100 g** of **alloy**.



# Deleading of a Cu-1wt%Pb alloy: Open calculation

**Setting** the final conditions for an **open** (i.e. **open** system) equilibrium calculation at **1200°C** and **0.001 atm** for **100** steps of incremental **<A> = 0.1**

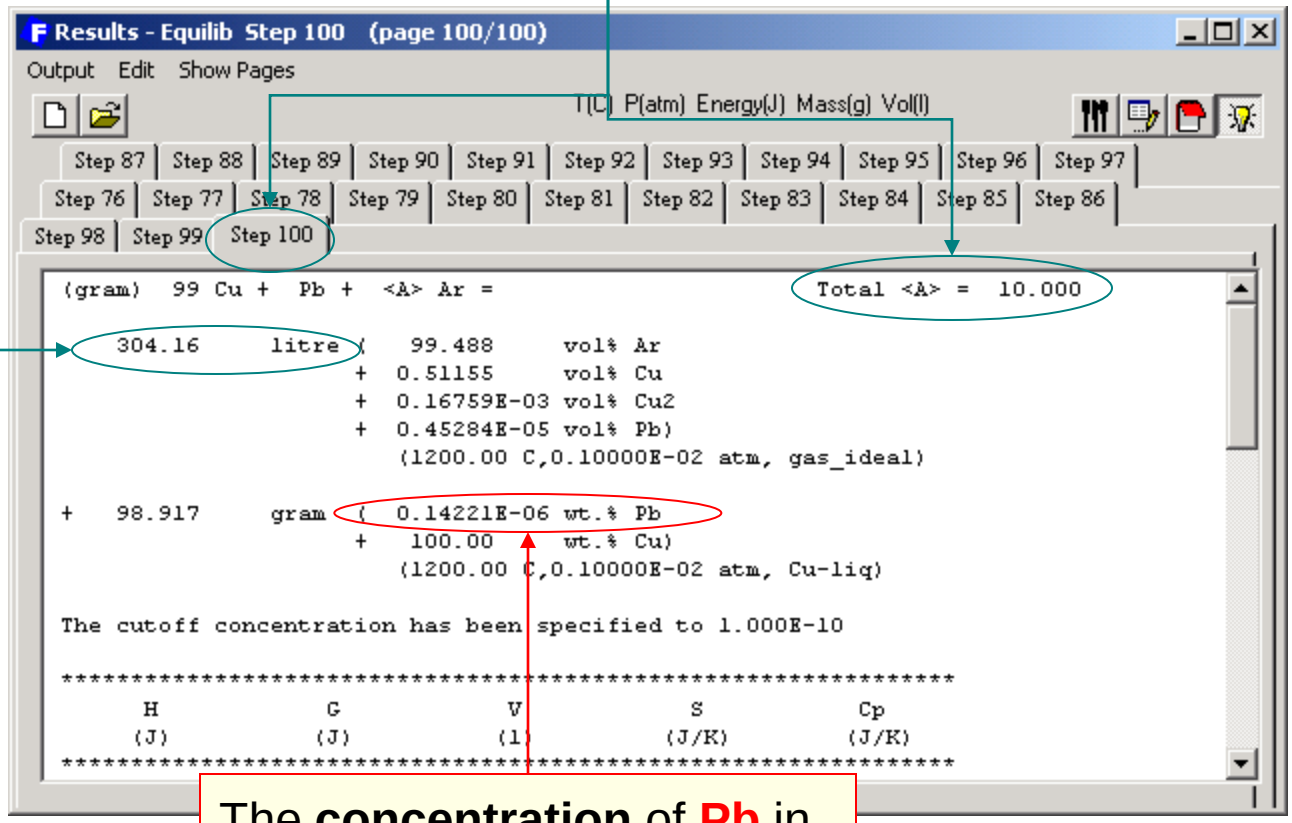
**1° Select open** in the **Equilibrium frame** to enable the **steps' Final Condition** input box




**2° Enter** the number of **steps** (here, **100**) and the amount **<A>** (here, **0.1** g of **Ar**) of reactant added to the system at each step at the end of which the gas phase is removed.

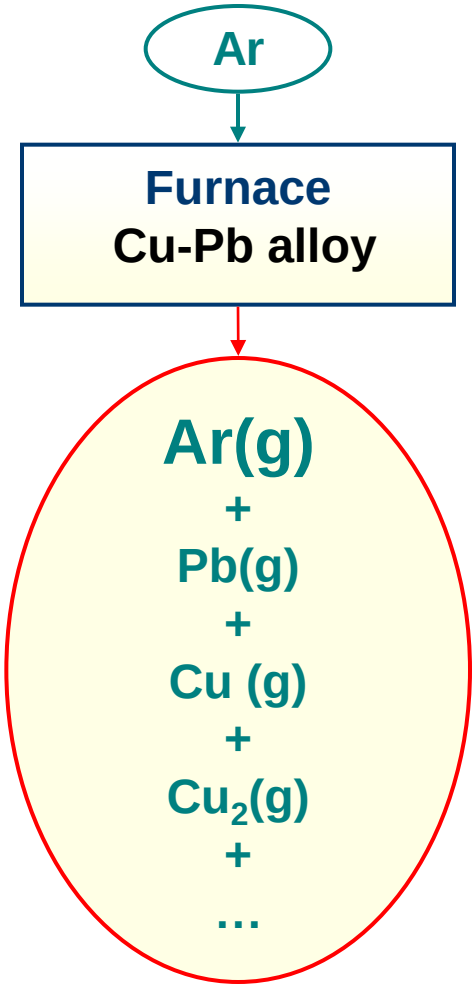
# Deleading of a Cu-1wt%Pb alloy: Open system equilibrium calculation

After 100 steps, A = **10.0**, i.e. **10** grams of **Ar** were added to **100** grams of **Cu-Pb alloy**



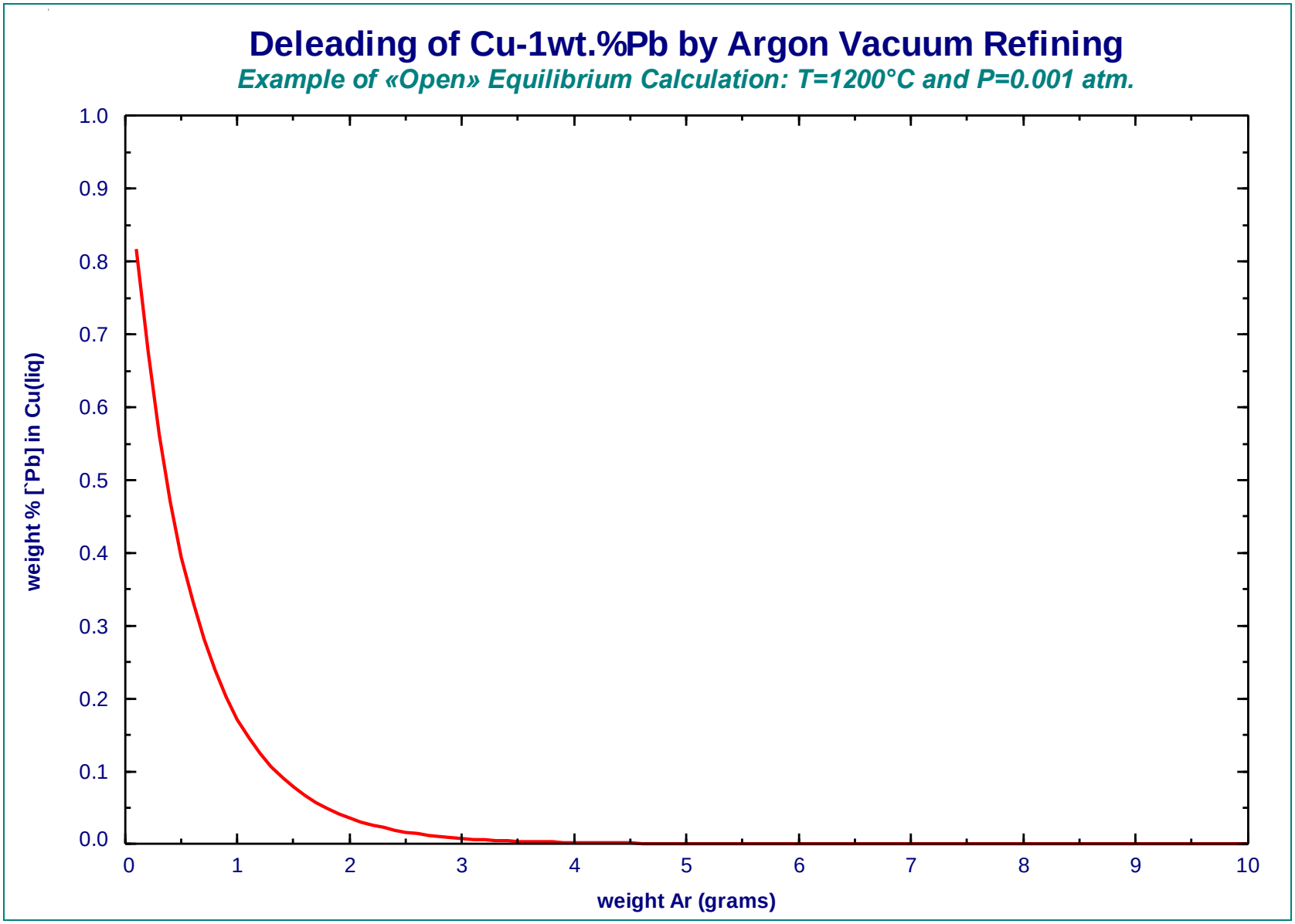

The **concentration** of **Pb** in **Cu(liq)** is **$1.4221 \times 10^{-7}$ wt.%**

in equilibrium with **304.16 l** of **gas**, mainly **Ar**.




**Note:**
The simulation is improved by specifying a smaller value of **<A>** (and a correspondingly larger number of steps).

# Deleading of a Cu-1wt%Pb alloy: Graphical Output



# Menu Window – Parameters menu

In the Parameters menu the user is given information on certain overall parameter values, e.g. the dimensions of the major data arrays.

The user may also modify certain parameters which relate to output lists or which permit the interference with the execution of the calculations.

The following slide shows the Parameter screen as a whole. Further slides are used to give details on the use of the parameters.

# Menu Window – Parameters menu

Dimensions frame

Target Limits frame

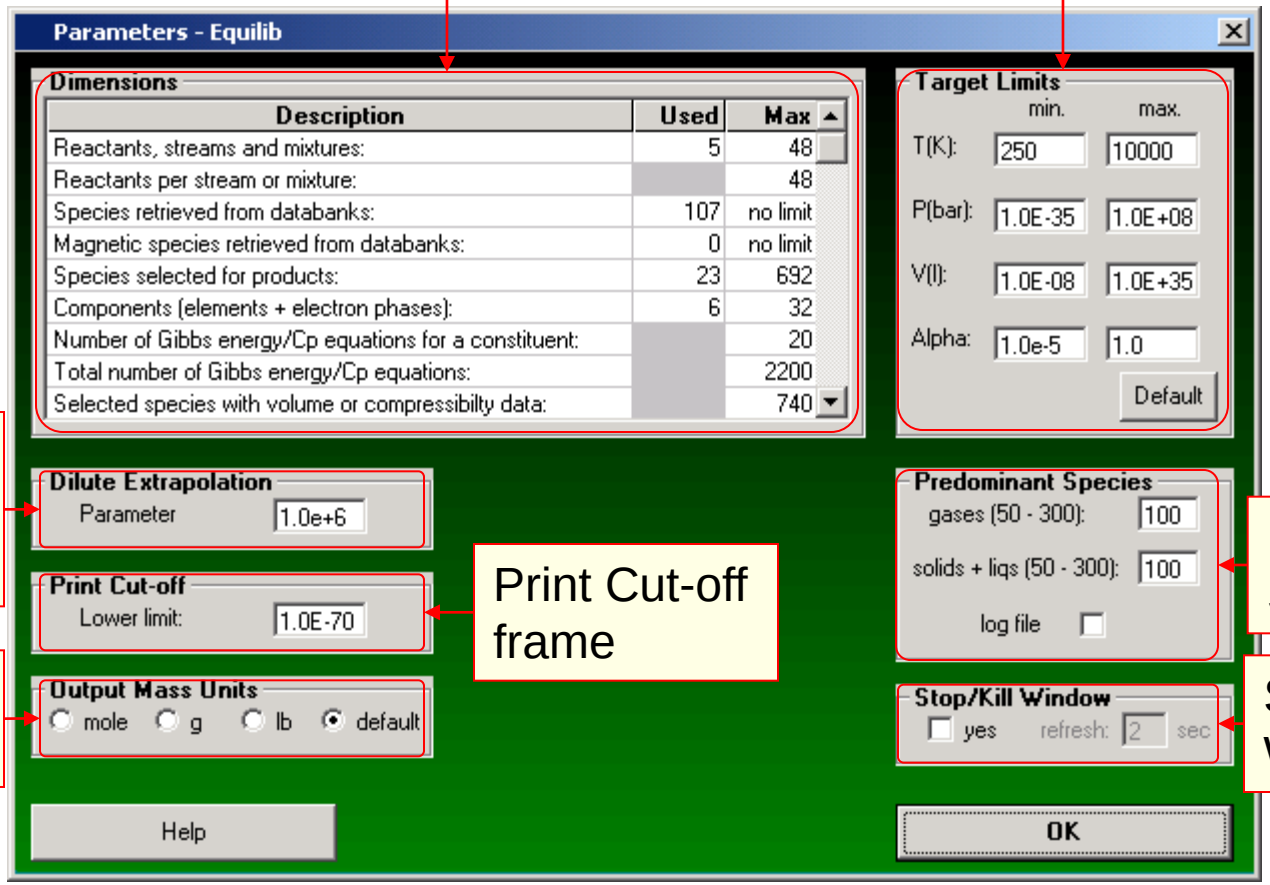
Dilute extrapolation frame

Print Cut-off frame

Predominant Species frame

Output Mass Units frame

Stop/Kill Window frame




**Help**

Additional information and extended menus are available for many of the items. Point to a frame heading or input box and then click the mouse-right-button.

# Parameters menu: Dimensions Frame

The following slide gives information on the Dimensions Frame.

This part of the Parameters menu is strictly for information of the user. NO changes may be made.

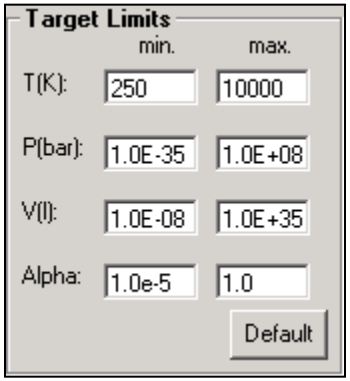
**Dimensions**

| Description | Used | Max |
|---|---|---|
| Reactants, streams and mixtures: | 5 | 48 |
| Reactants per stream or mixture: | | 48 |
| Species retrieved from databanks: | 107 | no limit |
| Magnetic species retrieved from databanks: | 0 | no limit |
| Species selected for products: | 23 | 692 |
| Components (elements + electron phases): | 6 | 32 |
| Number of Gibbs energy/Cp equations for a constituent: | | 20 |
| Total number of Gibbs energy/Cp equations: | | 2200 |
| Selected species with volume or compressibilty data: | | 740 |

- The dimensions table lists the current and maximum size of some commonly used variables. The maximum values are fixed during compilation and can not be modified without recompilation.
- Increasing a maximum value would increase the size of the program and reduce execution speed. Except for «Species selected for products», «Components», and «Total selected solutions», please contact us if you consider that a particular dimension is too small.

# Parameters menu: Target Limits Frame and Stop/Kill Button

The following slides shows how Target limits may be changed and how the Stop/Kill button is activated/deactivated.




## Target Limits

- These values are the lower and upper limits of temperature, pressure, volume and alpha when these values are being calculated by Equilib. It is recommended that the default settings be used.
- Click on the «Target» frame in the Menu Window for details on how to specify a target.

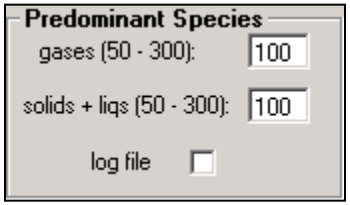
## Stop and Kill Button

- When «checked» you are able to follow the progress of the equilibrium calculation and have the option to «stop» or «kill» the calculation should the program get hung up.
- This feature is only really useful for large and lengthy calculations, or those cases where the program is unable to converge.

# Parameters menu: Predominant Species Frame

The following slide shows how the Predominant Species frame is made use of.

This input controls the execution of equilibrium calculations in which the number of species to be used exceeds the maximum number of species that may be used simultaneously.




## Predominant Species

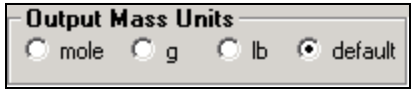
- These are the number of predominant gaseous species (50 to 300) and pure solid and liquid species (50 to 300) that will be calculated when the **Equilibrium** option «**Predominant**» is selected.
- To improve the chances of convergence it is recommended that you use «**300**» in both cases. If you must reduce the number (for example because you have selected more than 100 solution species) then you should retain «**300 gas**» species and reduce only the number of solid and liquid species.
- The «log file» records the progress of the predominant calculation. If you get the message **«- unable to calculate the standard state element(s)**» it may be useful to consult this file. The log file will appear in the Results Window only if the «**log file**» box is checked.

# Parameters menu: Dilute Extrapolation-Print Cut-off-Output Mass Units Frames

This slide shows how use is made of the Dilute Extrapolation, the Print Cut-off and the Output Mass units frames.

- This value is used for extrapolating solute data outside its normal dilute concentration range stored in its solution database.
- The parameter is an advanced feature of the program and should not be modified from its default value (1.0e+6).

- In the Results Window, equilibrium products below this value are not printed.
- This is useful in large calculations where you want to limit unwanted output for insignificant species.
- The value must be in the range 1.0e-70 to 0.01
- The value has no effect upon the results of the calculation.




- Normally the input reactants and output results are both in moles and mole fractions, or grams and weight per cent.
- This option enables you to have input moles and output weight, or vice versa. The equilibrium results are still the same, just the method of presenting the results is changed.
- Note, the same effect can be obtained using the "gram" and "mole" formats in the List Window.

# Reactants screen options

The following sixteen slides show how use is made of various options that can be found in the Reactants screen of the ***Equilib*** module.

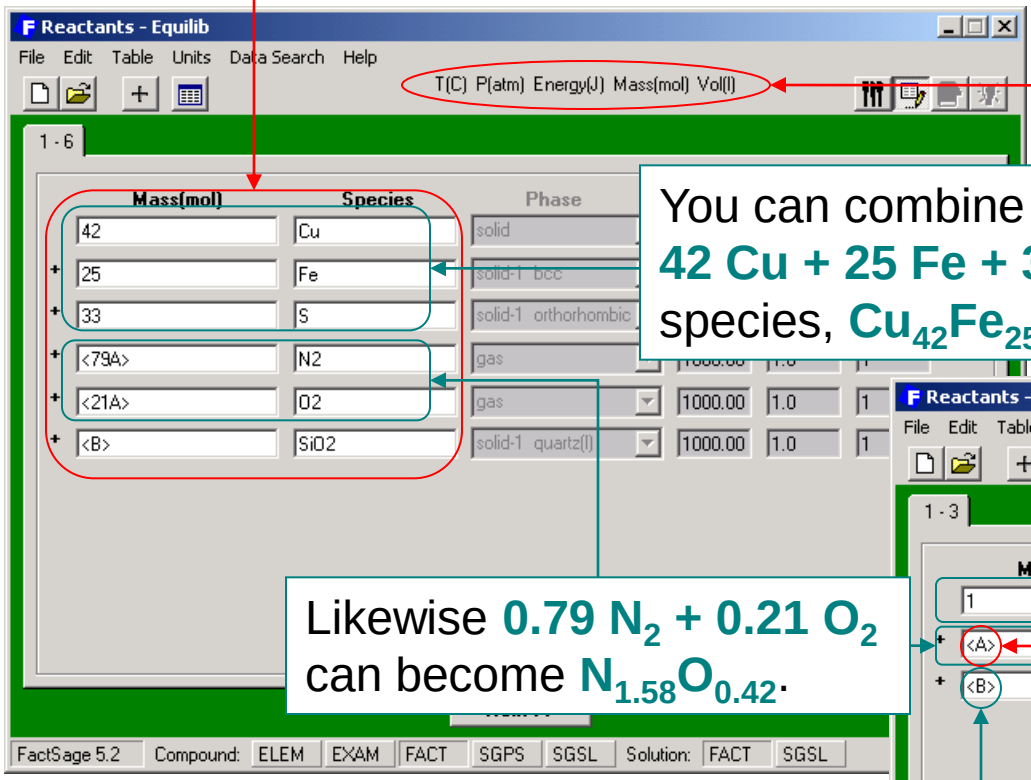
The use of arbitrary species formulae is shown in the following slide.

Note that this option is very useful when only the input amount of the «arbitrary» species is important for the calculation. As soon as extensive property changes are to be calculated this kind of input is not permitted since the «arbitrary» species has a chemical formula but no thermodynamic properties. Thus the input cannot be used to calculate the state properties of the reactants.

# Combining reactants into one composite chemical species

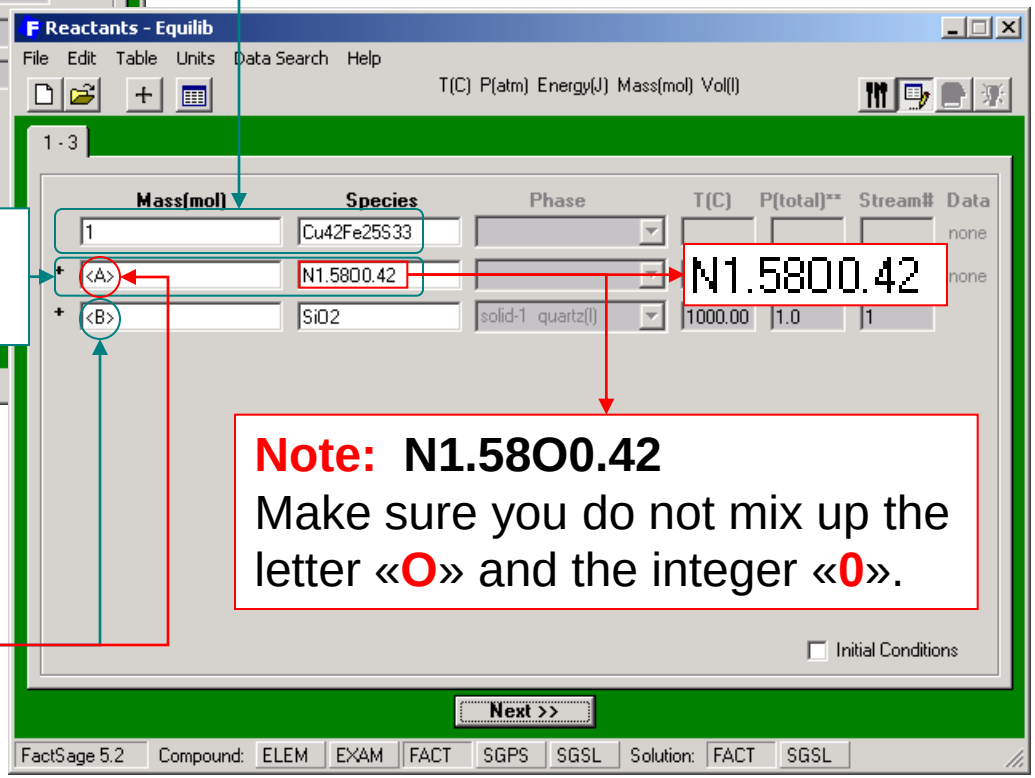
There are 6 reactants

The units are **T (°C)** and **Mass (mol)**




You can combine the 3 matte components, **42 Cu + 25 Fe + 33 S**, into one composite species, $Cu_{42}Fe_{25}S_{33}$.

Likewise **0.79 $N_2$ + 0.21 $O_2$** can become $N_{1.58}O_{0.42}$.




**Note: N1.58O0.42**
Make sure you do not mix up the letter «**O**» and the integer «**0**».

**<A>** is a **variable** corresponding to the number of moles of **air**, **<B>** is a **constant** amount of **$SiO_2$** defined in the **Menu Window**.

# Converting reactant mass units (mol g or lb)

The input of mass units in the Reactants screen is not fixed to the use of the unit that was chosen as default.

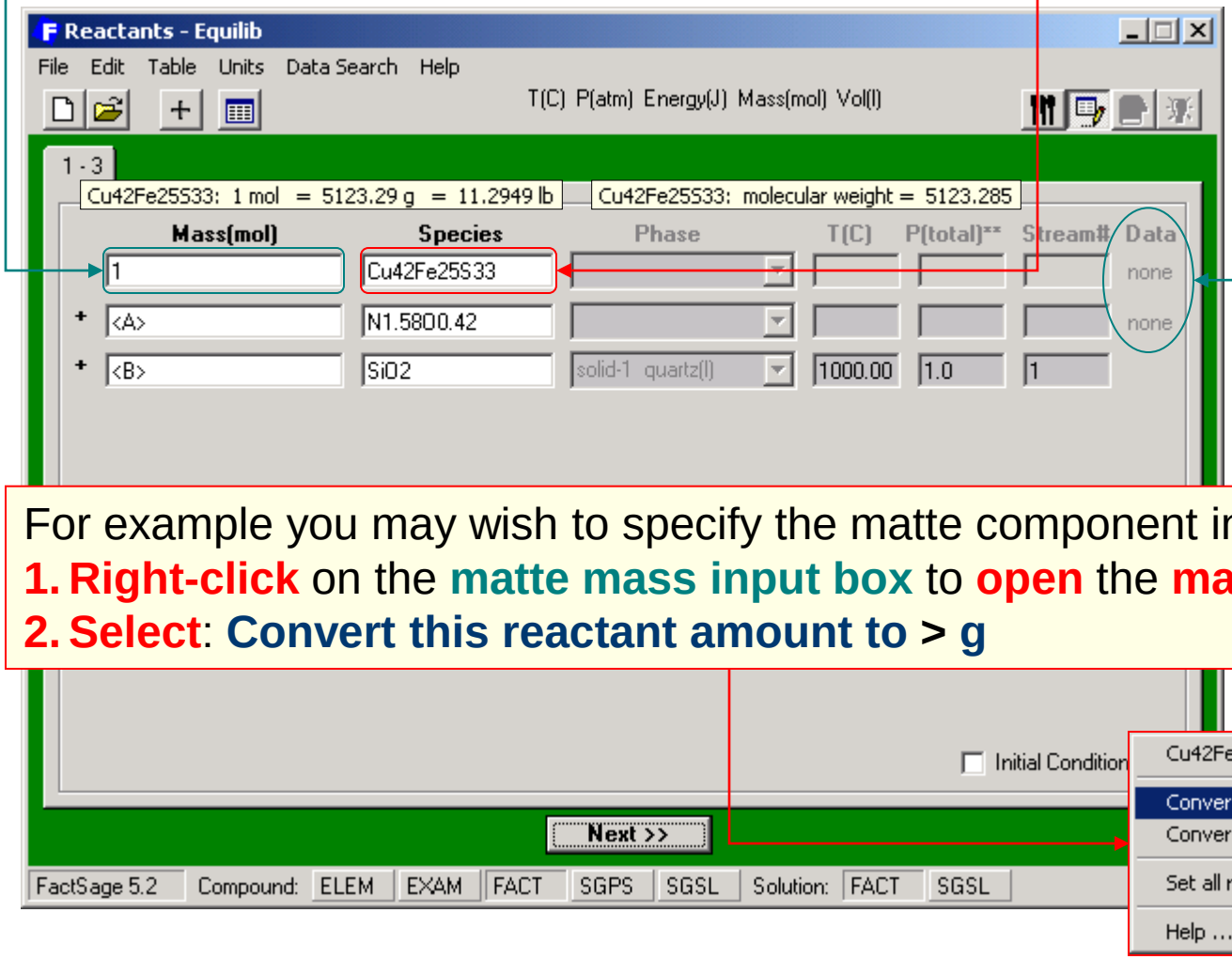
It is possible to «mix» mass units, i.e. to use the default for some and specific chosen units for others of the input substances.

The following two slides show how this is achieved.

# Converting reactant mass units (mol, g or lb)

Point the arrow in the mass input box to view the mass conversion.

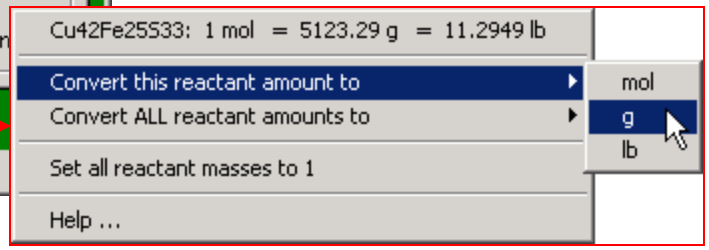
Point the arrow in the species input box to view the molecular weight.




**Note** that no data are available for the **composite chemical species**.

For example you may wish to specify the matte component in grams.

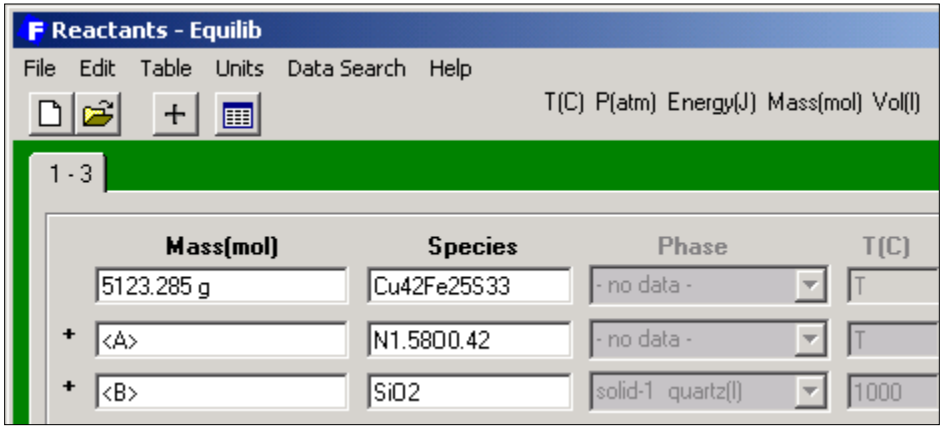
1. **Right-click** on the **matte mass input box** to **open** the **mass menu**.
2. **Select**: **Convert this reactant amount to > g**



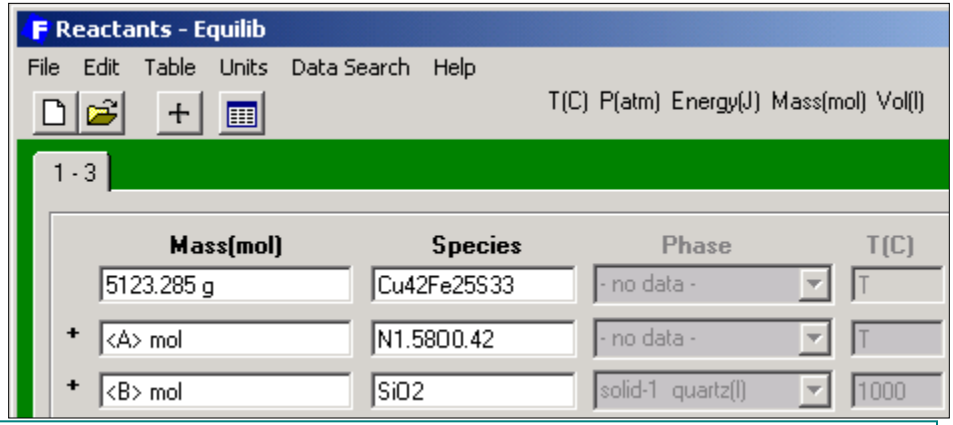
# Mixing reactant mass units of mol g and lb

You can mix the mass units by including a 'mol', 'g' or 'lb' in the reactant amount.

If the default mass units is mol, the following is equivalent to the above system:




Or if you like, you can always **explicitly** specify the mass units for each reactant amount to make your reactants data entry **independent** of the default mass units.




**Note:**

When creating a composite species (for example $Cu_{42}Fe_{25}S_{33}$ and $N_{1.58}O_{0.42}$)

- option «**initial conditions**» (Delta H, etc.) is **disabled** since there are no data for the species.
- the species is limited to 7 elements. For more than 7 elements use a mixture - refer to the ***Mixture*** module.

# Importing a stream or mixture

In addition to entering input substances by name/formula in the Reactants screen it is also possible to enter «groups» of substances as a whole package.

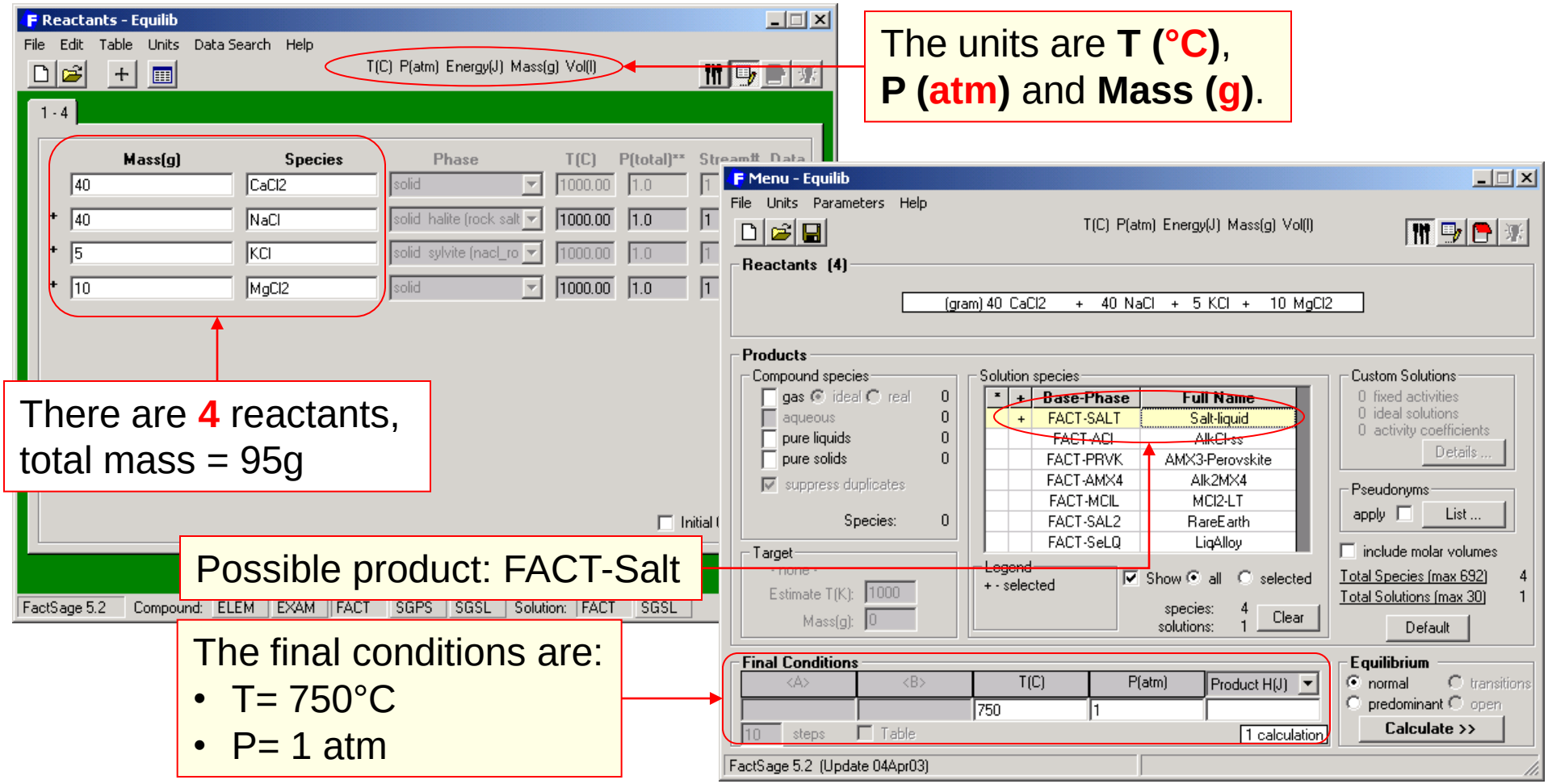
Such groups can be either Mixtures or Streams. For the generation of Mixtures see the Slide Show on the Mixture Module. For the generation of Stream see below (slides 11.4.1 and 11.4.2).

The following five slides (11.4.3 to 11.4.7) show the details of making use of Streams and Mixture in the Equilib input.

# Exporting and importing an equilibrated molten salt stream - $CaCl_2$-NaCl-KCl-$MgCl_2$

This example:

- **creates** and **saves** an equilibrated stream - $CaCl_2$-NaCl-KCl-$MgCl_2$ at 750°C.
- **imports** the stream into a new reaction
- **performs** various isothermal and adiabatic heat balances using the imported stream




The units are **T (°C)**, **P (atm)** and **Mass (g)**.

There are **4** reactants, total mass = 95g

Possible product: FACT-Salt

The final conditions are:

- T= 750°C
- P= 1 atm

# Saving an equilibrated stream

Results - Equilib 750 C

Output Edit Show Pages

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

```
(gram)  40 CaCl2 +  40 NaCl +  5 KCl +  10 MgCl2 =

    95.000      gram  (   42.105      wt.% NaCl
                      +   5.2632      wt.% KCl
                      +   10.526      wt.% MgCl2
                      +   42.105      wt.% CaCl2)
                         (750.00 C, 1 atm, Salt-liquid)
                      Mole fraction of sublattice constituents in Salt-liquid:
                      Na            0.56242
                      K             0.55112E-01
                      Mg            0.86307E-01
                      Ca            0.29616
                      ------------------------
                      Cl             1.0000

*****************************************************************
      H            G            V            S            Cp
     (J)          (J)          (l)         (J/K)        (J/K)
*****************************************************************
-5.78317E+05 -8.25636E+05  0.00000E+00  2.41724E+02  1.00273E+02
```

Equilibrated molten salt

Output

- Save or Print
- Plot
- Equilib Results file
- Stream File
  - Save stream file
    - Save gas phase ...
    - Save liquids ...
    - Save aqueous phase ...
    - Save solids ...
    - Save solution
      - FACT-SALT
  - Stream file properties ...
  - Summary of streams
  - Directory (C:\FACT-51\) ...
- Format

Save File in C:\FACT-51\Mixt*.dat

Enter the stream file number (1 - 9999)

OK

Cancel

12

Save File

Saving file 12

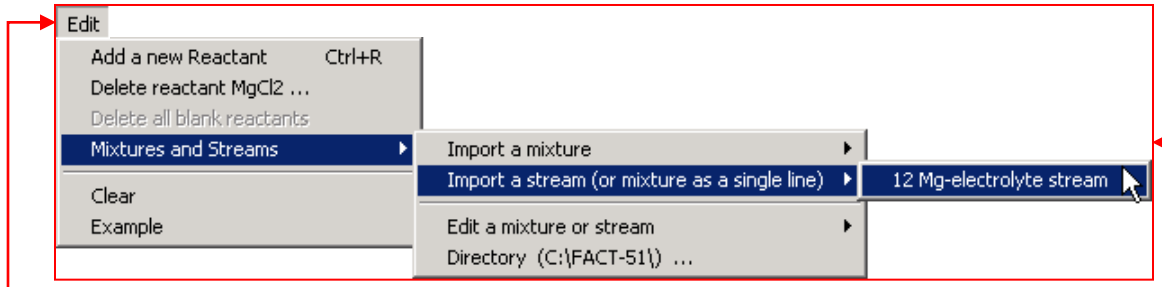
Enter the name of the stream (upto 26 characters)
ex: Roaster Gas, Cu Matte, Slag

OK

Cancel

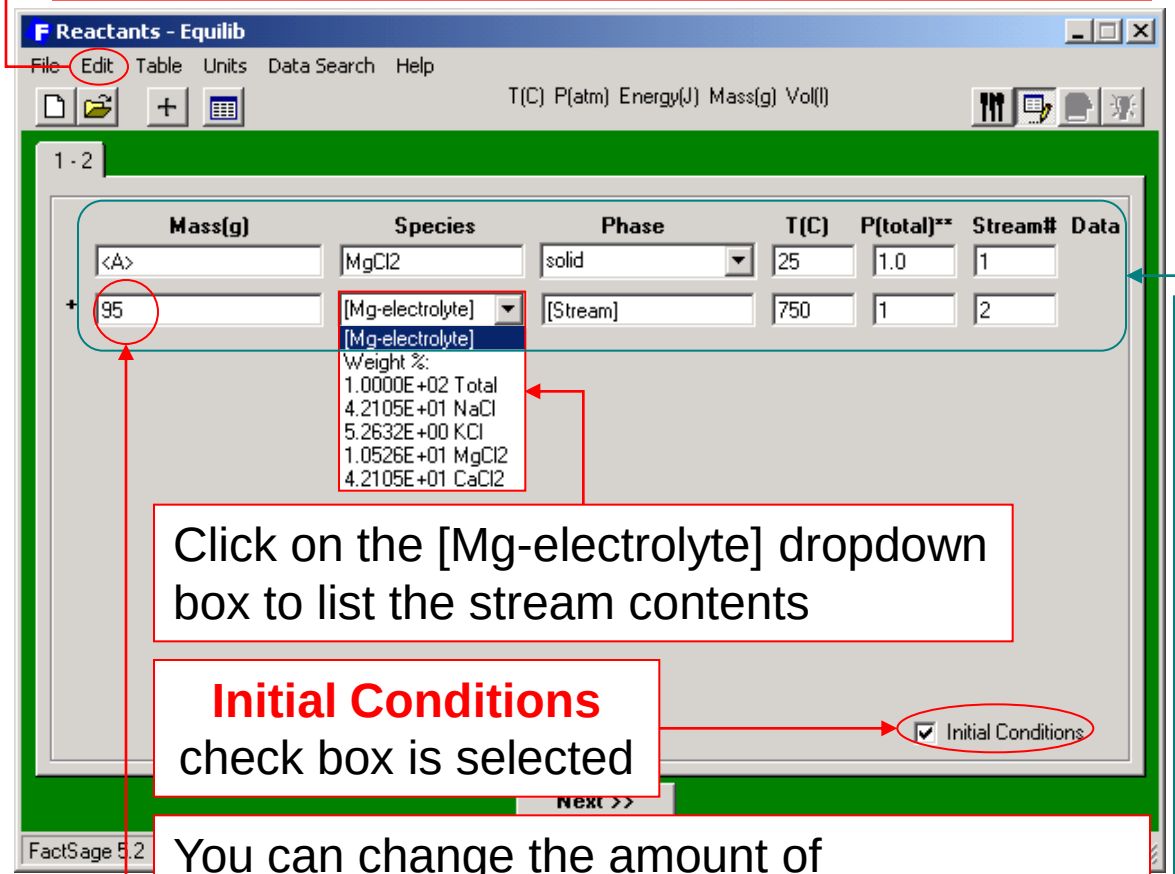
Mg-electrolyte

# Importing the stream into a reaction




**Import** the **Mg-electrolyte stream** by **selecting** it in the **Edit Menu**

There are now **2 reactants**:
**<A> $MgCl_2$(s,25°C)** +
**95 [Mg-electrolyte] (stream,750°C)**
i.e. <A + 95> grams total.




Click on the [Mg-electrolyte] dropdown box to list the stream contents

**Initial Conditions** check box is selected

You can change the amount of [**Mg-electrolyte**] from its default value (95 g)

**Note:** You cannot change the initial T (750°C) or P (1 atm) of the [Mg-electrolyte] stream - these values, together with selected stream thermodynamic properties (H, S, G, $C_p$, V), are stored in the stream file (mixt12.dat) and are imported into the calculation when **Initial Conditions** (ΔH, etc.) is checked.

# Equilibrated <0> and <5> $MgCl_2$ + 95g [Mg-electrolyte] stream at 750°C

In the **Menu Window** **FACT-Salt** is the only possible product. Set <**A**> = '**0 5**' (i.e. alpha = 0 and 5), **T = 750°C** and **P = 1 atm**. The **Results** are:

F Results - Equilib 750 C, A=0 (page 1/2)

Output Edit Show Pages

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

750 C, A=0 | 750 C, A=5

```
(gram)  <A> MgCl2 +  95 [Mg-electrolyte] =
 (25,1,s,#1) (750,1,stream,#2)

    95.000      gram  (   42.105      wt.% NaCl
                      +   5.2632      wt.% KCl
                      +   10.526      wt.% MgCl2
                      +   42.105      wt.% CaCl2)
                         (750.00 C, 1 atm, Salt-liquid)
                      Mole fraction of sublattice constituents in Salt-liquid:
                      Na            0.56242
                      K             0.55112E-01
                      Mg            0.86307E-01
                      Ca            0.29616
                      ------------------------
                      Cl             1.0000

where "A" on the reactant side is 0.0000

*****************************************************************************
  DELTA H       DELTA G       DELTA V       DELTA S       DELTA Cp      PROD V
    (J)           (J)           (1)           (J/K)         (J/K)         (1)
*****************************************************************************
0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+0
```

A = 0

Calculated **ΔH=0** – imported and equilibrated streams are the same.

Calculated **ΔH=4415 J** – this is the total energy required to heat 5 g $MgCl_2$ from 25 to 750°C and dissolve it into the molten salt.

F Results - Equilib 750 C, A=5 (page 2/2)

Output Edit Show Pages

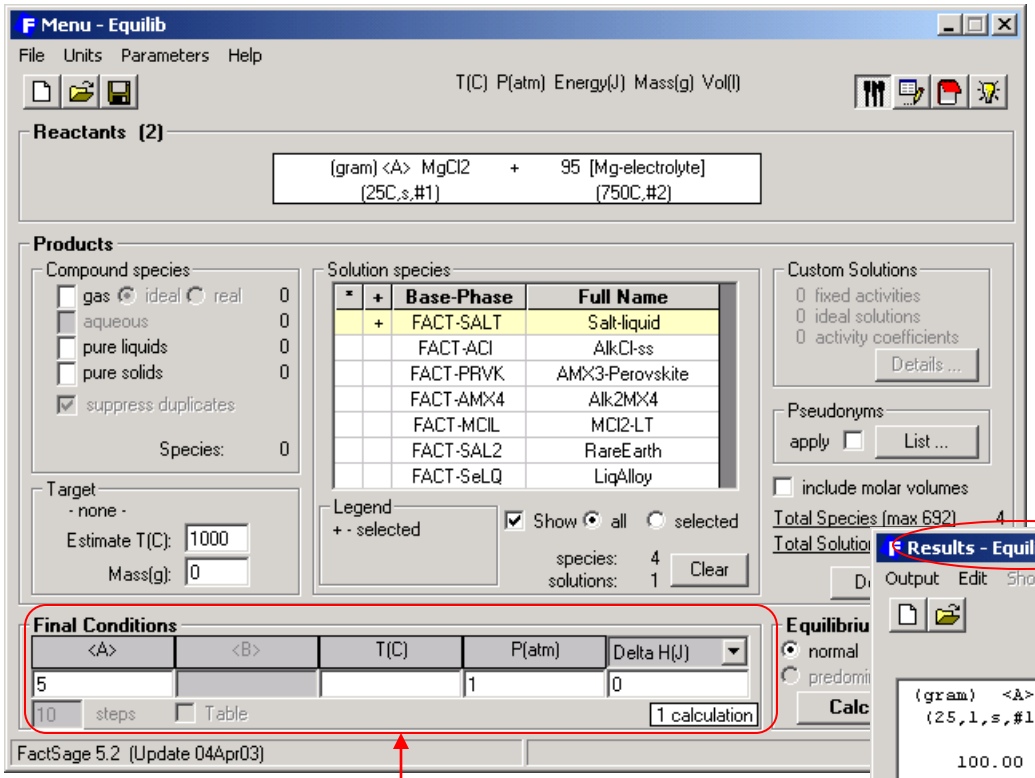
T(C) P(atm) Energy(J) Mass(g) Vol(l)

750 C, A=0 | 750 C, A=5

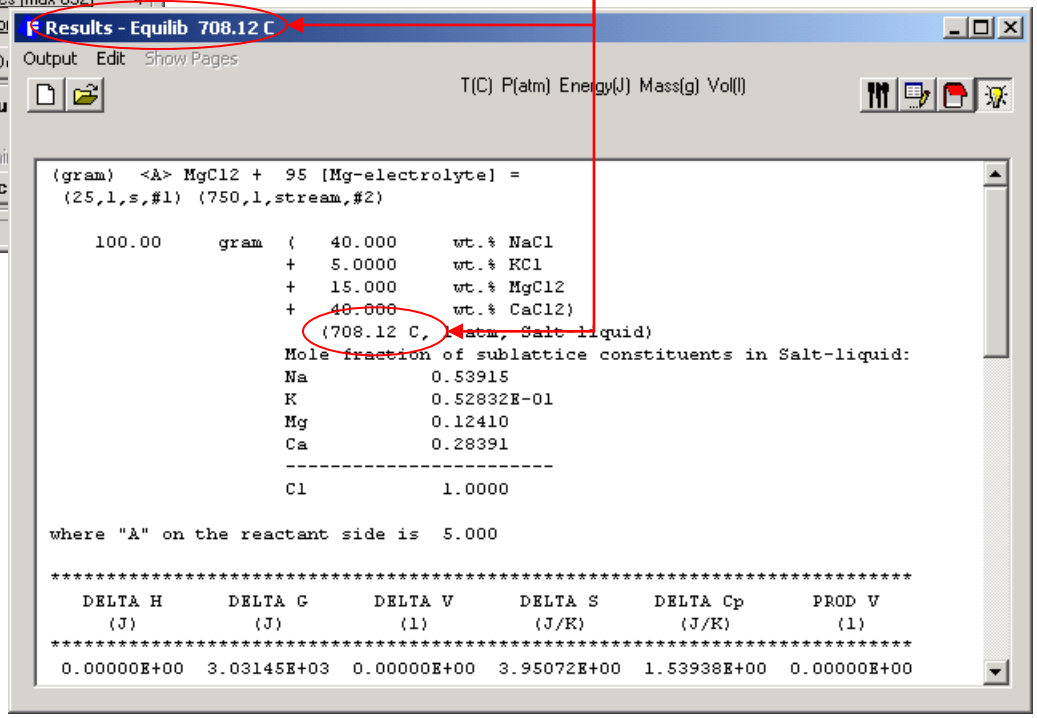
```
(gram)  <A> MgCl2 +  95 [Mg-electrolyte] =
 (25,1,s,#1) (750,1,stream,#2)

    100.00      gram  (   40.000      wt.% NaCl
                      +   5.0000      wt.% KCl
                      +   15.000      wt.% MgCl2
                      +   40.000      wt.% CaCl2)
                         (750.00 C, 1 atm, Salt-liquid)
                      Mole fraction of sublattice constituents in Salt-liquid:
                      Na            0.53915
                      K             0.52832E-01
                      Mg            0.12410
                      Ca            0.28391
                      ------------------------
                      Cl             1.0000

where "A" on the reactant side is  5.000

*****************************************************************************
  DELTA H       DELTA G       DELTA V       DELTA S       DELTA Cp      PROD V
    (J)           (J)           (1)           (J/K)         (J/K)         (1)
*****************************************************************************
4.41494E+03  -7.54762E+03   0.00000E+00   8.35660E+00   1.25388E+00   0.00000E+00
```

A = 5

# Adiabatic <5> $MgCl_2$ (solid, 25°C) + 95 g [Mg-electrolyte] stream

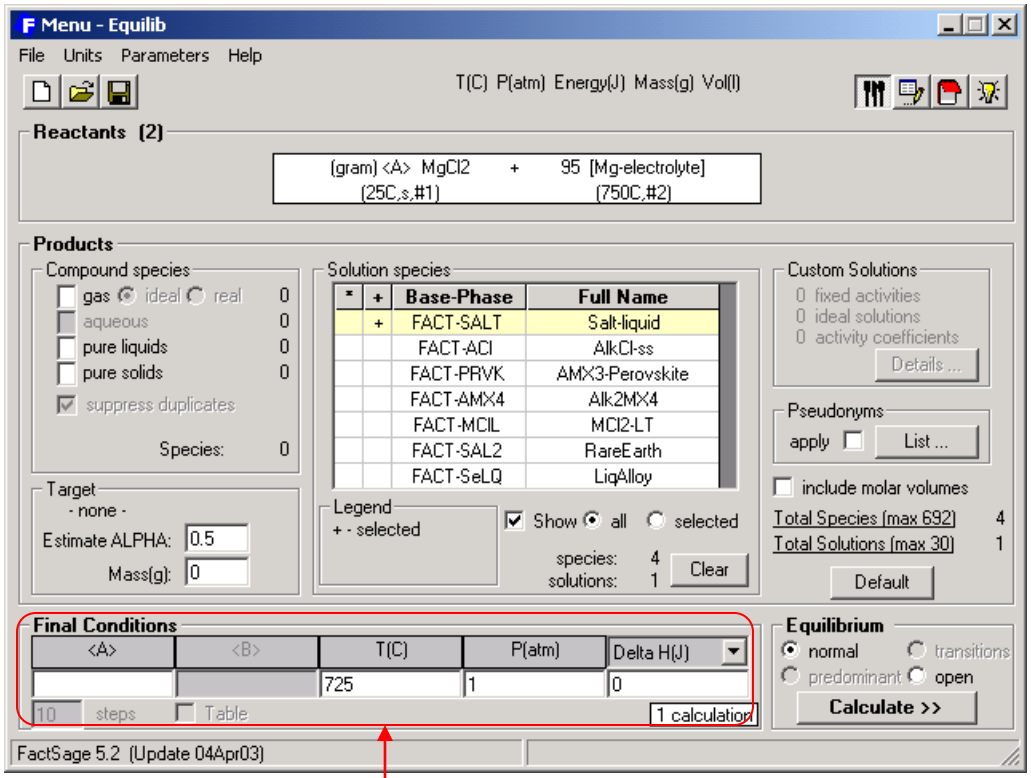



The output shows a calculated **adiabatic** temperature of **708.12°C**.




Return to the **Menu Window**, **set** <**A**> = **5** and **T(C)** undefined ('**blank**') then specify an adiabatic reaction: **ΔH = 0**.

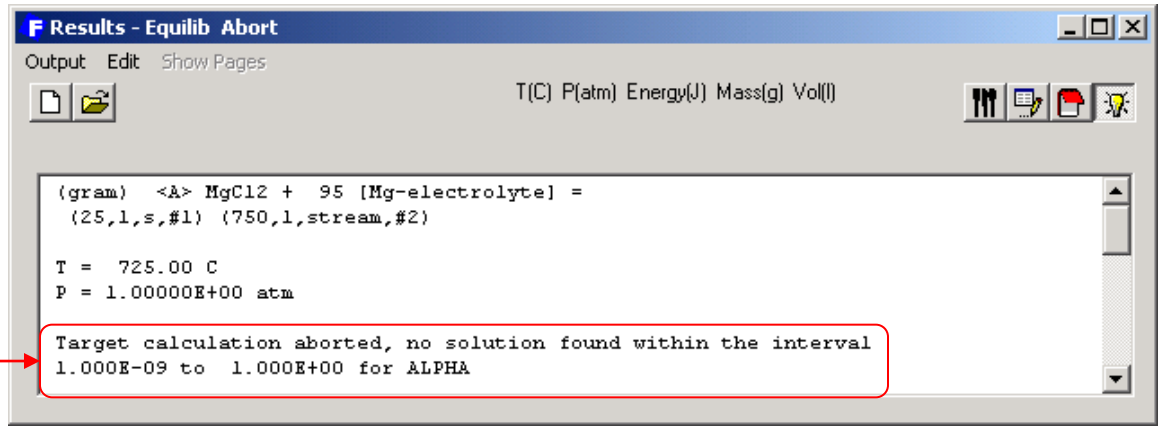
# Adiabatic <A> $MgCl_2$ (solid, 25°C)+ 95 g [Mg-electrolyte] stream at 725°C



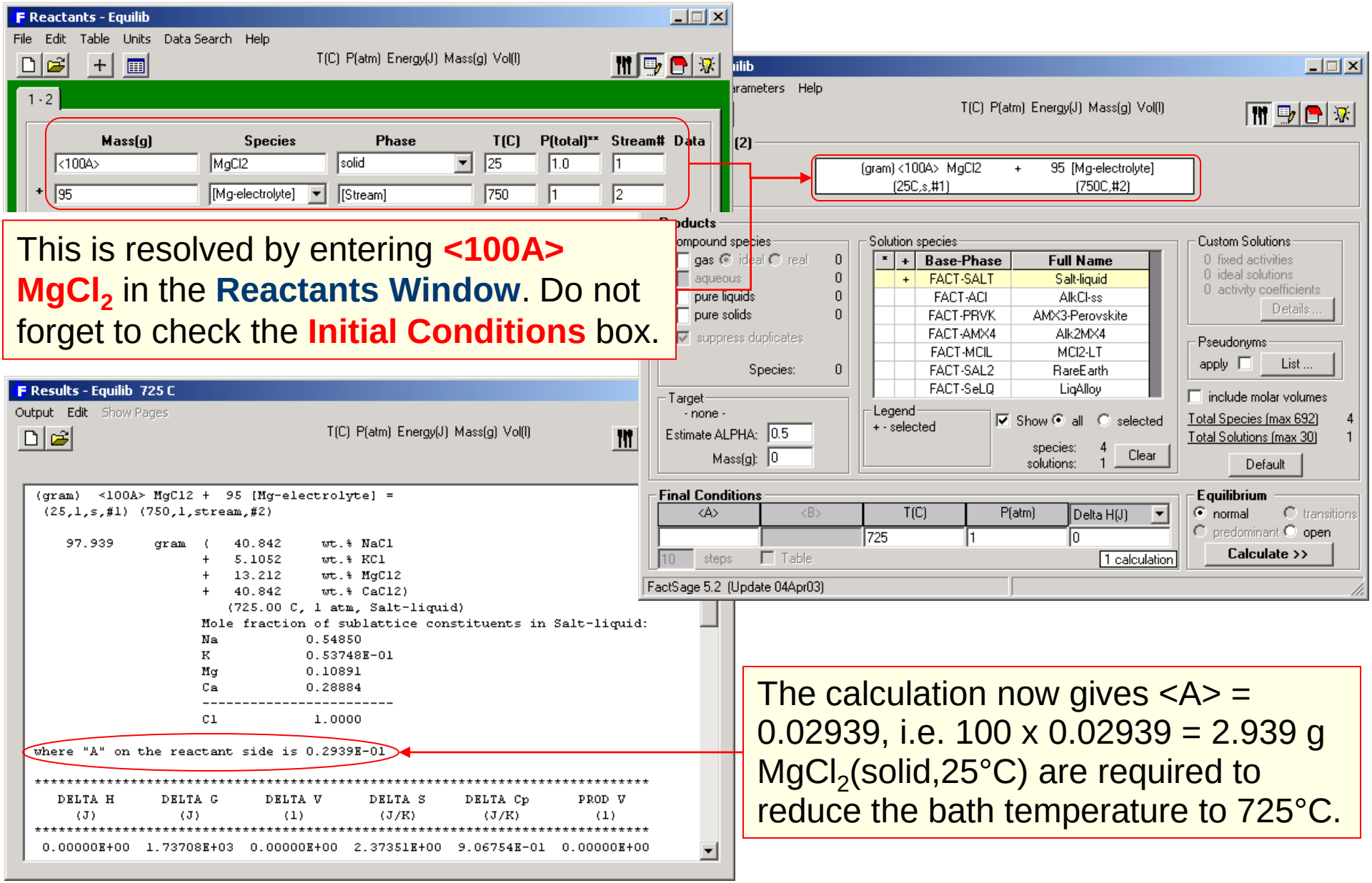

From the previous **Results** we know that the value of <A> should be 2 - 3 g. But ***Equilib*** requires that the calculated <A> be no more than 1.0.

Return to the **Menu Window**, set <**A**> undefined ('**blank**'), set **T(C) = 725°C** , and specify an adiabatic reaction: **ΔH = 0**.

The output shows:



# Adiabatic <100A> $MgCl_2$ (solid, 25°C)+ 95 g [Mg-electrolyte] stream at 725°C




This is resolved by entering **<100A>** **$MgCl_2$** in the **Reactants Window**. Do not forget to check the **Initial Conditions** box.

The calculation now gives <A> = 0.02939, i.e. 100 x 0.02939 = 2.939 g $MgCl_2$(solid,25°C) are required to reduce the bath temperature to 725°C.

# Using Reaction Table input

In addition to the two «group input» methods outlined above it is also possible to employ Reaction Tables from which the input amounts are read.

Such Reaction Tables provide the opportunity to enter input amounts for cases in which non-linear changes of the amounts are needed. In the table each line contains for a given set of input substances the irregularly changing amounts.

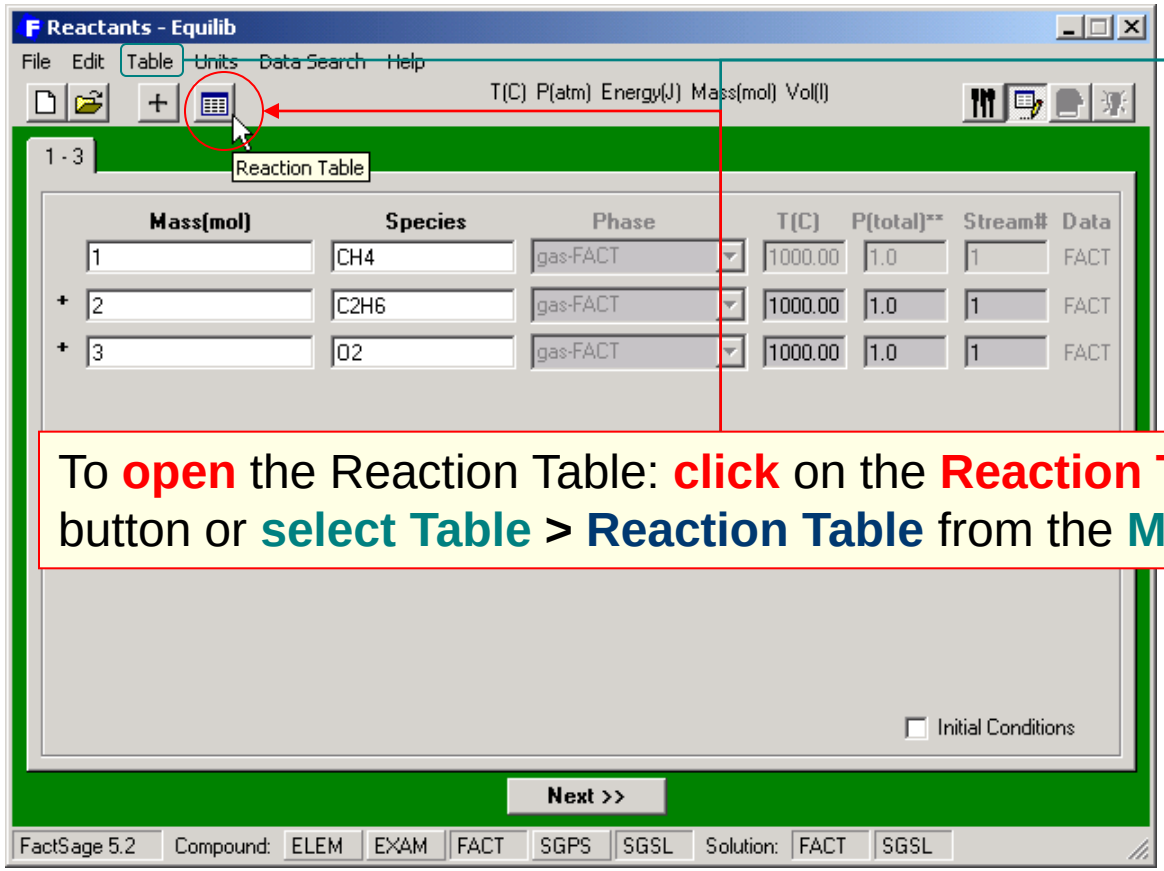
In the calculations the line number (Page number) will be treated as the independent parameter in order to sort the result tables.

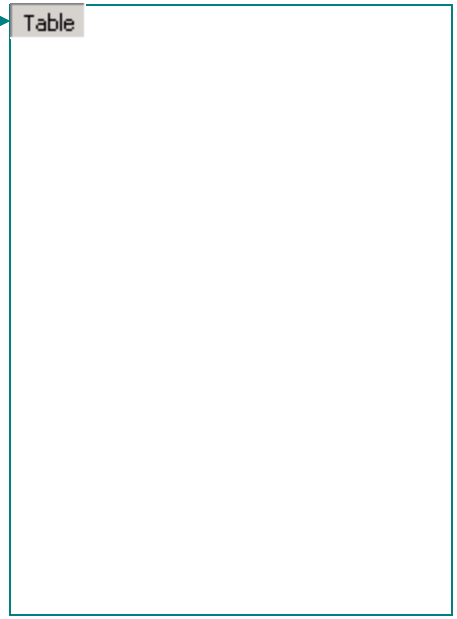
The Page number can also be used as an axis variable in the ***Result*** module.

# Reaction Table

In the **Reactants Window** you specify a set of reactant amounts, for example: 1 mol $CH_4$ + 2 mol $C_2H_6$ + 3 mol $O_2$:

With the **Reaction Table** you can specify many different sets of reactant amounts as well as their product temperatures and pressures - each resulting in a separate equilibrium calculation.

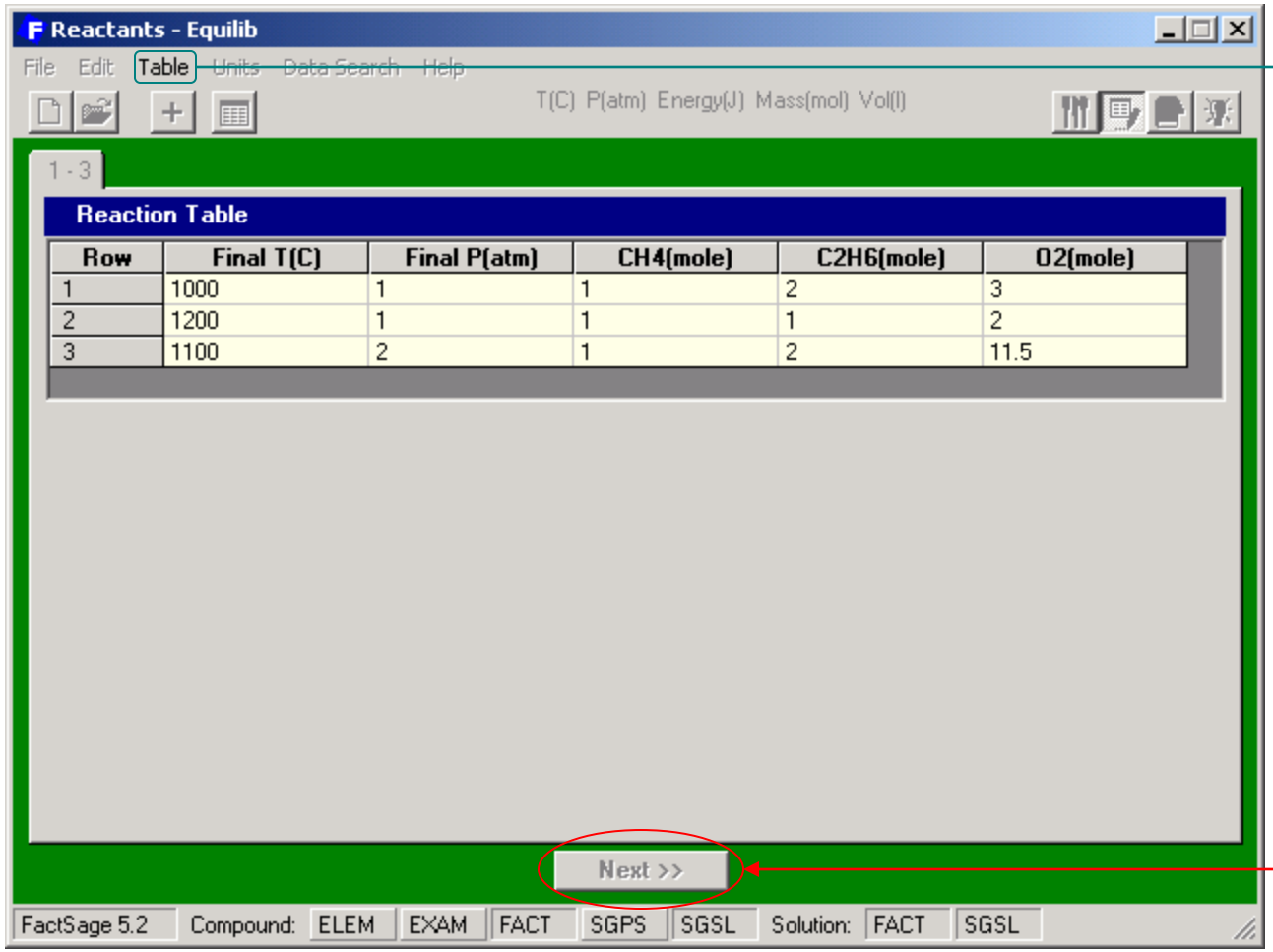


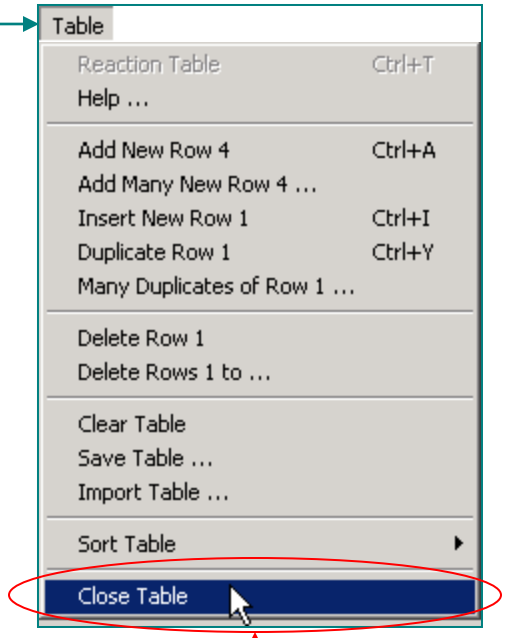

To **open** the Reaction Table: **click** on the **Reaction Table** button or **select Table > Reaction Table** from the **Menu Bar**.

# Editing the Reaction Table

Each set (row in the **Reaction Table**) generates a page in the **Results Window**. There is no limit to the number of sets. The **Reaction Table** may be created and edited here, or imported via a simple text or Excel spreadsheet.

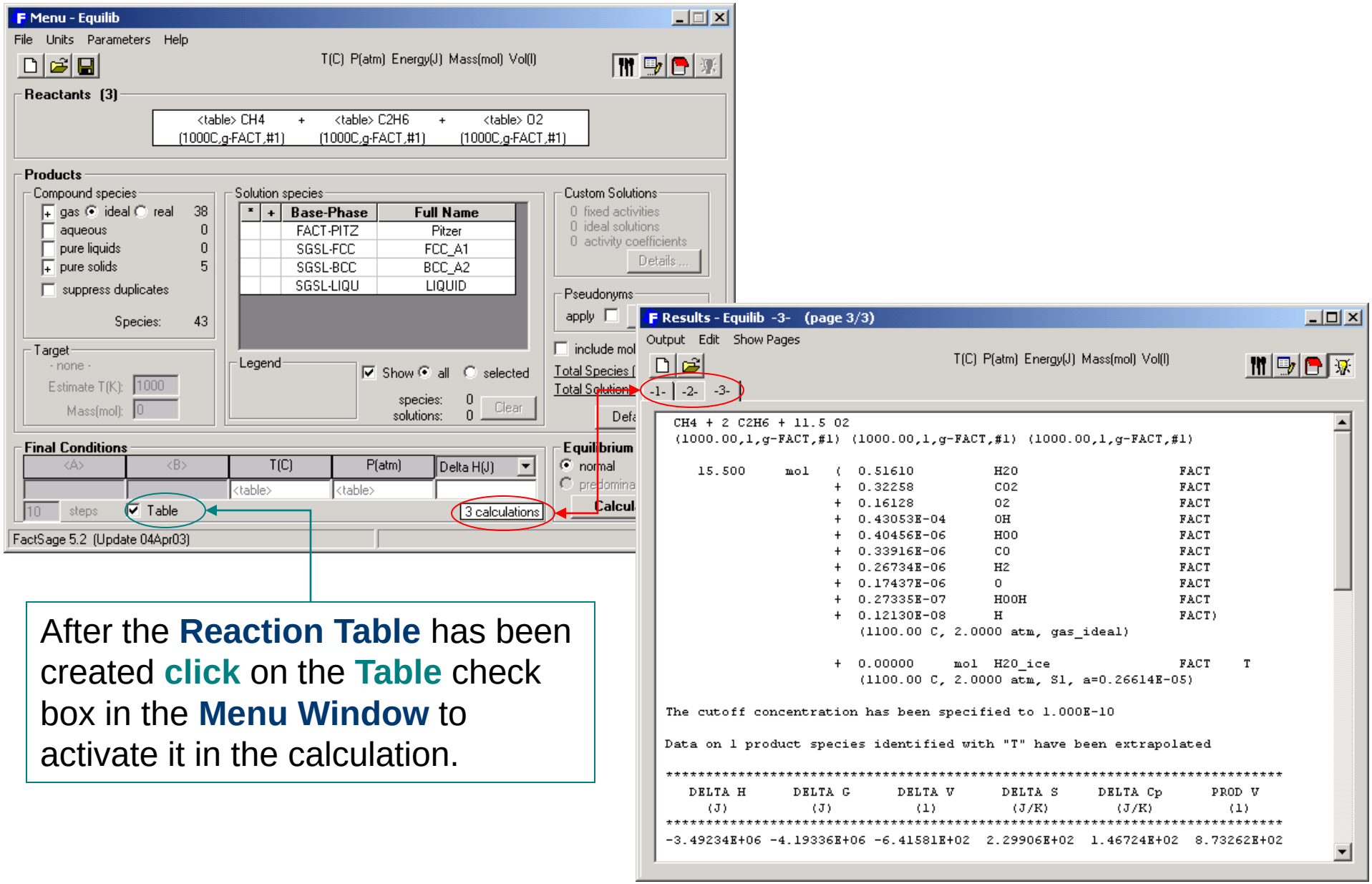



| Row | Final T(C) | Final P(atm) | CH4(mole) | C2H6(mole) | O2(mole) |
|---|---|---|---|---|---|
| 1 | 1000 | 1 | 1 | 2 | 3 |
| 2 | 1200 | 1 | 1 | 1 | 2 |
| 3 | 1100 | 2 | 1 | 2 | 11.5 |




After creating the table, **Close** it and **press Next >>**

# Reaction Table – Results Window



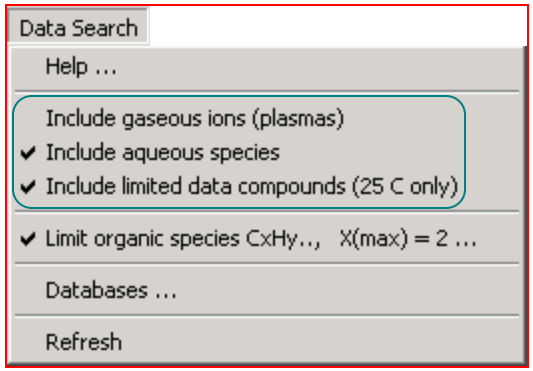

After the **Reaction Table** has been created **click** on the **Table** check box in the **Menu Window** to activate it in the calculation.

# Data search options

The following three slides show how the various options in the Data Search menu are employed to select/deselect specific data entries in a database.

It is shown how the Gas Ions, Aqueous Species, Limited Data and CxHy options are made use of.

# Data Search Menu: gas ions, aqueous species, limited data




- **Include gaseous ions (plasmas):**

  Gaseous ion concentrations are only significant at high temperatures and only meaningful in plasma calculations. Gaseous ions add a component (the electron) to the calculation and increase the total number of gaseous species. This increases slightly the calculation time. For most practical calculations gaseous ions have no effect and so it is safe not to include them in the data search.

  **Debye Shielding** is automatically taken into account for plasmas in *FactSage* versions 5.5 and higher.

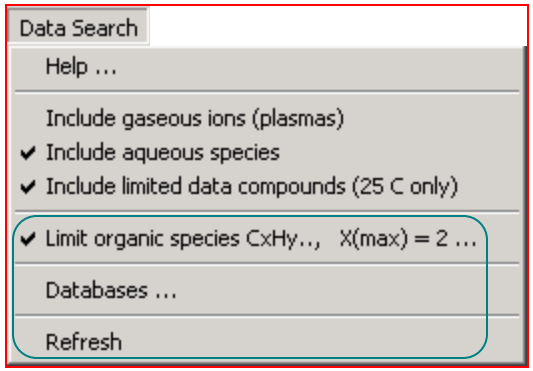
- **Include aqueous species:**

  Including aqueous species is only meaningful in aqueous (hydrometallurgical) calculations at or near room temperature. If your calculations are above 300°C there is no point in including the aqueous species. This option has no effect upon gaseous ions (plasmas).

- **Include limited data compound (25°C/298K data only):**

  Some solid and liquid compound species only have limited data - typically the Gibbs energy of formation at 298.15 K but without Cp and enthalpy data. In Equilib these compounds are flagged as '25°C or 298 K only' in the List Window. Such species are automatically dropped from the calculation if the final temperature is above 25°C. In such a case the "activity" column in the List Window is blank. Since most of these species are unimportant and in most cases ignored anyway then there is little need to select this option.

# Reactants window – Data Search Menu: $C_xH_y$, databases




- **Limit organic species $C_xH_y$:**

  The main compound substances database contains several hundred organic species $C_xH_y$… where the stoichiometric factor "x" can be large. These large organic molecules have little use in most inorganic calculations and are unlikely products in most equilibrium calculations. To drop large organic species from the data search you set "x" to the desired upper limit. For most calculations it is recommended you set x = 2, which means that organic molecules with 3 or more carbon atoms will be dropped from the data search.

- **Databases:**

  **Opens** the databases window.

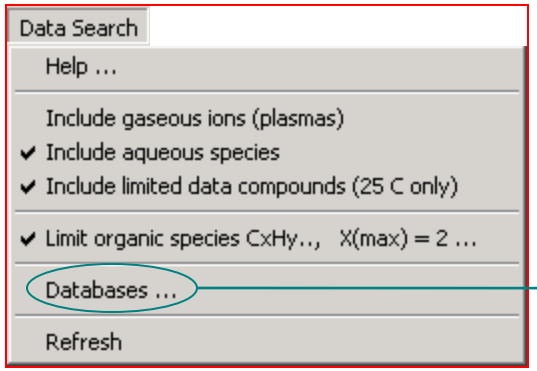
  Databases may be added to or removed from the data search. For example private data entered through the Compound and Solution programs, or other commercial databases such as Thermo-Tech. If you have both FACT and SGTE databases then you use this option to tell the program to search both databases or search only one.

  Note: Clicking on the databases bar also opens the Databases window.

  **Refresh:**

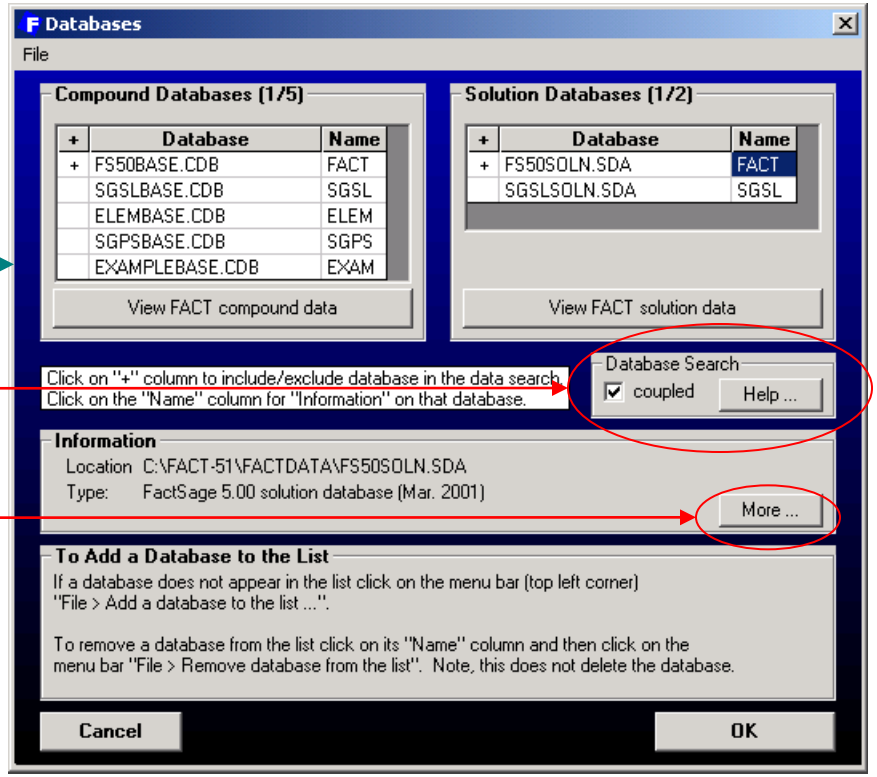
  In the Data Search menu when you change a search option (gaseous ions, aqueous species, limited data) or database selection then ***Equilib*** will automatically 'refresh' the system with the new options and data. However, if changes to the databases are made via another program (for example Compound and Solution) you must click on “Refresh" to update the current system.

# Databases Window




More information about coupled databases

More information about the selected database.




If '**coupled**' is checked (this is the recommended setting) then compound and solution databases with the same nickname (for example ***FACT*** or SGSL) are treated as a group.

For example, if you click on the '+' column in order to include the ***FACT*** compound database in the data search then the program automatically includes the ***FACT*** solution database. Likewise if you remove the SGSL solution database from the data search the program automatically excludes the SGSL intermetallic compound database.

If 'coupled' is NOT checked then the databases can be included or excluded independently. However this is not recommeded since it can lead to misleading results.

# *Equilib* Cooling Calculations

The ***Equilib*** module enables you to perform cooling calculations and display the phase transitions and compositions during

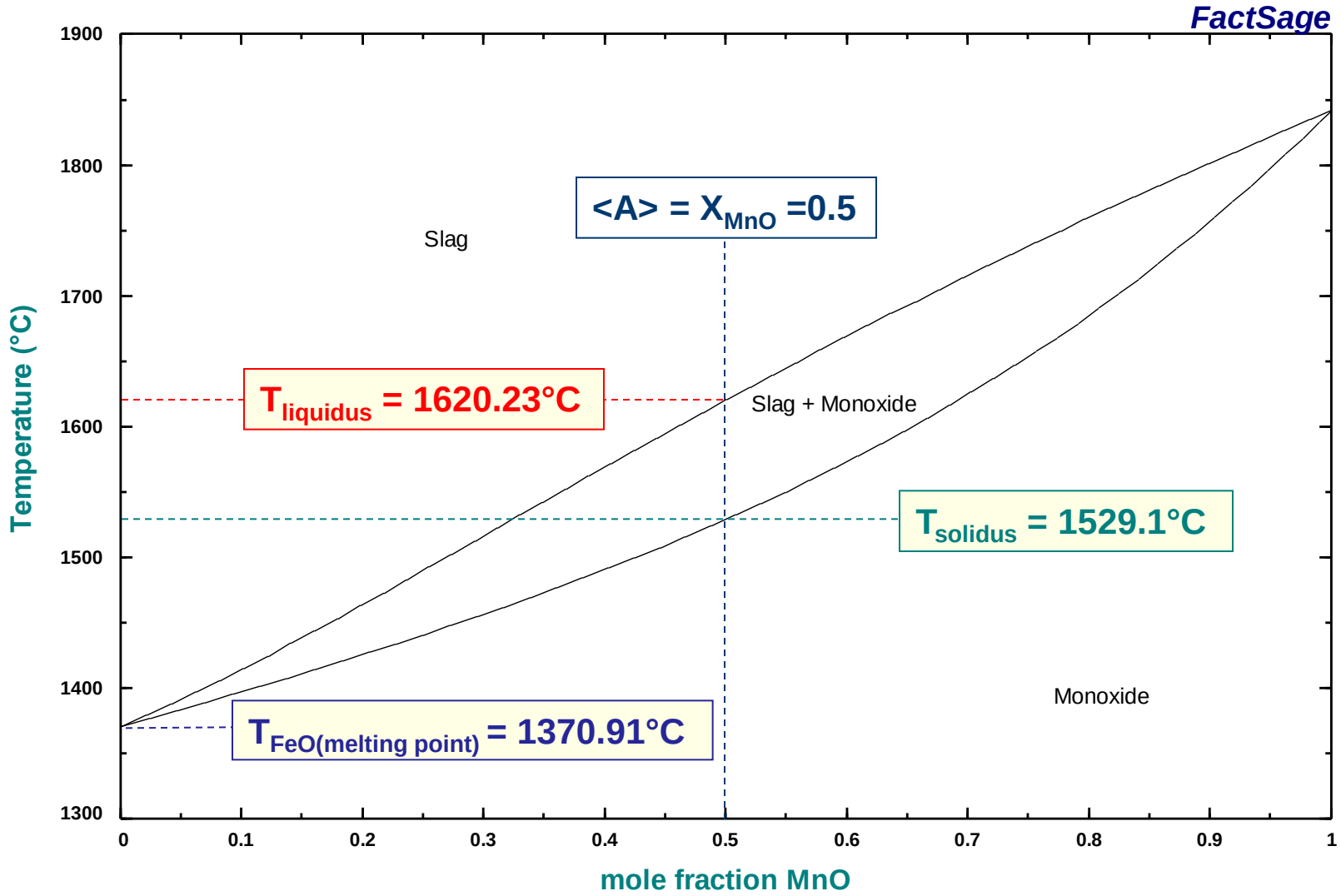
- **Equilibrium cooling**
- **Scheil-Gulliver cooling**
- **Full annealing of cast alloys**

## Cooling Calculations - Table of Contents


**Section 13.1** Table of Contents
**Section 13.2** Phase transitions : FeO-MnO
**Section 13.3** Simple equilibrium cooling : FeO-MnO
**Section 13.4** Simple Scheil-Gulliver cooling : FeO-MnO
**Section 13.5** Equilibrium cooling, plots: Al-Mg-Zn
**Section 13.6** Scheil-Gulliver cooling, annealing casted alloy : Al-Mg-Zn-Mn

# FeO-MnO : Phase transitions - binary phase diagram

**FeO-MnO** binary phase diagram calculated by ***Phase Diagram***



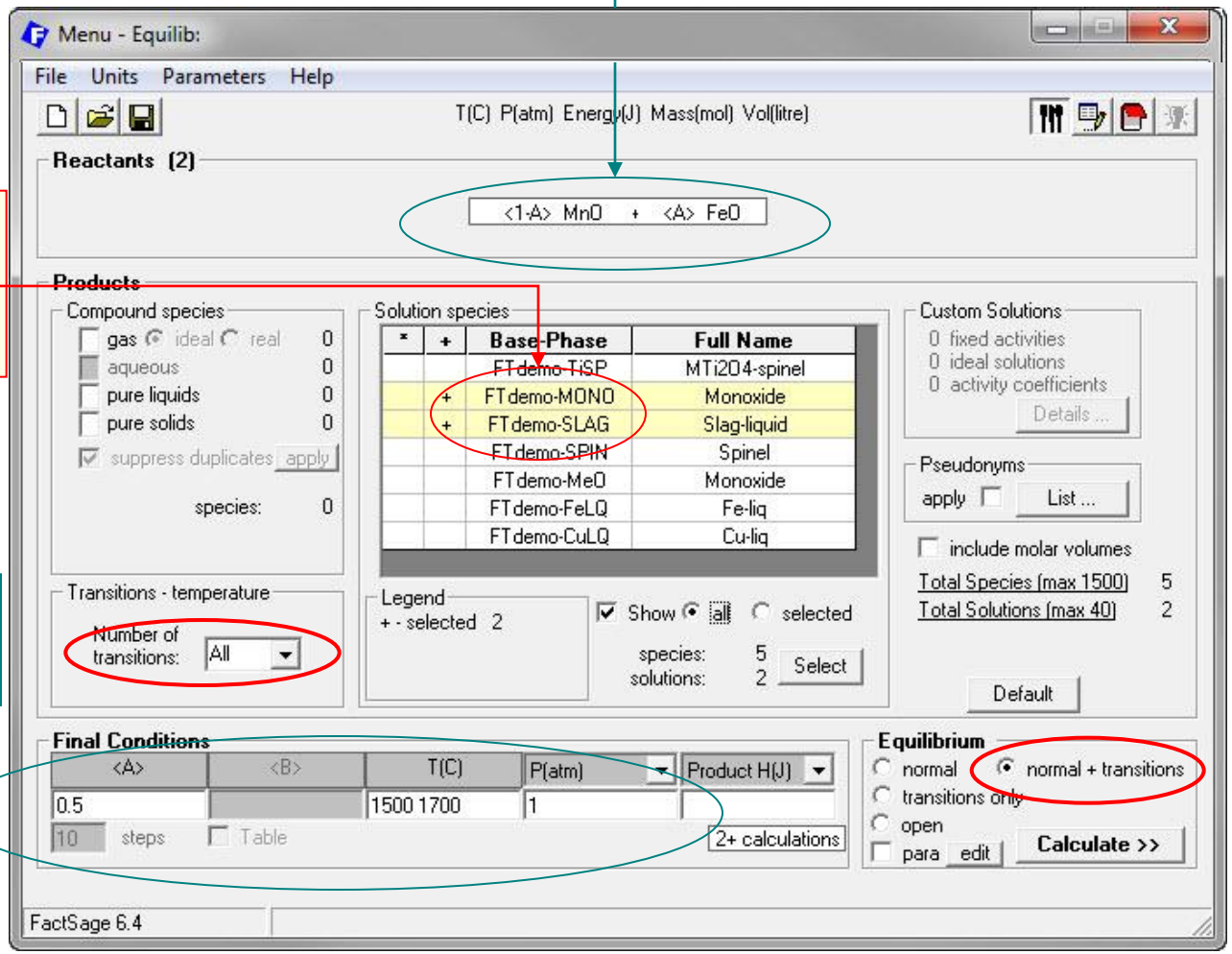
# FeO-MnO : Equilibrium phase transitions at $X_{FeO}$ = 0.5

**1°** Binary system <1-A> MnO + <A> FeO .

**2°** Possible products:

- solid solution (**MONO**)
- liquid Slag (**SLAG**)

**3°** <A> = **0.5**
T (°C) = **1500** and **1700**




**Equilib** will calculate the **equilibrium** at $X_{FeO}$ **= 0.5** for temperatures varying from **1500°C** to **1700°C** and will search for **All** phase **transitions**.

# FeO-MnO : Phase transitions showing liquidus and solidus

Results - Equilib 1620.23 C (page 3/4)

Output Edit Show Pages

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

1500 C | 1529.11 C | - 1620.23 C - | 1700 C

```
<1-A> MnO +  <A> FeO =

 1.0000      mol    Slag-liquid
 (71.392 gram, 1.0000 mol)
         (1620.23 C, 1 atm,      a=1.0000)
         ( 0.50000          FeO
         + 0.50000          MnO)

+ 0.00000     mol    Monoxide
         (1620.23 C, 1 atm,      a=1.(
         ( 0.30796          FeO
         + 0.69204          MnO)

where "A" on the reactant side is 0.5(

The cutoff concentration has been spe(

*************************************
      H            G            V
     (J)          (J)        (litre)
*************************************
-1.91102E+05 -5.49403E+05  0.00000E+0(
```

**Equilibrium liquidus**

Results - Equilib 1529.11 C (page 2/4)

Output Edit Show Pages

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

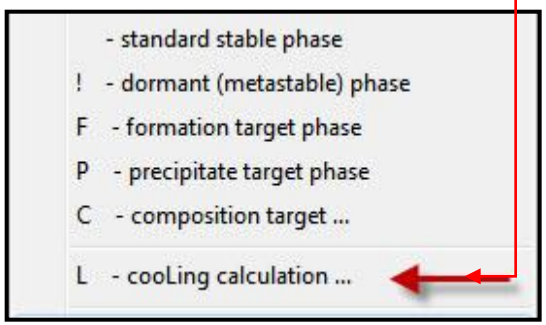
1500 C | - 1529.11 C - | 1620.23 C | 1700 C

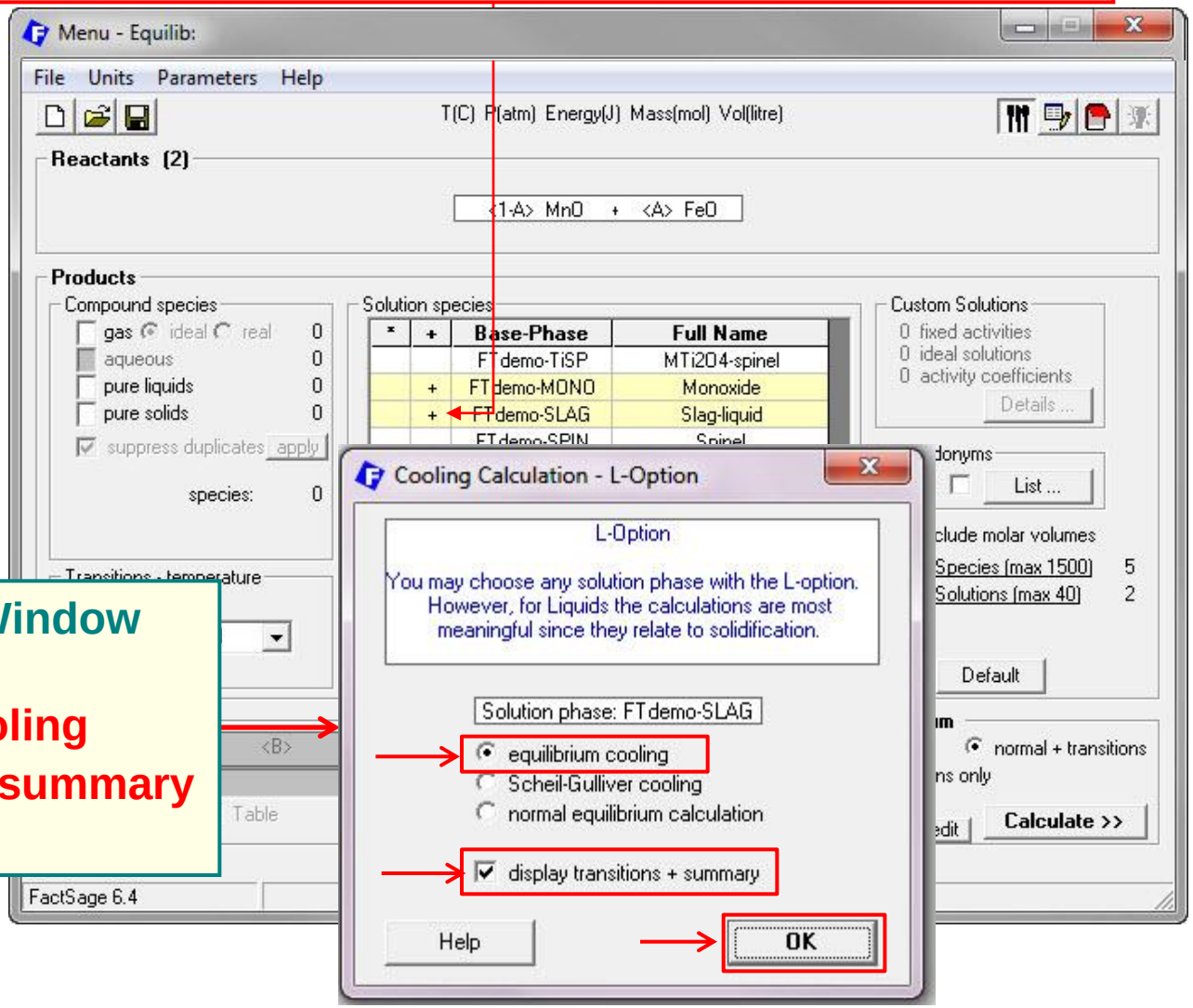
```
<1-A> MnO +  <A> FeO =

1.0000      mol    Monoxide
(71.392 gram, 1.0000 mol)
        (1529.11 C, 1 atm,      a=1.0000)
        ( 0.50000          FeO
        + 0.50000          MnO)

+ 0.00000     mol    Slag-liquid
        (1529.11 C, 1 atm,      a=1.0000)
        ( 0.67618          FeO
        + 0.32382          MnO)

where "A" on the reactant side is 0.50000

The cutoff concentration has been specified to 1.0000E-75

*****************************************************************
      H            G            V            S            Cp
     (J)          (J)        (litre)      (J/K)        (J/K)
*****************************************************************
-2.38118E+05 -5.33297E+05  0.00000E+00  1.63783E+02  6.63565E+01
```

**Equilibrium solidus**

# FeO-MnO : Simple equilibium cooling – L-Option

1° **Right-click** on the '+' column to open the **SLAG** extended menu and **select** **L– cooLing calculation**.to open the ***Cooling Calculation Window***



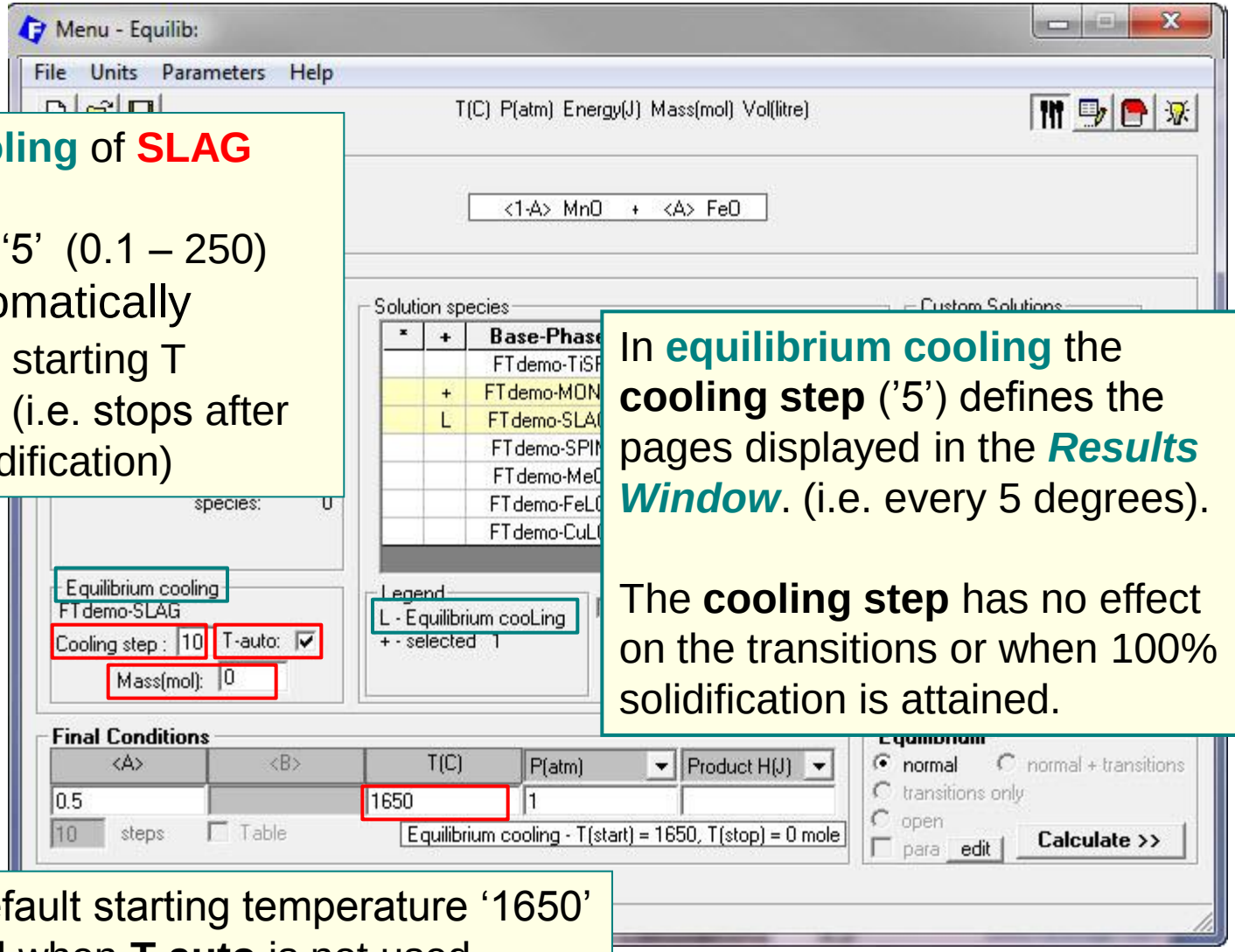

2° **Cooling Calculation Window**

- **select equilibrium cooling**
- **check √ transitions + summary**
- **click OK** to close.

# FeO-MnO : Simple equilibium cooling – step, T-auto and stop

**Equilibrium Cooling** of **SLAG**

- **cooling step** '5' (0.1 – 250)
- **T-auto** √ automatically calculates the starting T
- **final mass** '0' (i.e. stops after complete solidification)




In **equilibrium cooling** the **cooling step** ('5') defines the pages displayed in the ***Results Window***. (i.e. every 5 degrees).

The **cooling step** has no effect on the transitions or when 100% solidification is attained.

**Enter** default starting temperature '1650' – applied when **T-auto** is not used

# FeO-MnO : Equilibrium cooling – Summary and Transitions

Results - Equilib Summary (page-1/13)

Output Edit Show Pages

**Summary**

(mol) Vol(litre)

1550 C | 1540 C | 1530 C | 1529.11 C |

- Summary - | Transitions | 1630 C | 1620.23 C | 1620 C | 1610 C | 1600 C | 1590 C | 1580 C | 1570 C | 1560 C |

```
CONSTITUENTS AND PHASES AT 1529.11 C
(temperature of final disappearance of Slag-l
CONS.  PHASE                          TOTAL AMT/mol
  1    1 Monoxide                       2.0000E+00

('Double-Click' on any phase listed above to

SUMMARY OF REACTIONS

Cooling
1630 to 1620.23 C        (DELTA H = -6.3525E+02
Slag-liquid cooling

Constituent 1
1620.23 to 1529.11 C     (DELTA H = -4.7017E+04
Slag-liquid -> Monoxide

COMPOSITION OF PHASES IN CONSTITUENTS AT 1529
(temperature of final disappearance of Slag-l

Constituent 1
Monoxide
                                MOLE FRACTION  MA
Fe                                2.5000E-01
Mn                                2.5000E-01
O                                 5.0000E-01
                                TOTAL AMT/mol  TO
                                  2.0000E+00
```

Results - Equilib Transitions (page 0/13)

Output Edit Show Pages

**Transitions**

Vol(litre)

1550 C | 1540 C | 1530 C | 1529.11 C |

Summary | - Transitions - | 1630 C | 1620.23 C | 1620 C | 1610 C | 1600 C | 1590 C | 1580 C | 1570 C | 1560 C |

```
Temperature of transition -> 1620.23 C

EQUILIBRIUM COMPOSITION OF PHASES
Slag-liquid
                                MOLE FRACTION  MASS FRACTION
Fe                                2.5000E-01     3.9112E-01
Mn                                2.5000E-01     3.8477E-01
O                                 5.0000E-01     2.2411E-01
                                TOTAL AMT/mol  TOTAL AMT/gram
                                  2.0000E+00     7.1391E+01

-------------------------------------------------------------

Temperature of final disappearance of Slag-liquid -> 1529.11 C

EQUILIBRIUM COMPOSITION OF PHASES
Monoxide
                                MOLE FRACTION  MASS FRACTION
Fe                                2.5000E-01     3.9112E-01
Mn                                2.5000E-01     3.8477E-01
O                                 5.0000E-01     2.2411E-01
                                TOTAL AMT/mol  TOTAL AMT/gram
                                  2.0000E+00     7.1391E+01

AVERAGE COMPOSITION OF ALL PRODUCT PHASES TAKEN TOGETHER
                                MOLE FRACTION  MASS FRACTION
Fe                                2.5000E-01     3.9112E-01
Mn                                2.5000E-01     3.8477E-01
O                                 5.0000E-01     2.2411E-01
```

# FeO-MnO : Equilibrium cooling - Liquidus and Solidus

Results - Equilib 1620.23 C (page 2/13)

Output Edit Show Pages

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

1550 C | 1540 C | 1530 C | 1529.11 C | Summary | Transitions | 1630 C | - 1620.23 C - | 1620 C | 1610 C | 1600 C | 1590 C | 1580 C | 1570 C | 1560 C

```
<1-A> MnO +  <A> FeO =                                  [Equilibrium Cooling]

 1.0000      mol    Slag-liquid
 (71.391 gram, 1.0000 mol)
          (1620.23 C, 1 atm,      a=1.0000)
          ( 0.50000          FeO
          + 0.50000          MnO)

          System component        Mole fracti
          Fe                        0.25000
          Mn                        0.25000
          O                         0.50000

+ 0          mol    Monoxide
          (1620.23 C, 1 atm,      a=1.0000)
          ( 0.30796          FeO
          + 0.69204          MnO)

          System component        Mole fracti
          Fe                        0.15398
          Mn                        0.34602
          O                         0.50000

where "A" on the reactant side is 0.50000
```

**Liquidus**

Results - Equilib 1529.11 C (page 13/13)

Output Edit Show Pages

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

Summary | Transitions | 1630 C | 1620.23 C | 1620 C | 1610 C | 1600 C | 1590 C | 1580 C | 1570 C | 1560 C | 1550 C | 1540 C | 1530 C | - 1529.11 C -

```
<1-A> MnO +  <A> FeO =                                  [Equilibrium Cooling]

 1.0000      mol    Monoxide
 (71.391 gram, 1.0000 mol)
          (1529.11 C, 1 atm,      a=1.0000)
          ( 0.50000          FeO
          + 0.50000          MnO)

          System component        Mole fraction  Mass fraction
          Fe                        0.25000        0.39112
          Mn                        0.25000        0.38477
          O                         0.50000        0.22411

+ 0          mol    Slag-liquid
          (1529.11 C, 1 atm,      a=1.0000)
          ( 0.67618          FeO
          + 0.32382          MnO)

          System component        Mole fraction  Mass fraction
          Fe                        0.33809        0.52776
          Mn                        0.16191        0.24863
          O                         0.50000        0.22361

where "A" on the reactant side is 0.50000
```

**Solidus**

# Scheil target phase

The program performs a **Gulliver-Scheil cooling** calculation. That is, as phases precipitate from the **Scheil target phase** they are dropped from the total mass balance.

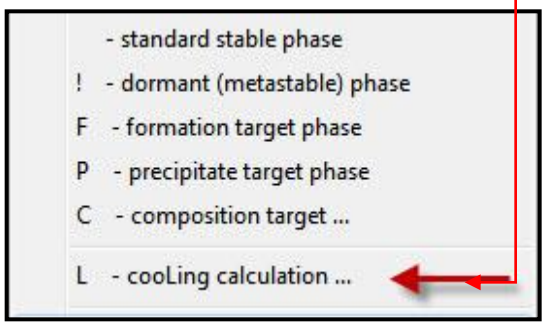
Generally a value of **T** (the initial temperature) and a cooling step must be specified in the **Final Conditions** frame. Normally, the Scheil calculation is repeated until the Scheil Target phase disappears. However it is possible to stop the calculation by either specifying a second temperature in the Final Conditions frame, or by specifying a target mass.

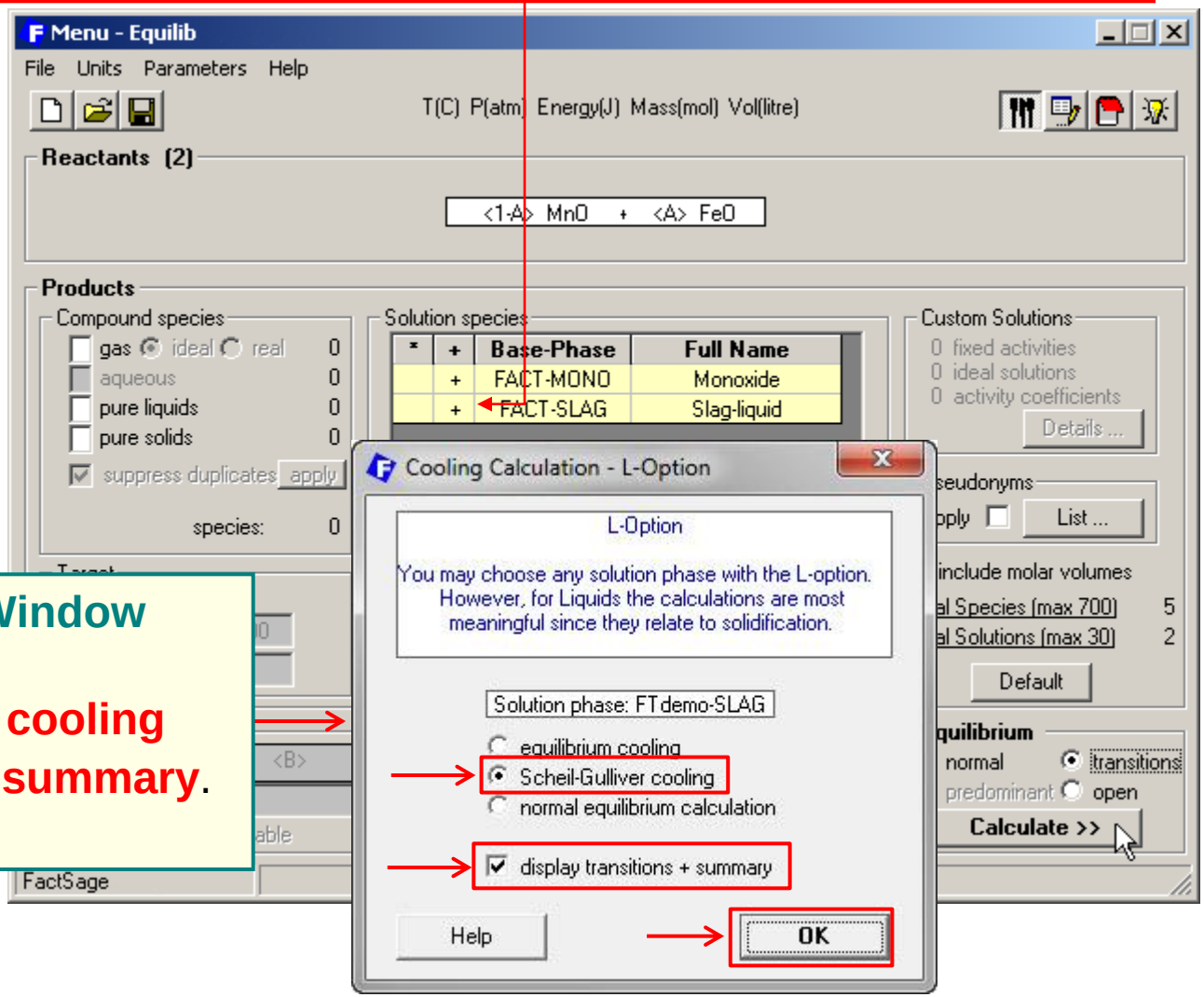
The **Scheil target phase** must be the gas phase or a real solution. If it is a liquid phase (such as FToxid-SLAG and Ftsalt-liquid) then the precipitates are generally solids - it would be unusual in this case to select and include other liquids or the gas phase in the calculation.

If the **Scheil target phase** is the **gas phase** then the precipitates could be any or all of the other compound and solution phases. To activate a Scheil target gas phase, first select the gas species in the usual way. Then with the mouse-right-button click on the gas '+' check box in the compound species frame of the Menu Window - this will open the Species Selection window. Point to the '+' column of any selected gas species and then click with the mouse-right-button and then select «Scheil cooling gas phase».

# FeO-MnO : Scheil-Gulliver cooling – L-Option

1° **Right-click** on the '+' column to open the **FACT-SLAG** extended menu and **select L– cooLing calculation**.to open the ***Cooling Calculation Window***




2° **Cooling Calculation Window**

- **select Scheil-Gulliver cooling**
- **check √ transitions + summary**.
- **click OK** to close.

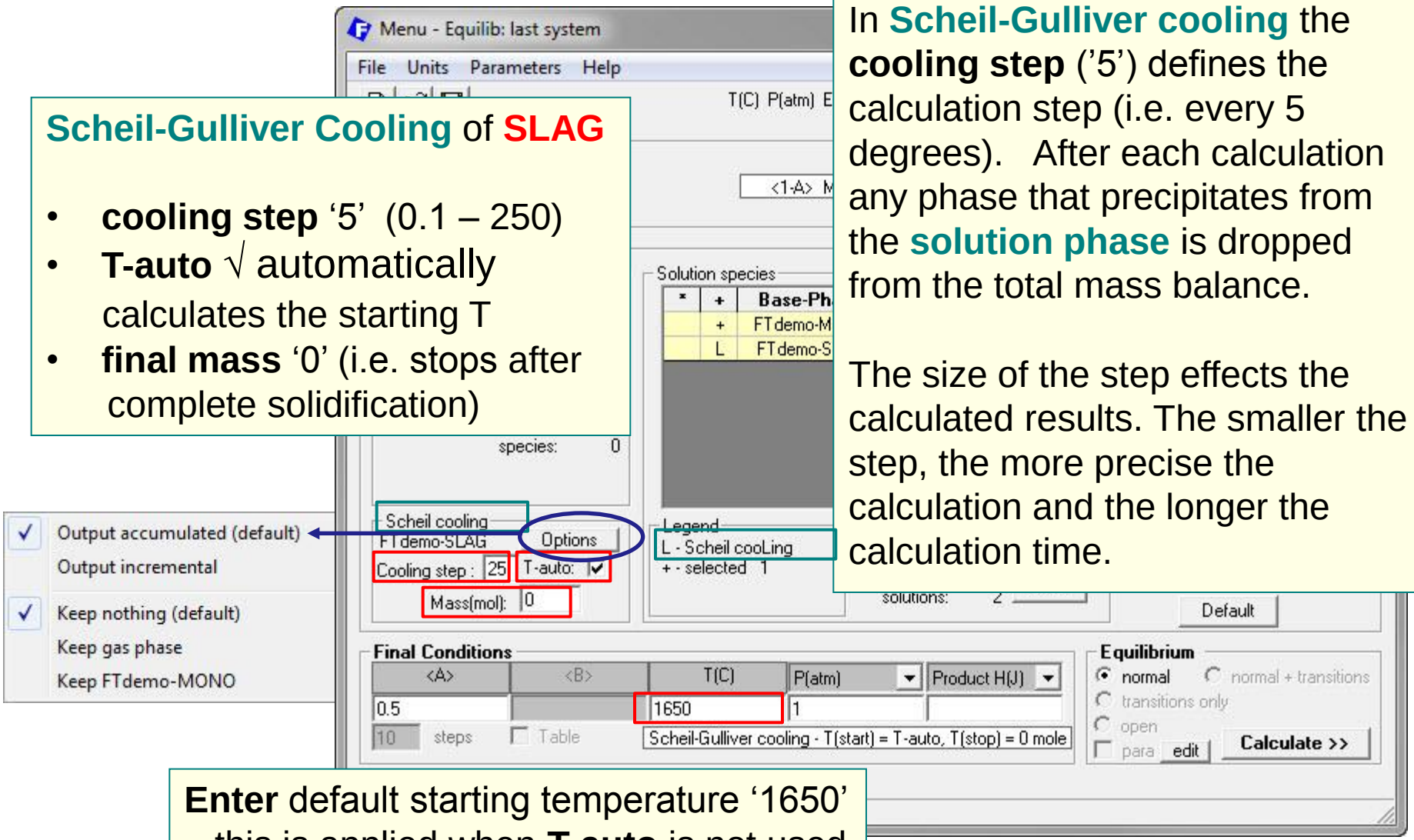
# FeO-MnO : Scheil-Gulliver cooling – step, T-auto and stop

## Scheil-Gulliver Cooling of SLAG

- **cooling step** '5' (0.1 – 250)
- **T-auto** √ automatically calculates the starting T
- **final mass** '0' (i.e. stops after complete solidification)

In **Scheil-Gulliver cooling** the **cooling step** ('5') defines the calculation step (i.e. every 5 degrees). After each calculation any phase that precipitates from the **solution phase** is dropped from the total mass balance.

The size of the step effects the calculated results. The smaller the step, the more precise the calculation and the longer the calculation time.




**Enter** default starting temperature '1650' – this is applied when **T-auto** is not used

# FeO-MnO : Scheil cooling – Summary and Transitions

Results - Equilib Summary (page-1/11)

Output Edit Show Pages

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

1425 C | 1403.47 C

Summary | Transitions | 1625 C | 1620.23 C | 1600 C | 1575 C | 1550 C | 1525 C | 1500 C | 1475 C | 1450 C

```
SCHEIL-GULLIVER COOLING

CONSTITUENTS AND PHASES AT 1403.47 C
(temperature of final disappearance of Slag-liquid)
CONS.  PHASE                    TOTAL AMT/mol   TOTAL AMT
  1    1 Monoxide                 2.0000E+00      7.1391E

('Double-Click' on any phase listed above to recycle it

SUMMARY OF REACTIONS

Cooling
1625 to 1620.23 C       (DELTA H = -3.1022E+02 J)
Slag-liquid cooling

Constituent 1
1620.23 to 1403.47 C    (DELTA H = -8.5425E+03 J)
Slag-liquid -> Monoxide

COMPOSITION OF PHASES IN CONSTITUENTS AT 1403.47 C
(temperature of final disappearance of Slag-liquid)

Constituent 1
Monoxide
                            MOLE FRACTION   MASS FRACTIO
Fe                            2.5000E-01      3.9112E-01
Mn                            2.5000E-01      3.8477E-01
O                             5.0000E-01      2.2411E-01
                            TOTAL AMT/mol   TOTAL AMT/gr
```

**Summary**

Results - Equilib Transitions (page 0/11)

Output Edit Show Pages

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

1425 C | 1403.47 C

Summary | - Transitions - | 1625 C | 1620.23 C | 1600 C | 1575 C | 1550 C | 1525 C | 1500 C | 1475 C | 1450 C

```
Temperature of final disappearance of Slag-liquid -> 1403.47 C

AVERAGE COMPOSITION OF ALL PRODUCT PHASES TAKEN TOGETHER
                            MOLE FRACTION   MASS FRACTION
Fe                            2.5000E-01      3.9112E-01
Mn                            2.5000E-01      3.8477E-01
O                             5.0000E-01      2.2411E-01
                            TOTAL AMT/mol   TOTAL AMT/gram
                              2.0000E+00      7.1391E+01

REACTION BETWEEN 1620.23 C AND 1403.47 C

Slag-liquid -> Monoxide

Reactants
                            TOTAL AMT/mol   TOTAL AMT/gram
Slag-liquid                  -2.0000E+00     -7.1391E+01

Products (Constituent 1)
Monoxide
                            MOLE FRACTION   MASS FRACTION
Fe                            2.5000E-01      3.9112E-01
Mn                            2.5000E-01      3.8477E-01
O                             5.0000E-01      2.2411E-01
                            TOTAL AMT/mol   TOTAL AMT/gram
                              2.0000E+00      7.1391E+01

CONSTITUENTS AND PHASES AT 1403.47 C
```

**Transitions**

# FeO-MnO : Scheil cooling – Start and Stop

Results - Equilib Summary (page-1/11)

Output Edit Show Pages

T(C) P(atm) Energy(J) Mass(mol) Vo

1425 C | 1403.47 C |

Summary | Transitions | 1625 C | 1620.23 C | 1600 C | 1575 C | 1550 C | 1525 C | 1500 C | 1475 C | 1450 C |

```
SCHEIL-GULLIVER COOLING

CONSTITUENTS AND PHASES AT 1403.47 C
(temperature of final disappearance of Slag-liquid)
CONS.  PHASE                    TOTAL AMT/mol   TOTAL AMT
  1    1 Monoxide                 2.0000E+00      7.1391E

('Double-Click' on any phase listed above to recycle it

SUMMARY OF REACTIONS

Cooling
1625 to 1620.23 C       (DELTA H = -3.1022E+02 J)
Slag-liquid cooling

Constituent 1
1620.23 to 1403.47 C    (DELTA H = -8.5425E+03 J)
Slag-liquid -> Monoxide

COMPOSITION OF PHASES IN CONSTITUENTS AT 1403.47 C
(temperature of final disappearance of Slag-liquid)

Constituent 1
Monoxide
                        MOLE FRACTION  MASS FRACTIO
```

**Start of solidification at 1620.23°C**

Results - Equilib Transitions (page 0/11)

Output Edit Show Pages

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

1425 C | 1403.47 C |

Summary | Transitions | 1625 C | 1620.23 C | 1600 C | 1575 C | 1550 C | 1525 C | 1500 C | 1475 C | 1450 C |

```
Temperature of final disappearance of Slag-liquid -> 1403.47 C

AVERAGE COMPOSITION OF ALL PRODUCT PHASES TAKEN TOGETHER
                            MOLE FRACTION  MASS FRACTION
Fe                            2.5000E-01     3.9112E-01
Mn                            2.5000E-01     3.8477E-01
O                             5.0000E-01     2.2411E-01
                            TOTAL AMT/mol  TOTAL AMT/gram
                              2.0000E+00     7.1391E+01

REACTION BETWEEN 1620.23 C AND 1403.47 C

                            TOTAL AMT/mol  TOT
                             -2.0000E+00    -7.1391E+01

                            MOLE FRACTION  MASS FRACTION
                              2.5000E-01     3.9112E-01
                              2.5000E-01     3.8477E-01
                              5.0000E-01     2.2411E-01
                            TOTAL AMT/mol  TOTAL AMT/gram
                              2.0000E+00     7.1391E+01

CONSTITUENTS AND PHASES AT 1403.47 C
```

**End of solidification at 1376.68°C**

The size of the cooling step effects the calculated results. Here the step 5°C gives 1376.68°C. The end of Scheil solidification should be at 1370.91°C – the melting point of FeO. With a much smaller step, 0.1°C, one obtains ~ 1370.9°C..

# FeO-MnO : Scheil cooling – incremental vs. accumulated

**Incremental Scheil solidification at 1500°C**

Summary | Transitions | 1625 C | 1620.23 C | 1600 C | 1575 C | 1550 C | 1525 C | - 1500 C - | 1475 C | 1450 C

[Incremental Scheil]

```
<1-A> MnO +  <A> FeO =

 0.22360    mol   Slag-liquid
 (16.010 gram, 0.22360 mol)
         (1500 C, 1 atm,      a=1.0000)
         ( 0.73123          FeO
         + 0.26877          MnO)

         System component        Mole fraction  Mass fr
         Fe                        0.36561        0.570
         Mn                        0.13439        0.206
         O                         0.50000        0.223

+ 9.6740E-02 mol   Monoxide
 (6.9129 gram, 9.6740E-02 mol)
         (1500 C, 1 atm,      a=1.0000
         ( 0.57467          FeO
         + 0.42533          MnO)

         System component        Mole fraction  Mass fr
         Fe                        0.28734        0.449
         Mn                        0.21266        0.327
         O                         0.50000        0.223

where "A" on the reactant side is 0.50000

The cutoff concentration has been specified to 1.0000E-

Mass fraction precipitated according to Scheil-Gulliver
```

- Output accumulated (default)
- Output incremental
- Keep nothing (default)
- Keep gas phase
- Keep FTdemo-MONO

Results - Equilib 1500 C (page 7/11)

Output Edit Show Pages

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

1425 C | 1403.47 C

Summary | Transitions | 1625 C | 1620.23 C | 1600 C | 1575 C | 1550 C | 1525 C | - 1500 C - | 1475 C | 1450 C

[Accumulated Scheil]

```
<1-A> MnO +  <A> FeO =

 0.77640    mol   Monoxide
 (55.381 gram, 0.77640 mol)
         (1500 C, 1 atm,      a=1.0000)
         ( 0.43341          FeO
         + 0.56659          MnO)

         System component        Mole fraction  Mass fraction
         Fe                        0.21670        0.33932
         Mn                        0.28330        0.43638
         O                         0.50000        0.22430

+ 0.22360    mol   Slag-liquid
 (16.010 gram, 0.22360 mol)
         (1500 C, 1 atm,      a=1.0000)
         ( 0.73123          FeO
         + 0.26877          MnO)

         System component        Mole fraction  Mass fraction
         Fe                        0.36561        0.57032
         Mn                        0.13439        0.20623
         O                         0.50000        0.22345

where "A" on the reactant side is 0.50000

The cutoff concentration has been specified to 1.0000E-70

Mass fraction precipitated according to Scheil-Gulliver = 0.77574
```

**Accumulated Scheil solidification at 1500°C**

- Output accumulated (default)
- Output incremental
- Keep nothing (default)
- Keep gas phase
- Keep FTdemo-MONO

# Al-Mg-Zn : Equilibrium cooling $X_{Mg}$=0.8 $X_{Al}$=0.15 $X_{Zn}$=0.05

**Al-Mg-Zn** polythermal liquidus projection calculated by ***Phase Diagram*** with data taken from **FTlite – FACT light alloy databases**

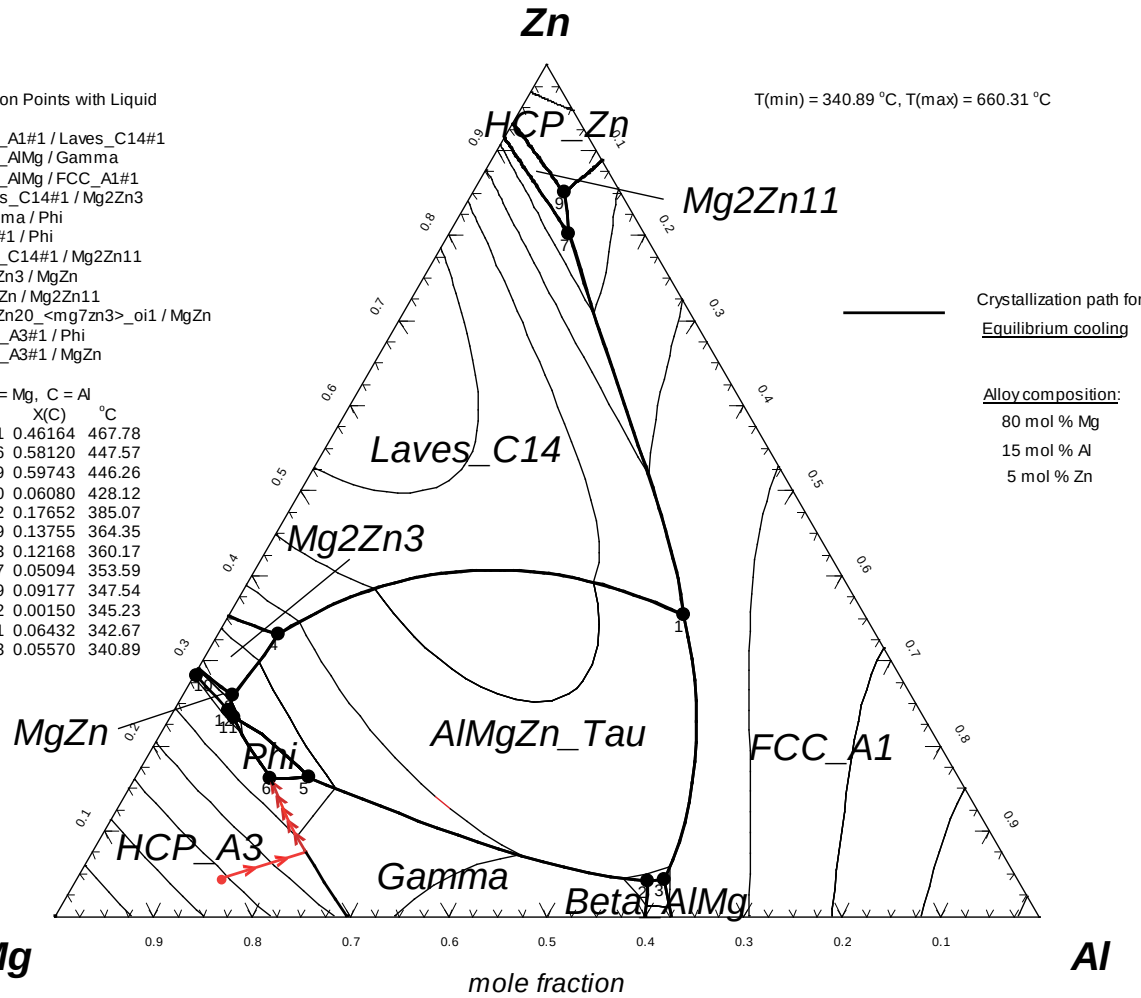
Four-Phase Intersection Points with Liquid

1: AlMgZn_Tau / FCC_A1#1 / Laves_C14#1
2: AlMgZn_Tau / Beta_AlMg / Gamma
3: AlMgZn_Tau / Beta_AlMg / FCC_A1#1
4: AlMgZn_Tau / Laves_C14#1 / Mg2Zn3
5: AlMgZn_Tau / Gamma / Phi
6: Gamma / HCP_A3#1 / Phi
7: FCC_A1#1 / Laves_C14#1 / Mg2Zn11
8: AlMgZn_Tau / Mg2Zn3 / MgZn
9: FCC_A1#1 / HCP_Zn / Mg2Zn11
10: HCP_A3#1 / Mg51Zn20_<mg7zn3>_oi1 / MgZn
11: AlMgZn_Tau / HCP_A3#1 / Phi
12: AlMgZn_Tau / HCP_A3#1 / MgZn

A = Zn, B = Mg, C = Al

| | X(A) | X(B) | X(C) | °C |
|---|---|---|---|---|
| 1: | 0.35365 | 0.18471 | 0.46164 | 467.78 |
| 2: | 0.04094 | 0.37786 | 0.58120 | 447.57 |
| 3: | 0.04248 | 0.36009 | 0.59743 | 446.26 |
| 4: | 0.33110 | 0.60810 | 0.06080 | 428.12 |
| 5: | 0.16296 | 0.66052 | 0.17652 | 385.07 |
| 6: | 0.16267 | 0.69979 | 0.13755 | 364.35 |
| 7: | 0.80148 | 0.07683 | 0.12168 | 360.17 |
| 8: | 0.25899 | 0.69007 | 0.05094 | 353.59 |
| 9: | 0.85034 | 0.05789 | 0.09177 | 347.54 |
| 10: | 0.28328 | 0.71522 | 0.00150 | 345.23 |
| 11: | 0.23357 | 0.70211 | 0.06432 | 342.67 |
| 12: | 0.24168 | 0.70263 | 0.05570 | 340.89 |

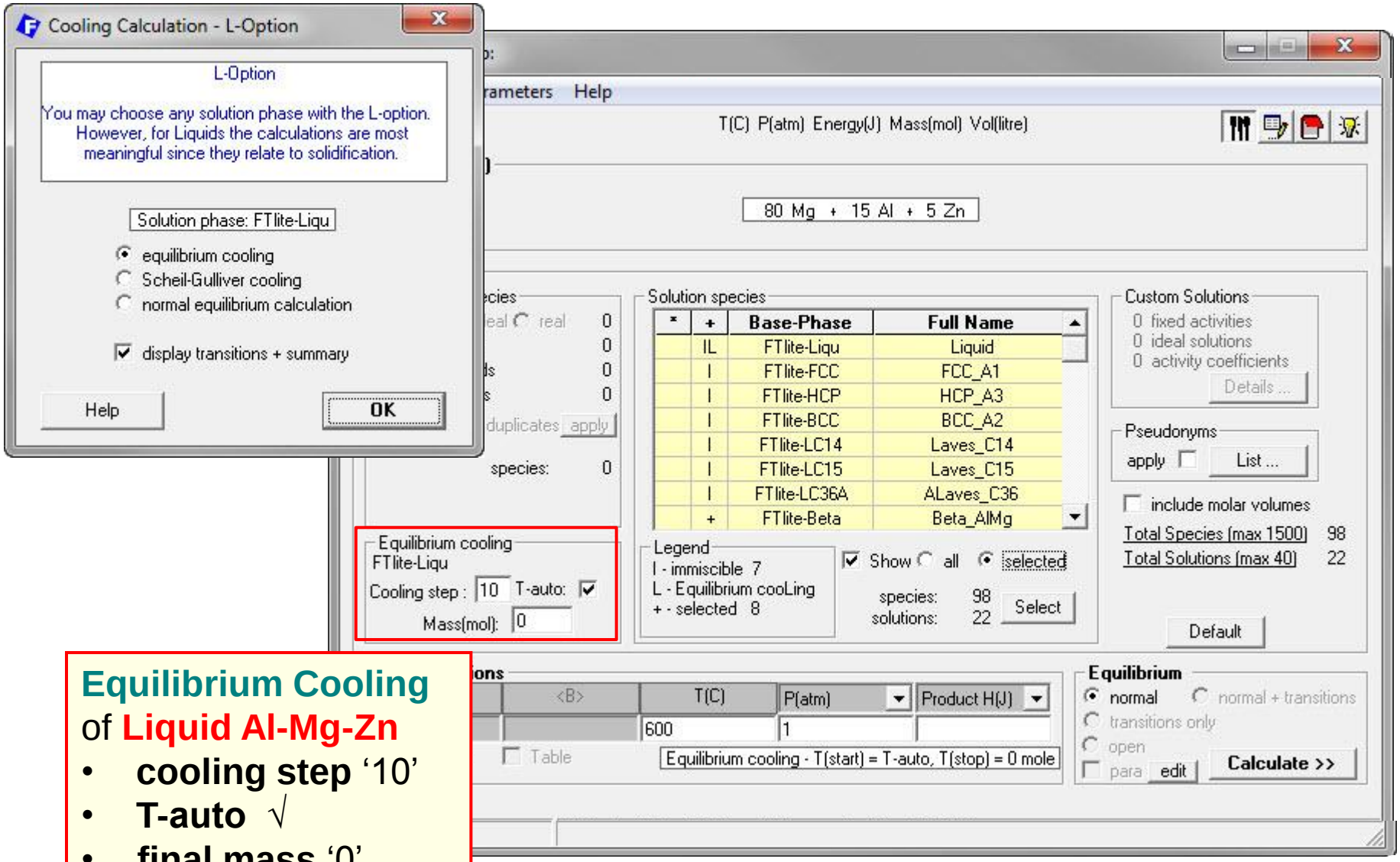
T(min) = 340.89 °C, T(max) = 660.31 °C




Crystallization path for Equilibrium cooling

Alloy composition:
80 mol % Mg
15 mol % Al
5 mol % Zn

# Al-Mg-Zn : Equilibium cooling – L-Option




**Equilibrium Cooling**
of **Liquid Al-Mg-Zn**

- **cooling step** '10'
- **T-auto** √
- **final mass** '0'

# Al-Mg-Zn : Equilibium cooling – Summary of Results

Liquidus temperature = **497.61°C**

**Constituent 1** is primary hcp formed between **497.61°C** and **404.48°C**

Microstructural **constituents**, and the phases in them

Results - Equilib Summary (page-1/18)

Output Edit Show Pages

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

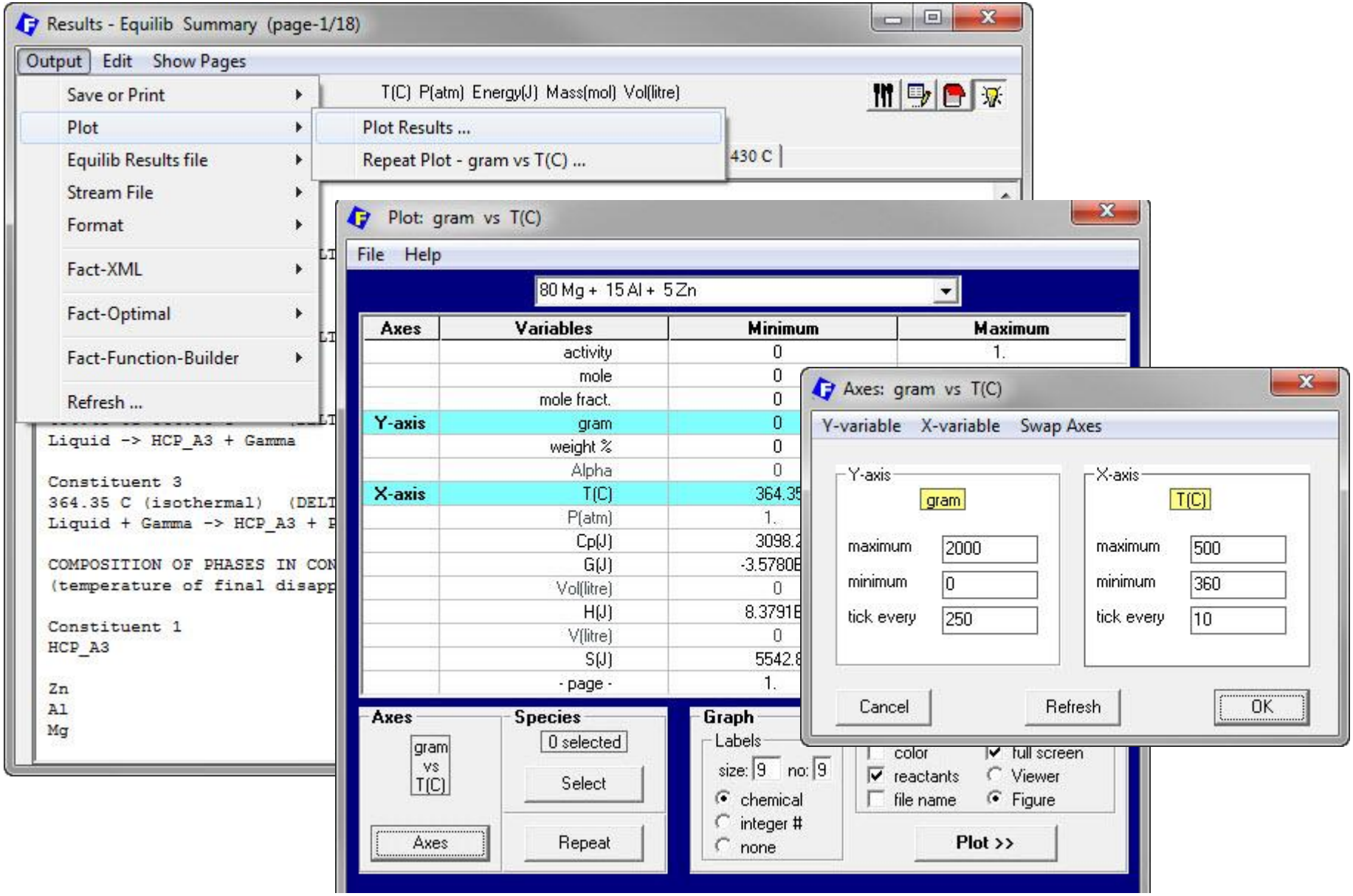
420 C | 410 C | 404.48 C | 400 C | 390 C | 380 C | 370 C | 364.35 C | 364.35 C

Summary | Transitions | 500 C | 497.61 C | 490 C | 480 C | 470 C | 460 C | 450 C | 440 C | 430 C

```
SUMMARY OF REACTIONS

Cooling
500 to 497.61 C        (DELTA H = -7.4229E+03 J)
Liquid cooling

Constituent 1
497.61 to 404.48 C     (DELTA H = -5.8385E+05 J)
Liquid -> HCP_A3

Constituent 2
404.48 to 364.35 C     (DELTA H = -4.2933E+05 J)
Liquid -> HCP_A3 + Gamma

Constituent 3
364.35 C (isothermal)  (DELTA H = -9.9422E+04 J)
Liquid + Gamma -> HCP_A3 + Phi

COMPOSITION OF PHASES IN CONSTITUENTS AT 364.35 C
(temperature of final disappearance of Liquid)

Constituent 1
HCP_A3
                          MOLE FRACTION  MASS FRACTION
Zn                          1.6531E-02     4.2984E-02
Al                          5.9743E-02     6.4109E-02
Mg                          9.2373E-01     8.9291E-01
                          TOTAL AMT/mol  TOTAL AMT/gram
```

**Constituent 2** is a binary eutectic formed between **404.48°C** and **364.35°C**

# Al-Mg-Zn : Equilibium cooling – Plot Results



# Al-Mg-Zn : Equilibium cooling – Plot Results

Selection of species to be plotted
- select all solids and elements for which **Gram (max)** > 0

Results - Equilib 600 C (page 1/31) FactSage 6.2 beta

Species Selection - EQUILIB Results: gram vs T(C)

File Show

| + | # | Species | Gram (min) | Gram (max) | Wt.% (min) | Wt.% (max) | Act. (min) | Act. (max) |
|---|---|---|---|---|---|---|---|---|
| | 126 | Mg51Zn20(s) | 0 | 0 | 0 | 0 | 3.2943E-26 | 9.6902E-07 |
| | | **SOLUTIONS** | | | | | | |
| | 127 | GAS | 0 | 0 | 0 | 0 | 0 | 0 |
| + | 128 | Liqu#1 | 0 | 2676.1 | 0 | 0 | 0.949003 | 1. |
| | 129 | Liqu#2 | 0 | 0 | 0 | 0 | 0.949003 | 1. |
| | 130 | FCC#1 | 0 | 0 | 0 | 0 | 0.66603 | 0.798147 |
| | 131 | FCC#2 | 0 | 0 | 0 | 0 | 0.66603 | 0.798147 |
| + | 132 | HCP#1 | 0 | 1575.7 | 0 | 0 | 0.876183 | 1. |
| | 133 | HCP#2 | 0 | 0 | 0 | 0 | 0.876183 | 1. |
| | 134 | BCC#1 | 0 | 0 | 0 | 0 | 0.740645 | 0.803598 |
| | 135 | BCC#2 | 0 | 0 | 0 | 0 | 0.740645 | 0.803598 |
| | 136 | LC14#1 | 0 | 0 | 0 | 0 | 9.7821E-02 | 0.375458 |
| | 137 | LC14#2 | 0 | 0 | 0 | 0 | 4.8940E-02 | 0.110639 |
| | 138 | LC15#1 | 0 | 0 | 0 | 0 | 3.8461E-02 | 8.4836E-02 |
| | 139 | LC15#2 | 0 | 0 | 0 | 0 | 3.1307E-02 | 8.4836E-02 |
| | 140 | LC36A#1 | 0 | 0 | 0 | 0 | 3.6789E-02 | 8.3827E-02 |
| | 141 | LC36A#2 | 0 | 0 | 0 | 0 | 3.2212E-04 | 8.3827E-02 |
| | 142 | Beta | 0 | 0 | 0 | 0 | 3.4867E-11 | 1.5177E-02 |
| + | 143 | Gama | 0 | 777.29 | 0 | 0 | 1.3865E-08 | 1. |

Mass: mole / gram

Order: integer # / mass (max) / fraction (max) / activity (max)

source

Select Top 15

4 species selected

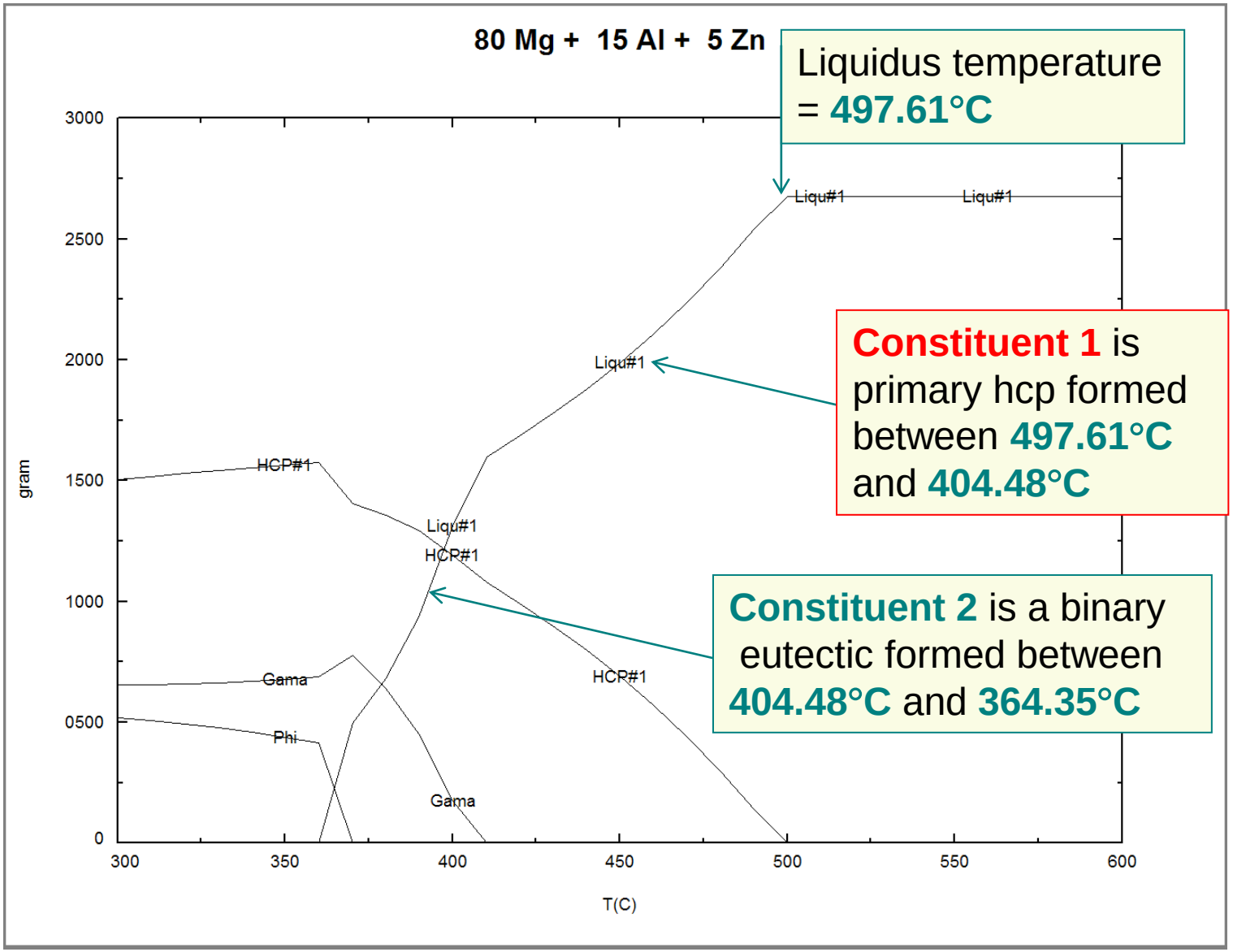
Clear

Refresh

OK

Click on the "+" column to add or remove species.

# Al-Mg-Zn : Equilibium cooling – Plot Results



# Al-Mg-Zn : Scheil cooling $X_{Mg}$=0.8 $X_{Al}$=0.15 $X_{Zn}$=0.05

**Al-Mg-Zn** polythermal liquidus projection calculated by ***Phase Diagram*** with data taken from **FTlite – FACT light alloy databases**

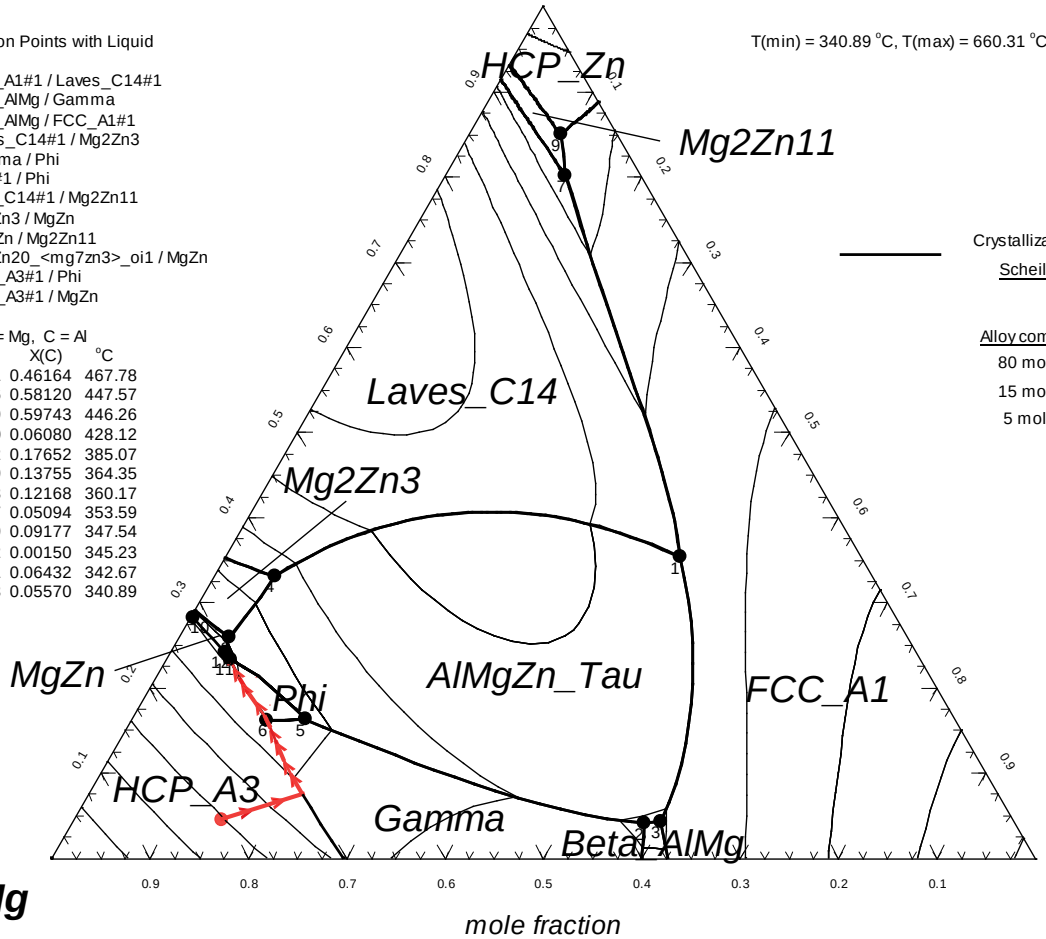
Four-Phase Intersection Points with Liquid

1: AlMgZn_Tau / FCC_A1#1 / Laves_C14#1
2: AlMgZn_Tau / Beta_AlMg / Gamma
3: AlMgZn_Tau / Beta_AlMg / FCC_A1#1
4: AlMgZn_Tau / Laves_C14#1 / Mg2Zn3
5: AlMgZn_Tau / Gamma / Phi
6: Gamma / HCP_A3#1 / Phi
7: FCC_A1#1 / Laves_C14#1 / Mg2Zn11
8: AlMgZn_Tau / Mg2Zn3 / MgZn
9: FCC_A1#1 / HCP_Zn / Mg2Zn11
10: HCP_A3#1 / Mg51Zn20_<mg7zn3>_oi1 / MgZn
11: AlMgZn_Tau / HCP_A3#1 / Phi
12: AlMgZn_Tau / HCP_A3#1 / MgZn

A = Zn, B = Mg, C = Al

| | X(A) | X(B) | X(C) | °C |
|---|---|---|---|---|
| 1: | 0.35365 | 0.18471 | 0.46164 | 467.78 |
| 2: | 0.04094 | 0.37786 | 0.58120 | 447.57 |
| 3: | 0.04248 | 0.36009 | 0.59743 | 446.26 |
| 4: | 0.33110 | 0.60810 | 0.06080 | 428.12 |
| 5: | 0.16296 | 0.66052 | 0.17652 | 385.07 |
| 6: | 0.16267 | 0.69979 | 0.13755 | 364.35 |
| 7: | 0.80148 | 0.07683 | 0.12168 | 360.17 |
| 8: | 0.25899 | 0.69007 | 0.05094 | 353.59 |
| 9: | 0.85034 | 0.05789 | 0.09177 | 347.54 |
| 10: | 0.28328 | 0.71522 | 0.00150 | 345.23 |
| 11: | 0.23357 | 0.70211 | 0.06432 | 342.67 |
| 12: | 0.24168 | 0.70263 | 0.05570 | 340.89 |

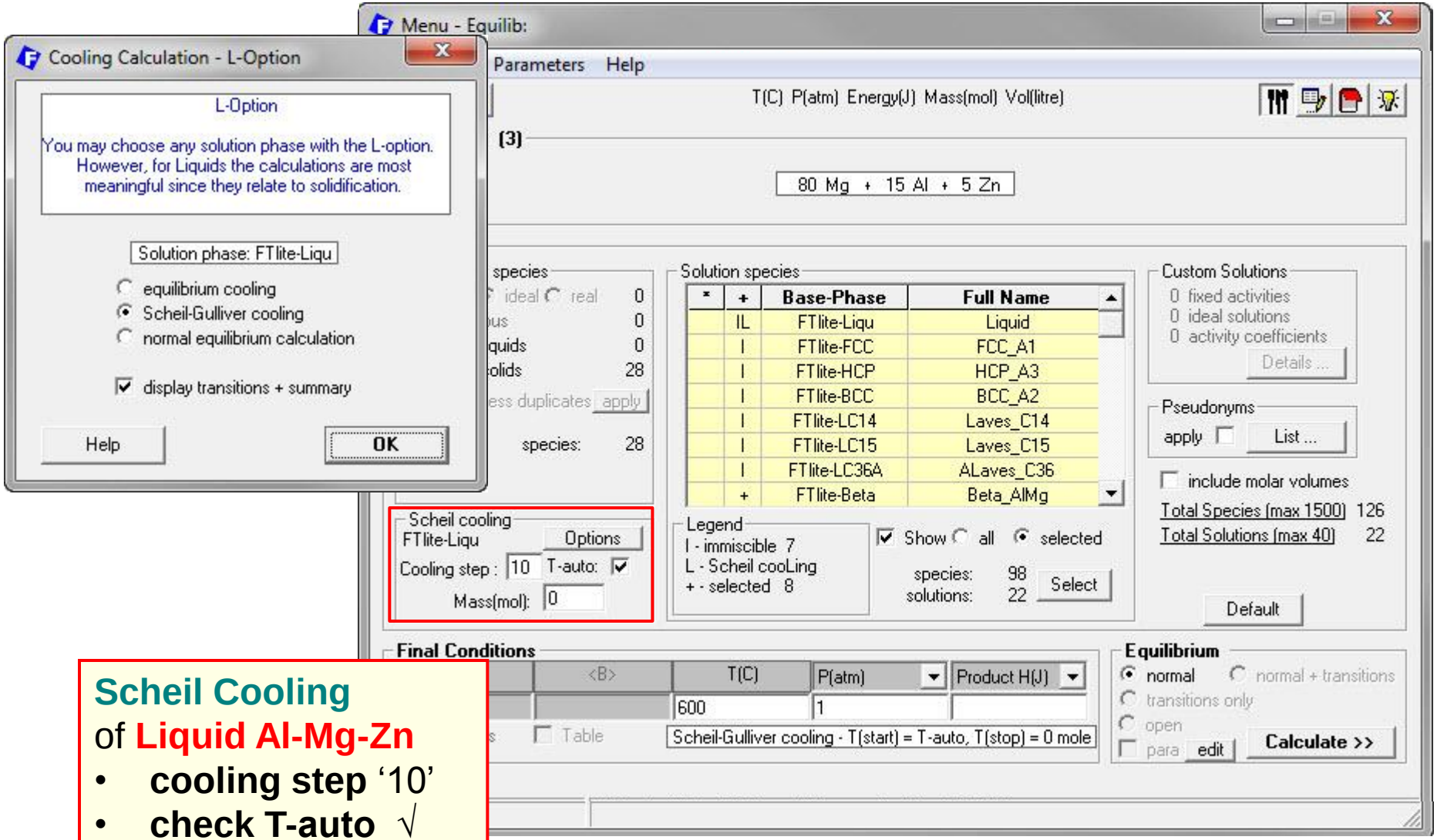
T(min) = 340.89 °C, T(max) = 660.31 °C




Crystallization path for Scheil cooling

Alloy composition:
80 mol % Mg
15 mol % Al
5 mol % Zn

# Al-Mg-Zn : Scheil-Gulliver cooling – L-Option

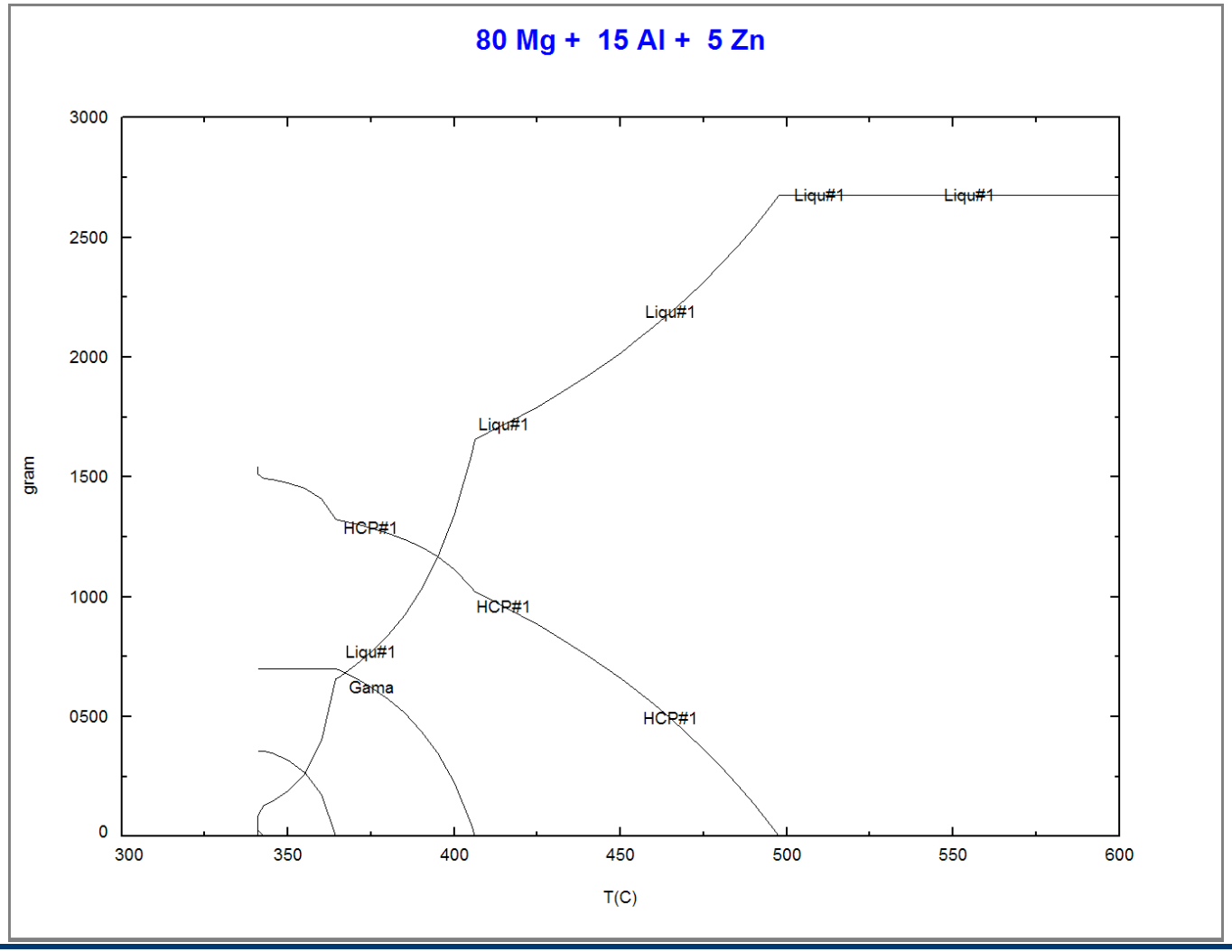



**Scheil Cooling**
of **Liquid Al-Mg-Zn**

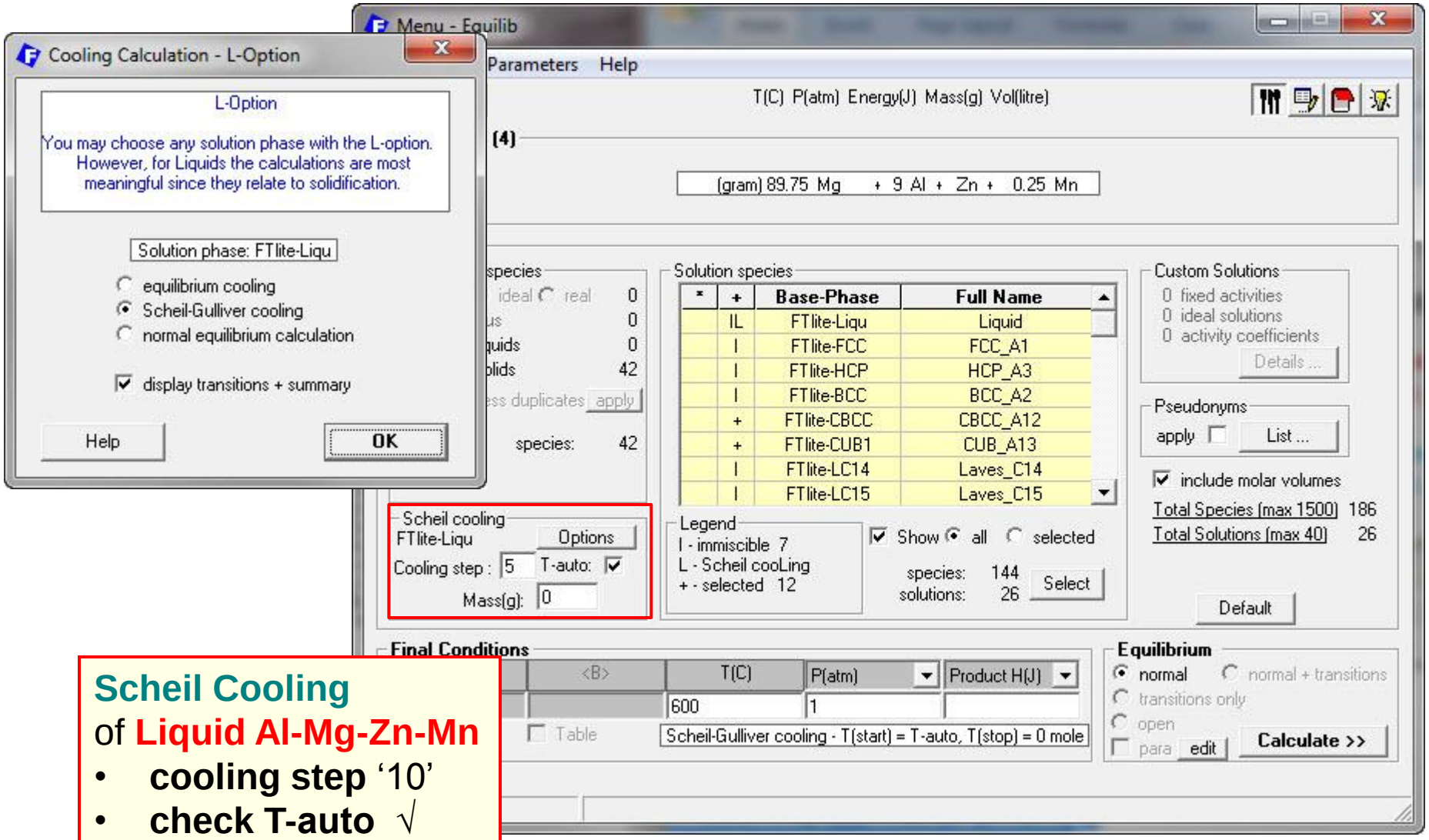
- **cooling step '10'**
- **check T-auto √**
- **enter final mass '0'**

# Graphical output of Scheil target calculation

Calculation ends at temperature of final disappearance of liquid.
Graph shows phase distribution



# Al-Mg-Zn-Mn : Scheil cooling AZ91 + 0.25 wt.% Mn alloy




**Scheil Cooling**
of **Liquid Al-Mg-Zn-Mn**

- **cooling step** '10'
- **check T-auto** √
- **enter final mass** '0'

# Al-Mg-Zn-Mn : Scheil cooling – Summary and Transitions

**AZ91 + 0.25 wt.% Mn alloy:**

89.75Al-9Mg-Zn-0.25Mg (wt%)

Results - Equilib Summary (page-1/60)

Output Edit Show Pages

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

510 C | 505 C | 500 C |

560 C | 555 C | 550 C | 545 C | 540 C | 535 C | 530 C | 525 C | 524.12 C | 520 C | 515 C |

- Summary - | Transitions | 595 C | 594.16 C | 594.07 C | 590 C | 585 C | 580 C | 575 C | 570 C | 565 C |

**Summary**

```
SCHEIL-GULLIVER COOLING

CONSTITUENTS AND PHASES AT 340.89 C
(temperature of final disappearance of Liquid)
CONS.  PHASE                          TOTAL AMT/mol   TOTAL AMT/gram
  1    1 Al8Mn5_D810                   1.3055E-05      5.0230E-04

  2    1 HCP_A3                        2.6553E+00      6.4835E+01
  2    2 Al8Mn5_D810                   7.5208E-03      2.8466E-01

  3    1 HCP_A3                        6.3501E-01      1.5580E+01
  3    2 Mn4Al11_s1(s)                 4.2235E-03      1.4544E-01

  4    1 HCP_A3                        6.8848E-02      1.6956E+00
  4    2 MnAl4_s1(s)                   5.4346E-04      1.7702E-02

  5    1 HCP_A3                        1.9793E-01      4.8919E+00
  5    2 Gamma                         4.5374E-01      1.1829E+01
  5    3 MnAl4_s1(s)                   8.0662E-04      2.6274E-02

  6    1 HCP_A3                        7.1873E-03      1.8150E-01
  6    2 Phi                           1.0940E-02      3.7598E-01
  6    3 Mn4Al11_s1(s)                 1.3741E-06      4.7318E-05

  7    1 HCP_A3                        7.7250E-04      1.9639E-02
  7    2 AlMgZn_Tau                    6.7948E-04      2.9038E-02
  7    3 Mn4Al11_s1(s)                 3.4950E-08      1.2035E-06

  8    1 HCP_A3                        1.2677E-03      3.2228E-02
  8    2 MgZn                          9.0976E-04      3.9438E-02
```

Results - Equilib Transitions (page 0/60)

Output Edit Show Pages

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

510 C | 505 C | 500 C |

560 C | 555 C | 550 C | 545 C | 540 C | 535 C | 530 C | 525 C | 524.12 C | 520 C | 515 C |

Summary | - Transitions - | 595 C | 594.16 C | 594.07 C | 590 C | 585 C | 580 C | 575 C | 570 C | 565 C |

**Transitions**

```
SCHEIL-GULLIVER COOLING

Starting temperature -> 595 C
Cooling step -> 5 C

COMPOSITION OF Liquid
                              MOLE FRACTION   MASS FRACTION
Zn                              3.7803E-03      1.0000E-02
Mn                              1.1247E-03      2.5000E-03
Al                              8.2441E-02      9.0000E-02
Mg                              9.1265E-01      8.9750E-01
                              TOTAL AMT/mol   TOTAL AMT/gram
                                4.0461E+00      1.0000E+02

-------------------------------------------------------------

Temperature of transition -> 594.16 C

COMPOSITION OF Liquid
                              MOLE FRACTION   MASS FRACTION
Zn                              3.7803E-03      1.0000E-02
Mn                              1.1247E-03      2.5000E-03
Al                              8.2441E-02      9.0000E-02
Mg                              9.1265E-01      8.9750E-01
                              TOTAL AMT/mol   TOTAL AMT/gram
                                4.0461E+00      1.0000E+02

-------------------------------------------------------------

Temperature of transition -> 594.07 C
```

# Al-Mg-Zn-Mn : Scheil cooling - Microstructure Constituents

Summary & Transitions

**Microstructure constituents of AZ91 + 0.25 wt.% Mn alloy after Scheil cooling.**

Results - Equilib Summary (page-1/60)

Output Edit Show Pages

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

510 C | 505 C | 500 C |

560 C | 555 C | 550 C | 545 C | 540 C | 535 C | 530 C | 525 C | 524.12 C | 520 C | 515 C |

- Summary - | Transitions | 595 C | 594.16 C | 594.07 C | 590 C | 585 C | 580 C | 575 C | 570 C

```
SCHEIL-GULLIVER COOLING

CONSTITUENTS AND PHASES AT 340.89 C
(temperature of final disappearance of Liquid)
CONS.  PHASE                    TOTAL AMT/mol   TOTAL AMT/gram  TOTAL W
  1    1 Al8Mn5_D810             1.3055E-05      5.0230E-04      0.00
  2    1 HCP_A3                  2.6553E+00      6.4835E+01      3.73
  2    2 Al8Mn5_D810             7.5208E-03      2.8466E-01      0.00
  3    1 HCP_A3                  6.3501E-01      1.5580E+01      8.93
  3    2 Mn4Al11_s1(s)           4.2235E-03      1.4544E-01      3.91
  4    1 HCP_A3                  6.8848E-02      1.6956E+00      9.65
  4    2 MnAl4_s1(s)             5.4346E-04      1.7702E-02      5.13
  5    1 HCP_A3                  1.9793E-01      4.8919E+00      2.78
  5    2 Gamma                   4.5374E-01      1.1829E+01      5.85
  5    3 MnAl4_s1(s)             8.0662E-04      2.6274E-02      7.61
  6    1 HCP_A3                  7.1873E-03      1.8150E-01      1.01
  6    2 Phi                     1.0940E-02      3.7598E-01      1.39
  6    3 Mn4Al11_s1(s)           1.3741E-06      4.7318E-05      1.27
  7    1 HCP_A3                  7.7250E-04      1.9639E-02      1.08
  7    2 AlMgZn_Tau              6.7948E-04      2.9038E-02      7.67
  7    3 Mn4Al11_s1(s)           3.4950E-08      1.2035E-06      3.23
  8    1 HCP_A3                  1.2677E-03      3.2228E-02      1.78
  8    2 MgZn                    9.0976E-04      3.9438E-02      1.08
```

| CONS | | PHASE | TOTAL AMT/Wt.% | DESCRIPTION |
|---|---|---|---|---|
| 1 | 1 | Al8Mn5_D810 | 0.05% | Constituent 1 594.16 to 594.07 C<br>Liquid -> Al8Mn5_D810 |
| 2 | 1 | HCP_A3 | 6483.50% | Constituent 2 594.07 to 524.12 C |
| 2 | 2 | Al8Mn5_D810 | 28.47% | Liquid -> HCP_A3 + Al8Mn5_D810 |
| 3 | 1 | HCP_A3 | 1558.00% | Constituent 3 524.12 to 447.41 C |
| 3 | 2 | Mn4Al11_s1(s) | 14.54% | Liquid -> HCP_A3 + Mn4Al11_s1(s) |
| 4 | 1 | HCP_A3 | 169.56% | Constituent 4 447.41 to 431.70 C |
| 4 | 2 | MnAl4_s1(s) | 1.77% | Liquid -> HCP_A3 + MnAl4_s1(s) |
| 5 | 1 | HCP_A3 | 489.19% | Constituent 5 431.70 to 364.34 C |
| 5 | 2 | Gamma | 1182.90% | Liquid -> HCP_A3 + Gamma + MnAl4_s1(s) |
| 5 | 3 | MnAl4_s1(s) | 2.63% | |
| 6 | 1 | HCP_A3 | 18.15% | Constituent 6 364.34 to 342.67 C |
| 6 | 2 | Phi | 37.60% | Liquid -> HCP_A3 + Phi + Mn4Al11_s1(s) |
| 6 | 3 | Mn4Al11_s1(s) | 0.00% | |
| 7 | 1 | HCP_A3 | 1.96% | Constituent 7 342.67 to 340.89 C |
| 7 | 2 | AlMgZn_Tau | 2.90% | Liquid -> HCP_A3 + AlMgZn_Tau + Mn4Al11_s1(s) |
| 7 | 3 | Mn4Al11_s1(s) | 0.00% | |
| 8 | 1 | HCP_A3 | 3.22% | |
| 8 | 2 | MgZn | 3.94% | Constituent 8 340.89 C (isothermal) |
| 8 | 3 | AlMgZn_Tau | 1.64% | Liquid -> HCP_A3 + MgZn + AlMgZn_Tau + Mn4Al11_s1(s) |
| 8 | 4 | Mn4Al11_s1(s) | 0.00% | |

**Final disappearance of liquid at 340.89°C**

# Al-Mg-Zn-Mn : Scheil cooling and fully annealing cast alloy

Scheil cooling and post equilibration (annealing) of Scheil microstructure: **AZ91 alloy + 0.25 wt.% Mn**

**Tracking microstructure constituents**

**Output : Solidification temperature of 340.89°C**

| CONS. | PHASE | TOTAL AMT/gram |
|---|---|---|
| 1 | 1 'Al8Mn5' | 5.2241E-04 |
| 2 | 1 HCP | 6.4599E+01 |
| 2 | 2 'Al8Mn5' | 2.8231E-01 |
| 3 | 1 HCP | 1.5644E+01 |
| 3 | 2 Al11Mn4 | 1.4638E-01 |
| 4 | 1 HCP | 1.7084E+00 |
| 4 | 2 'Al4Mn' | 1.7892E-02 |
| 5 | 1 HCP | 4.9213E+00 |
| 5 | 2 'Al12Mg17' | 1.1878E+01 |
| 5 | 3 'Al4Mn' | 2.6558E-02 |
| 6 | 1 HCP | 1.9669E-01 |
| 6 | 2 Phi | 4.0423E-01 |
| 6 | 3 'Al4Mn' | 1.7904E-05 |
| 6 | 4 Al11Mn4 | 3.8196E-05 |
| 7 | 1 HCP | 2.4177E-02 |
| 7 | 2 Tau | 3.5706E-02 |
| 7 | 3 Al11Mn4 | 1.4894E-06 |
| 8 | 1 HCP | 4.2084E-02 |
| 8 | 2 MgZn | 5.1501E-02 |
| 8 | 3 Tau | 2.1364E-02 |
| 8 | 4 Al11Mn4 | 2.3786E-06 |

Amount & Average Composition of the **HCP phase**

| | wt. % | Mg | Al | Zn | Mn |
|---|---|---|---|---|---|
| 2 | 64.599 | 96.19 | 3.67 | 0.125 | 195 ppm |
| 3 | 15.644 | 92.25 | 7.45 | 0.298 | 14.7 ppm |
| 4 | 1.708 | 89.22 | 10.34 | 0.440 | 1.2 ppm |
| 5 | 4.921 | 88.95 | 10.03 | 1.021 | 0.7 ppm |
| 6 | 0.197 | 89.77 | 5.14 | 5.086 | 0.1 ppm |
| 7 | 0.024 | 90.55 | 2.93 | 6.519 | 0.2 ppm |
| 8 | 0.042 | 90.57 | 2.90 | 6.538 | 0.2 ppm |

# Al-Mg-Zn-Mn : selecting HCP phase for full annealing

Results - Equilib Summary (page-1/60)

Output Edit Show Pages

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

510 C | 505 C | 500 C |

560 C | 555 C | 550 C | 545 C | 540 C | 535 C | 530 C | 525 C | 524.12 C | 520 C | 515 C |

- Summary - | Transitions | 595 C | 594.16 C | 594.07 C | 590 C | 585 C | 580 C | 575 C | 570 C | 565 C |

SCHEIL-GULLIVER COOLING

CONSTITUENTS AND PHASES AT 340.89 C
(temperature of final disappearance of Liquid)

| CONS. | PHASE | TOTAL AMT/mol | TOTAL AMT/gram | TOTAL VOL/dm3 |
|---|---|---|---|---|
| 1 | 1 Al8Mn5_D810 | 1.3055E-05 | 5.0230E-04 | 0.0000E+00 |
| 2 | 1 HCP_A3 | 2.6553E+00 | 6.4835E+01 | 3.7348E-02 |
| 2 | 2 Al8Mn5_D810 | 7.5208E-03 | 2.8466E-01 | 0.0000E+00 |
| 3 | 1 HCP_A3 | 6.3501E-01 | 1.5580E+01 | 8.9318E-03 |
| [illegible] | [illegible] | [illegible] | [illegible] | 3.9104E-05 |
| [illegible] | [illegible] | [illegible] | [illegible] | 9.6839E-04 |
| [illegible] | [illegible] | [illegible] | [illegible] | 5.1305E-06 |
| [illegible] | [illegible] | [illegible] | [illegible] | 2.7840E-03 |
| 5 | 2 Gamma | 4.5374E-01 | 1.1829E+01 | 5.8586E-03 |
| 5 | 3 MnAl4_s1(s) | 8.0662E-04 | 2.6274E-02 | 7.6148E-06 |
| 6 | 1 HCP_A3 | 7.1873E-03 | 1.8150E-01 | 1.0109E-04 |
| 6 | 2 Phi | 1.0940E-02 | 3.7598E-01 | 1.3952E-04 |
| 6 | [illegible] | [illegible] | [illegible] | 1.2722E-08 |
| 7 | [illegible] | [illegible] | [illegible] | 1.0866E-05 |
| 7 | 2 AlMgZn_Tau | 6.7948E-04 | 2.9038E-02 | 7.6777E-06 |
| 7 | 3 Mn4Al11_s1(s) | 3.4950E-08 | 1.2035E-06 | 3.2358E-10 |
| 8 | 1 HCP_A3 | 1.2677E-03 | 3.2228E-02 | 1.7831E-05 |
| 8 | 2 MgZn | 9.0976E-04 | 3.9438E-02 | 1.0892E-05 |

1° **Point mouse** to **constituent 2 HCP_A3** and **double-click**

2° Click **OK** to recycle **HCP_A3**

FactSage 6.3: Equilib

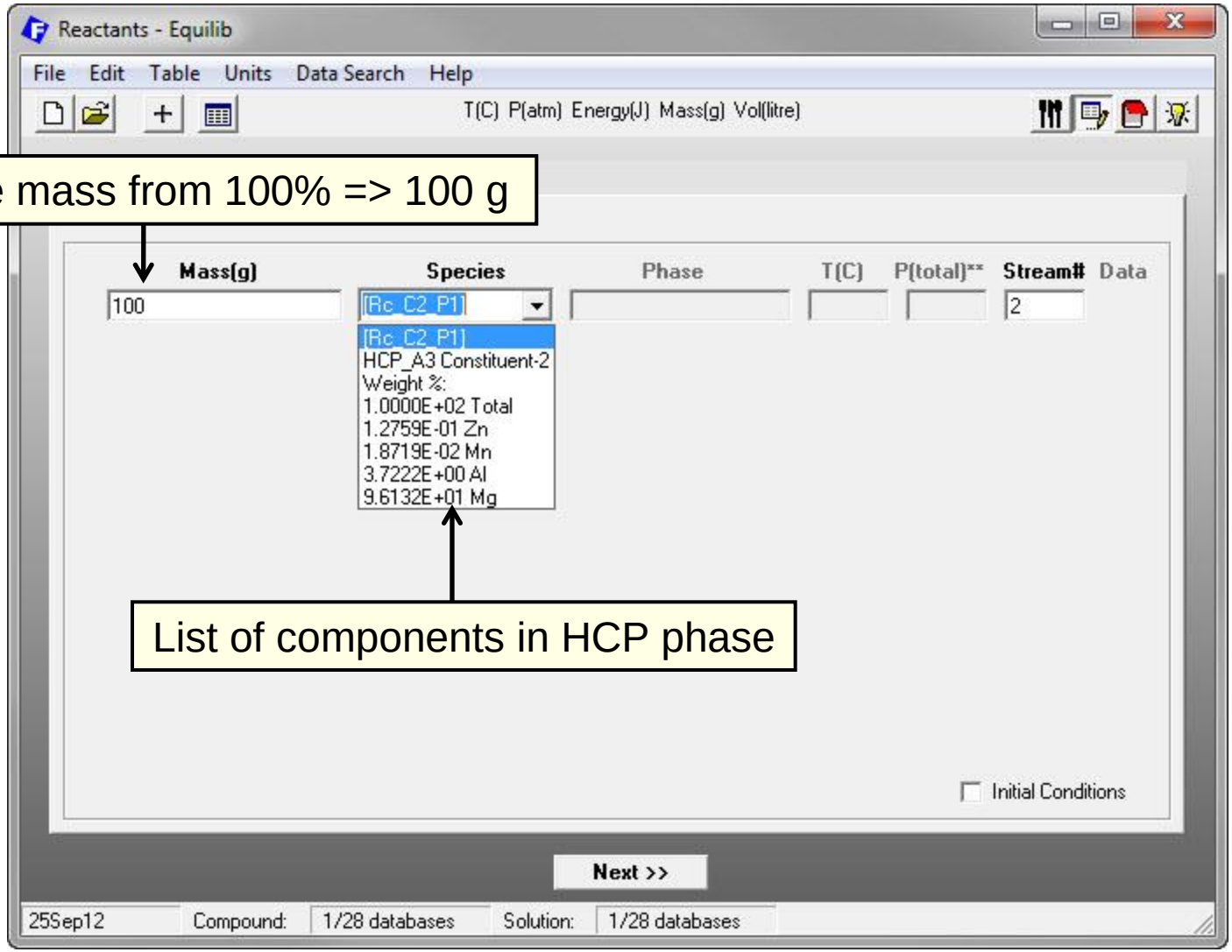
Do you wish to recycle Phase 1 of Constituent 2?

HCP_A3

| | MOLE FRACTION | MASS FRACTION |
|---|---|---|
| Zn | 4.7652E-04 | 1.2759E-03 |
| Mn | 8.3198E-05 | 1.8719E-04 |
| Al | 3.3684E-02 | 3.7222E-02 |
| Mg | 9.6576E-01 | 9.6132E-01 |
| | TOTAL AMT/mol | TOTAL AMT/gram |
| | 2.6553E+00 | 6.4835E+01 |

OK Cancel

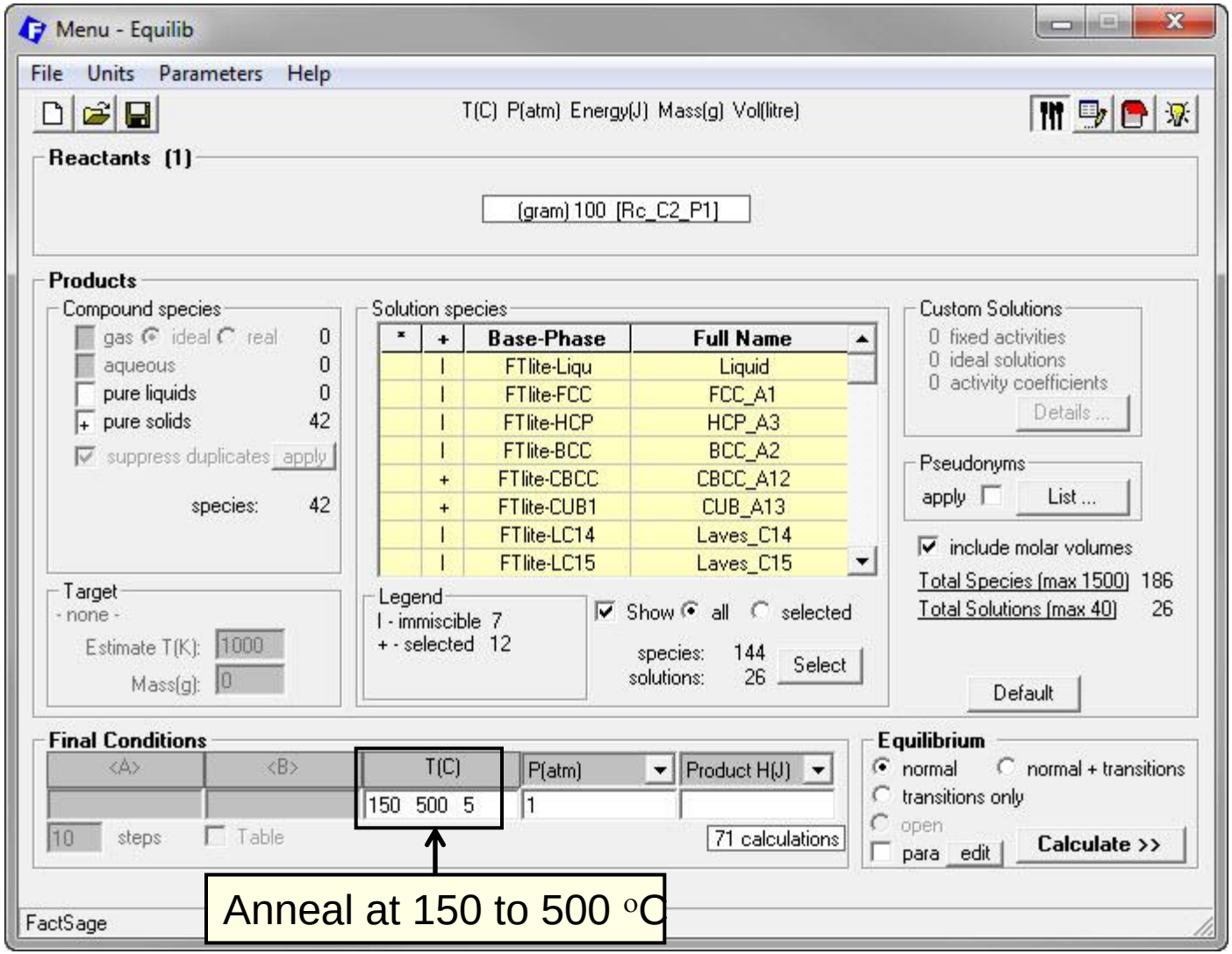
# Al-Mg-Zn-Mn : HCP phase imported into *Reactant Window*



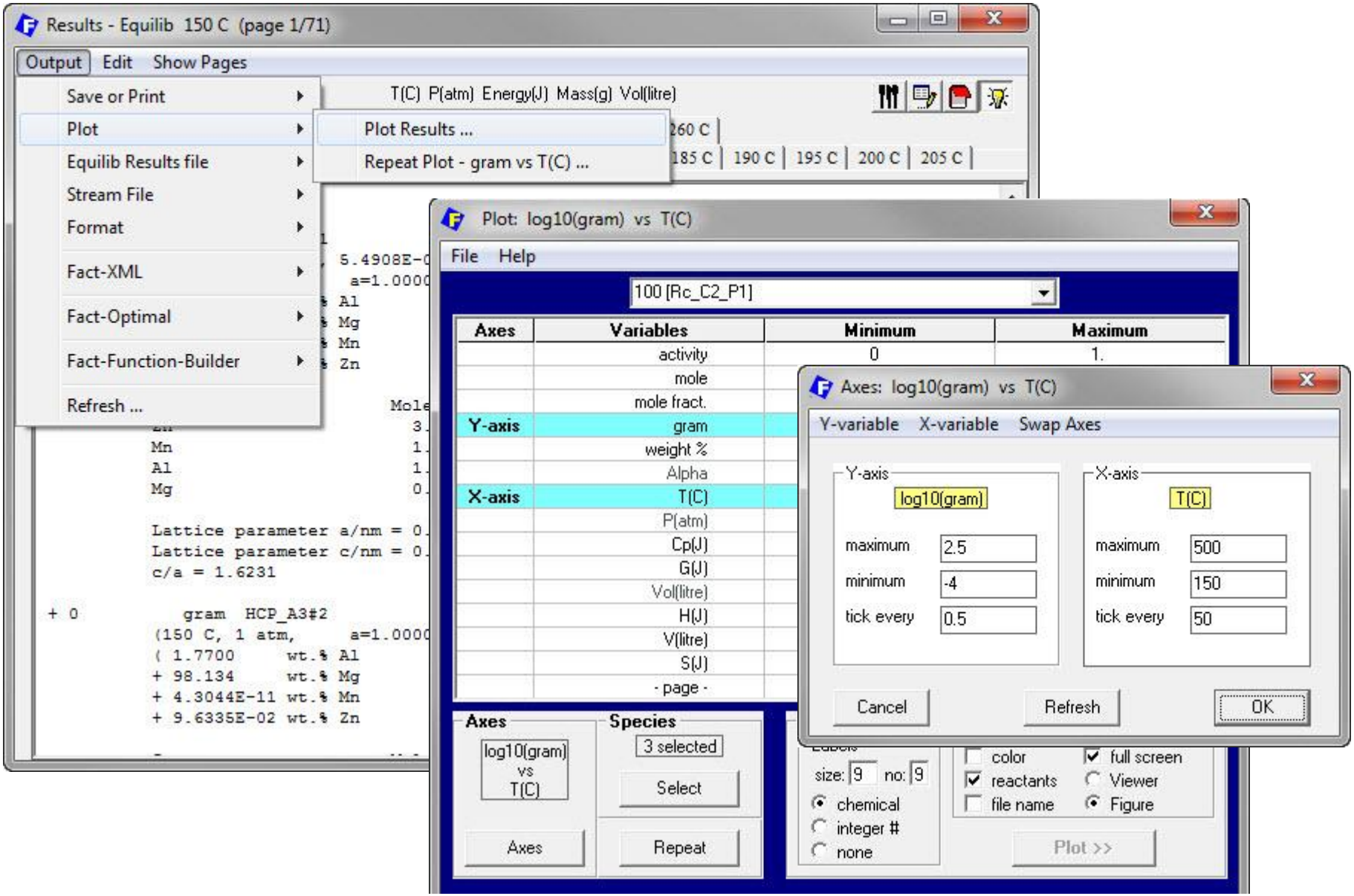

Change mass from 100% => 100 g

List of components in HCP phase

# Al-Mg-Zn-Mn : Equilibrium calculation – full annealing of HCP

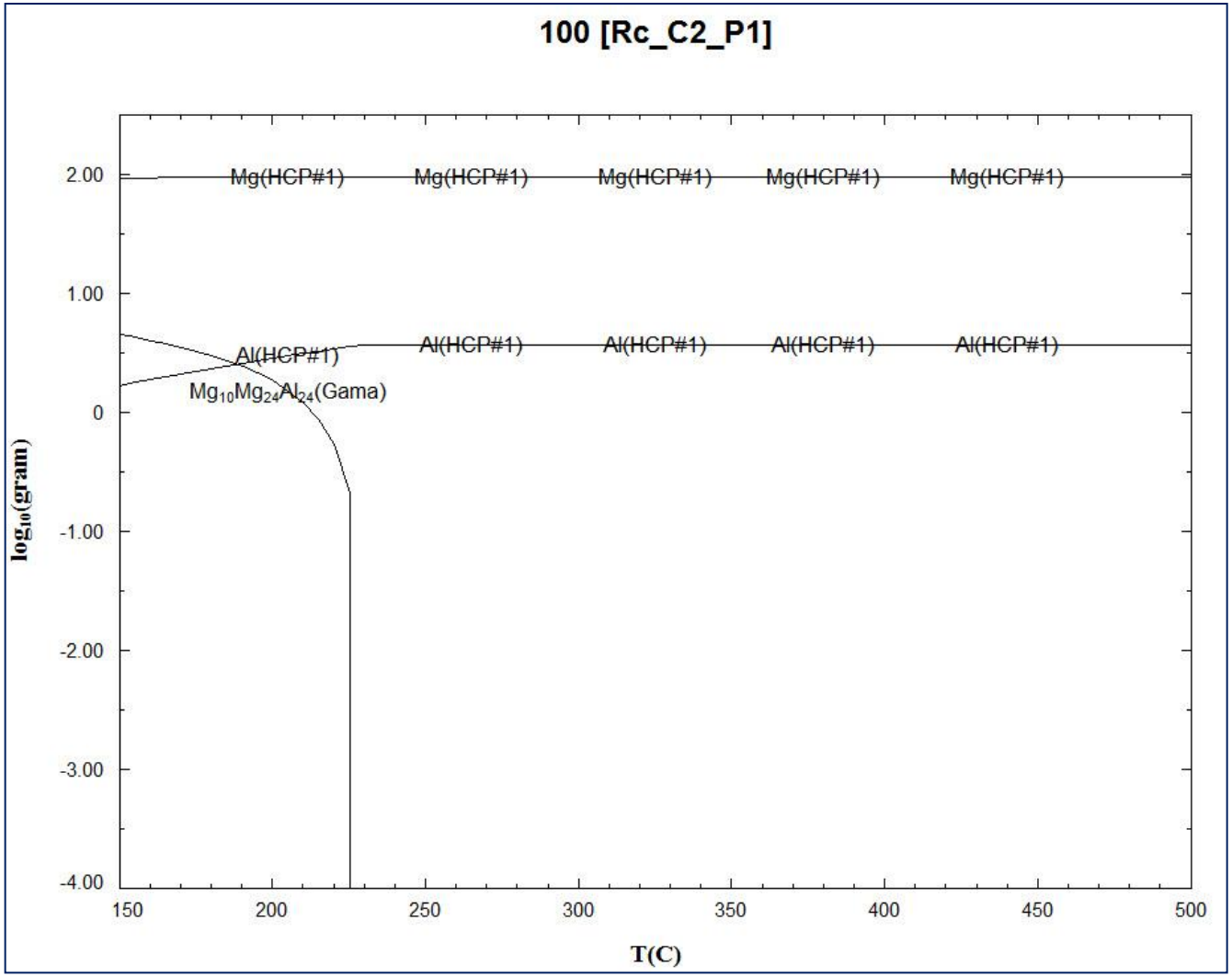


# Al-Mg-Zn-Mn : Plotting fully annealed HCP phase



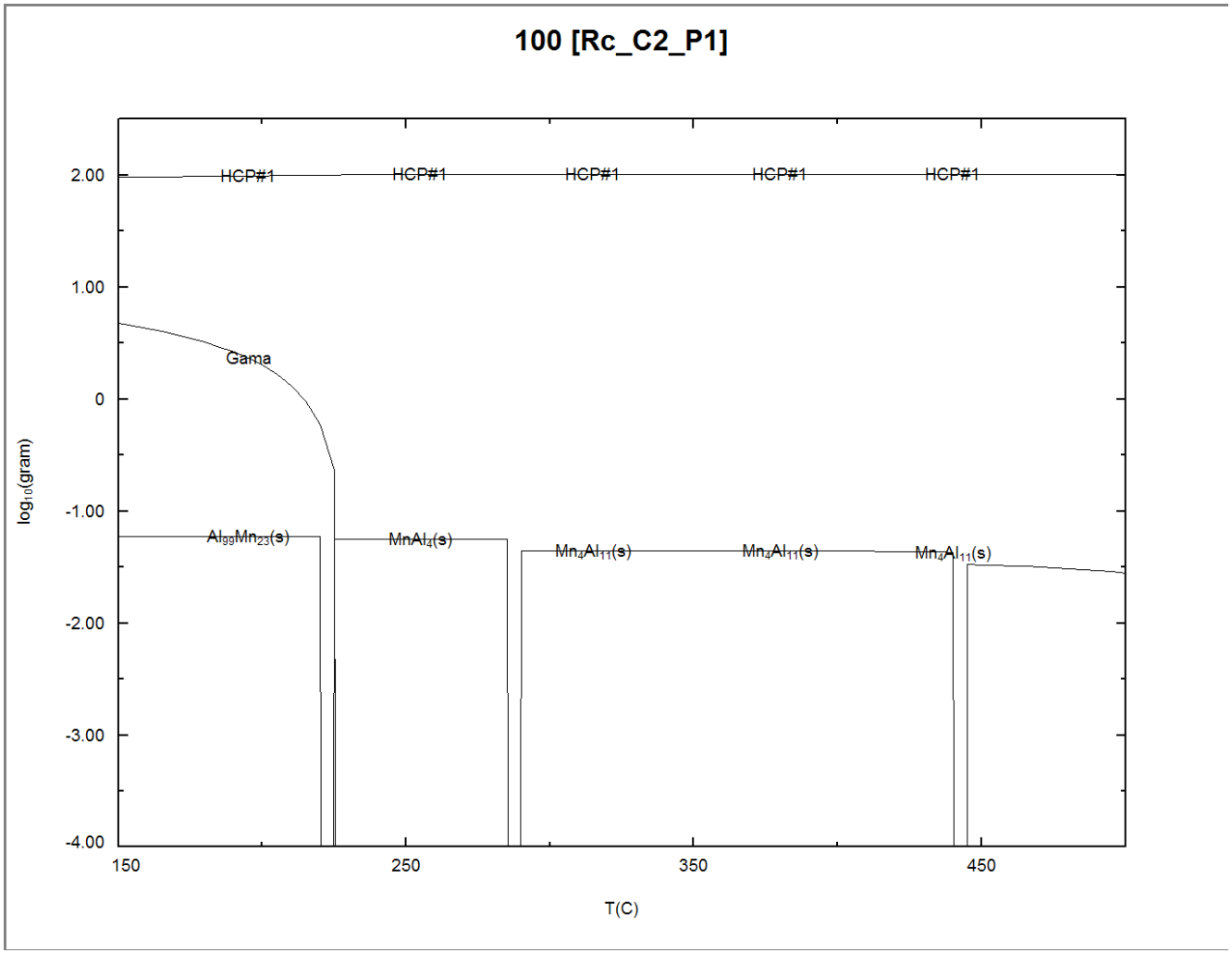
# Al-Mg-Zn-Mn : Graph of fully annealed HCP phase

Equilibrium phase distribution in HCP phase of constituent 2 after annealing (HCP + precipitates)



# Al-Mg-Zn-Mn : Graph of fully annealed HCP phase

Equilibrium phase distribution in HCP phase of constituent 2 after annealing (HCP + precipitates)



# Al-Mg-Zn-Mn : Tracking microstructure constituents

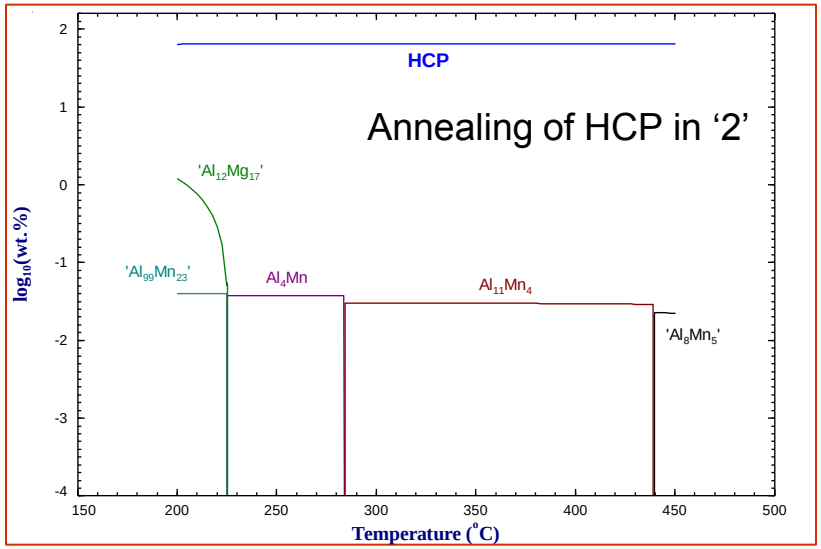
Scheil cooling and post equilibration (annealing) of Scheil microstructure: AZ91 alloy + 0.25 wt.% Mn

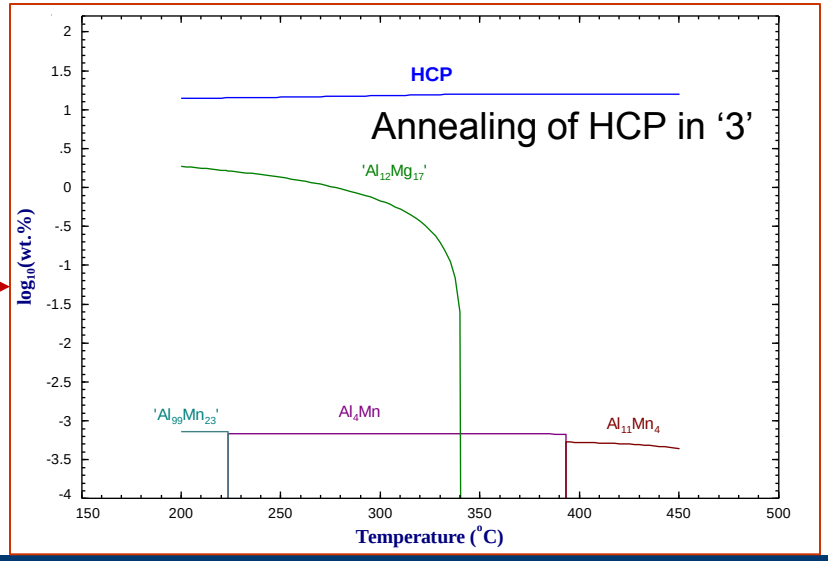
Tracking microstructure constituents

Annealing:
Phases *vs* T for HCP in the different microstructural constituents

Amount & Average Composition of the **HCP phase** at 340.89°C

| | wt. % | Mg | Al | Zn | Mn |
|---|---|---|---|---|---|
| 2 | 64.599 | 96.19 | 3.67 | 0.125 | 195 ppm |
| 3 | 15.644 | 92.25 | 7.45 | 0.298 | 14.7 ppm |
| 4 | 1.708 | 89.22 | 10.34 | 0.440 | 1.2 ppm |
| 5 | 4.921 | 88.95 | 10.03 | 1.021 | 0.7 ppm |
| 6 | 0.197 | 89.77 | 5.14 | 5.086 | 0.1 ppm |
| 7 | 0.024 | 90.55 | 2.93 | 6.519 | 0.2 ppm |
| 8 | 0.042 | 90.57 | 2.90 | 6.538 | 0.2 ppm |



# Paraequilibrium and minimum Gibbs energy calculations

- In certain solid systems, some elements diffuse much faster than others. Hence, if an initially homogeneous single-phase system at high temperature is quenched rapidly and then held at a lower temperature, a temporary **paraequilibrium state** may result in which the rapidly diffusing elements have reached equilibrium, but the more slowly diffusing elements have remained essentially immobile.

- The best known, and most industrially important, example occurs when homogeneous austenite is quenched and annealed. Interstitial elements such as C and N are much more mobile than the metallic elements.

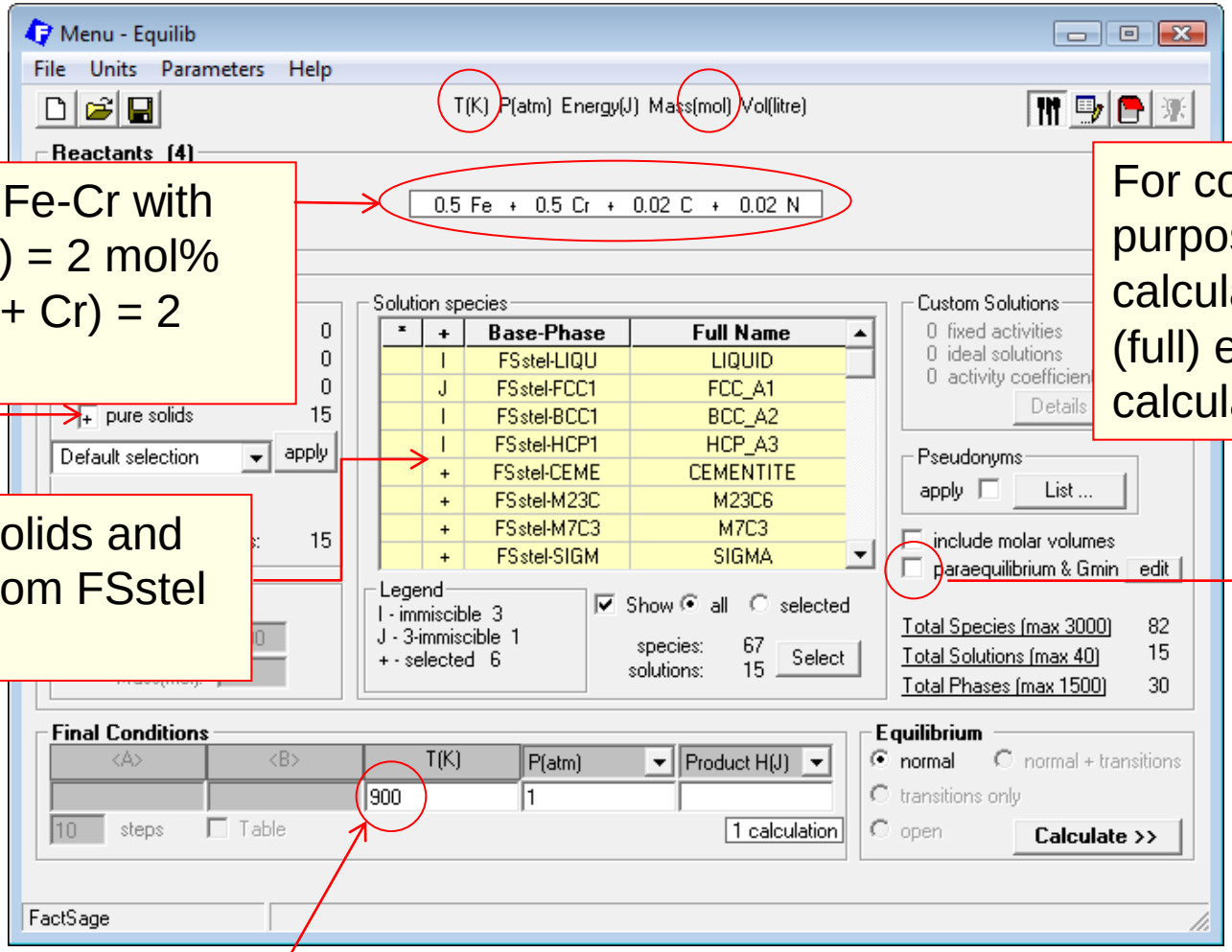
- At paraequilibrium, the ratios of the slowly diffusing elements in all phases are the same and are equal to their ratios in the initial single-phase alloy. The algorithm used to calculate paraequilibrium in FactSage is based upon this fact. That is, the algorithm minimizes the Gibbs energy of the system under this constraint.

- If a paraequilibrium calculation is performed specifying that no elements diffuse quickly, then the ratios of all elements are the same as in the initial homogeneous state. In other words, such a calculation will simply yield the single homogeneous phase with the minimum Gibbs energy at the temperature of the calculation. Such a calculation may be of practical interest in **physical vapour deposition** where deposition from the vapour phase is so rapid that phase separation cannot occur, resulting in a single-phase solid deposit.

- Paraequilibrium phase diagrams and minimum Gibbs energy diagrams may be calculated with the **Phase Diagram Module**. See the Phase Diagram slide show.

# Paraequilibrium and minimum Gibbs energy calculations

## Fe-Cr-C-N system at 900K




Equimolar Fe-Cr with C/(Fe + Cr) = 2 mol% and N/(Fe + Cr) = 2 mol%

Select all solids and solutions from FSstel database

For comparison purposes, our first calculation is a normal (full) equilibrium calculation

T = 900K

# Paraequilibrium and minimum Gibbs energy calculations

## Output for a normal (full) equilibrium calculation

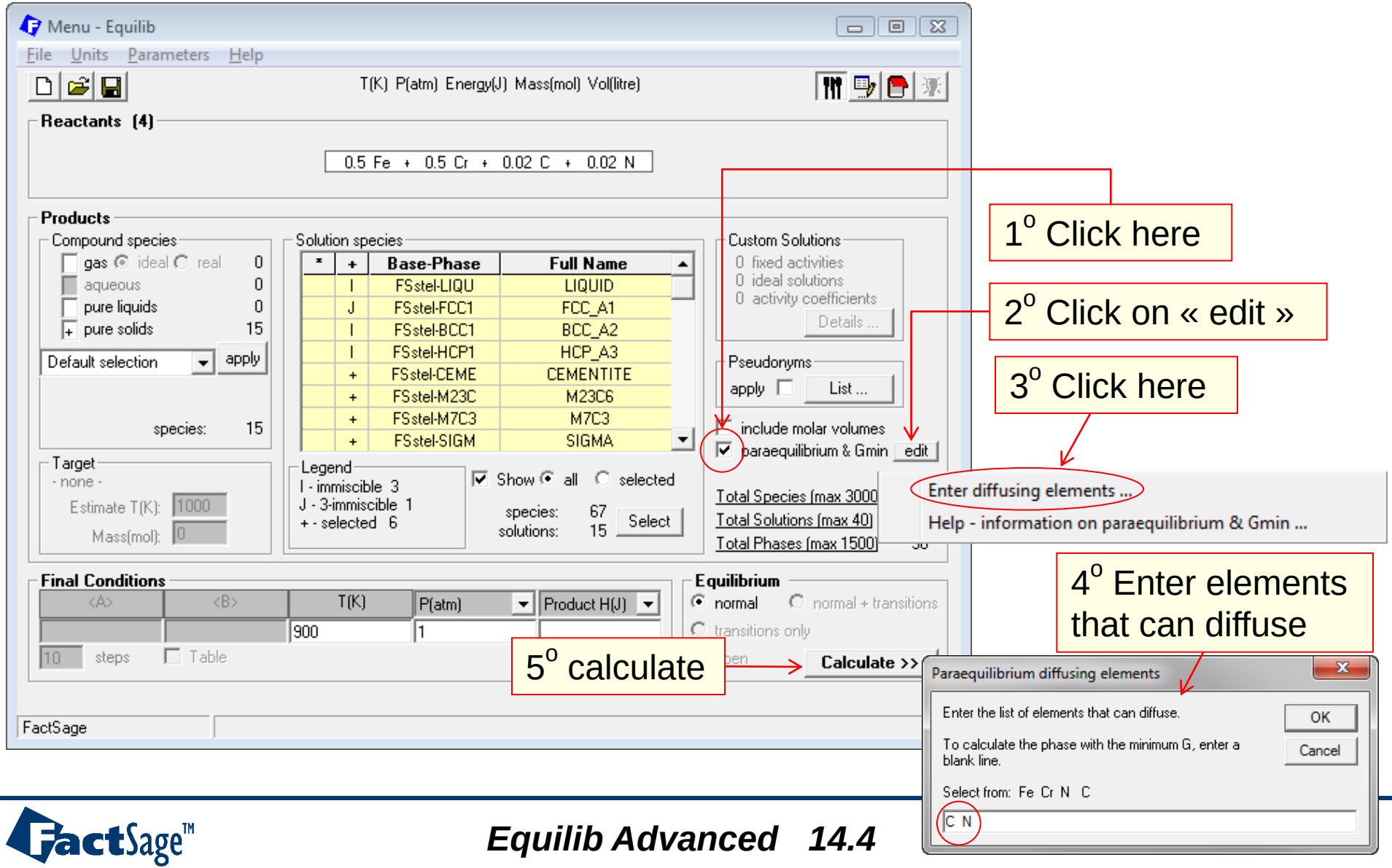
```
0.5 Fe +  0.5 Cr +  0.02 C +  0.02 N =

  7.4396E-02 mol   BCC_A2#1
  (4.0866 gram, 7.4396E-02 mol)
        (900 K, 1 atm,     a=1.0000)
        ( 9.6768E-07      Cr1C3
        + 3.1056E-06      Fe1C3
        + 5.0286E-07      Cr1N3
        + 1.6138E-06      Fe1N3
        + 0.23757         Cr1Va3
        + 0.76243         Fe1Va3)

  + 2.6944E-02 mol   SIGMA
  (43.703 gram, 2.6944E-02 mol)
        (900 K, 1 atm,     a=1.0000)
        ( 0.54775         Fe8Cr4Cr18
        + 0.45225         Fe8Cr4Fe18)

        + 2.1157E-02 mol   HCP_A3#1
  (2.4859 gram, 2.1157E-02 mol)
        (900 K, 1 atm,     a=1.0000)
        ( 2.0659E-02      Cr2C
        + 4.3490E-05      Fe2C
        + 0.94329         Cr2N
        + 1.9858E-03      Fe2N
        + 3.3949E-02      Cr2Va
        + 7.1468E-05      Fe2Va)

+ 3.2602E-03 mol   M23C6
  (4.1658 gram, 3.2602E-03 mol)
        (900 K, 1 atm,     a=1.0000)
        ( 0.81351         Cr20Cr3C6
        + 0.10610         Fe20Cr3C6
        + 7.1113E-02      Cr20Fe3C6
        + 9.2748E-03      Fe20Fe3C6)
```

**4 phases are formed at full equilibrium**

# Paraequilibrium and minimum Gibbs energy calculations

## Fe-Cr-C-N system at 900K

## when only C and N are permitted to diffuse



# Paraequilibrium and minimum Gibbs energy calculations

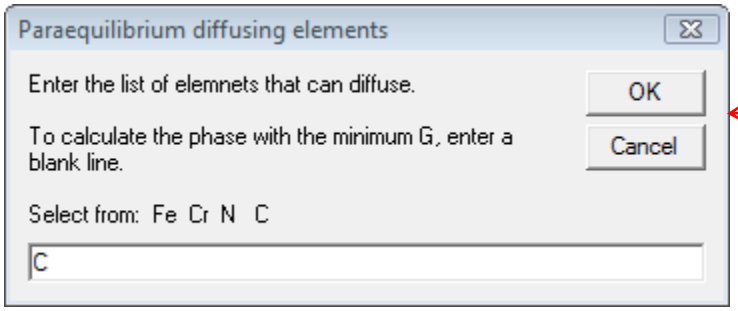
## Output when only C and N are permitted to diffuse

```
0.5 Fe +  0.5 Cr +  0.02 C +  0.02 N =

  0.14857    mol   FCC_A1#1
  (8.2952 gram, 0.14857 mol)
        (900 K, 1 atm,     a=1.0000)
        ( 1.1737E-03      Cr1C1
        + 1.1737E-03      Fe1C1
        + 6.7310E-02      Cr1N1
        + 6.7310E-02      Fe1N1
        + 0.43152         Cr1Va1
        + 0.43152         Fe1Va1)

        System component                Mole fraction  Mass fraction
        Fe                              0.43977        0.50010
        Cr                              0.43977        0.46563
        N                               0.11840        3.3771E-02
        C                               2.0646E-03     5.0496E-04

 + 2.5870E-02 mol   SIGMA
  (41.848 gram, 2.5870E-02 mol)
        (900 K, 1 atm,     a=1.0000)
        ( 0.61111         Fe8Cr4Cr18
        + 0.38889         Fe8Cr4Fe18)

        System component                Mole fraction  Mass fraction
        Fe                              0.50000        0.51785
        Cr                              0.50000        0.48215

 + 3.2752E-03 mol   M23C6
  (4.2978 gram, 3.2752E-03 mol)
        (900 K, 1 atm,     a=1.0000)
        ( 0.25000         Cr20Cr3C6
        + 0.25000         Fe20Cr3C6
        + 0.25000         Cr20Fe3C6
        + 0.25000         Fe20Fe3C6)

        System component                Mole fraction  Mass fraction
        Fe                              0.39655        0.48941
        Cr                              0.39655        0.45568
        C                               0.20690        5.4917E-02
```

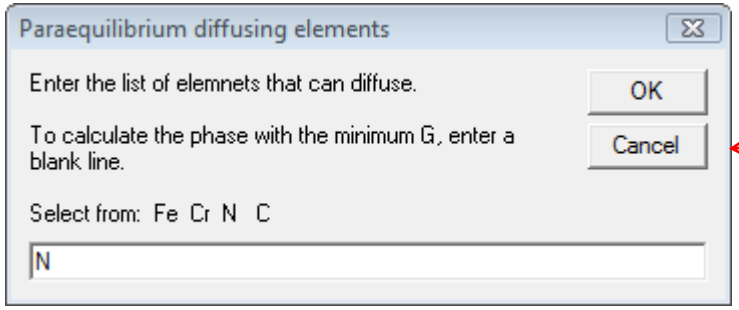
**Fe/Cr** molar ratio = **1/1** in all phases

**3 phases are formed at paraequilibrium when only C and N are permitted to diffuse**

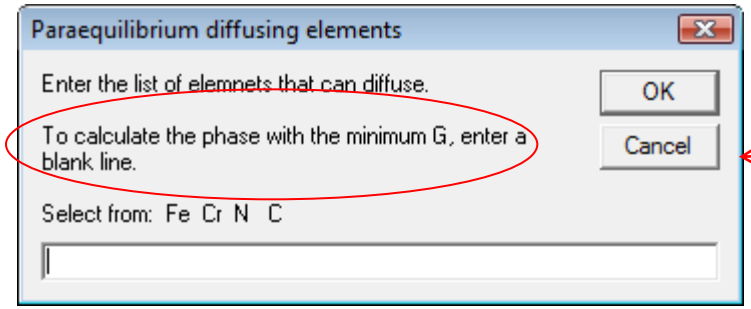
# Paraequilibrium and minimum Gibbs energy calculations




**Input when only C is permitted to diffuse**




**Input when only N is permitted to diffuse**




**Input when no elements are permitted to diffuse (minimum Gibbs energy calculation)**

# Paraequilibrium and minimum Gibbs energy calculations

## Output when only C is permitted to diffuse

```
0.5 Fe +  0.5 Cr +  0.02 C +  0.02 N =

 0.94732    mol   BCC_A2#1
 (51.387 gram, 0.94732 mol)
        (900 K, 1 atm,     a=1.0000)
        ( 6.1460E-04      Cr1C3
        + 6.1460E-04      Fe1C3
        + 3.3333E-03      Cr1N3
        + 3.3333E-03      Fe1N3
        + 0.49605         Cr1Va3
        + 0.49605         Fe1Va3)

        System component          Mole fraction  Mass fraction
        Fe                        0.48843        0.51475
        Cr                        0.48843        0.47927
        N                         1.9537E-02     5.1642E-03
        C                         3.6023E-03     8.1649E-04

+ 1.7560E-02 mol   CEMENTITE
 (3.0536 gram, 1.7560E-02 mol)
        (900 K, 1 atm,     a=1.0000)
        ( 0.47000         Cr3C1
        + 0.47000         Fe3C1
        + 3.0000E-02      Cr3N1
        + 3.0000E-02      Fe3N1)

        System component          Mole fraction  Mass fraction
        Fe                        0.37500        0.48172
        Cr                        0.37500        0.44852
        N                         1.5000E-02     4.8329E-03
        C                         0.23500        6.4926E-02
```

**Fe/Cr** molar ratio = **1/1** in all phases

**N/(Fe+Cr)** molar ratio = **0.02** in all phases

**2 phases are formed at paraequilibrium**

# Paraequilibrium and minimum Gibbs energy calculations

## Output when only N is permitted to diffuse

```
FactSage 6.4
 0.5 Fe +  0.5 Cr +  0.02 C +  0.02 N =

  0.81037    mol   BCC_A2#1
  (43.892 gram, 0.81037 mol)
        (900 K, 1 atm,     a=1.0000)
        ( 3.3333E-03      Cr1C3
        + 3.3333E-03      Fe1C3
        + 2.4375E-05      Cr1N3
        + 2.4375E-05      Fe1N3
        + 0.49664         Cr1Va3
        + 0.49664         Fe1Va3)

        System component          Mole fraction  Mass fraction
        Fe                         0.49013        0.51553
        Cr                        0.49013        0.48000
        N                         1.4336E-04     3.7820E-05
        C                         1.9605E-02     4.4350E-03

 + 0.18963    mol   FCC_A1#1
  (10.549 gram, 0.18963 mol)
        (900 K, 1 atm,     a=1.0000)
        ( 1.0000E-02      Cr1C1
        + 1.0000E-02      Fe1C1
        + 5.2423E-02      Cr1N1
        + 5.2423E-02      Fe1N1
        + 0.43758         Cr1Va1
        + 0.43758         Fe1Va1)

        System component          Mole fraction  Mass fraction
        Fe                        0.44451        0.50194
        Cr                        0.44451        0.46734
        N                         9.3209E-02     2.6399E-02
        C                         1.7780E-02     4.3181E-03
```

**Fe/Cr** molar ratio = **1/1** in all phases

**C/(Fe+Cr)** molar ratio = **0.02** in all phases

**2 phases are formed at paraequilibrium**

# Paraequilibrium and minimum Gibbs energy calculations

## Minimum Gibbs energy calculation (no elements permitted to diffuse)

0.5 Fe + 0.5 Cr + 0.02 C + 0.02 N =

1.0000 mol BCC_A2#1
(54.441 gram, 1.0000 mol)
(900 K, 1 atm, a=1.0000)
( 3.3333E-03 Cr1C3
+ 3.3333E-03 Fe1C3
+ 3.3333E-03 Cr1N3
+ 3.3333E-03 Fe1N3
+ 0.49333 Cr1Va3
+ 0.49333 Fe1Va3)

| System component | Mole fraction | Mass fraction |
|---|---|---|
| Fe | 0.48077 | 0.51290 |
| Cr | 0.48077 | 0.47755 |
| N | 1.9231E-02 | 5.1457E-03 |
| C | 1.9231E-02 | 4.4124E-03 |

**The phase with the lowest Gibbs energy of this composition at 900K is the bcc phase**