Advanced features of *Equilib*

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

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(continued)

Advanced features of *Equilib* - Table of Contents (continued)

(continued)

Advanced features of *Equilib* - Table of Contents (continued)

Target phase options

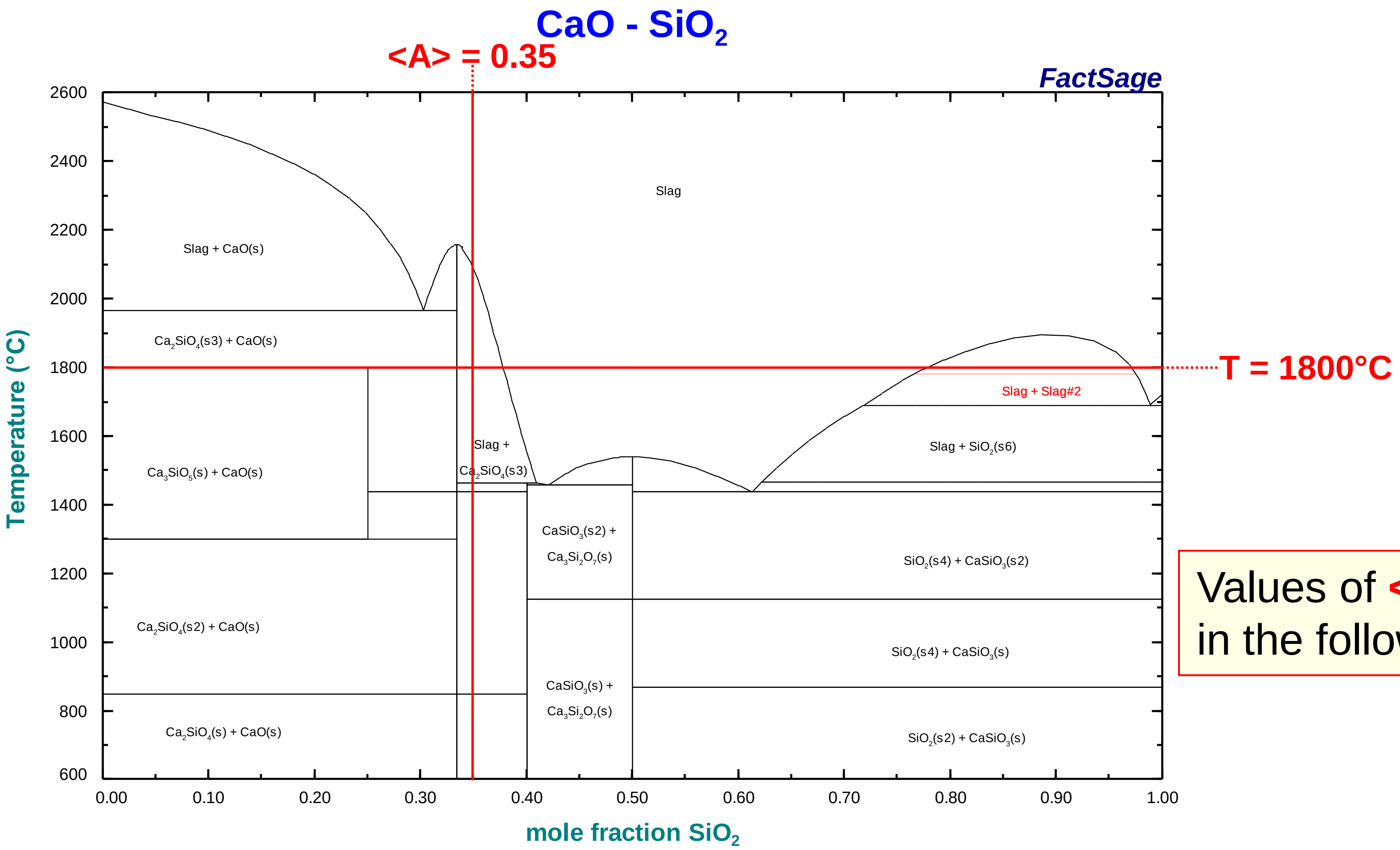
A species or solution phase may be declared as a Target phase. There are several types of target phases:

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).


CaO - SiO_2

<A> = 0.35

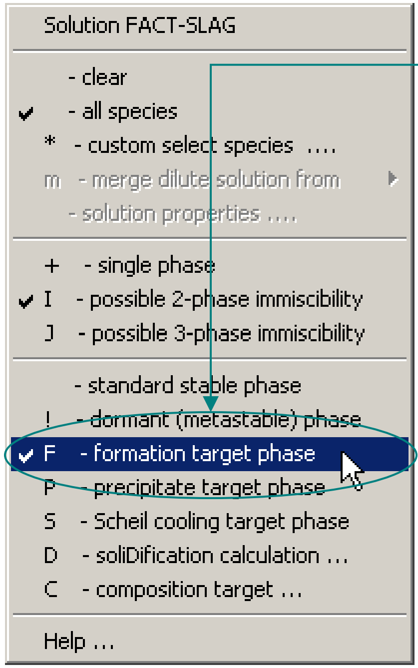
T = 1800°C

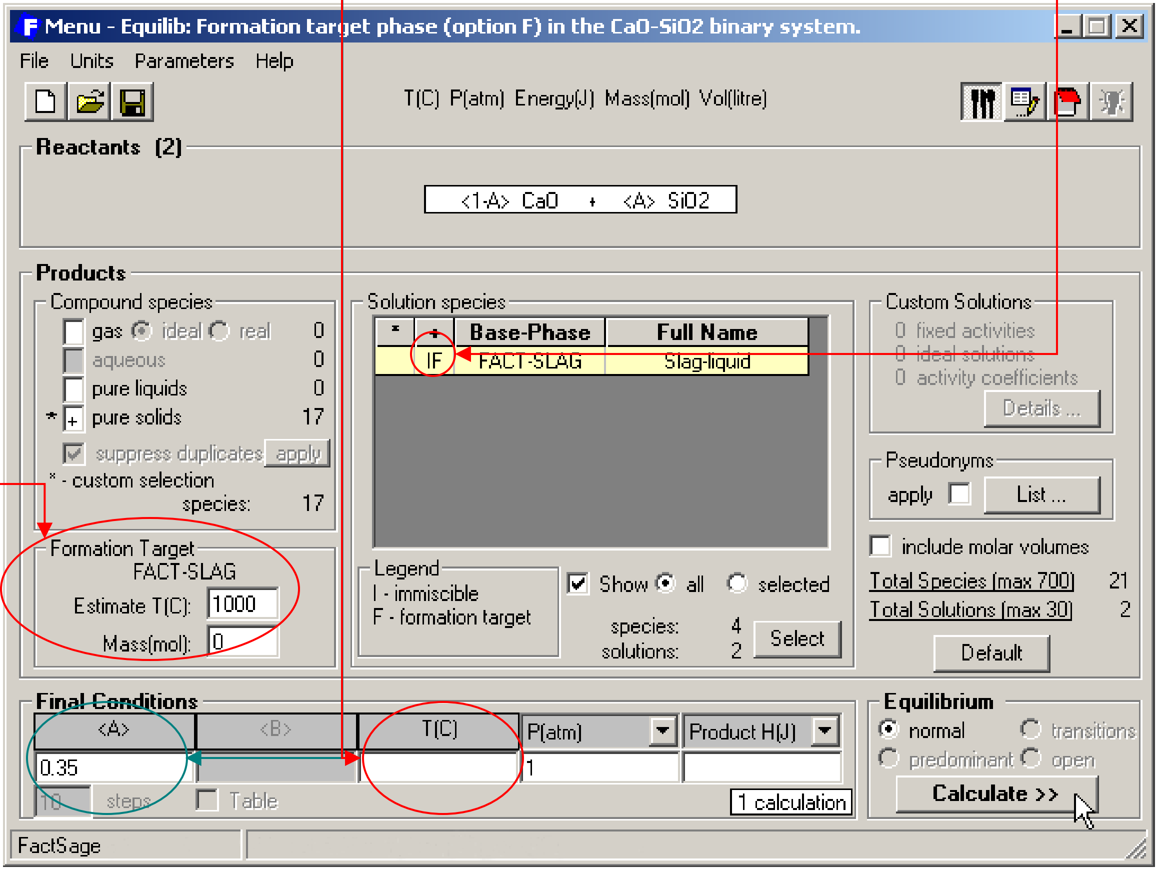
Values of **<A>** and **T** used in the following example.

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.





Reactants (2): <1-A> CaO + <A> SiO2

Compound species:

☐ gas ● ideal ○ real	0
☐ aqueous	0
☐ pure liquids	0
* ☑ pure solids	17

☑ suppress duplicates apply

* - custom selection species: 17

Solution species:

*	+	Base-Phase	Full Name
	IF	FACT-SLAG	Slag-liquid

Custom Solutions: 0 fixed activities; 0 ideal solutions; 0 activity coefficients; Details ...

Pseudonyms: apply ☐ List ...

☐ include molar volumes

Total Species (max 700) 21

Total Solutions (max 30) 2

Default

Formation Target FACT-SLAG

Estimate T(C): 1000

Mass(mol): 0

Legend: I - immiscible; F - formation target

☑ Show ● all ○ selected

species: 4

solutions: 2

Select

Final Conditions:

<A>	<B>	T(C)	P(atm)	Product H(J)
0.35			1	

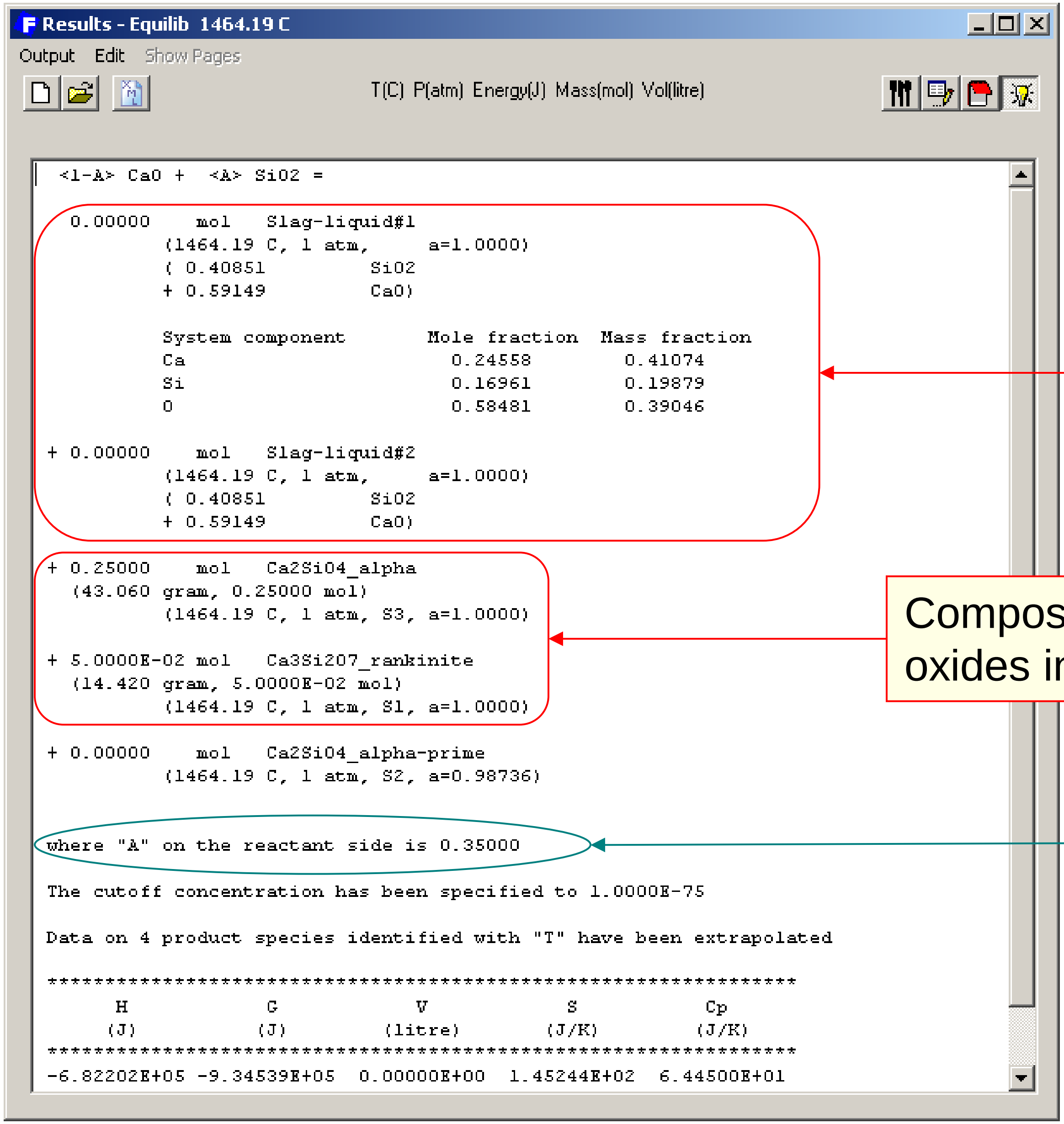
10 steps ☐ Table 1 calculation

Equilibrium: ● normal ○ transitions ○ predominant ○ open

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



```
 <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
```

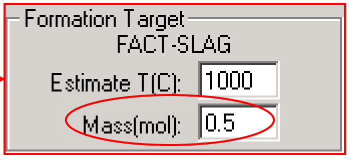
Note:
activity = 1.0
number of moles = 0
for the slag phase (liquid)
i.e. FACT-SLAG is just
beginning to form.

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

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

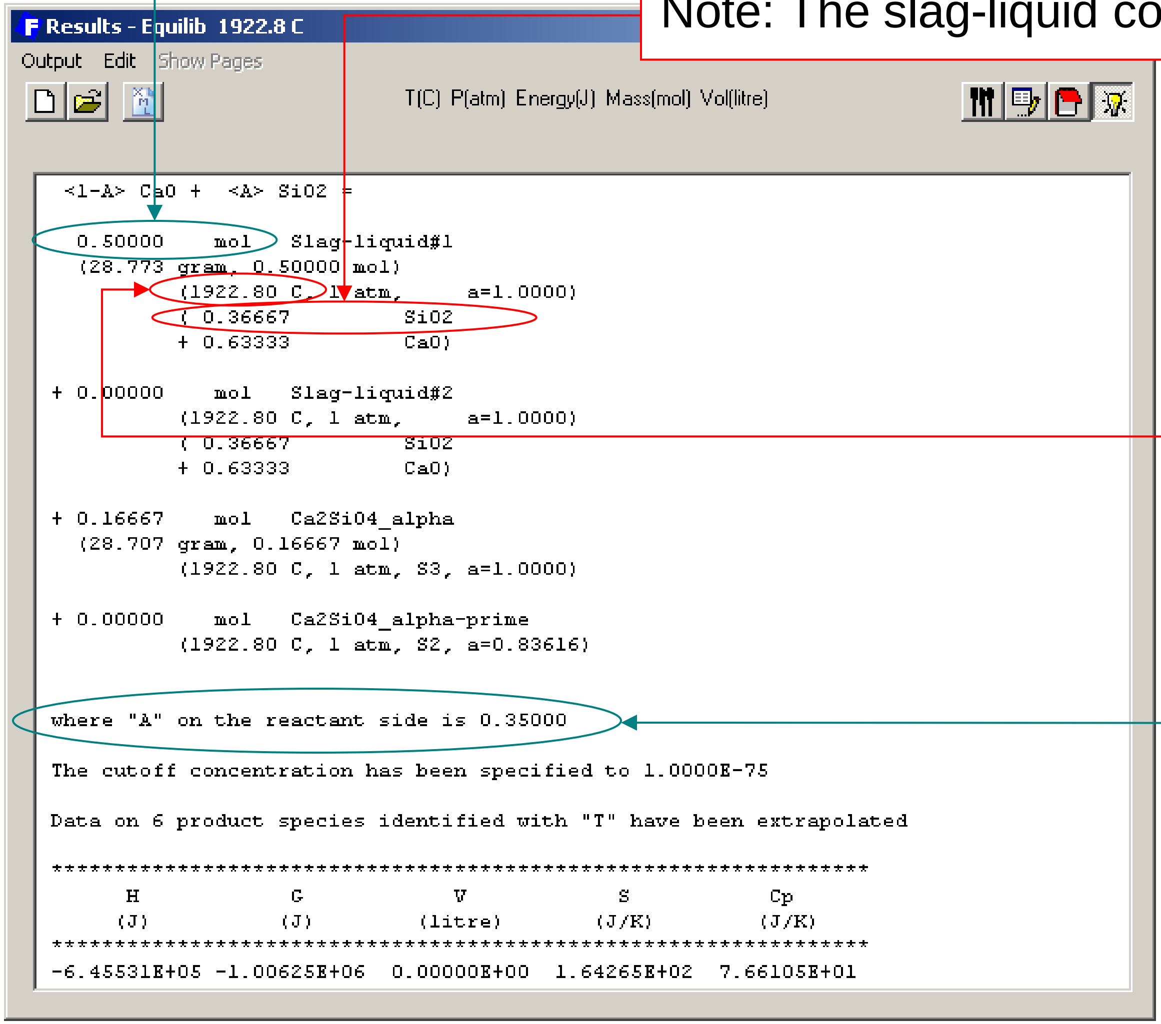
Formation Target phase: specifying the target phase mass

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



```
 <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
```

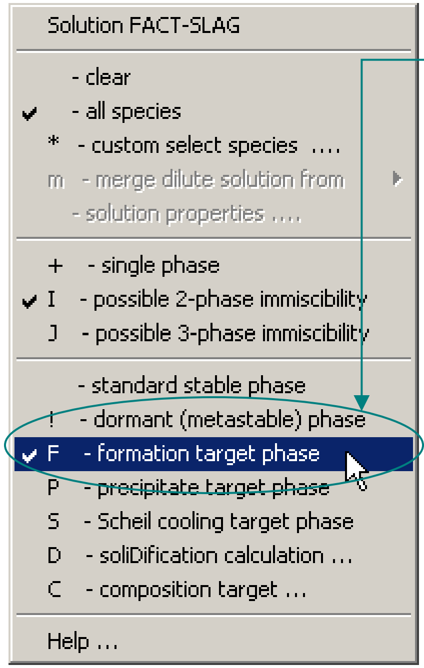
and the temperature has increased to: T = 1922.80°C

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

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

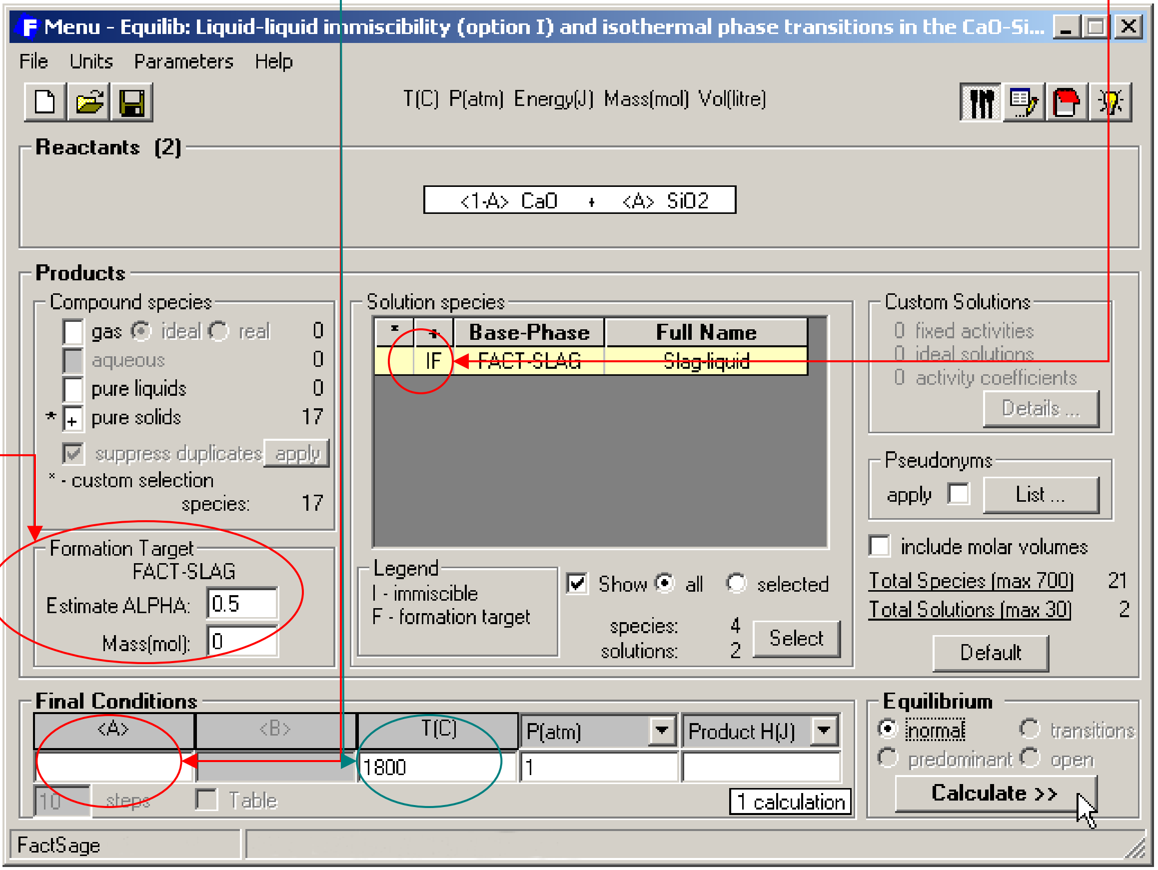
1° Right-click on the + column to open the **FACT-SLAG** extended menu and **select** F –formation target phase.

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).



Reactants (2): <1-A> CaO + <A> SiO2

Compound species: ☐ gas ● ideal ○ real 0; ☐ aqueous 0; ☐ pure liquids 0; * ☒ pure solids 17; ☑ suppress duplicates apply; * - custom selection species: 17

*	+	Base-Phase	Full Name
	IF	FACT-SLAG	Slag-liquid

Legend: I - immiscible; F - formation target

☑ Show ● all ○ selected; species: 4; solutions: 2; Select

Custom Solutions: 0 fixed activities; 0 ideal solutions; 0 activity coefficients; Details ...

Pseudonyms: apply ☐ List ...

☐ include molar volumes

Total Species (max 700) 21

Total Solutions (max 30) 2

Default

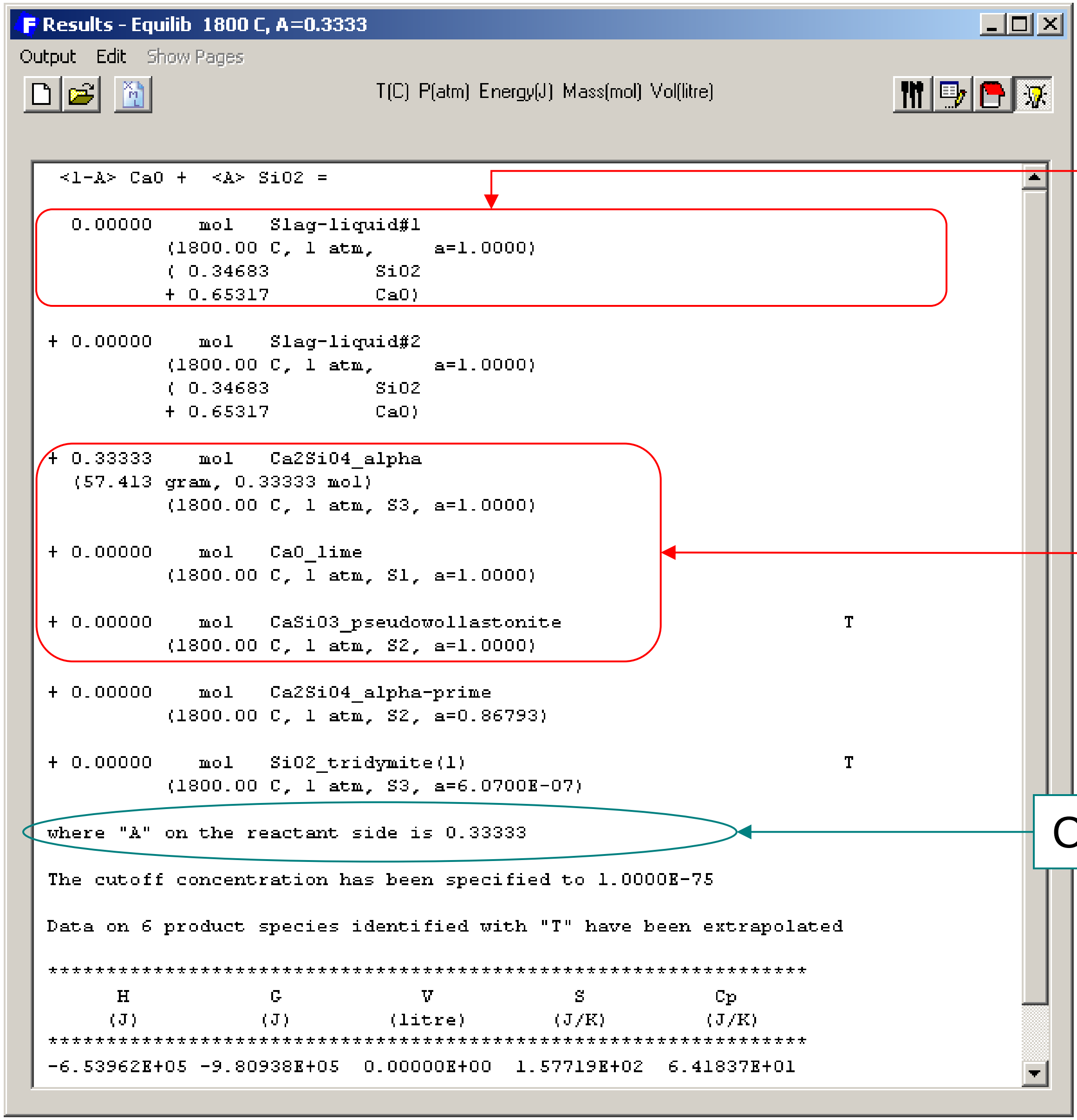
Formation Target FACT-SLAG
Estimate ALPHA: 0.5
Mass(mol): 0

<A>	<B>	T(C)	P(atm)	Product H(J)
		1800	1	

10 steps ☐ Table; 1 calculation

Equilibrium: ● normal ○ transitions ○ predominant ○ open

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



```
 <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.

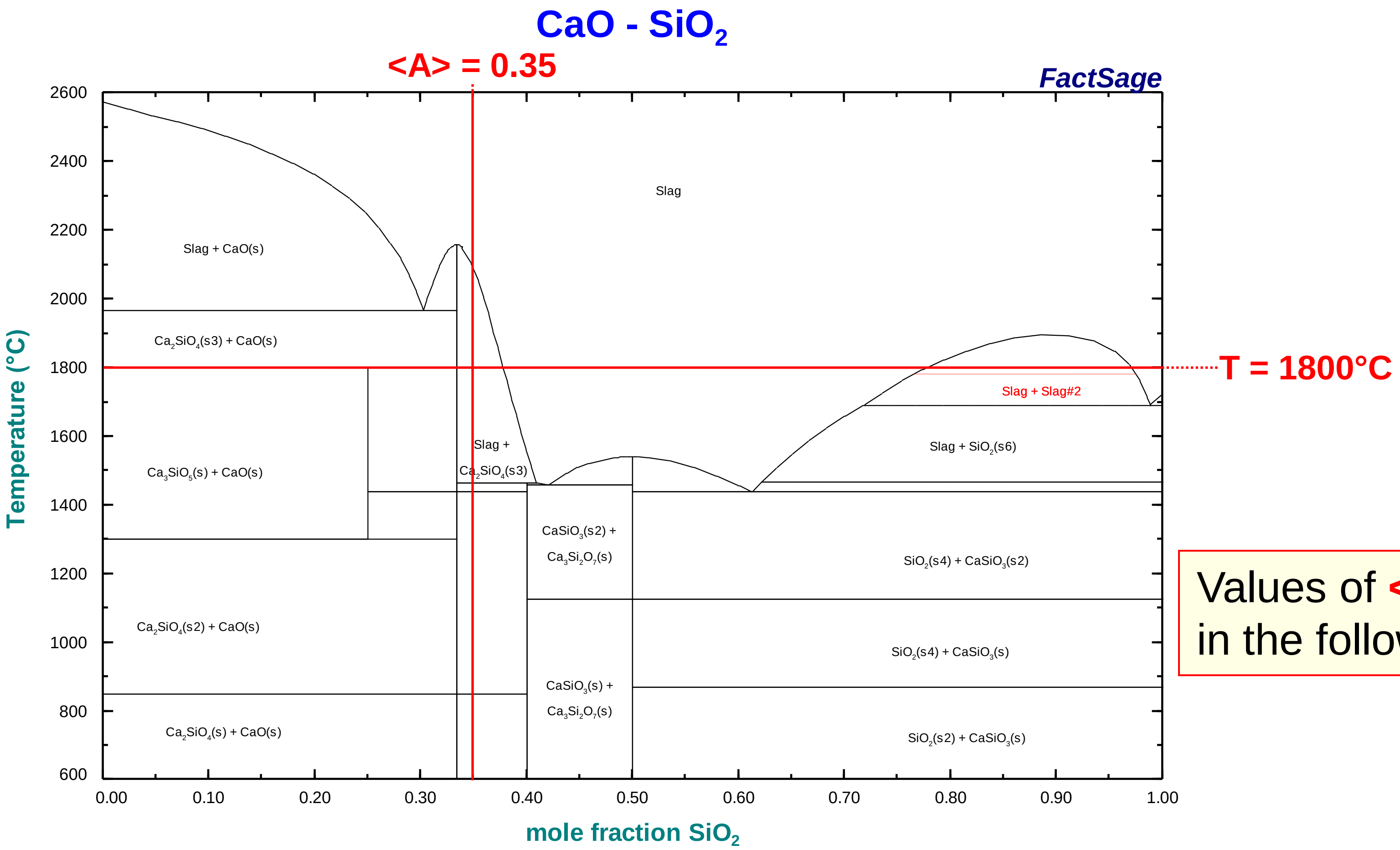
Compositions and quantities of the solid phases in equilibrium (activity =1) with FACT-SLAG.

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.

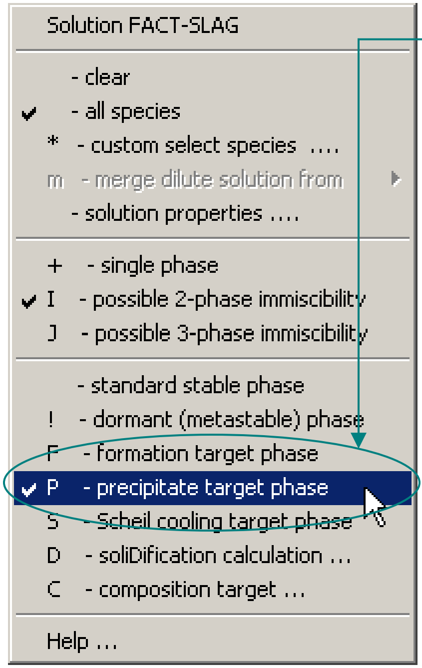


Values of **<A>** and **T** used in the following example.

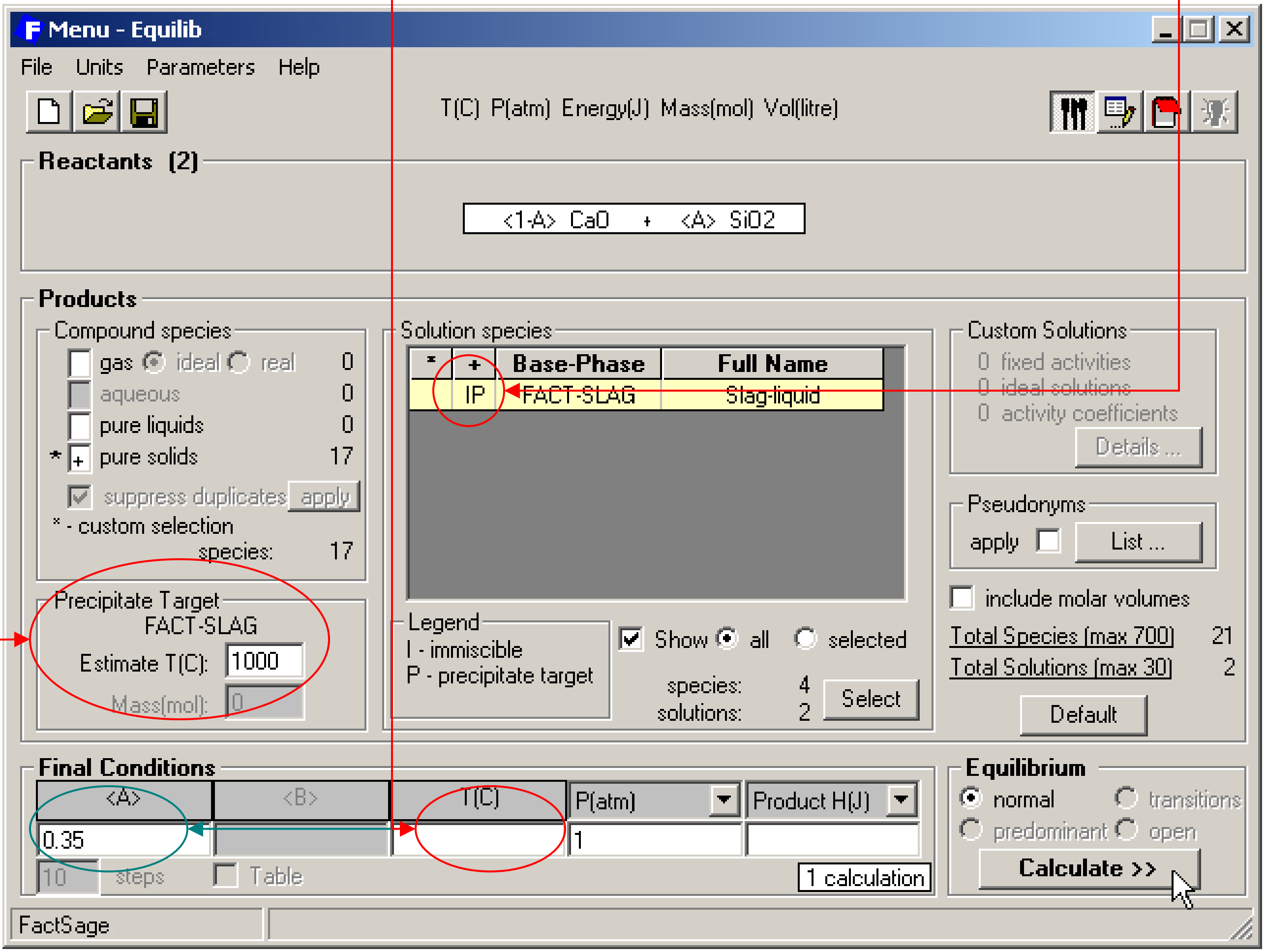
Setting a **FACT-SLAG** precipitate target at a given composition

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**.



Reactants (2): <1-A> CaO + <A> SiO2

Compound species: ☐ gas ● ideal ○ real 0; ☐ aqueous 0; ☐ pure liquids 0; * ☑ pure solids 17; ☑ suppress duplicates apply; * - custom selection species: 17

Solution species:

*	+	Base-Phase	Full Name
	IP	FACT-SLAG	Slag-liquid

Custom Solutions: 0 fixed activities; 0 ideal solutions; 0 activity coefficients; Details ...

Pseudonyms: apply ☐ List ...

☐ include molar volumes

Total Species (max 700) 21

Total Solutions (max 30) 2

Default

Precipitate Target FACT-SLAG
Estimate T(C): 1000
Mass(mol): 0

Legend: I - immiscible; P - precipitate target

☑ Show ● all ○ selected

species: 4

solutions: 2

Select

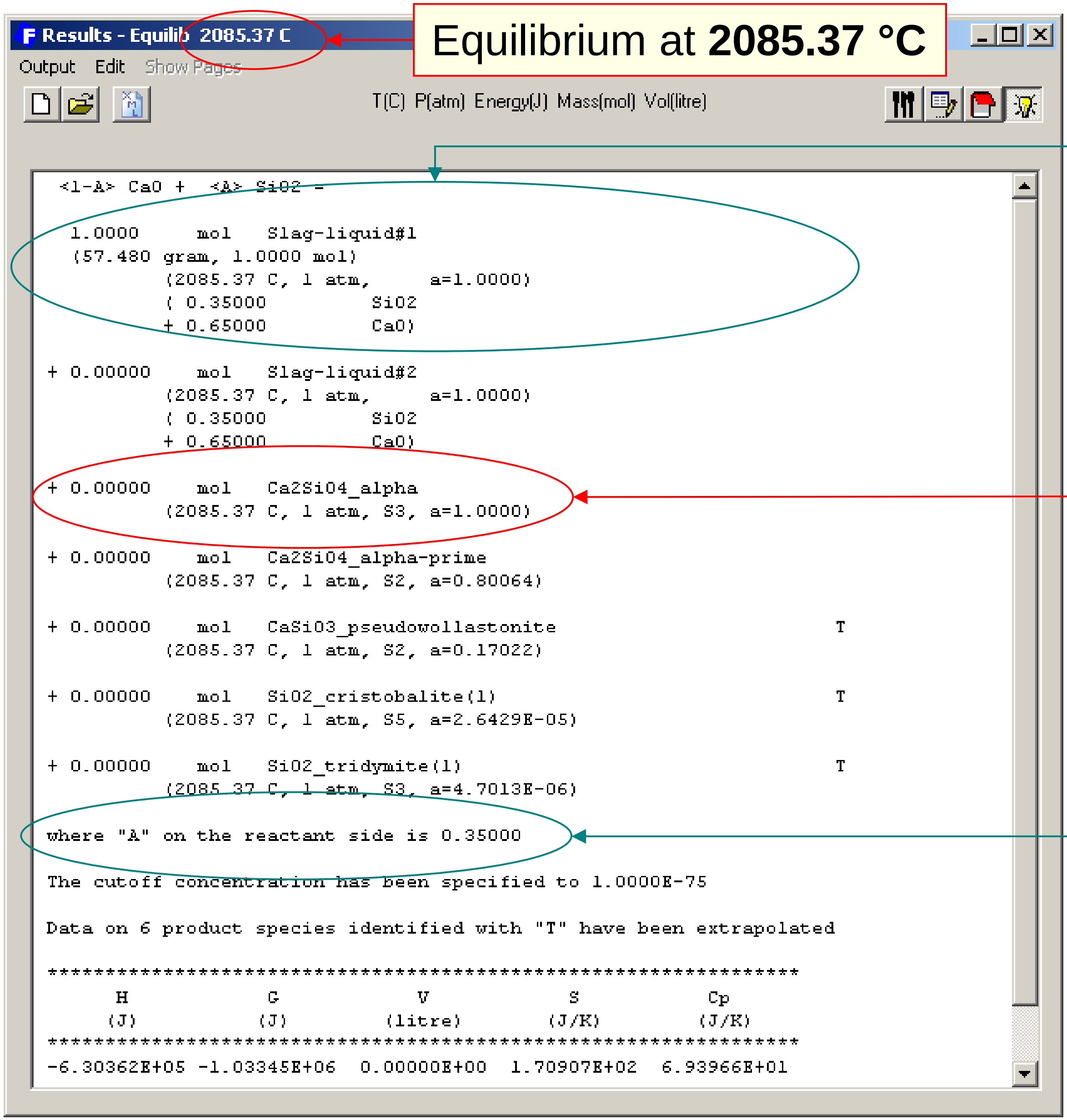
Final Conditions:

<A>	<B>	T(C)	P(atm)	Product H(J)
0.35			1	

10 steps ☐ Table 1 calculation

Equilibrium: ● normal ○ transitions ○ predominant ○ open

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



```
 <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**

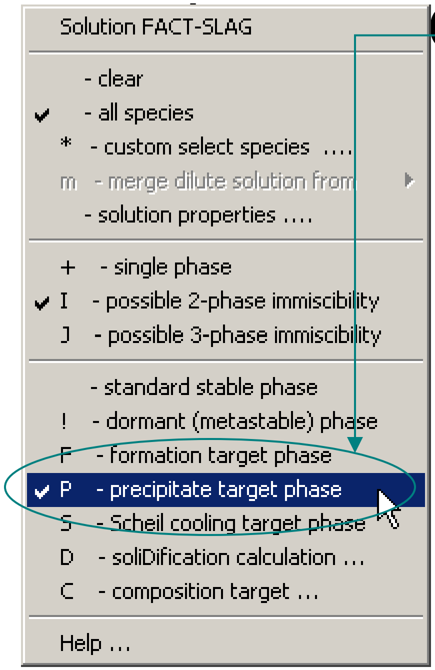
Note:
activity = **1.0**
number of moles =**1** (100%)
for the first phase:
the slag phase (liquid).

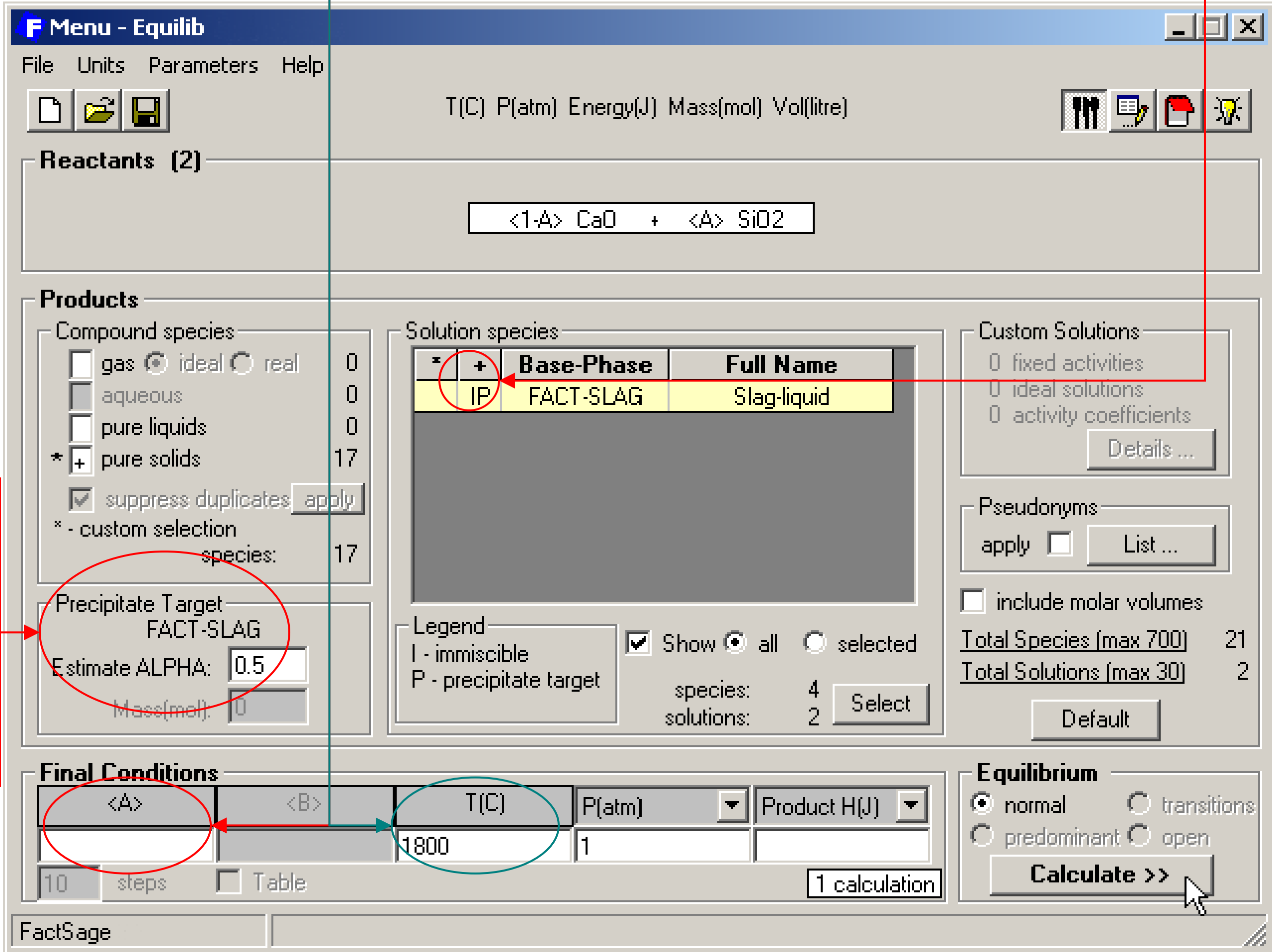
First precipitate to deposit from the slag phase
activity = **1.0**
number of moles = **0**.

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

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**.





Reactants (2): <1-A> CaO + <A> SiO2

Compound species:
- ☐ gas ● ideal ○ real 0
- ☐ aqueous 0
- ☐ pure liquids 0
- * ☐+ pure solids 17
- ☑ suppress duplicates apply
- * - custom selection species: 17

Solution species:

*	+	Base-Phase	Full Name
	IP	FACT-SLAG	Slag-liquid

Precipitate Target FACT-SLAG

Estimate ALPHA: 0.5

Mass(mol):

☑ Show ● all ○ selected

species: 4

solutions: 2

Select

Custom Solutions: 0 fixed activities; 0 ideal solutions; 0 activity coefficients; Details ...

Pseudonyms apply ☐ List ...

☐ include molar volumes

Total Species (max 700) 21

Total Solutions (max 30) 2

Default

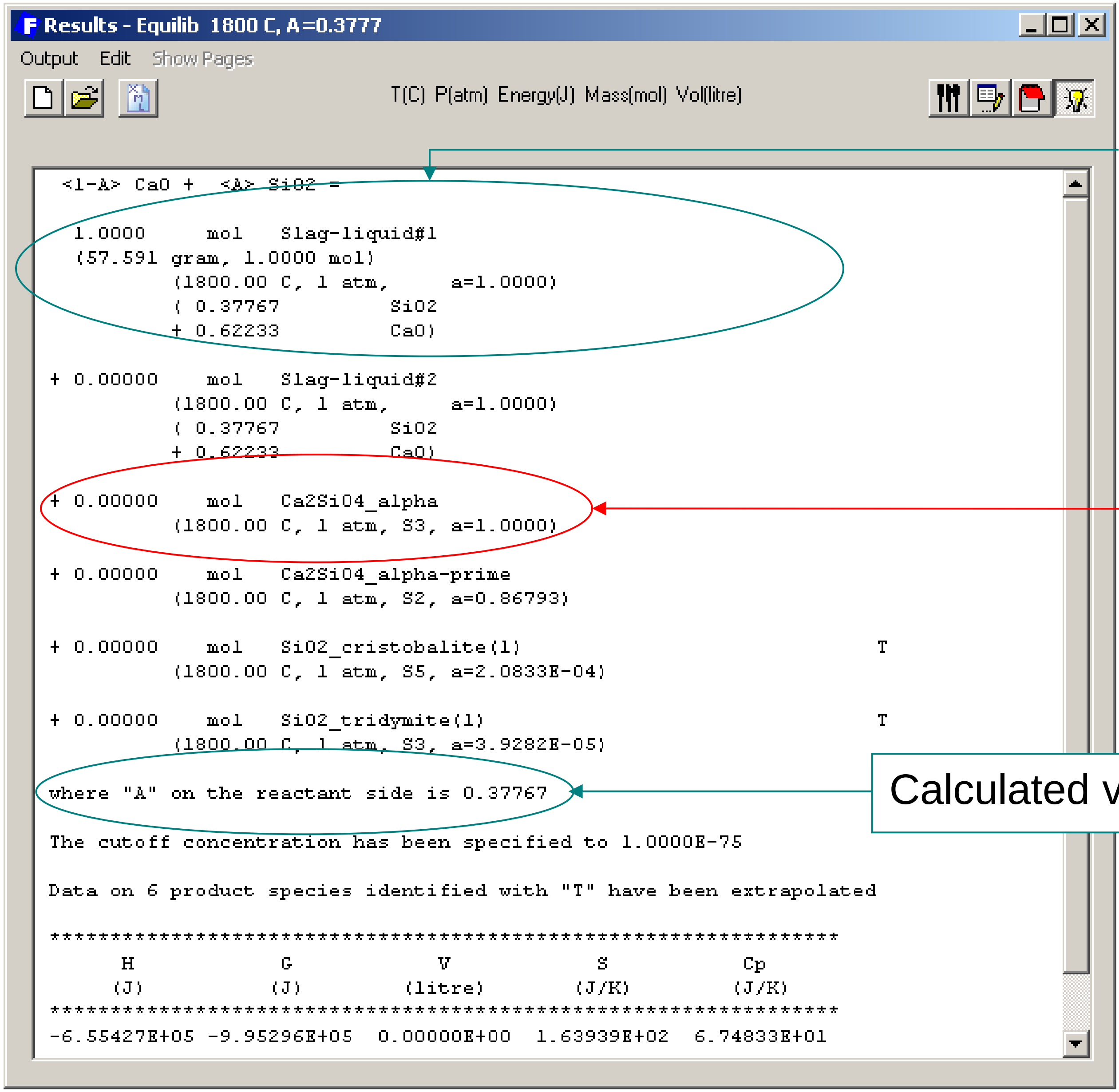
<A>	<B>	T(C)	P(atm)	Product H(J)
		1800	1	

10 steps ☐ Table 1 calculation

Equilibrium: ● normal ○ transitions ○ predominant ○ open

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



```
 <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**.

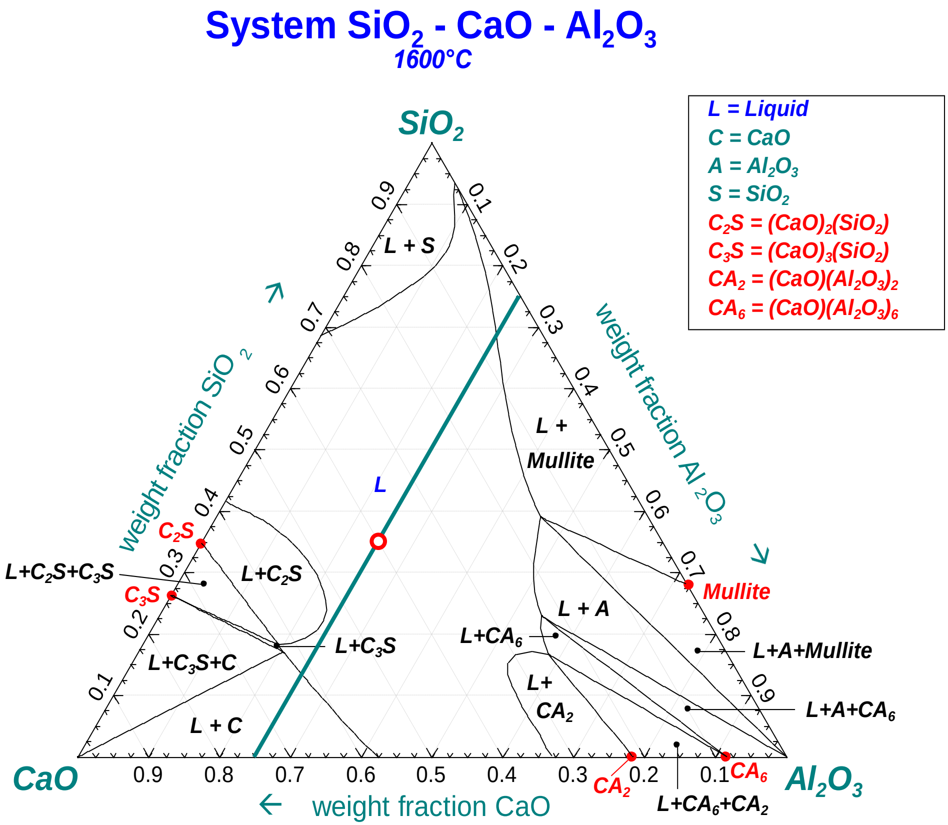
Calculated value of **<A>**, **X_{SiO_2} = 0.3767**.

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

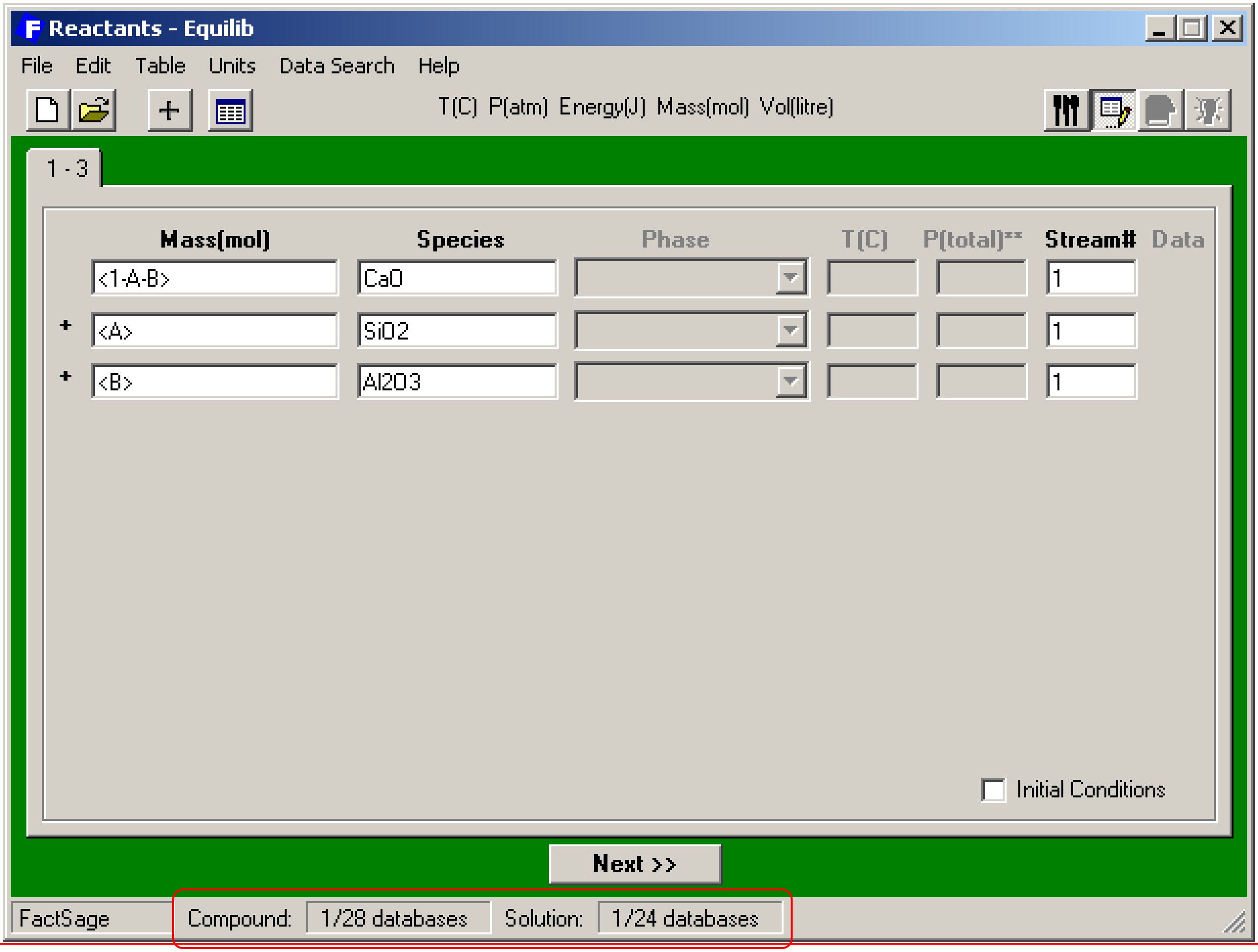
Teal line for <B> = 25% (2nd example)

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 %.



	Mass(mol)	Species	Phase	T(C)	P(total)**	Stream#	Data
	<1-A-B>	CaO				1	
+	<A>	SiO2				1	
+	<B>	Al2O3				1	

☐ Initial Conditions

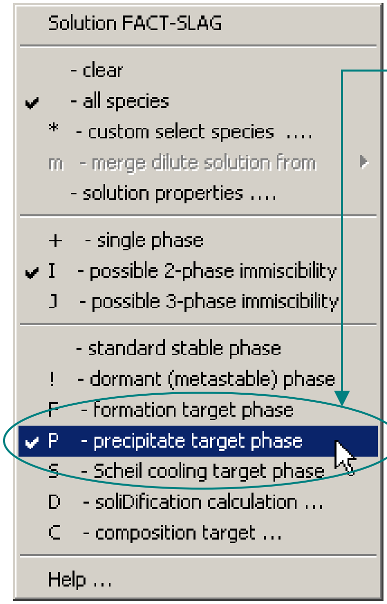
Compound: 1/28 databases Solution: 1/24 databases

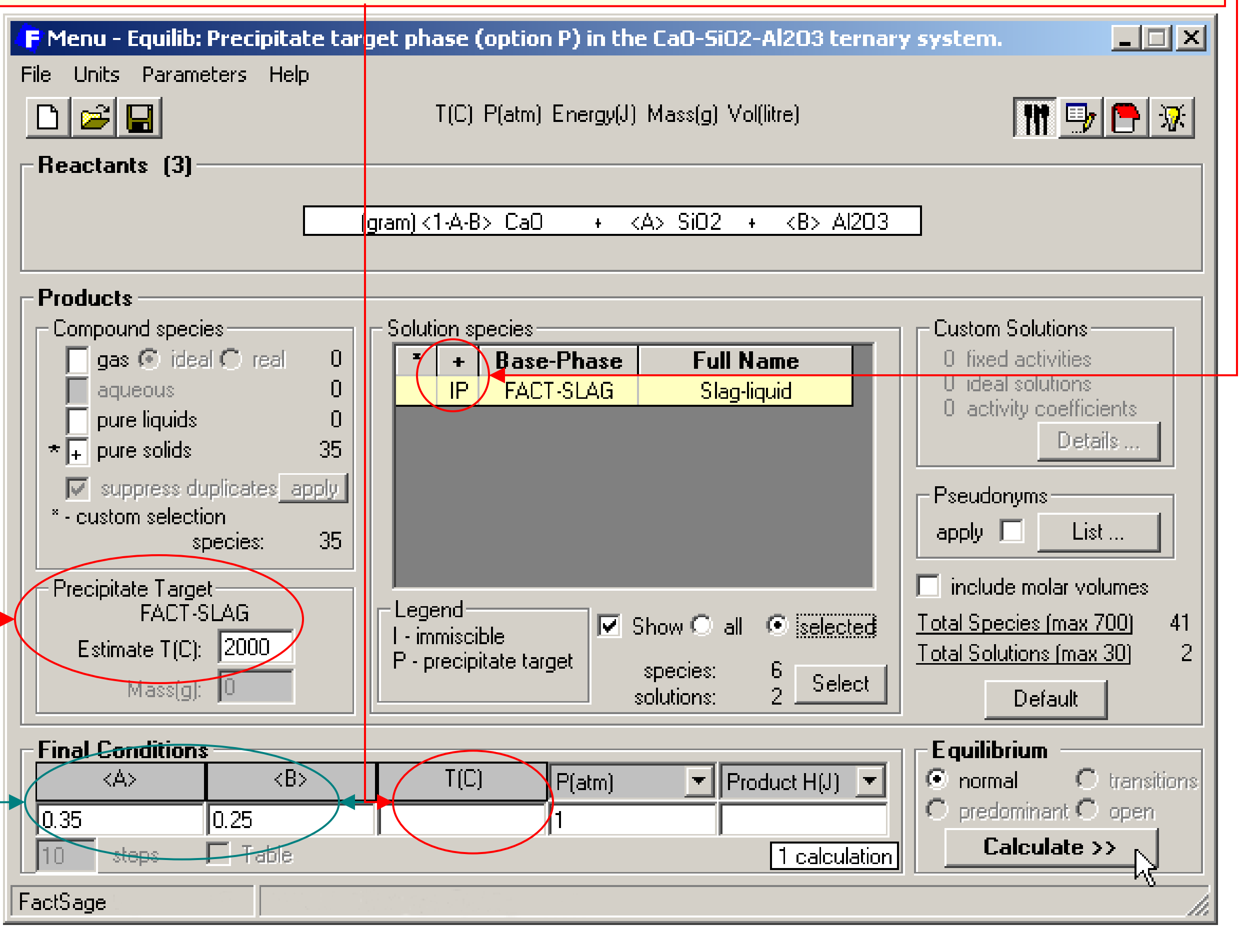
All data taken from the ***FACT*** **compound** and **solution databases**.

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**.





Reactants (3): (gram) <1-A-B> CaO + <A> SiO2 + <B> Al2O3

Compound species: ☐ gas ● ideal ○ real 0; ☐ aqueous 0; ☐ pure liquids 0; * ☐+ pure solids 35; ☑ suppress duplicates apply; * - custom selection species: 35

Solution species:

*	+	Base-Phase	Full Name
	IP	FACT-SLAG	Slag-liquid

Show ☑ ○ all ● selected; species: 6; solutions: 2; Select

Custom Solutions: 0 fixed activities; 0 ideal solutions; 0 activity coefficients; Details ...

Pseudonyms: apply ☐ List ...

☐ include molar volumes

Total Species (max 700) 41

Total Solutions (max 30) 2

Default

Precipitate Target: FACT-SLAG; Estimate T(C): 2000; Mass(g): 0

Final Conditions:

<A>	<B>	T(C)	P(atm)	Product H(J)
0.35	0.25		1	

10 steps ☐ Table; 1 calculation

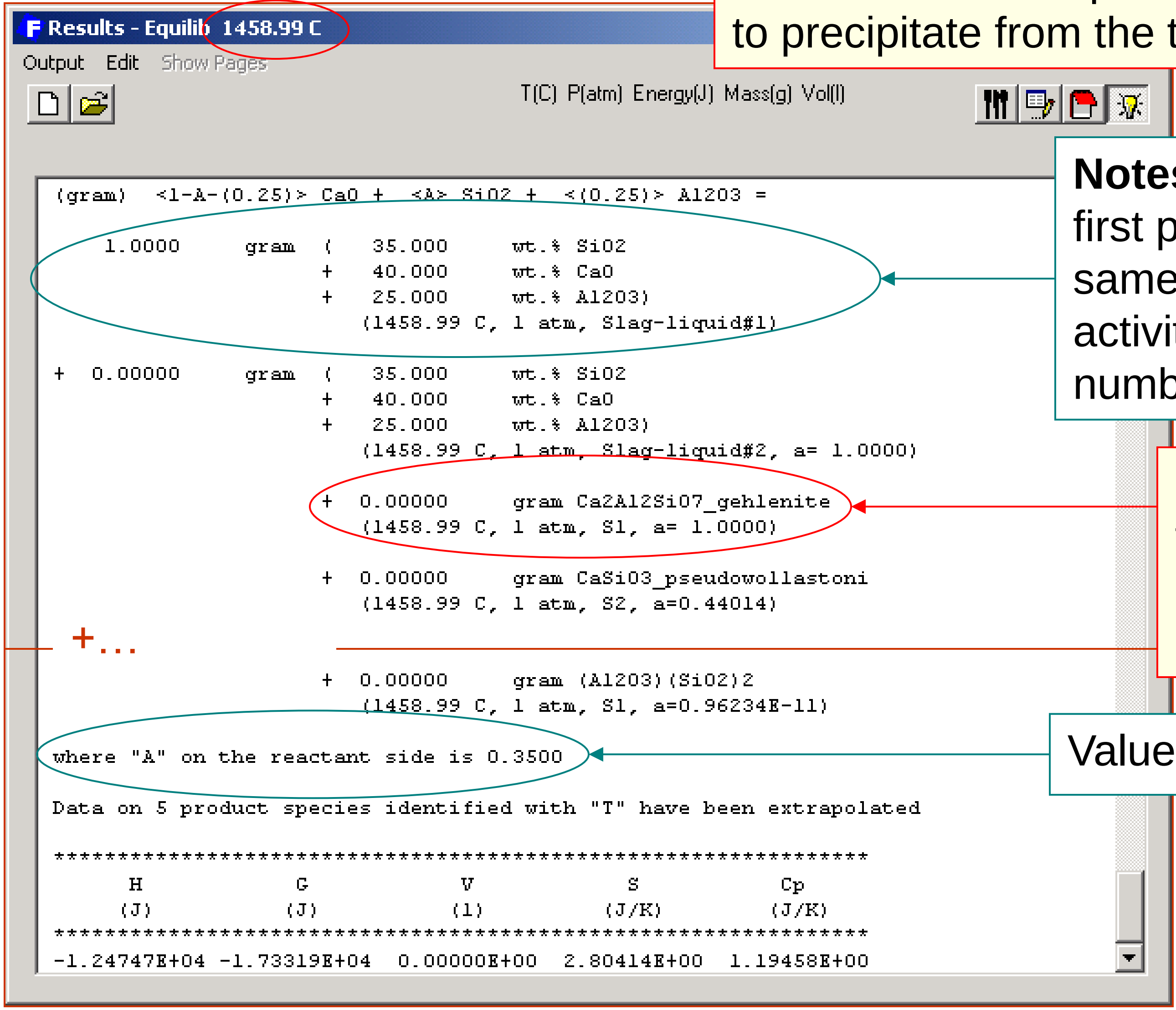
Equilibrium: ● normal ○ transitions ○ predominant ○ open

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**).



```
(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)          (l)        (J/K)        (J/K)
****************************************************************
-1.24747E+04 -1.73319E+04  0.00000E+00  2.80414E+00  1.19458E+00
```

+...

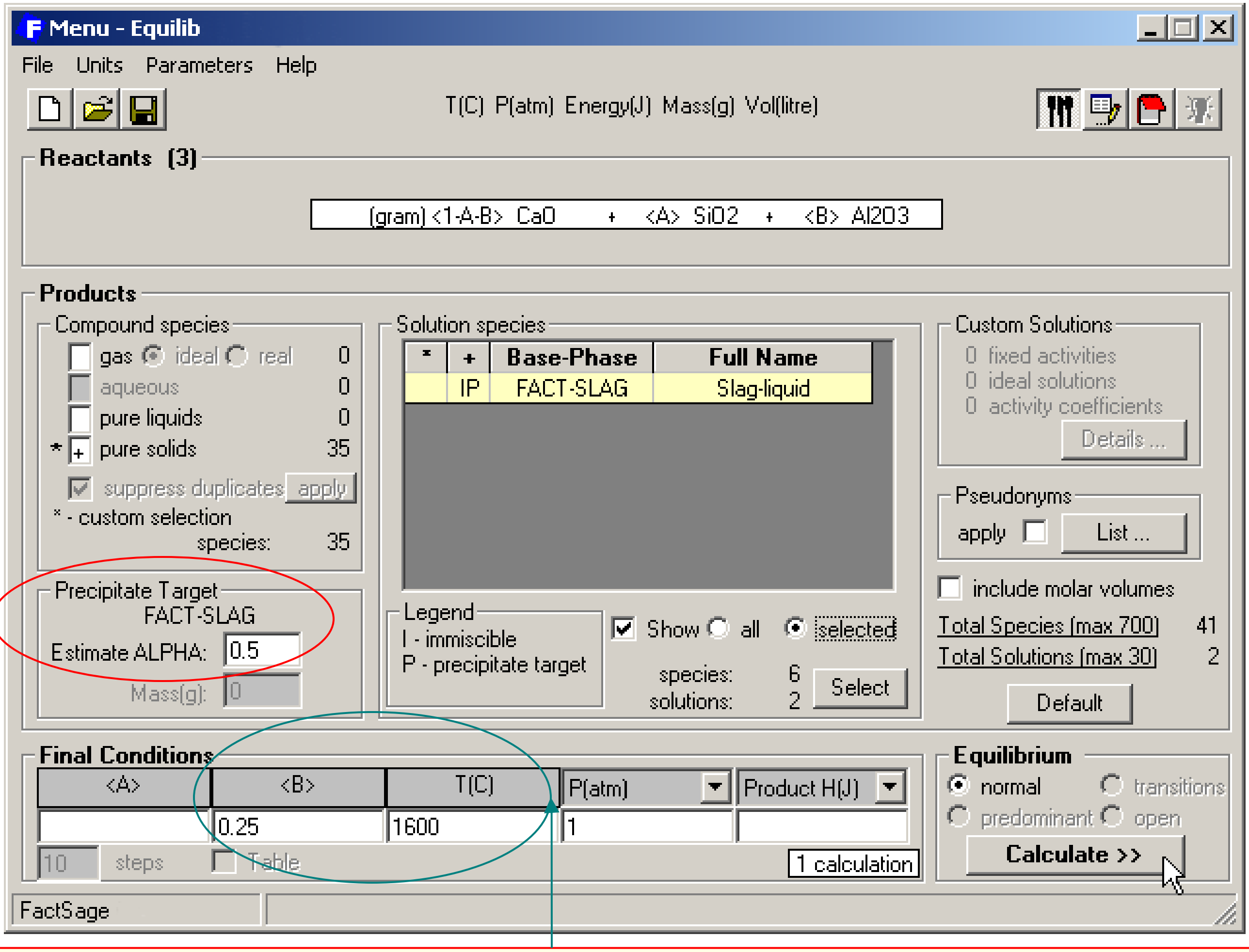
Notes: the composition of the first phase (Slag-liquid) is the same as the input values.
activity = **1.0**
number of grams = **1** (i.e. 100%)

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)**.



Reactants (3): (gram) <1-A-B> CaO + <A> SiO2 + <B> Al2O3

Compound species:
- ☐ gas ● ideal ○ real 0
- ☐ aqueous 0
- ☐ pure liquids 0
- * ☐+ pure solids 35
- ☑ suppress duplicates apply
- * - custom selection
- species: 35

*	+	Base-Phase	Full Name
	IP	FACT-SLAG	Slag-liquid

Legend: I - immiscible; P - precipitate target

☑ Show ○ all ● selected

species: 6
solutions: 2

Custom Solutions: 0 fixed activities; 0 ideal solutions; 0 activity coefficients

Pseudonyms: apply ☐

☐ include molar volumes

Total Species (max 700) 41
Total Solutions (max 30) 2

Precipitate Target: FACT-SLAG
Estimate ALPHA: 0.5
Mass(g): 0

<A>	<B>	T(C)	P(atm)	Product H(J)
	0.25	1600	1	

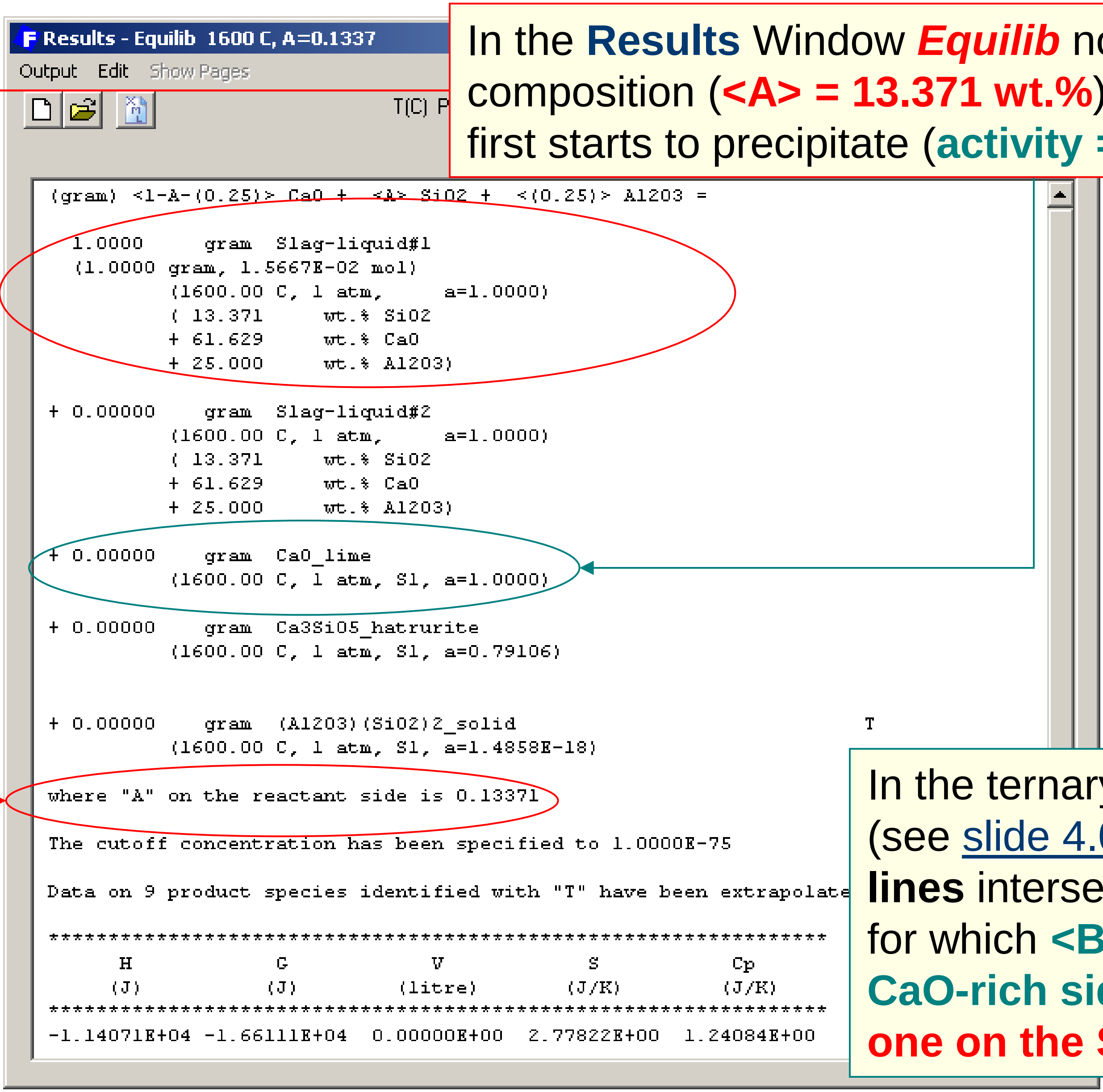
10 steps ☐ Table — 1 calculation

Equilibrium: ● normal ○ transitions ○ predominant ○ open

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**)

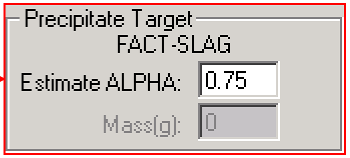


```
(gram) <1-A-(0.25)> CaO +  <A> SiO2 +  <(0.25)> Al2O3 =

  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

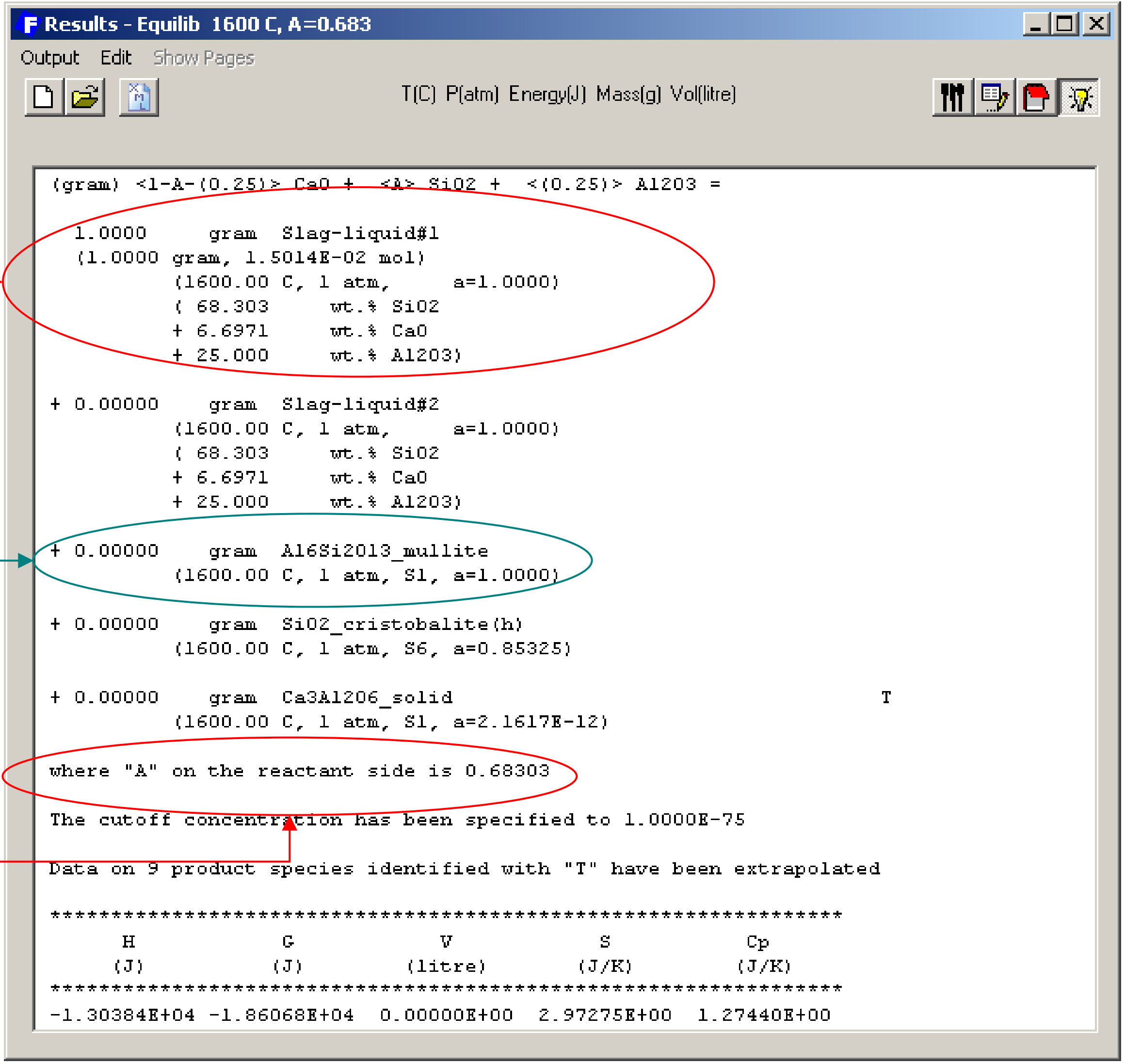
By setting (in the **Menu Window**) another estimate for ALPHA <A> on the **SiO_2-rich side**, one can calculate the other value of <A> for which a precipitate starts to form.



Estimate ALPHA: 0.75

Mass(g): 0

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**).



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

   1.0000     gram  Slag-liquid#1
   (1.0000 gram, 1.5014E-02 mol)
           (1600.00 C, 1 atm,      a=1.0000)
           ( 68.303      wt.% SiO2
           + 6.6971      wt.% CaO
           + 25.000      wt.% Al2O3)

+ 0.00000     gram  Slag-liquid#2
           (1600.00 C, 1 atm,      a=1.0000)
           ( 68.303      wt.% SiO2
           + 6.6971      wt.% CaO
           + 25.000      wt.% Al2O3)

+ 0.00000     gram  Al6Si2O13_mullite
           (1600.00 C, 1 atm, S1, a=1.0000)

+ 0.00000     gram  SiO2_cristobalite(h)
           (1600.00 C, 1 atm, S6, a=0.85325)

+ 0.00000     gram  Ca3Al2O6_solid                            T
           (1600.00 C, 1 atm, S1, a=2.1617E-12)

where "A" on the reactant side is 0.68303

The cutoff concentration has been specified to 1.0000E-75

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

*****************************************************************
      H             G             V             S            Cp
     (J)           (J)         (litre)        (J/K)        (J/K)
*****************************************************************
-1.30384E+04 -1.86068E+04  0.00000E+00  2.97275E+00  1.27440E+00
```

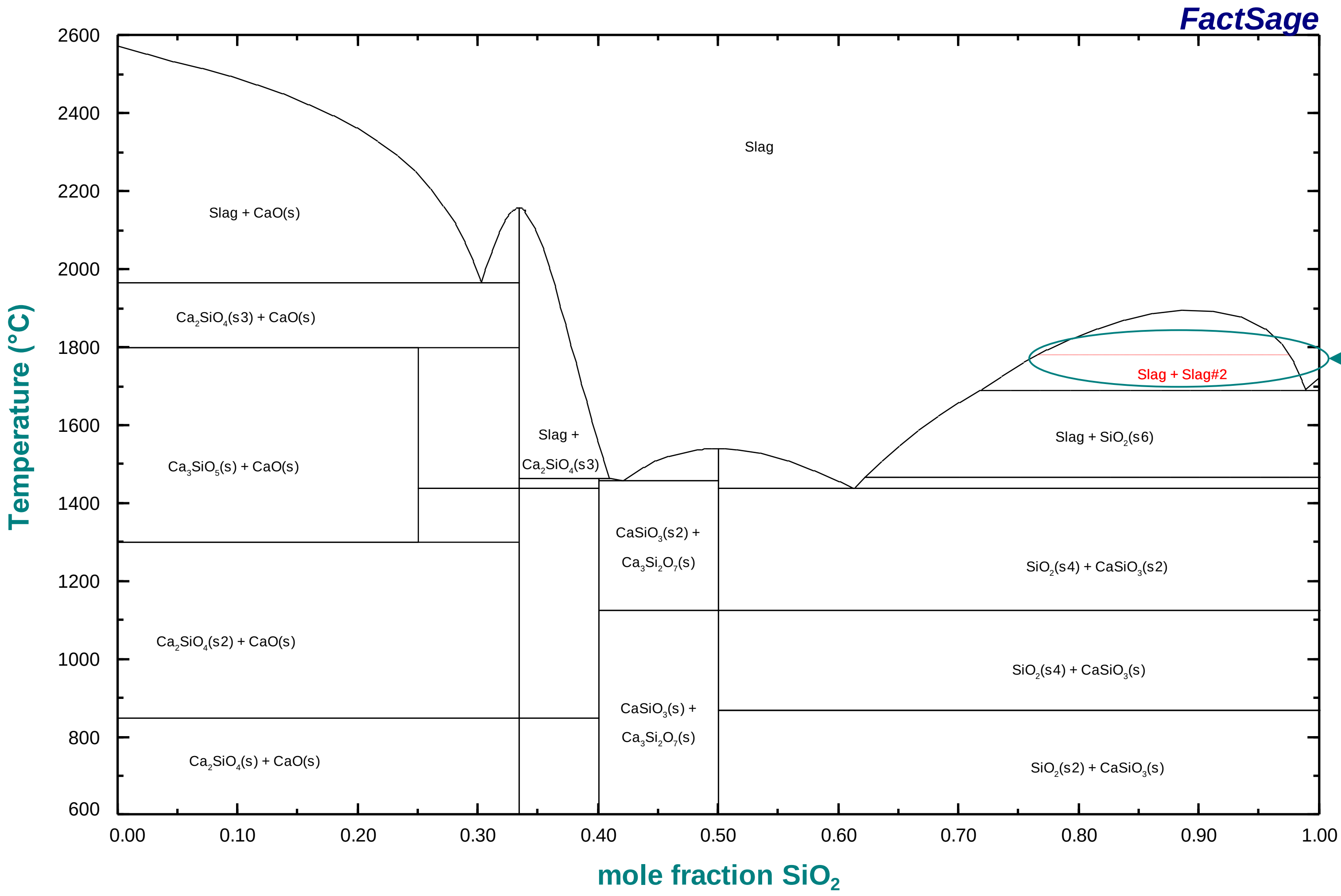
Compostion target phase

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.

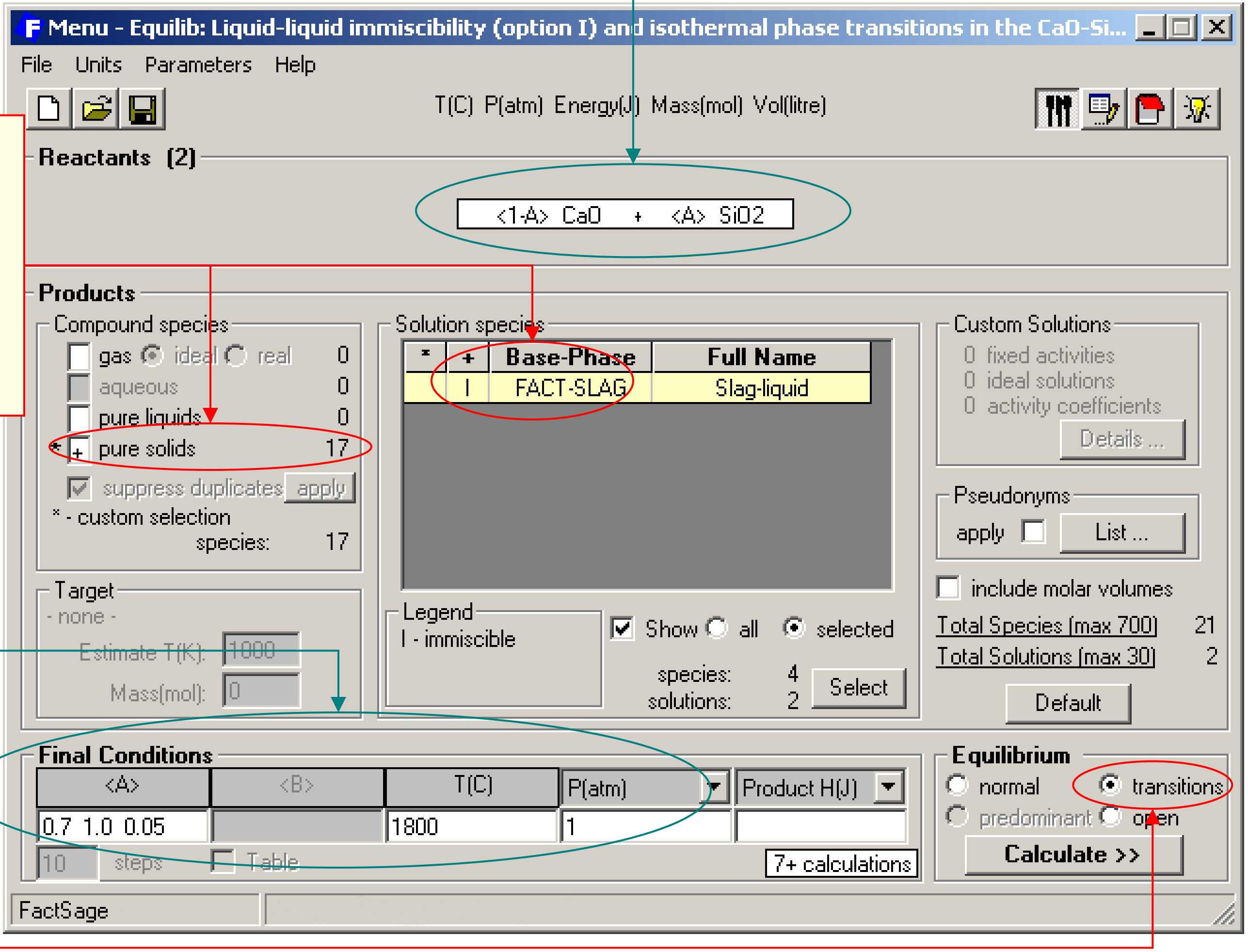
CaO - SiO_2



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)**



Menu - Equilib: Liquid-liquid immiscibility (option I) and isothermal phase transitions in the CaO-Si...

Reactants (2)

<1-A> CaO + <A> SiO2

Products

Compound species

☐ gas ● ideal ○ real		0
☐ aqueous		0
☐ pure liquids		0
* + pure solids		17

☑ suppress duplicates apply

* - custom selection

species: 17

Solution species

*	+	Base-Phase	Full Name
	I	FACT-SLAG	Slag-liquid

Legend

I - immiscible

☑ Show ○ all ● selected

species: 4

solutions: 2

Custom Solutions

0 fixed activities

0 ideal solutions

0 activity coefficients

Pseudonyms

apply ☐ List ...

☐ include molar volumes

Total Species (max 700) 21

Total Solutions (max 30) 2

Target

\- none -

Estimate T(K): 1000

Mass(mol): 0

Final Conditions

<A>	<B>	T(C)	P(atm)	Product H(J)
0.7 1.0 0.05		1800	1	

10 steps ☐ Table

7+ calculations

Equilibrium

○ normal ● transitions

○ predominant ○ open

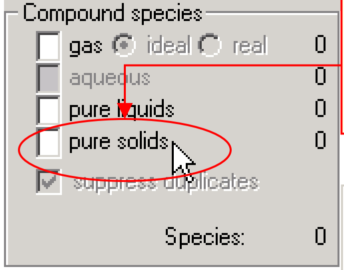
3° <A> = 0.7, 0.75, …, 1.0
T (°C) = 1800

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.



Compound species

☐ gas ● ideal ○ real 0

☐ aqueous 0

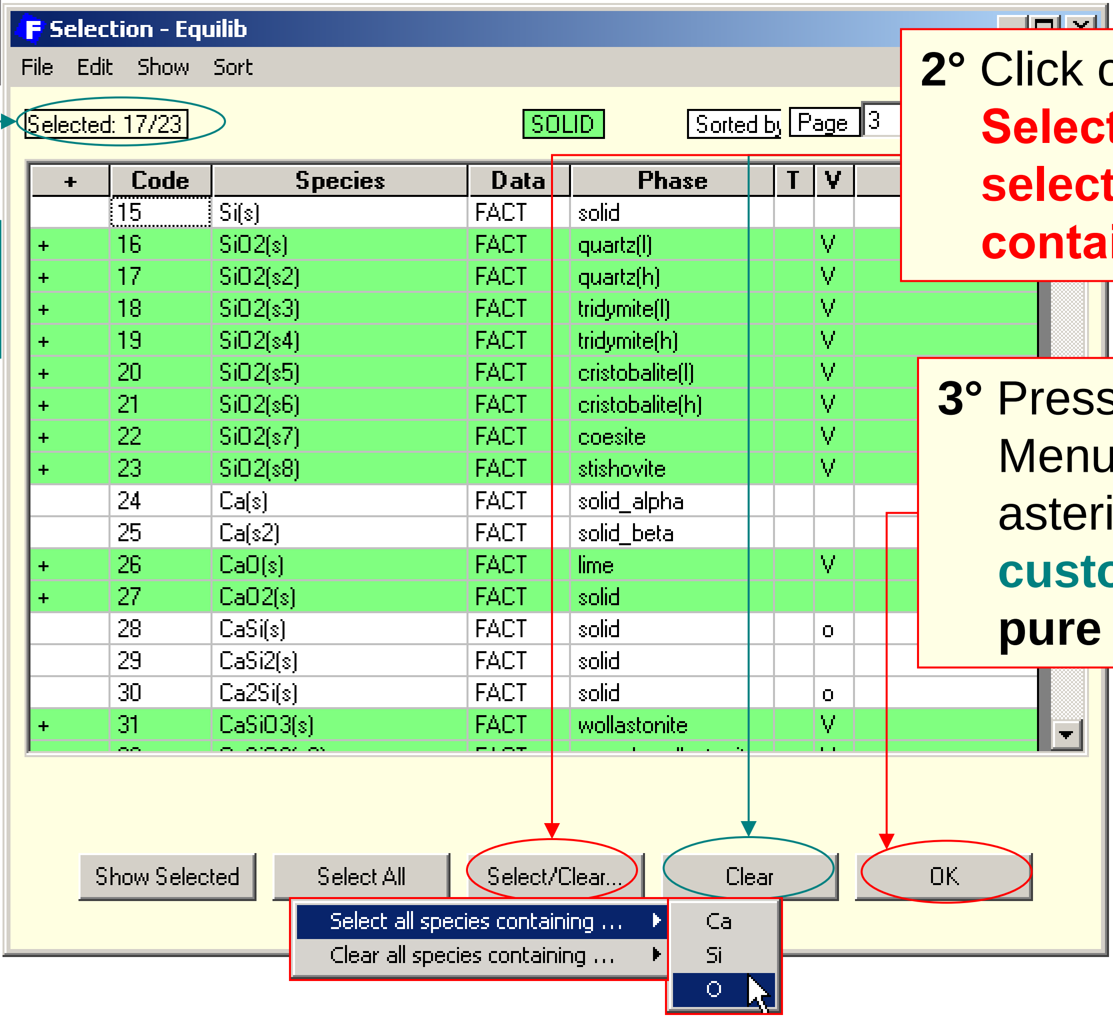
☐ pure liquids 0

☐ pure solids 0

☑ suppress duplicates

Species: 0

17 pure solid oxides

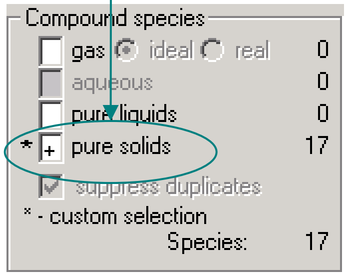


Selected: 17/23 SOLID Sorted by Page 3

+	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**.



Compound species

☐ gas ● ideal ○ real 0

☐ aqueous 0

☐ pure liquids 0

* ☐+ pure solids 17

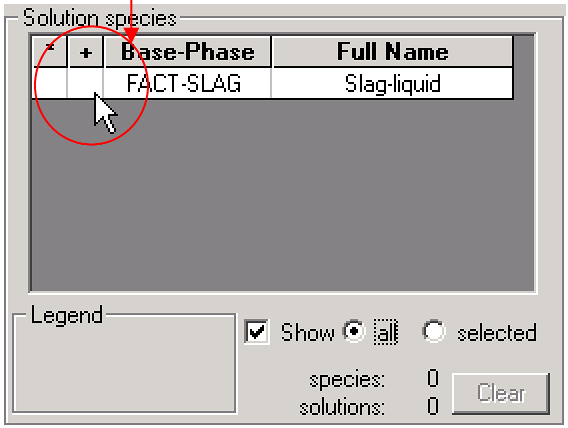
☑ suppress duplicates

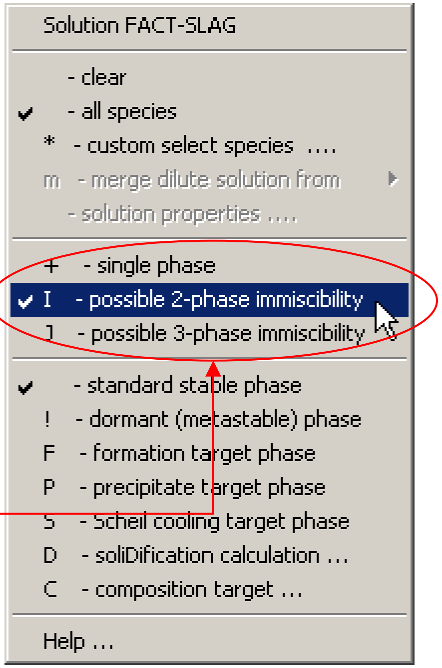
* - custom selection

Species: 17

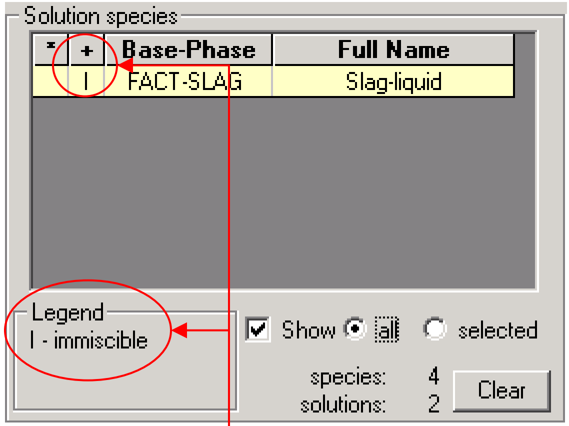
Step 2°: Products Selection – solution species

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**.

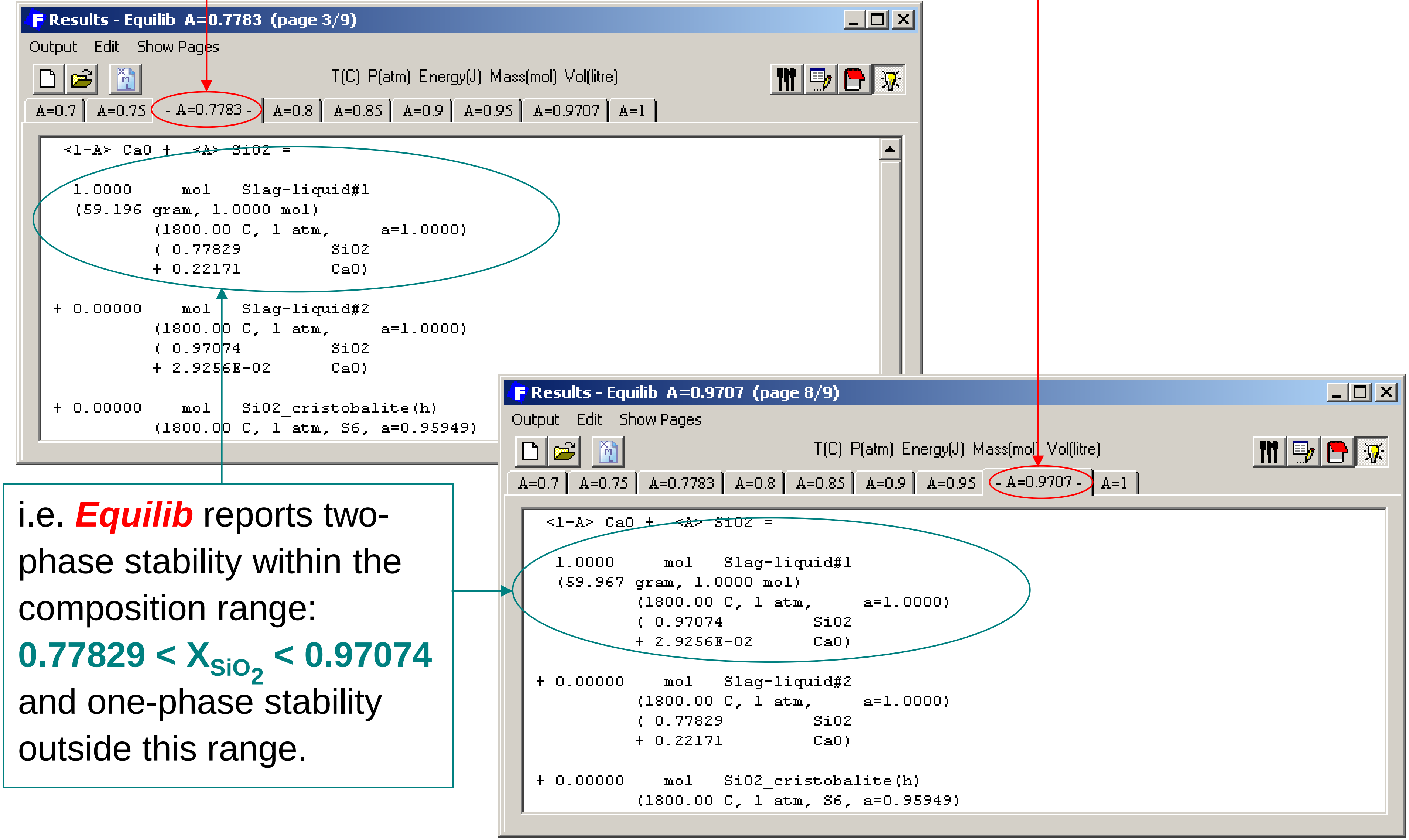


3° The **I** indicates a possible **2-phase immiscible** region.

- **[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.



```
 <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)
```

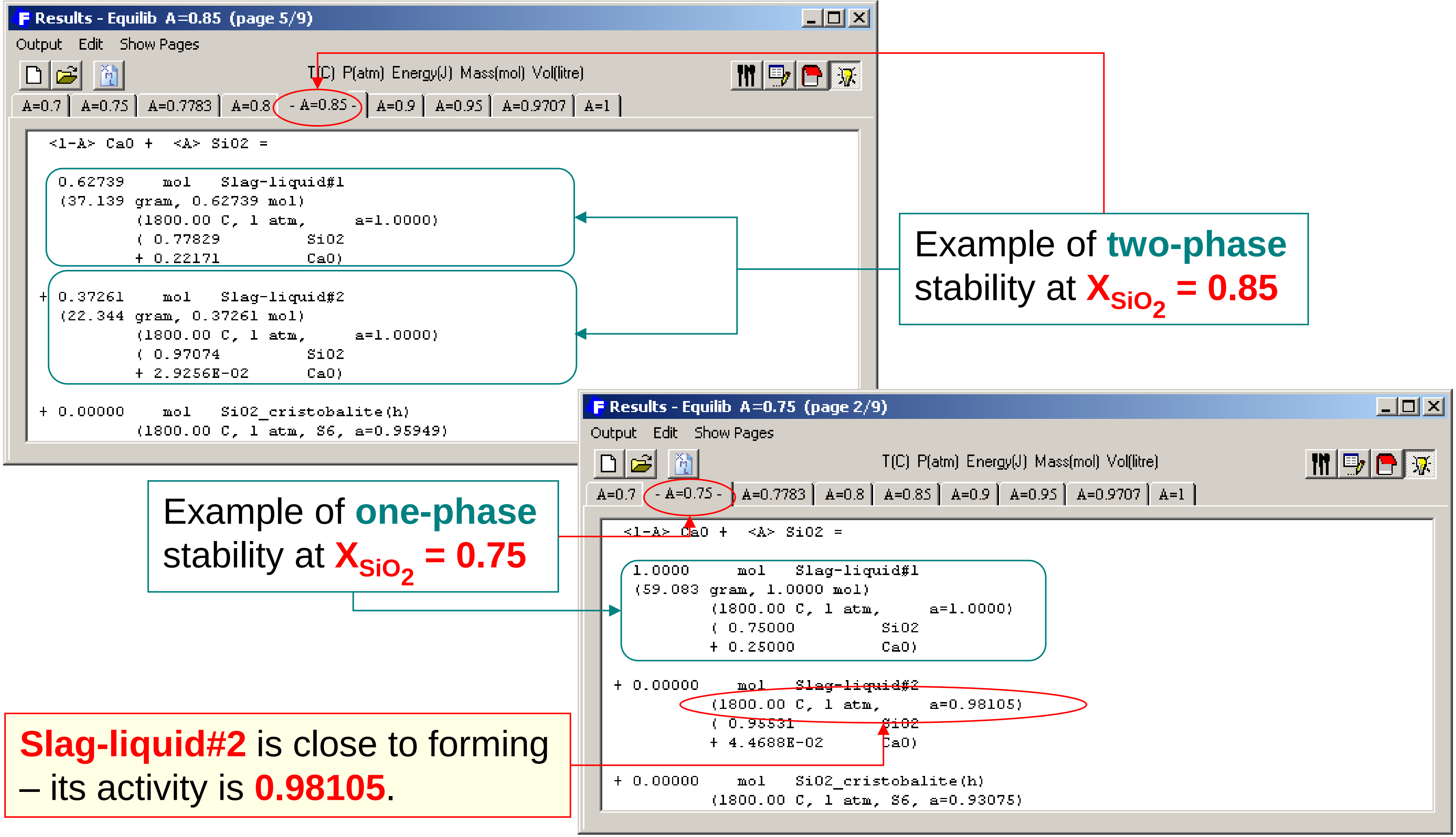
```
 <1-A> CaO +  <A> SiO2 =

  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



```
 <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**

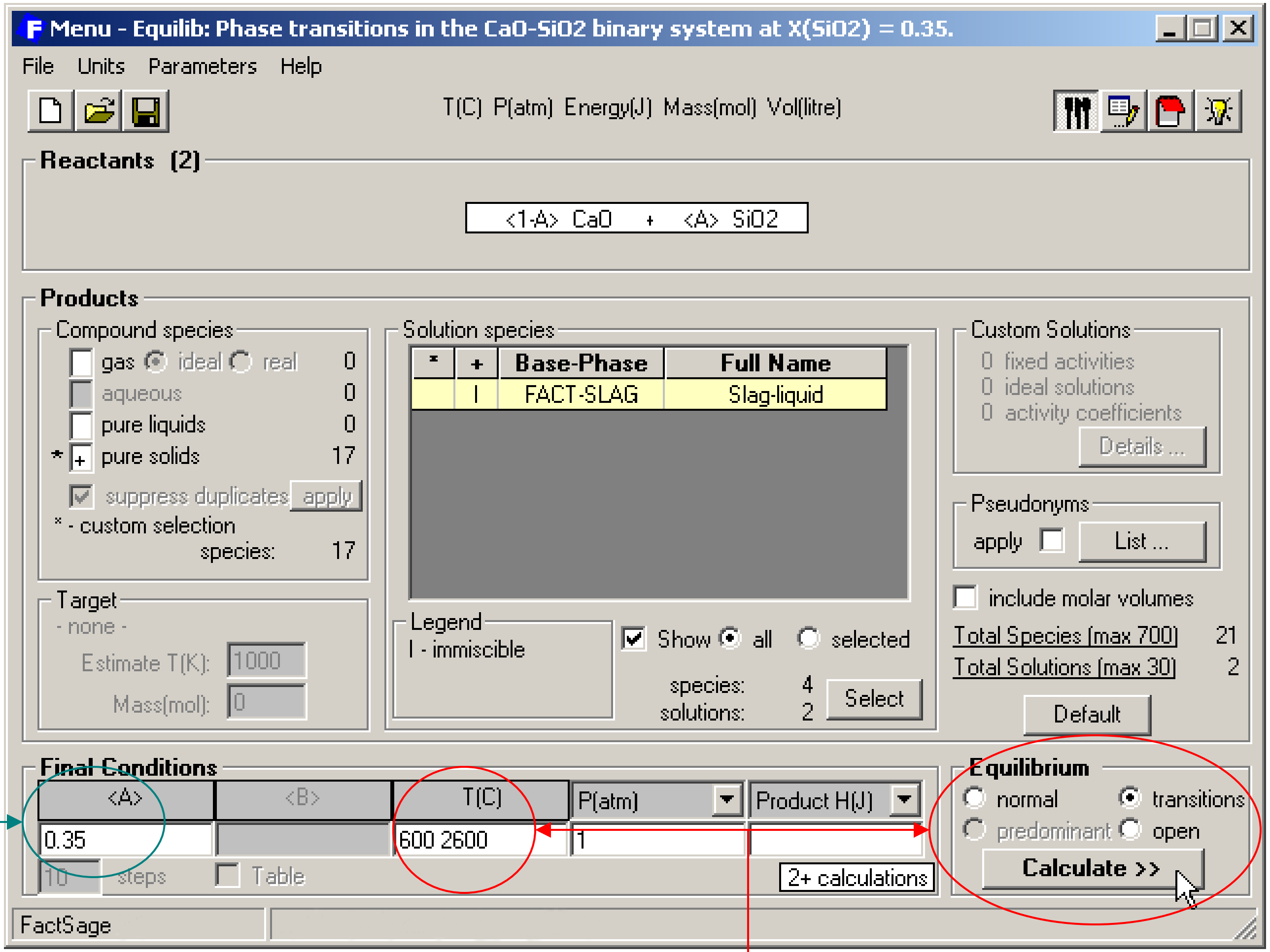
```
 <1-A> CaO +  <A> SiO2 =

  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 **$CaO\text{-}SiO_2$** binary system



Menu - Equilib: Phase transitions in the CaO-SiO2 binary system at X(SiO2) = 0.35.

File Units Parameters Help

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

Reactants (2)

<1-A> CaO + <A> SiO2

Products

Compound species

- ☐ gas ● ideal ○ real 0
- ☐ aqueous 0
- ☐ pure liquids 0
- * ☒ pure solids 17
- ☑ suppress duplicates apply

* - custom selection

species: 17

Target

\- none -

Estimate T(K): 1000

Mass(mol): 0

Solution species

*	+	Base-Phase	Full Name
	I	FACT-SLAG	Slag-liquid

Legend

I - immiscible

☑ Show ● all ○ selected

species: 4

solutions: 2

Select

Custom Solutions

0 fixed activities

0 ideal solutions

0 activity coefficients

Details ...

Pseudonyms

apply ☐ List ...

☐ include molar volumes

Total Species (max 700) 21

Total Solutions (max 30) 2

Default

Final Conditions

<A>	<B>	T(C)	P(atm)	Product H(J)
0.35		600 2600	1	

10 steps ☐ Table 2+ calculations

Equilibrium

○ normal ● transitions

○ predominant ○ open

Calculate >>

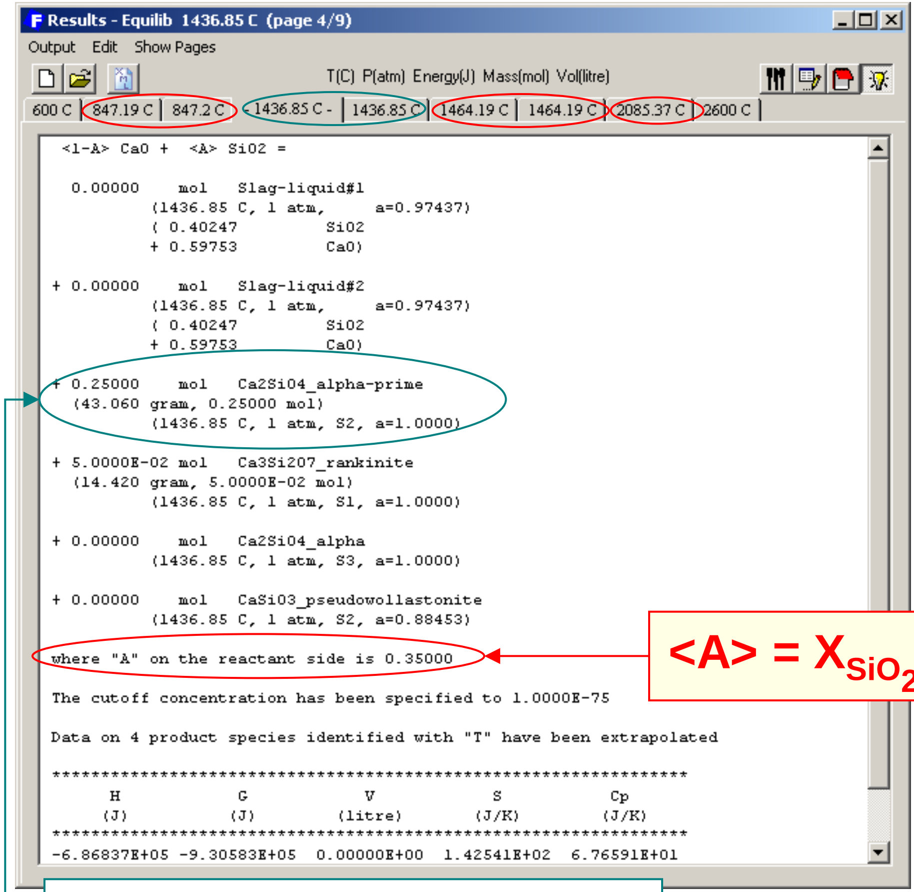
FactSage

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.

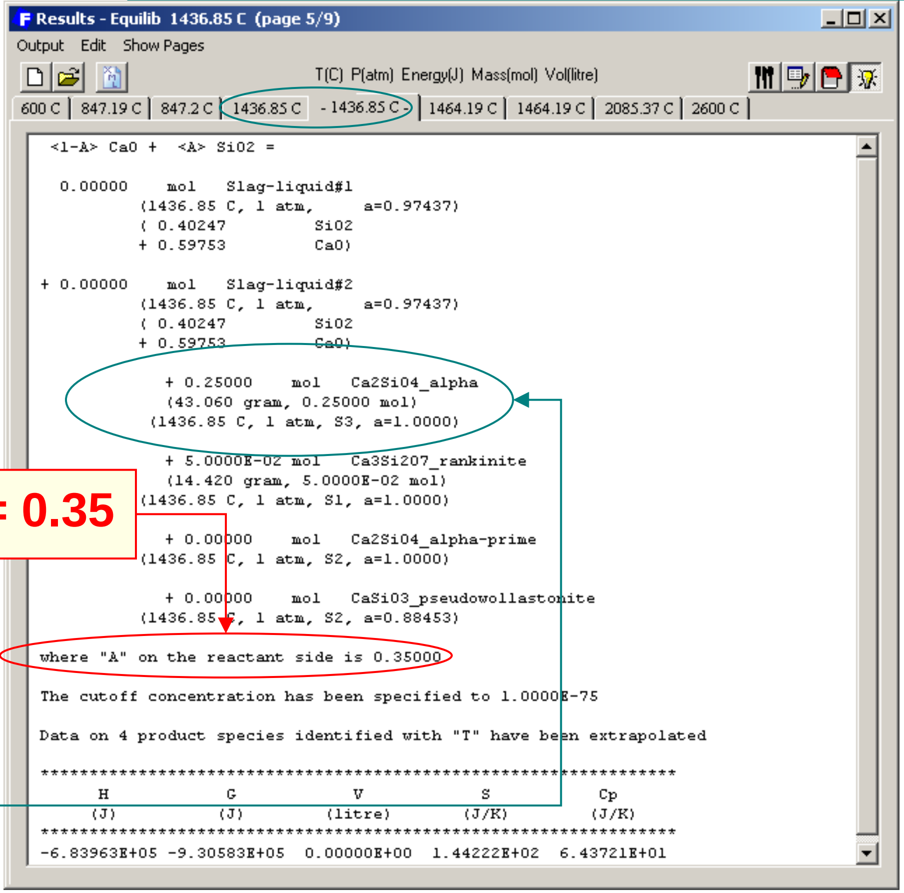
Transition Temperatures for X_{SiO_2} = 0.35 in CaO-SiO_2

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.



```
 <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
```

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

<A> = X_{SiO_2} = 0.35

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

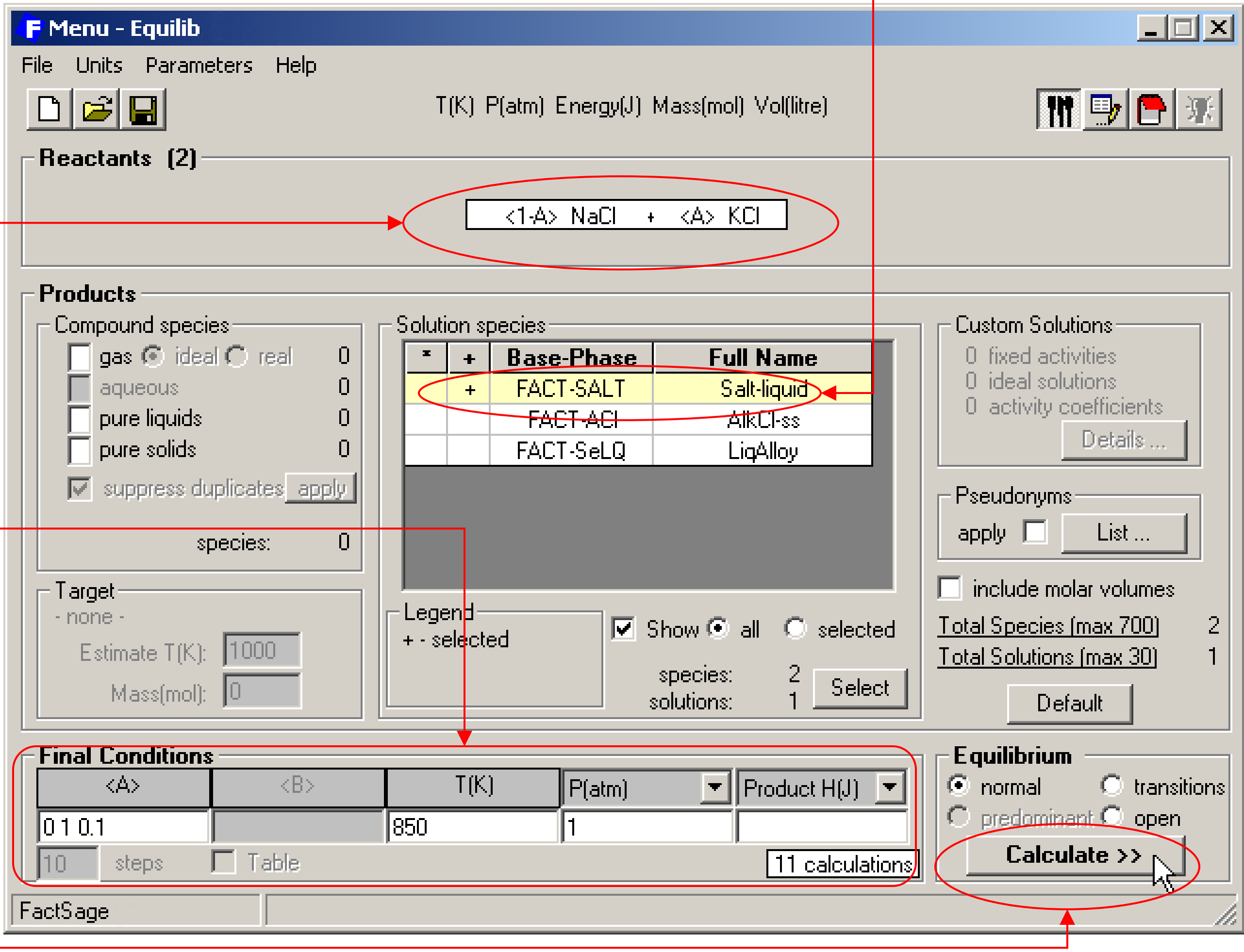
1° The reactants are <1-A> NaCl + <A> KCl – i.e. the NaCl-KCl binary system where <A> varies from 0 to 1.

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



Reactants (2)

<1-A> NaCl + <A> KCl

Products

Compound species
- ☐ gas ● ideal ○ real 0
- ☐ aqueous 0
- ☐ pure liquids 0
- ☐ pure solids 0
- ☑ suppress duplicates

species: 0

Solution species

*	+	Base-Phase	Full Name
	+	FACT-SALT	Salt-liquid
		FACT-ACl	AlkCl-ss
		FACT-SeLQ	LiqAlloy

Legend
+ - selected

☑ Show ● all ○ selected

species: 2
solutions: 1

Custom Solutions
0 fixed activities
0 ideal solutions
0 activity coefficients

Pseudonyms
apply ☐

☐ include molar volumes

Total Species (max 700) 2
Total Solutions (max 30) 1

Target
- none -
Estimate T(K): 1000
Mass(mol): 0

Final Conditions

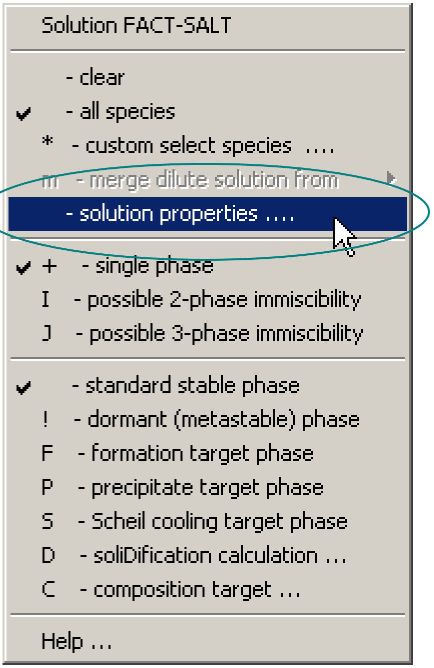
<A>	<B>	T(K)	P(atm)	Product H(J)
0 1 0.1		850	1	

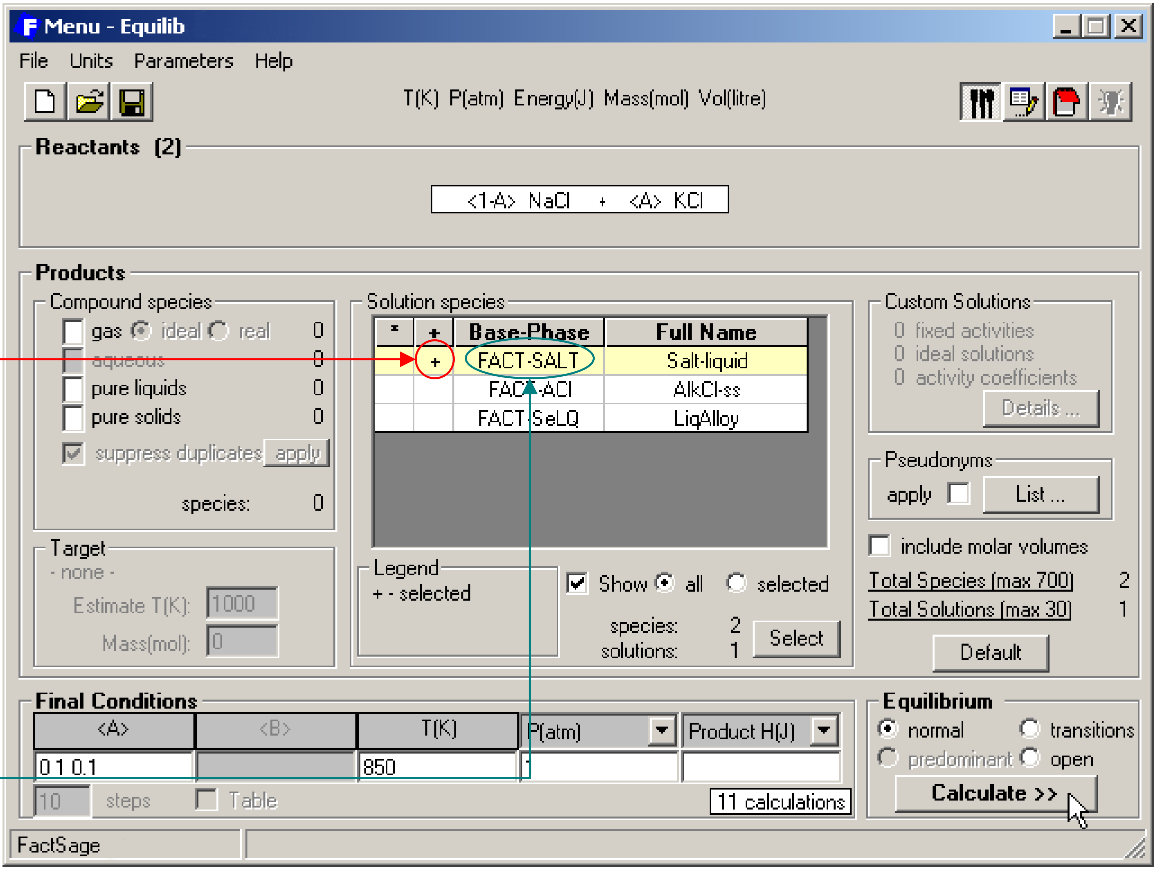
10 steps ☐ Table 11 calculations

Equilibrium
- ● normal ○ transitions
- ○ predominant ○ open

Solution Properties: opening the window

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





Reactants (2): <1-A> NaCl + <A> KCl

Compound species: ☐ gas ● ideal ○ real 0; ☐ aqueous 0; ☐ pure liquids 0; ☐ pure solids 0; ☑ suppress duplicates apply; species: 0

Solution species:

*	+	Base-Phase	Full Name
	+	FACT-SALT	Salt-liquid
		FACT-ACl	AlkCl-ss
		FACT-SeLQ	LiqAlloy

Legend: + - selected

☑ Show ● all ○ selected; species: 2; solutions: 1

Custom Solutions: 0 fixed activities; 0 ideal solutions; 0 activity coefficients

Pseudonyms: apply ☐

☐ include molar volumes

Total Species (max 700) 2

Total Solutions (max 30) 1

Target: - none -; Estimate T(K): 1000; Mass(mol): 0

Final Conditions:

<A>	<B>	T(K)	P(atm)	Product H(J)
0 1 0.1		850	1	

10 steps ☐ Table; 11 calculations

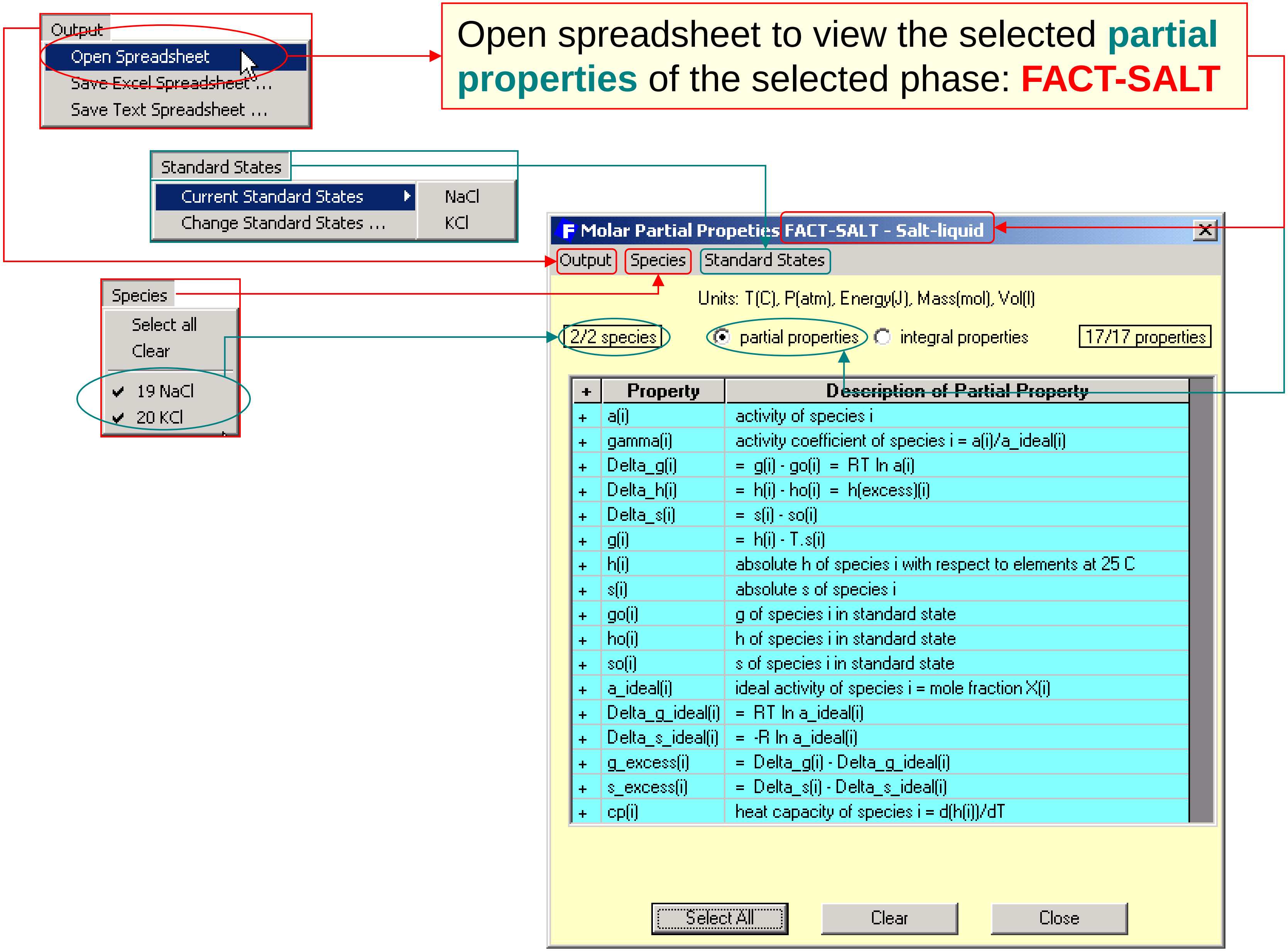
Equilibrium: ● normal ○ transitions ○ predominant ○ open

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**



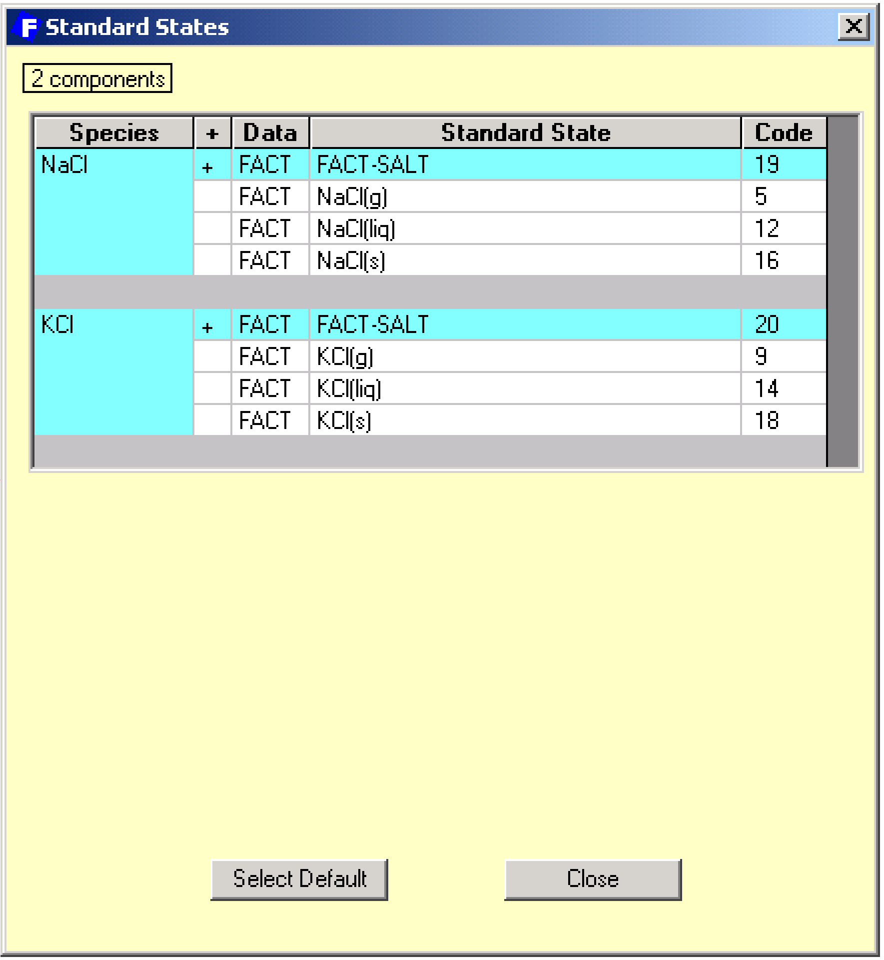
Units: T(C), P(atm), Energy(J), Mass(mol), Vol(l)

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

Solution Properties: **Changing** Standard States

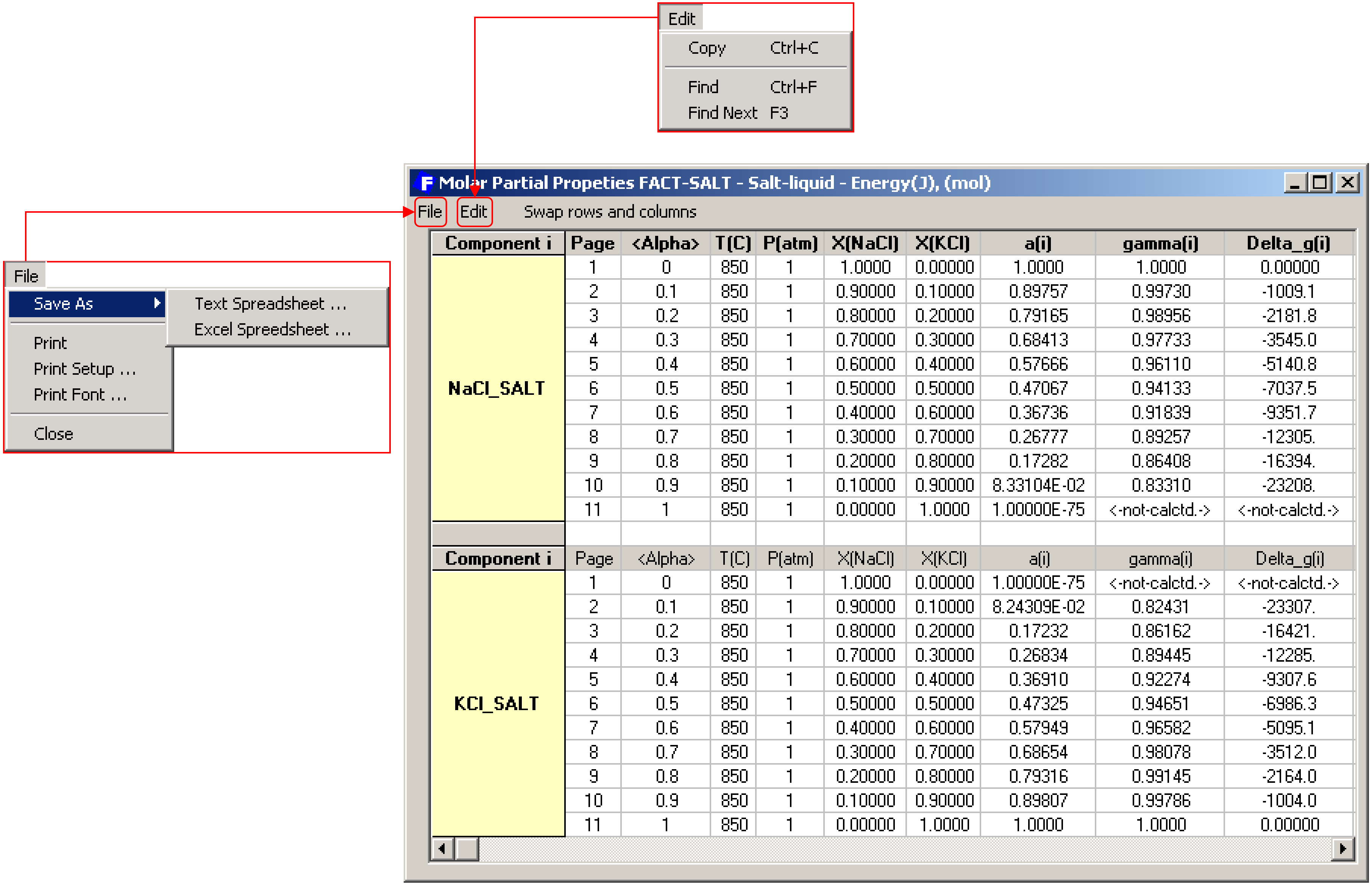
In the **solution properties** window menu, **select Standard States > Change Standard States…** and **click** in the **+** column to **select** the new standard state.



2 components

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

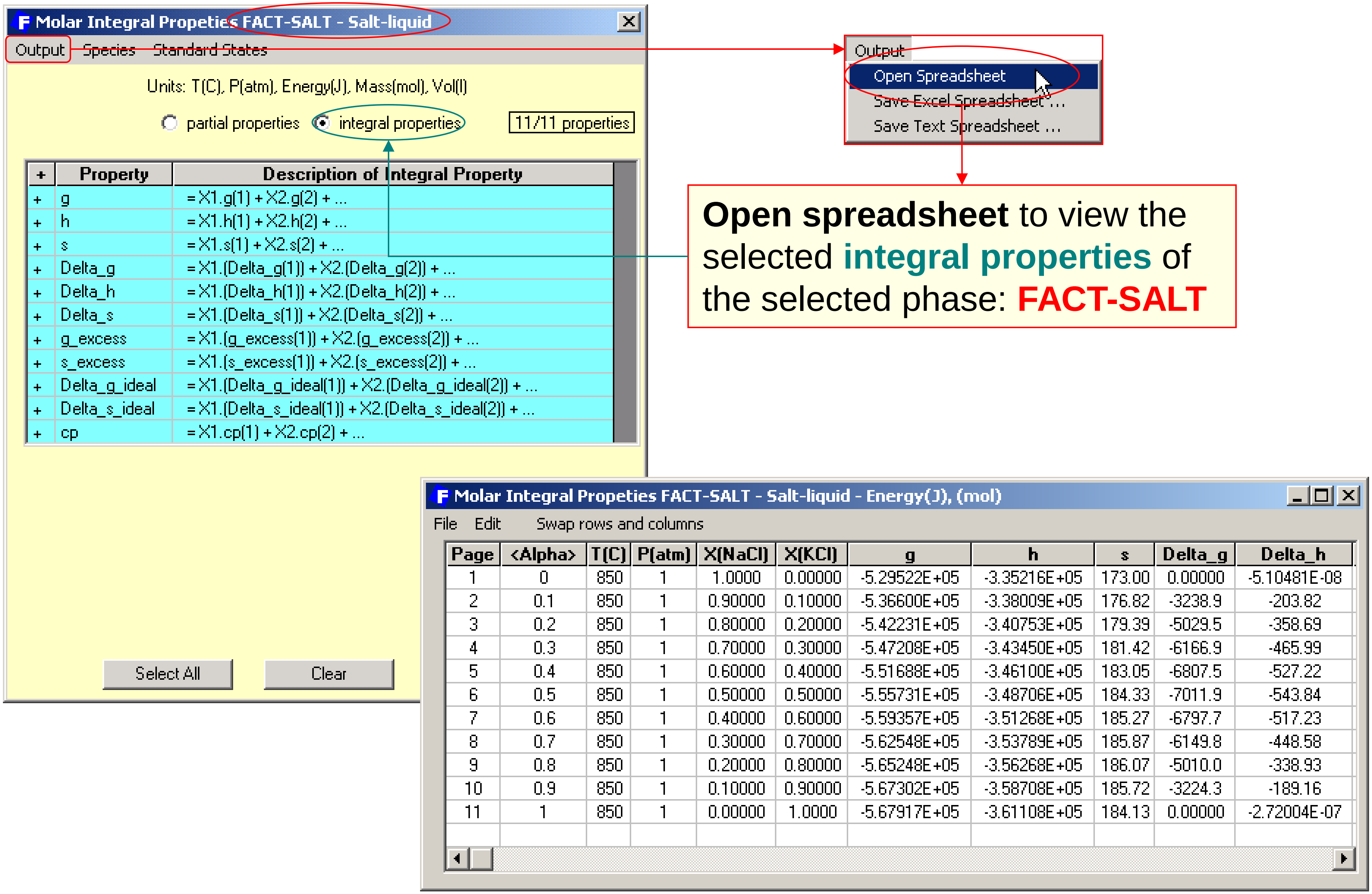
Solution Properties: Molar Partial Properties Spreadsheet



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



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

○ partial properties ● integral properties

11/11 properties

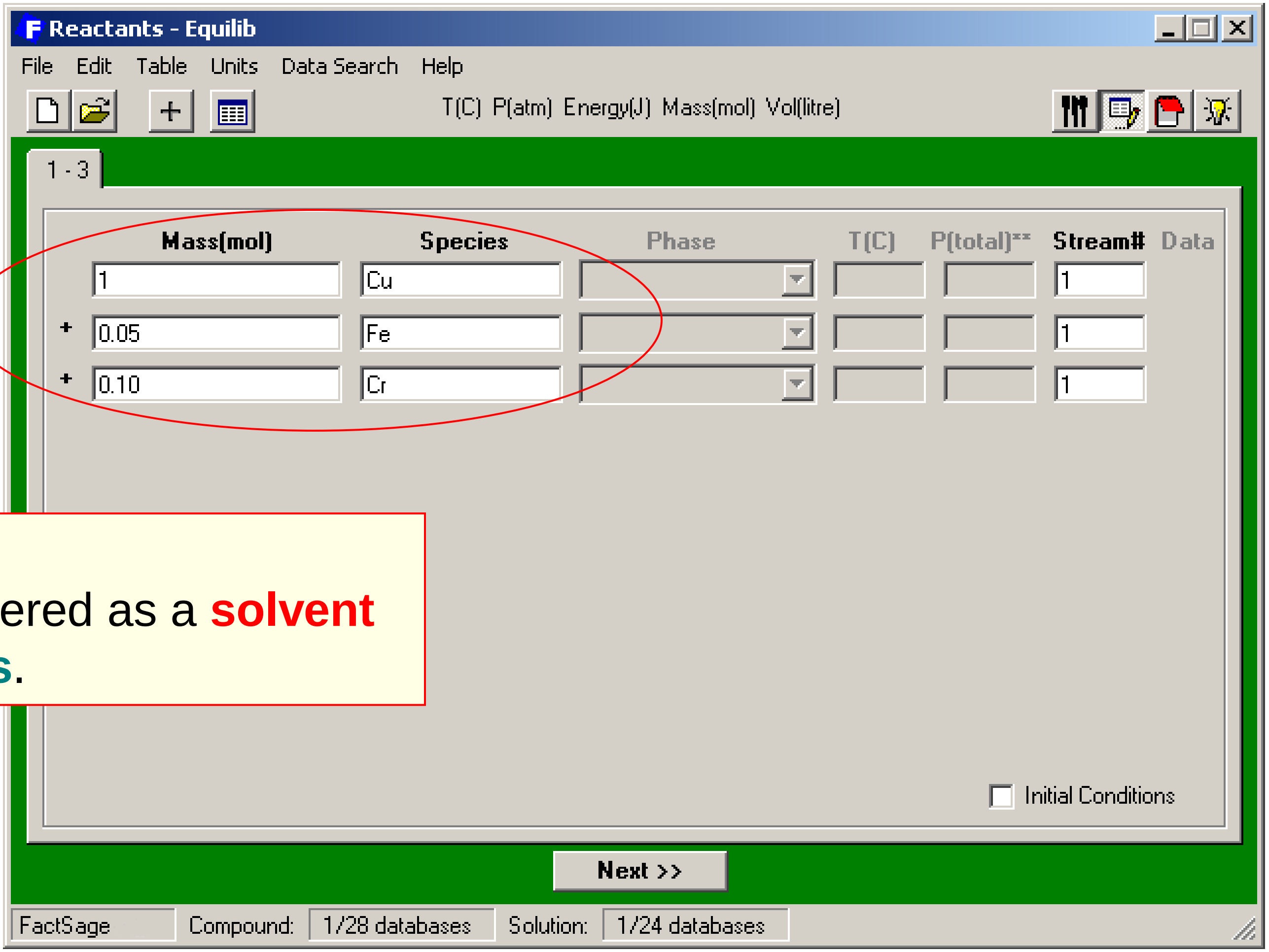
+	Property	Description of Integral Property
+	g	= X1.g(1) + X2.g(2) + ...
+	h	= X1.h(1) + X2.h(2) + ...
+	s	= X1.s(1) + X2.s(2) + ...
+	Delta_g	= X1.(Delta_g(1)) + X2.(Delta_g(2)) + ...
+	Delta_h	= X1.(Delta_h(1)) + X2.(Delta_h(2)) + ...
+	Delta_s	= X1.(Delta_s(1)) + X2.(Delta_s(2)) + ...
+	g_excess	= 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) + ...

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

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**.

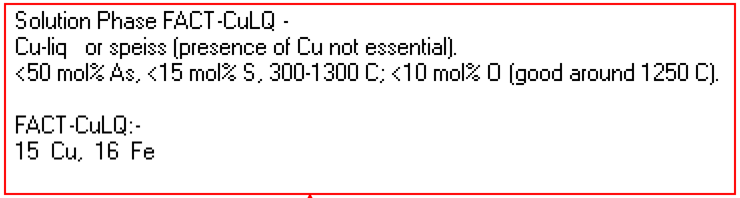


	Mass(mol)	Species	Phase	T(C)	P(total)**	Stream#	Data
	1	Cu				1	
+	0.05	Fe				1	
+	0.10	Cr				1	

☐ Initial Conditions

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).

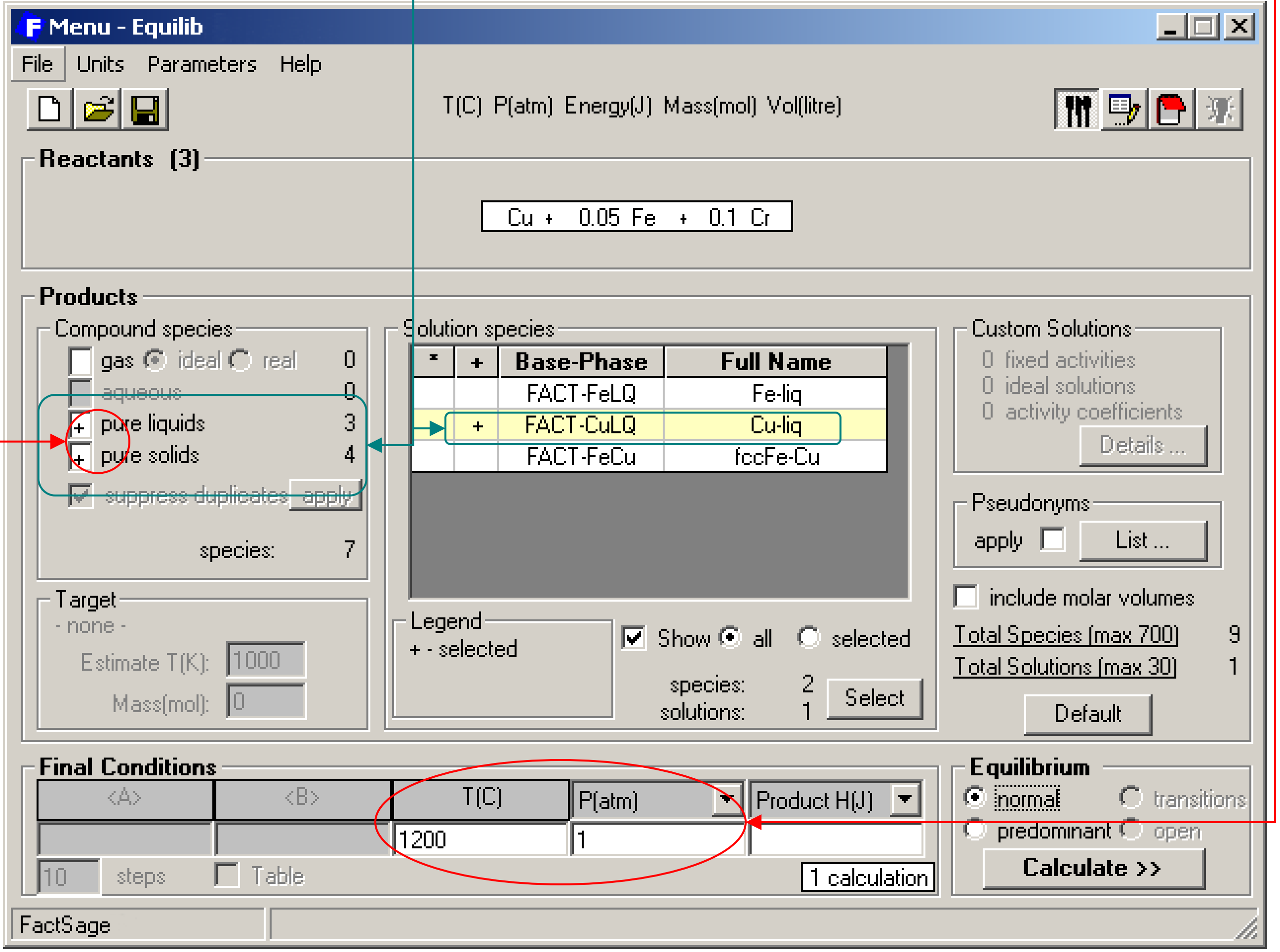
FACT-CuLQ:-
15 Cu, 16 Fe

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**



Reactants (3)

Cu + 0.05 Fe + 0.1 Cr

Products

Compound species

☐ gas ● ideal ○ real		0
☐ aqueous		0
+ pure liquids		3
+ pure solids		4
☑ suppress duplicates	apply	
species:		7

Solution species

*	+	Base-Phase	Full Name
		FACT-FeLQ	Fe-liq
	+	FACT-CuLQ	Cu-liq
		FACT-FeCu	fccFe-Cu

Legend
+ - selected

☑ Show ● all ○ selected

species: 2
solutions: 1

Custom Solutions
0 fixed activities
0 ideal solutions
0 activity coefficients

Pseudonyms
apply ☐

☐ include molar volumes

Total Species (max 700) 9
Total Solutions (max 30) 1

Target
- none -
Estimate T(K): 1000
Mass(mol): 0

Final Conditions

<A>	<B>	T(C)	P(atm)	Product H(J)
		1200	1	

10 steps ☐ Table

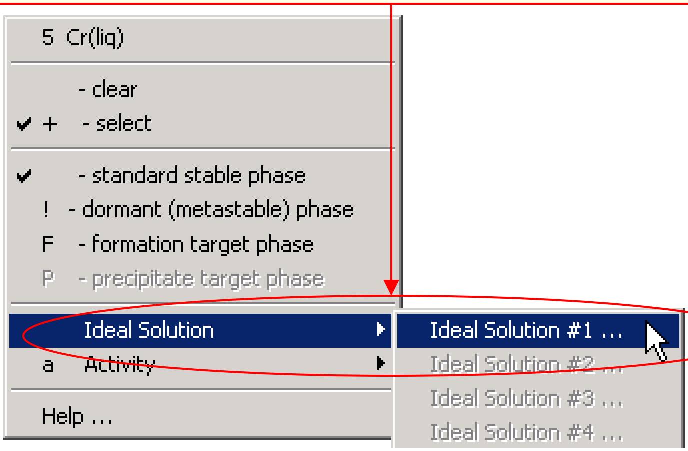
1 calculation

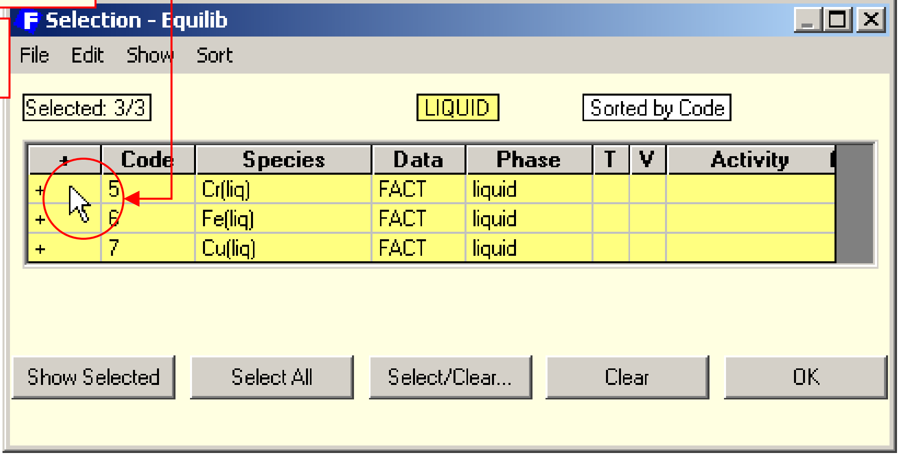
Equilibrium
● normal ○ transitions
○ predominant ○ open

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…





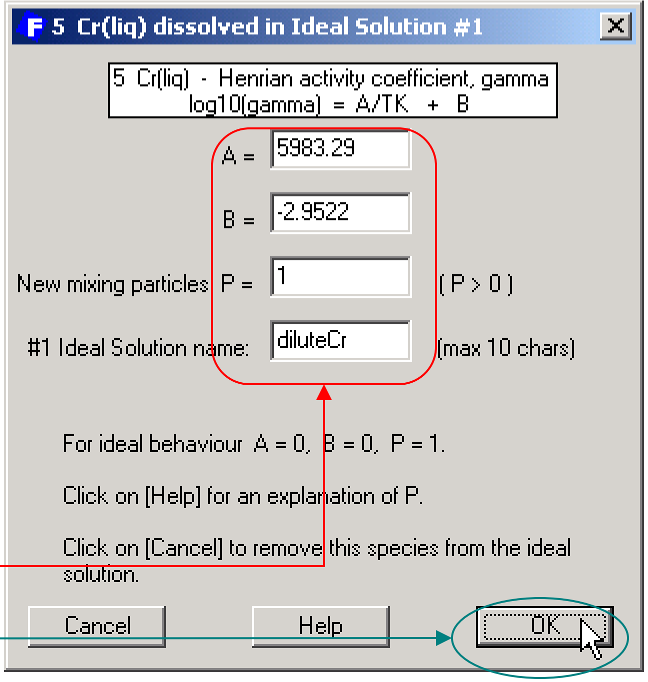
Selected: 3/3 LIQUID Sorted by Code

+	Code	Species	Data	Phase	T	V	Activity
+	5	Cr(liq)	FACT	liquid			
+	6	Fe(liq)	FACT	liquid			
+	7	Cu(liq)	FACT	liquid			

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:

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

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**.



5 Cr(liq) - Henrian activity coefficient, gamma
log10(gamma) = A/TK + B

A = 5983.29

B = -2.9522

New mixing particles P = 1 (P > 0)

#1 Ideal Solution name: diluteCr (max 10 chars)

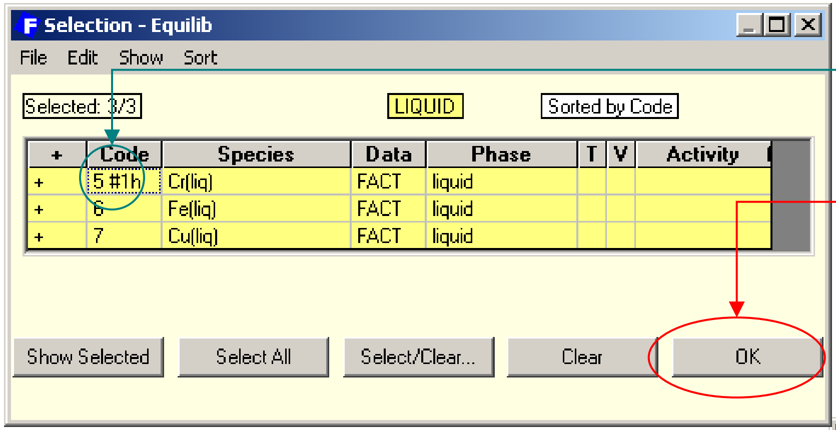
For ideal behaviour A = 0, B = 0, P = 1.

Click on [Help] for an explanation of P.

Click on [Cancel] to remove this species from the ideal solution.

4° **Press OK**

Merging the **ideal solution diluteCr** and **FACT-CuLQ**



Selected: 3/3 LIQUID Sorted by Code

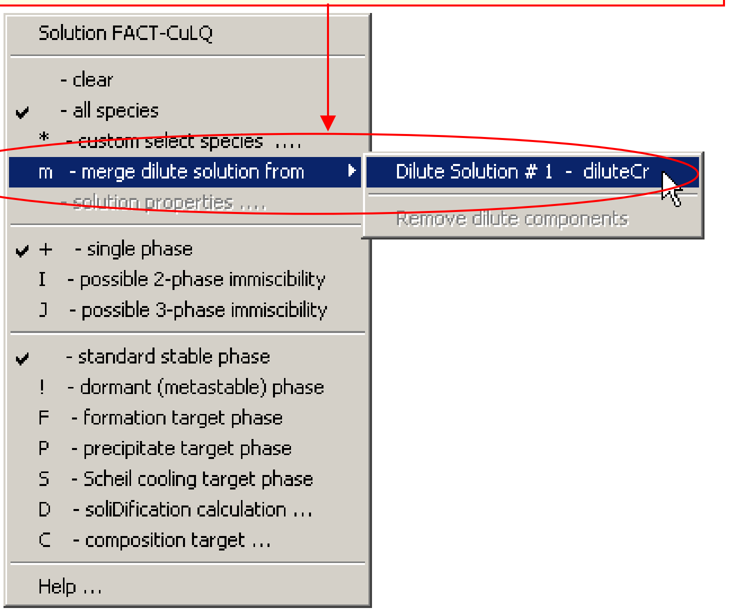
+	Code	Species	Data	Phase	T	V	Activity
+	5 #1h	Cr(liq)	FACT	liquid			
+	6	Fe(liq)	FACT	liquid			
+	7	Cu(liq)	FACT	liquid			

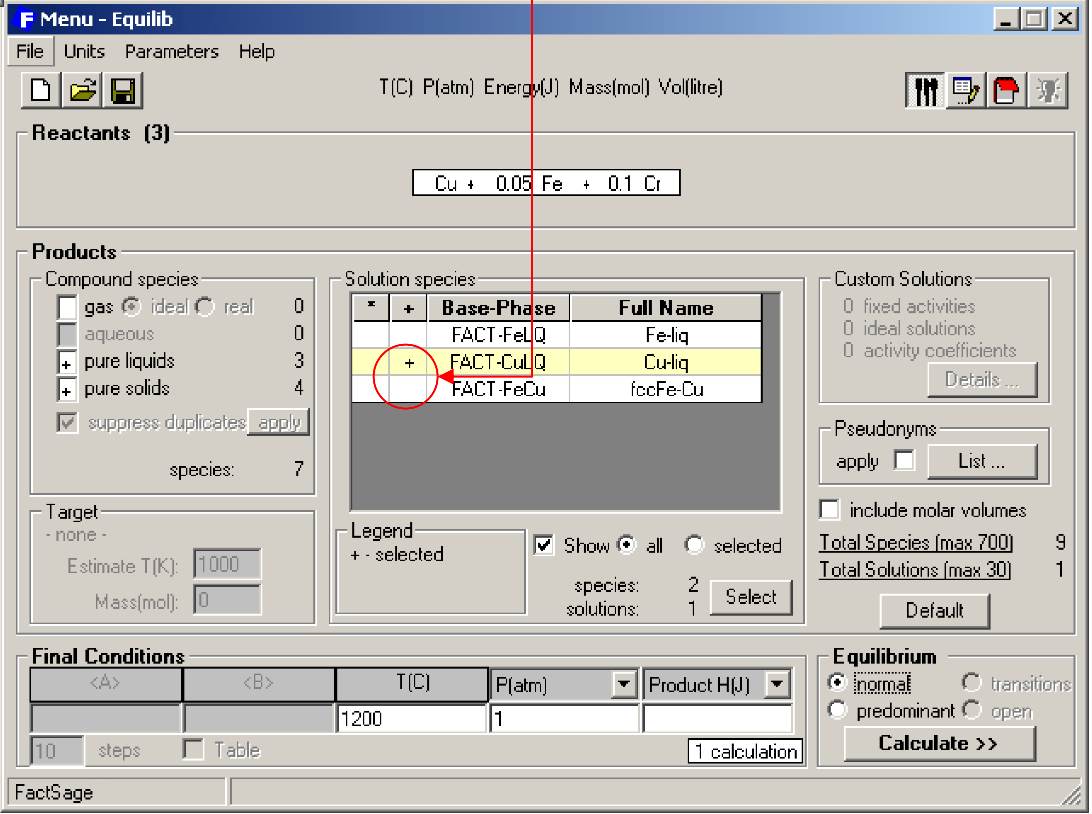
# denotes species also used in ideal solution **1** and **h** indicates an henrian activity coefficient

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





Reactants (3)

Cu + 0.05 Fe + 0.1 Cr

Compound species:

- ☐ gas ● ideal ○ real 0
- ☐ aqueous 0
- + pure liquids 3
- + pure solids 4
- ☑ suppress duplicates apply
- species: 7

Solution species:

*	+	Base-Phase	Full Name
		FACT-FeLQ	Fe-liq
	+	FACT-CuLQ	Cu-liq
		FACT-FeCu	fccFe-Cu

☑ Show ● all ○ selected

species: 2
solutions: 1

Custom Solutions:

- 0 fixed activities
- 0 ideal solutions
- 0 activity coefficients

Pseudonyms: apply ☐

☐ include molar volumes

Total Species (max 700)	9
Total Solutions (max 30)	1

Target: Estimate T(K): 1000 Mass(mol): 0

Final Conditions:

<A>	<B>	T(C)	P(atm)	Product H(J)
		1200	1	

10 steps ☐ Table 1 calculation

Equilibrium: ● normal ○ transitions ○ predominant ○ open

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

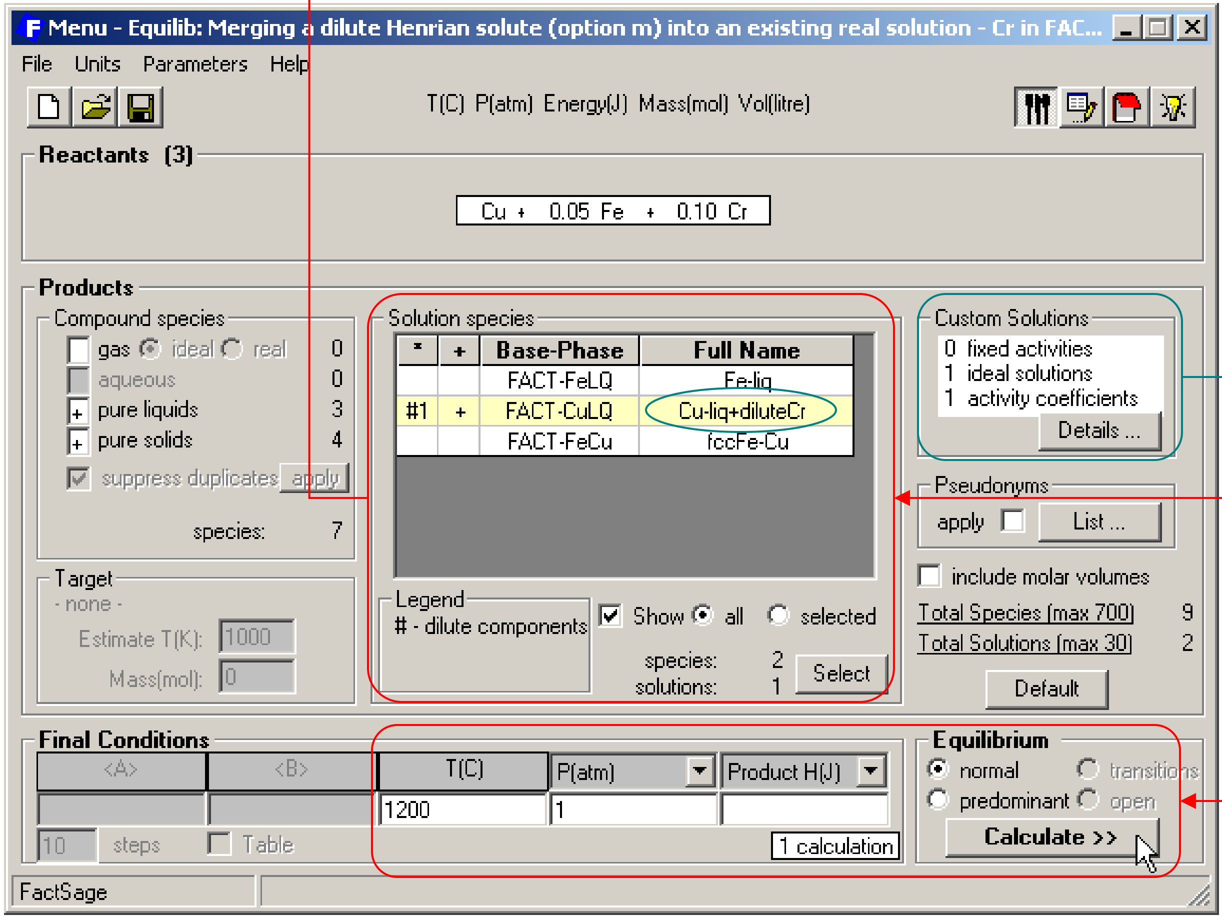
Solution Phase FACT-CuLQ -
Cu-liq or speiss (presence of Cu not essential).
<50 mol% As, <15 mol% S, 300-1300 C; <10 mol% O (good around 1250 C).

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:

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

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



Menu - Equilib: Merging a dilute Henrian solute (option m) into an existing real solution - Cr in FAC...

File Units Parameters Help

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

Reactants (3)

Cu + 0.05 Fe + 0.10 Cr

Products

Compound species
- ☐ gas ● ideal ○ real 0
- ☐ aqueous 0
- ☐+ pure liquids 3
- ☐+ pure solids 4
- ☑ suppress duplicates apply

species: 7

Target
- none -
Estimate T(K): 1000
Mass(mol): 0

Solution species

*	+	Base-Phase	Full Name
		FACT-FeLQ	Fe-liq
#1	+	FACT-CuLQ	Cu-liq+diluteCr
		FACT-FeCu	fccFe-Cu

Legend
- dilute components

☑ Show ● all ○ selected
species: 2
solutions: 1
Select

Custom Solutions
0 fixed activities
1 ideal solutions
1 activity coefficients
Details ...

Pseudonyms
apply ☐ List ...

☐ include molar volumes
Total Species (max 700) 9
Total Solutions (max 30) 2
Default

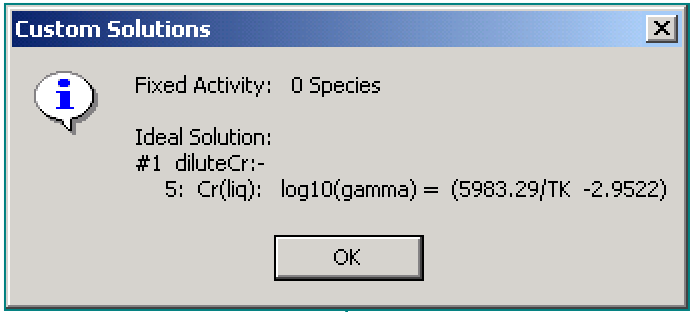
Final Conditions

<A>	<B>	T(C)	P(atm)	Product H(J)
		1200	1	

10 steps ☐ Table 1 calculation

Equilibrium
● normal ○ transitions
○ predominant ○ open
Calculate >>

FactSage



Custom Solutions

Fixed Activity: 0 Species

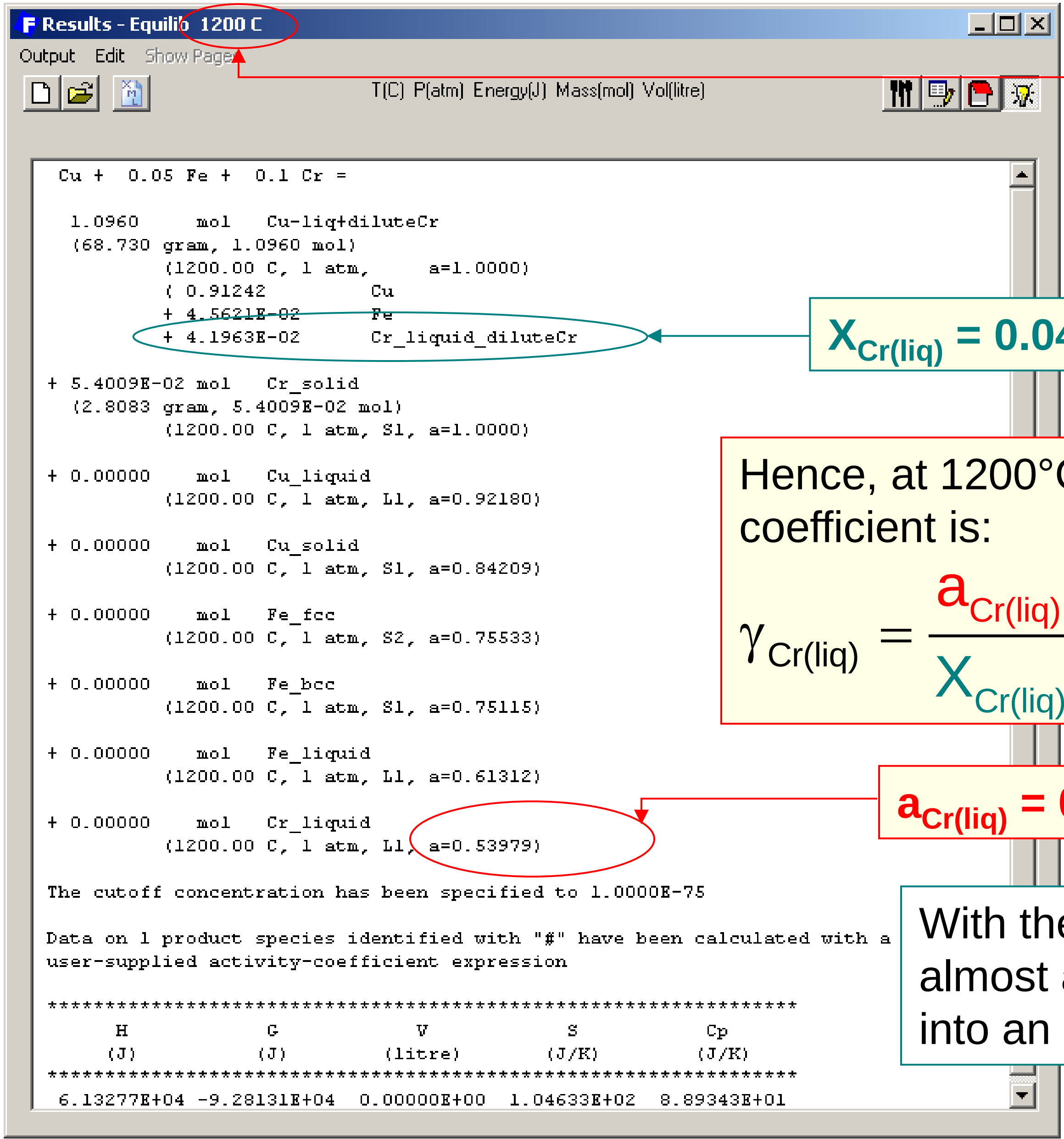
Ideal Solution:
#1 diluteCr:-
5: Cr(liq): log10(gamma) = (5983.29/TK -2.9522)

OK

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



```
 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

$X_{Cr(liq)} = 0.041963$

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

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

$a_{Cr(liq)} = 0.53979$

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**.

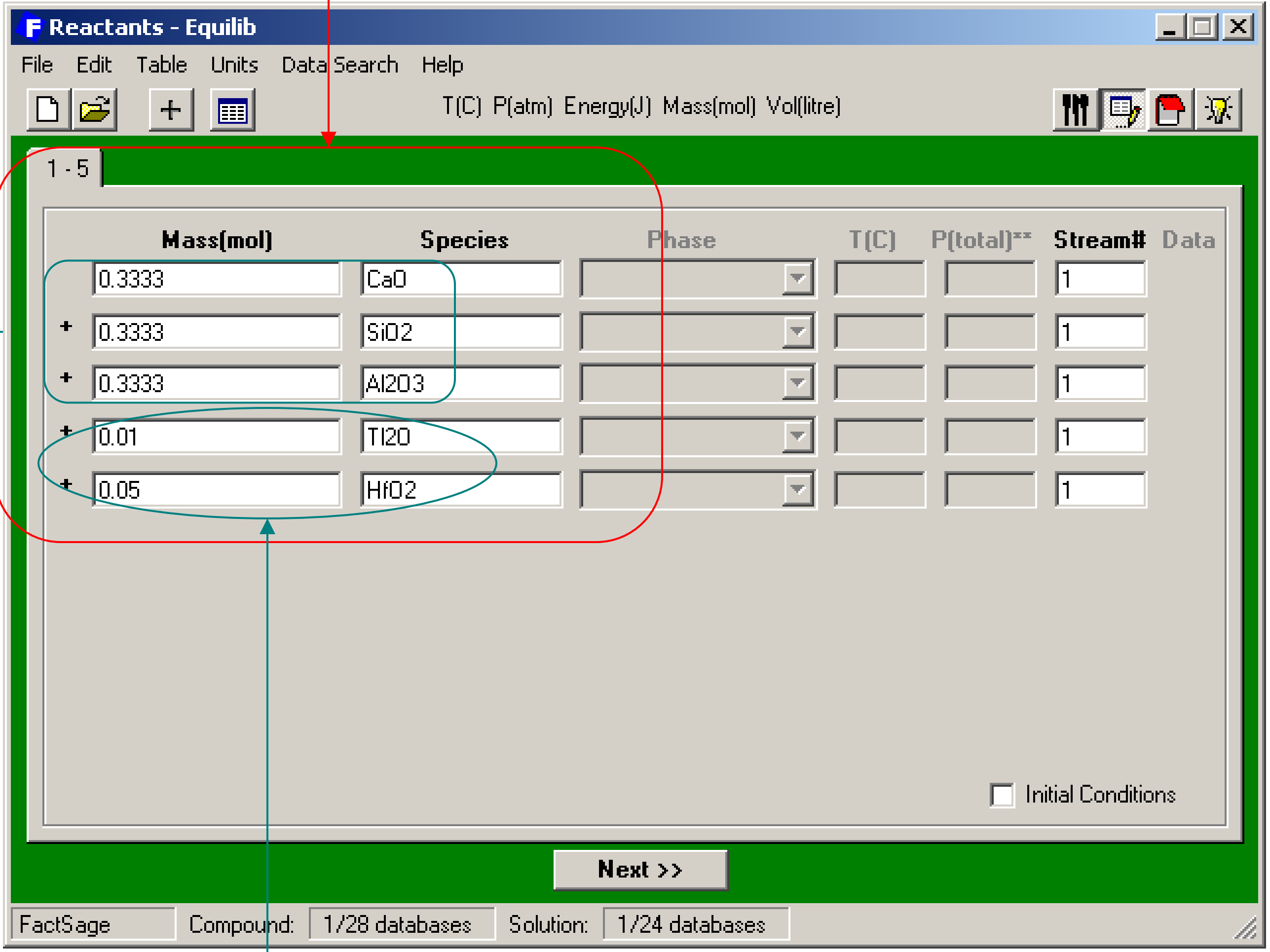
It is assumed that the activity coefficients (defined as $\gamma = a/X$ where a = activity and X = mole fraction) of the **dilute** constituents are independent of composition. That is, the dilute components obey **Henry's Law**. Also, for demonstration purposes let us assume that the activity coefficient 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…

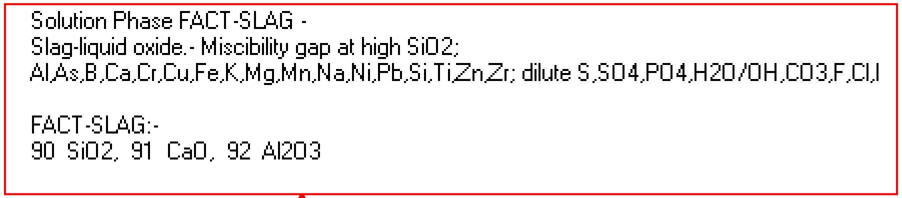


	Mass(mol)	Species	Phase	T(C)	P(total)**	Stream#	Data
	0.3333	CaO				1	
+	0.3333	SiO2				1	
+	0.3333	Al2O3				1	
+	0.01	Tl2O				1	
+	0.05	HfO2				1	

☐ Initial Conditions

…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

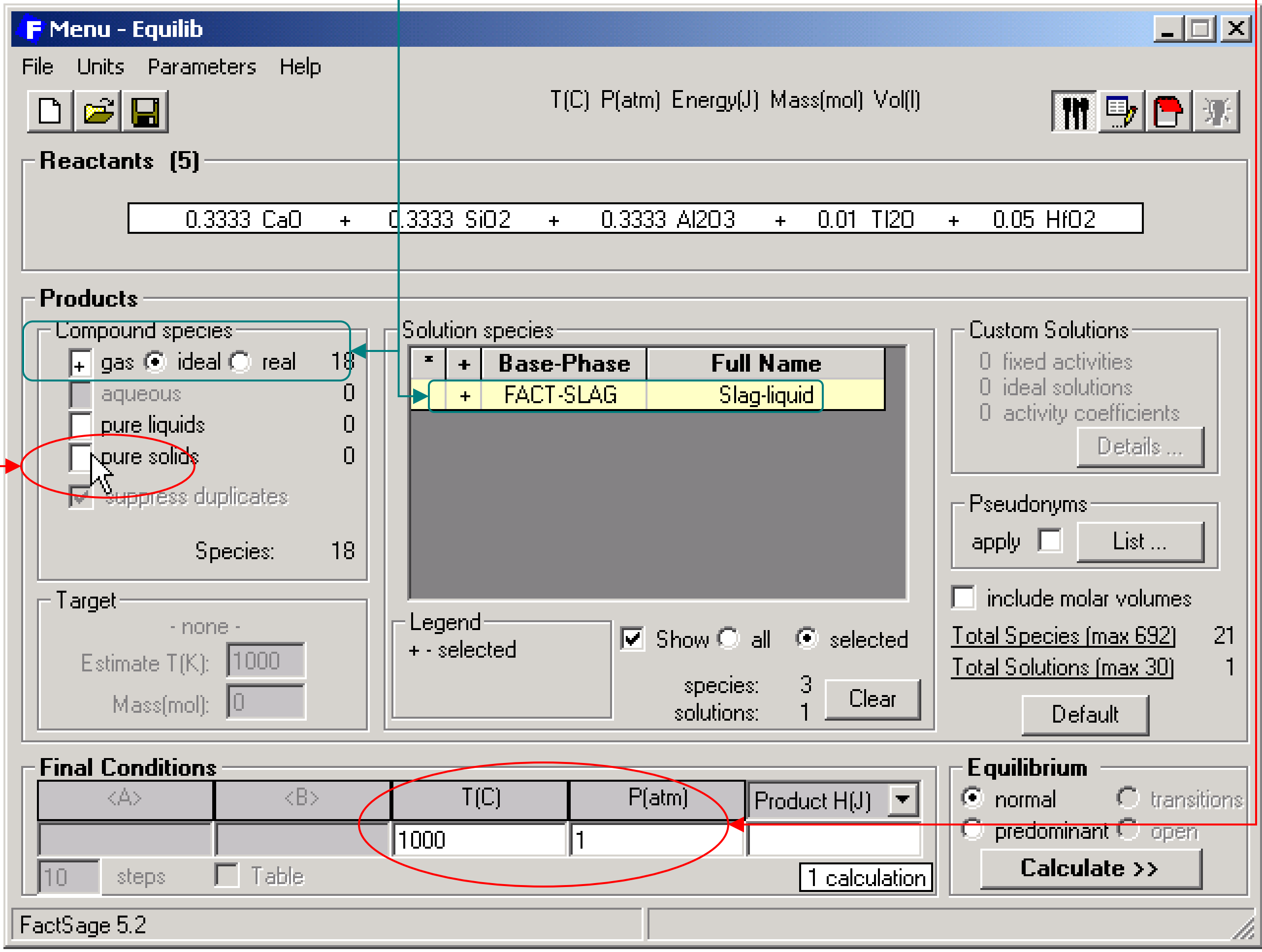
FACT-SLAG:-
90 SiO2, 91 CaO, 92 Al2O3

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

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

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

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



Reactants (5)

0.3333 CaO + 0.3333 SiO2 + 0.3333 Al2O3 + 0.01 Tl2O + 0.05 HfO2

Products

Compound species

- ☐ gas ● ideal ○ real 18
- ☐ aqueous 0
- ☐ pure liquids 0
- ☐ pure solids 0
- ☑ suppress duplicates

Species: 18

Target: - none -
Estimate T(K): 1000
Mass(mol): 0

Solution species

*	+	Base-Phase	Full Name
	+	FACT-SLAG	Slag-liquid

Legend: + - selected

☑ Show ○ all ● selected

species: 3
solutions: 1

Custom Solutions
0 fixed activities
0 ideal solutions
0 activity coefficients

Pseudonyms: apply ☐

☐ include molar volumes

Total Species (max 692) 21
Total Solutions (max 30) 1

Final Conditions

<A>	<B>	T(C)	P(atm)	Product H(J)
		1000	1	

10 steps ☐ Table — 1 calculation

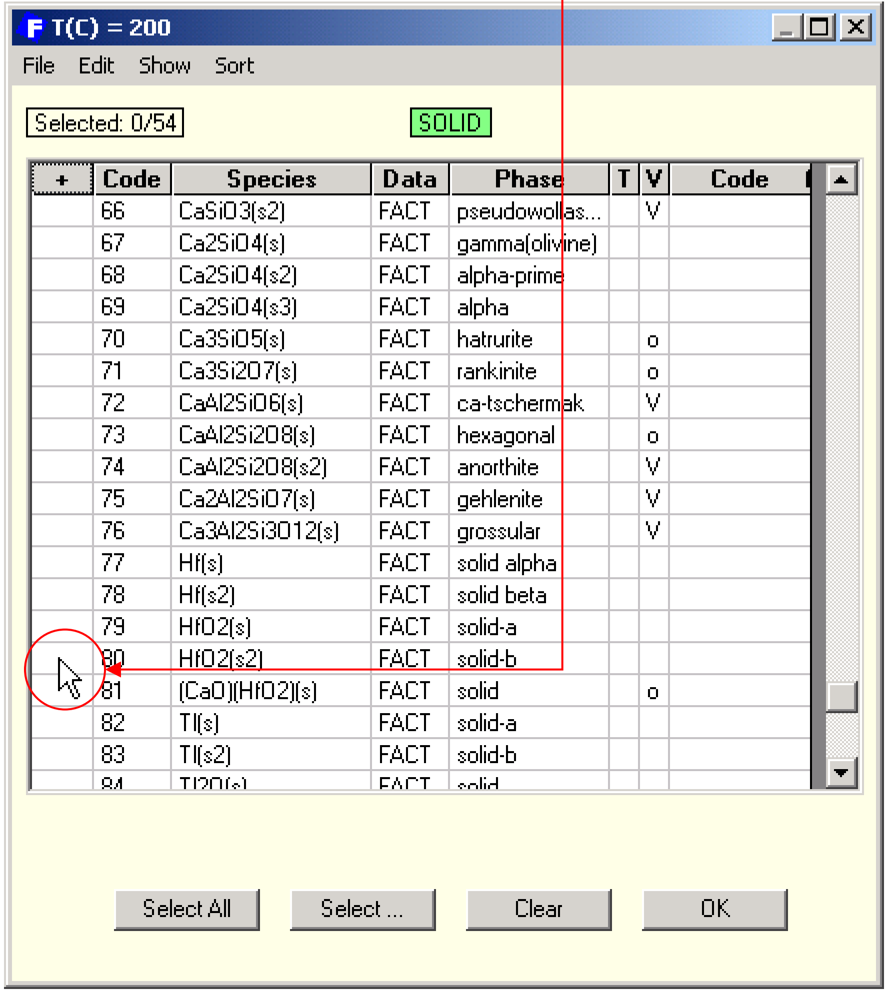
Equilibrium: ● normal ○ transitions ○ predominant ○ open

FactSage 5.2

Creating an **ideal Henrian solution** of HfO_2(s)

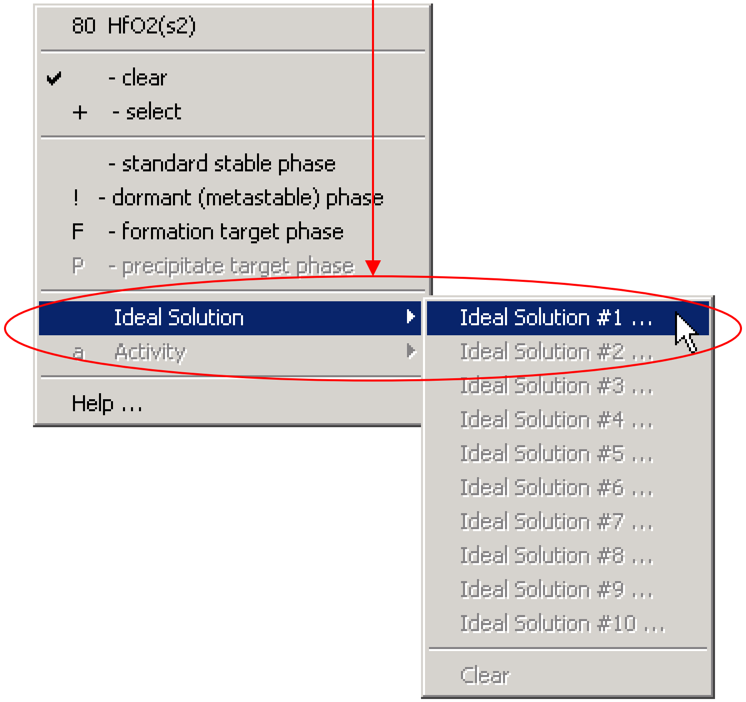
1° **Right-click** to open the HfO_2(s2) extended menu

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



Selected: 0/54

+	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			



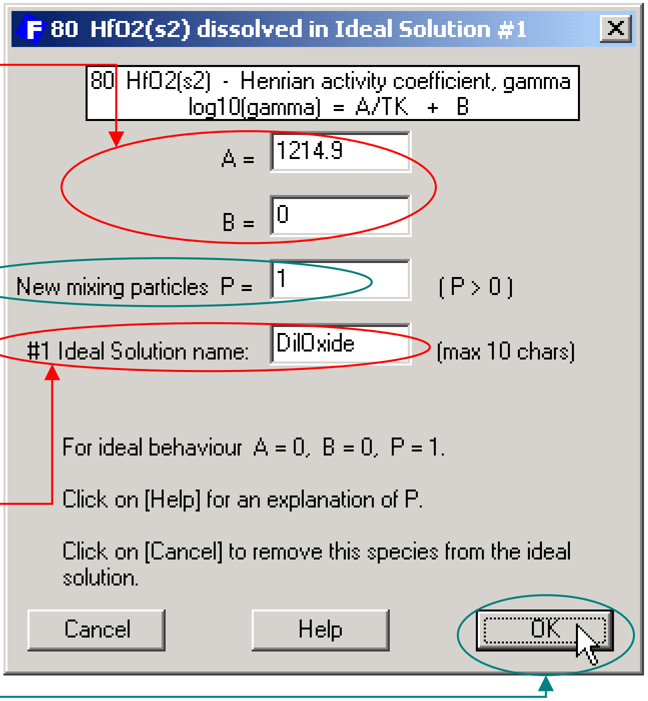
Creating an **ideal Henrian solution** of **HfO_2(s)** – setting γ

3° **Enter** $\log_{10} [\gamma_{HfO_2(s2)}] = \mathbf{1214.9}/T(K) + \mathbf{0}$
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**.



80 HfO2(s2) dissolved in Ideal Solution #1

80 HfO2(s2) - Henrian activity coefficient, gamma
log10(gamma) = A/TK + B

A = 1214.9

B = 0

New mixing particles P = 1 (P > 0)

#1 Ideal Solution name: DilOxide (max 10 chars)

For ideal behaviour A = 0, B = 0, P = 1.

Click on [Help] for an explanation of P.

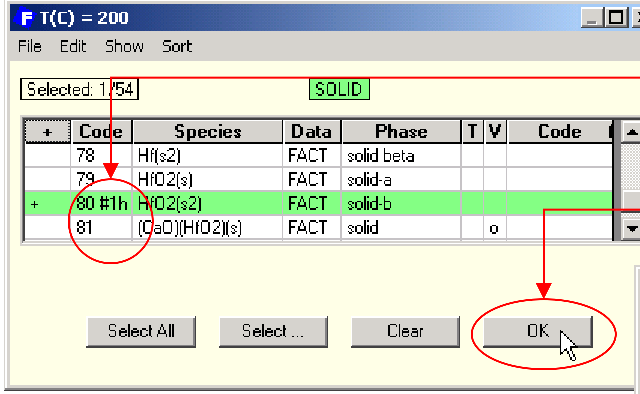
Click on [Cancel] to remove this species from the ideal solution.

Notes:

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

Adding $Tl_2O(l)$ to the ideal solution

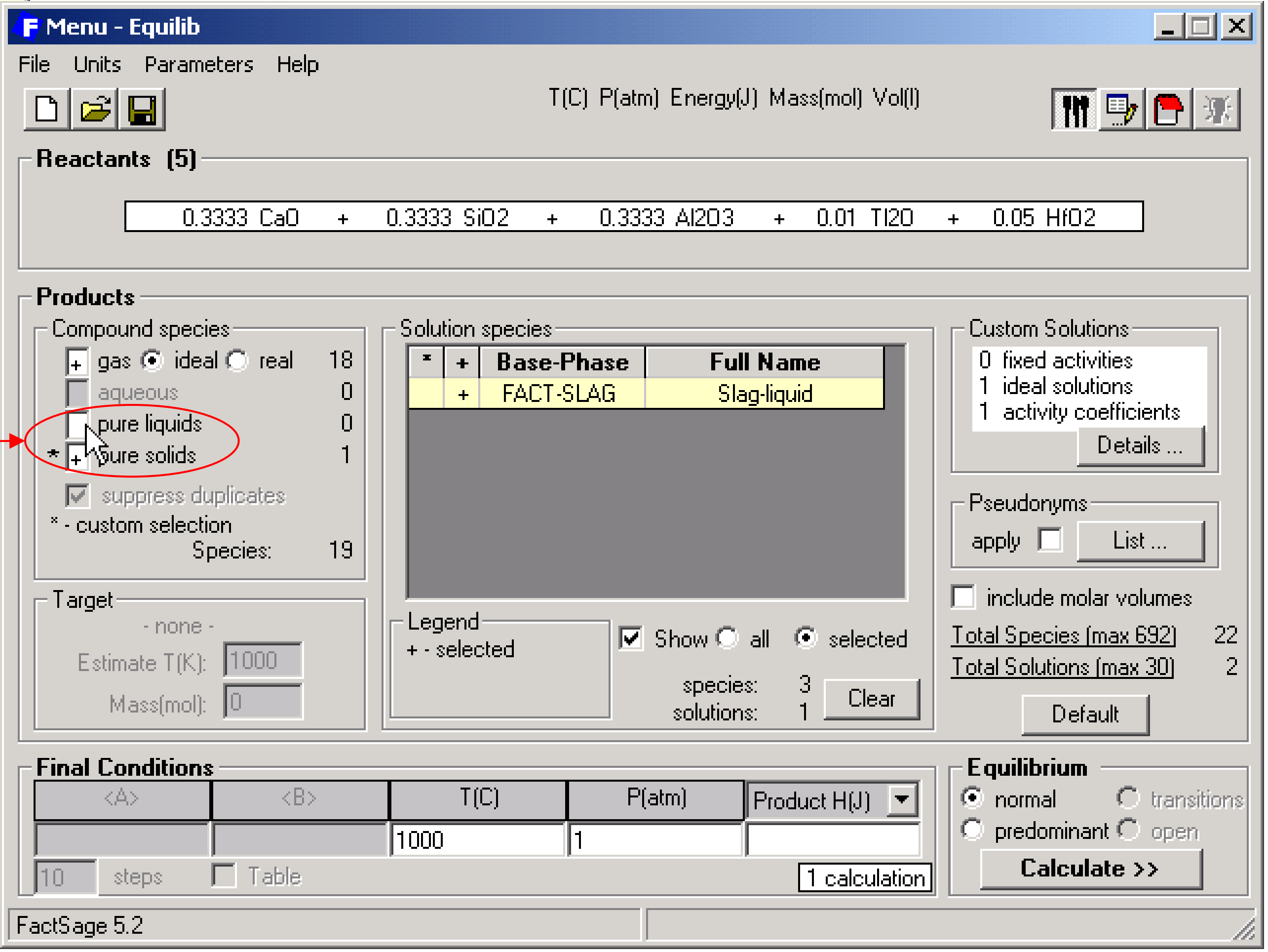
# denotes species also used in ideal solution **1** and **h** indicates an henrian activity coefficient



Selected: 1/54 SOLID

+	Code	Species	Data	Phase	T	V	Code
	78	Hf(s2)	FACT	solid beta			
	79	HfO2(s)	FACT	solid-a			
+	80 #1h	HfO2(s2)	FACT	solid-b			
	81	(CaO)(HfO2)(s)	FACT	solid		o	

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



Reactants (5)

0.3333 CaO + 0.3333 SiO2 + 0.3333 Al2O3 + 0.01 Tl2O + 0.05 HfO2

Products

Compound species
☐+ gas ● ideal ○ real 18
☐ aqueous 0
☐ pure liquids 0
* ☐+ pure solids 1
☑ suppress duplicates
* - custom selection
Species: 19

Solution species

*	+	Base-Phase	Full Name
	+	FACT-SLAG	Slag-liquid

Legend
\+ - selected

☑ Show ○ all ● selected
species: 3
solutions: 1

Custom Solutions
0 fixed activities
1 ideal solutions
1 activity coefficients

Pseudonyms
apply ☐

☐ include molar volumes
Total Species (max 692) 22
Total Solutions (max 30) 2

Target
\- none -
Estimate T(K): 1000
Mass(mol): 0

Final Conditions

<A>	<B>	T(C)	P(atm)	Product H(J)
		1000	1	

10 steps ☐ Table 1 calculation

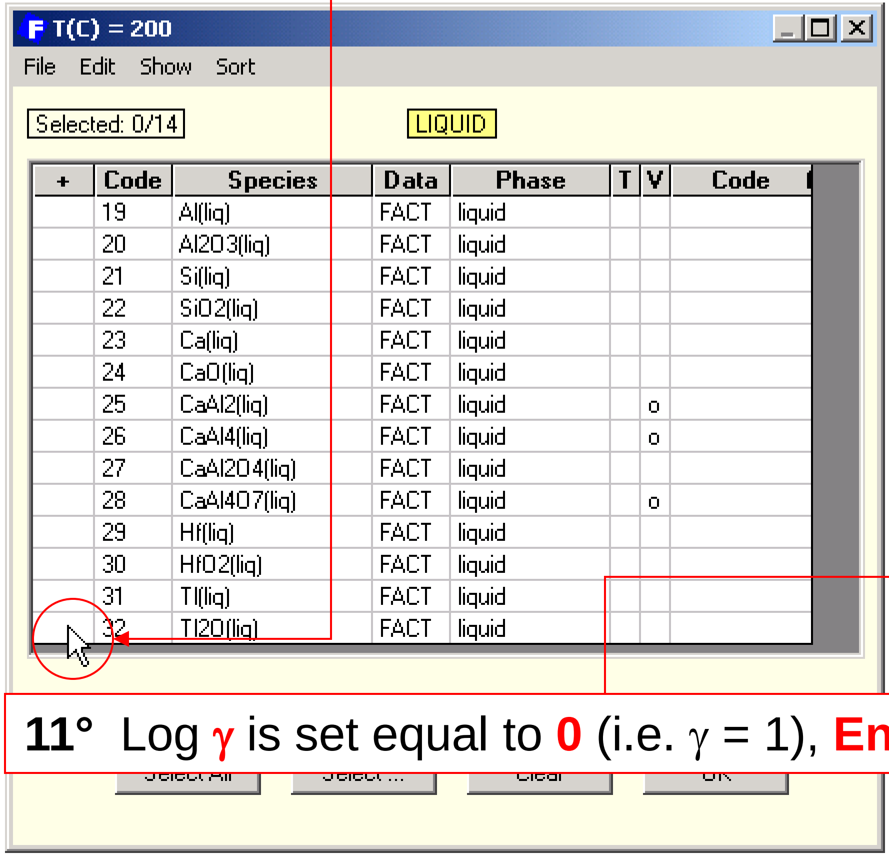
Equilibrium
● normal ○ transitions
○ predominant ○ open

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

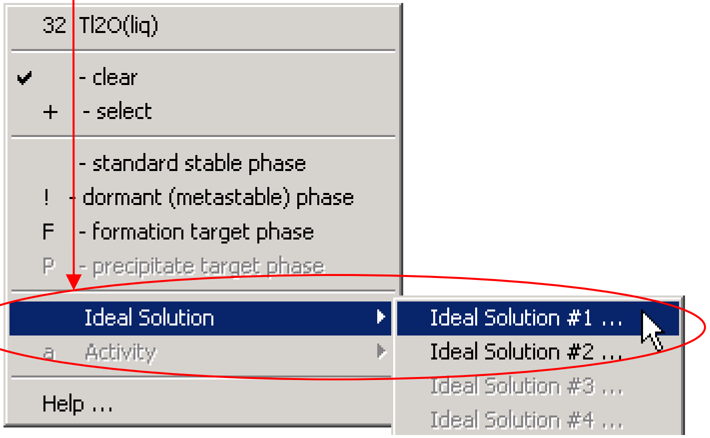
Adding $Tl_2O(l)$ to the ideal solution – setting γ

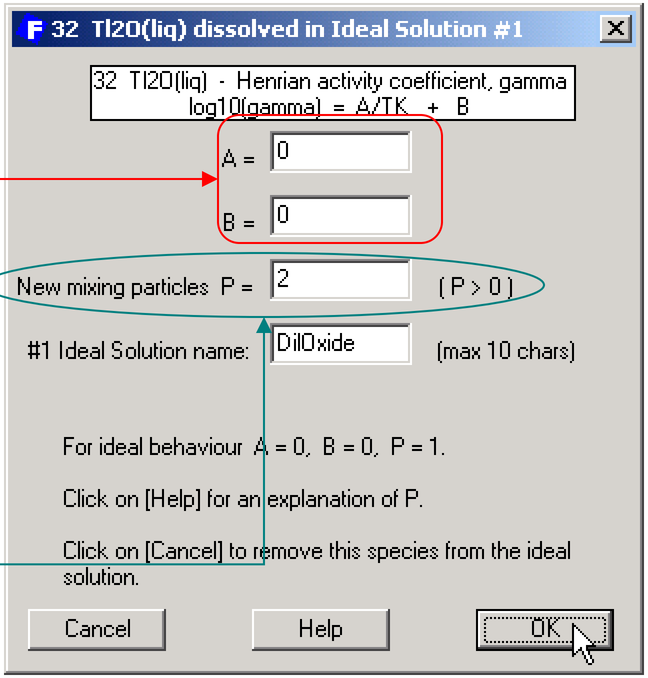
9° **Right-click** to open the $Tl_2O(liq)$ extended menu

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



+	Code	Species	Data	Phase	T	V	Code
	19	Al(liq)	FACT	liquid			
	20	Al2O3(liq)	FACT	liquid			
	21	Si(liq)	FACT	liquid			
	22	SiO2(liq)	FACT	liquid			
	23	Ca(liq)	FACT	liquid			
	24	CaO(liq)	FACT	liquid			
	25	CaAl2(liq)	FACT	liquid		o	
	26	CaAl4(liq)	FACT	liquid		o	
	27	CaAl2O4(liq)	FACT	liquid			
	28	CaAl4O7(liq)	FACT	liquid		o	
	29	Hf(liq)	FACT	liquid			
	30	HfO2(liq)	FACT	liquid			
	31	Tl(liq)	FACT	liquid			
	32	Tl2O(liq)	FACT	liquid			





32 Tl2O(liq) - Henrian activity coefficient, gamma
log10(gamma) = A/TK + B

A = 0

B = 0

New mixing particles P = 2 (P > 0)

#1 Ideal Solution name: DilOxide (max 10 chars)

For ideal behaviour A = 0, B = 0, P = 1.

Click on [Help] for an explanation of P.

Click on [Cancel] to remove this species from the ideal solution.

11° Log γ is set equal to **0** (i.e. γ = 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, γ and new mixing particles, **P**

A **dilute solute** in an **ideal solution** may have a Henrian activity coefficient, γ, 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:

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

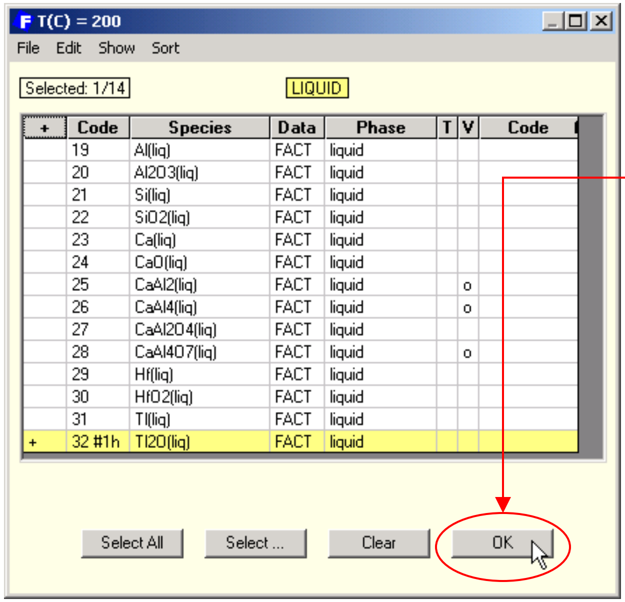
Merging the **ideal Henrian solution DilOxide** and **FACT-Slag**

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

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

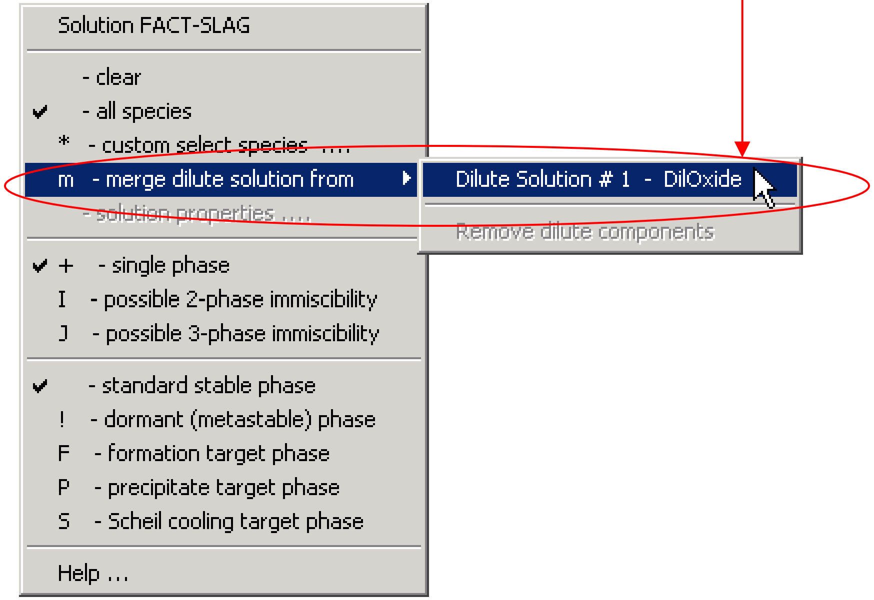
14° **Right-click** in the **+** column of **FACT-Slag** to open its extended menu.

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



Selected: 1/14 LIQUID

+	Code	Species	Data	Phase	T	V	Code
	19	Al(liq)	FACT	liquid			
	20	Al2O3(liq)	FACT	liquid			
	21	Si(liq)	FACT	liquid			
	22	SiO2(liq)	FACT	liquid			
	23	Ca(liq)	FACT	liquid			
	24	CaO(liq)	FACT	liquid			
	25	CaAl2(liq)	FACT	liquid		o	
	26	CaAl4(liq)	FACT	liquid		o	
	27	CaAl2O4(liq)	FACT	liquid			
	28	CaAl4O7(liq)	FACT	liquid		o	
	29	Hf(liq)	FACT	liquid			
	30	HfO2(liq)	FACT	liquid			
	31	Tl(liq)	FACT	liquid			
+	32 #1h	Tl2O(liq)	FACT	liquid			

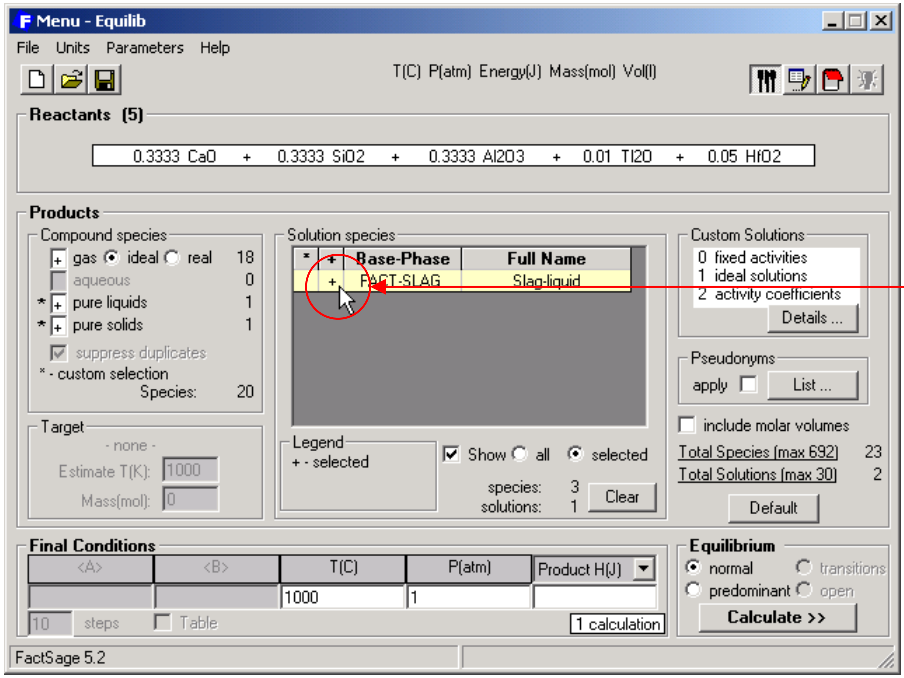

Solution FACT-SLAG

- clear
✓ - all species
* - custom select species ....
m - merge dilute solution from ▸ Dilute Solution # 1 - DilOxide
- solution properties ....
Remove dilute components

✓ + - single phase
I - possible 2-phase immiscibility
J - possible 3-phase immiscibility

✓ - standard stable phase
! - dormant (metastable) phase
F - formation target phase
P - precipitate target phase
S - Scheil cooling target phase

Help ...



Reactants (5)

0.3333 CaO + 0.3333 SiO2 + 0.3333 Al2O3 + 0.01 Tl2O + 0.05 HfO2

Products

Compound species: ☐ gas ● ideal ○ real 18; ☐ aqueous 0; * ☐ pure liquids 1; * ☐ pure solids 1; ☑ suppress duplicates; * - custom selection; Species: 20

Solution species:

*	+	Base-Phase	Full Name
	+	FACT-SLAG	Slag-liquid

Custom Solutions: 0 fixed activities; 1 ideal solutions; 2 activity coefficients; Details ...

Pseudonyms: apply ☐ List ...

☐ include molar volumes

Total Species (max 692) 23

Total Solutions (max 30) 2

Default

Target: - none -; Estimate T(K): 1000; Mass(mol): 0

Legend: + - selected; ☑ Show ○ all ● selected; species: 3; solutions: 1; Clear

Final Conditions

<A>	<B>	T(C)	P(atm)	Product H(J)
		1000	1	

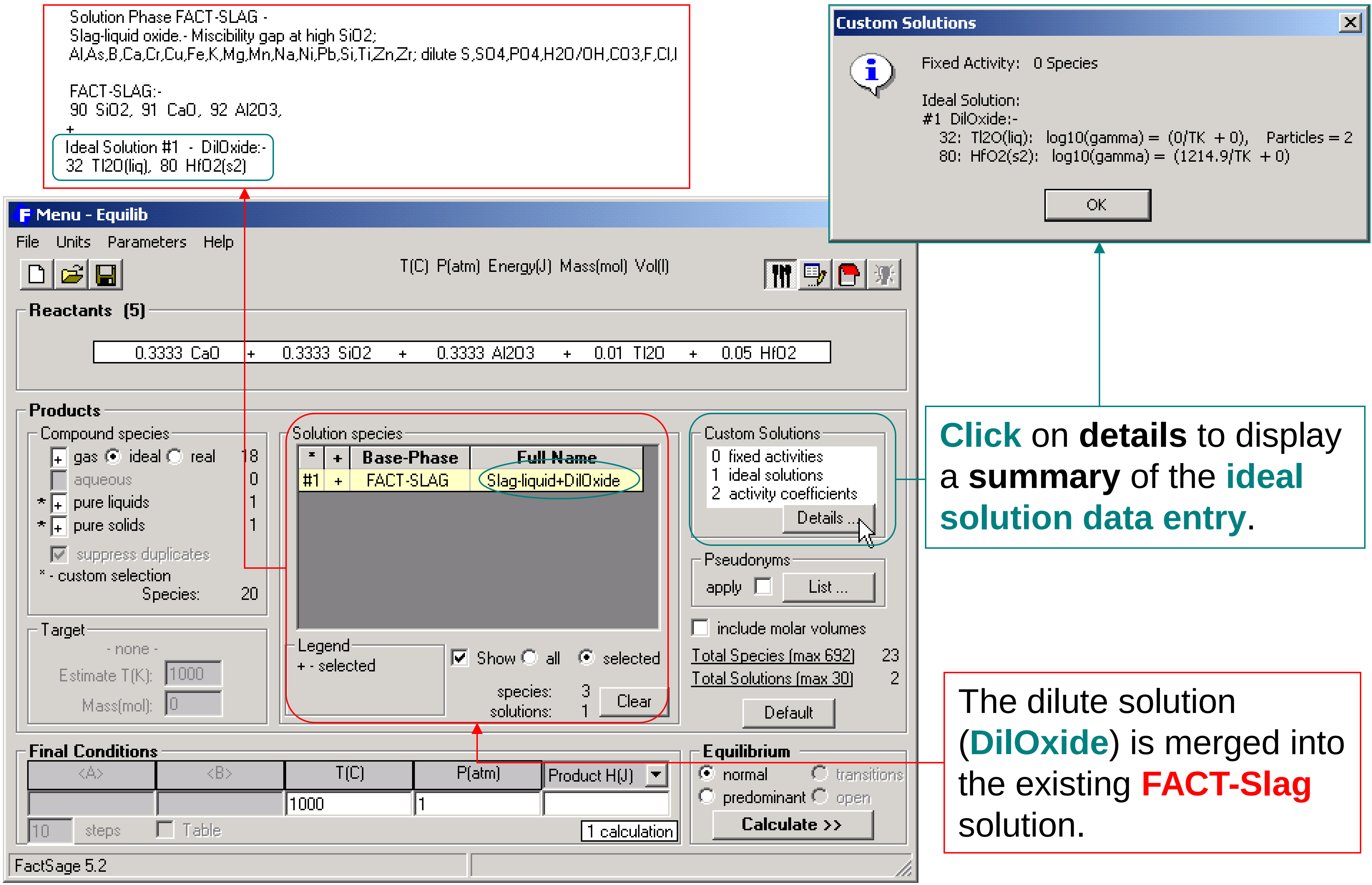
10 steps ☐ Table 1 calculation

Equilibrium: ● normal ○ transitions ○ predominant ○ open

Calculate >>

FactSage 5.2

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)

Custom Solutions

Fixed Activity: 0 Species

Ideal Solution:
#1 DilOxide:-
32: Tl2O(liq): log10(gamma) = (0/TK + 0), Particles = 2
80: HfO2(s2): log10(gamma) = (1214.9/TK + 0)

Menu - Equilib

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

Reactants (5)

0.3333 CaO + 0.3333 SiO2 + 0.3333 Al2O3 + 0.01 Tl2O + 0.05 HfO2

Products

Compound species
- ☒ gas ● ideal ○ real 18
- ☐ aqueous 0
- * ☒ pure liquids 1
- * ☒ pure solids 1
- ☑ suppress duplicates
- * - custom selection
- Species: 20

Target
- none -
Estimate T(K): 1000
Mass(mol): 0

Solution species

*	+	Base-Phase	Full Name
#1	+	FACT-SLAG	Slag-liquid+DilOxide

Legend
+ - selected

☑ Show ○ all ● selected
species: 3
solutions: 1

Custom Solutions
0 fixed activities
1 ideal solutions
2 activity coefficients

Pseudonyms
apply ☐

☐ include molar volumes

Total Species (max 692) 23
Total Solutions (max 30) 2

Final Conditions

<A>	<B>	T(C)	P(atm)	Product H(J)
		1000	1	

10 steps ☐ Table 1 calculation

Equilibrium
● normal ○ transitions
○ predominant ○ open

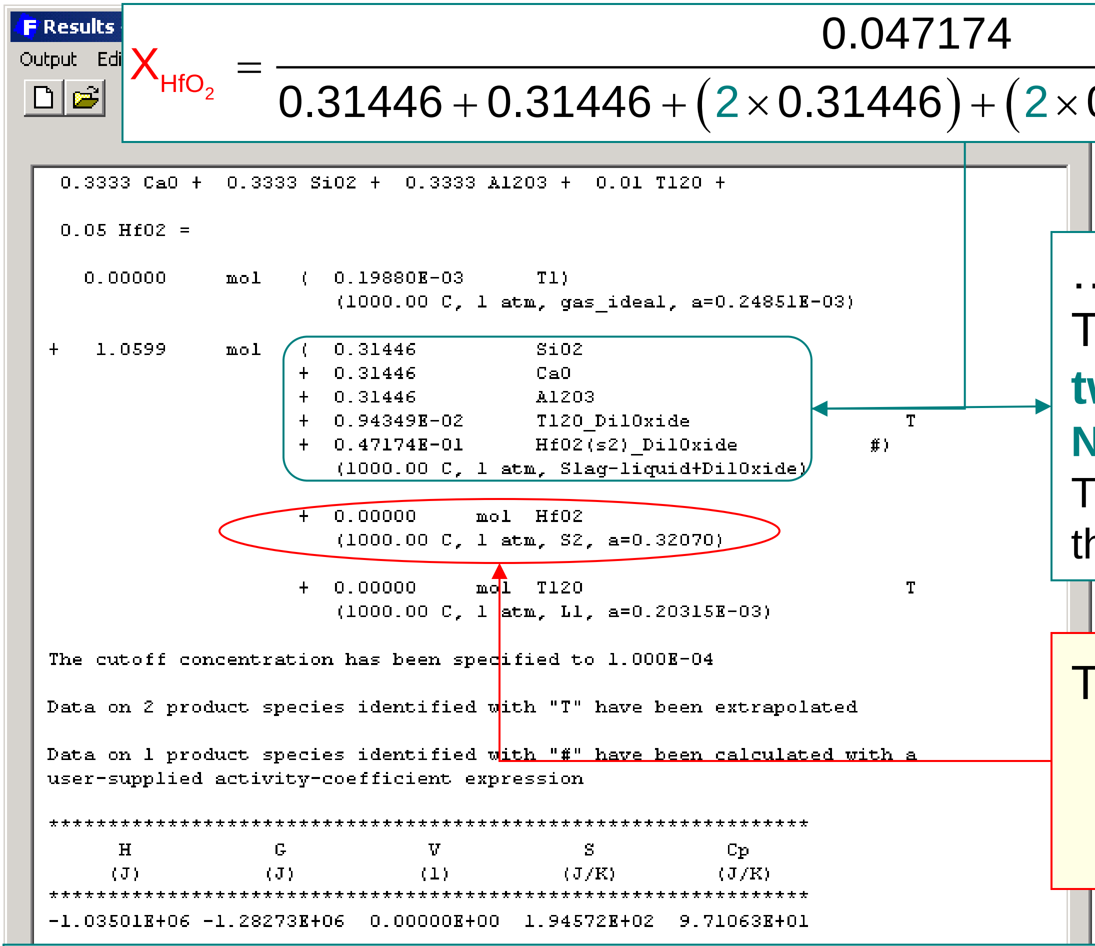
FactSage 5.2

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-SiO_2-Al_2O_3 slag: **Results** (***FACT*** format)

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



```
 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: $\mathbf{Al_2O_3 \rightarrow 2\ Al^{3+} + 3\ O^{2-}}$

Note:

This information about Al_2O_3 is included in the FACT-SLAG database.

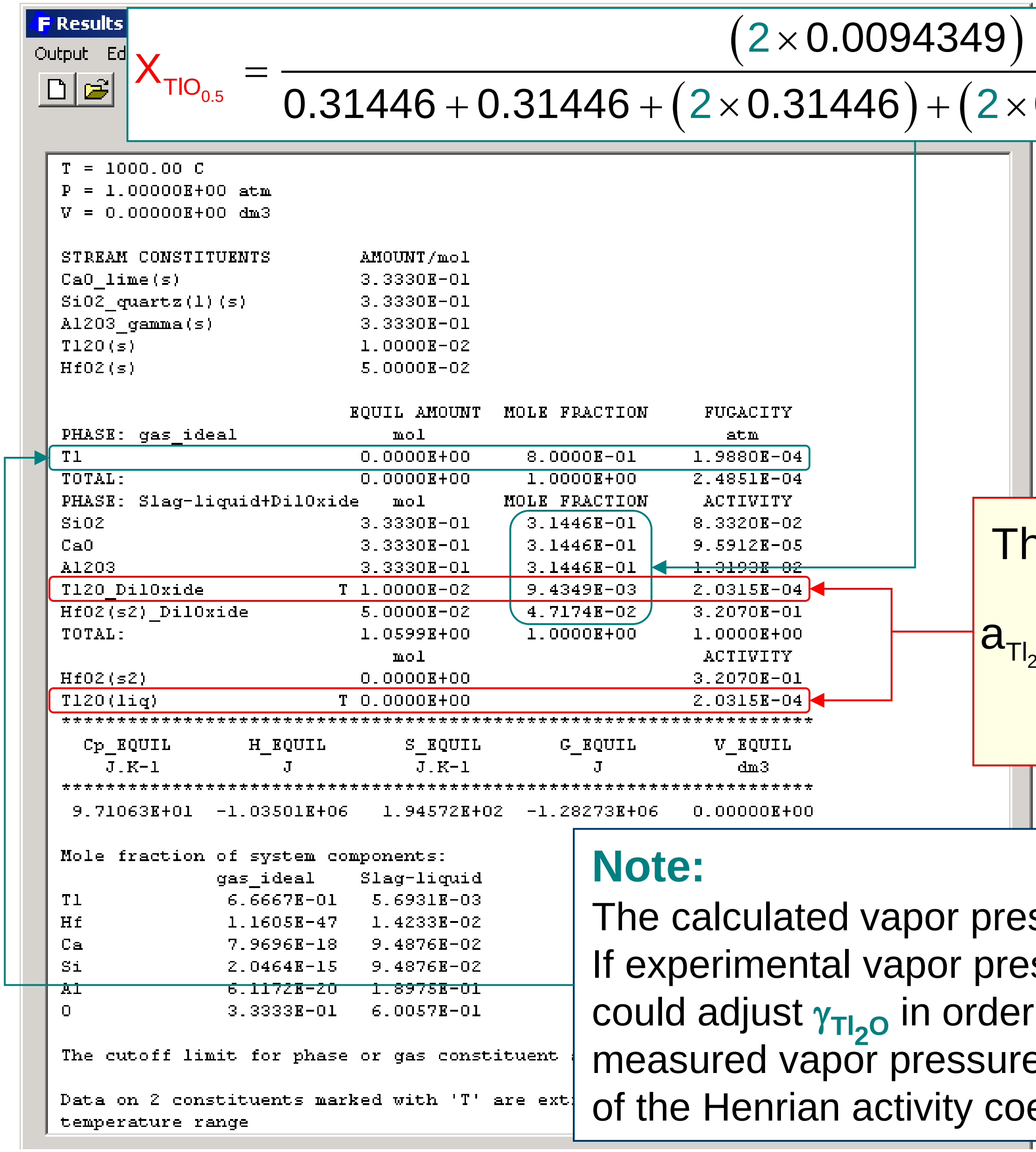
The calculated **activity** of HfO_2(s2) is:

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

Note:

If we increase γ_{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 γ_{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)



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

```
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 × 10^{-4} atm. If experimental vapor pressure data were available, then one could adjust γ_{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.

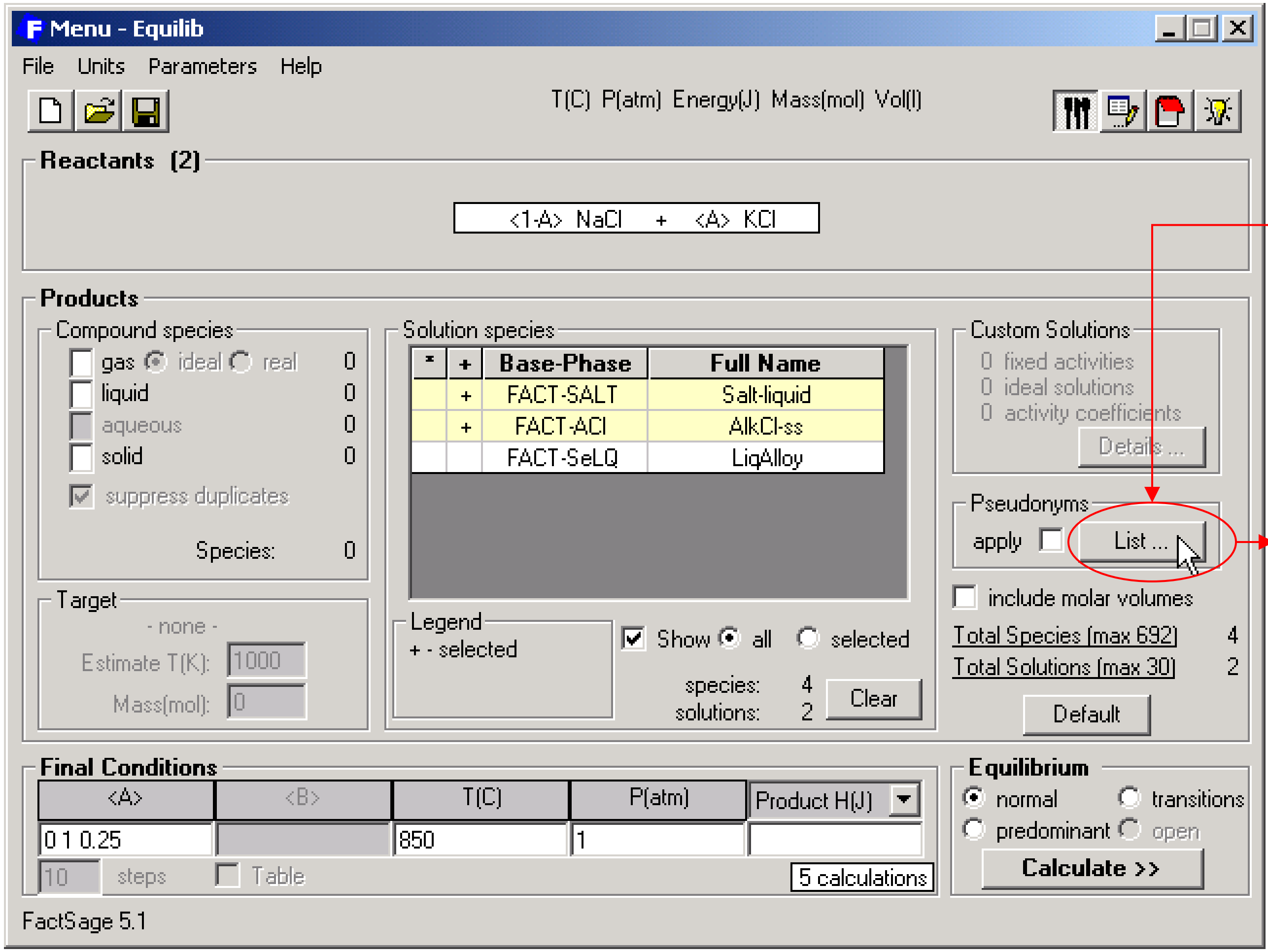
Using Pseudonyms

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-A> NaCl + <A> KCl

*	+	Base-Phase	Full Name
	+	FACT-SALT	Salt-liquid
	+	FACT-ACl	AlkCl-ss
		FACT-SeLQ	LiqAlloy

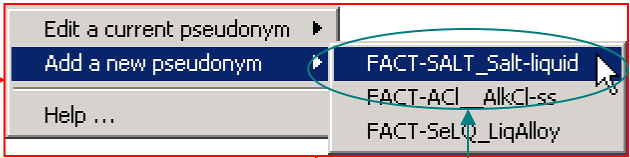
species: 4
solutions: 2

Total Species (max 692) 4
Total Solutions (max 30) 2

<A>	<B>	T(C)	P(atm)	Product H(J)
0.1 0.25		850	1	

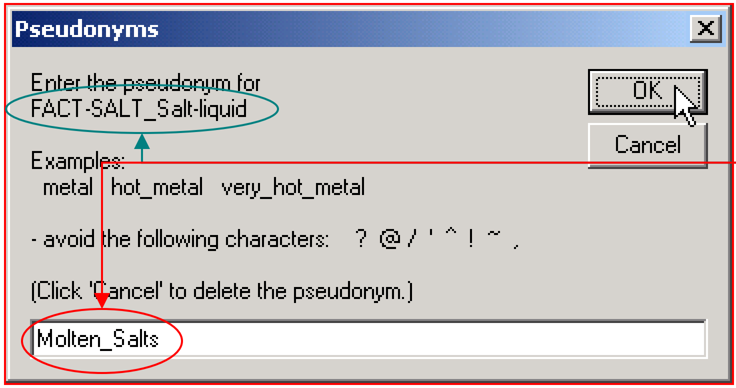
10 steps ☐ Table 5 calculations

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



Pseudonyms

Enter the pseudonym for
FACT-SALT_Salt-liquid

Examples:
metal hot_metal very_hot_metal

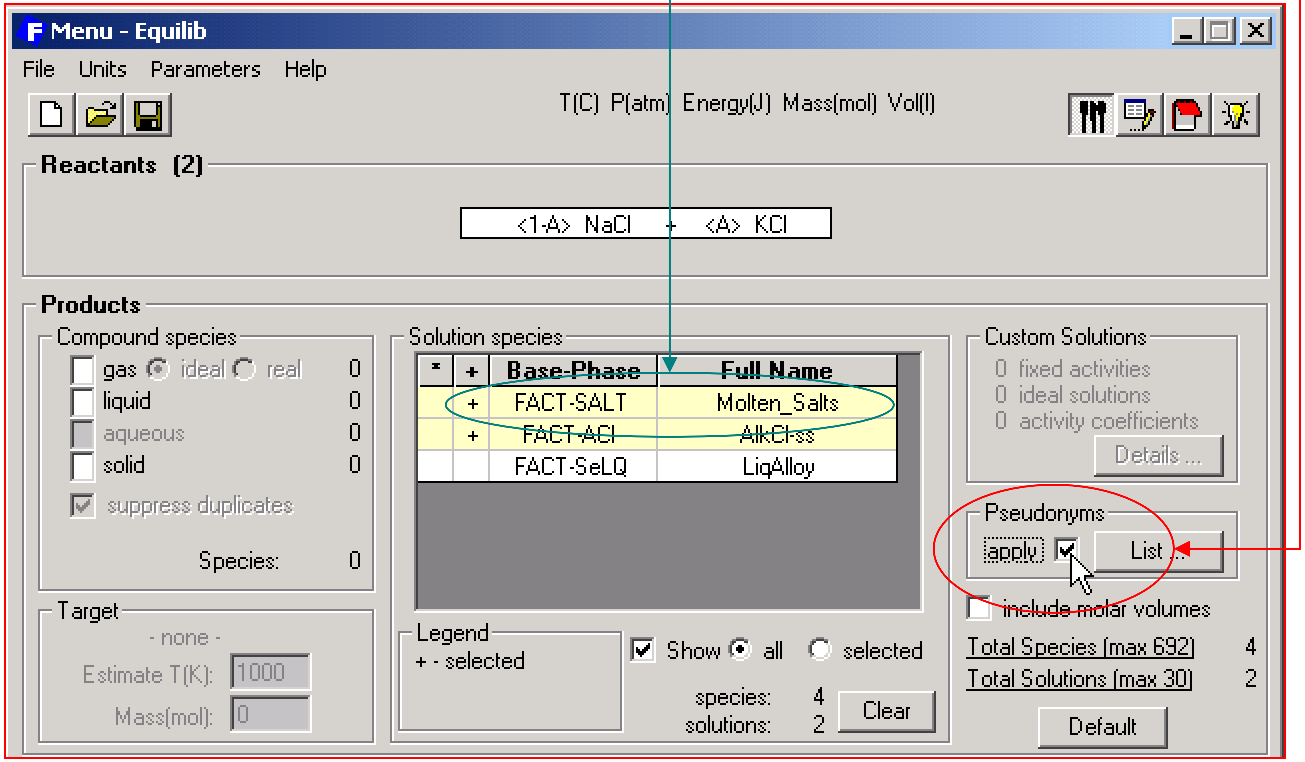
- avoid the following characters: ? @ / ' ^ ! ~ ,

(Click 'Cancel' to delete the pseudonym.)

Molten_Salts

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**.



Menu - Equilib

Reactants (2)

<1-A> NaCl + <A> KCl

Products

Compound species

- ☐ gas ● ideal ○ real 0
- ☐ liquid 0
- ☐ aqueous 0
- ☐ solid 0
- ☑ suppress duplicates

Species: 0

Solution species

*	+	Base-Phase	Full Name
	+	FACT-SALT	Molten_Salts
	+	FACT-ACl	AlkCl-ss
		FACT-SeLQ	LiqAlloy

Custom Solutions

0 fixed activities
0 ideal solutions
0 activity coefficients

Pseudonyms

apply ☑

☐ include molar volumes

Total Species (max 692) 4
Total Solutions (max 30) 2

Target

- none -
Estimate T(K): 1000
Mass(mol): 0

Legend
+ - selected

☑ Show ● all ○ selected

species: 4
solutions: 2

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.

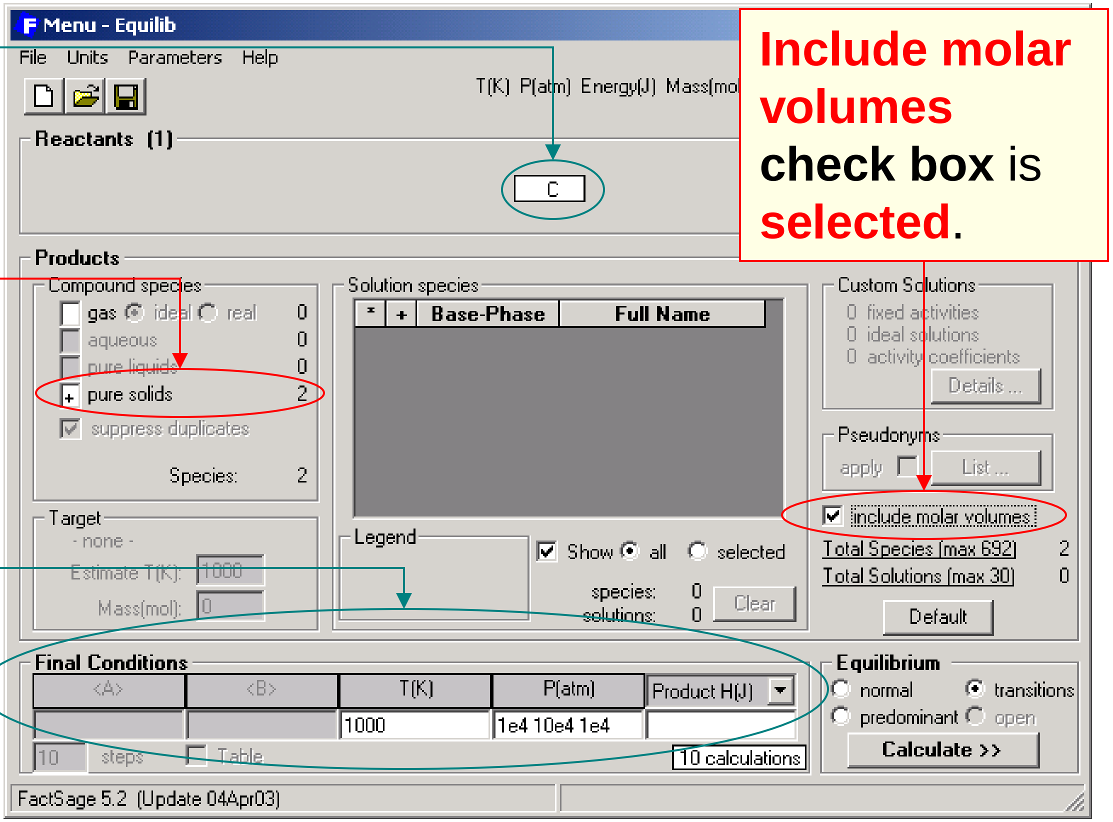
Include **molar volumes** : **graphite** to **diamond** transition

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) = **1×10^4 atm**, **2×10^4 atm**, …, **1×10^5 atm**



Reactants (1)
C

Products
Compound species
☐ gas ● ideal ○ real 0
☐ aqueous 0
☐ pure liquids 0
+ pure solids 2
☑ suppress duplicates
Species: 2

☑ include molar volumes
Total Species (max 692) 2
Total Solutions (max 30) 0

Final Conditions

T(K)	P(atm)
1000	1e4 10e4 1e4

10 calculations

Equilibrium
○ normal ● transitions
○ predominant ○ open

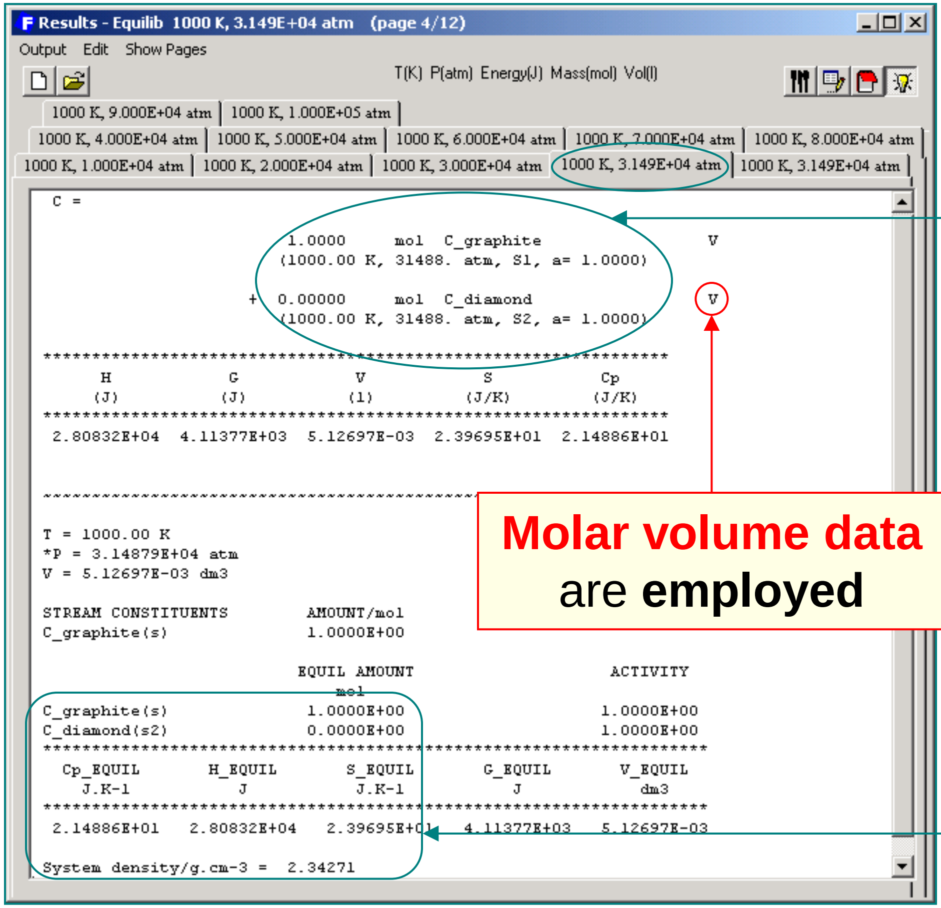
FactSage 5.2 (Update 04Apr03)

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

The program will calculate the equilibrium at **1000K** for pressures varying from **1×10^4 atm** to **1×10^5 atm** in increments of **1×10^4 atm** and will search for all phase **transitions**.

Graphite to **diamond** **transition**: equilibrium calculation

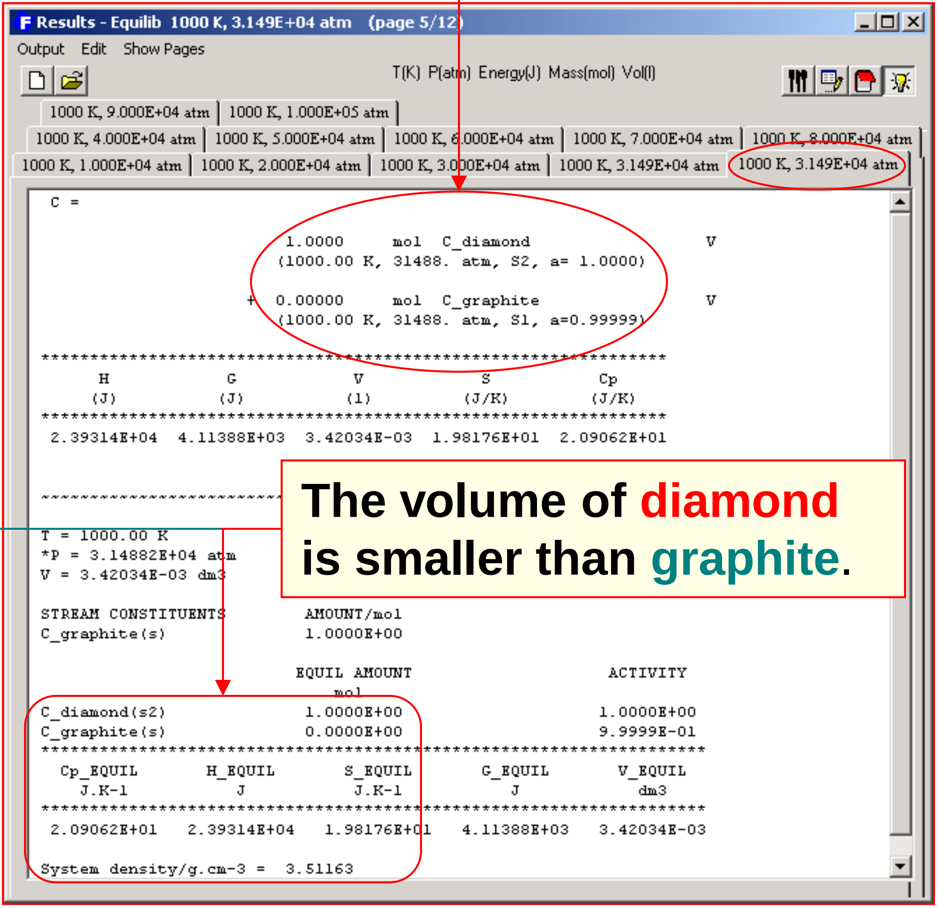
Note: If molar volumes are **not** included then **no** transitions are found.



```
 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
```

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

Molar volume data are **employed**



```
 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
```

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.

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.

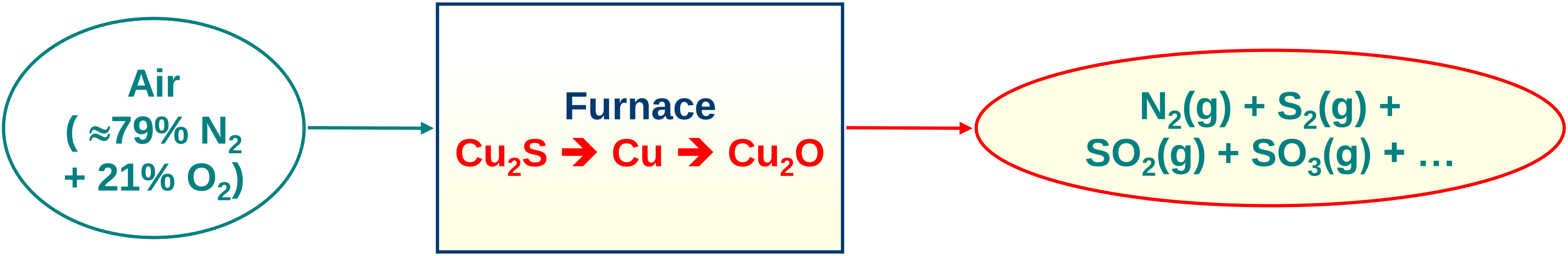
The following slide explains the general procedure in more detail. In sections 9.1 and 9.2 two example applications are shown.

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.



Air
(≈79% N_2 + 21% O_2)

Furnace
$Cu_2S \rightarrow Cu \rightarrow Cu_2O$

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

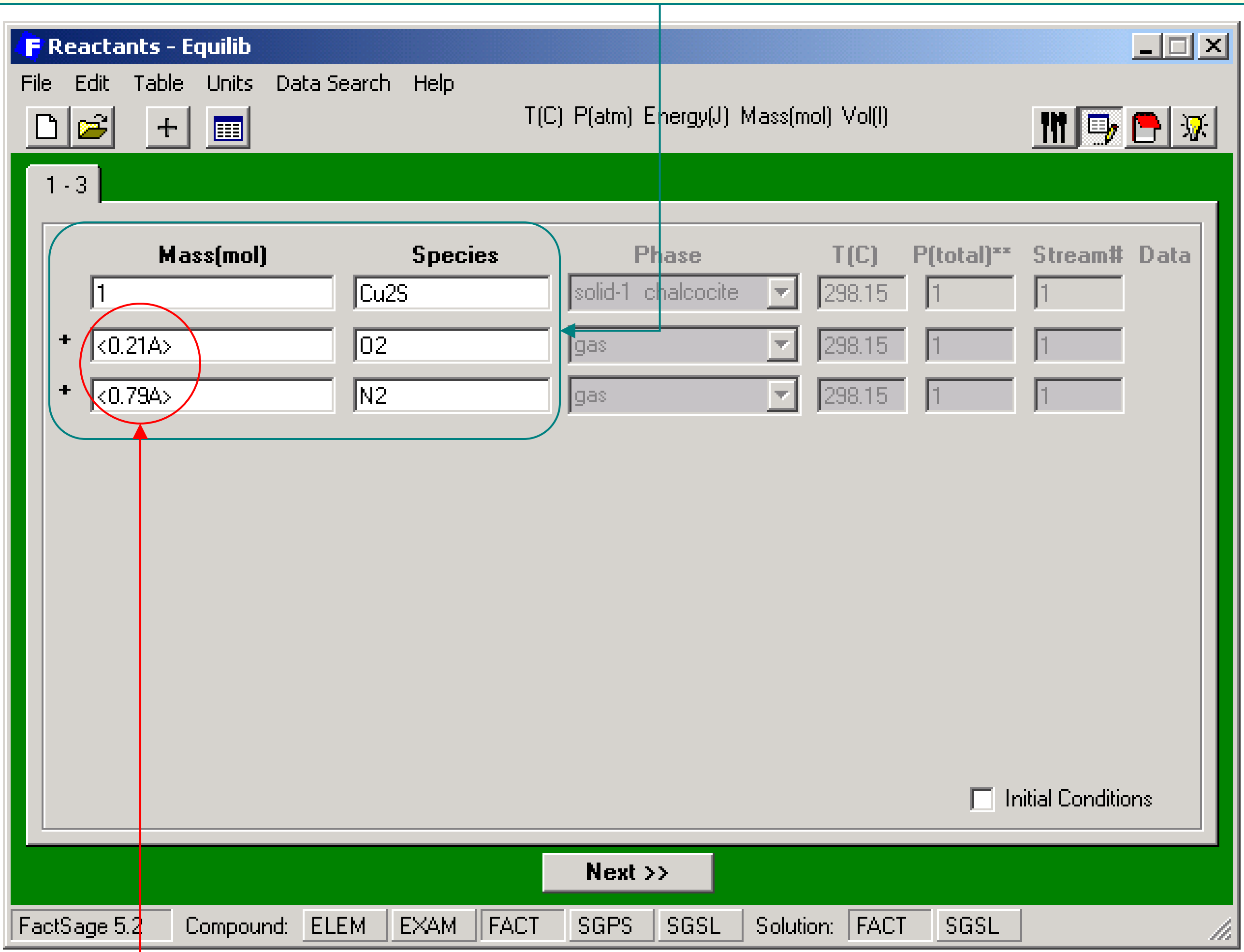
Desulphuring of Cu_2S

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**.



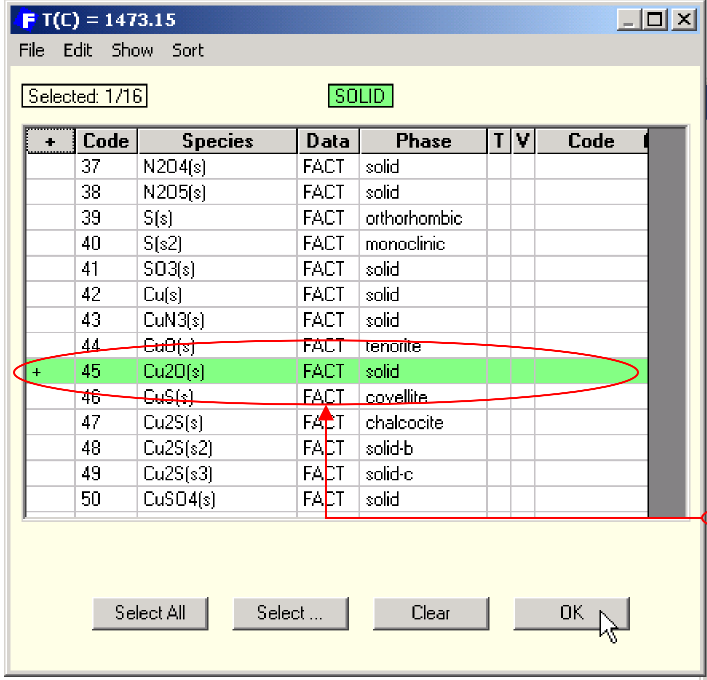
	Mass(mol)	Species
	1	Cu2S
+	<0.21A>	O2
+	<0.79A>	N2

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:

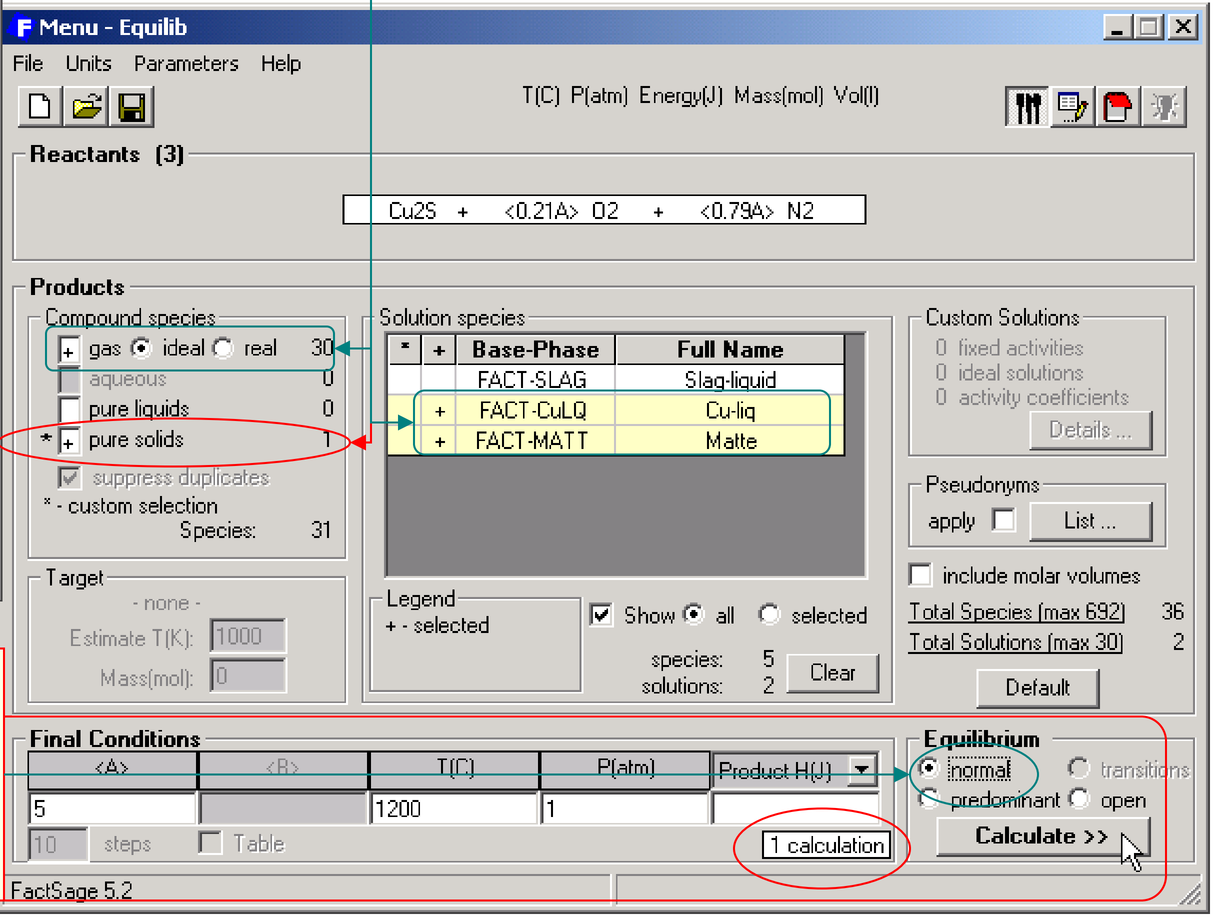
- **Solution species: FACT-CuLQ, FACT-MATT**
- **Compound species: ideal gas, $Cu_2O(s)$**



T(C) = 1473.15

Selected: 1/16 SOLID

+	Code	Species	Data	Phase	T	V	Code
	37	N2O4(s)	FACT	solid			
	38	N2O5(s)	FACT	solid			
	39	S(s)	FACT	orthorhombic			
	40	S(s2)	FACT	monoclinic			
	41	SO3(s)	FACT	solid			
	42	Cu(s)	FACT	solid			
	43	CuN3(s)	FACT	solid			
	44	~~CuO(s)~~	~~FACT~~	~~tenorite~~			
+	45	Cu2O(s)	FACT	solid			
	46	~~CuS(s)~~	~~FACT~~	~~covellite~~			
	47	Cu2S(s)	FACT	chalcocite			
	48	Cu2S(s2)	FACT	solid-b			
	49	Cu2S(s3)	FACT	solid-c			
	50	CuSO4(s)	FACT	solid			



Menu - Equilib

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

Reactants (3)

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

Products

Compound species

☐+ gas ● ideal ○ real 30
☐ aqueous 0
☐ pure liquids 0
* ☐+ pure solids 1
☑ suppress duplicates
* - custom selection
Species: 31

Solution species

*	+	Base-Phase	Full Name
		FACT-SLAG	Slag-liquid
	+	FACT-CuLQ	Cu-liq
	+	FACT-MATT	Matte

Legend
+ - selected

☑ Show ● all ○ selected
species: 5
solutions: 2

Custom Solutions
0 fixed activities
0 ideal solutions
0 activity coefficients

Pseudonyms
apply ☐

☐ include molar volumes
Total Species (max 692) 36
Total Solutions (max 30) 2

Target
- none -
Estimate T(K): 1000
Mass(mol): 0

Final Conditions

<A>	<B>	T(C)	P(atm)	Product H(J)
5		1200	1	

10 steps ☐ Table 1 calculation

Equilibrium

● normal ○ transitions
○ predominant ○ open

FactSage 5.2

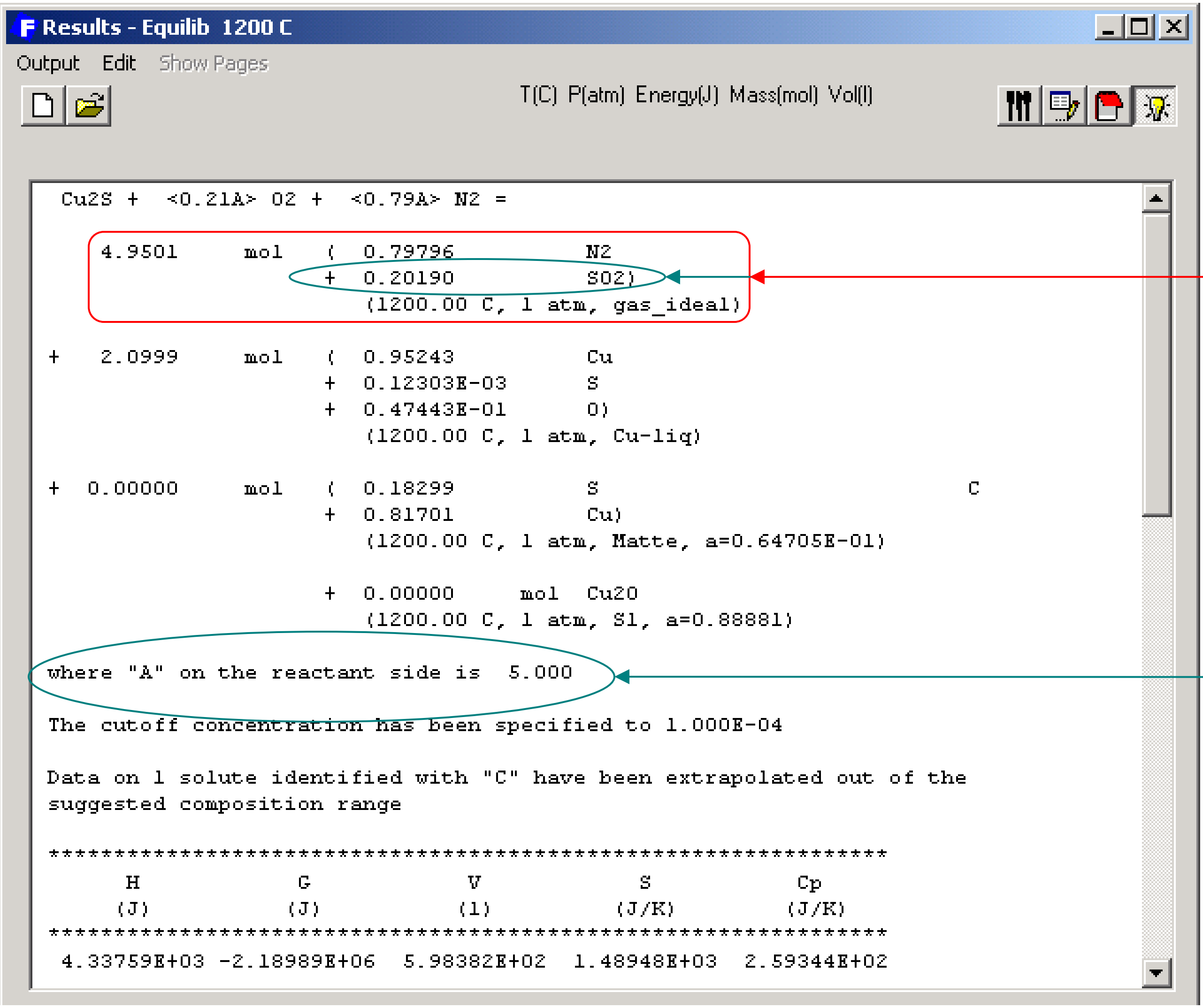
Setting the final conditions for a **normal** (i.e. **closed** system) equilibrium calculation at **1200°C** and **1 atm** for **<A> = 5**

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 ➔ Cu ➔ Cu_2O



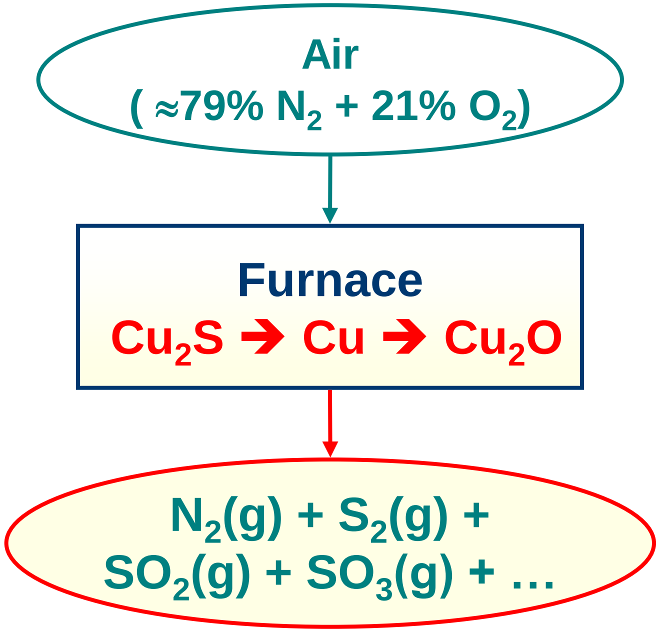
```
 Cu2S +  <0.21A> O2 +  <0.79A> N2 =

   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, S1, 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

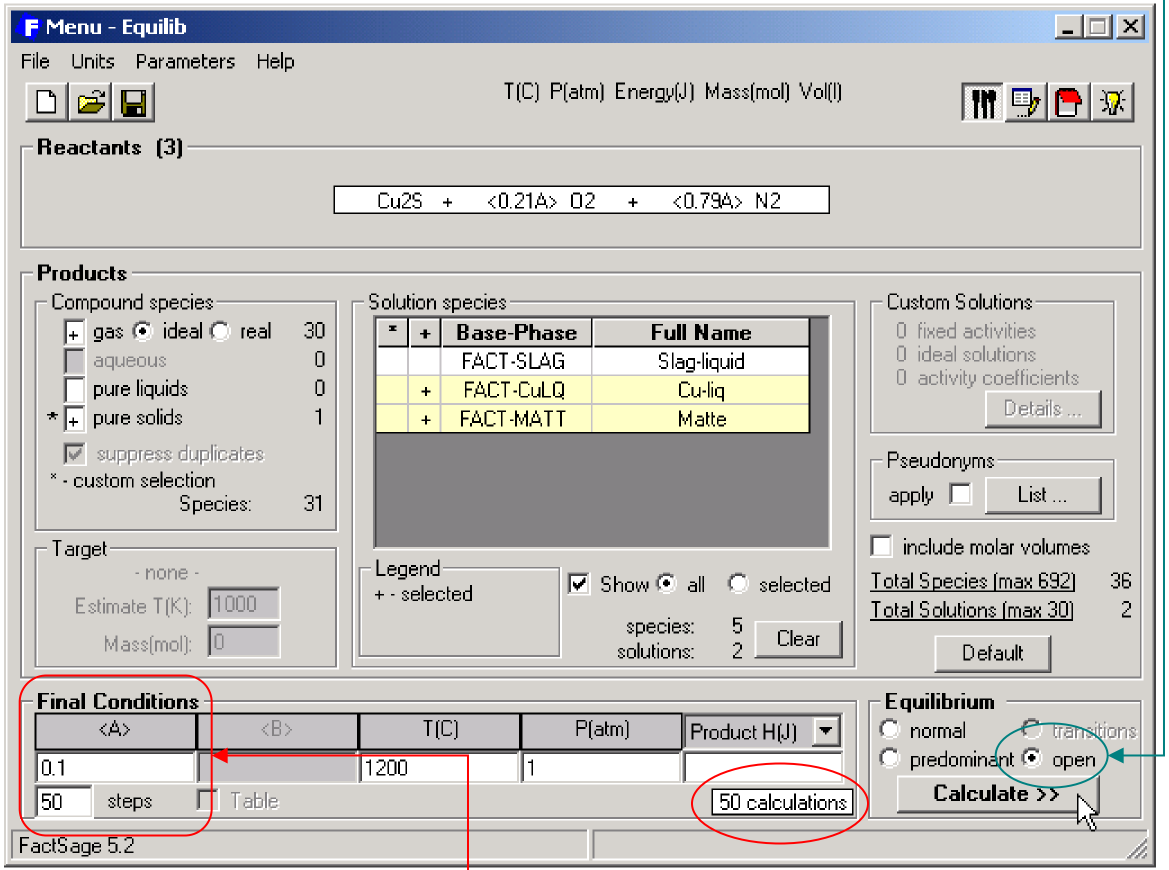
(≈79% N_2 + 21% O_2)

Furnace

Cu_2S → Cu → Cu_2O

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

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



Reactants (3)

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

Products

Compound species

- ☒ gas ● ideal ○ real 30
- ☐ aqueous 0
- ☐ pure liquids 0
- * ☒ pure solids 1
- ☑ suppress duplicates
- * - custom selection
- Species: 31

Solution species

*	+	Base-Phase	Full Name
		FACT-SLAG	Slag-liquid
	+	FACT-CuLQ	Cu-liq
	+	FACT-MATT	Matte

Legend: + - selected

☑ Show ● all ○ selected

species: 5
solutions: 2

Custom Solutions

- 0 fixed activities
- 0 ideal solutions
- 0 activity coefficients

Pseudonyms: apply ☐

☐ include molar volumes

Total Species (max 692) 36

Total Solutions (max 30) 2

Target: - none -

Estimate T(K): 1000

Mass(mol): 0

Final Conditions

<A>	<B>	T(C)	P(atm)	Product H(J)
0.1		1200	1	

50 steps ☐ Table

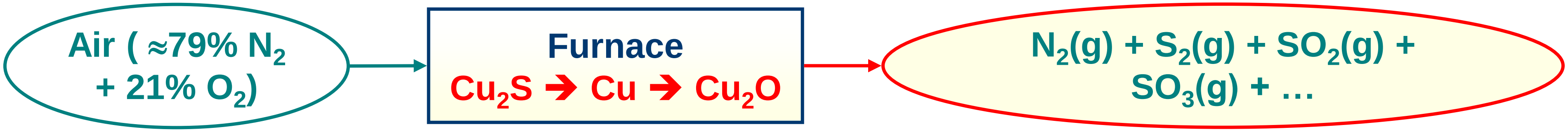
50 calculations

Equilibrium

○ normal ○ transitions
○ predominant ● open

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

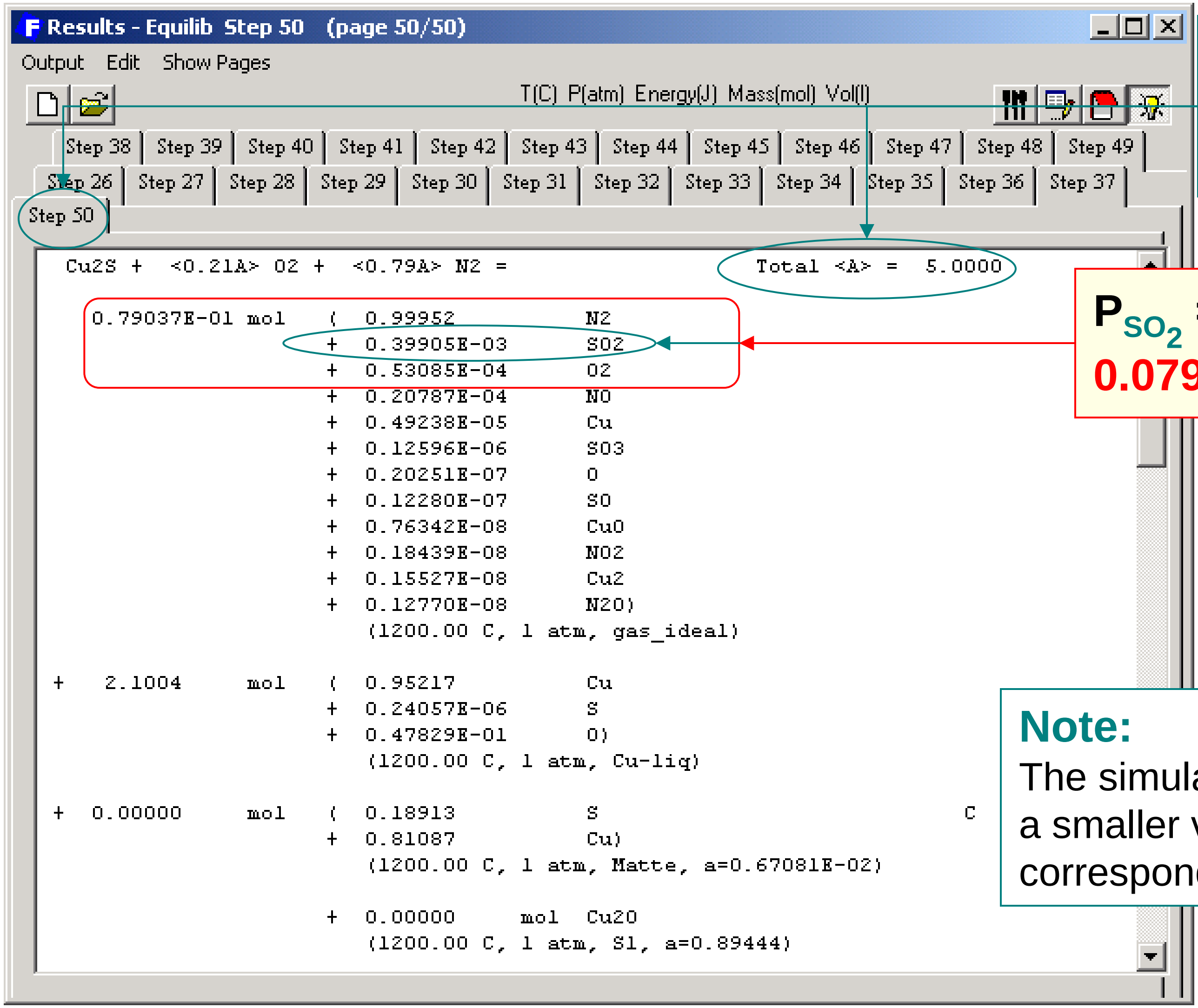


Air (≈79% N_2 + 21% O_2)

Furnace

$Cu_2S \rightarrow Cu \rightarrow Cu_2O$

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



```
 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, S1, a=0.89444)
```

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

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

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.

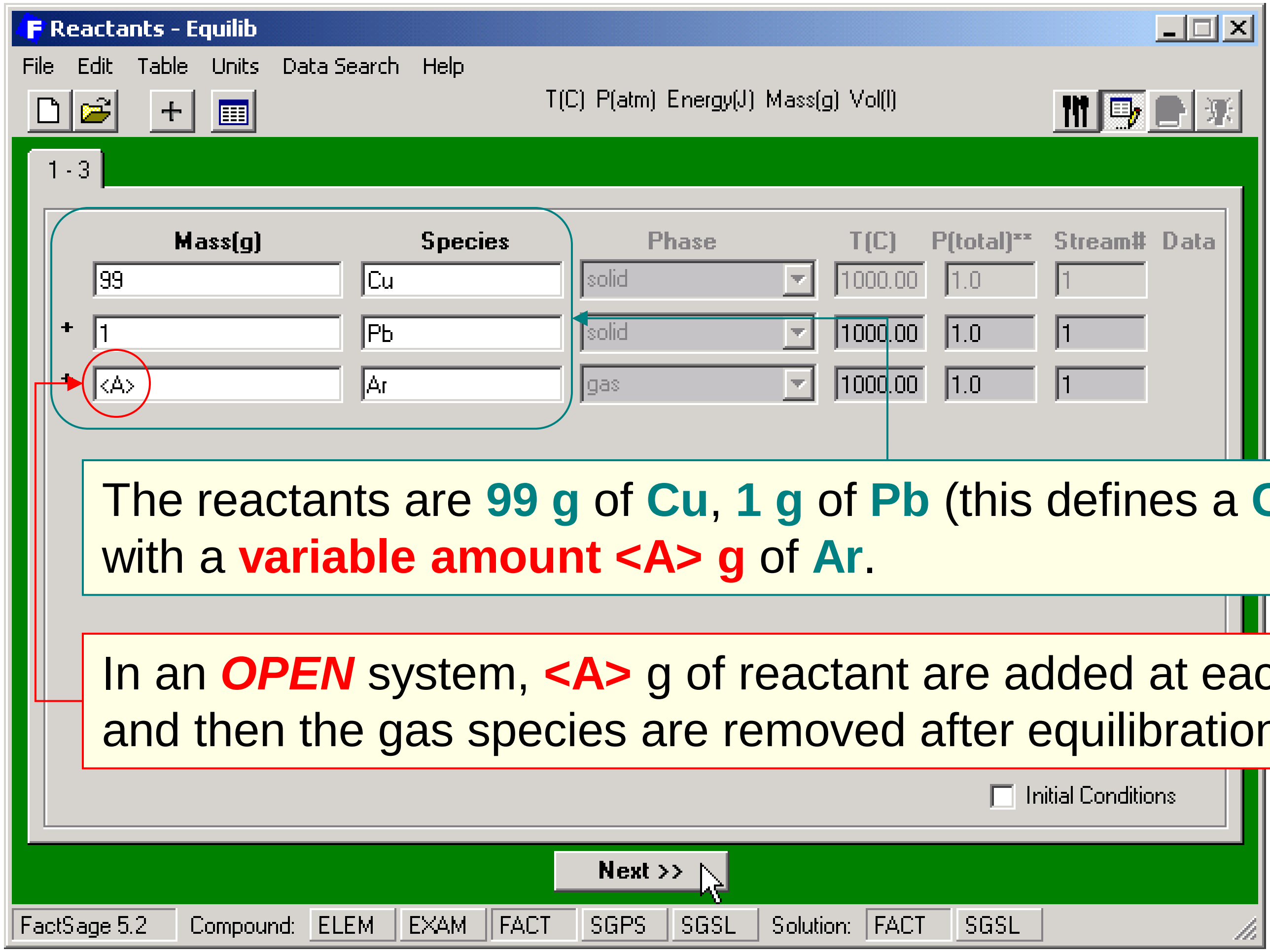
The following six slides show how the Open command can be employed to simulate the process.

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.



	Mass(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
	99	Cu	solid	1000.00	1.0	1	
+	1	Pb	solid	1000.00	1.0	1	
+	<A>	Ar	gas	1000.00	1.0	1	

☐ Initial Conditions

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**.

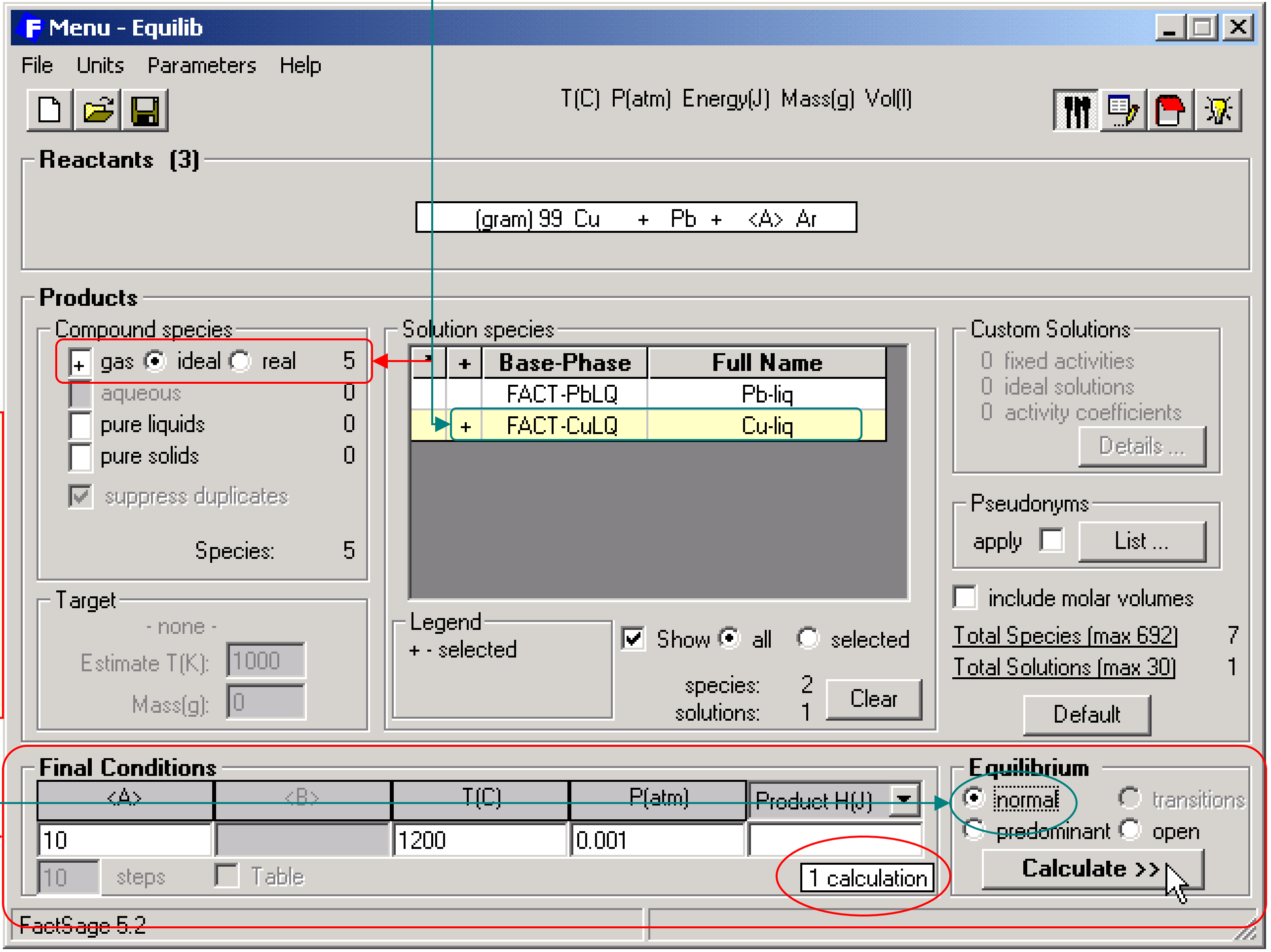
In an ***OPEN*** system, **<A>** g of reactant are added at each step and then the gas species are removed after equilibration.

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**



Menu - Equilib

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

Reactants (3)

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

Products

Compound species

☐ +	gas ● ideal ○ real	5
☐	aqueous	0
☐	pure liquids	0
☐	pure solids	0
☑	suppress duplicates	
	Species:	5

Solution species

+	Base-Phase	Full Name
	FACT-PbLQ	Pb-liq
+	FACT-CuLQ	Cu-liq

Legend: + - selected

☑ Show ● all ○ selected

species: 2

solutions: 1

Custom Solutions: 0 fixed activities, 0 ideal solutions, 0 activity coefficients

Pseudonyms: apply ☐

☐ include molar volumes

Total Species (max 692) 7

Total Solutions (max 30) 1

Target: - none -; Estimate T(K): 1000; Mass(g): 0

Final Conditions

<A>	<B>	T(C)	P(atm)	Product H(J)
10		1200	0.001	

10 steps ☐ Table

1 calculation

Equilibrium

● normal ○ transitions

○ predominant ○ open

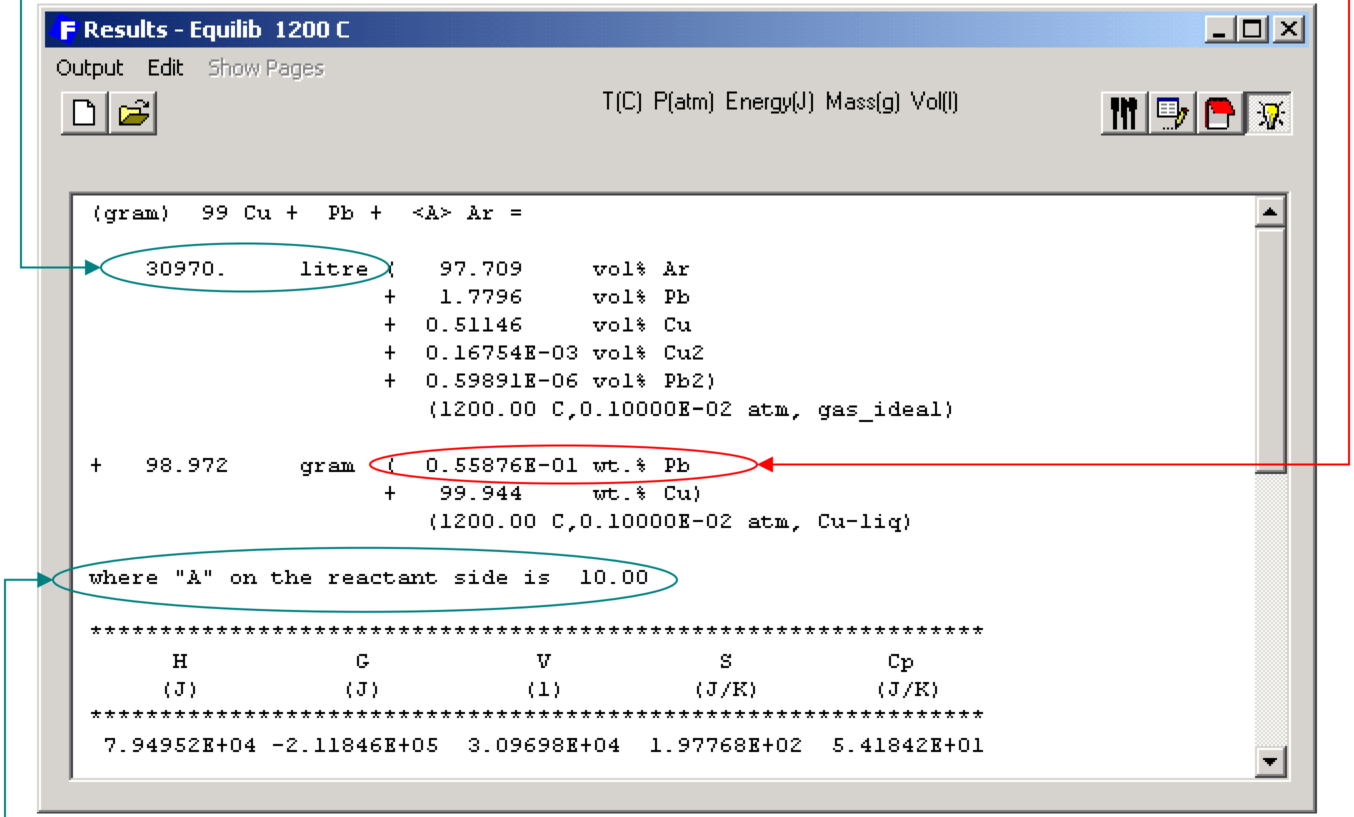
Calculate >>

FactSage 5.2

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

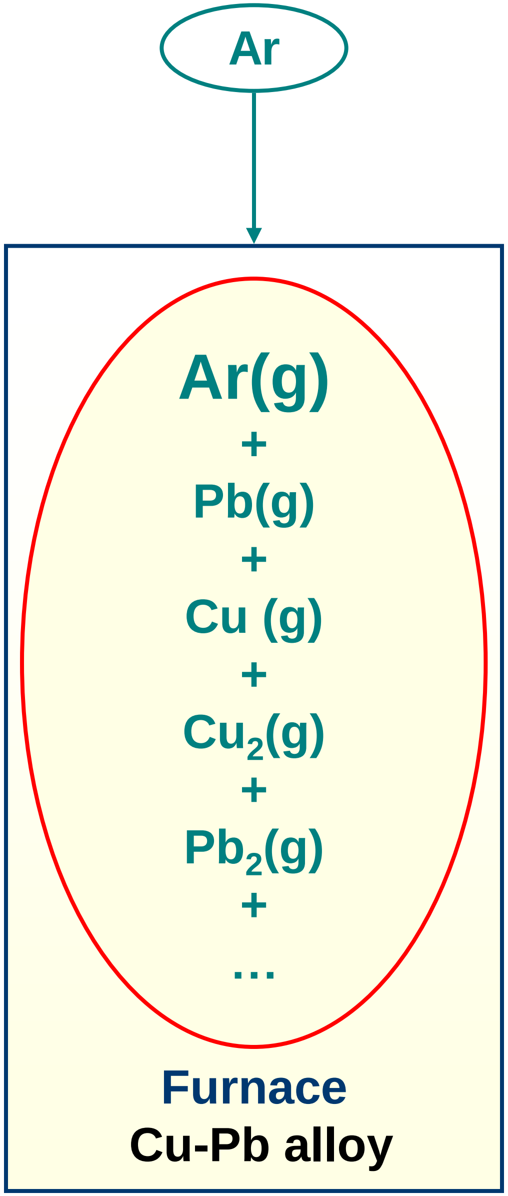
The **concentration** of **Pb** in **Cu(liq)** is **5.5876 × 10^{-2} wt.%**

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



```
(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**.



Ar

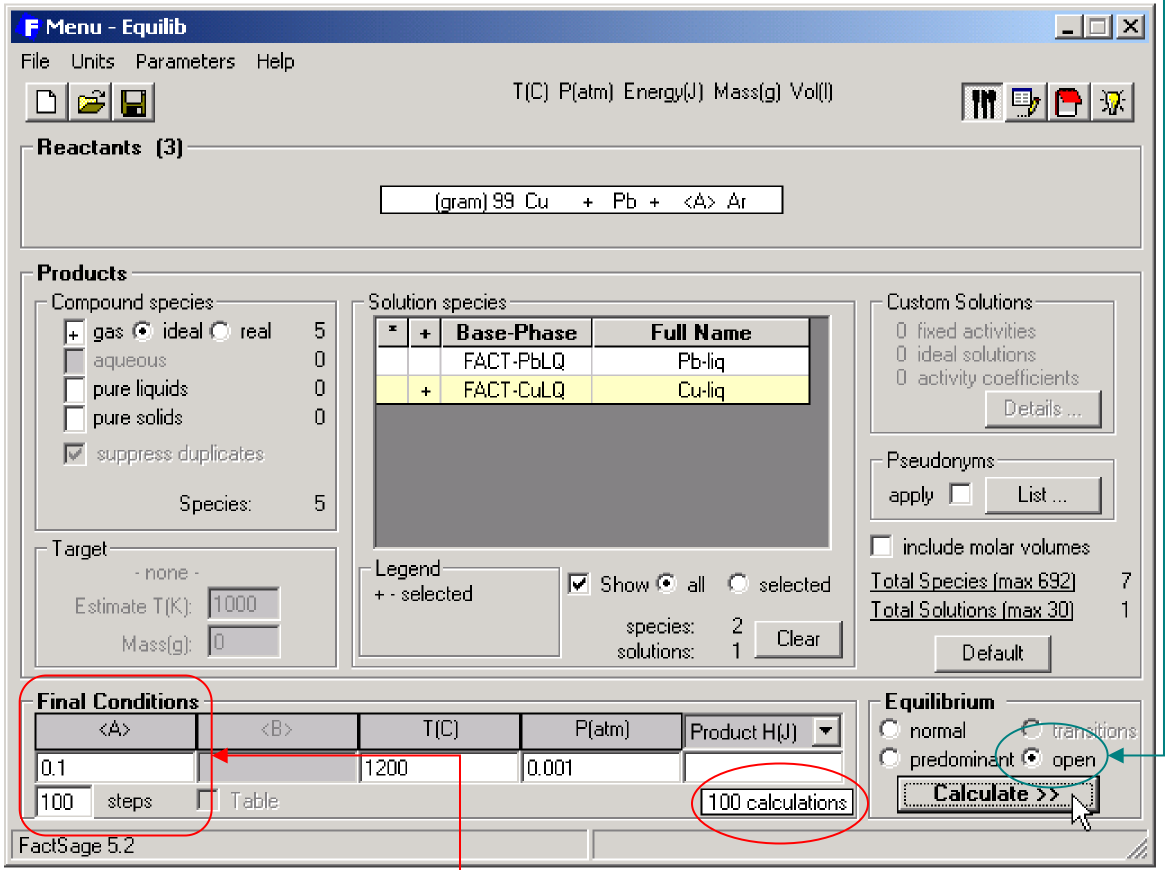
$Ar(g)$
+
$Pb(g)$
+
$Cu(g)$
+
$Cu_2(g)$
+
$Pb_2(g)$
+
…

Furnace
Cu-Pb 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



Reactants (3)

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

Compound species

- ☑ gas ● ideal ○ real 5
- ☐ aqueous 0
- ☐ pure liquids 0
- ☐ pure solids 0
- ☑ suppress duplicates

Species: 5

Solution species

*	+	Base-Phase	Full Name
		FACT-PbLQ	Pb-liq
	+	FACT-CuLQ	Cu-liq

Final Conditions

<A>	<B>	T(C)	P(atm)	Product H(J)
0.1		1200	0.001	

100 steps ☐ Table — 100 calculations

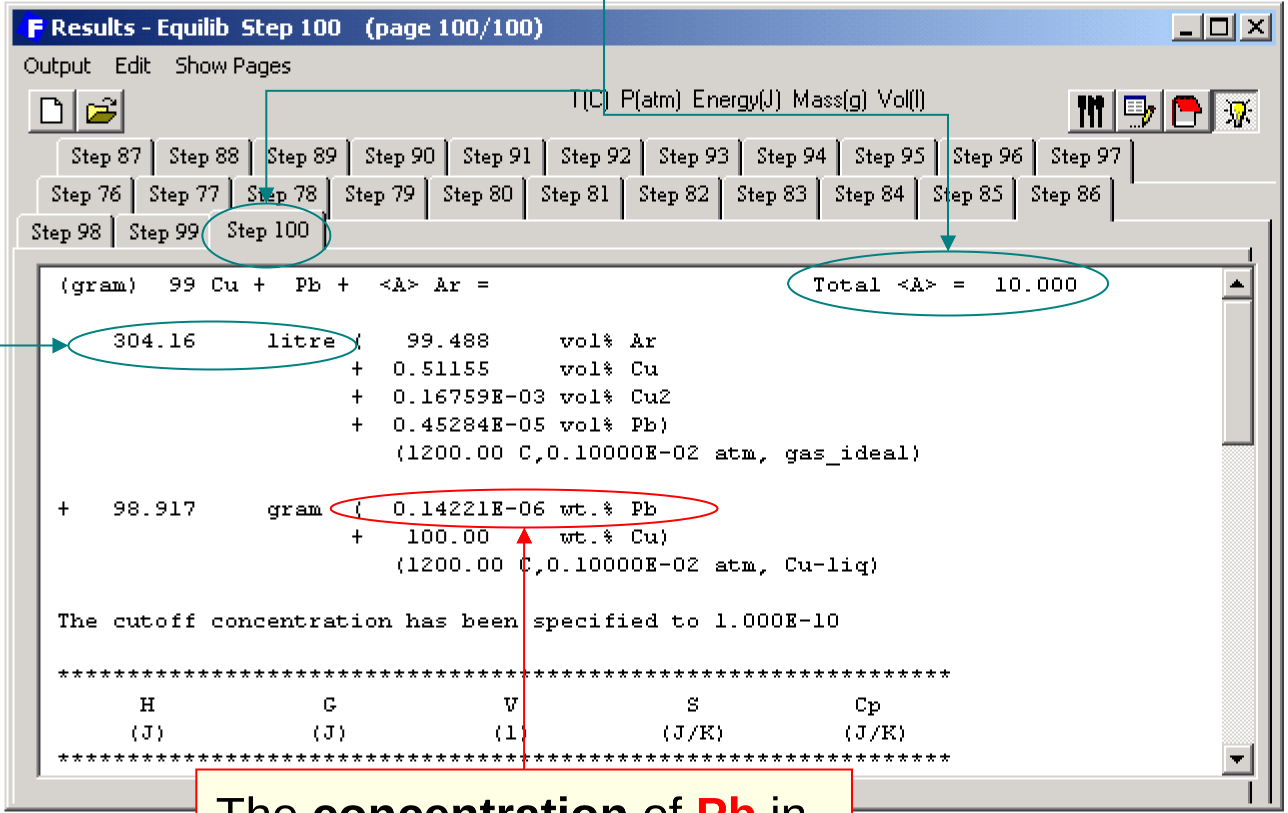
Equilibrium

○ normal ○ transitions ○ predominant ● open

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

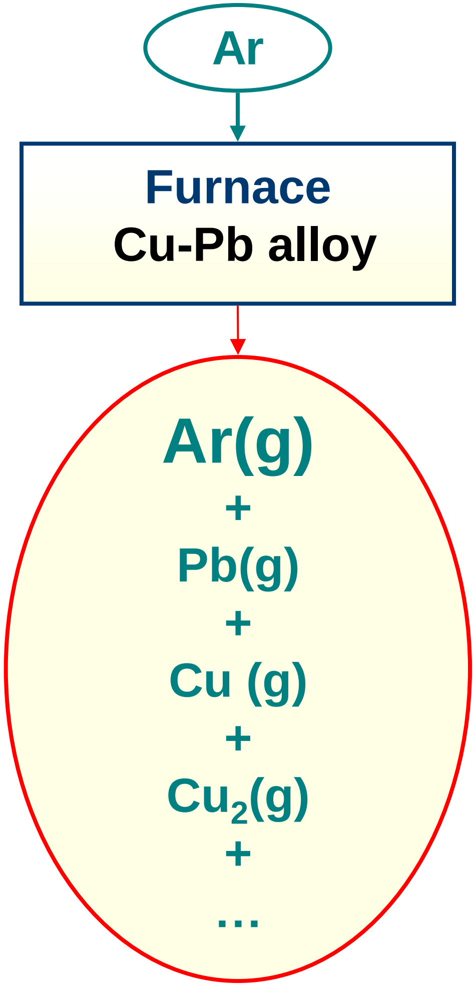
After 100 steps, A = **10.0**, i.e. **10** grams of **Ar** were added to **100** grams of **Cu-Pb alloy**



```
 (gram)   99 Cu +   Pb +   <A> Ar =                       Total <A> =   10.000

     304.16       litre (    99.488      vol% Ar
                        +  0.51155      vol% Cu
                        +  0.16759E-03 vol% Cu2
                        +  0.45284E-05 vol% Pb)
                         (1200.00 C,0.10000E-02 atm, gas_ideal)

 +   98.917       gram  (  0.14221E-06 wt.% Pb
                        +    100.00      wt.% Cu)
                         (1200.00 C,0.10000E-02 atm, Cu-liq)

 The cutoff concentration has been specified to 1.000E-10

 *****************************************************************
      H             G             V             S             Cp
     (J)           (J)           (l)          (J/K)         (J/K)
 *****************************************************************
```

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

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



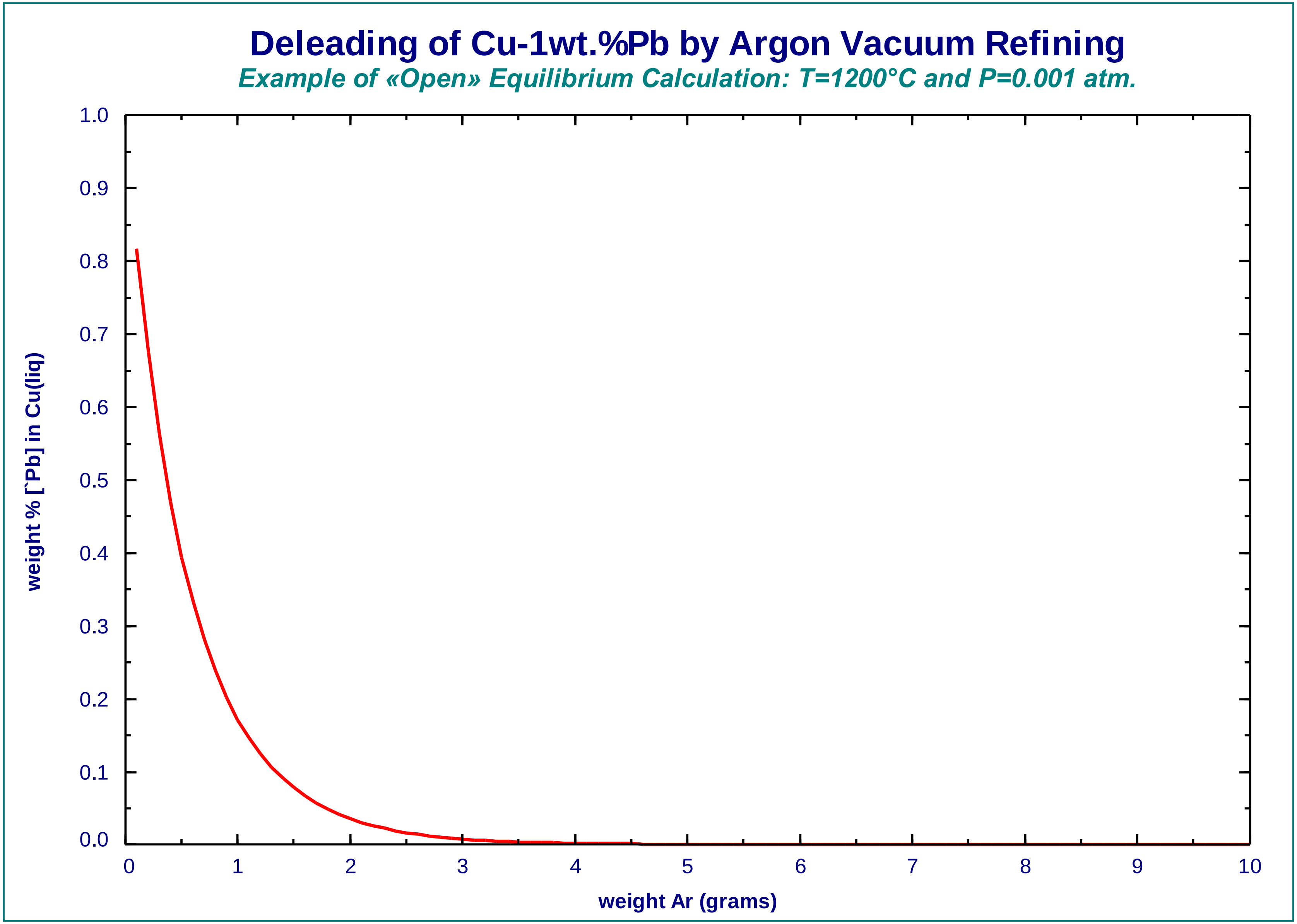
Ar

Furnace
Cu-Pb alloy

Ar(g)
+
Pb(g)
+
Cu (g)
+
Cu_2(g)
+
…

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



Equilib Advanced 9.2.6

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

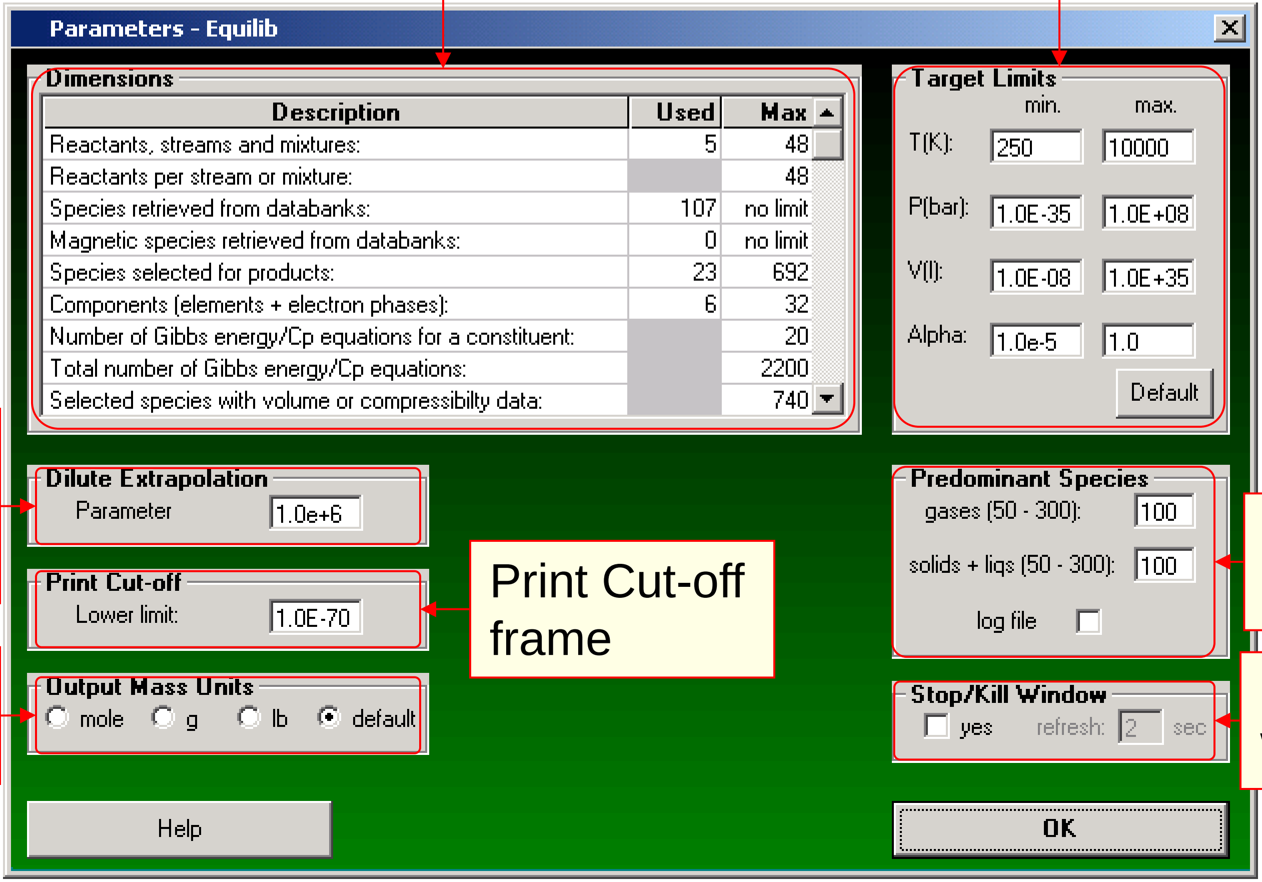
Dilute extrapolation frame

Output Mass Units frame

Print Cut-off frame

Predominant Species frame

Stop/Kill Window frame



Parameters - Equilib

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

Target Limits

	min.	max.
T(K):	250	10000
P(bar):	1.0E-35	1.0E+08
V(l):	1.0E-08	1.0E+35
Alpha:	1.0e-5	1.0

Dilute Extrapolation

Parameter 1.0e+6

Print Cut-off

Lower limit: 1.0E-70

Output Mass Units

○ mole ○ g ○ lb ● default

Predominant Species

gases (50 - 300): 100

solids + liqs (50 - 300): 100

log file ☐

Stop/Kill Window

☐ yes refresh: 2 sec

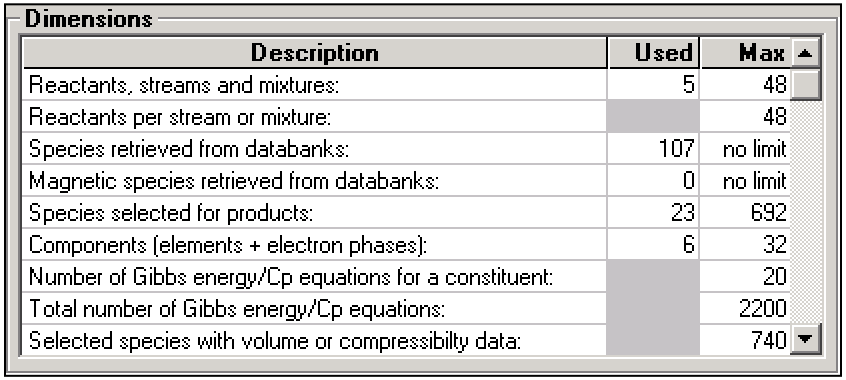
Help

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.



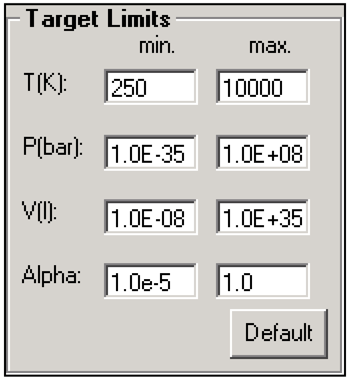
Dimensions

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

	min.	max.
T(K):	250	10000
P(bar):	1.0E-35	1.0E+08
V(l):	1.0E-08	1.0E+35
Alpha:	1.0e-5	1.0

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/Kill Window

☐ yes refresh: 2 sec

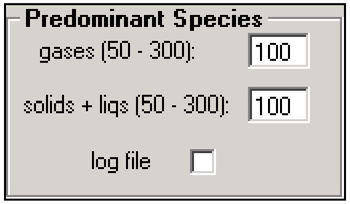
Stop and Kill Button

- 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

gases (50 - 300): 100

solids + liqs (50 - 300): 100

log file ☐

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.

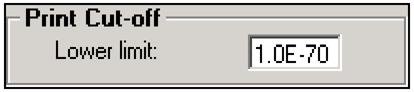
Parameters menu: Dilute Extrapolation-Print Cut-off-Output Mass Units Frames

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

Dilute Extrapolation

Parameter 1.0e+6

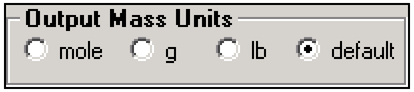
- This value is used for extrapolating solute data outside its normal dilute concentration range stored in its solution database.
- The parameter is an advanced feature of the program and should not be modified from its default value (1.0e+6).



Print Cut-off

Lower limit: 1.0E-70

- 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.



Output Mass Units

○ mole ○ g ○ lb ● default

- 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.

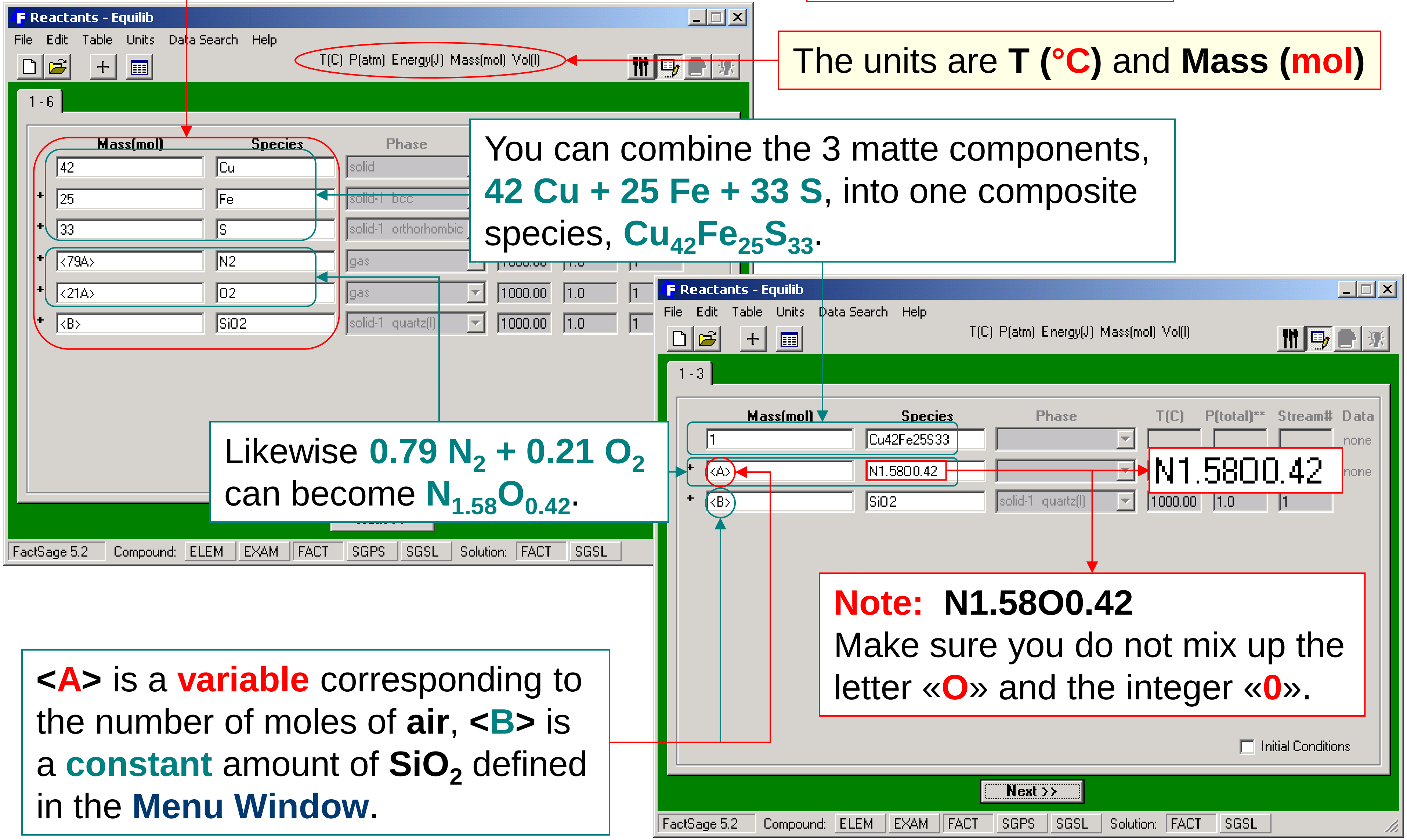
Reactants screen options

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



	Mass(mol)	Species	Phase			
	42	Cu	solid			
+	25	Fe	solid-1 bcc			
+	33	S	solid-1 orthorhombic			
+	<79A>	N2	gas	1000.00	1.0	1
+	<21A>	O2	gas	1000.00	1.0	1
+	<B>	SiO2	solid-1 quartz(l)	1000.00	1.0	1

	Mass(mol)	Species	Phase	T(C)	P(total)**	Stream#	Data
	1	Cu42Fe25S33					none
+	<A>	N1.58O0.42					none
+	<B>	SiO2	solid-1 quartz(l)	1000.00	1.0	1	

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 **$N_{1.58}O_{0.42}$**.

N1.58O0.42

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.

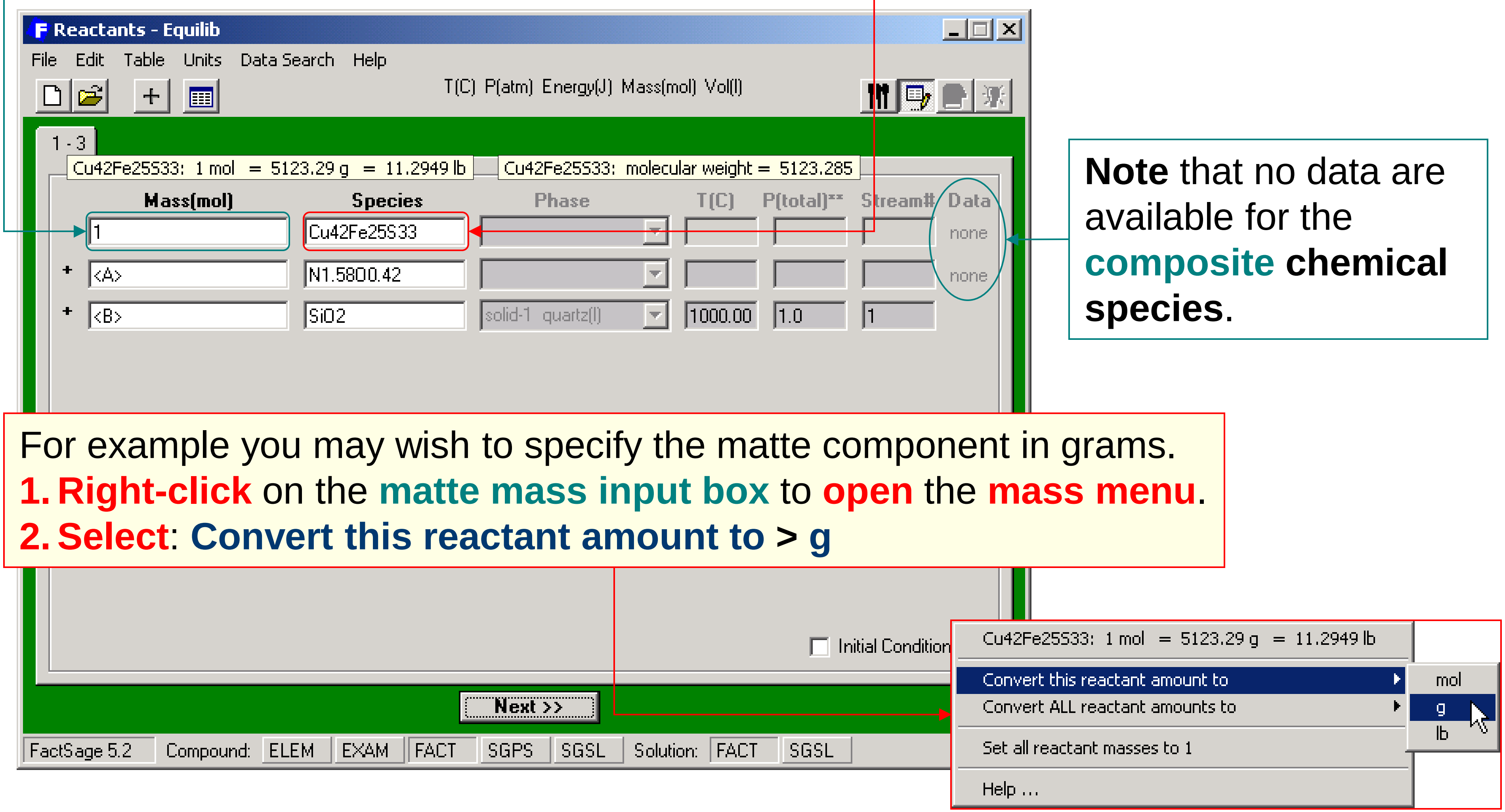
It is possible to «mix» mass units, i.e. to use the default for some and specific chosen units for others of the input substances.

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.



Cu42Fe25S33: 1 mol = 5123.29 g = 11.2949 lb

Cu42Fe25S33: molecular weight = 5123.285

	Mass(mol)	Species	Phase	T(C)	P(total)**	Stream#	Data
	1	Cu42Fe25S33					none
+	<A>	N1.58O0.42					none
+	<B>	SiO2	solid-1 quartz(l)	1000.00	1.0	1	

☐ Initial Conditions

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

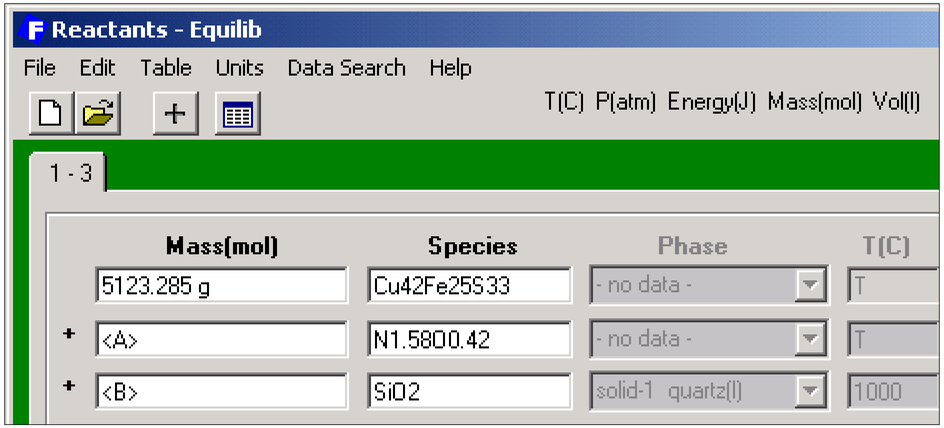
For example you may wish to specify the matte component in grams.

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

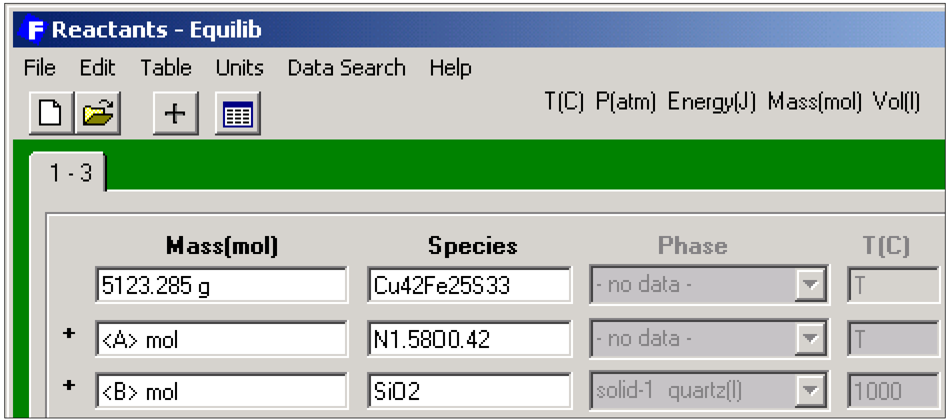
You can mix the mass units by including a 'mol', 'g' or 'lb' in the reactant amount.

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



	Mass(mol)	Species	Phase	T(C)
	5123.285 g	Cu42Fe25S33	- no data -	T
+	<A>	N1.58O0.42	- no data -	T
+	<B>	SiO2	solid-1 quartz(l)	1000

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.



	Mass(mol)	Species	Phase	T(C)
	5123.285 g	Cu42Fe25S33	- no data -	T
+	<A> mol	N1.58O0.42	- no data -	T
+	<B> mol	SiO2	solid-1 quartz(l)	1000

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.

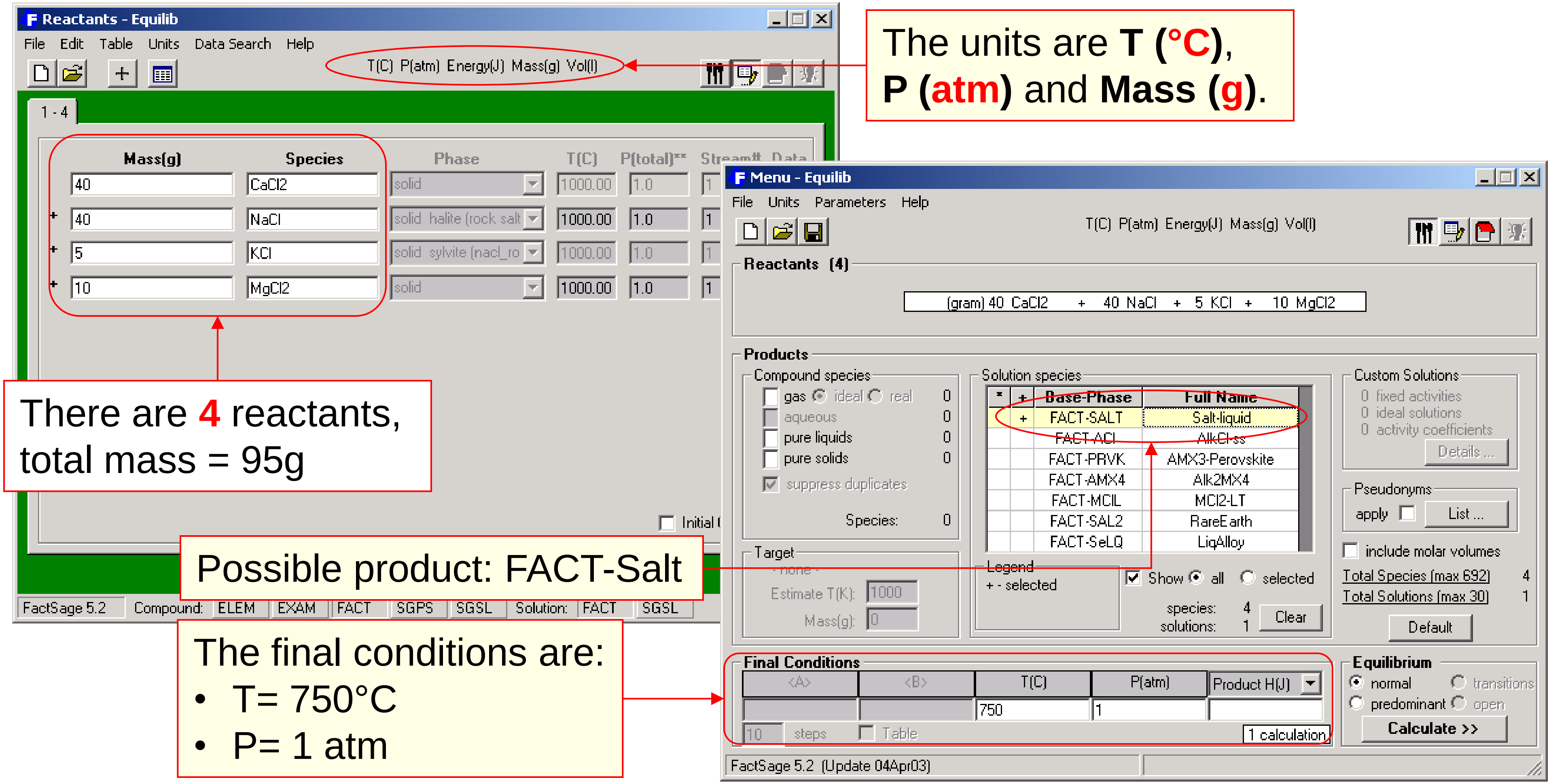
Such groups can be either Mixtures or Streams. For the generation of Mixtures see the Slide Show on the Mixture Module. For the generation of Stream see below (slides 11.4.1 and 11.4.2).

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



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

Mass(g)	Species	Phase	T(C)	P(total)**	Stream# Data
40	CaCl2	solid	1000.00	1.0	1
+ 40	NaCl	solid halite (rock salt	1000.00	1.0	1
+ 5	KCl	solid sylvite (nacl_ro	1000.00	1.0	1
+ 10	MgCl2	solid	1000.00	1.0	1

Reactants (4)

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

☐ gas ● ideal ○ real 0
☐ aqueous 0
☐ pure liquids 0
☐ pure solids 0
☑ suppress duplicates
Species: 0

Target - none -
Estimate T(K): 1000
Mass(g): 0

Solution species

*	+	Base-Phase	Full Name
	+	FACT-SALT	Salt-liquid
		FACT-ACL	AlkCl-ss
		FACT-PRVK	AMX3-Perovskite
		FACT-AMX4	Alk2MX4
		FACT-MCIL	MCl2-LT
		FACT-SAL2	RareEarth
		FACT-SeLQ	LiqAlloy

☑ Show ● all ○ selected
species: 4
solutions: 1

0 fixed activities
0 ideal solutions
0 activity coefficients
Details ...
Pseudonyms apply ☐ List ...
☐ include molar volumes
Total Species (max 692) 4
Total Solutions (max 30) 1

Final Conditions

<A>	<B>	T(C)	P(atm)	Product H(J)
		750	1	

10 steps ☐ Table 1 calculation

Equilibrium
● normal ○ transitions
○ predominant ○ open

FactSage 5.2 (Update 04Apr03)

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

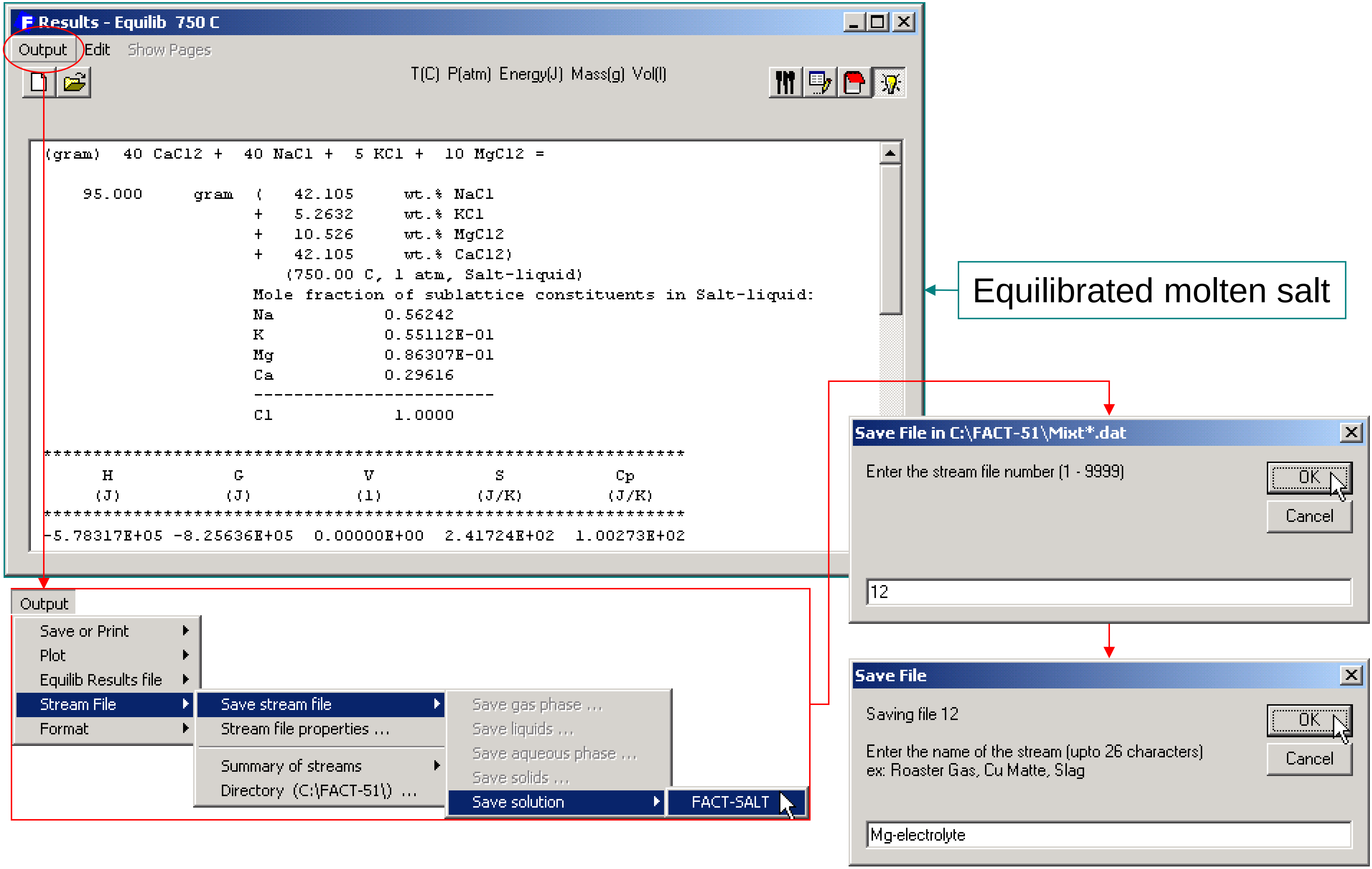
There are **4** reactants, total mass = 95g

Possible product: FACT-Salt

The final conditions are:

- T= 750°C
- P= 1 atm

Saving an equilibrated stream



```
(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

Enter the stream file number (1 - 9999)

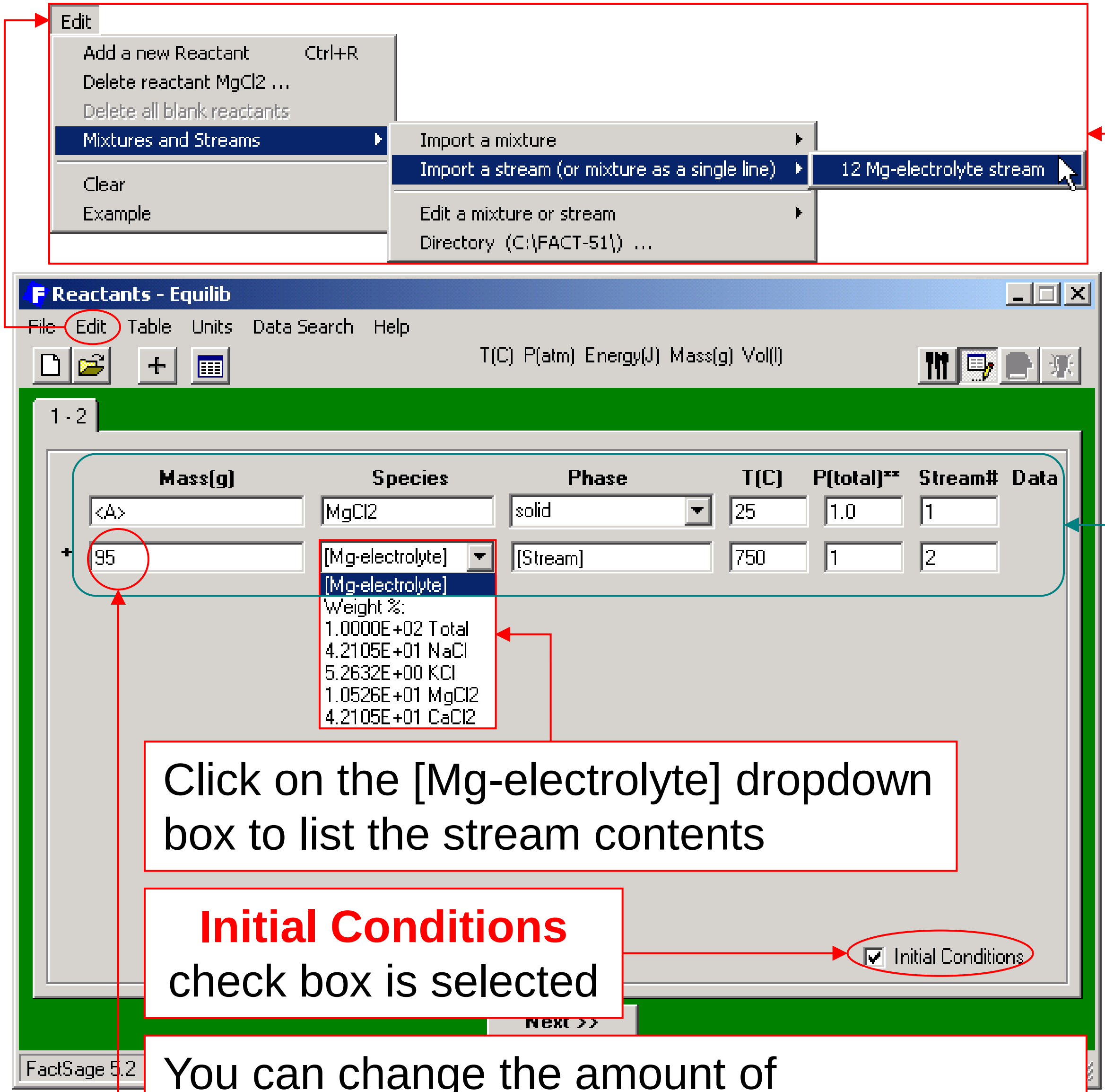
12

Saving file 12

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

Mg-electrolyte

Importing the stream into a reaction



Mass(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
<A>	MgCl2	solid	25	1.0	1	
+ 95	[Mg-electrolyte]	[Stream]	750	1	2	

[Mg-electrolyte]
Weight %:
1.0000E+02 Total
4.2105E+01 NaCl
5.2632E+00 KCl
1.0526E+01 MgCl2
4.2105E+01 CaCl2

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

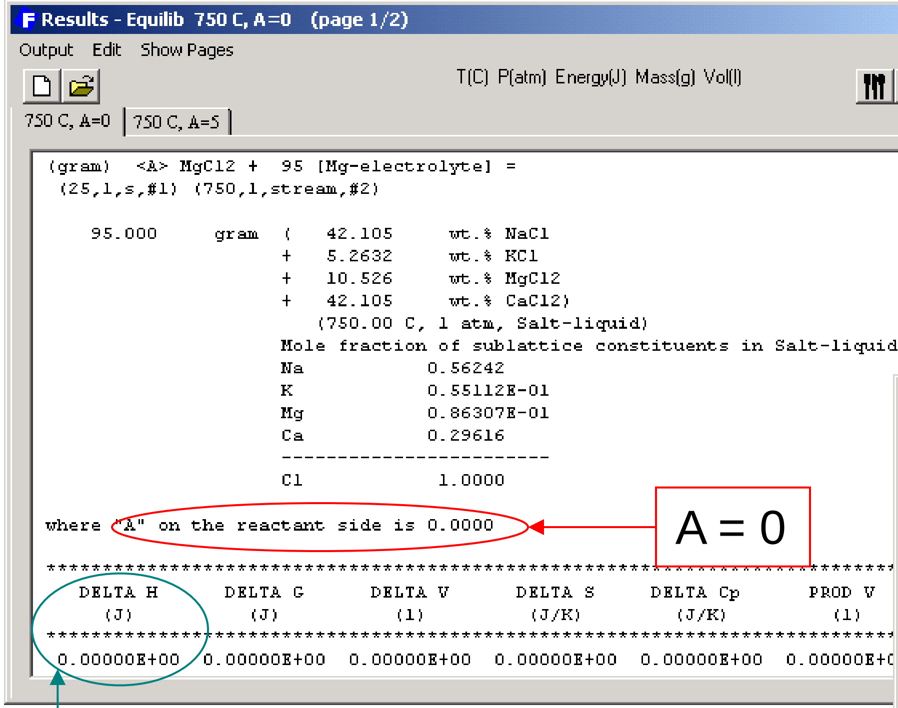
Initial Conditions check box is selected

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:

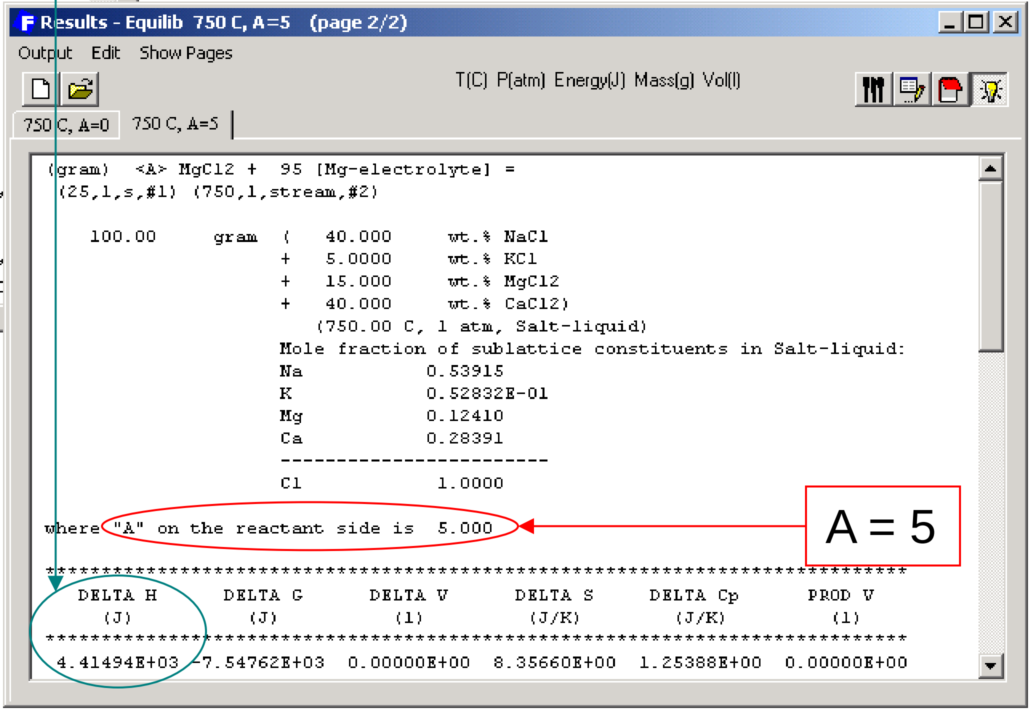


```
 (gram)  <A> MgCl2 +  95 [Mg-electrolyte] =
  (25,1,s,#1) (750,1,stream,#2)

    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)           (l)          (J/K)         (J/K)          (l)
 ***************************************************************************
  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.

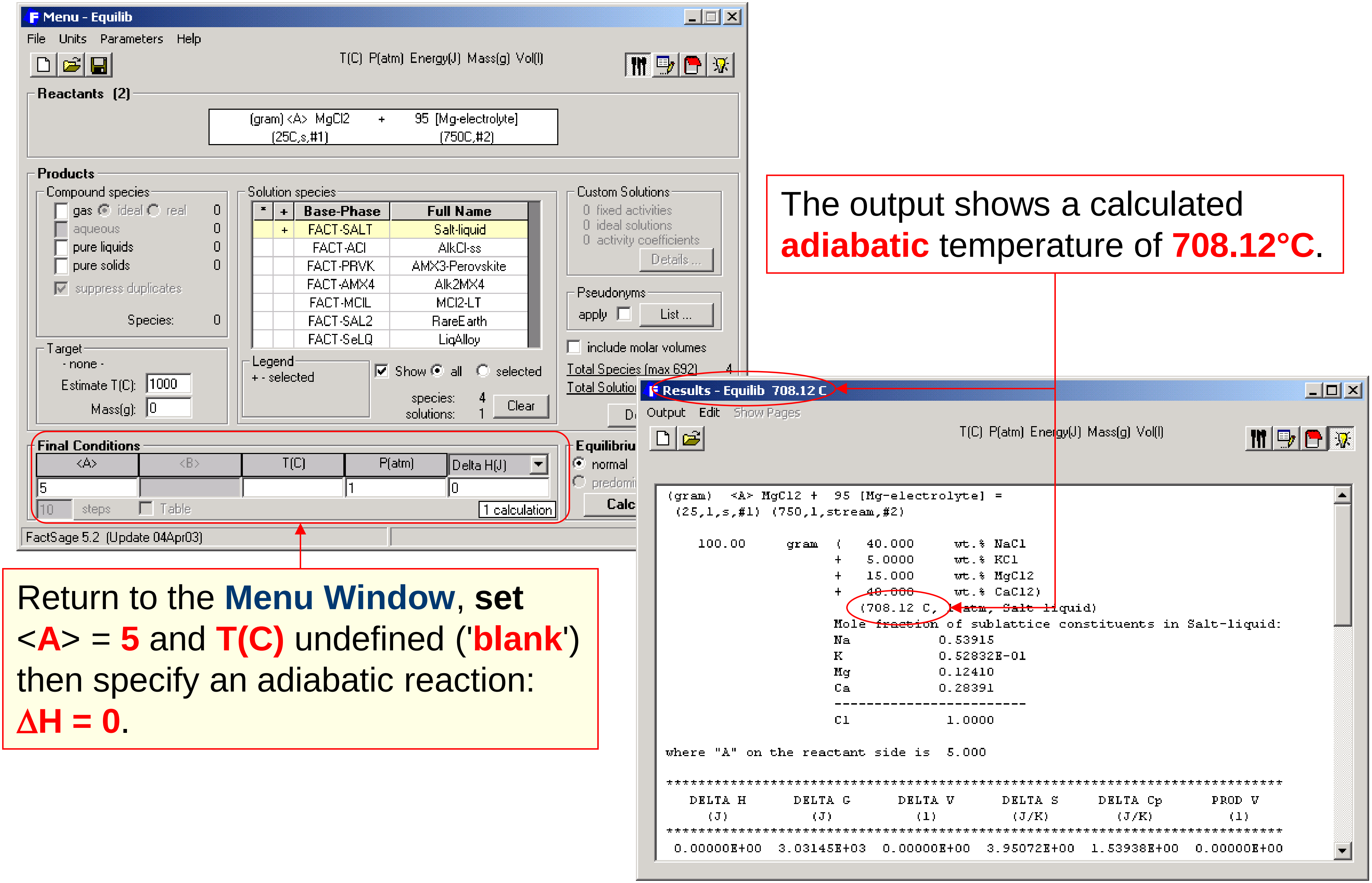
Calculated **ΔH=4415 J** – this is the total energy required to heat 5 g $MgCl_2$ from 25 to 750°C and dissolve it into the molten salt.



```
 (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)           (l)          (J/K)         (J/K)          (l)
 ***************************************************************************
  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



Reactants (2)

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

Products

Compound species

- ☐ gas ● ideal ○ real 0
- ☐ aqueous 0
- ☐ pure liquids 0
- ☐ pure solids 0
- ☑ suppress duplicates

Species: 0

Solution species

*	+	Base-Phase	Full Name
	+	FACT-SALT	Salt-liquid
		FACT-ACl	AlkCl-ss
		FACT-PRVK	AMX3-Perovskite
		FACT-AMX4	Alk2MX4
		FACT-MCIL	MCl2-LT
		FACT-SAL2	RareEarth
		FACT-SeLQ	LiqAlloy

Legend
+ - selected

☑ Show ● all ○ selected

species: 4
solutions: 1

Custom Solutions
0 fixed activities
0 ideal solutions
0 activity coefficients

Pseudonyms
apply ☐

☐ include molar volumes

Total Species (max 692) 4

Target
- none -
Estimate T(C): 1000
Mass(g): 0

Final Conditions

<A>	<B>	T(C)	P(atm)	Delta H(J)
5			1	0

10 steps ☐ Table 1 calculation

Equilibrium
● normal
○ predomi

FactSage 5.2 (Update 04Apr03)

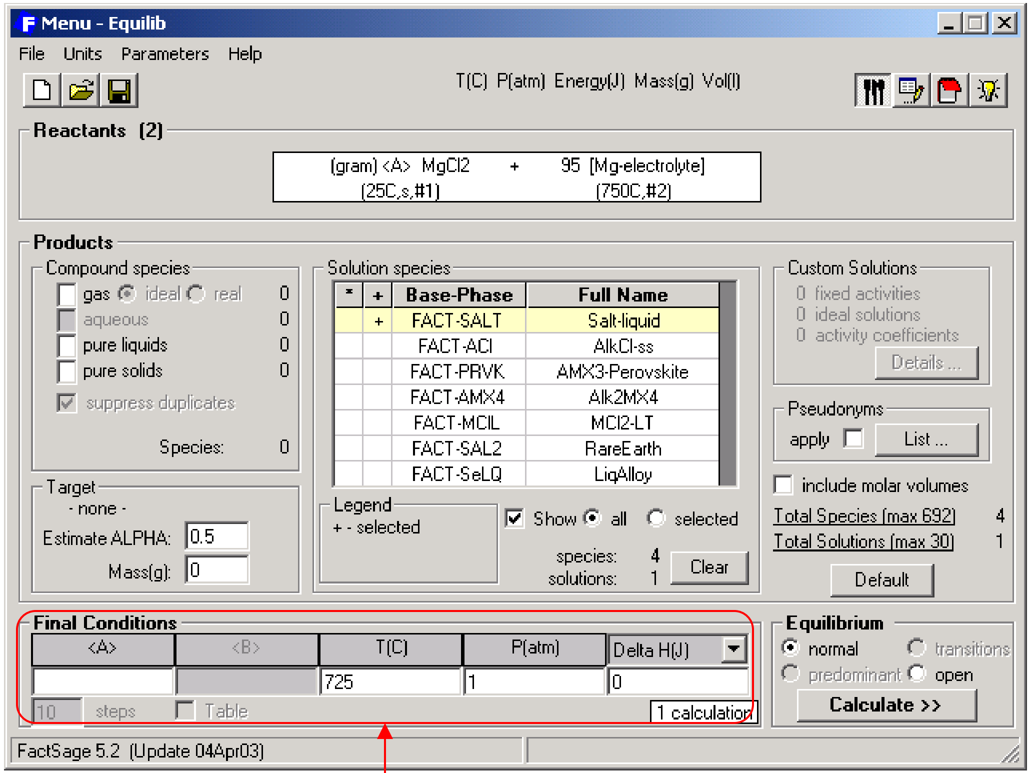
Results - Equilib 708.12 C

```
(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)
                        (708.12 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)           (l)          (J/K)         (J/K)         (l)
*************************************************************************
 0.00000E+00  3.03145E+03  0.00000E+00  3.95072E+00  1.53938E+00  0.00000E+00
```

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



Reactants (2)

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

Products

Compound species
- ☐ gas ● ideal ○ real 0
- ☐ aqueous 0
- ☐ pure liquids 0
- ☐ pure solids 0
- ☑ suppress duplicates
- Species: 0

Solution species

*	+	Base-Phase	Full Name
	+	FACT-SALT	Salt-liquid
		FACT-ACl	AlkCl-ss
		FACT-PRVK	AMX3-Perovskite
		FACT-AMX4	Alk2MX4
		FACT-MCIL	MCl2-LT
		FACT-SAL2	RareEarth
		FACT-SeLQ	LiqAlloy

Legend: + - selected

☑ Show ● all ○ selected

species: 4
solutions: 1

Custom Solutions
- 0 fixed activities
- 0 ideal solutions
- 0 activity coefficients

Pseudonyms: apply ☐

☐ include molar volumes

Total Species (max 692) 4
Total Solutions (max 30) 1

Target: - none -
Estimate ALPHA: 0.5
Mass(g): 0

Final Conditions

<A>	<B>	T(C)	P(atm)	Delta H(J)
		725	1	0

10 steps ☐ Table 1 calculation

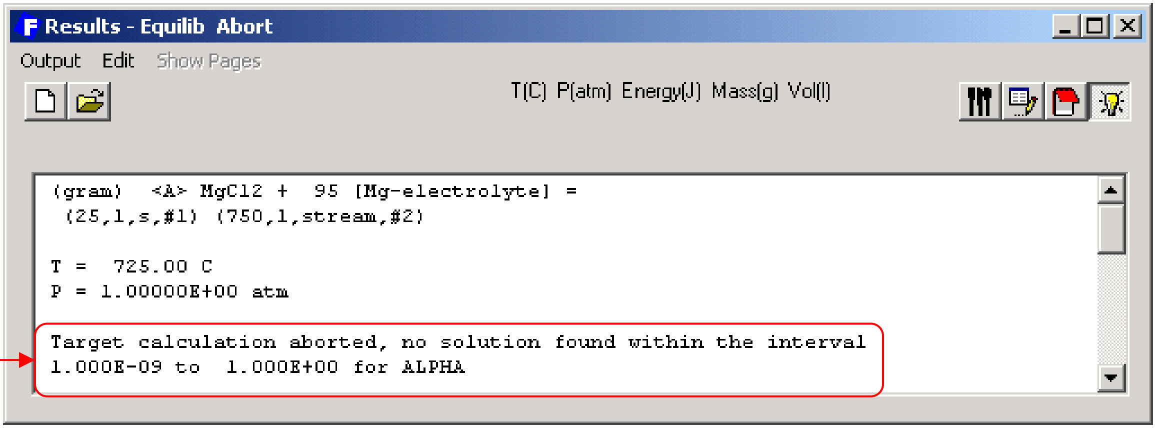
Equilibrium
- ● normal ○ transitions
- ○ predominant ○ open

Calculate >>

FactSage 5.2 (Update 04Apr03)

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.

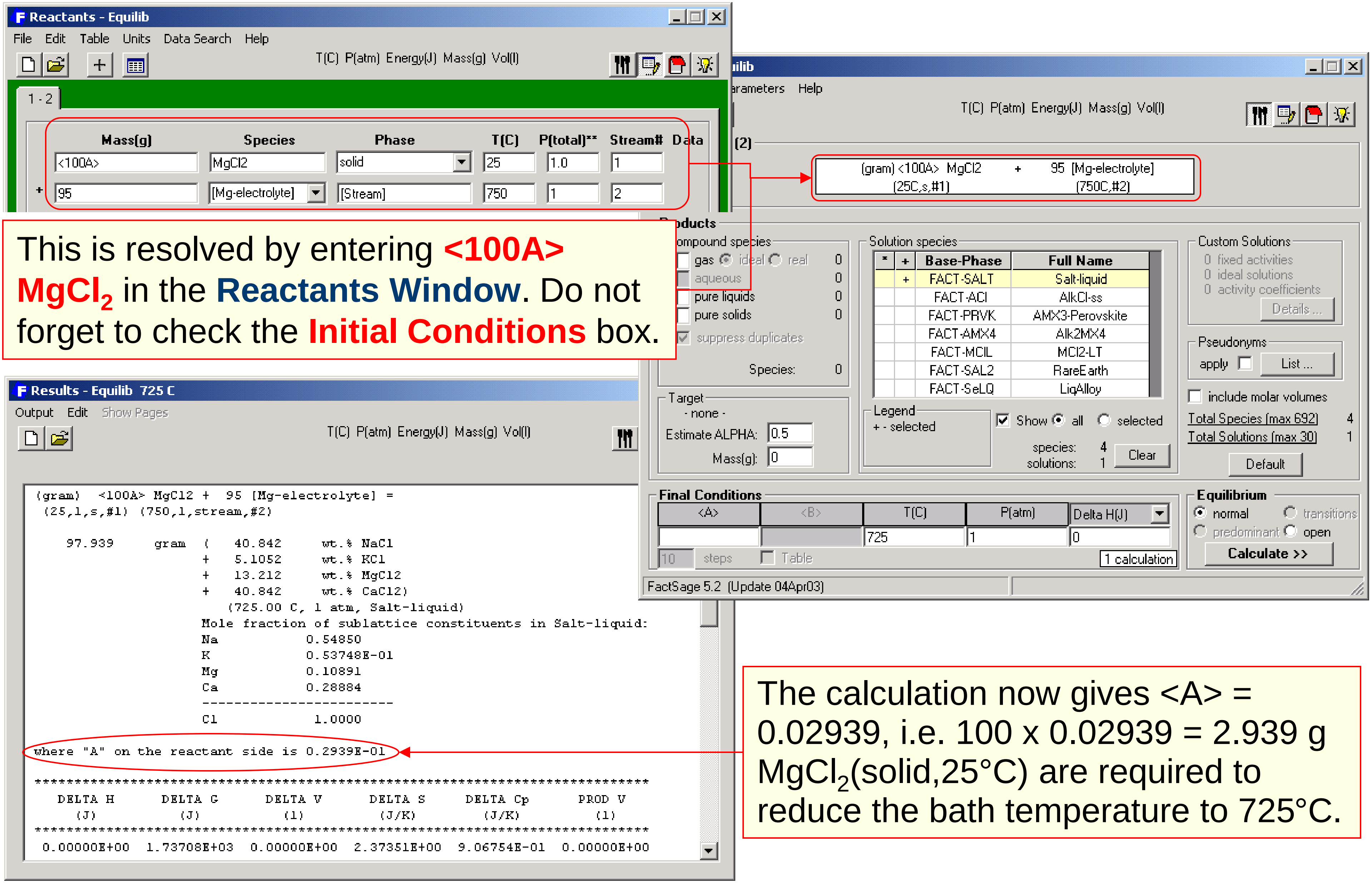
Return to the **Menu Window**, set <**A**> undefined ('**blank**'), set **T(C) = 725°C** , and specify an adiabatic reaction: **ΔH = 0**.



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

T =   725.00 C
P = 1.00000E+00 atm

Target calculation aborted, no solution found within the interval
1.000E-09 to  1.000E+00 for ALPHA
```

The output shows:

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



	Mass(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
	<100A>	MgCl2	solid	25	1.0	1	
+	95	[Mg-electrolyte]	[Stream]	750	1	2	

(gram) <100A> MgCl2 + 95 [Mg-electrolyte]
(25C,s,#1) (750C,#2)

*	+	Base-Phase	Full Name
	+	FACT-SALT	Salt-liquid
		FACT-ACl	AlkCl-ss
		FACT-PRVK	AMX3-Perovskite
		FACT-AMX4	Alk2MX4
		FACT-MCIL	MCl2-LT
		FACT-SAL2	RareEarth
		FACT-SeLQ	LiqAlloy

Estimate ALPHA: 0.5
Mass(g): 0
species: 4
solutions: 1
Total Species (max 692) 4
Total Solutions (max 30) 1

Final Conditions

<A>	<B>	T(C)	P(atm)	Delta H(J)
		725	1	0

10 steps ☐ Table 1 calculation

Equilibrium
● normal ○ transitions
○ predominant ○ open
Calculate >>

FactSage 5.2 (Update 04Apr03)

```
(gram)  <100A> MgCl2 +  95 [Mg-electrolyte] =
 (25,1,s,#1)  (750,1,stream,#2)

   97.939      gram   (   40.842      wt.% NaCl
                      +    5.1052     wt.% KCl
                      +   13.212      wt.% MgCl2
                      +   40.842      wt.% CaCl2)
                          (725.00 C, 1 atm, Salt-liquid)
                      Mole fraction of sublattice constituents in Salt-liquid:
                      Na            0.54850
                      K             0.53748E-01
                      Mg            0.10891
                      Ca            0.28884
                      ------------------------
                      Cl             1.0000

where "A" on the reactant side is 0.2939E-01

***********************************************************************
  DELTA H      DELTA G      DELTA V      DELTA S      DELTA Cp     PROD V
   (J)          (J)          (l)         (J/K)        (J/K)        (l)
***********************************************************************
 0.00000E+00  1.73708E+03  0.00000E+00  2.37351E+00  9.06754E-01  0.00000E+00
```

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.

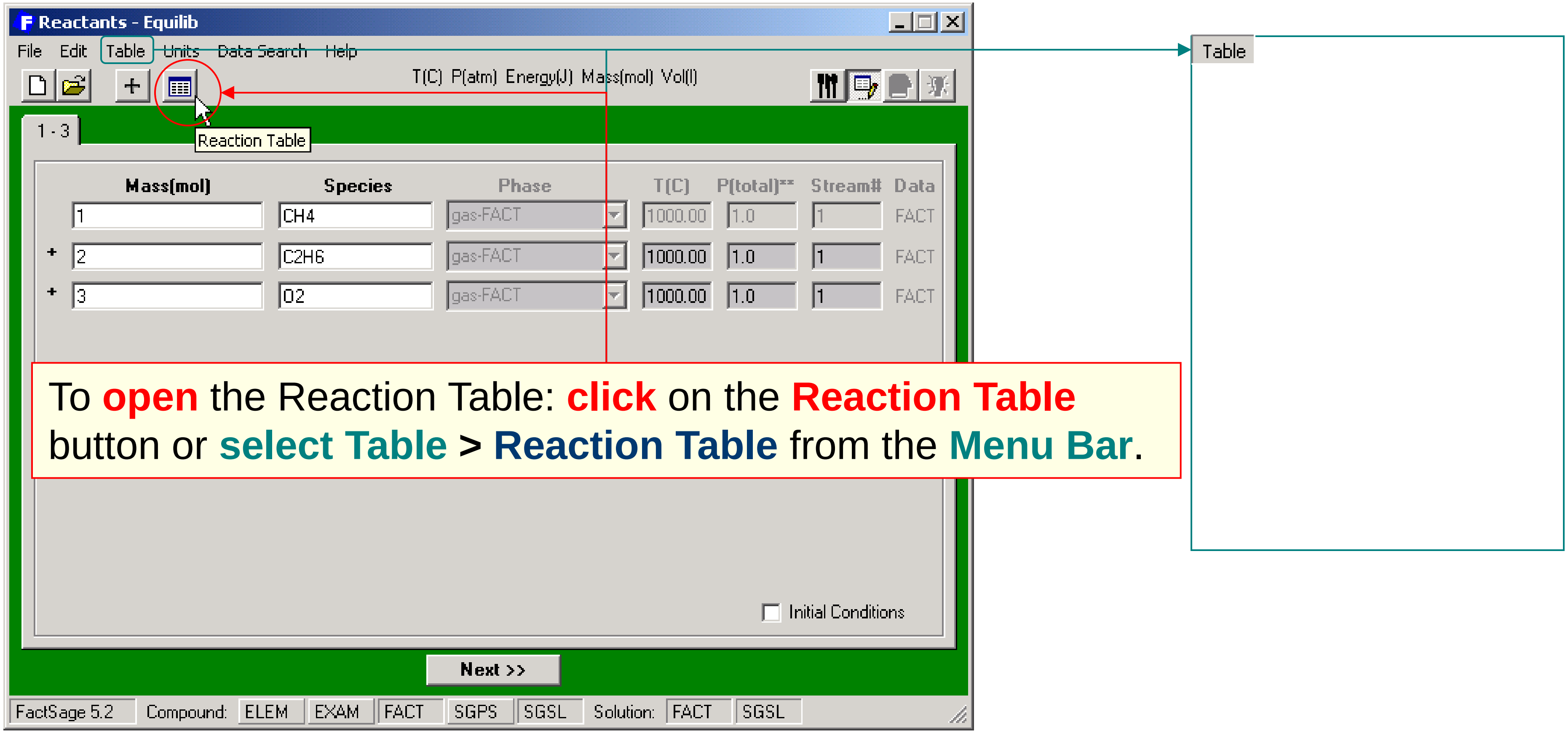
In the calculations the line number (Page number) will be treated as the independent parameter in order to sort the result tables.

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.

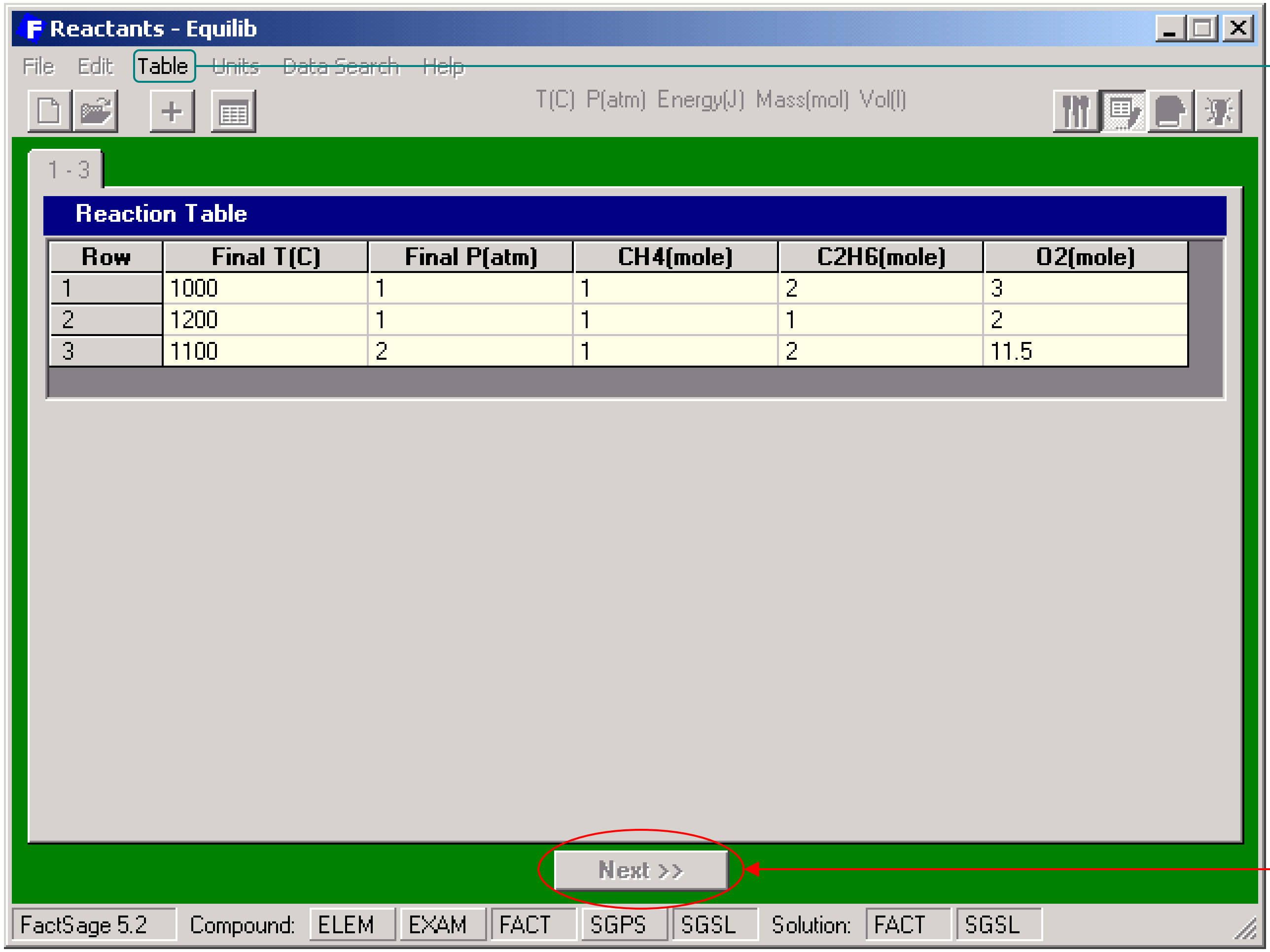


	Mass(mol)	Species	Phase	T(C)	P(total)**	Stream#	Data
	1	CH4	gas-FACT	1000.00	1.0	1	FACT
+	2	C2H6	gas-FACT	1000.00	1.0	1	FACT
+	3	O2	gas-FACT	1000.00	1.0	1	FACT

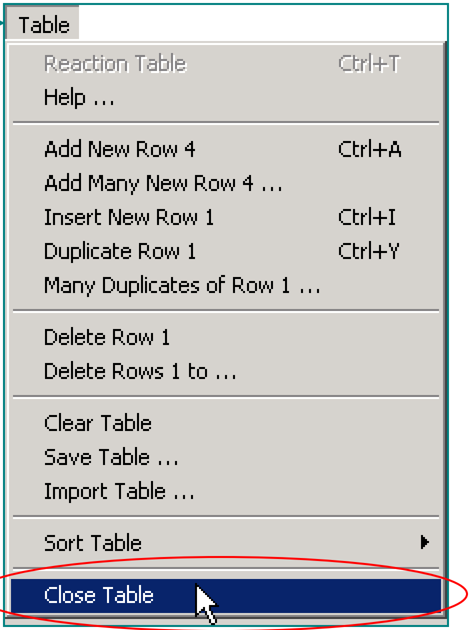
To **open** the Reaction Table: **click** on the **Reaction Table** button or **select Table > Reaction Table** from the **Menu Bar**.

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.

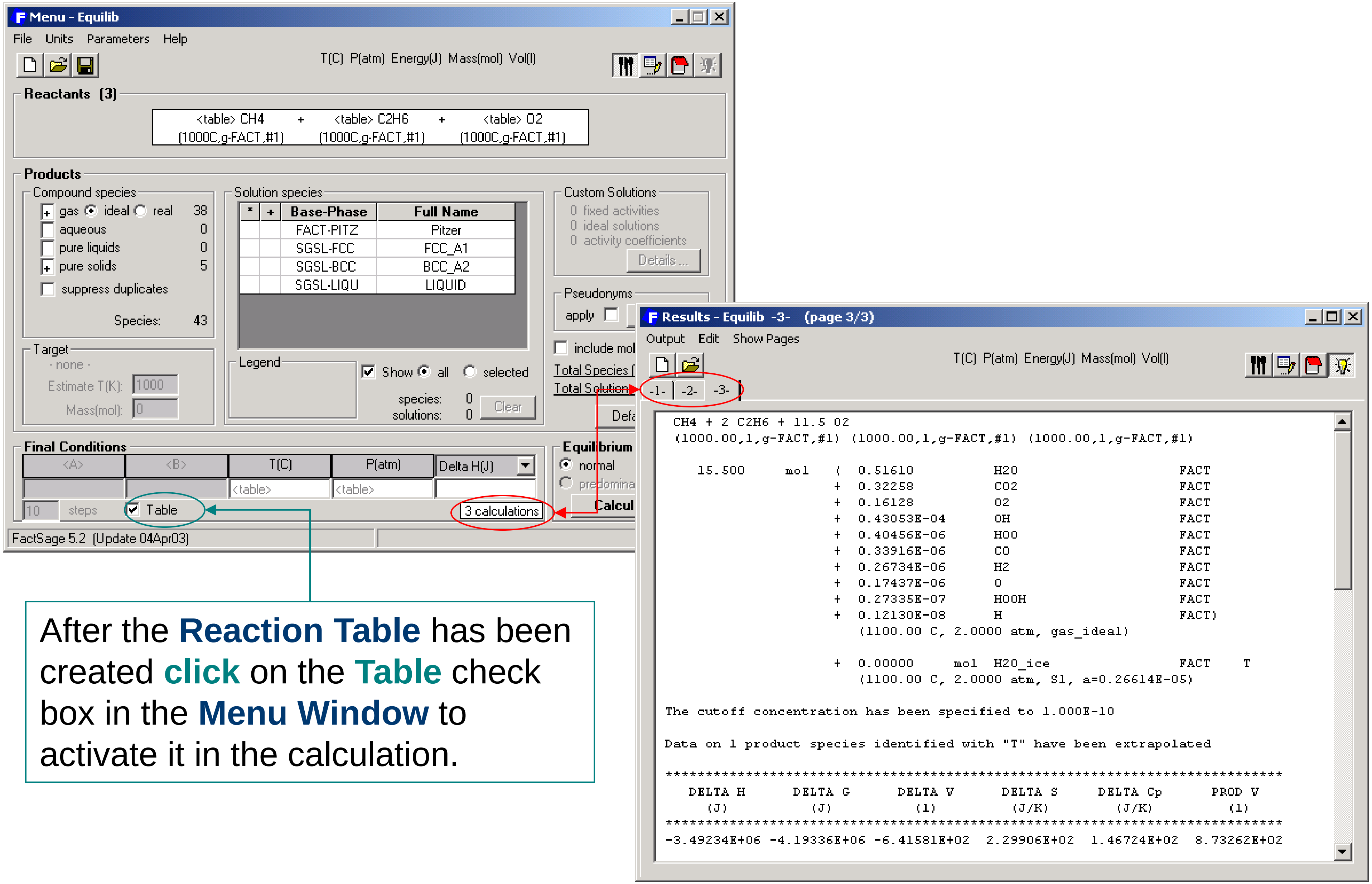


Row	Final T(C)	Final P(atm)	CH4(mole)	C2H6(mole)	O2(mole)
1	1000	1	1	2	3
2	1200	1	1	1	2
3	1100	2	1	2	11.5



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

Reaction Table – Results Window



Reactants (3): <table> CH4 (1000C,g-FACT,#1) + <table> C2H6 (1000C,g-FACT,#1) + <table> O2 (1000C,g-FACT,#1)

Compound species:

- ☒ gas ● ideal ○ real 38
- ☐ aqueous 0
- ☐ pure liquids 0
- ☒ pure solids 5
- ☐ suppress duplicates
- Species: 43

Solution species:

*	+	Base-Phase	Full Name
		FACT-PITZ	Pitzer
		SGSL-FCC	FCC_A1
		SGSL-BCC	BCC_A2
		SGSL-LIQU	LIQUID

Custom Solutions: 0 fixed activities, 0 ideal solutions, 0 activity coefficients

Pseudonyms: apply ☐

☐ include mol

Total Species (

Total Solution

Target: - none - ; Estimate T(K): 1000 ; Mass(mol): 0

Legend: ☑ Show ● all ○ selected ; species: 0 ; solutions: 0

Final Conditions:

<A>	<B>	T(C)	P(atm)	Delta H(J)
		<table>	<table>	

10 steps ☑ Table ; 3 calculations

Equilibrium: ● normal ○ predomina

FactSage 5.2 (Update 04Apr03)

```
 CH4 + 2 C2H6 + 11.5 O2
(1000.00,1,g-FACT,#1) (1000.00,1,g-FACT,#1) (1000.00,1,g-FACT,#1)

   15.500     mol   (  0.51610         H2O                  FACT
                     +  0.32258         CO2                  FACT
                     +  0.16128         O2                   FACT
                     +  0.43053E-04     OH                   FACT
                     +  0.40456E-06     HOO                  FACT
                     +  0.33916E-06     CO                   FACT
                     +  0.26734E-06     H2                   FACT
                     +  0.17437E-06     O                    FACT
                     +  0.27335E-07     HOOH                 FACT
                     +  0.12130E-08     H                    FACT)
                       (1100.00 C, 2.0000 atm, gas_ideal)

                     +  0.00000    mol  H2O_ice              FACT    T
                       (1100.00 C, 2.0000 atm, S1, a=0.26614E-05)

The cutoff concentration has been specified to 1.000E-10

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

************************************************************************
  DELTA H      DELTA G      DELTA V      DELTA S      DELTA Cp     PROD V
    (J)          (J)          (l)         (J/K)        (J/K)        (l)
************************************************************************
-3.49234E+06 -4.19336E+06 -6.41581E+02  2.29906E+02  1.46724E+02  8.73262E+02
```

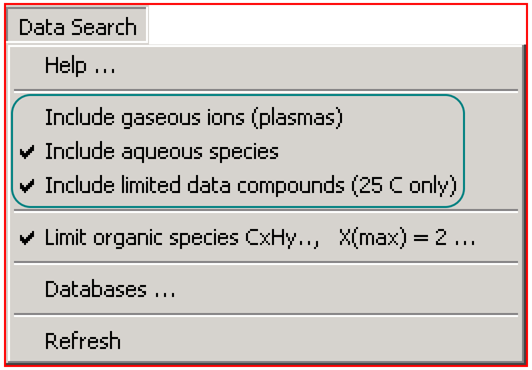
After the **Reaction Table** has been created **click** on the **Table** check box in the **Menu Window** to activate it in the calculation.

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.

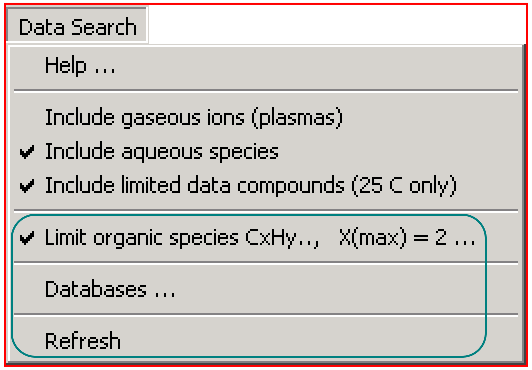
- **Include aqueous species:**

  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.

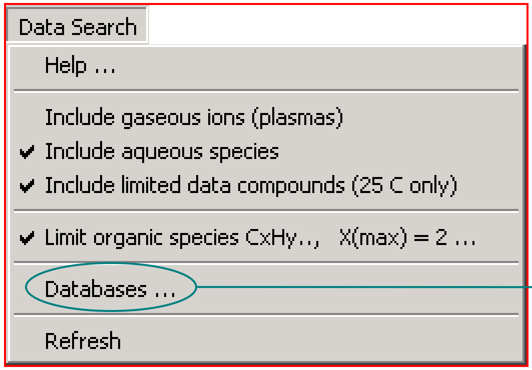
Databases may be added to or removed from the data search. For example private data entered through the Compound and Solution programs, or other commercial databases such as Thermo-Tech. If you have both FACT and SGTE databases then you use this option to tell the program to search both databases or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



Data Search

Help ...

Include gaseous ions (plasmas)

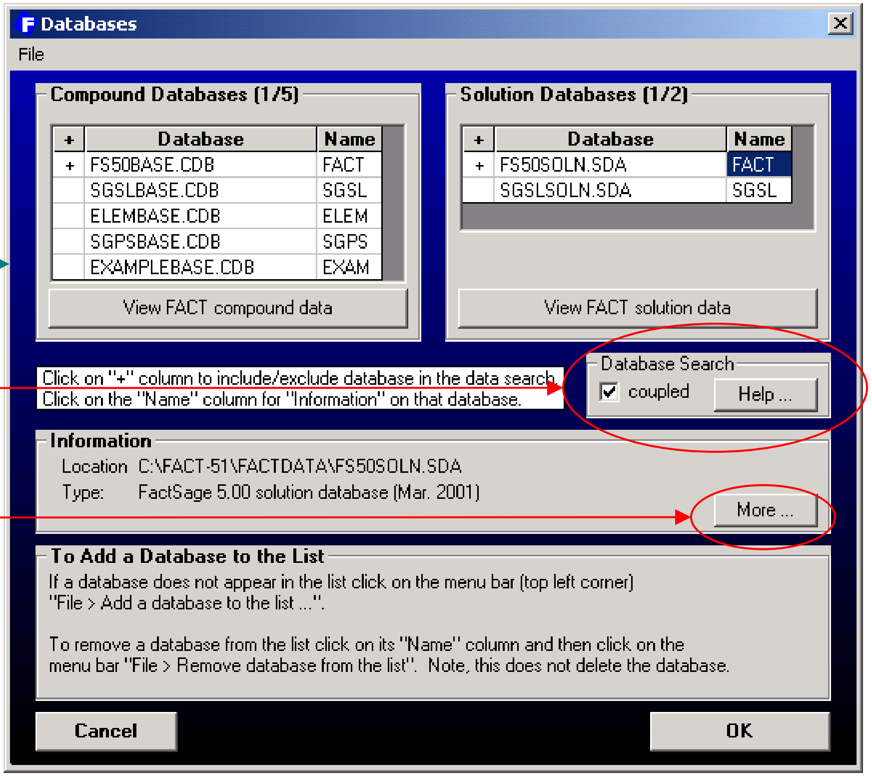
✓ Include aqueous species

✓ Include limited data compounds (25 C only)

✓ Limit organic species CxHy.., X(max) = 2 ...

Databases ...

Refresh



Databases

File

Compound Databases (1/5)

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

Solution Databases (1/2)

+	Database	Name
+	FS50SOLN.SDA	FACT
	SGSLSOLN.SDA	SGSL

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

Database Search

☑ coupled

Information

Location C:\FACT-51\FACTDATA\FS50SOLN.SDA

Type: FactSage 5.00 solution database (Mar. 2001)

To Add a Database to the List

If a database does not appear in the list click on the menu bar (top left corner) "File > Add a database to the list ...".

To remove a database from the list click on its "Name" column and then click on the menu bar "File > Remove database from the list". Note, this does not delete the database.

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.

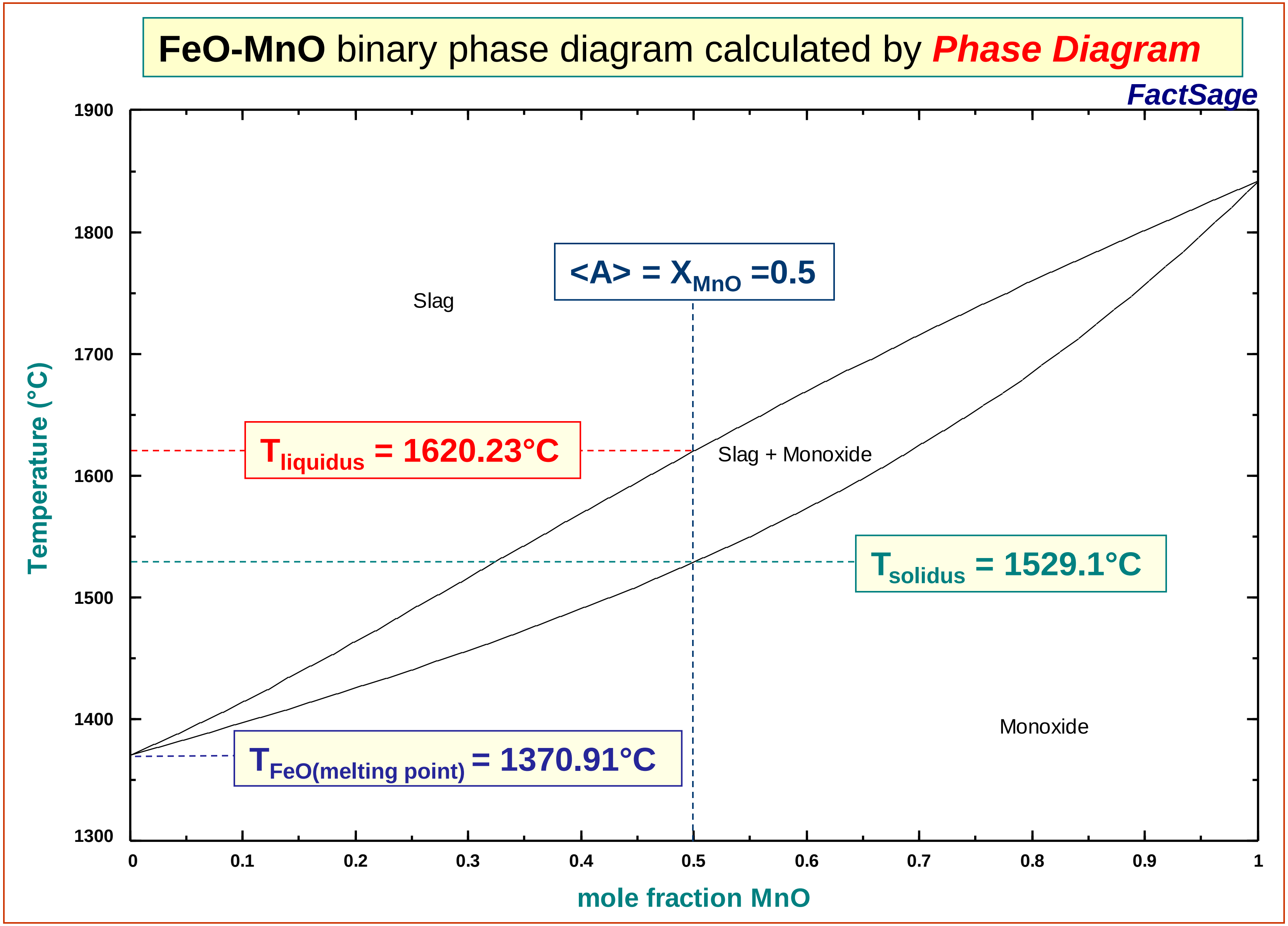
Equilib Cooling Calculations

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

- **Equilibrium cooling**
- **Scheil-Gulliver cooling with or without back diffusion**
- **Full annealing of cast alloys**

Cooling Calculations - Table of Contents

FeO-MnO : **Phase transitions** - binary phase diagram

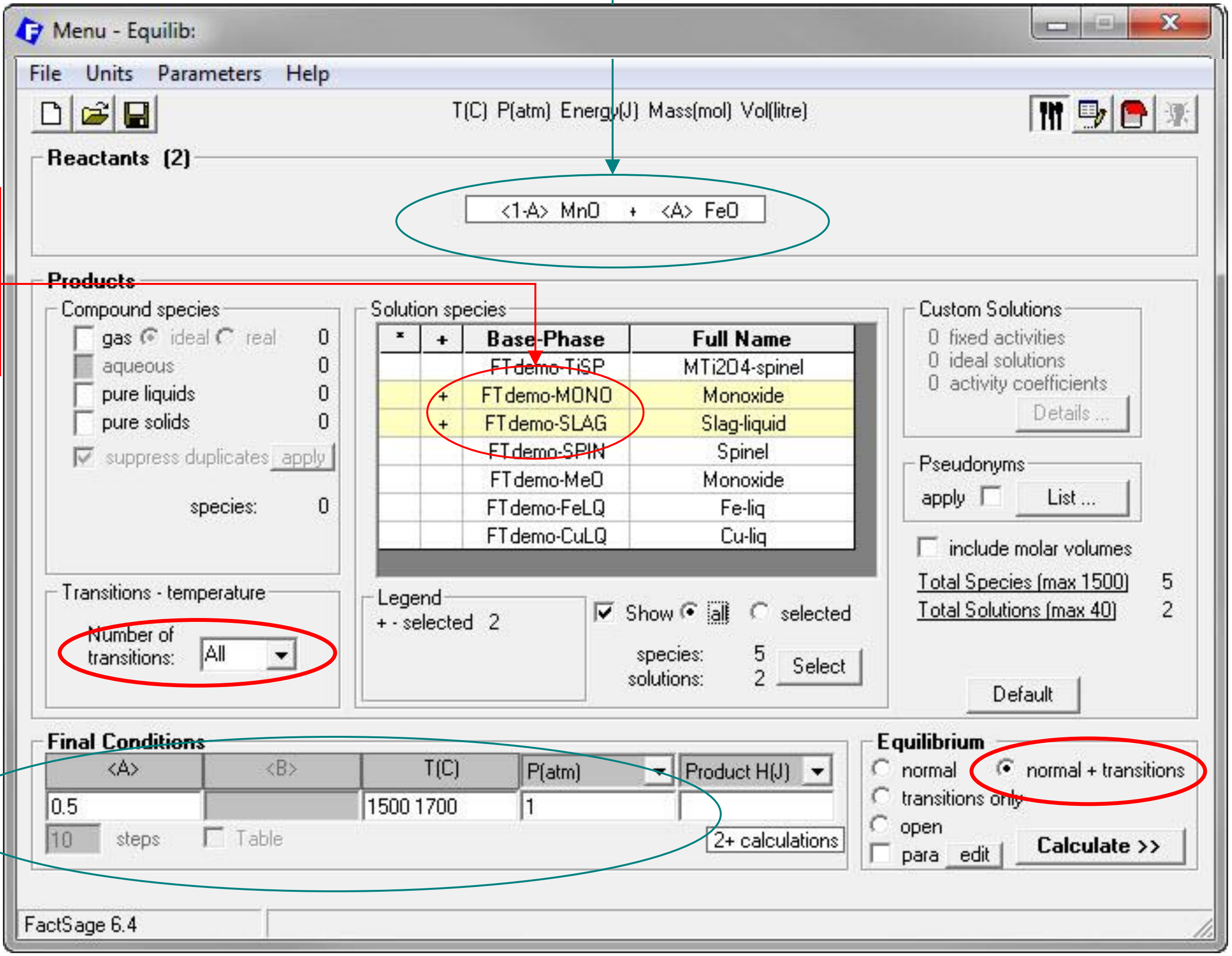


FeO-MnO : Equilibrium phase transitions at X_{FeO} = 0.5

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**



Menu - Equilib:

File Units Parameters Help

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

Reactants (2)

<1-A> MnO + <A> FeO

Products

Compound species
☐ gas ● ideal ○ real 0
☐ aqueous 0
☐ pure liquids 0
☐ pure solids 0
☑ suppress duplicates apply
species: 0

Solution species

*	+	Base-Phase	Full Name
		FTdemo-TiSP	MTi2O4-spinel
	+	FTdemo-MONO	Monoxide
	+	FTdemo-SLAG	Slag-liquid
		FTdemo-SPIN	Spinel
		FTdemo-MeO	Monoxide
		FTdemo-FeLQ	Fe-liq
		FTdemo-CuLQ	Cu-liq

Custom Solutions
0 fixed activities
0 ideal solutions
0 activity coefficients
Details ...

Pseudonyms
apply ☐ List ...

☐ include molar volumes
Total Species (max 1500) 5
Total Solutions (max 40) 2

Transitions - temperature
Number of transitions: All

Legend
+ - selected 2

☑ Show ● all ○ selected
species: 5
solutions: 2
Select

Default

Final Conditions

<A>	<B>	T(C)	P(atm)	Product H(J)
0.5		1500 1700	1	

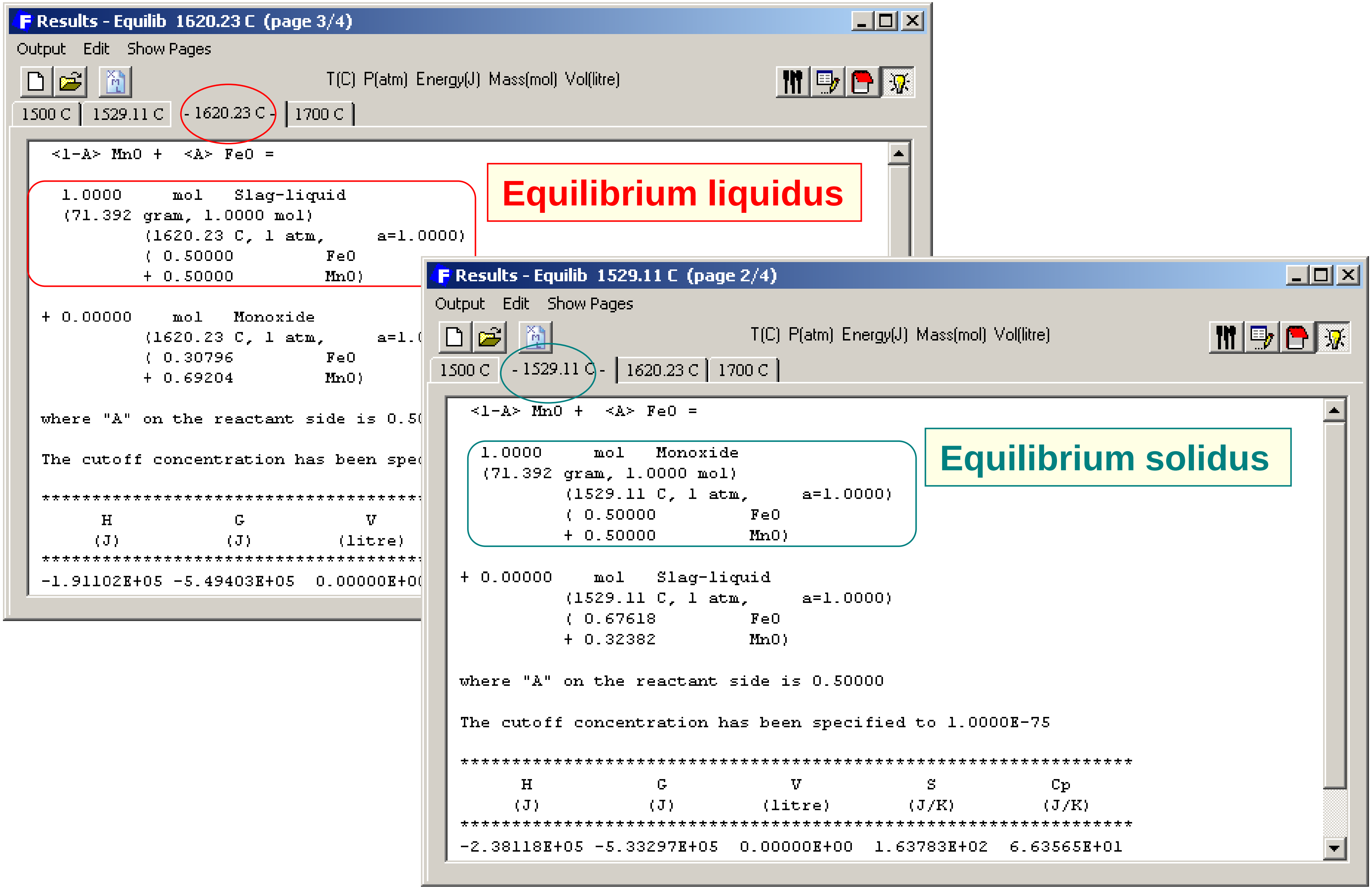
10 steps ☐ Table 2+ calculations

Equilibrium
○ normal ● normal + transitions
○ transitions only
○ open
☐ para edit
Calculate >>

FactSage 6.4

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



Equilibrium liquidus

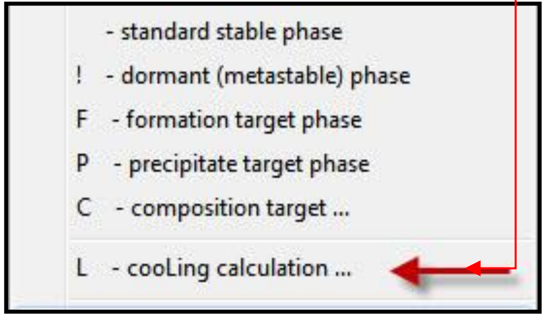
```
 <1-A> MnO +  <A> FeO =

   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 spec

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

Equilibrium solidus

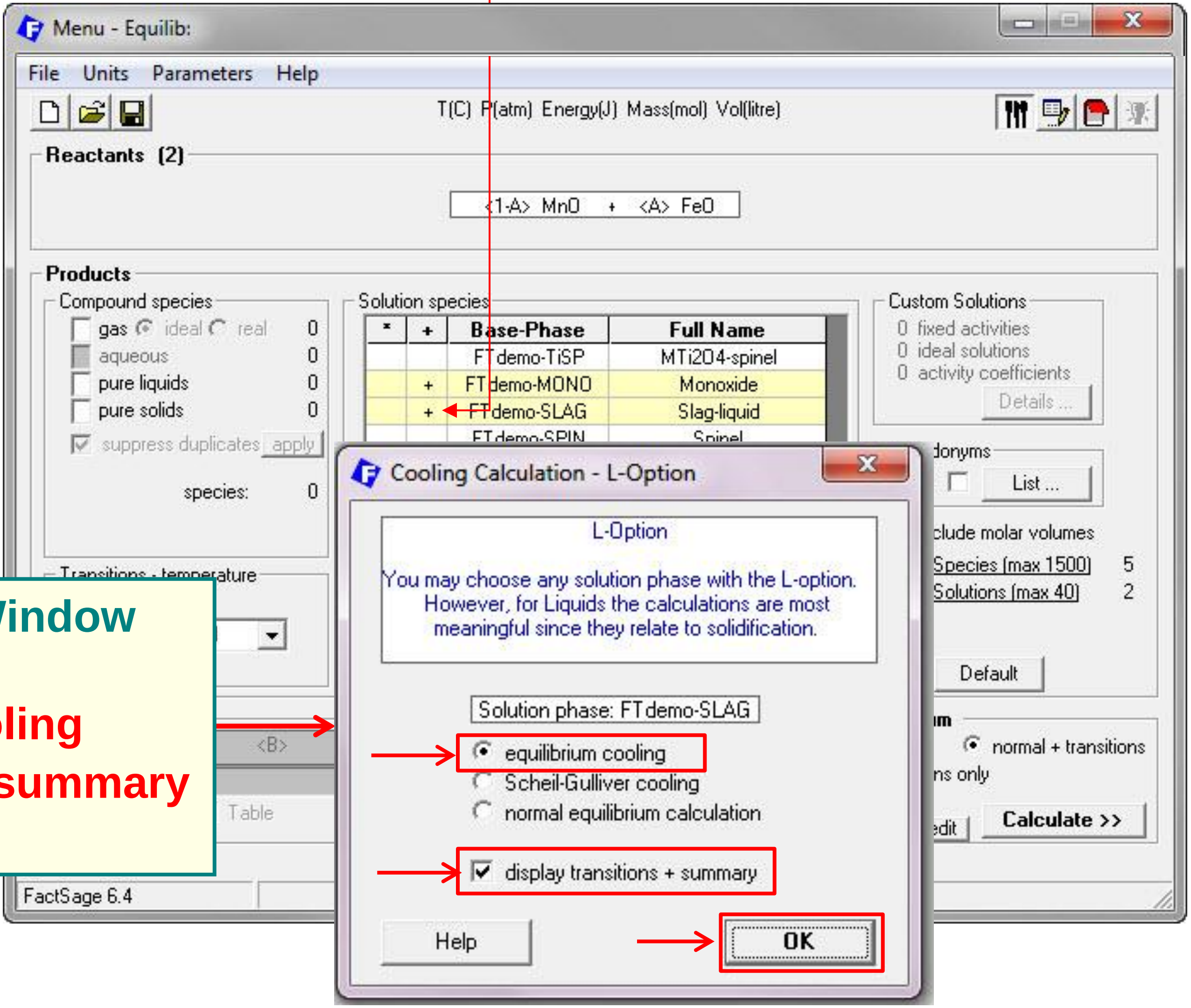
```
 <1-A> MnO +  <A> FeO =

   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
```

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***



- standard stable phase
! - dormant (metastable) phase
F - formation target phase
P - precipitate target phase
C - composition target ...
L - cooLing calculation ...



<1-A> MnO + <A> FeO

*	+	Base-Phase	Full Name
		FTdemo-TiSP	MTi2O4-spinel
	+	FTdemo-MONO	Monoxide
	+	FTdemo-SLAG	Slag-liquid
		FTdemo-SPIN	Spinel

Species (max 1500) 5
Solutions (max 40) 2

FactSage 6.4

Cooling Calculation - L-Option

L-Option

You may choose any solution phase with the L-option. However, for Liquids the calculations are most meaningful since they relate to solidification.

Solution phase: FTdemo-SLAG

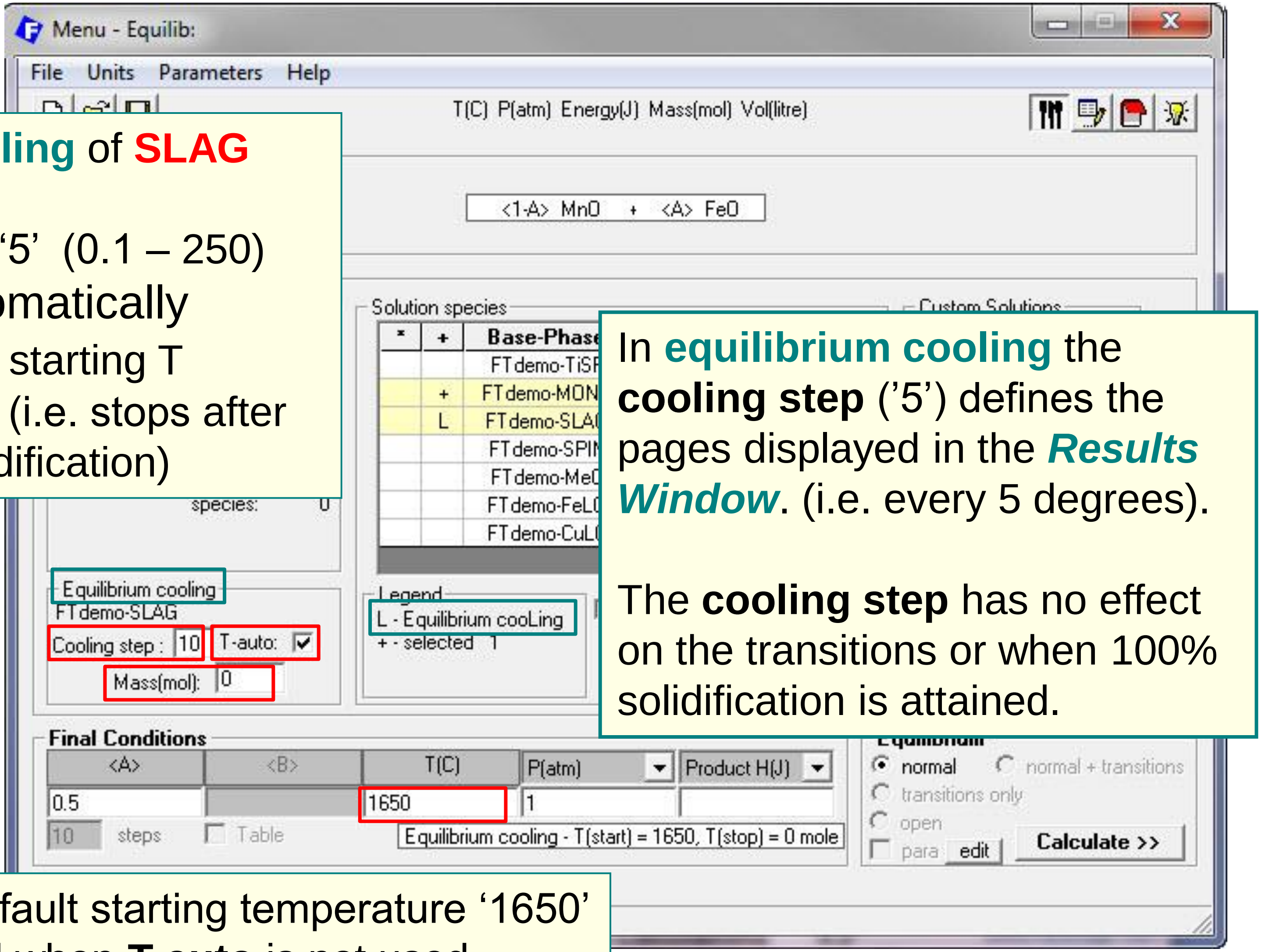
● equilibrium cooling
○ Scheil-Gulliver cooling
○ normal equilibrium calculation

☑ display transitions + summary

2° **Cooling Calculation Window**

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

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



<1-A> MnO + <A> FeO

*	+	Base-Phase
		FTdemo-TiSF
	+	FTdemo-MON
	L	FTdemo-SLA
		FTdemo-SPIN
		FTdemo-MeO
		FTdemo-FeLQ
		FTdemo-CuLQ

species: 0

Equilibrium cooling
FTdemo-SLAG
Cooling step : 10 T-auto: ☑
Mass(mol): 0

L - Equilibrium cooLing
+ - selected 1

<A>	<B>	T(C)	P(atm)	Product H(J)
0.5		1650	1	

10 steps ☐ Table

Equilibrium cooling - T(start) = 1650, T(stop) = 0 mole

Equilibrium
● normal ○ normal + transitions
○ transitions only
○ open
☐ para edit

Equilibrium Cooling of **SLAG**

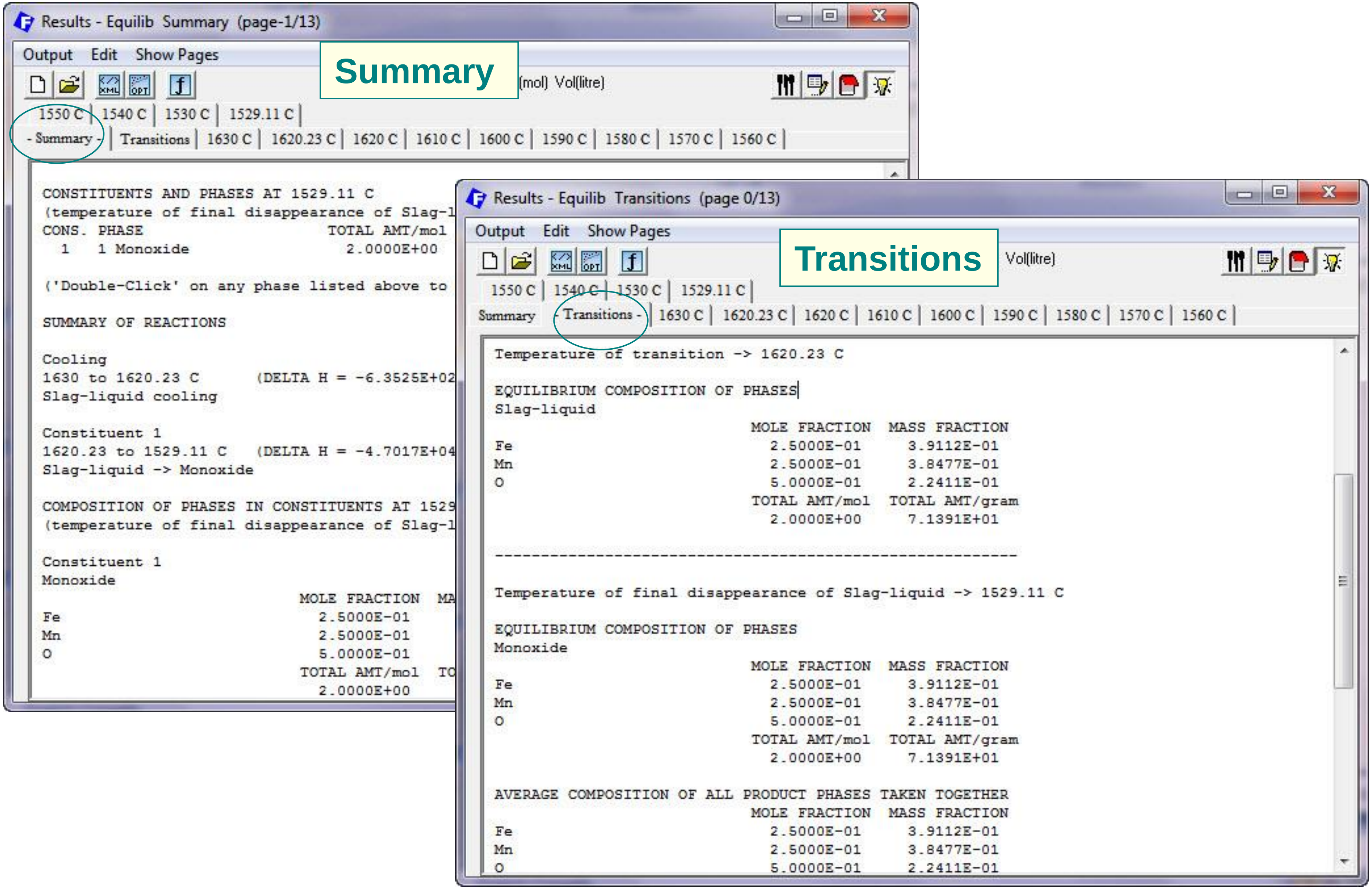
- **cooling step** ‘5’ (0.1 – 250)
- **T-auto** √ automatically calculates the starting T
- **final mass** ‘0’ (i.e. stops after complete solidification)

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

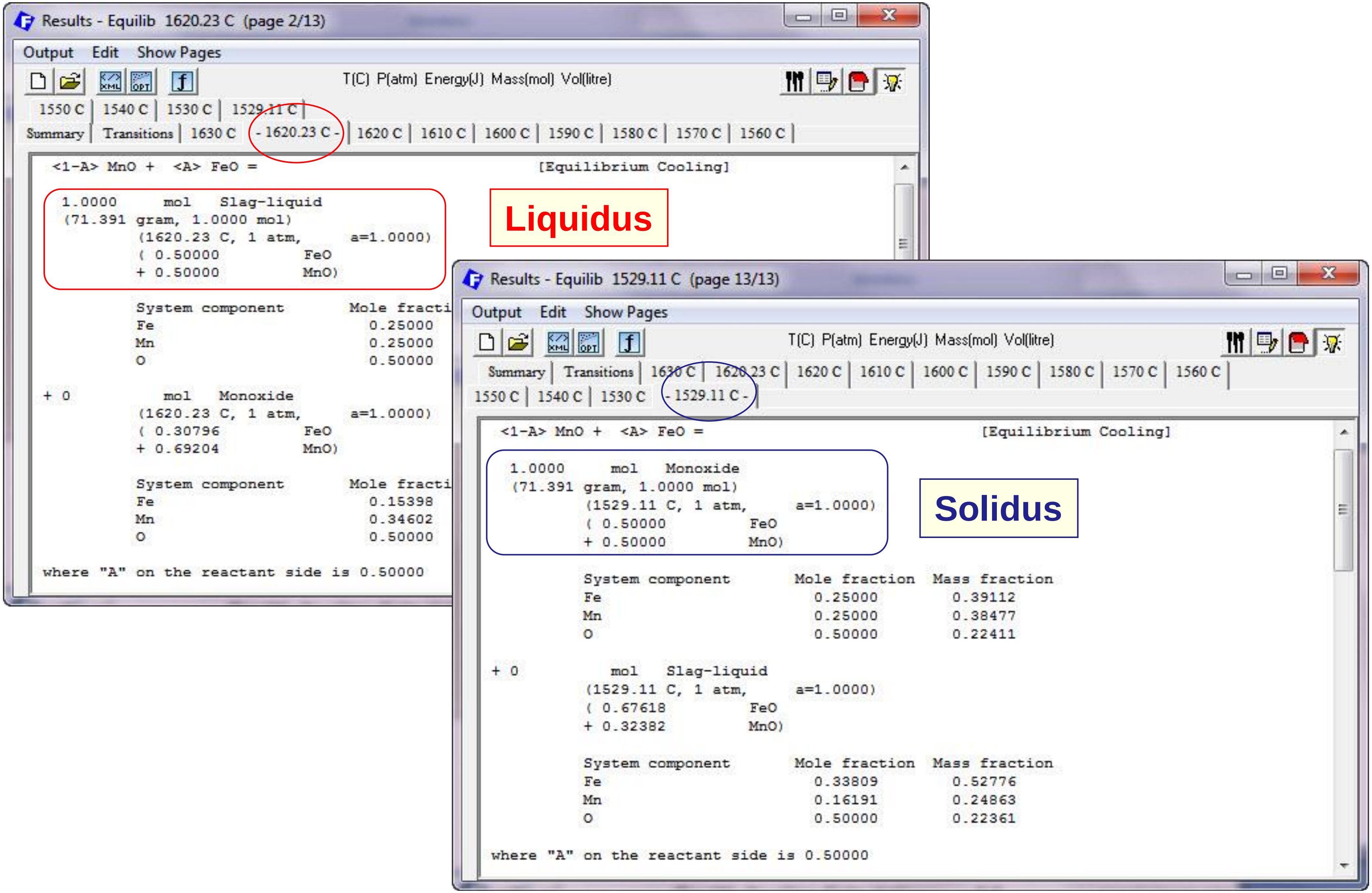
FeO-MnO : Equilibrium cooling – Summary and Transitions



```
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
```

```
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



```
 <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

```
 <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.

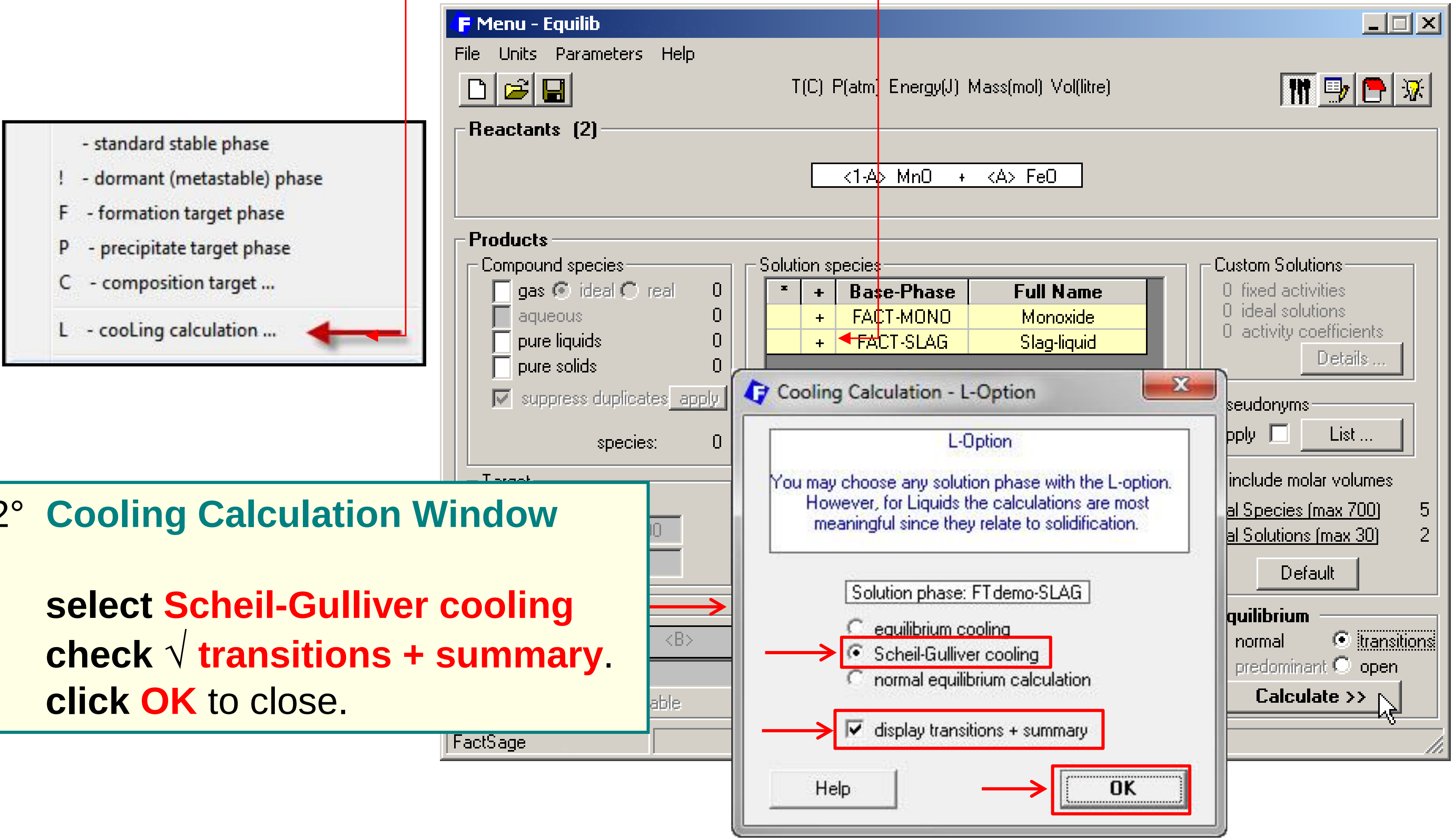
Generally a value of **T** (the initial temperature) and a cooling step must be specified in the **Final Conditions** frame. Normally, the Scheil calculation is repeated until the Scheil Target phase disappears. However it is possible to stop the calculation by either specifying a second temperature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



- standard stable phase
! - dormant (metastable) phase
F - formation target phase
P - precipitate target phase
C - composition target ...
L - cooLing calculation ...

Menu - Equilib

Reactants (2)

<1-A> MnO + <A> FeO

Products

Solution species

*	+	Base-Phase	Full Name
	+	FACT-MONO	Monoxide
	+	FACT-SLAG	Slag-liquid

Cooling Calculation - L-Option

L-Option

You may choose any solution phase with the L-option. However, for Liquids the calculations are most meaningful since they relate to solidification.

Solution phase: FTdemo-SLAG

○ equilibrium cooling
● Scheil-Gulliver cooling
○ normal equilibrium calculation

☑ display transitions + summary

2° Cooling Calculation Window

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

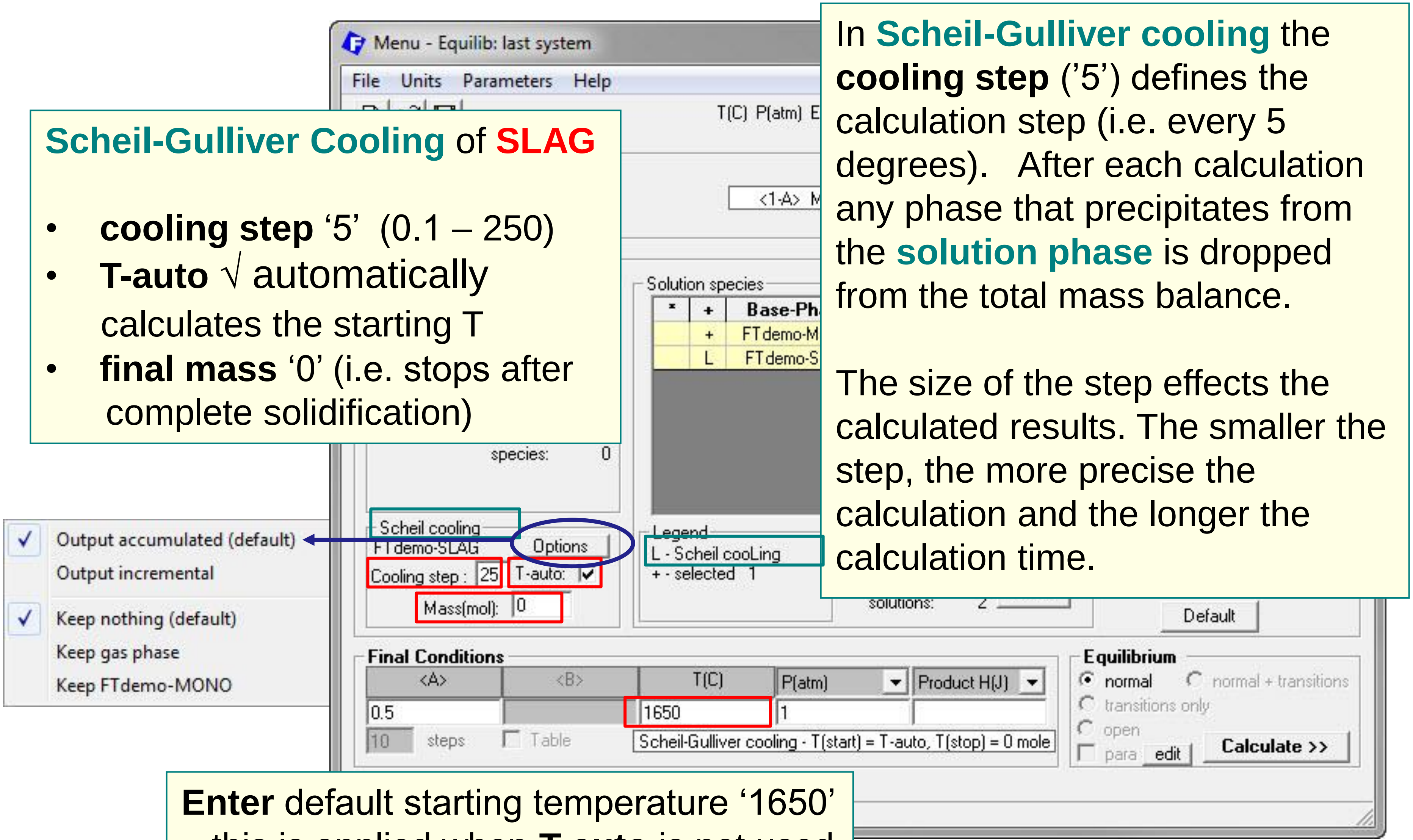
FeO-MnO : Scheil-Gulliver cooling – step, T-auto and stop

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.



Cooling step : 25

T-auto: ☑

Mass(mol): 0

<A>	<B>	T(C)	P(atm)	Product H(J)
0.5		1650	1	

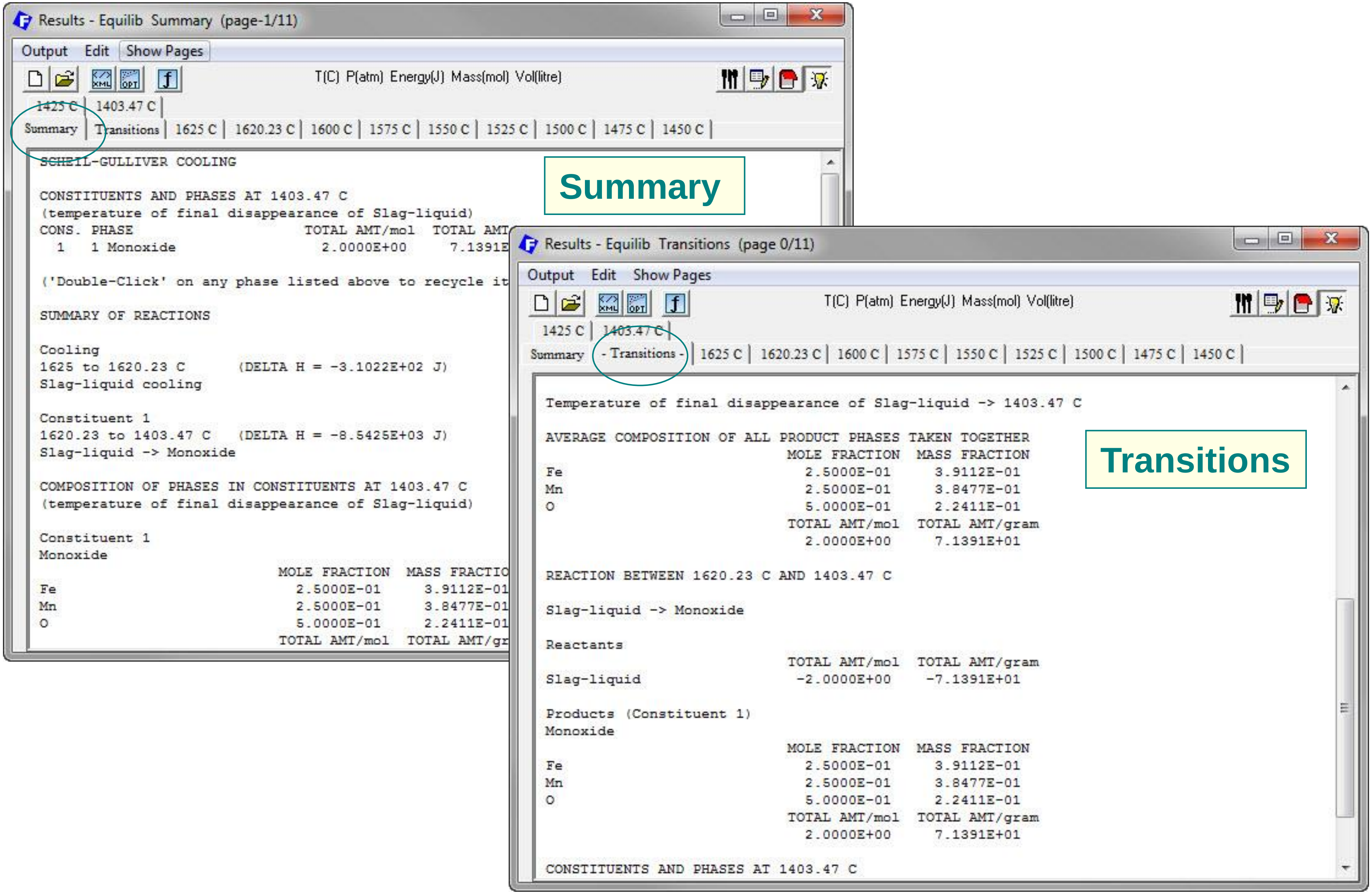
10 steps ☐ Table

Scheil-Gulliver cooling - T(start) = T-auto, T(stop) = 0 mole

● normal ○ normal + transitions
○ transitions only
○ open
☐ para

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

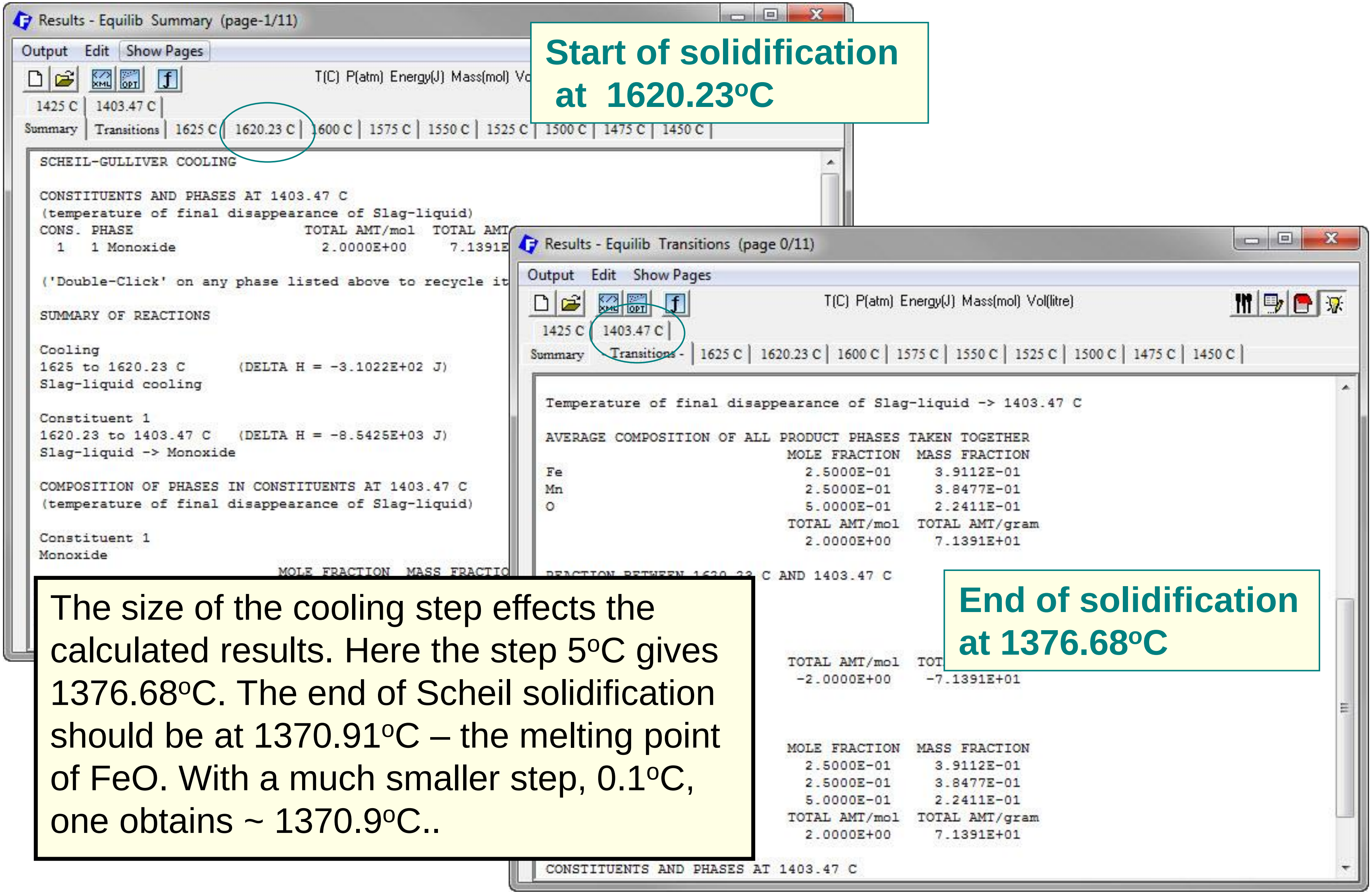
FeO-MnO : Scheil cooling – Summary and Transitions



```
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
```

```
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
```

FeO-MnO : Scheil cooling – Start and Stop



```
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
```

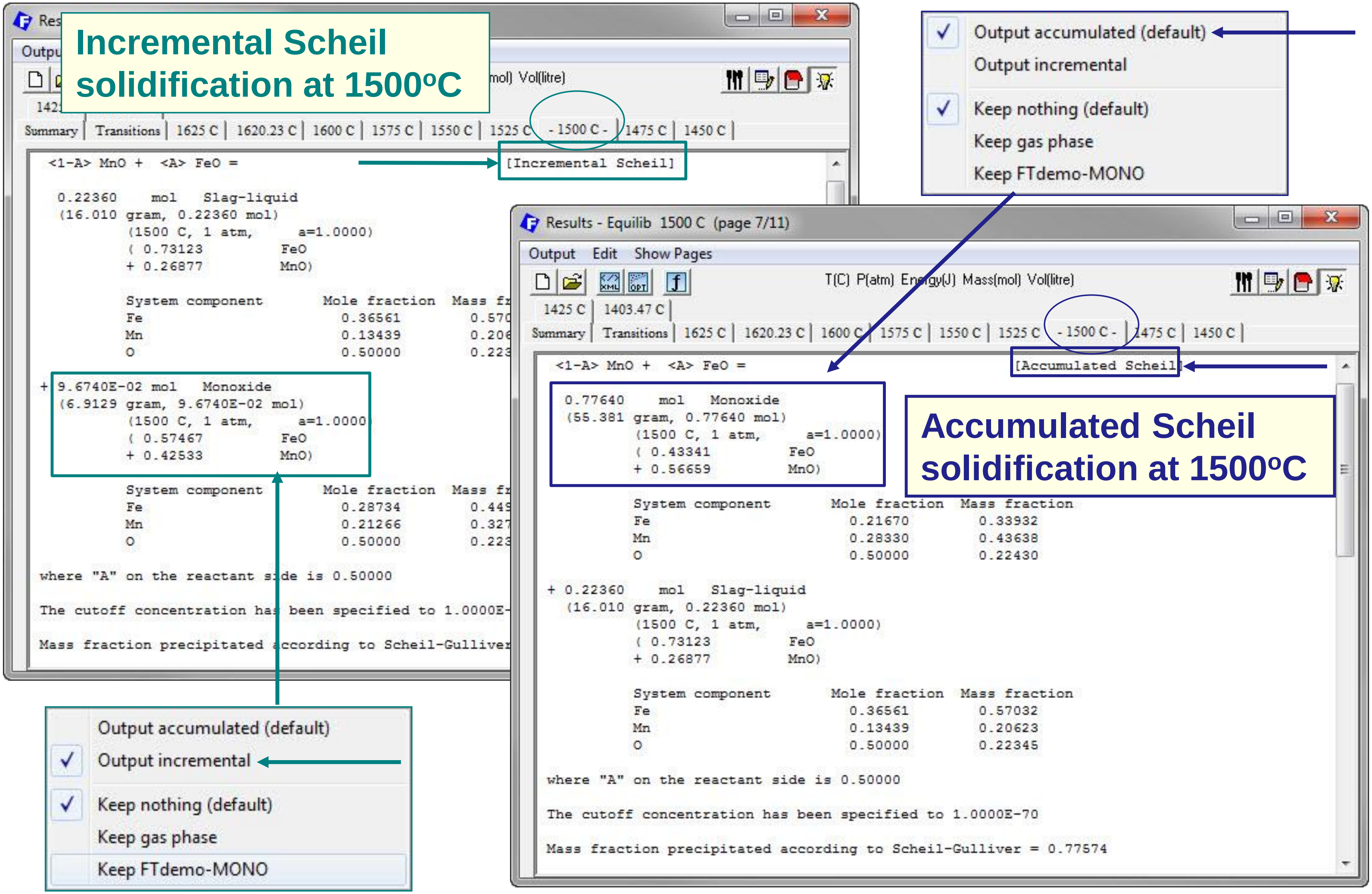
```
Temperature of final disappearance of Slag-liquid -> 1403.47 C

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
```

Start of solidification at 1620.23°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 1500ºC

```
<1-A> MnO +  <A> FeO =                            [Incremental Scheil]

  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

Accumulated Scheil solidification at 1500ºC

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

```
<1-A> MnO +  <A> FeO =                            [Accumulated Scheil]

  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
```

Scheil Cooling with Back Diffusion

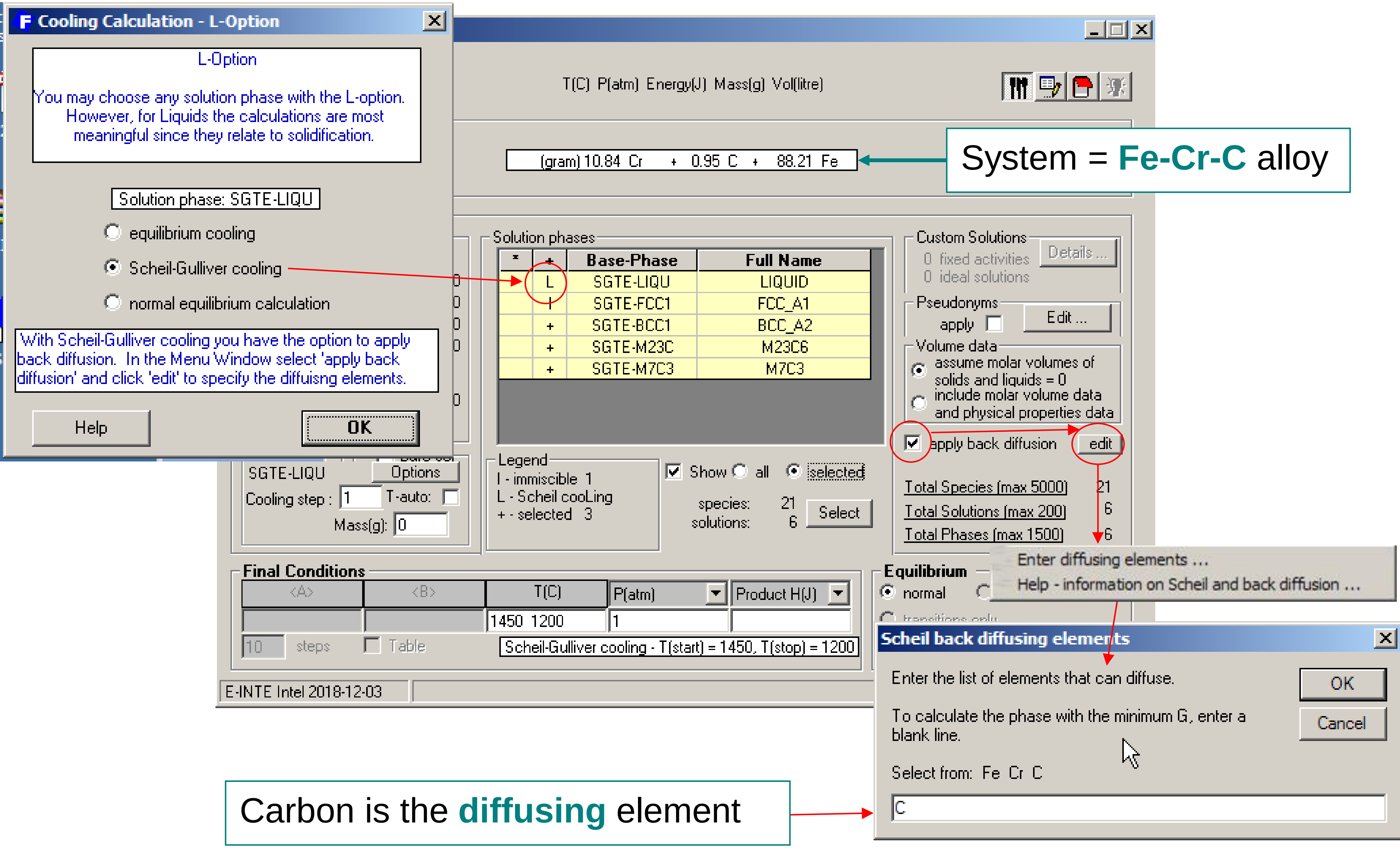
- In Scheil-Gulliver cooling with back diffusion, specified elements are permitted to equilibrate between phases during cooling. Other elements, once precipitated, remain in their solid phases and are removed from the mass balance as in regular Scheil cooling. After each incremental temperature decrease, ***Equilib*** permits exchange of only the diffusing elements among phases until their chemical potentials are the same in all phases.

- The following example is for an Fe-Cr-C alloy cooled from the liquid state with back diffusion of interstitial carbon.

- Input is exactly as in regular Scheil cooling except that the diffusing elements are specified.

- Output is similar to regular Scheil cooling.

Scheil Cooling with **Back Diffusion**



Cooling Calculation - L-Option

L-Option

You may choose any solution phase with the L-option. However, for Liquids the calculations are most meaningful since they relate to solidification.

Solution phase: SGTE-LIQU

○ equilibrium cooling

● Scheil-Gulliver cooling

○ normal equilibrium calculation

With Scheil-Gulliver cooling you have the option to apply back diffusion. In the Menu Window select 'apply back diffusion' and click 'edit' to specify the diffuisng elements.

(gram) 10.84 Cr + 0.95 C + 88.21 Fe

System = **Fe-Cr-C** alloy

Solution phases

*	+	Base-Phase	Full Name
	L	SGTE-LIQU	LIQUID
	I	SGTE-FCC1	FCC_A1
	+	SGTE-BCC1	BCC_A2
	+	SGTE-M23C	M23C6
	+	SGTE-M7C3	M7C3

Custom Solutions
0 fixed activities
0 ideal solutions

Pseudonyms
apply ☐

Volume data
● assume molar volumes of solids and liquids = 0
○ include molar volume data and physical properties data

☑ apply back diffusion

Total Species (max 5000) 21
Total Solutions (max 200) 6
Total Phases (max 1500) 6

Legend
I - immiscible 1
L - Scheil cooLing
+ - selected 3

☑ Show ○ all ● selected

species: 21
solutions: 6

SGTE-LIQU

Cooling step : 1 T-auto: ☐
Mass(g): 0

Final Conditions

<A>	<B>	T(C)	P(atm)	Product H(J)
		1450 1200	1	

10 steps ☐ Table

Scheil-Gulliver cooling - T(start) = 1450, T(stop) = 1200

Equilibrium
● normal
○ transitions only

E-INTE Intel 2018-12-03

Enter diffusing elements ...
Help - information on Scheil and back diffusion ...

Scheil back diffusing elements

Enter the list of elements that can diffuse.

To calculate the phase with the minimum G, enter a blank line.

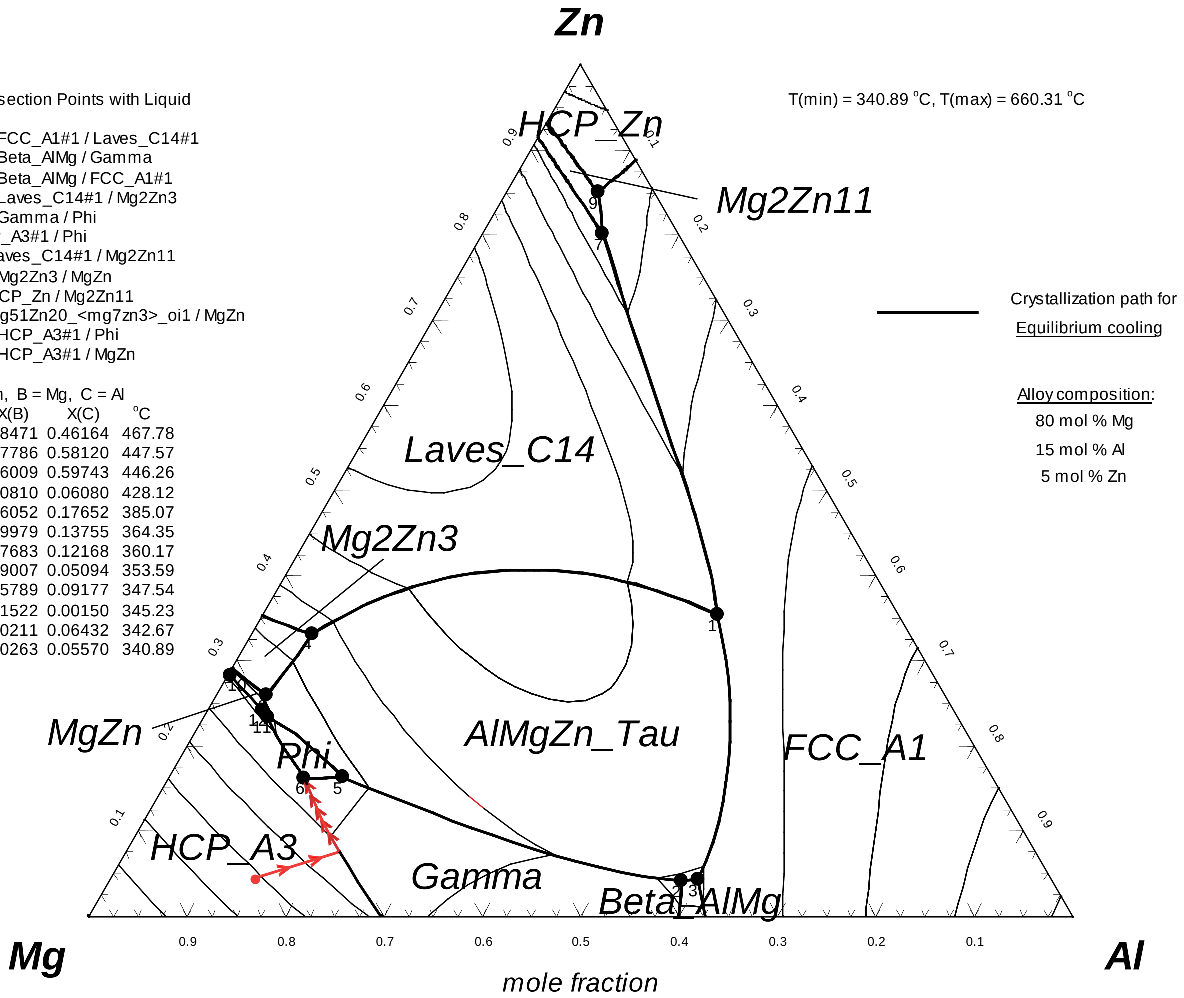
Select from: Fe Cr C

C

Carbon is the **diffusing** element

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

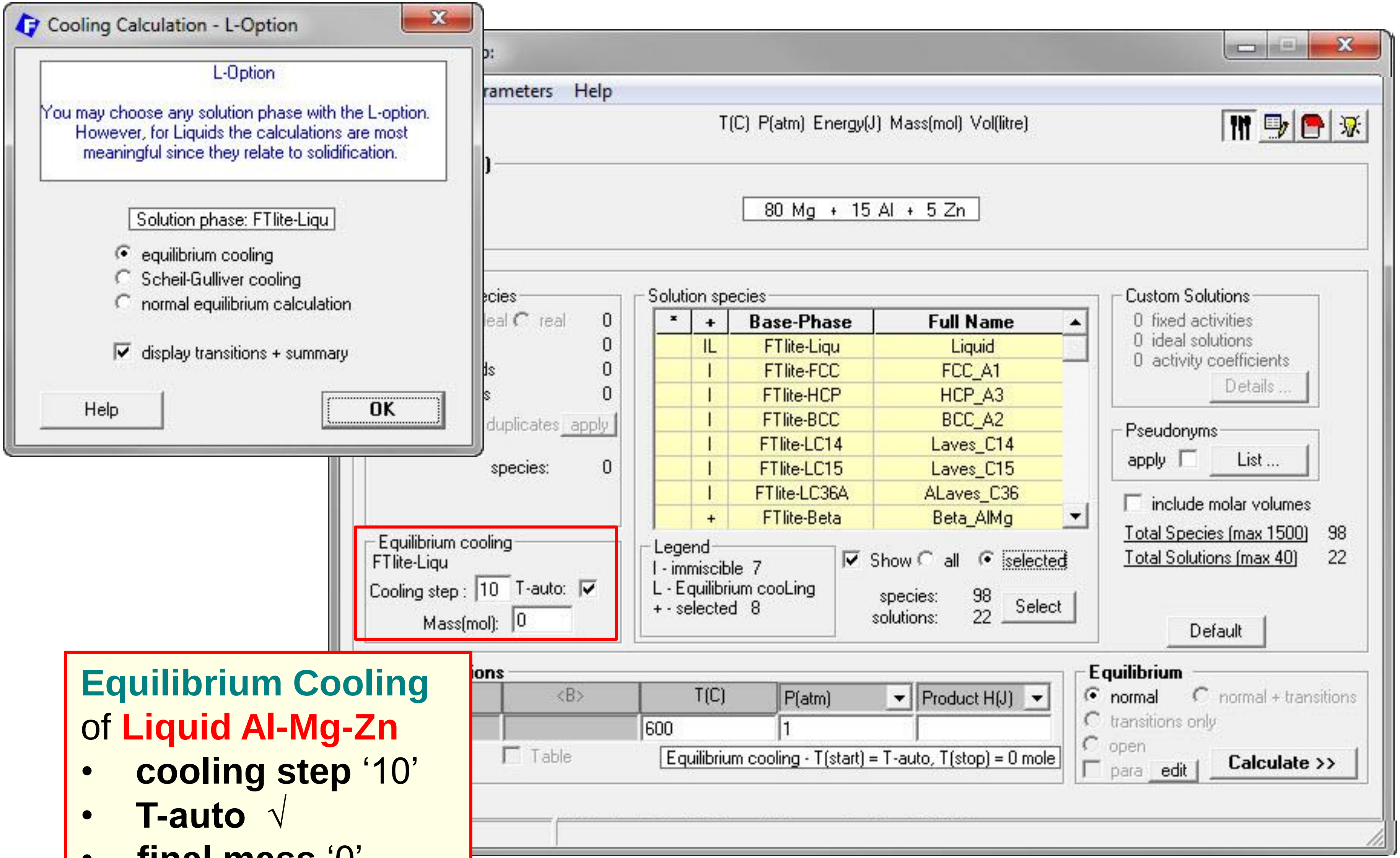
T(min) = 340.89 °C, T(max) = 660.31 °C

Crystallization path for
Equilibrium cooling

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

Equilib Advanced 13.4

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



Cooling Calculation - L-Option

L-Option

You may choose any solution phase with the L-option. However, for Liquids the calculations are most meaningful since they relate to solidification.

Solution phase: FTlite-Liqu

● equilibrium cooling
○ Scheil-Gulliver cooling
○ normal equilibrium calculation

☑ display transitions + summary

80 Mg + 15 Al + 5 Zn

Solution species

*	+	Base-Phase	Full Name
	IL	FTlite-Liqu	Liquid
	I	FTlite-FCC	FCC_A1
	I	FTlite-HCP	HCP_A3
	I	FTlite-BCC	BCC_A2
	I	FTlite-LC14	Laves_C14
	I	FTlite-LC15	Laves_C15
	I	FTlite-LC36A	ALaves_C36
	+	FTlite-Beta	Beta_AlMg

Legend
I - immiscible 7
L - Equilibrium cooLing
+ - selected 8

☑ Show ○ all ● selected

species: 98
solutions: 22

Custom Solutions
0 fixed activities
0 ideal solutions
0 activity coefficients

Pseudonyms
apply ☐

☐ include molar volumes

Total Species (max 1500) 98
Total Solutions (max 40) 22

Equilibrium cooling
FTlite-Liqu
Cooling step : 10 T-auto: ☑
Mass(mol): 0

<B>	T(C)	P(atm)	Product H(J)
	600	1	

☐ Table

Equilibrium cooling - T(start) = T-auto, T(stop) = 0 mole

Equilibrium
● normal ○ normal + transitions
○ transitions only
○ open
☐ para

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

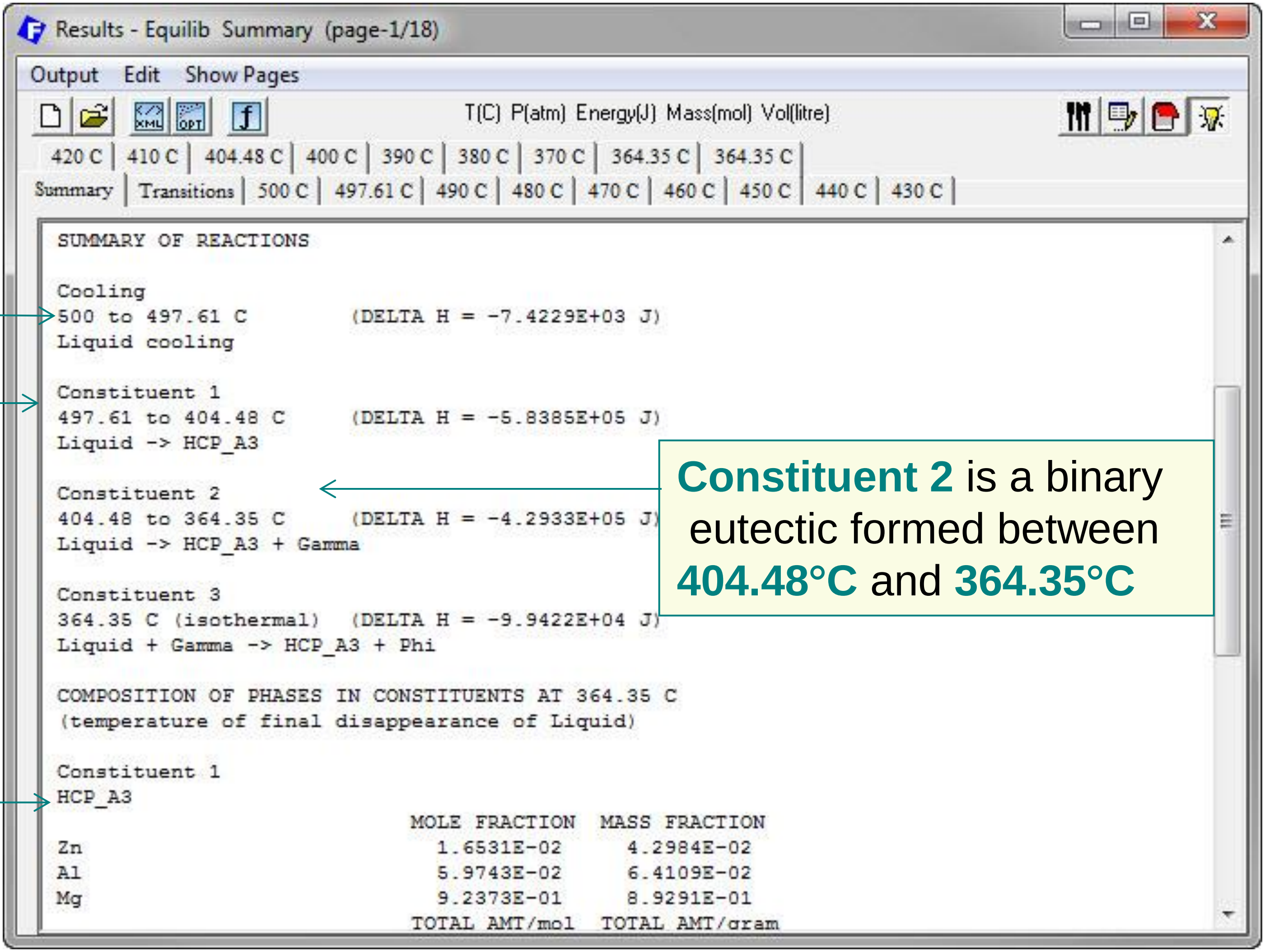
- **cooling step** ‘10’
- **T-auto** √
- **final mass** ‘0’

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**

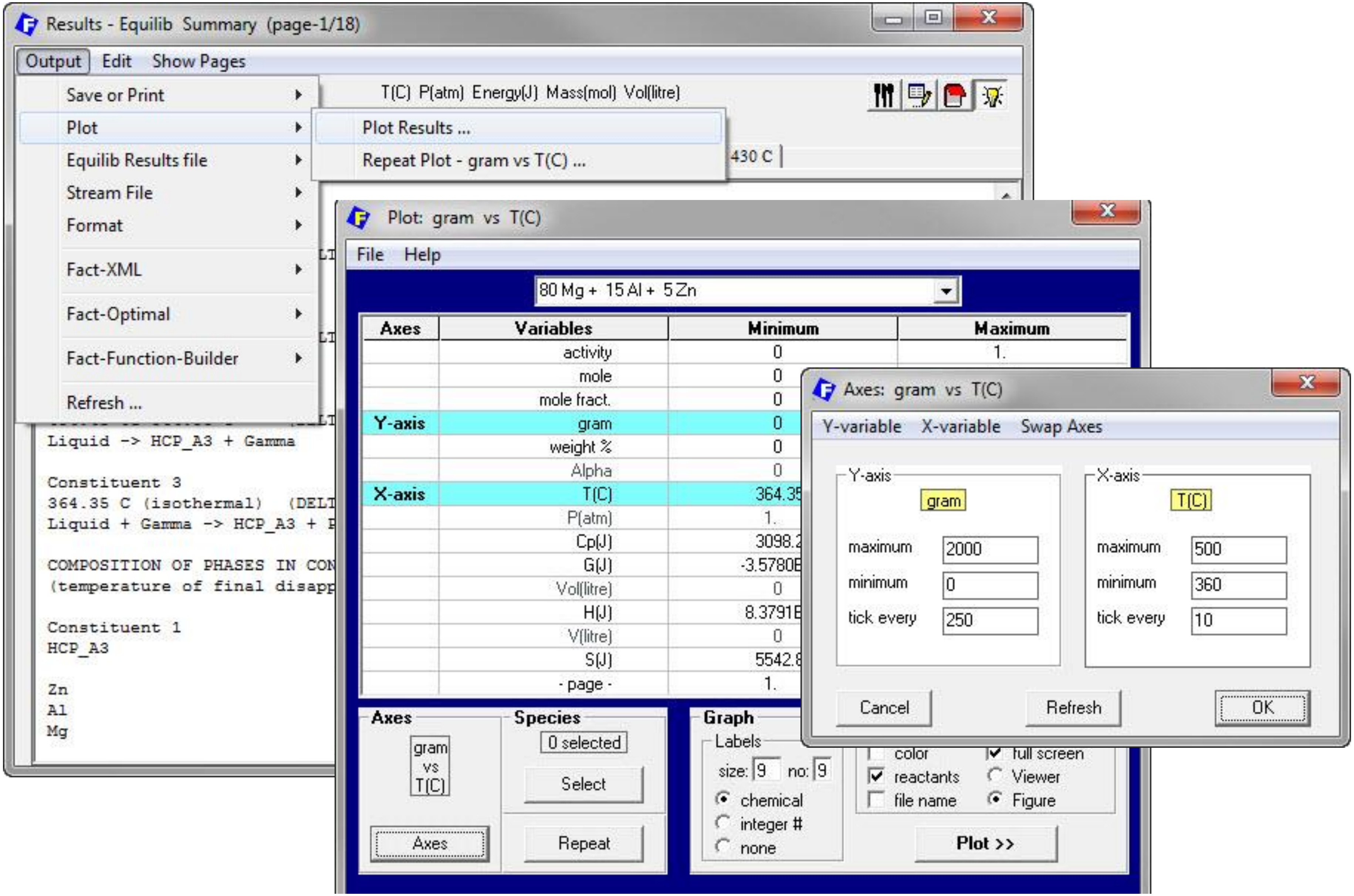
Microstructural **constituents**, and the phases in them



```
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



```
Liquid -> HCP_A3 + Gamma

Constituent 3
364.35 C (isothermal)   (DELT
Liquid + Gamma -> HCP_A3 + P

COMPOSITION OF PHASES IN CON
(temperature of final disapp

Constituent 1
HCP_A3

Zn
Al
Mg
```

80 Mg + 15 Al + 5 Zn

Axes	Variables	Minimum	Maximum
	activity	0	1.
	mole	0	
	mole fract.	0	
Y-axis	gram	0	
	weight %	0	
	Alpha	0	
X-axis	T(C)	364.35	
	P(atm)	1.	
	Cp(J)	3098.2	
	G(J)	-3.5780E	
	Vol(litre)	0	
	H(J)	8.3791E	
	V(litre)	0	
	S(J)	5542.8	
	- page -	1.	

Axes: gram vs T(C)

	Y-axis	X-axis
	gram	T(C)
maximum	2000	500
minimum	0	360
tick every	250	10

Axes: gram vs T(C)

Labels: size: 9 no: 9

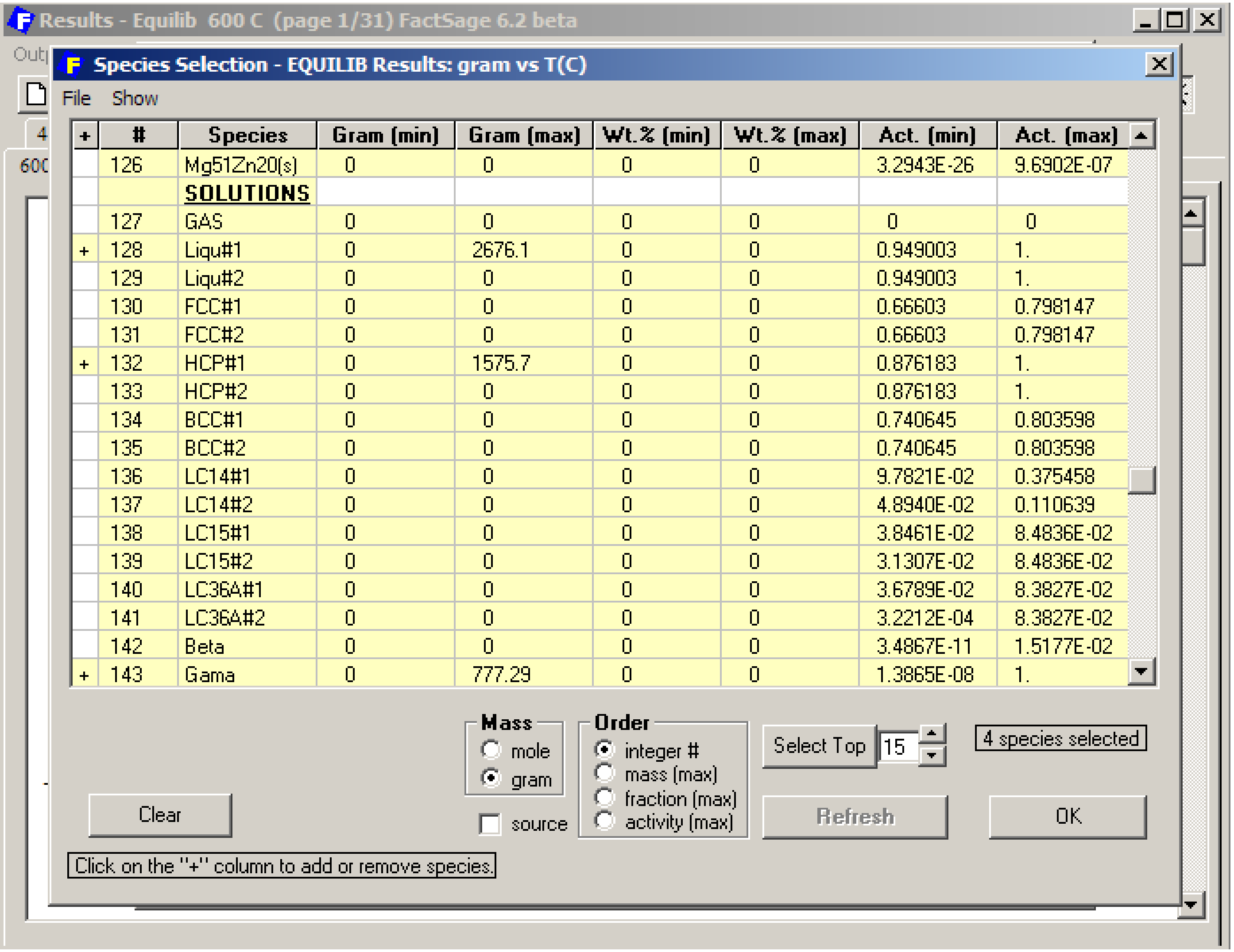
● chemical
○ integer #
○ none

☐ color
☑ reactants
☐ file name

☑ full screen
○ Viewer
● Figure

Al-Mg-Zn : Equilibium cooling – Plot Results

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



+	#	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

☐ source

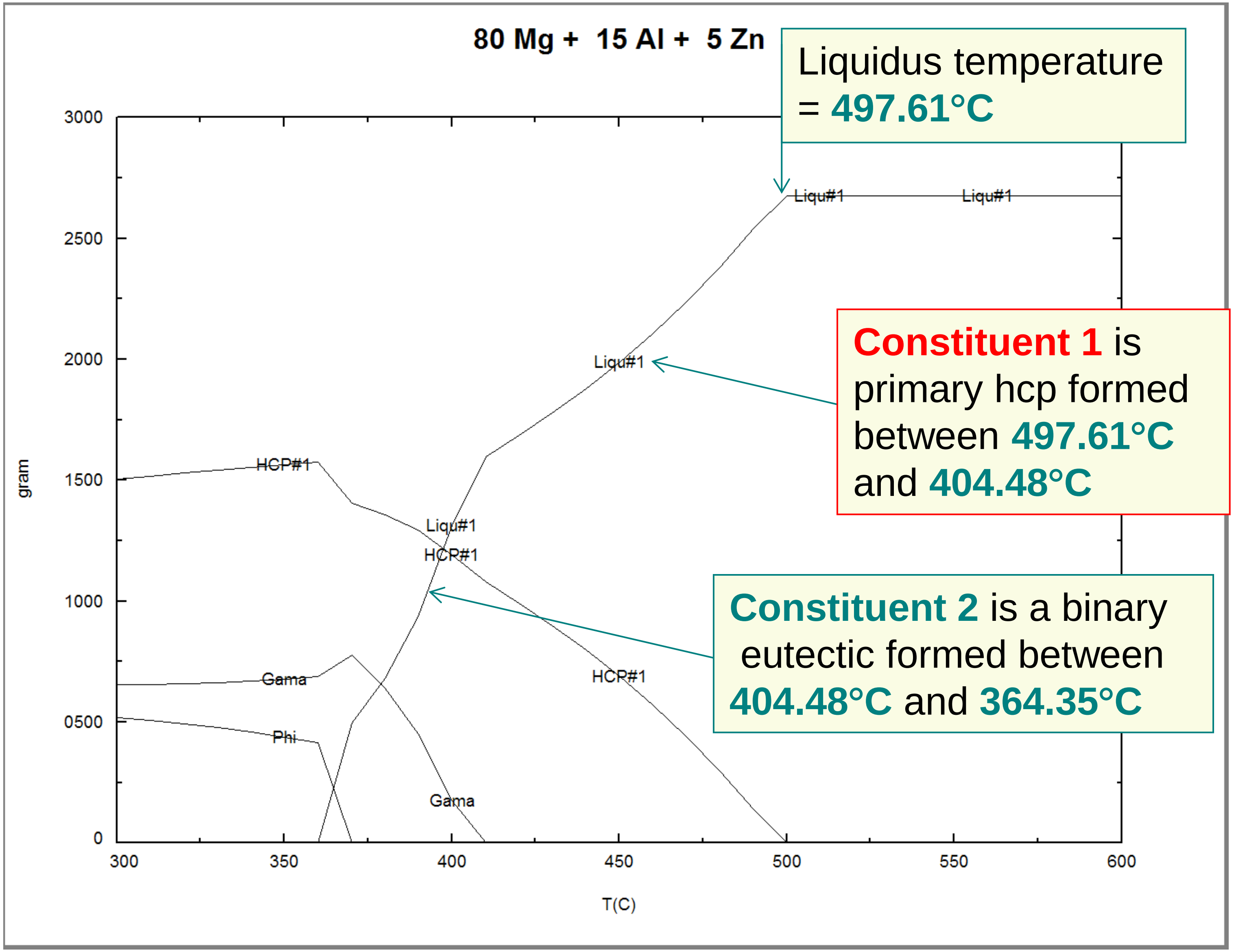
Order
● integer #
○ mass (max)
○ fraction (max)
○ activity (max)

Select Top 15

4 species selected

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

Al-Mg-Zn : Equilibium cooling – Plot Results



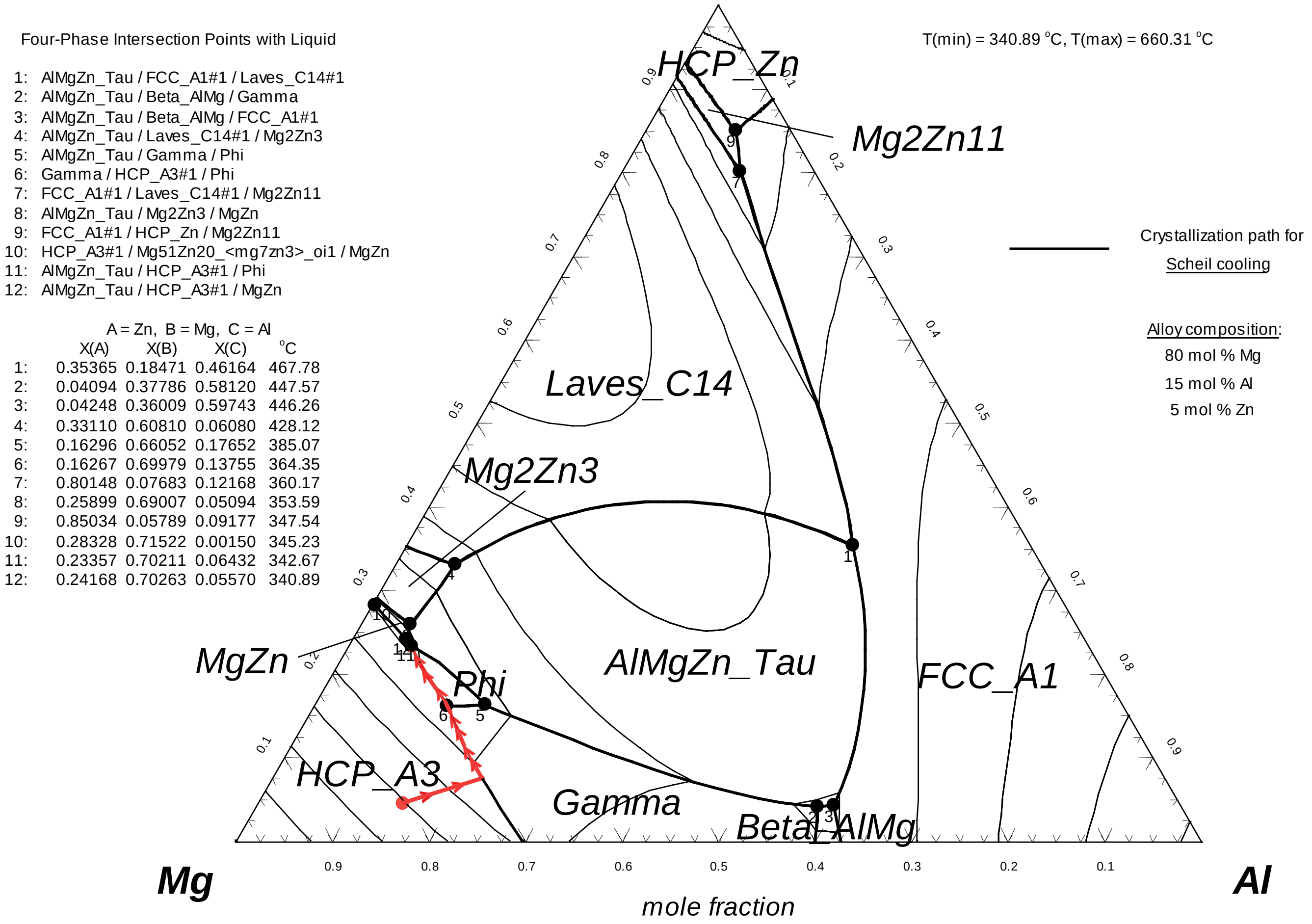
Liquidus temperature = **497.61°C**

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

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

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

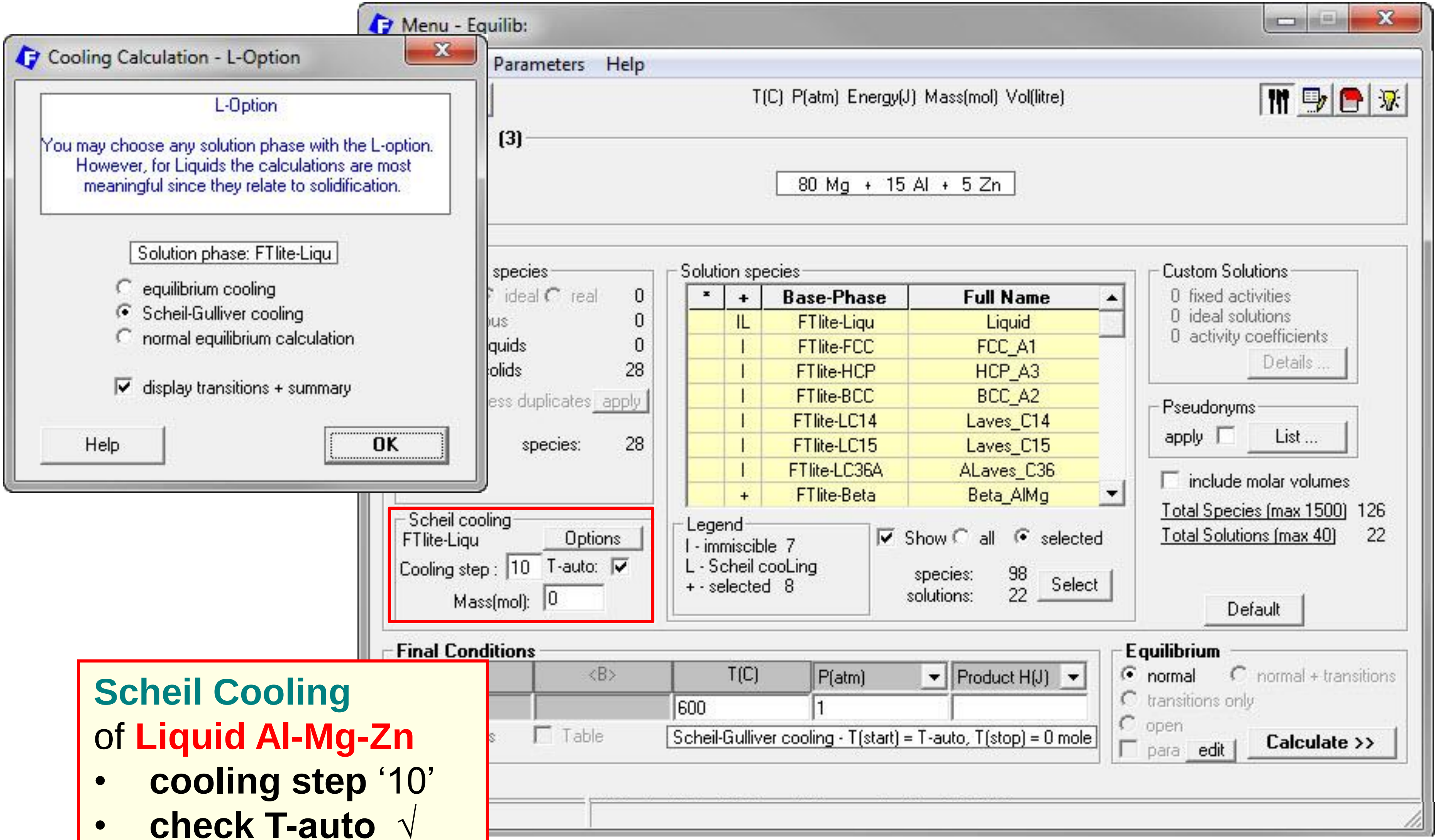
	X(A)	X(B)	X(C)	°C
1:	0.35365	0.18471	0.46164	467.78
2:	0.04094	0.37786	0.58120	447.57
3:	0.04248	0.36009	0.59743	446.26
4:	0.33110	0.60810	0.06080	428.12
5:	0.16296	0.66052	0.17652	385.07
6:	0.16267	0.69979	0.13755	364.35
7:	0.80148	0.07683	0.12168	360.17
8:	0.25899	0.69007	0.05094	353.59
9:	0.85034	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



Cooling Calculation - L-Option

L-Option

You may choose any solution phase with the L-option. However, for Liquids the calculations are most meaningful since they relate to solidification.

Solution phase: FTlite-Liqu

○ equilibrium cooling
● Scheil-Gulliver cooling
○ normal equilibrium calculation

☑ display transitions + summary

Menu - Equilib:

80 Mg + 15 Al + 5 Zn

Solution species

*	+	Base-Phase	Full Name
	IL	FTlite-Liqu	Liquid
	I	FTlite-FCC	FCC_A1
	I	FTlite-HCP	HCP_A3
	I	FTlite-BCC	BCC_A2
	I	FTlite-LC14	Laves_C14
	I	FTlite-LC15	Laves_C15
	I	FTlite-LC36A	ALaves_C36
	+	FTlite-Beta	Beta_AlMg

Legend
I - immiscible 7
L - Scheil cooLing
+ - selected 8

☑ Show ○ all ● selected
species: 98
solutions: 22

Total Species (max 1500) 126
Total Solutions (max 40) 22

Scheil cooling
FTlite-Liqu
Cooling step : 10 T-auto: ☑
Mass(mol): 0

Final Conditions

T(C)	P(atm)	Product H(J)
600	1	

Scheil-Gulliver cooling - T(start) = T-auto, T(stop) = 0 mole

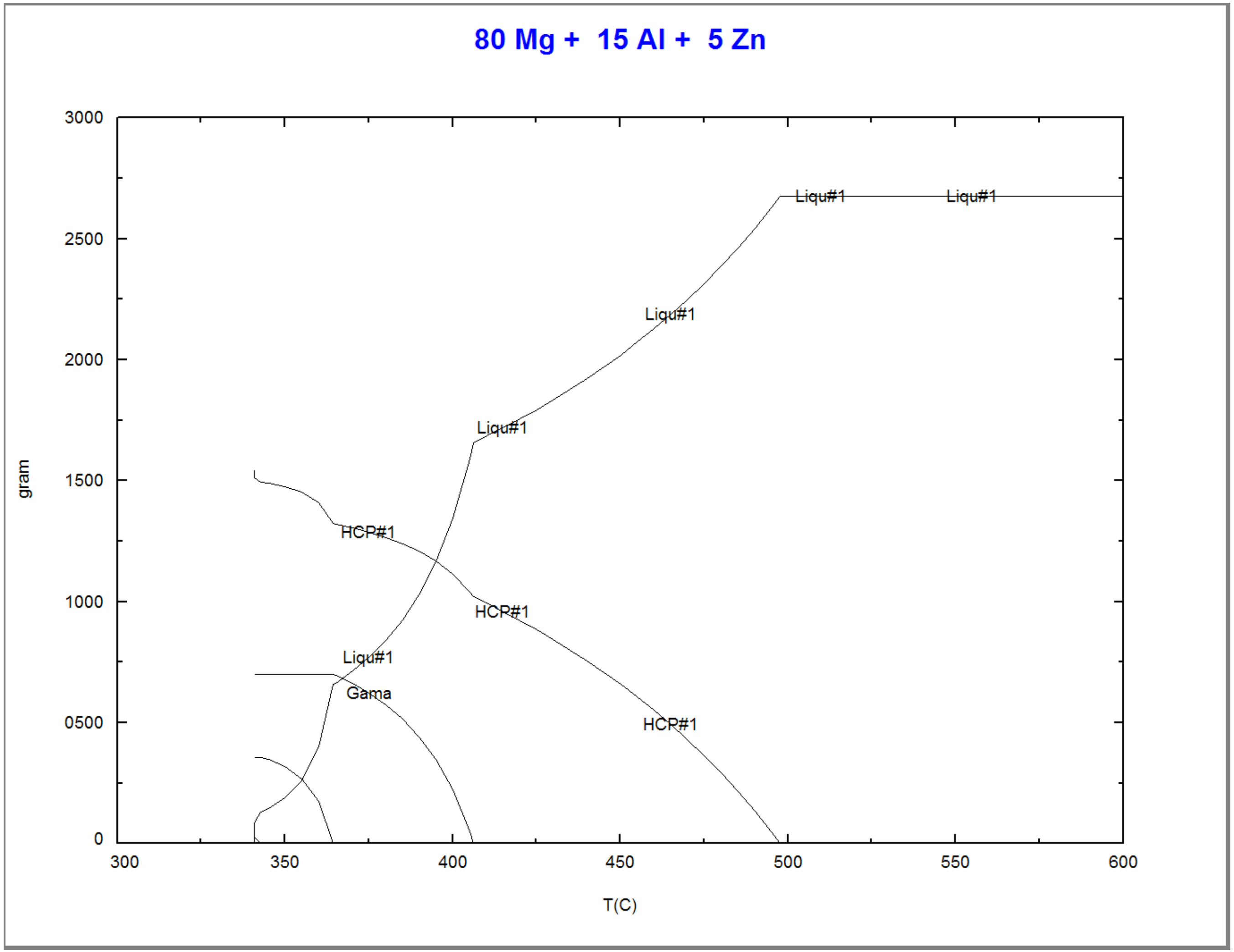
Equilibrium
● normal ○ normal + transitions
○ transitions only
○ open

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

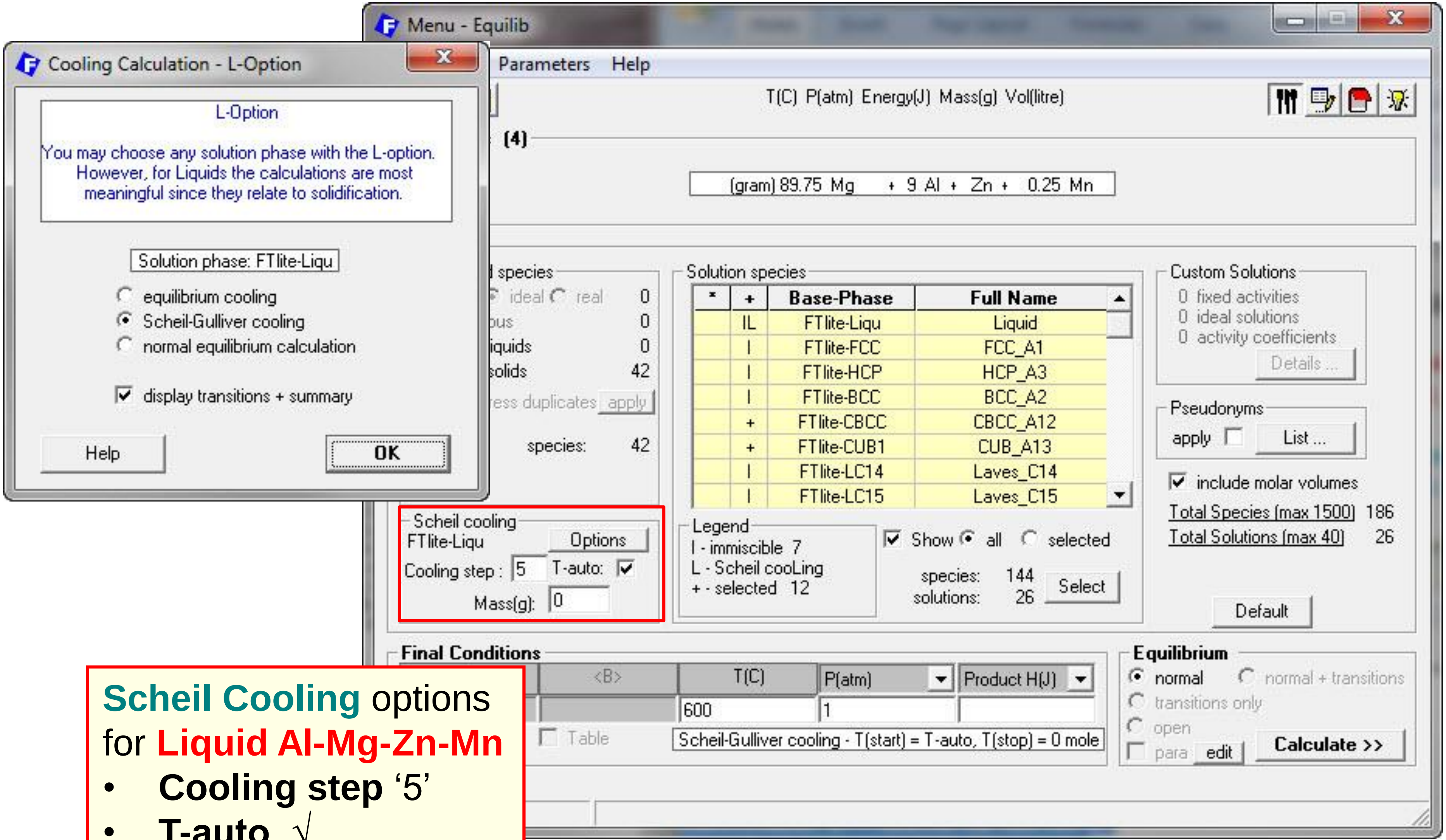
- **cooling step** ‘10’
- **check T-auto** √
- **enter final mass** ‘0’

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



Cooling Calculation - L-Option

L-Option

You may choose any solution phase with the L-option. However, for Liquids the calculations are most meaningful since they relate to solidification.

Solution phase: FTlite-Liqu

○ equilibrium cooling
● Scheil-Gulliver cooling
○ normal equilibrium calculation

☑ display transitions + summary

Menu - Equilib

(gram) 89.75 Mg + 9 Al + Zn + 0.25 Mn

Solution species

*	+	Base-Phase	Full Name
	IL	FTlite-Liqu	Liquid
	I	FTlite-FCC	FCC_A1
	I	FTlite-HCP	HCP_A3
	I	FTlite-BCC	BCC_A2
	+	FTlite-CBCC	CBCC_A12
	+	FTlite-CUB1	CUB_A13
	I	FTlite-LC14	Laves_C14
	I	FTlite-LC15	Laves_C15

Scheil cooling
FTlite-Liqu
Cooling step : 5 T-auto: ☑
Mass(g): 0

Legend
I - immiscible 7
L - Scheil cooLing
+ - selected 12

☑ Show ● all ○ selected
species: 144
solutions: 26

☑ include molar volumes
Total Species (max 1500) 186
Total Solutions (max 40) 26

Final Conditions

T(C)	P(atm)
600	1

Scheil-Gulliver cooling - T(start) = T-auto, T(stop) = 0 mole

Equilibrium
● normal ○ normal + transitions
○ transitions only
○ open

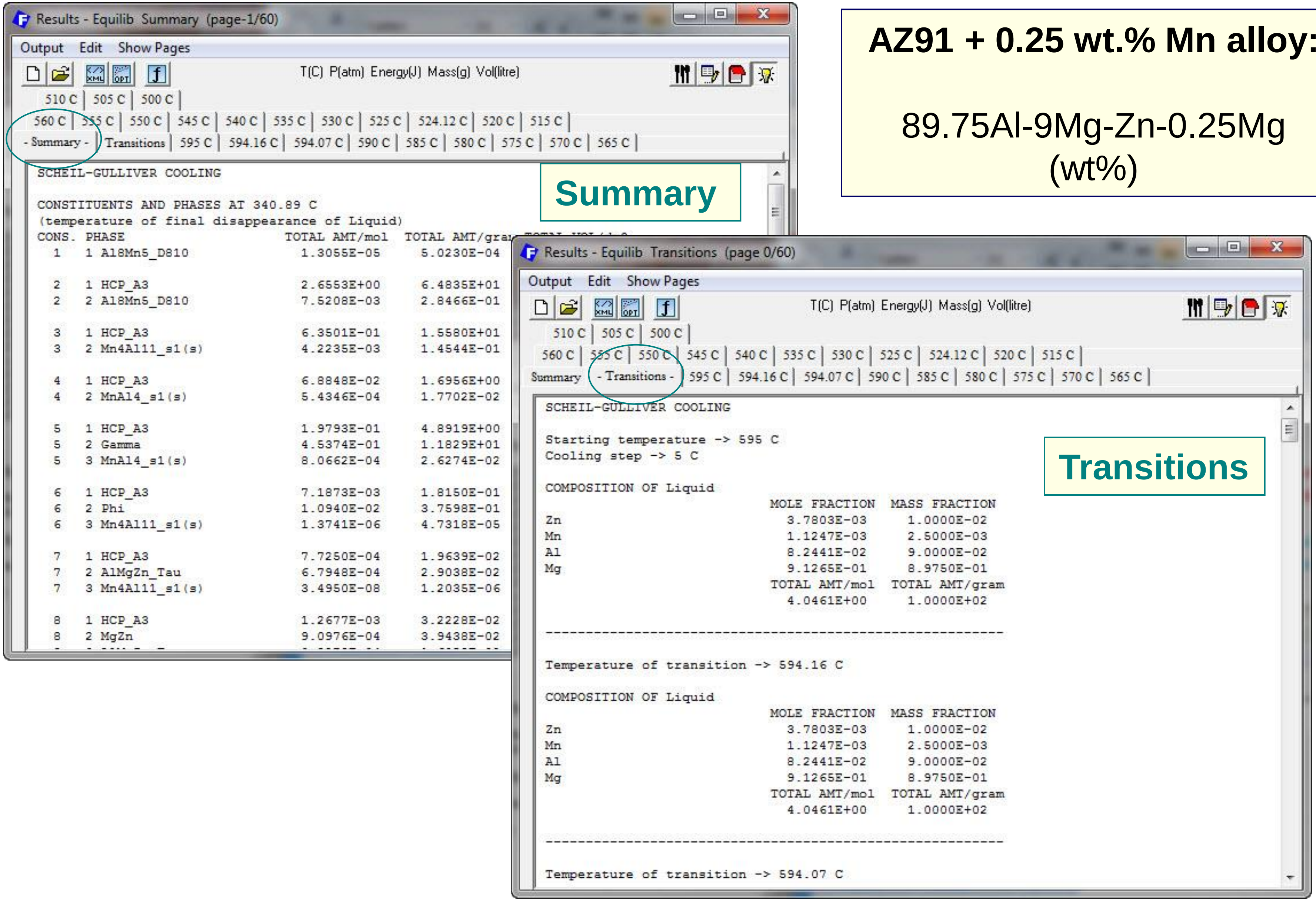
Scheil Cooling options for **Liquid Al-Mg-Zn-Mn**

- **Cooling step** ‘5’
- **T-auto** √
- **Final mass(g)** ‘0’

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

AZ91 + 0.25 wt.% Mn alloy:

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



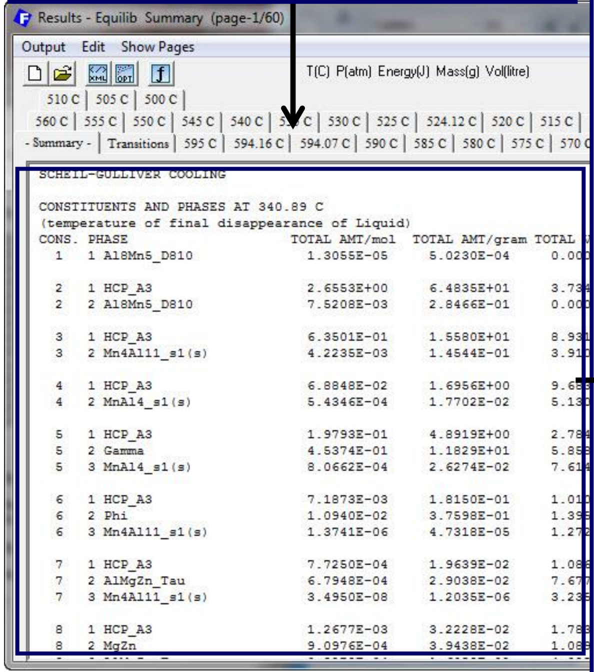
```
SCHEIL-GULLIVER COOLING

CONSTITUENTS AND PHASES AT 340.89 C
(temperature of final disappearance of Liquid)
CONS. PHASE                          TOTAL AMT/mol  TOTAL AMT/gra
  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
```

```
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.



```
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
  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     9.6
  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 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

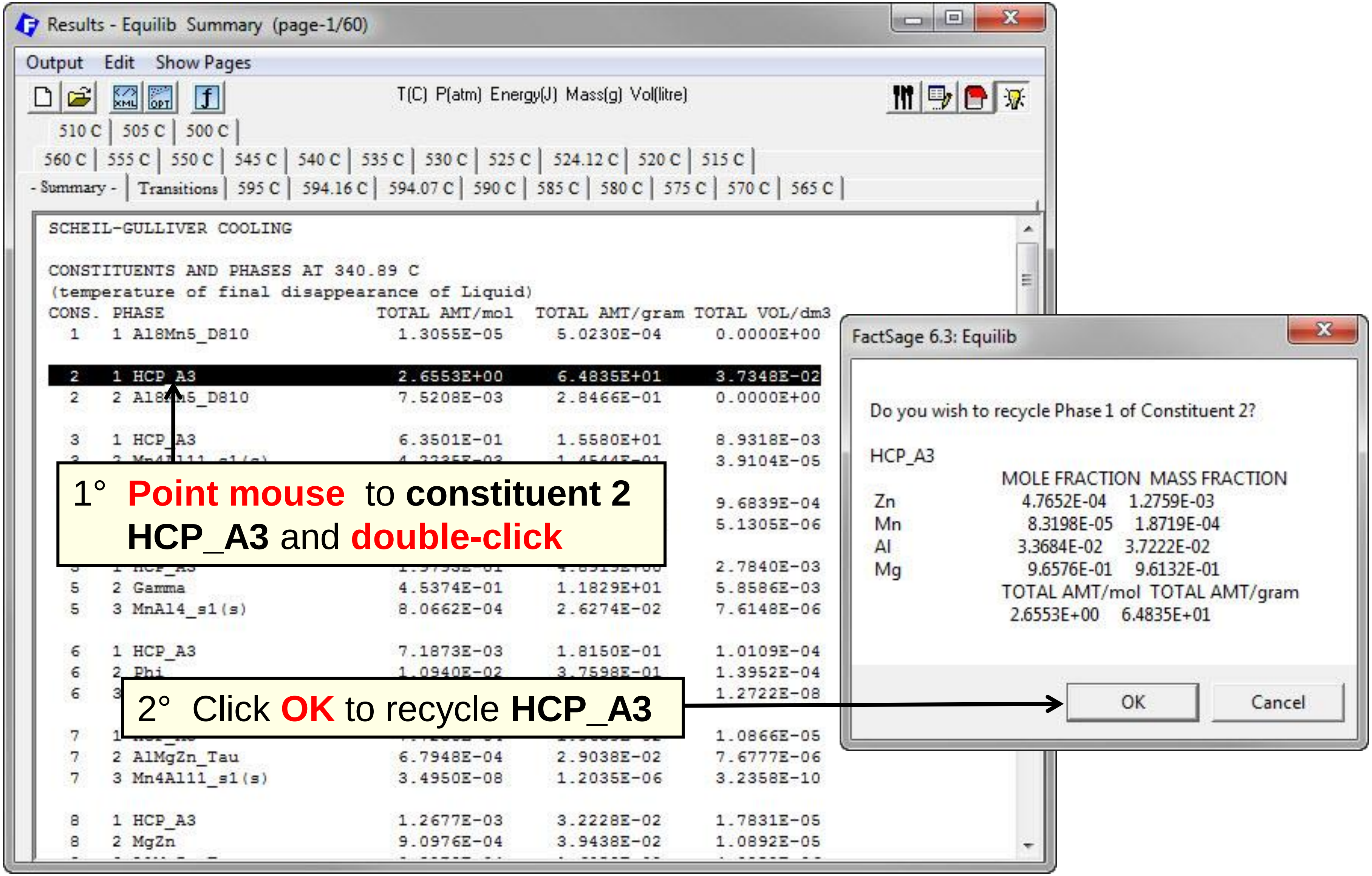
Output : Solidification temperature of 340.89°C

```
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



```
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
                                                               3.9104E-05

                                                               9.6839E-04
                                                               5.1305E-06

                                                               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                                                            1.3952E-04
  6                                                            1.2722E-08

  7                                                            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
```

Do you wish to recycle Phase 1 of Constituent 2?

HCP_A3

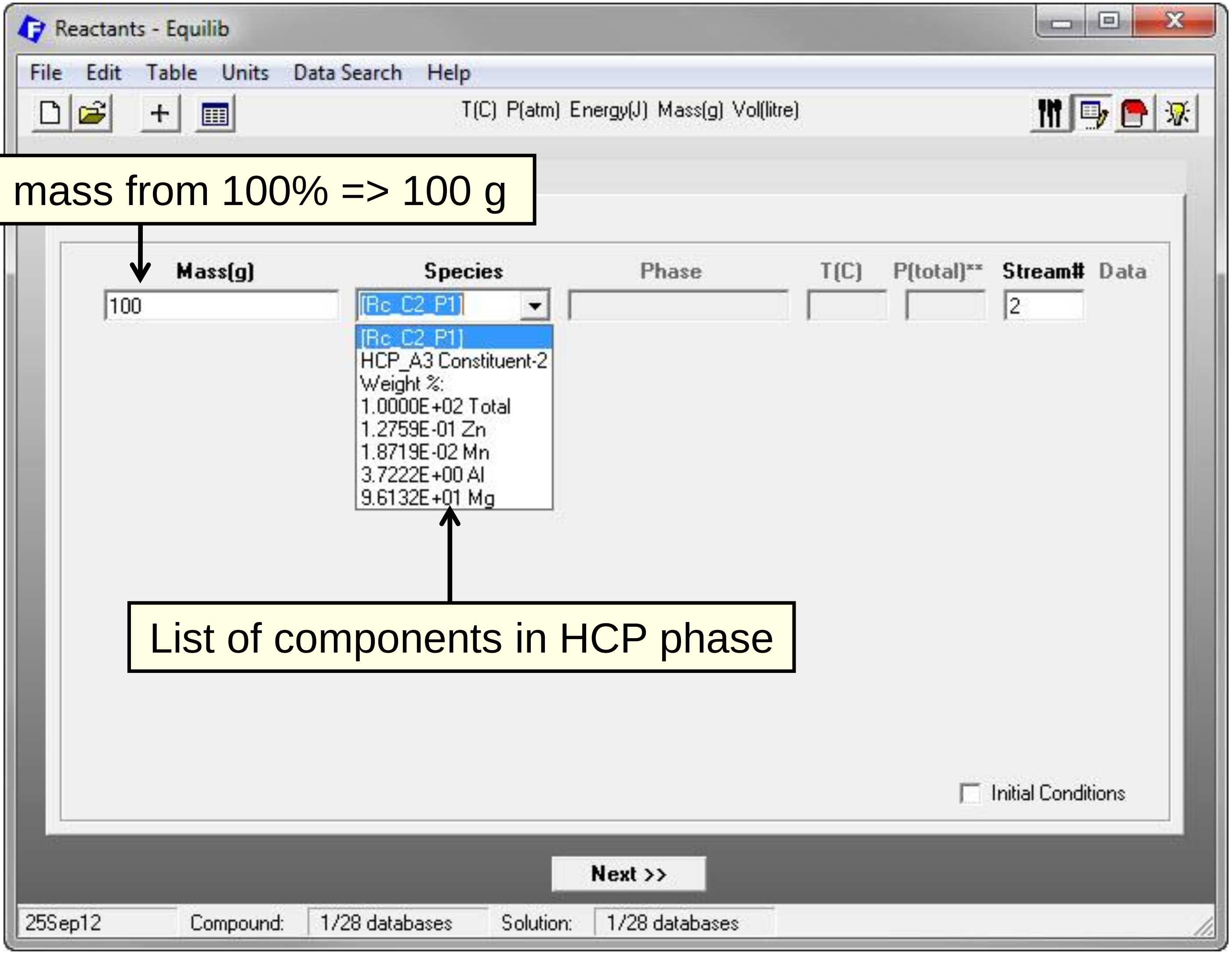
	MOLE FRACTION	MASS FRACTION
Zn	4.7652E-04	1.2759E-03
Mn	8.3198E-05	1.8719E-04
Al	3.3684E-02	3.7222E-02
Mg	9.6576E-01	9.6132E-01

TOTAL AMT/mol	TOTAL AMT/gram
2.6553E+00	6.4835E+01

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

2° Click **OK** to recycle **HCP_A3**

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



Mass(g): 100

Species: [Rc_C2_P1]

Stream#: 2

[Rc_C2_P1]
HCP_A3 Constituent-2
Weight %:
1.0000E+02 Total
1.2759E-01 Zn
1.8719E-02 Mn
3.7222E+00 Al
9.6132E+01 Mg

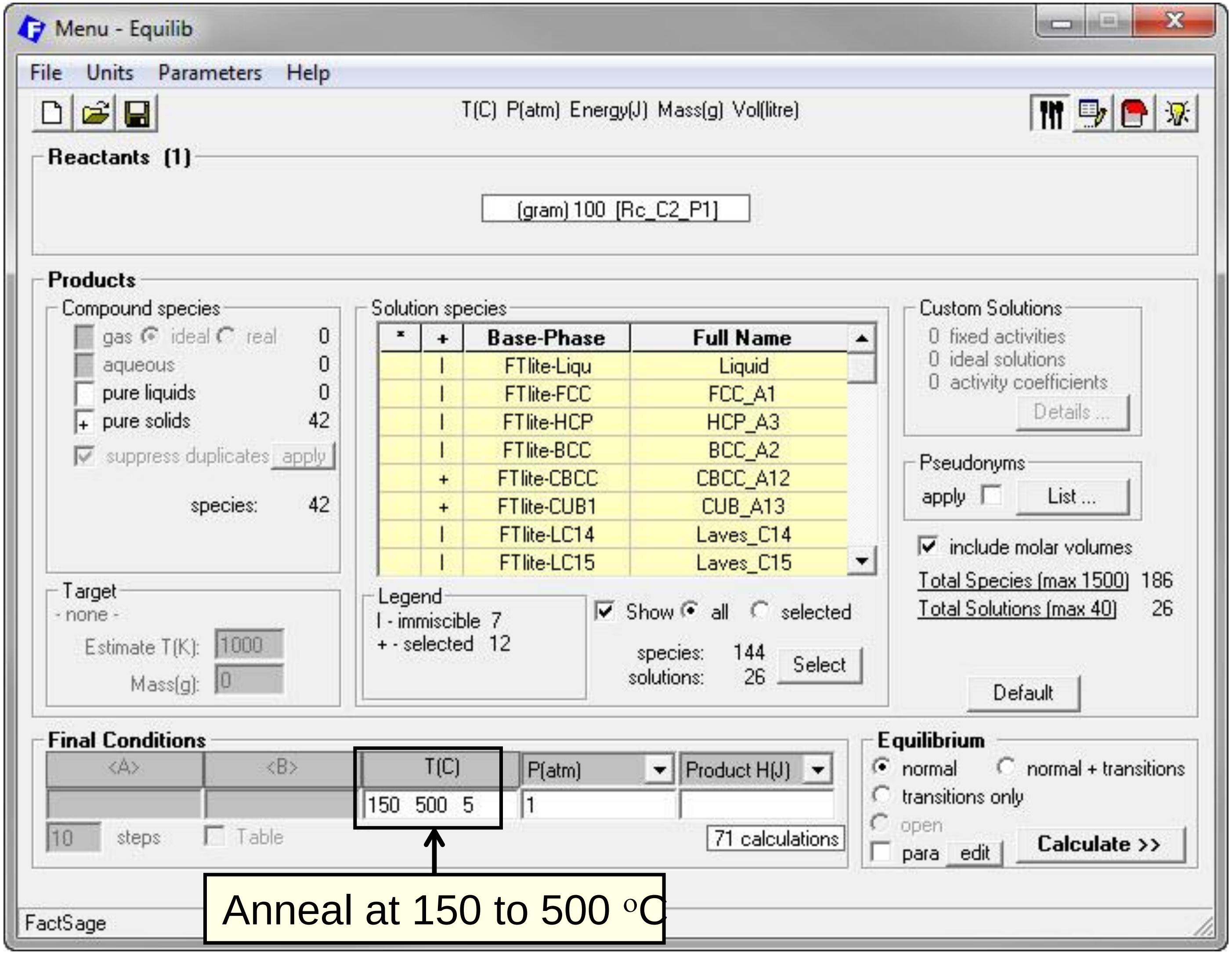
☐ Initial Conditions

25Sep12 Compound: 1/28 databases Solution: 1/28 databases

Change mass from 100% => 100 g

List of components in HCP phase

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



Reactants (1)

(gram) 100 [Rc_C2_P1]

Products

Compound species

☐ gas ● ideal ○ real 0
☐ aqueous 0
☐ pure liquids 0
+ pure solids 42
☑ suppress duplicates
species: 42

Solution species

*	+	Base-Phase	Full Name
	I	FTlite-Liqu	Liquid
	I	FTlite-FCC	FCC_A1
	I	FTlite-HCP	HCP_A3
	I	FTlite-BCC	BCC_A2
	+	FTlite-CBCC	CBCC_A12
	+	FTlite-CUB1	CUB_A13
	I	FTlite-LC14	Laves_C14
	I	FTlite-LC15	Laves_C15

Legend
I - immiscible 7
+ - selected 12

☑ Show ● all ○ selected
species: 144
solutions: 26

Custom Solutions
0 fixed activities
0 ideal solutions
0 activity coefficients

Pseudonyms
apply ☐

☑ include molar volumes
Total Species (max 1500) 186
Total Solutions (max 40) 26

Target
- none -
Estimate T(K): 1000
Mass(g): 0

Final Conditions

<A>	<B>	T(C)	P(atm)	Product H(J)
		150 500 5	1	

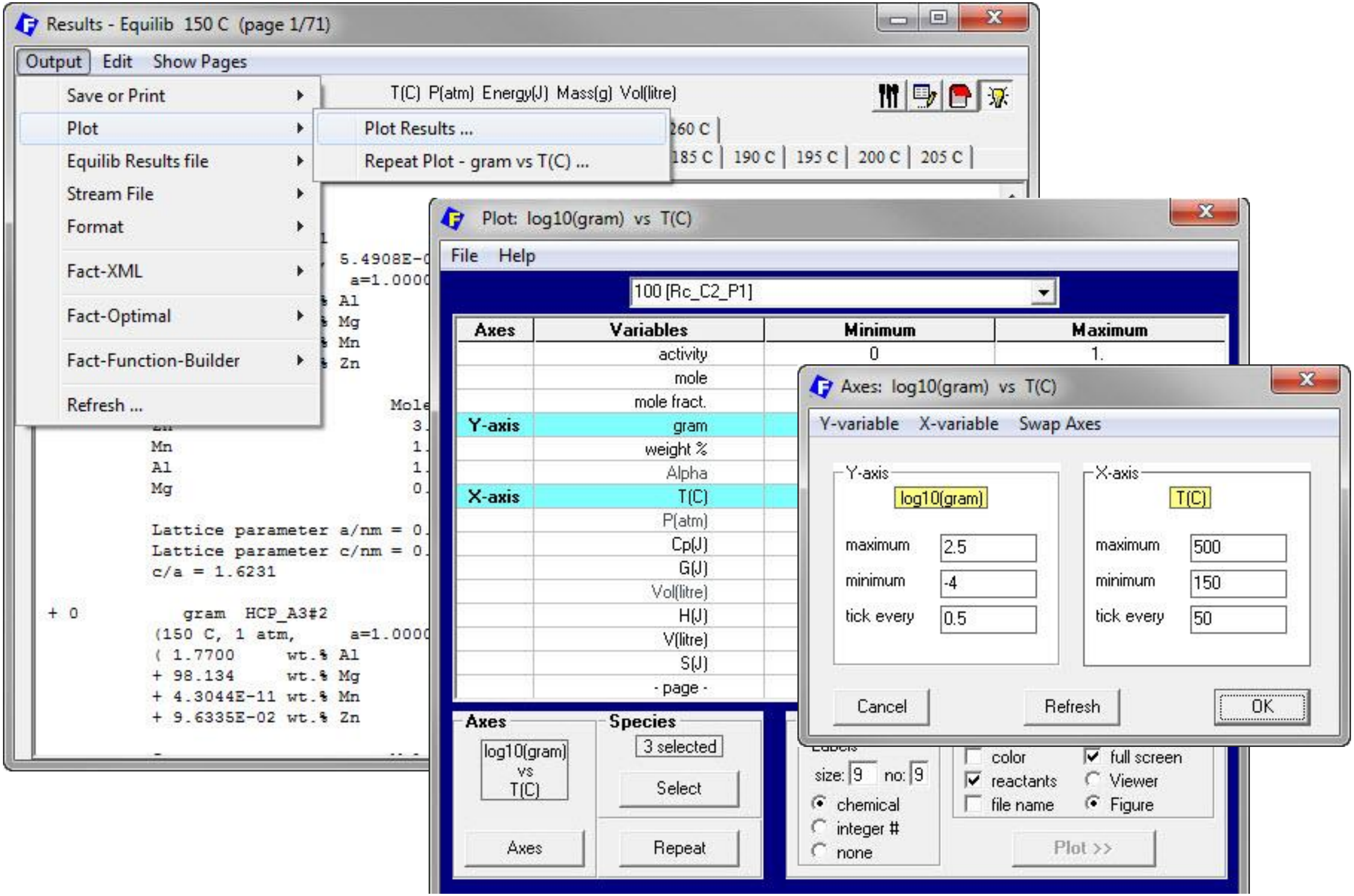
10 steps ☐ Table
71 calculations

Equilibrium

● normal ○ normal + transitions
○ transitions only
○ open
☐ para

Anneal at 150 to 500 °C

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



```
                                          1
                                        , 5.4908E-0
                                          a=1.0000
                                        % Al
                                        % Mg
                                        % Mn
                                        % Zn

                                    Mole
          Zn                          3.
          Mn                          1.
          Al                          1.
          Mg                          0.

          Lattice parameter a/nm = 0.
          Lattice parameter c/nm = 0.
          c/a = 1.6231

 + 0         gram  HCP_A3#2
          (150 C, 1 atm,          a=1.0000
          ( 1.7700      wt.% Al
          + 98.134      wt.% Mg
          + 4.3044E-11 wt.% Mn
          + 9.6335E-02 wt.% Zn
```

100 [Rc_C2_P1]

Axes	Variables	Minimum	Maximum
	activity	0	1.
	mole		
	mole fract.		
Y-axis	gram		
	weight %		
	Alpha		
X-axis	T(C)		
	P(atm)		
	Cp(J)		
	G(J)		
	Vol(litre)		
	H(J)		
	V(litre)		
	S(J)		
	- page -		

Axes: log10(gram) vs T(C)

Species: 3 selected

Labels: size: 9 no: 9

● chemical
○ integer #
○ none

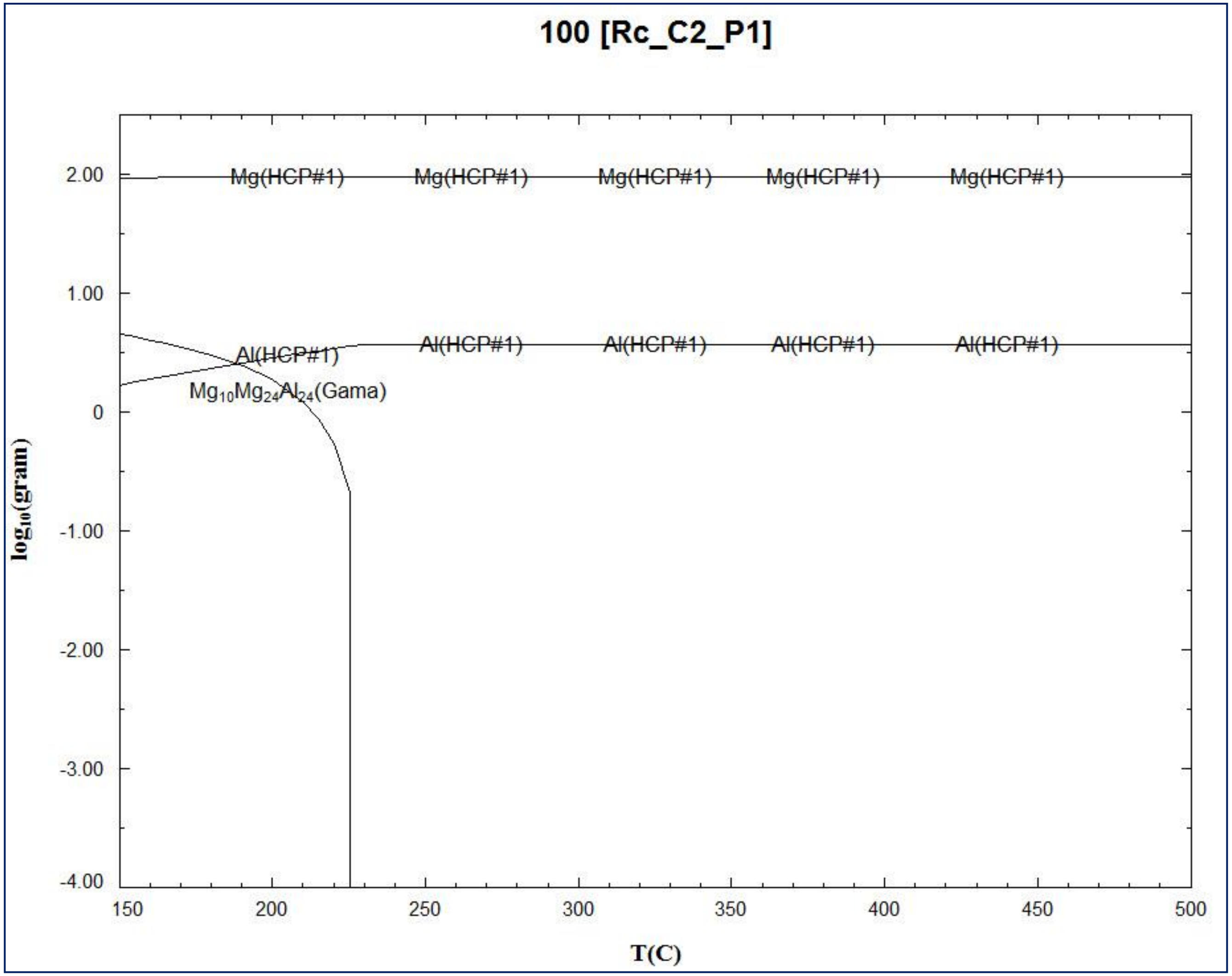
☐ color
☑ reactants
☐ file name

☑ full screen
○ Viewer
● Figure

	Y-axis	X-axis
	log10(gram)	T(C)
maximum	2.5	500
minimum	-4	150
tick every	0.5	50

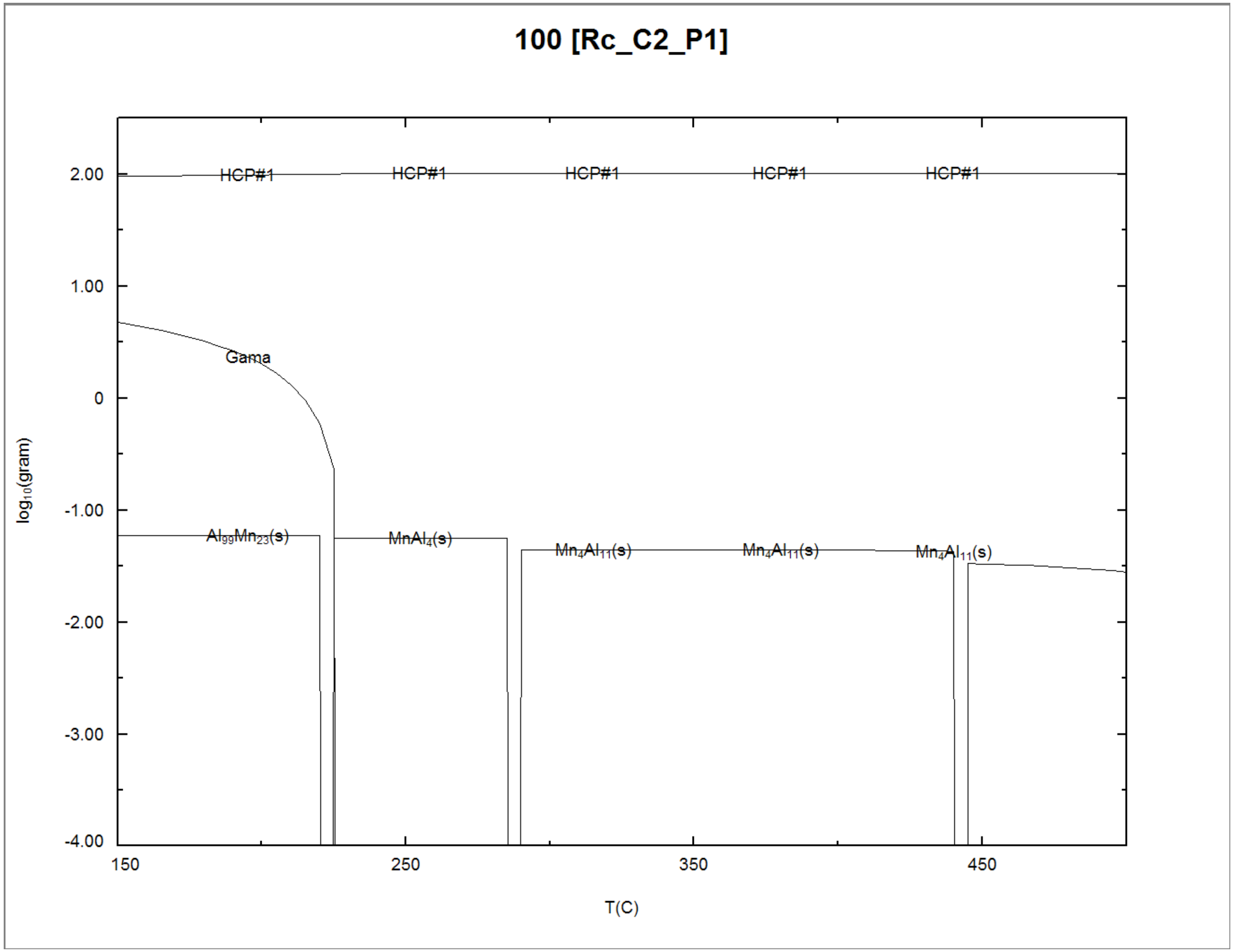
Al-Mg-Zn-Mn : Graph of fully annealed HCP phase

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

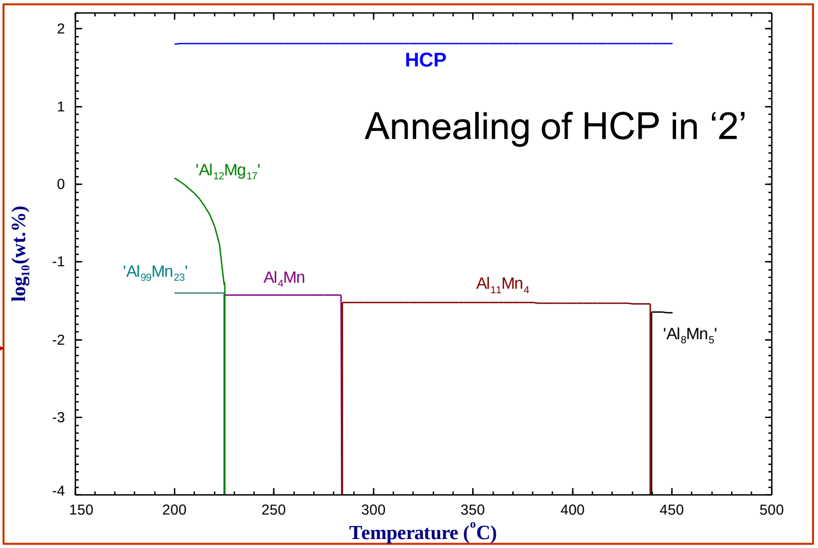
Scheil cooling and post equilibration (annealing) of Scheil microstructure: AZ91 alloy + 0.25 wt.% Mn

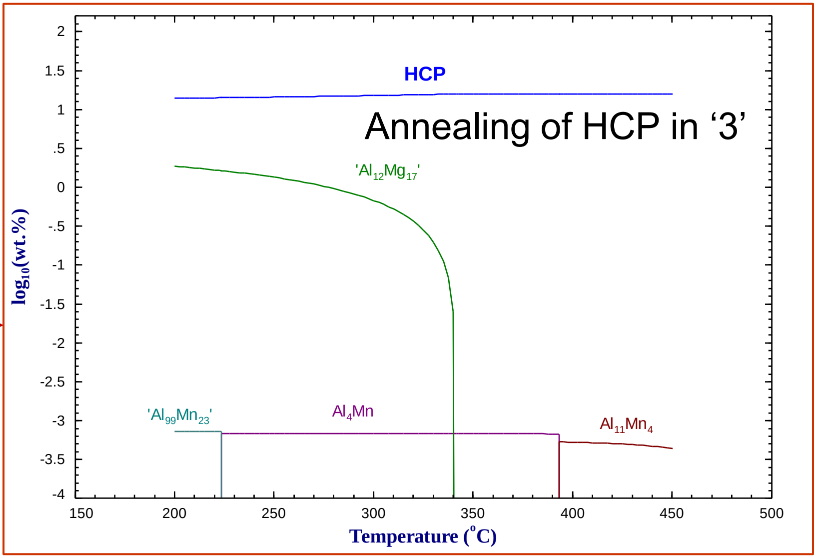
Tracking microstructure constituents

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.

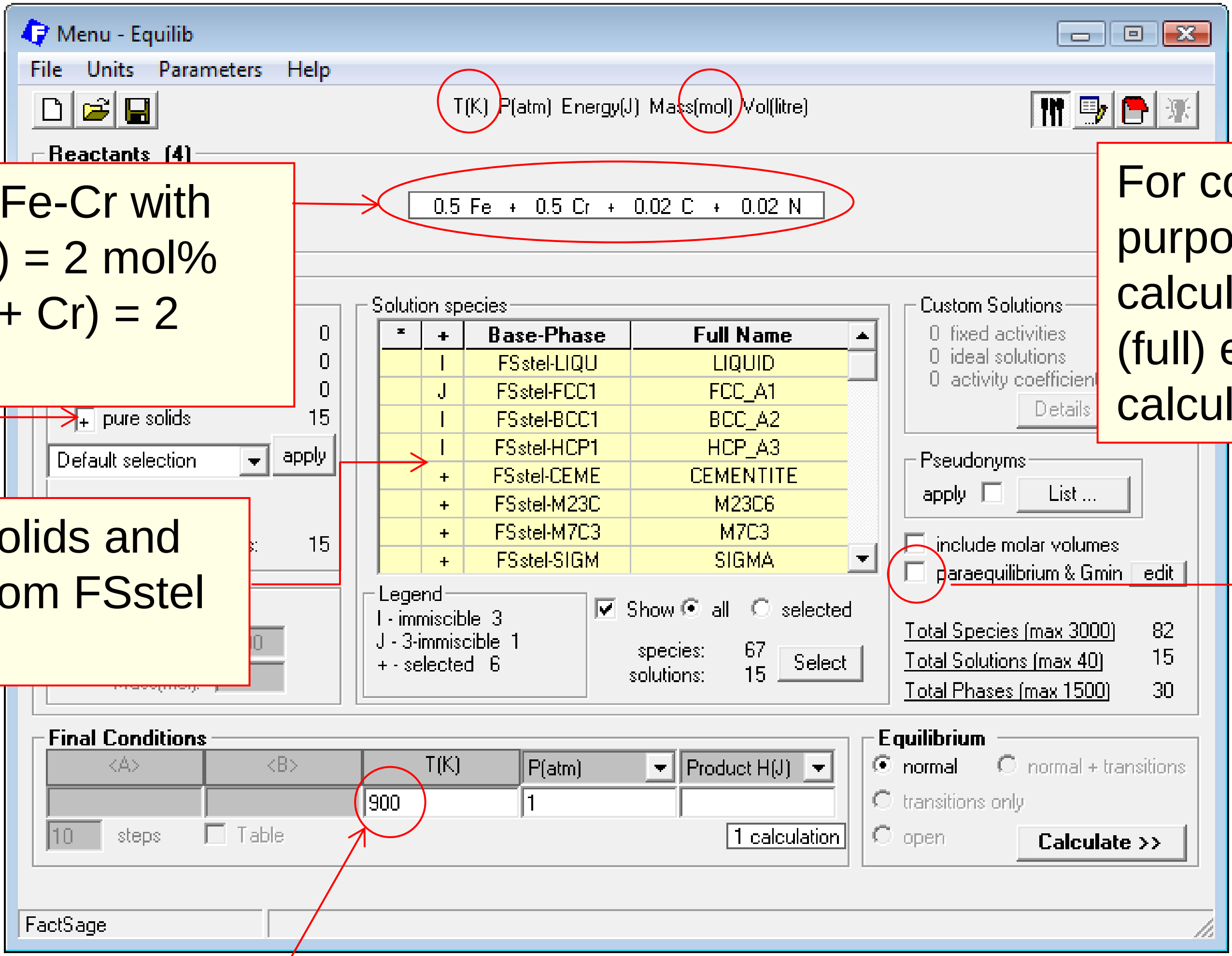
- At paraequilibrium, the ratios of the slowly diffusing elements in all phases are the same and are equal to their ratios in the initial single-phase alloy. The algorithm used to calculate paraequilibrium in FactSage is based upon this fact. That is, the algorithm minimizes the Gibbs energy of the system 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



Menu - Equilib

Reactants (4)

0.5 Fe + 0.5 Cr + 0.02 C + 0.02 N

☐+ pure solids 15

Default selection apply

Solution species

*	+	Base-Phase	Full Name
	I	FSstel-LIQU	LIQUID
	J	FSstel-FCC1	FCC_A1
	I	FSstel-BCC1	BCC_A2
	I	FSstel-HCP1	HCP_A3
	+	FSstel-CEME	CEMENTITE
	+	FSstel-M23C	M23C6
	+	FSstel-M7C3	M7C3
	+	FSstel-SIGM	SIGMA

Legend
I - immiscible 3
J - 3-immiscible 1
+ - selected 6

☑ Show ● all ○ selected

species: 67
solutions: 15

Select

Custom Solutions
0 fixed activities
0 ideal solutions
0 activity coefficien

Details

Pseudonyms
apply ☐ List ...

☐ include molar volumes
☐ paraequilibrium & Gmin edit

Total Species (max 3000) 82
Total Solutions (max 40) 15
Total Phases (max 1500) 30

Final Conditions

<A>	<B>	T(K)	P(atm)	Product H(J)
		900	1	

10 steps ☐ Table

1 calculation

Equilibrium
● normal ○ normal + transitions
○ transitions only
○ open

Calculate >>

FactSage

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

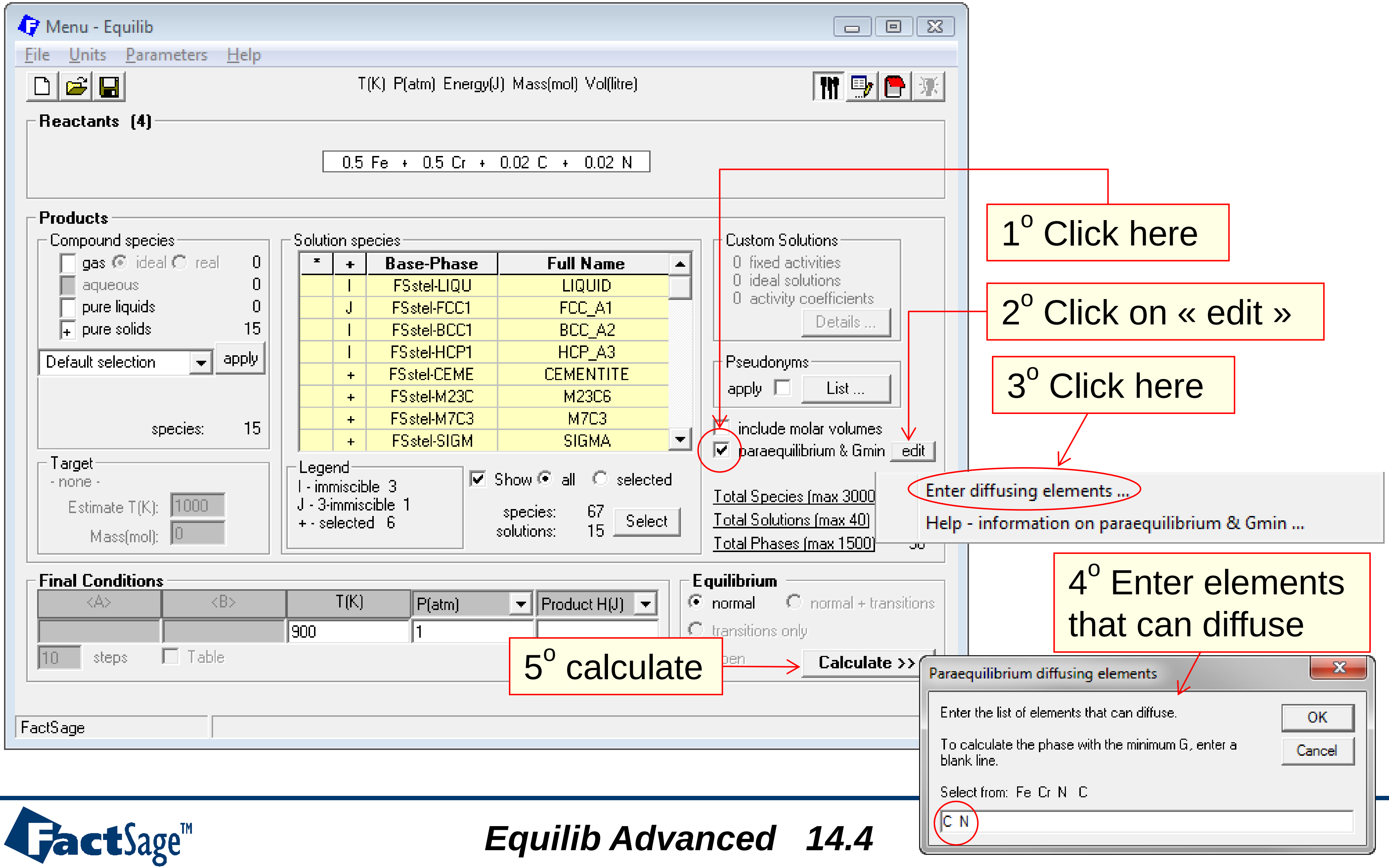
```
0.5 Fe +  0.5 Cr +  0.02 C +  0.02 N =

   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



Menu - Equilib

Reactants (4)

0.5 Fe + 0.5 Cr + 0.02 C + 0.02 N

Products

Compound species

☐ gas ● ideal ○ real	0
☐ aqueous	0
☐ pure liquids	0
☐+ pure solids	15

Default selection · apply

species: 15

Solution species

*	+	Base-Phase	Full Name
	I	FSstel-LIQU	LIQUID
	J	FSstel-FCC1	FCC_A1
	I	FSstel-BCC1	BCC_A2
	I	FSstel-HCP1	HCP_A3
	+	FSstel-CEME	CEMENTITE
	+	FSstel-M23C	M23C6
	+	FSstel-M7C3	M7C3
	+	FSstel-SIGM	SIGMA

Legend
I - immiscible 3
J - 3-immiscible 1
+ - selected 6

☑ Show ● all ○ selected

species: 67
solutions: 15

Custom Solutions
0 fixed activities
0 ideal solutions
0 activity coefficients

Pseudonyms
apply ☐ List ...

☐ include molar volumes
☑ paraequilibrium & Gmin · edit

Total Species (max 3000
Total Solutions (max 40)
Total Phases (max 1500)

Enter diffusing elements ...
Help - information on paraequilibrium & Gmin ...

Target
- none -
Estimate T(K): 1000
Mass(mol): 0

Final Conditions

<A>	<B>	T(K)	P(atm)	Product H(J)
		900	1	

10 steps ☐ Table

Equilibrium
● normal ○ normal + transitions
○ transitions only

Calculate >>

FactSage

Paraequilibrium diffusing elements

Enter the list of elements that can diffuse.

To calculate the phase with the minimum G, enter a blank line.

Select from: Fe Cr N C

C N

OK · Cancel

1^o Click here

2^o Click on « edit »

3^o Click here

4^o Enter elements that can diffuse

5^o calculate

Paraequilibrium and minimum Gibbs energy calculations

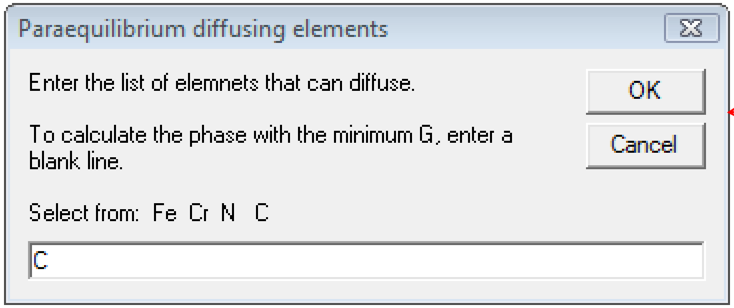
Output when only C and N are permitted to diffuse

```
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


Paraequilibrium diffusing elements

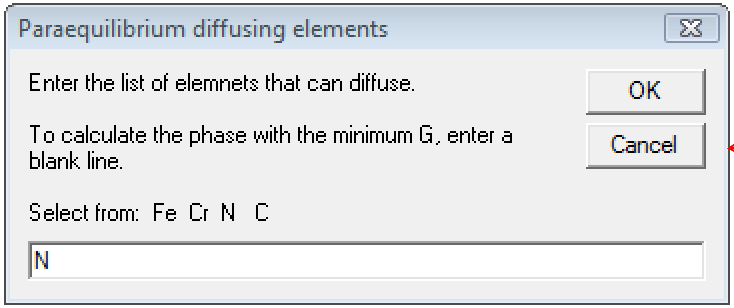
Enter the list of elemnets that can diffuse.

To calculate the phase with the minimum G, enter a blank line.

Select from: Fe Cr N C

C

Input when only C is permitted to diffuse


Paraequilibrium diffusing elements

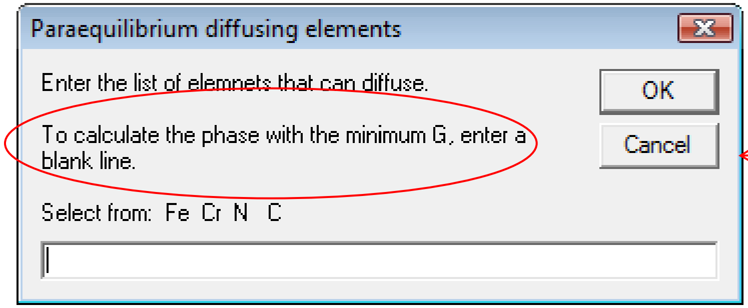
Enter the list of elemnets that can diffuse.

To calculate the phase with the minimum G, enter a blank line.

Select from: Fe Cr N C

N

Input when only N is permitted to diffuse


Paraequilibrium diffusing elements

Enter the list of elemnets that can diffuse.

To calculate the phase with the minimum G, enter a blank line.

Select from: Fe Cr N C

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
```

2 phases are formed at paraequilibrium

Fe/Cr molar ratio = **1/1** in all phases

N/(Fe+Cr) molar ratio = **0.02** in all phases

Paraequilibrium and minimum Gibbs energy calculations

Output when only N is permitted to diffuse

```
 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
```

2 phases are formed at paraequilibrium

Fe/Cr molar ratio = **1/1** in all phases

C/(Fe+Cr) molar ratio = **0.02** in all phases

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

Using Virtual Elements to Impose Constraints

- FactSage permits the use of “virtual elements” with chemical symbols Qa, Qb, Qc, …….., Qz with atomic weights of 0.0. Virtual elements may be used in the modules ***EQUILIB***, ***PHASE DIAGRAM***, ***COMPOUND*** and ***SOLUTION*** in the same way as real elements.

- The use of virtual elements provides a useful means of applying constraints to certain equilibrium calculations as will be illustrated in the examples in this Section.

- For many of these examples you will need to activate the databases VIRT and SURF which can be found in the **FACTBASE** sub-folder of your FactSage folder.

- For additional examples, see:

R. Pajarre, P. Koukkari and P. Kangas, Chem. Eng. Sci., 146 (2016) 244-258

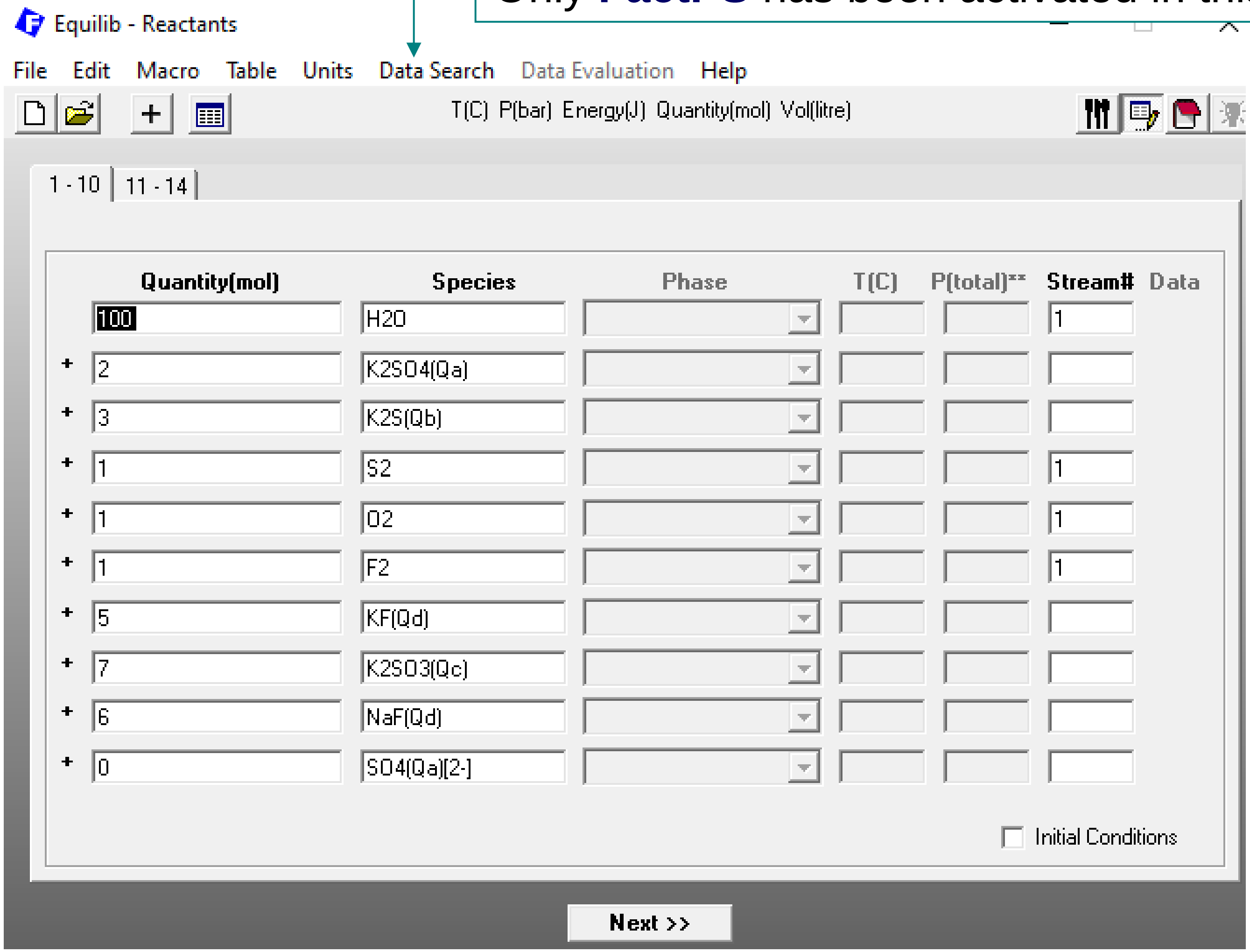
and

P. Koukkari, VTT Technology Bulletin 160 (2014), VTT Tech. Res. Ctr of Finland, Espoo, Finland.

Aqueous solution with redox reactions prohibited

- In aqueous solutions, redox reactions between oxidation states of elements (as, for example, between SO_4[2-], S[2-] and SO_3[2-] ions in solution) are often kinetically hindered. An unconstrained FactSage equilibrium calculation will always permit such reactions. In order to prohibit such reactions so that, for instance, the amount of SO_4[2-] in the output is equal to the amount of SO_4[2-] in the input, virtual elements can be employed to provide the required constraints.
- The present example considers an equilibrium between an aqueous solution, a gas phase and solid salts with such constraints applied.

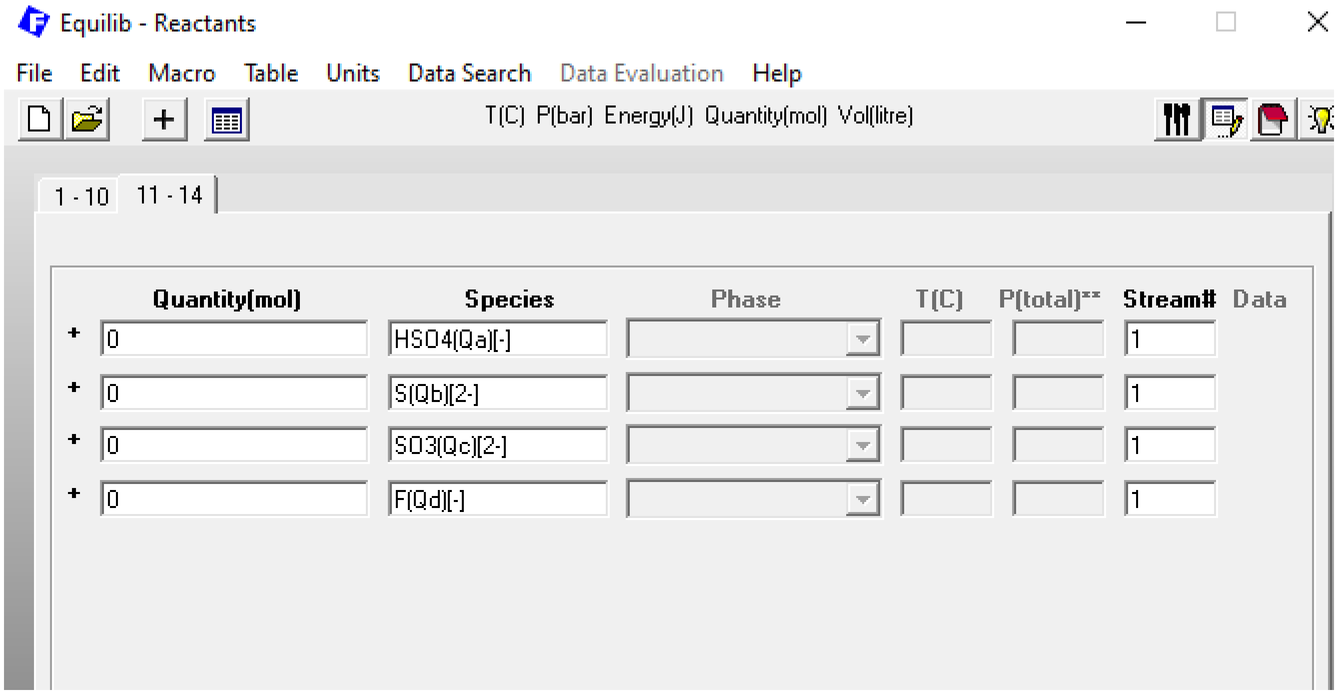
Only **FactPS** has been activated in this example



	Quantity(mol)	Species	Phase	T(C)	P(total)**	Stream#	Data
	100	H2O				1	
+	2	K2SO4(Qa)					
+	3	K2S(Qb)					
+	1	S2				1	
+	1	O2				1	
+	1	F2				1	
+	5	KF(Qd)					
+	7	K2SO3(Qc)					
+	6	NaF(Qd)					
+	0	SO4(Qa)[2-]					

☐ Initial Conditions

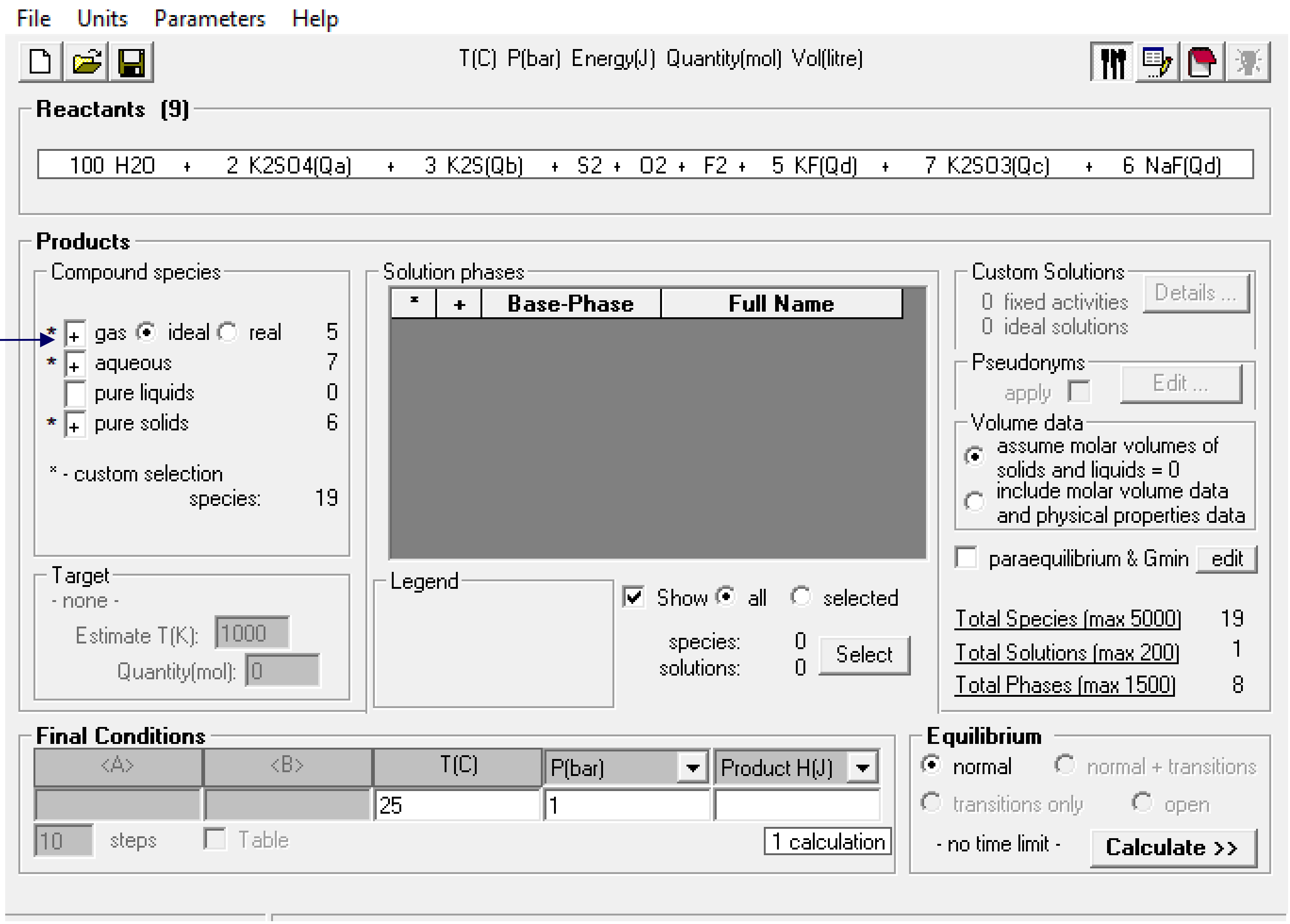
In the **Input,** all SO_4[2], S[2-], SO_3[2-] and F[-] ions are associated with equal amounts of Qa, Qb, Qc, and Qd virtual elements respectively



	Quantity(mol)	Species	Phase	T(C)	P(total)**	Stream#	Data
+	0	HSO4(Qa)[-]				1	
+	0	S(Qb)[2-]				1	
+	0	SO3(Qc)[2-]				1	
+	0	F(Qd)[-]				1	

Zero amounts of SO_4(Qa)[2-], HSO_4(Qa)[-], S(Qb)[2-],SO_3(Qc)[2-] and F(Qd)[-] species are entered in order for them to appear in the species selection lists on the menu window. (Note, that SO_4(Qa)[2-] and HSO_4(Qa)[-] are both associated with the same virtual element Qa.)

For simplicity, only O_2, F_2, S_2, SO_2 and SO_3 gases have been selected



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

Reactants (9)

100 H2O + 2 K2SO4(Qa) + 3 K2S(Qb) + S2 + O2 + F2 + 5 KF(Qd) + 7 K2SO3(Qc) + 6 NaF(Qd)

Products

Compound species

*	☐+	gas ● ideal ○ real	5
*	☐+	aqueous	7
	☐	pure liquids	0
*	☐+	pure solids	6

* - custom selection

species: 19

Solution phases

*	+	Base-Phase	Full Name

Custom Solutions

0 fixed activities

0 ideal solutions

Pseudonyms

apply ☐

Volume data

● assume molar volumes of solids and liquids = 0

○ include molar volume data and physical properties data

☐ paraequilibrium & Gmin

Target

- none -

Estimate T(K): 1000

Quantity(mol): 0

Legend

☑ Show ● all ○ selected

species: 0

solutions: 0

Total Species (max 5000) 19

Total Solutions (max 200) 1

Total Phases (max 1500) 8

Final Conditions

<A>	<B>	T(C)	P(bar)	Product H(J)
		25	1	

10 steps ☐ Table

1 calculation

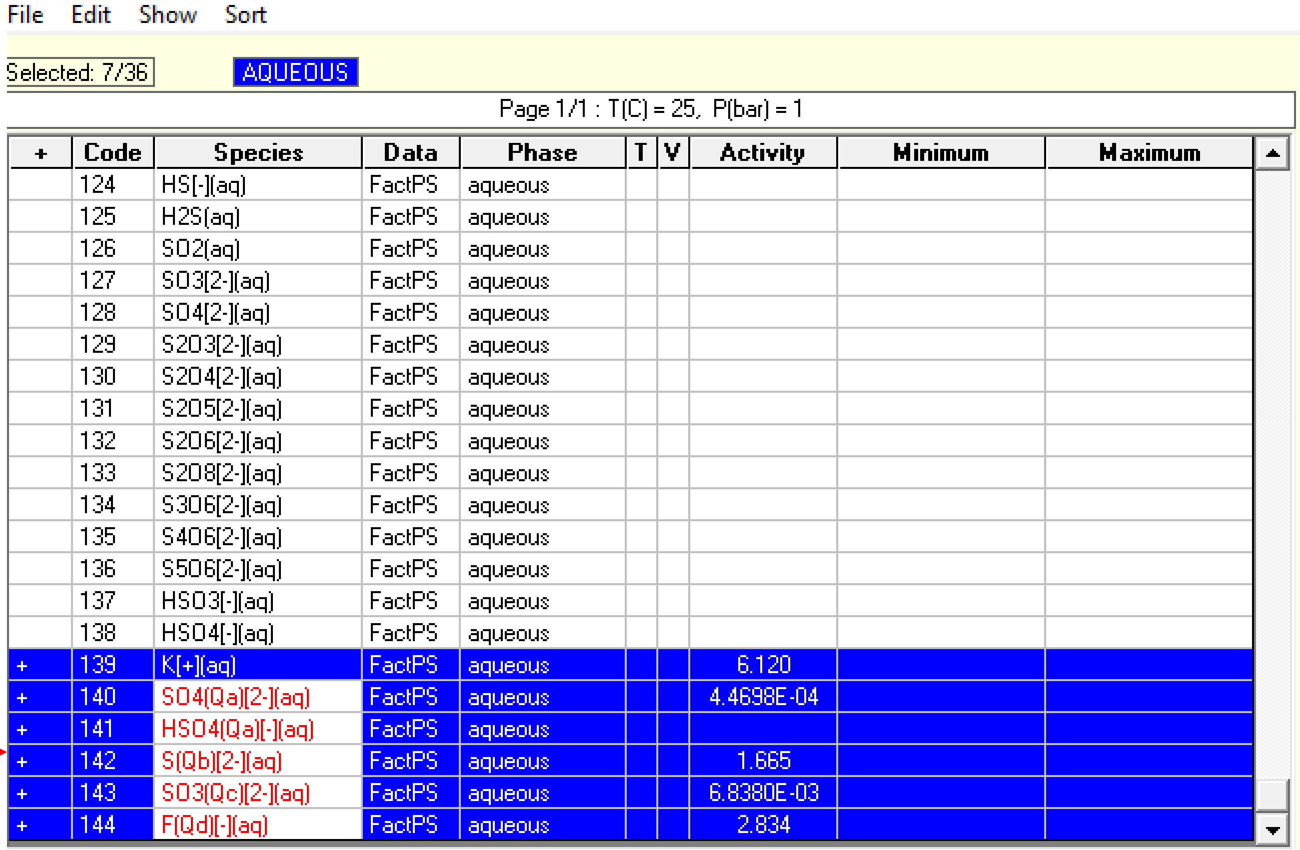
Equilibrium

● normal ○ normal + transitions

○ transitions only ○ open

- no time limit -

Aqueous species selection



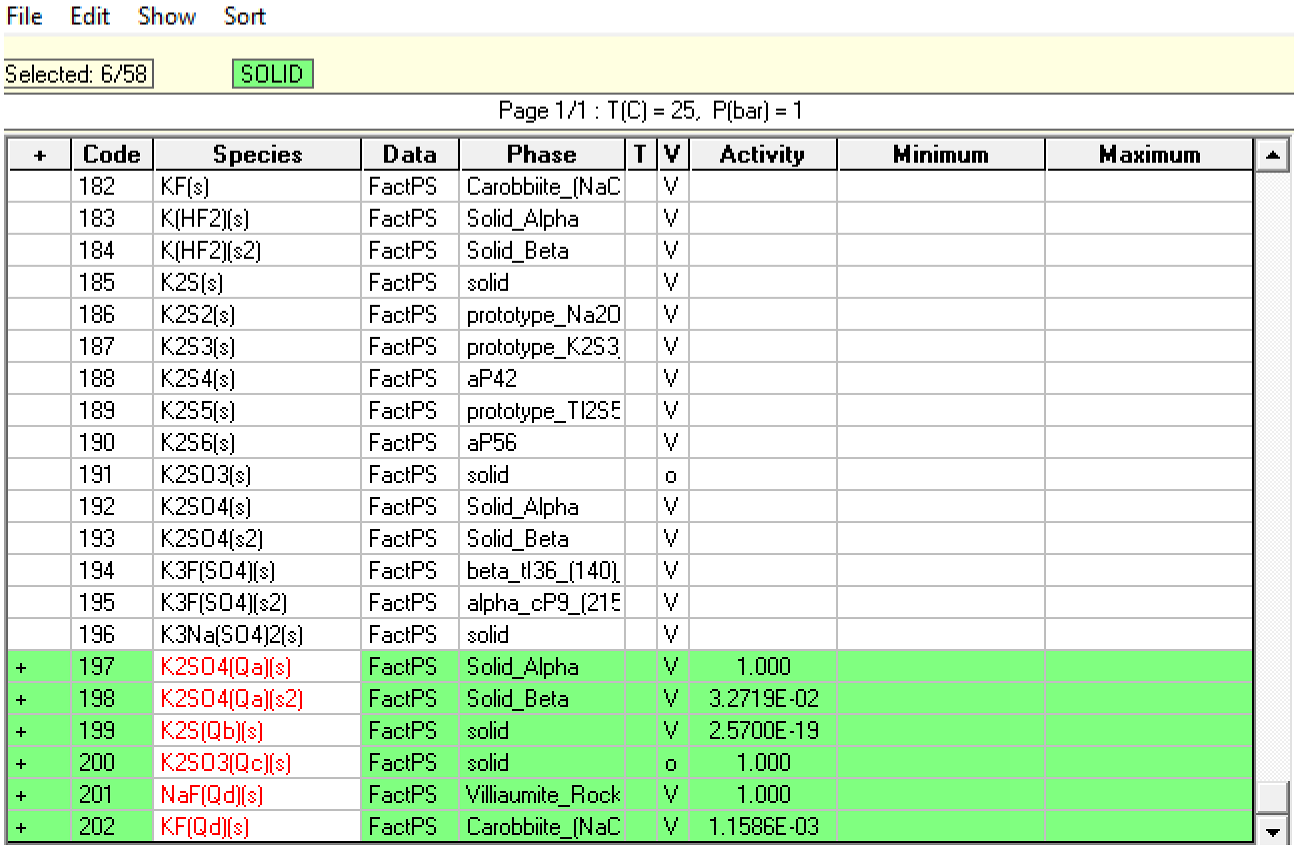
Page 1/1 : T(C) = 25, P(bar) = 1

+	Code	Species	Data	Phase	T	V	Activity	Minimum	Maximum
	124	HS[-](aq)	FactPS	aqueous					
	125	H2S(aq)	FactPS	aqueous					
	126	SO2(aq)	FactPS	aqueous					
	127	SO3[2-](aq)	FactPS	aqueous					
	128	SO4[2-](aq)	FactPS	aqueous					
	129	S2O3[2-](aq)	FactPS	aqueous					
	130	S2O4[2-](aq)	FactPS	aqueous					
	131	S2O5[2-](aq)	FactPS	aqueous					
	132	S2O6[2-](aq)	FactPS	aqueous					
	133	S2O8[2-](aq)	FactPS	aqueous					
	134	S3O6[2-](aq)	FactPS	aqueous					
	135	S4O6[2-](aq)	FactPS	aqueous					
	136	S5O6[2-](aq)	FactPS	aqueous					
	137	HSO3[-](aq)	FactPS	aqueous					
	138	HSO4[-](aq)	FactPS	aqueous					
+	139	K[+](aq)	FactPS	aqueous			6.120		
+	140	SO4(Qa)[2-](aq)	FactPS	aqueous			4.4698E-04		
+	141	HSO4(Qa)[-](aq)	FactPS	aqueous					
+	142	S(Qb)[2-](aq)	FactPS	aqueous			1.665		
+	143	SO3(Qc)[2-](aq)	FactPS	aqueous			6.8380E-03		
+	144	F(Qd)[-](aq)	FactPS	aqueous			2.834		

Only these species (and Na[+]) are selected.

FactSage automatically assigns the properties of SO_4[2-] to SO_4(Qa)[2-], the properties of HSO_4[-] to HSO_4(Qa)[-], etc.

Solid species selection



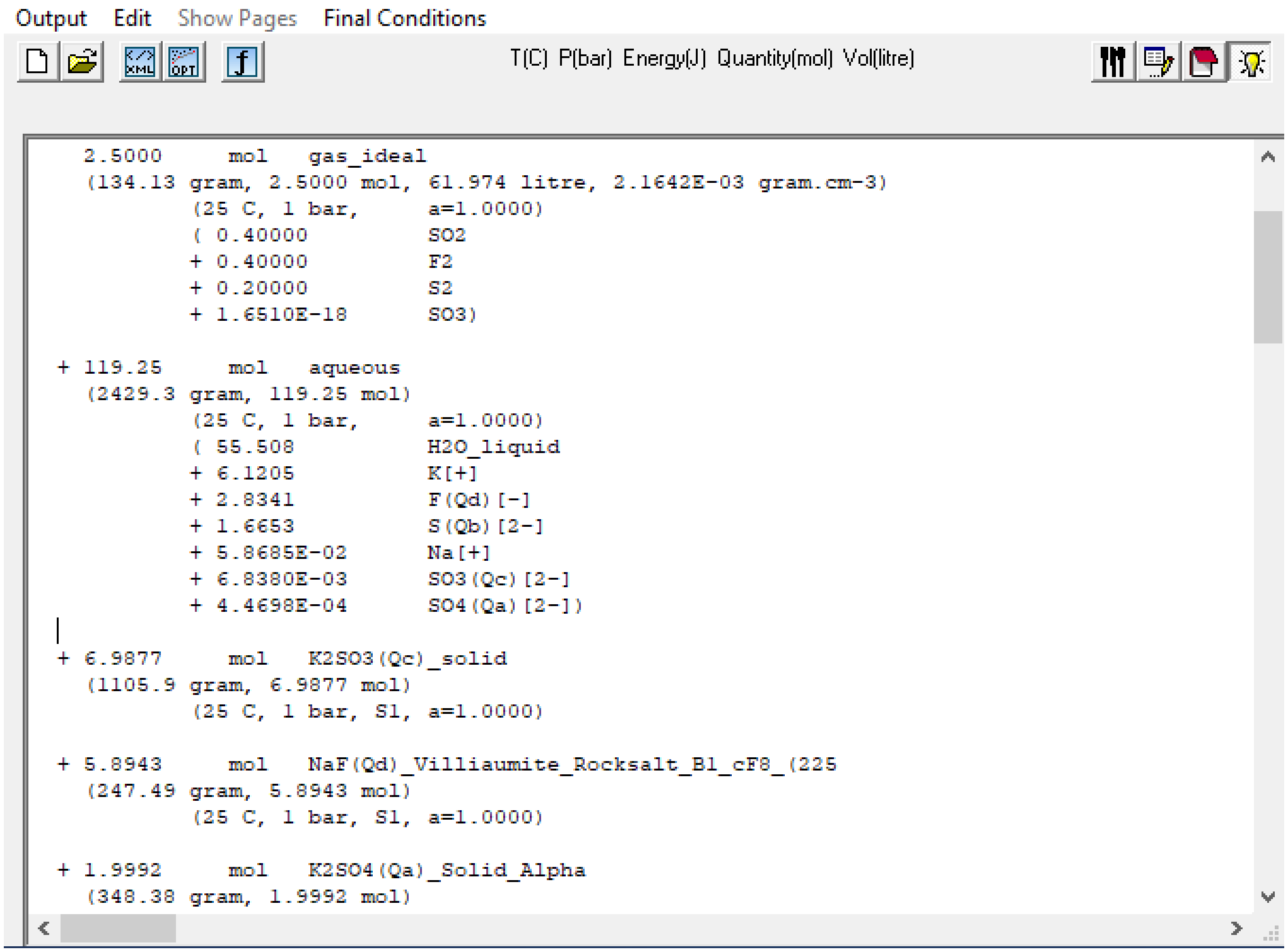
Selected: 6/58

Page 1/1 : T(C) = 25, P(bar) = 1

+	Code	Species	Data	Phase	T	V	Activity	Minimum	Maximum
	182	KF(s)	FactPS	Carobbiite_(NaC		V			
	183	K(HF2)(s)	FactPS	Solid_Alpha		V			
	184	K(HF2)(s2)	FactPS	Solid_Beta		V			
	185	K2S(s)	FactPS	solid		V			
	186	K2S2(s)	FactPS	prototype_Na2O		V			
	187	K2S3(s)	FactPS	prototype_K2S3		V			
	188	K2S4(s)	FactPS	aP42		V			
	189	K2S5(s)	FactPS	prototype_Tl2S5		V			
	190	K2S6(s)	FactPS	aP56		V			
	191	K2SO3(s)	FactPS	solid		o			
	192	K2SO4(s)	FactPS	Solid_Alpha		V			
	193	K2SO4(s2)	FactPS	Solid_Beta		V			
	194	K3F(SO4)(s)	FactPS	beta_tI36_(140)		V			
	195	K3F(SO4)(s2)	FactPS	alpha_cP9_(215		V			
	196	K3Na(SO4)2(s)	FactPS	solid		V			
+	197	K2SO4(Qa)(s)	FactPS	Solid_Alpha		V	1.000		
+	198	K2SO4(Qa)(s2)	FactPS	Solid_Beta		V	3.2719E-02		
+	199	K2S(Qb)(s)	FactPS	solid		V	2.5700E-19		
+	200	K2SO3(Qc)(s)	FactPS	solid		o	1.000		
+	201	NaF(Qd)(s)	FactPS	Villiaumite_Rock		V	1.000		
+	202	KF(Qd)(s)	FactPS	Carobbiite_(NaC		V	1.1586E-03		

Only these species (and Na[+]) are selected.

FactSage automatically assigns the properties of K_2SO_4(s) to K_2SO_4(Qa)(s), etc.

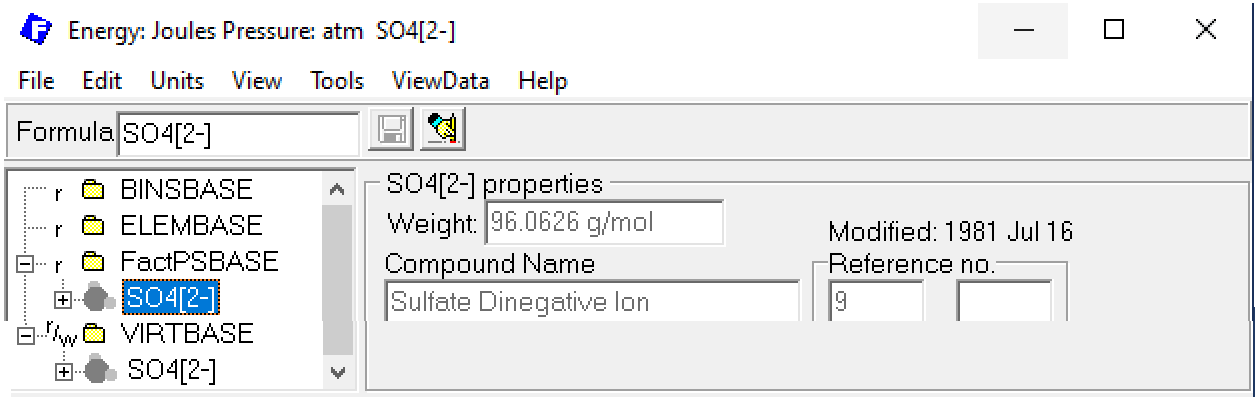


```
   2.5000      mol   gas_ideal
   (134.13 gram, 2.5000 mol, 61.974 litre, 2.1642E-03 gram.cm-3)
           (25 C, 1 bar,     a=1.0000)
           ( 0.40000         SO2
           + 0.40000         F2
           + 0.20000         S2
           + 1.6510E-18      SO3)

 + 119.25      mol   aqueous
   (2429.3 gram, 119.25 mol)
           (25 C, 1 bar,     a=1.0000)
           ( 55.508          H2O_liquid
           + 6.1205          K[+]
           + 2.8341          F(Qd)[-]
           + 1.6653          S(Qb)[2-]
           + 5.8685E-02      Na[+]
           + 6.8380E-03      SO3(Qc)[2-]
           + 4.4698E-04      SO4(Qa)[2-])

 + 6.9877      mol   K2SO3(Qc)_solid
   (1105.9 gram, 6.9877 mol)
           (25 C, 1 bar, S1, a=1.0000)

 + 5.8943      mol   NaF(Qd)_Villiaumite_Rocksalt_B1_cF8_(225
   (247.49 gram, 5.8943 mol)
           (25 C, 1 bar, S1, a=1.0000)

 + 1.9992      mol   K2SO4(Qa)_Solid_Alpha
   (348.38 gram, 1.9992 mol)
```

All redox reactions have been prohibited, both between phases and within the aqueous phase. For example, the total amount of SO_3 is (100/55.508) * 0.006838 + 6.9877 = 7.000 mol as entered on the reactants window

Entering data in a private COMPOUND (cdb) database for species containing virtual elements

- Rather than entering 0.0 moles of species such as S(Qb)[2-], SO_3(Qc)[2-], etc. on the reactants window in order for them to appear in the species selection lists as in the previous example, they may be entered and stored in a private database just like any other compounds.
- The following slides show how the species SO_4(Qa)[2-] may be entered and stored in a private database with the properties of SO_4[2-]aq copied from **FactPS**.



Energy: Joules Pressure: atm SO4[2-]

Formula SO4[2-]

SO4[2-] properties

Weight: 96.0626 g/mol

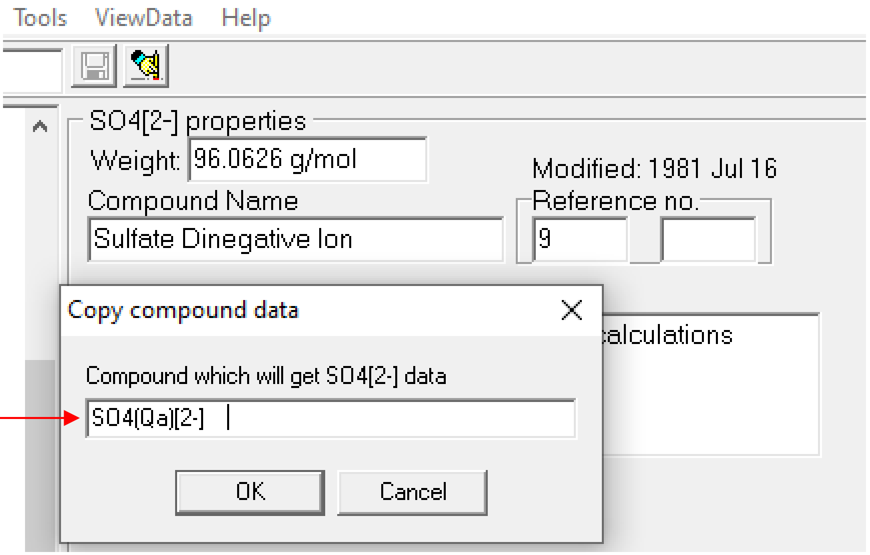
Modified: 1981 Jul 16

Compound Name: Sulfate Dinegative Ion

Reference no. 9

- Open FACTDATA/VIRTBASE.cdb which you will find in your FactSage folder.
- Drag and drop SO4[2-] from **FactPSBASE** to VIRTBASE

Click "Tools", then, in the dropdown menu that appears, click on "Copy data to new compound"



SO4[2-] properties

Weight: 96.0626 g/mol

Modified: 1981 Jul 16

Compound Name

Sulfate Dinegative Ion

Reference no.

9

alculations

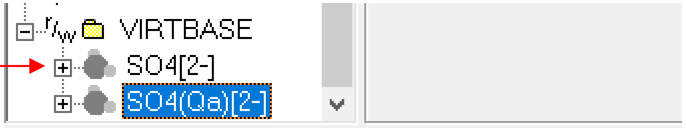
Copy compound data

Compound which will get SO4[2-] data

SO4(Qa)[2-]

Enter new name

Now delete SO4[2-] from VIRTBASE

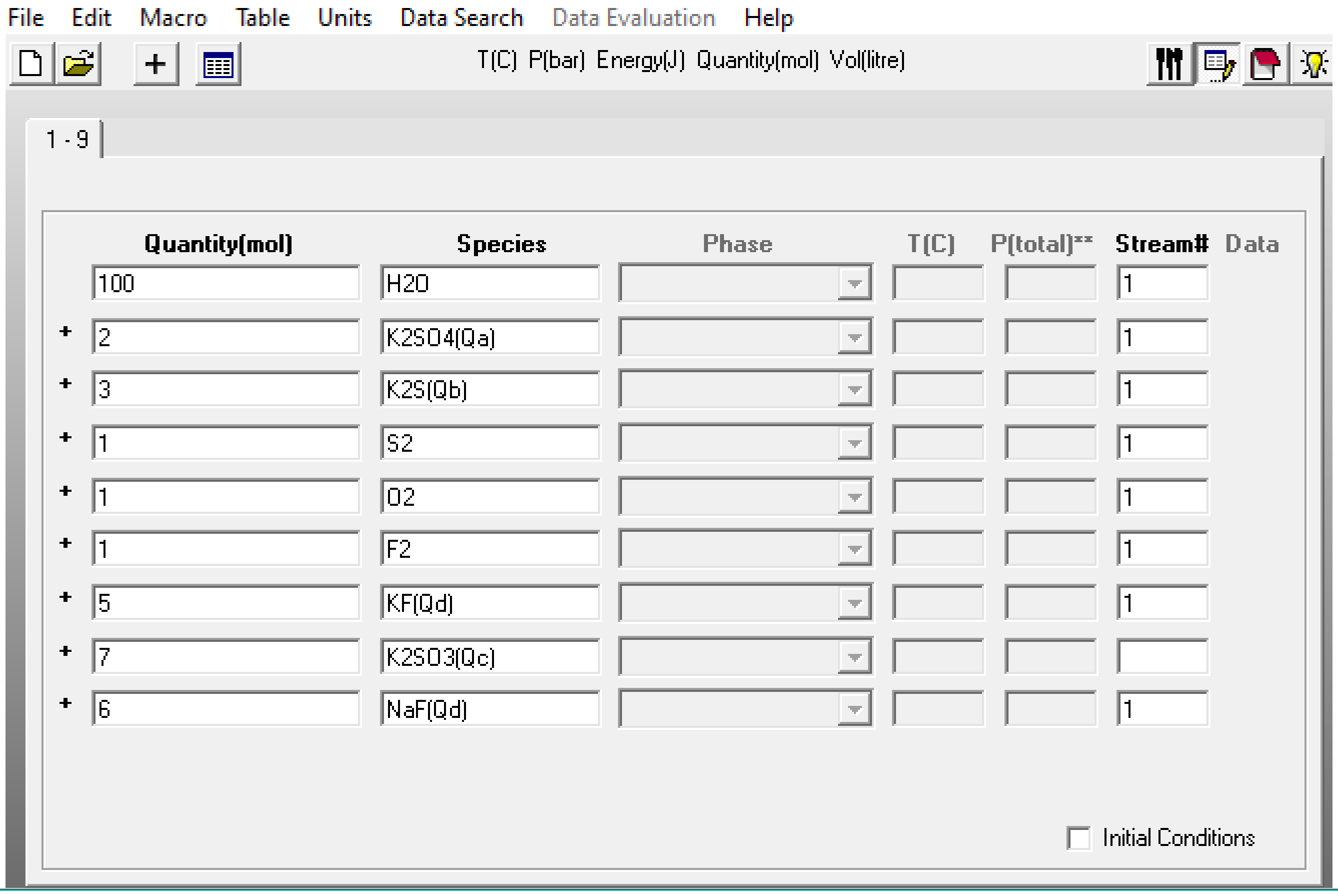


SO4(Qa)[2-] now in VIRTBASE

Aqueous solution with redox reactions prohibited

This is the same example as in Section 15.2, but with data taken from the private database **VIRTBASE**

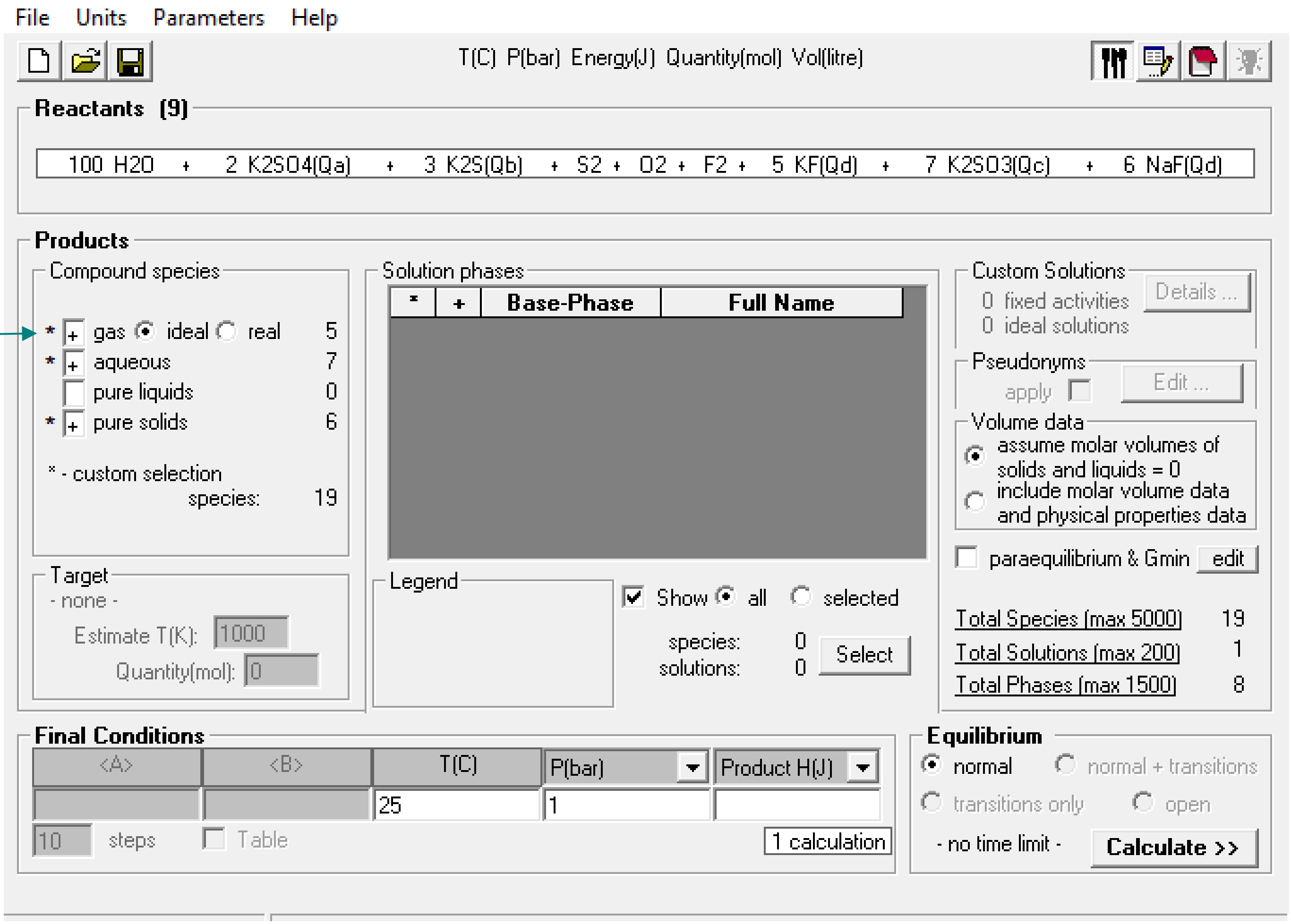
Add **FACTDATA/VIRTBASE** (which is in your **FACTSage** folder) to your list of active databases and check the "VIRT" box



	Quantity(mol)	Species	Phase	T(C)	P(total)**	Stream#	Data
	100	H2O				1	
+	2	K2SO4(Qa)				1	
+	3	K2S(Qb)				1	
+	1	S2				1	
+	1	O2				1	
+	1	F2				1	
+	5	KF(Qd)				1	
+	7	K2SO3(Qc)					
+	6	NaF(Qd)				1	

It is not necessary to enter 0.0 moles of SO4(Qa)[2-], etc. as in the previous example since the data will be taken from **FACTDATA/VIRTBASE**

For simplicity, only O_2, F_2, S_2, SO_2 and SO_3 gases have been selected



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

Reactants (9)

100 H2O + 2 K2SO4(Qa) + 3 K2S(Qb) + S2 + O2 + F2 + 5 KF(Qd) + 7 K2SO3(Qc) + 6 NaF(Qd)

Products

Compound species

*	☒ gas ● ideal ○ real		5
*	☒ aqueous		7
	☐ pure liquids		0
*	☒ pure solids		6

* - custom selection

species: 19

Solution phases

*	+	Base-Phase	Full Name

Target

- none -

Estimate T(K): 1000

Quantity(mol): 0

Legend

☑ Show ● all ○ selected

species: 0

solutions: 0

Custom Solutions

0 fixed activities

0 ideal solutions

Pseudonyms

apply ☐

Volume data

● assume molar volumes of solids and liquids = 0

○ include molar volume data and physical properties data

☐ paraequilibrium & Gmin

Total Species (max 5000) 19

Total Solutions (max 200) 1

Total Phases (max 1500) 8

Final Conditions

<A>	<B>	T(C)	P(bar)	Product H(J)
		25	1	

10 steps ☐ Table

1 calculation

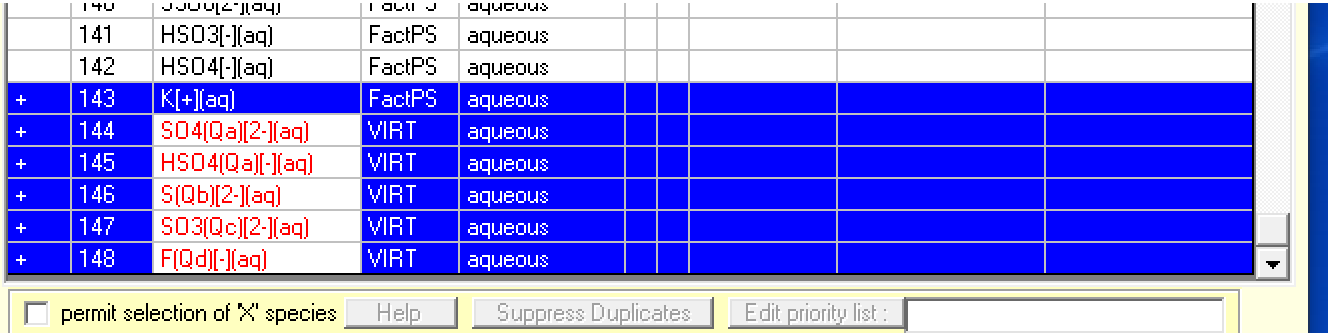
Equilibrium

● normal ○ normal + transitions

○ transitions only ○ open

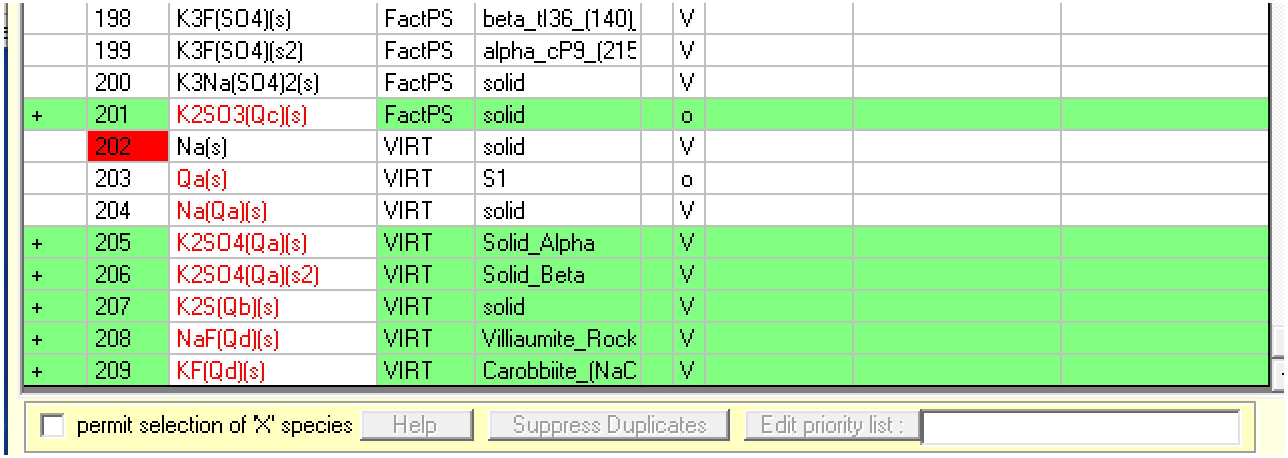
- no time limit -

All required data have already been entered in **FACTDATA/VIRTBASE.cdb**.
Select only these aqueous and solid species.
Output will be identical to slide 15.2.6



	141	HSO3[-](aq)	FactPS	aqueous
	142	HSO4[-](aq)	FactPS	aqueous
+	143	K[+](aq)	FactPS	aqueous
+	144	SO4(Qa)[2-](aq)	VIRT	aqueous
+	145	HSO4(Qa)[-](aq)	VIRT	aqueous
+	146	S(Qb)[2-](aq)	VIRT	aqueous
+	147	SO3(Qc)[2-](aq)	VIRT	aqueous
+	148	F(Qd)[-](aq)	VIRT	aqueous

☐ permit selection of 'X' species



	198	K3F(SO4)(s)	FactPS	beta_tI36_(140)	V
	199	K3F(SO4)(s2)	FactPS	alpha_cP9_(215	V
	200	K3Na(SO4)2(s)	FactPS	solid	V
+	201	K2SO3(Qc)(s)	FactPS	solid	o
	202	Na(s)	VIRT	solid	V
	203	Qa(s)	VIRT	S1	o
	204	Na(Qa)(s)	VIRT	solid	V
+	205	K2SO4(Qa)(s)	VIRT	Solid_Alpha	V
+	206	K2SO4(Qa)(s2)	VIRT	Solid_Beta	V
+	207	K2S(Qb)(s)	VIRT	solid	V
+	208	NaF(Qd)(s)	VIRT	Villiaumite_Rock	V
+	209	KF(Qd)(s)	VIRT	Carobbiite_(NaC	V

☐ permit selection of 'X' species

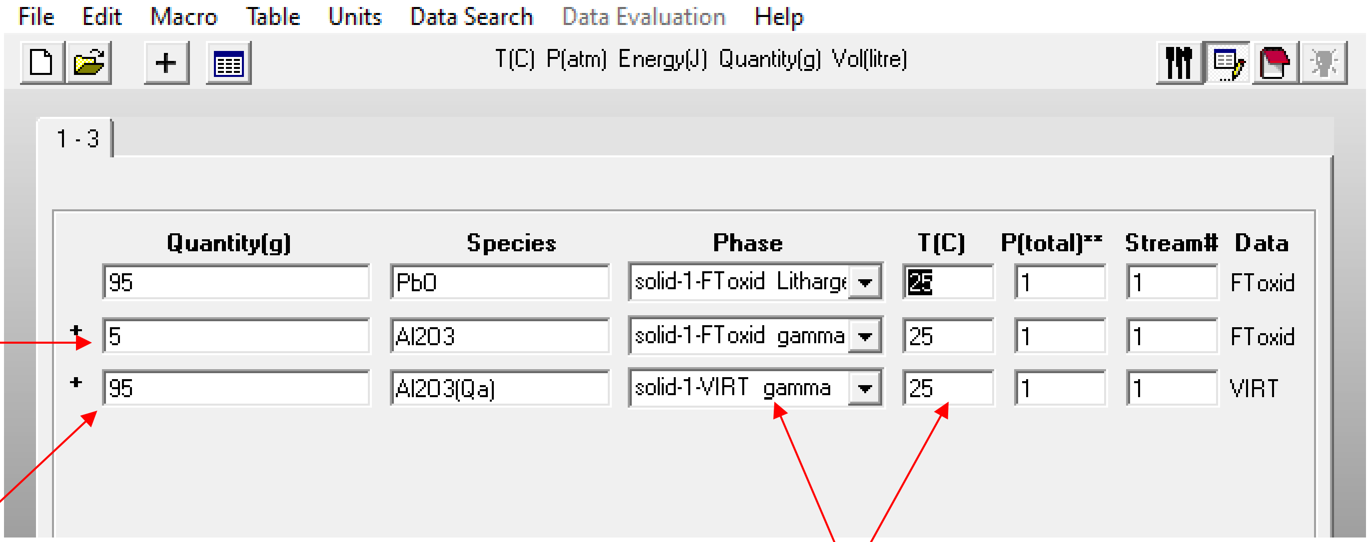
Heating in a crucible which partially reacts with its contents

- 100 g of PbO are placed in an Al_2O_3 crucible at 25 ^oC and heated to 1200^{o}C. The crucible weighs 100 g.

- Calculate the heat required (assuming no heat losses) if only 5 g of Al_2O_3 dissolve in the PbO. (That is, the liquid PbO does not become saturated in Al_2O_3.)

- This calculation can be performed by associating Qa with the Al_2O_3 which does not dissolve.

Activate **FACTDATA/VIRTBASE** in which Al_2O_3(Qa) has been stored with the properties of Al_2O_3 (corundum)



	Quantity(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
	95	PbO	solid-1-FToxid Litharge	25	1	1	FToxid
+	5	Al2O3	solid-1-FToxid gamma	25	1	1	FToxid
+	95	Al2O3(Qa)	solid-1-VIRT gamma	25	1	1	VIRT

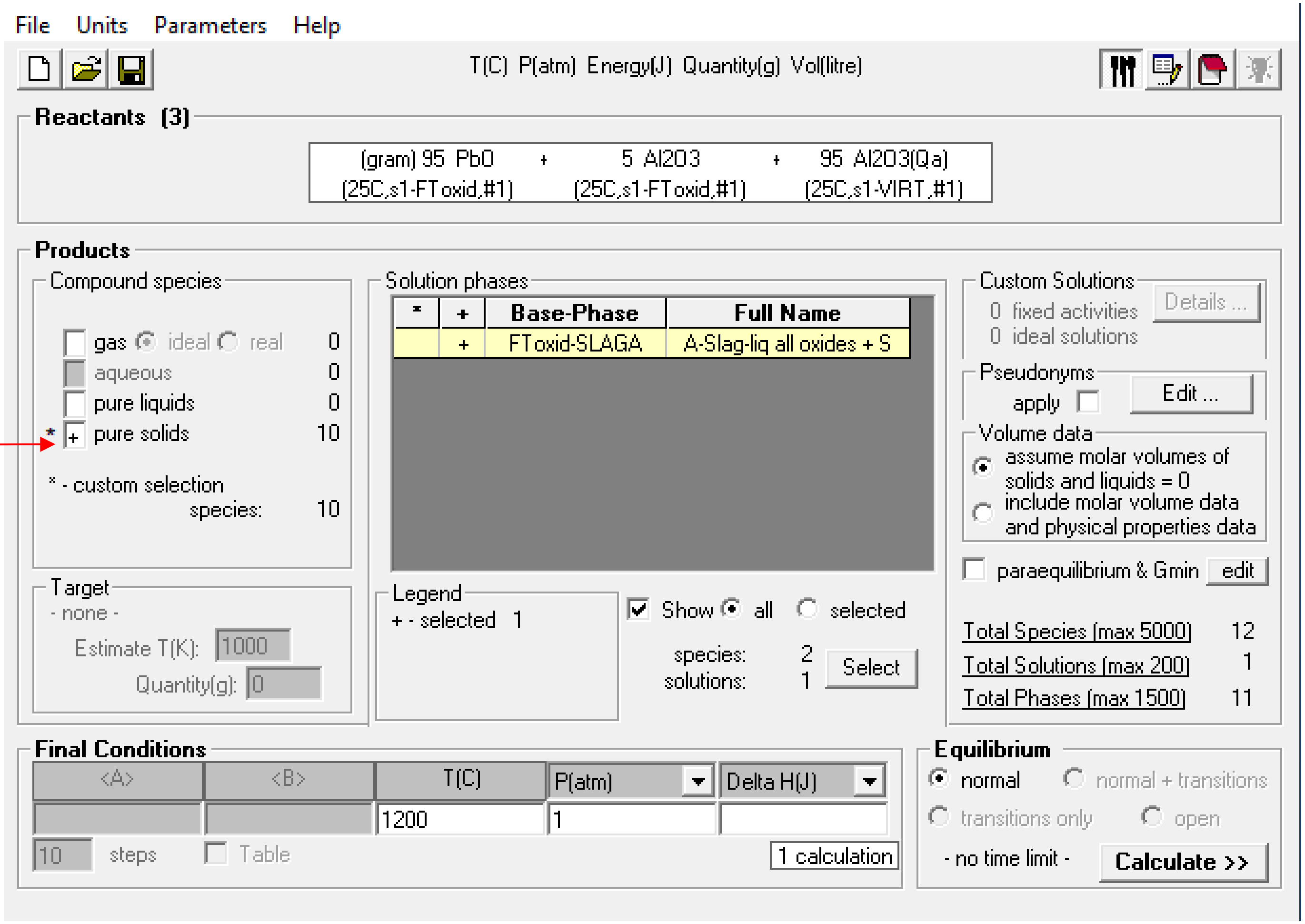
5 g of Al_2O_3 dissolve

95 g of Al_2O_3 do not dissolve

Initial Conditions

(<u>Note</u>: If an initial condition for a species containing a virtual element such as Al_2O_3(Qa) is to be selected, then the compound must first be entered in a compound (cdb) database.)

Select only Al_2O_3(Qa)



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

Reactants (3)

(gram) 95 PbO [25C,s1-FToxid,#1] + 5 Al2O3 [25C,s1-FToxid,#1] + 95 Al2O3(Qa) [25C,s1-VIRT,#1]

Products

Compound species

☐ gas ● ideal ○ real 0
☐ aqueous 0
☐ pure liquids 0
* ☑ pure solids 10

* - custom selection species: 10

Target
- none -
Estimate T(K): 1000
Quantity(g): 0

Solution phases

*	+	Base-Phase	Full Name
	+	FToxid-SLAGA	A-Slag-liq all oxides + S

Legend
\+ - selected 1

☑ Show ● all ○ selected

species: 2
solutions: 1

Custom Solutions
0 fixed activities
0 ideal solutions

Pseudonyms
apply ☐

Volume data
● assume molar volumes of solids and liquids = 0
○ include molar volume data and physical properties data

☐ paraequilibrium & Gmin

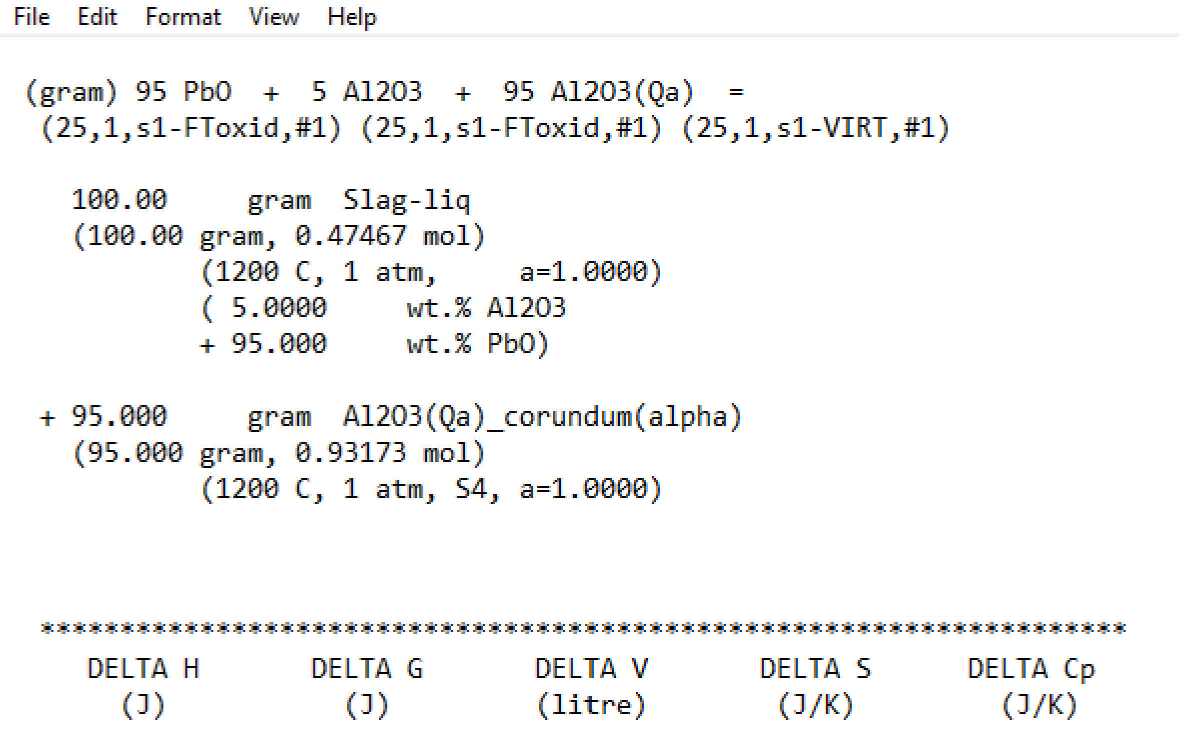
Total Species (max 5000) 12
Total Solutions (max 200) 1
Total Phases (max 1500) 11

Final Conditions

<A>	<B>	T(C)	P(atm)	Delta H(J)
		1200	1	

10 steps ☐ Table 1 calculation

Equilibrium
● normal ○ normal + transitions
○ transitions only ○ open
- no time limit -



```
(gram) 95 PbO  +  5 Al2O3  +  95 Al2O3(Qa)  =
 (25,1,s1-FToxid,#1) (25,1,s1-FToxid,#1) (25,1,s1-VIRT,#1)

   100.00     gram  Slag-liq
   (100.00 gram, 0.47467 mol)
           (1200 C, 1 atm,     a=1.0000)
           ( 5.0000     wt.% Al2O3
           + 95.000     wt.% PbO)

 + 95.000     gram  Al2O3(Qa)_corundum(alpha)
   (95.000 gram, 0.93173 mol)
           (1200 C, 1 atm, S4, a=1.0000)



 ********************************************************************
     DELTA H       DELTA G       DELTA V       DELTA S       DELTA Cp
       (J)           (J)         (litre)        (J/K)         (J/K)
 ********************************************************************
  1.60492E+05  -2.64604E+05   0.00000E+00   2.24696E+02   5.74004E+01
```

The required enthalpy

Preventing Unwanted Reactions and adding virtual elements to end-members of solutions

- **The 8.1 version of the FTsalt database contains** data for solid compounds, solid solutions and a molten salt phase in the system $NaNO_3$, $NaNO_2$, $NaClO_4$, NaCl.

- In a calculation with unconstrained Gibbs energy minimization, the following reaction will occur:

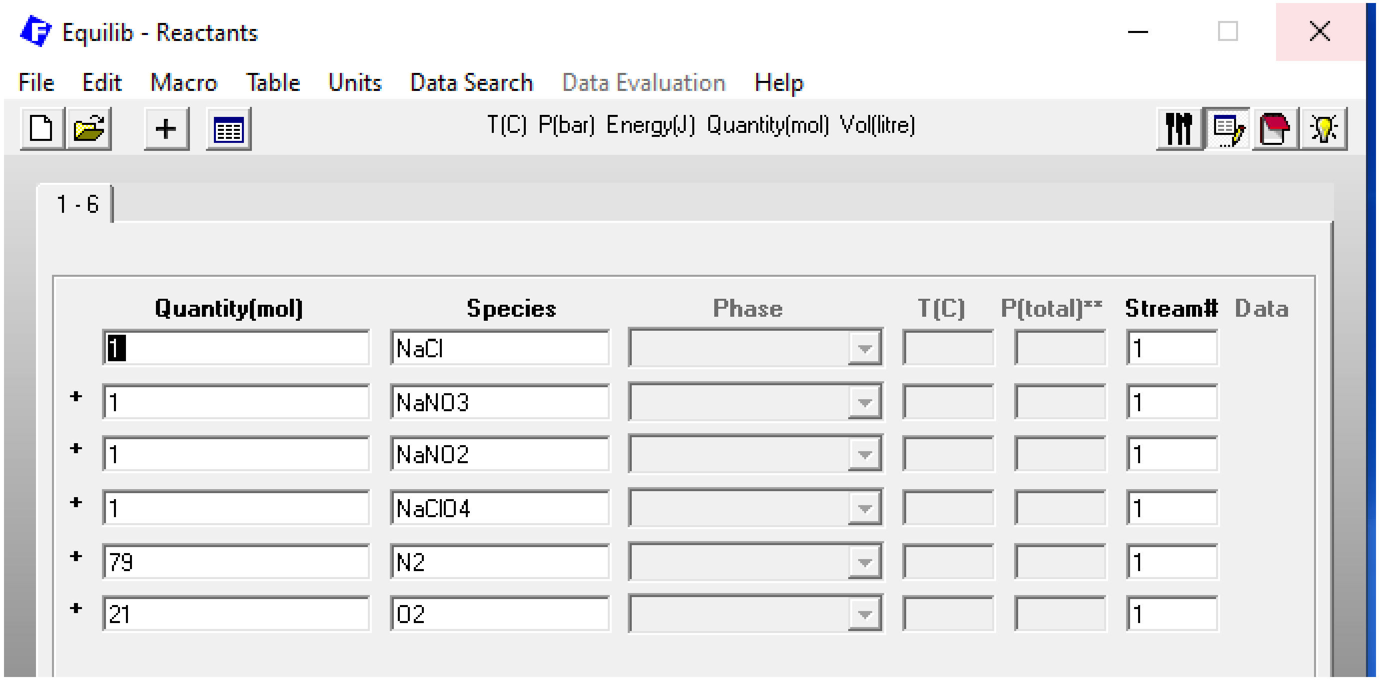
$$4NaNO_2 + NaClO_4 = 4NaNO_3 + NaCl$$

  Furthermore, if air is present, the salt will react with N_2 and O_2.

- In reality, the amounts of NO_2^-, NO_3^-, ClO_4^- and Cl^- remain constant. This constraint can be applied through the use of virtual elements.

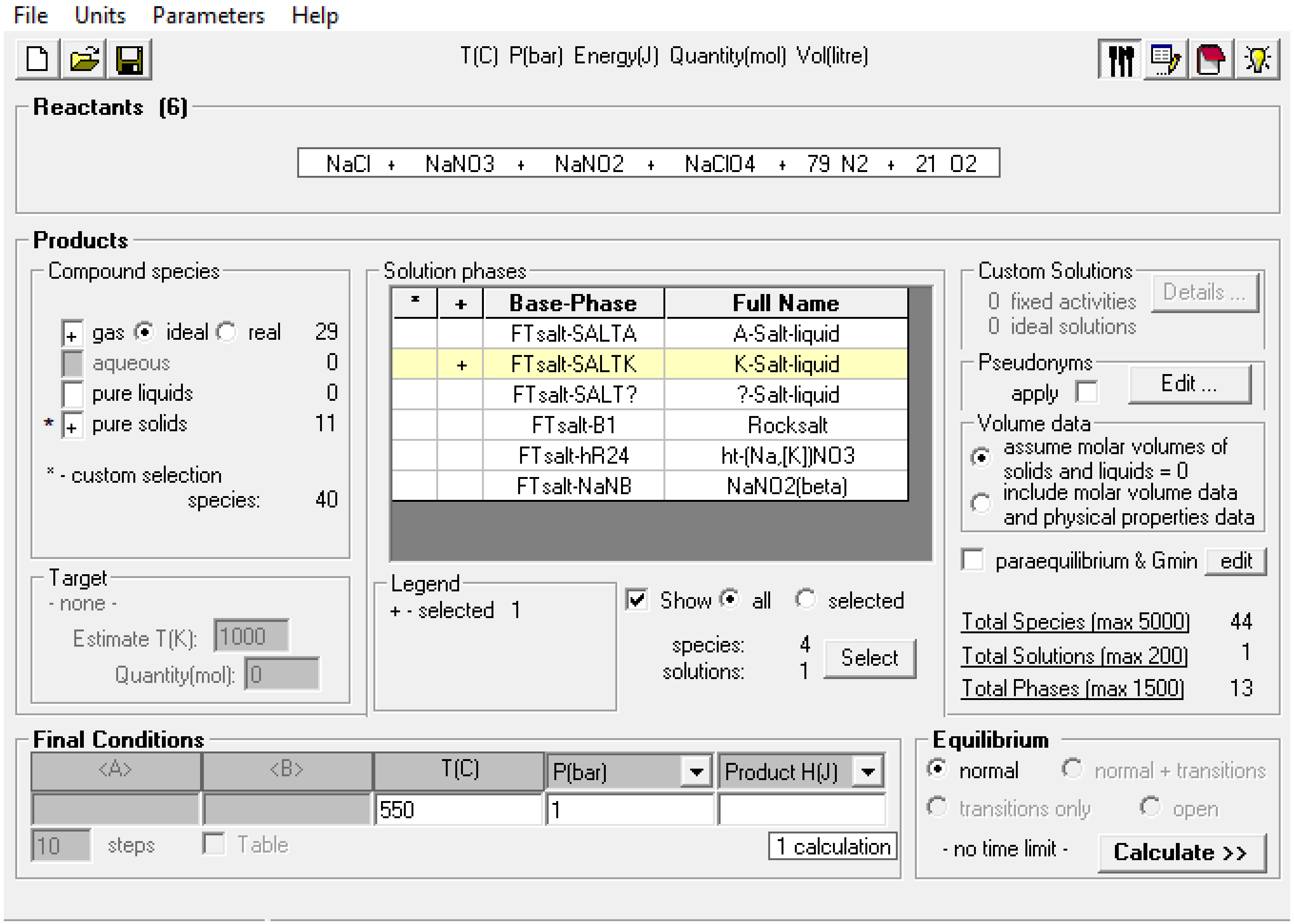
The next three slides illustrate the results when the equilibria are unconstrained

Input equimolar $NaNO_3$, $NaNO_2$, $NaClO_4$, NaCl plus air



	Quantity(mol)	Species	Phase	T(C)	P(total)**	Stream#	Data
	1	NaCl				1	
+	1	NaNO3				1	
+	1	NaNO2				1	
+	1	NaClO4				1	
+	79	N2				1	
+	21	O2				1	

Calculation of unconstrained equilibrium



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

Reactants (6)

NaCl + NaNO3 + NaNO2 + NaClO4 + 79 N2 + 21 O2

Products

Compound species

	☐+ gas ● ideal ○ real		29
	☐ aqueous		0
	☐ pure liquids		0
*	☐+ pure solids		11

* - custom selection
species: 40

Target
- none -
Estimate T(K): 1000
Quantity(mol): 0

Solution phases

*	+	Base-Phase	Full Name
		FTsalt-SALTA	A-Salt-liquid
	+	FTsalt-SALTK	K-Salt-liquid
		FTsalt-SALT?	?-Salt-liquid
		FTsalt-B1	Rocksalt
		FTsalt-hR24	ht-(Na,[K])NO3
		FTsalt-NaNB	NaNO2(beta)

Legend
+ - selected 1

☑ Show ● all ○ selected

species: 4
solutions: 1

Custom Solutions
0 fixed activities
0 ideal solutions

Pseudonyms
apply ☐

Volume data
● assume molar volumes of solids and liquids = 0
○ include molar volume data and physical properties data

☐ paraequilibrium & Gmin

Total Species (max 5000) 44
Total Solutions (max 200) 1
Total Phases (max 1500) 13

Final Conditions

<A>	<B>	T(C)	P(bar)	Product H(J)
		550	1	

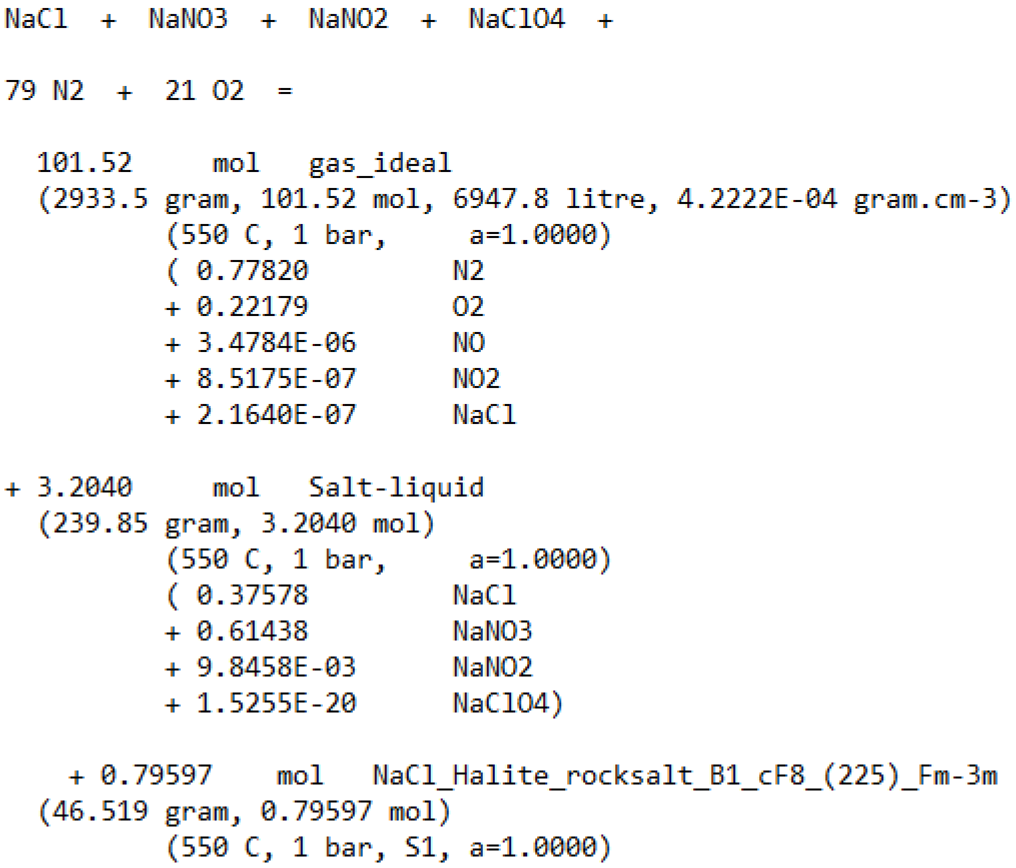
10 steps ☐ Table 1 calculation

Equilibrium

● normal ○ normal + transitions
○ transitions only ○ open
- no time limit -

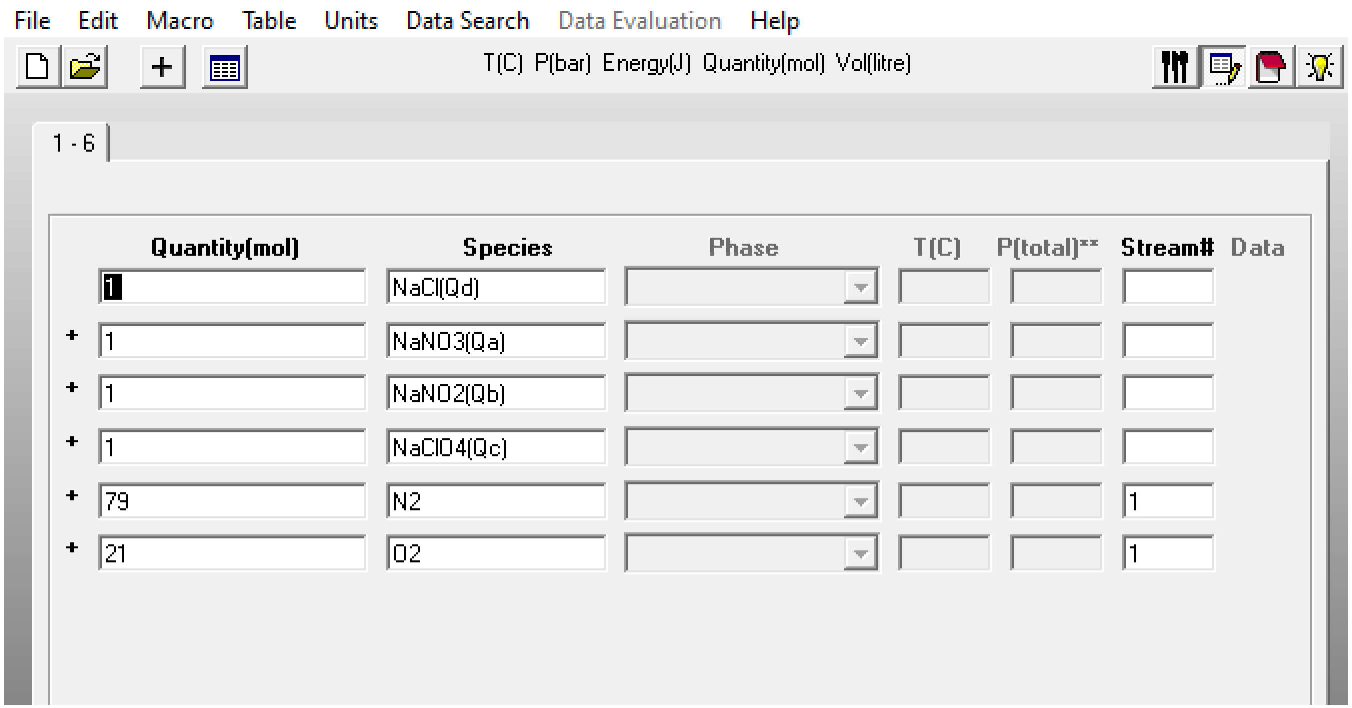
With unconstrained equilibrium

it can be seen that there is virtually complete reaction of ClO_4^- as well as reaction between salt and gas



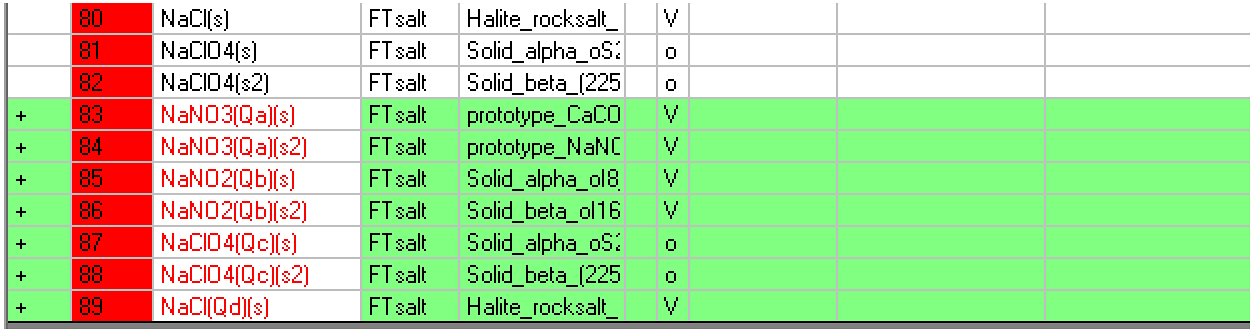
```
NaCl   +   NaNO3   +   NaNO2   +   NaClO4   +

79 N2   +   21 O2   =

  101.52      mol    gas_ideal
  (2933.5 gram, 101.52 mol, 6947.8 litre, 4.2222E-04 gram.cm-3)
          (550 C, 1 bar,      a=1.0000)
          ( 0.77820          N2
          + 0.22179          O2
          + 3.4784E-06       NO
          + 8.5175E-07       NO2
          + 2.1640E-07       NaCl

+ 3.2040      mol    Salt-liquid
  (239.85 gram, 3.2040 mol)
          (550 C, 1 bar,      a=1.0000)
          ( 0.37578          NaCl
          + 0.61438          NaNO3
          + 9.8458E-03       NaNO2
          + 1.5255E-20       NaClO4)

    + 0.79597     mol    NaCl_Halite_rocksalt_B1_cF8_(225)_Fm-3m
  (46.519 gram, 0.79597 mol)
          (550 C, 1 bar, S1, a=1.0000)
```

The following slides illustrate the use of virtual elements to maintain the amounts of NO_2^-, NO_3^-, ClO_4^- and Cl^- constant. A different virtual element is associated with each anion.



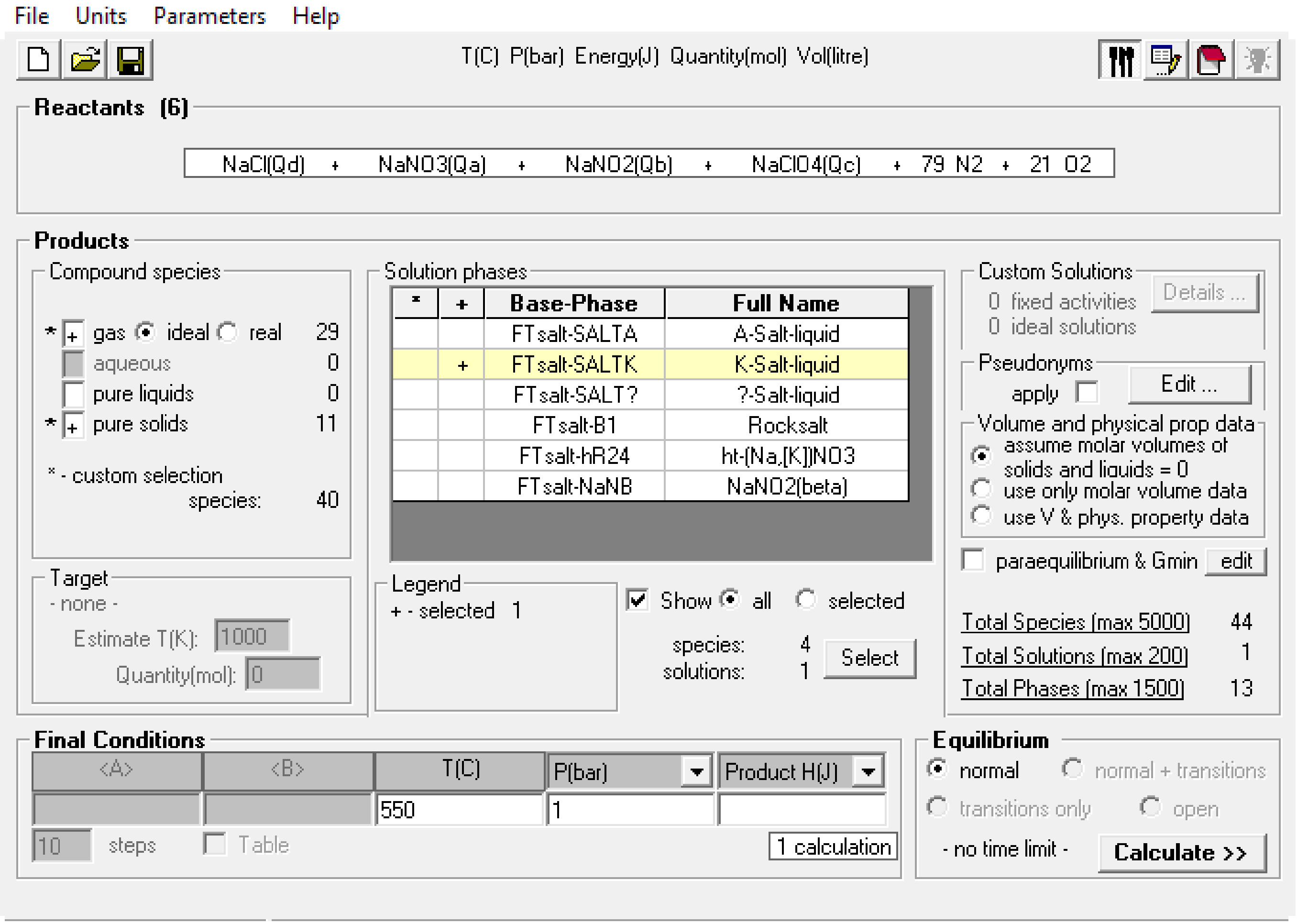
	Quantity(mol)	Species	Phase	T(C)	P(total)**	Stream#	Data
	1	NaCl(Qd)					
+	1	NaNO3(Qa)					
+	1	NaNO2(Qb)					
+	1	NaClO4(Qc)					
+	79	N2				1	
+	21	O2				1	

Solid compound selection



	80	NaCl(s)	FTsalt	Halite_rocksalt_		V
	81	NaClO4(s)	FTsalt	Solid_alpha_oS		o
	82	NaClO4(s2)	FTsalt	Solid_beta_(225		o
+	83	NaNO3(Qa)(s)	FTsalt	prototype_CaCO		V
+	84	NaNO3(Qa)(s2)	FTsalt	prototype_NaN		V
+	85	NaNO2(Qb)(s)	FTsalt	Solid_alpha_oI8		V
+	86	NaNO2(Qb)(s2)	FTsalt	Solid_beta_oI16		V
+	87	NaClO4(Qc)(s)	FTsalt	Solid_alpha_oS		o
+	88	NaClO4(Qc)(s2)	FTsalt	Solid_beta_(225		o
+	89	NaCl(Qd)(s)	FTsalt	Halite_rocksalt_		V

These species are those entered in the reactants window. They are automatically and temporarily created in **FTsalt** with the same properties as the corresponding compounds without the virtual elements.



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

Reactants (6)

NaCl(Qd) + NaNO3(Qa) + NaNO2(Qb) + NaClO4(Qc) + 79 N2 + 21 O2

Products

Compound species

* ☑	gas ● ideal ○ real	29
☐	aqueous	0
☐	pure liquids	0
* ☑	pure solids	11

* - custom selection
species: 40

Solution phases

*	+	Base-Phase	Full Name
		FTsalt-SALTA	A-Salt-liquid
	+	FTsalt-SALTK	K-Salt-liquid
		FTsalt-SALT?	?-Salt-liquid
		FTsalt-B1	Rocksalt
		FTsalt-hR24	ht-(Na,[K])NO3
		FTsalt-NaNB	NaNO2(beta)

Legend
+ - selected 1

☑ Show ● all ○ selected

species: 4
solutions: 1

Custom Solutions
0 fixed activities
0 ideal solutions

Pseudonyms
apply ☐

Volume and physical prop data
● assume molar volumes of solids and liquids = 0
○ use only molar volume data
○ use V & phys. property data

☐ paraequilibrium & Gmin

Total Species (max 5000) 44
Total Solutions (max 200) 1
Total Phases (max 1500) 13

Target
- none -
Estimate T(K): 1000
Quantity(mol): 0

Final Conditions

<A>	<B>	T(C)	P(bar)	Product H(J)
		550	1	

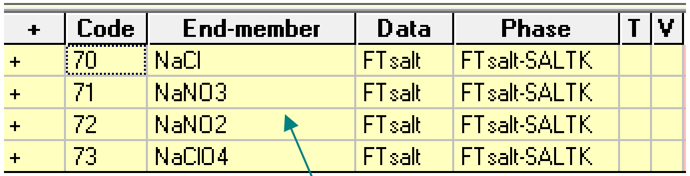
10 steps ☐ Table
1 calculation

Equilibrium
● normal ○ normal + transitions
○ transitions only ○ open
- no time limit -

The end-members of the solutions must now also be associated with the virtual elements. This could be done by creating a private solution (sln) file with the **SOLUTION** module, but can also be done during execution as shown on the next slide.

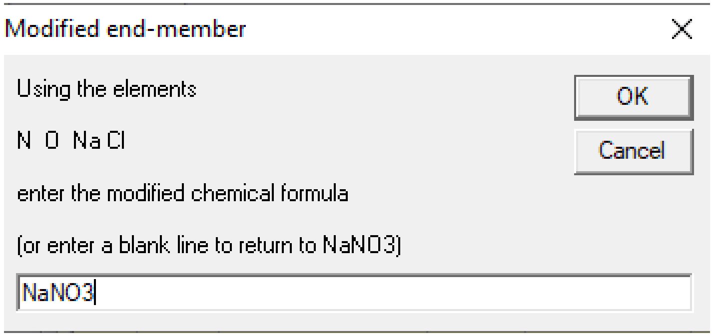
Adding virtual elements to the end-members of a solution

1) Right click on the name **FTsalt-SALTK** on the menu window (previous slide).



+	Code	End-member	Data	Phase	T	V
+	70	NaCl	FTsalt	FTsalt-SALTK		
+	71	NaNO3	FTsalt	FTsalt-SALTK		
+	72	NaNO2	FTsalt	FTsalt-SALTK		
+	73	NaClO4	FTsalt	FTsalt-SALTK		

2) Click on the name of an end-member



Using the elements

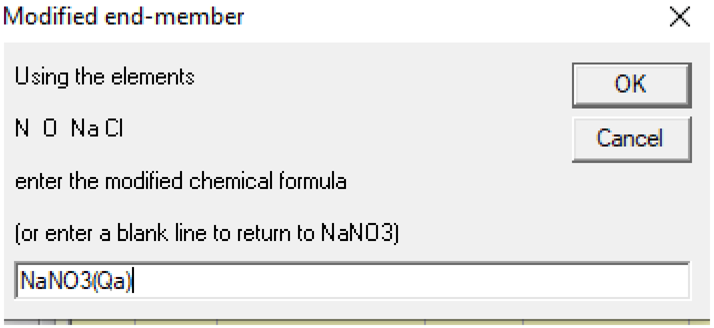
N O Na Cl

enter the modified chemical formula

(or enter a blank line to return to NaNO3)

NaNO3

3) Ready for editing



Using the elements

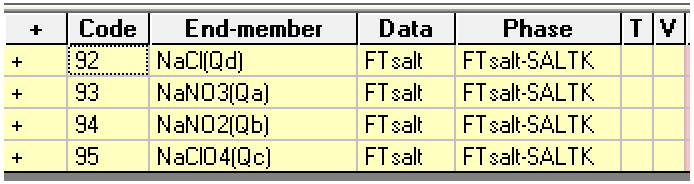
N O Na Cl

enter the modified chemical formula

(or enter a blank line to return to NaNO3)

NaNO3(Qa)

4) Enter modified chemical formula

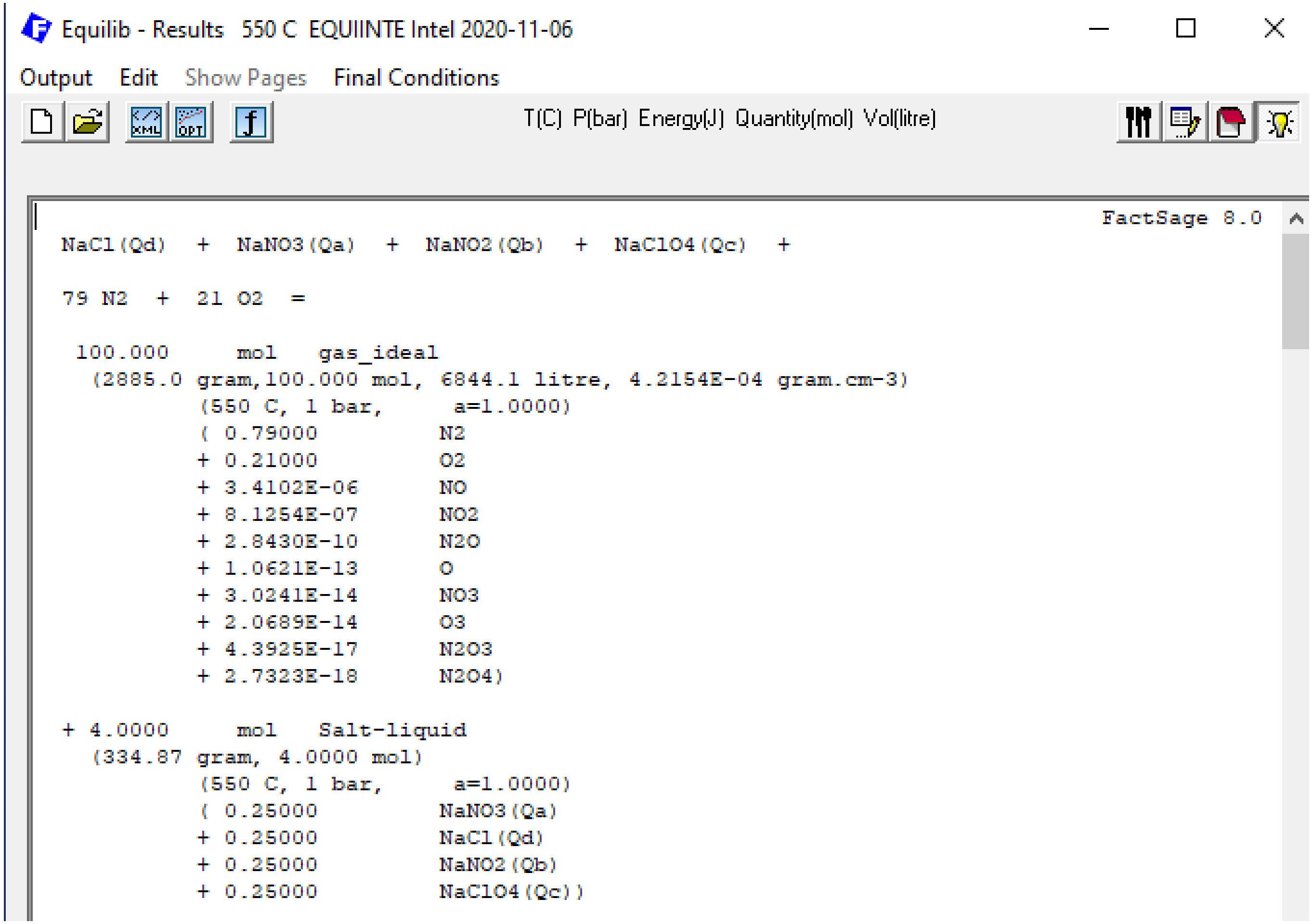


+	Code	End-member	Data	Phase	T	V
+	92	NaCl(Qd)	FTsalt	FTsalt-SALTK		
+	93	NaNO3(Qa)	FTsalt	FTsalt-SALTK		
+	94	NaNO2(Qb)	FTsalt	FTsalt-SALTK		
+	95	NaClO4(Qc)	FTsalt	FTsalt-SALTK		

5) Repeat for other end-members

- The end-members of the three solid solutions (see previous slide) are modified in a similar fashion

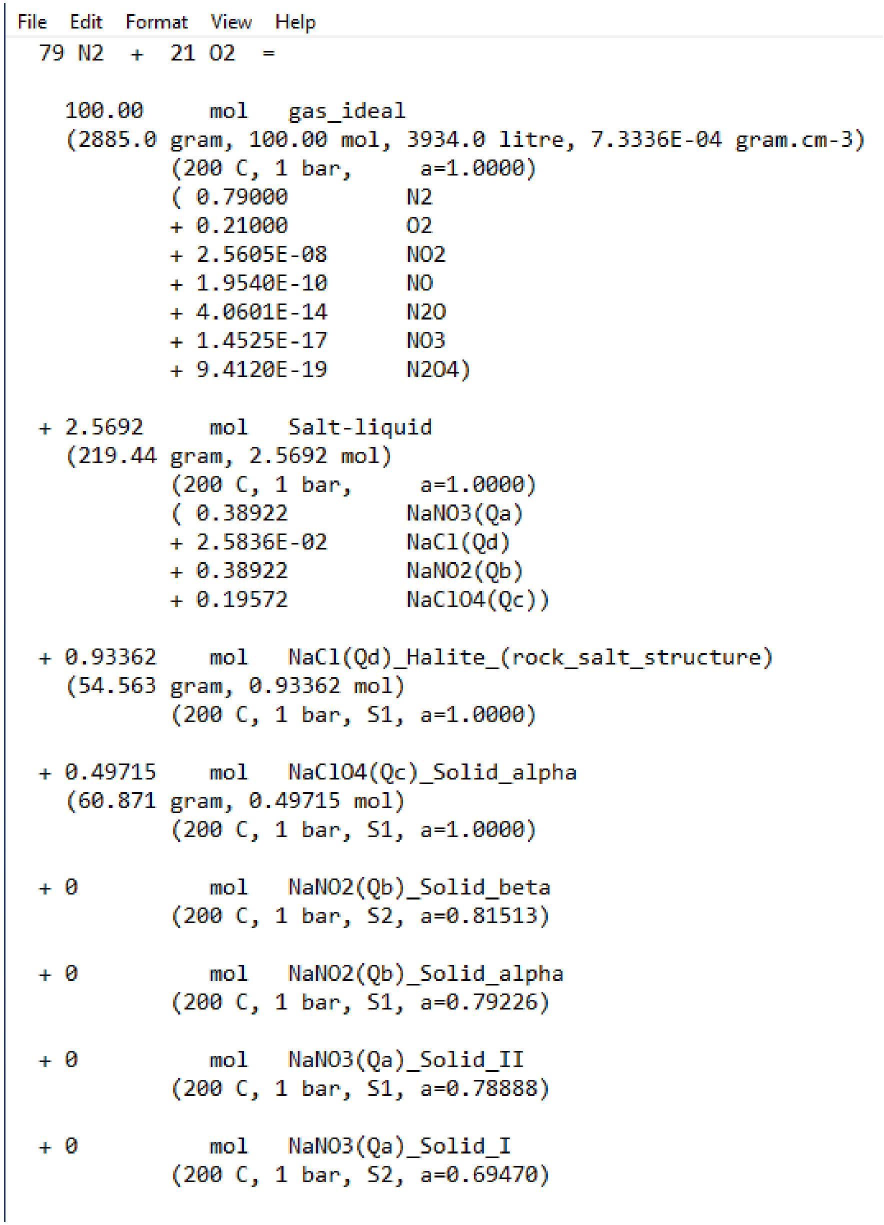
Output at 550ºC. No reactions within the salt or with the gas occur



```
                                                           FactSage 8.0
 NaCl(Qd)  +  NaNO3(Qa)  +  NaNO2(Qb)  +  NaClO4(Qc)  +

 79 N2  +  21 O2  =

  100.000     mol   gas_ideal
   (2885.0 gram,100.000 mol, 6844.1 litre, 4.2154E-04 gram.cm-3)
           (550 C, 1 bar,     a=1.0000)
           ( 0.79000          N2
           + 0.21000          O2
           + 3.4102E-06       NO
           + 8.1254E-07       NO2
           + 2.8430E-10       N2O
           + 1.0621E-13       O
           + 3.0241E-14       NO3
           + 2.0689E-14       O3
           + 4.3925E-17       N2O3
           + 2.7323E-18       N2O4)

 + 4.0000     mol   Salt-liquid
   (334.87 gram, 4.0000 mol)
           (550 C, 1 bar,     a=1.0000)
           ( 0.25000          NaNO3(Qa)
           + 0.25000          NaCl(Qd)
           + 0.25000          NaNO2(Qb)
           + 0.25000          NaClO4(Qc))
```

Output at 200°C

Solid compounds appear, but numbers of moles of each anion remain constant. For example, the number of moles of ClO_4^- is 2.5692(0.19572) + 0.49715 = 1.000 mol as entered in the reactants window.



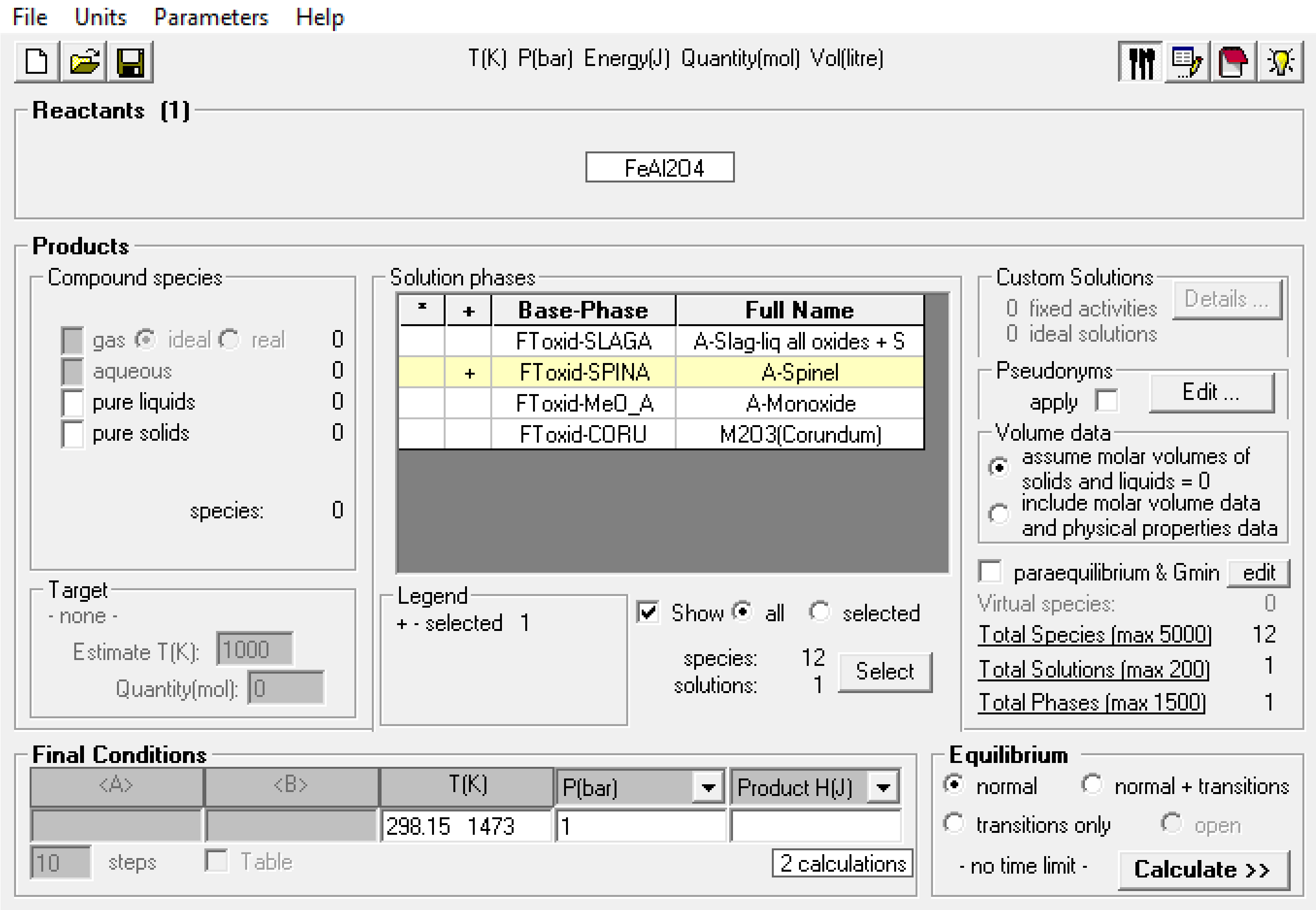
```
79 N2  +  21 O2   =

  100.00     mol   gas_ideal
  (2885.0 gram, 100.00 mol, 3934.0 litre, 7.3336E-04 gram.cm-3)
          (200 C, 1 bar,     a=1.0000)
          ( 0.79000         N2
          + 0.21000         O2
          + 2.5605E-08      NO2
          + 1.9540E-10      NO
          + 4.0601E-14      N2O
          + 1.4525E-17      NO3
          + 9.4120E-19      N2O4)

+ 2.5692     mol   Salt-liquid
  (219.44 gram, 2.5692 mol)
          (200 C, 1 bar,     a=1.0000)
          ( 0.38922         NaNO3(Qa)
          + 2.5836E-02      NaCl(Qd)
          + 0.38922         NaNO2(Qb)
          + 0.19572         NaClO4(Qc))

+ 0.93362    mol   NaCl(Qd)_Halite_(rock_salt_structure)
  (54.563 gram, 0.93362 mol)
          (200 C, 1 bar, S1, a=1.0000)

+ 0.49715    mol   NaClO4(Qc)_Solid_alpha
  (60.871 gram, 0.49715 mol)
          (200 C, 1 bar, S1, a=1.0000)

+ 0          mol   NaNO2(Qb)_Solid_beta
          (200 C, 1 bar, S2, a=0.81513)

+ 0          mol   NaNO2(Qb)_Solid_alpha
          (200 C, 1 bar, S1, a=0.79226)

+ 0          mol   NaNO3(Qa)_Solid_II
          (200 C, 1 bar, S1, a=0.78888)

+ 0          mol   NaNO3(Qa)_Solid_I
          (200 C, 1 bar, S2, a=0.69470)
```

Preventing internal equilibria within a spinel phase

In this example,

$FeAl_2O_4$ spinel is cooled rapidly from 1473 K to 298.15 K in a calorimeter. Calculate the heat evolved, given that the equilibrium cation distribution between tetrahedral and octahedral sites at 1473 K is retained metastably at 298.15 K.

Input to calculate equilibrium cation distribution



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

Reactants (1)

FeAl2O4

Products

Compound species

☐ gas ● ideal ○ real 0
☐ aqueous 0
☐ pure liquids 0
☐ pure solids 0

species: 0

Solution phases

*	+	Base-Phase	Full Name
		FToxid-SLAGA	A-Slag-liq all oxides + S
	+	FToxid-SPINA	A-Spinel
		FToxid-MeO_A	A-Monoxide
		FToxid-CORU	M2O3(Corundum)

Custom Solutions
0 fixed activities
0 ideal solutions

Pseudonyms
apply ☐

Volume data
● assume molar volumes of solids and liquids = 0
○ include molar volume data and physical properties data

☐ paraequilibrium & Gmin

Virtual species: 0
Total Species (max 5000) 12
Total Solutions (max 200) 1
Total Phases (max 1500) 1

Target
- none -
Estimate T(K): 1000
Quantity(mol): 0

Legend
+ - selected 1

☑ Show ● all ○ selected

species: 12
solutions: 1

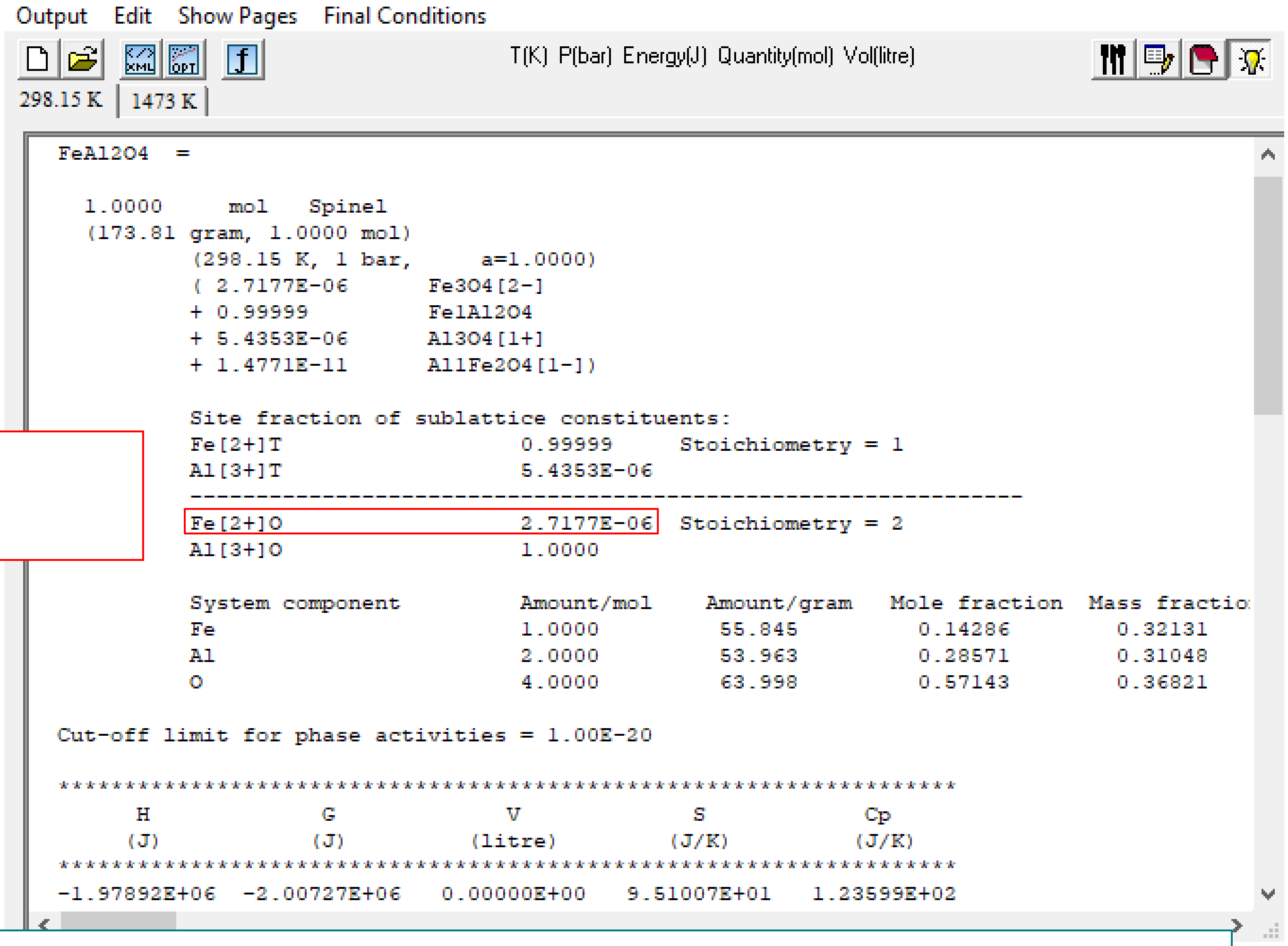
Final Conditions

<A>	<B>	T(K)	P(bar)	Product H(J)
		298.15 1473	1	

10 steps ☐ Table
2 calculations

Equilibrium
● normal ○ normal + transitions
○ transitions only ○ open
- no time limit -

Equilibrium cation distribution at 298.15 K

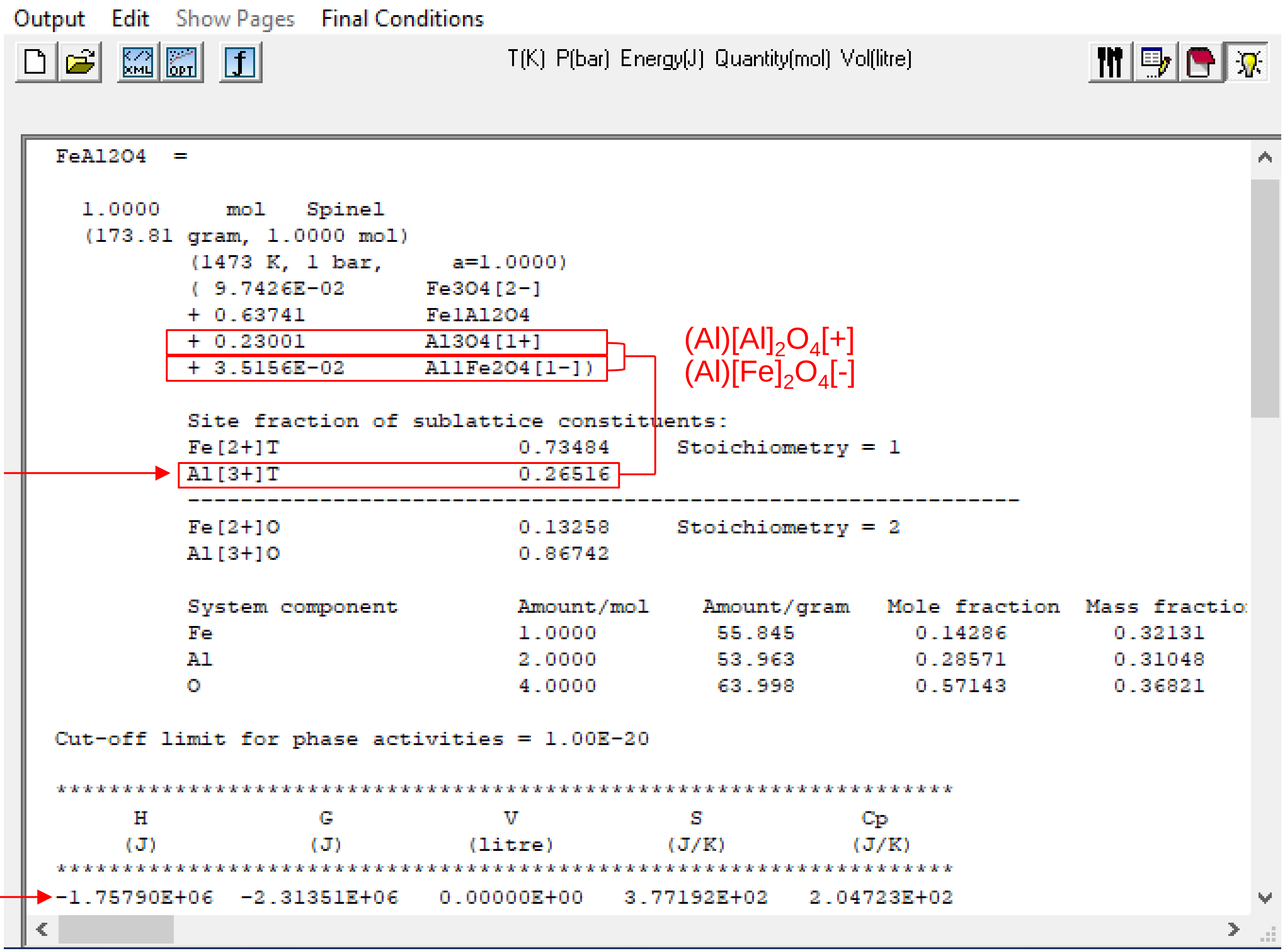


```
FeAl2O4  =

  1.0000     mol   Spinel
  (173.81 gram, 1.0000 mol)
          (298.15 K, 1 bar,      a=1.0000)
          ( 2.7177E-06       Fe3O4[2-]
          + 0.99999          Fe1Al2O4
          + 5.4353E-06       Al3O4[1+]
          + 1.4771E-11       Al1Fe2O4[1-])

          Site fraction of sublattice constituents:
          Fe[2+]T                   0.99999     Stoichiometry = 1
          Al[3+]T                   5.4353E-06
          ----------------------------------------------------------------
          Fe[2+]O                   2.7177E-06  Stoichiometry = 2
          Al[3+]O                   1.0000

          System component          Amount/mol    Amount/gram   Mole fraction  Mass fractio
          Fe                        1.0000         55.845         0.14286        0.32131
          Al                        2.0000         53.963         0.28571        0.31048
          O                         4.0000         63.998         0.57143        0.36821

Cut-off limit for phase activities = 1.00E-20

*********************************************************************
     H             G              V              S            Cp
    (J)           (J)          (litre)         (J/K)        (J/K)
*********************************************************************
-1.97892E+06  -2.00727E+06   0.00000E+00   9.51007E+01   1.23599E+02
```

Degree of inversion
Al[3+]T = 0.00

At equilibrium at 298.15 K the degree of inversion is 0.00.
That is, no tetrahedral sites are occupied by Al^{3+} ions: $(Fe)[Al]_2O_4$

Equilibrium cation distribution at 1473 K



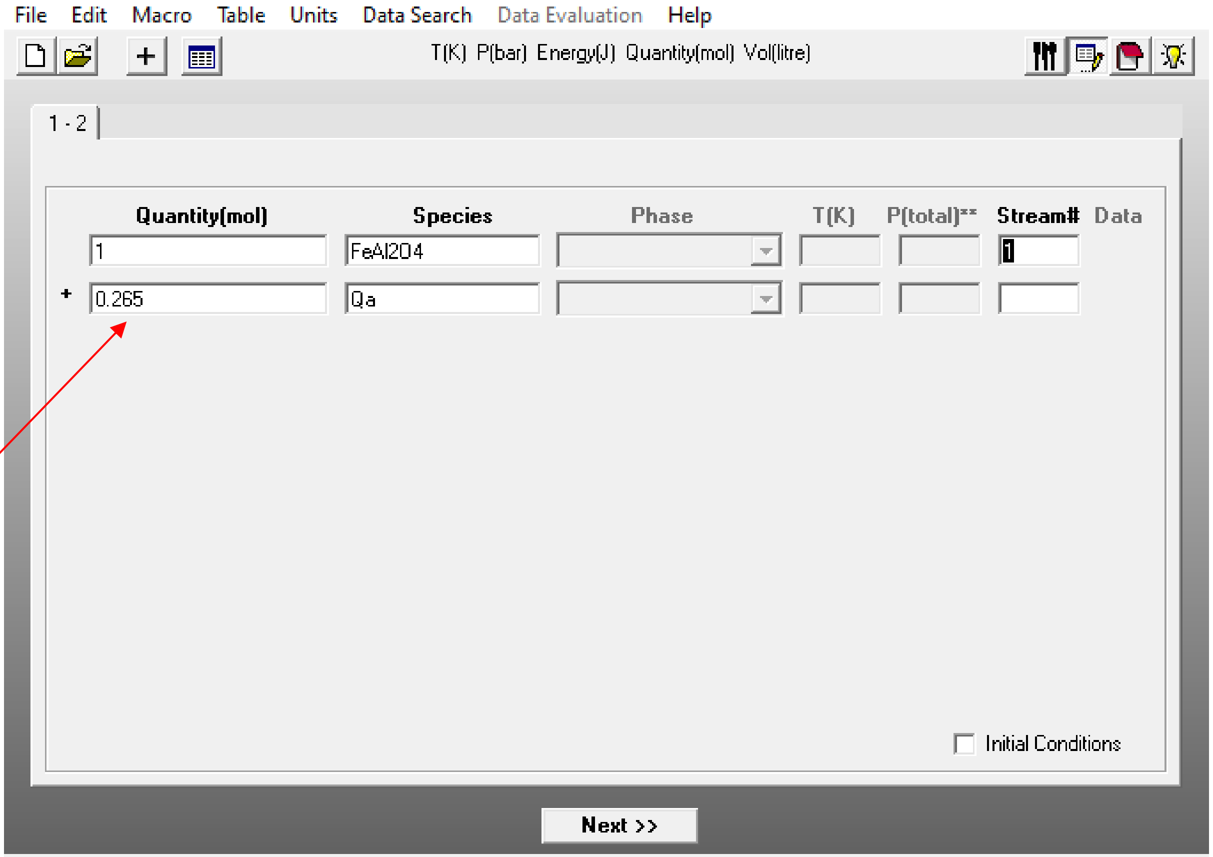
```
 FeAl2O4  =

   1.0000      mol   Spinel
   (173.81 gram, 1.0000 mol)
           (1473 K, 1 bar,      a=1.0000)
           ( 9.7426E-02       Fe3O4[2-]
           + 0.63741          Fe1Al2O4
           + 0.23001          Al3O4[1+]
           + 3.5156E-02       Al1Fe2O4[1-])

           Site fraction of sublattice constituents:
           Fe[2+]T                   0.73484     Stoichiometry = 1
           Al[3+]T                   0.26516
           ---------------------------------------------------------------
           Fe[2+]O                   0.13258     Stoichiometry = 2
           Al[3+]O                   0.86742

           System component          Amount/mol    Amount/gram   Mole fraction  Mass fractio
           Fe                        1.0000         55.845         0.14286        0.32131
           Al                        2.0000         53.963         0.28571        0.31048
           O                         4.0000         63.998         0.57143        0.36821

 Cut-off limit for phase activities = 1.00E-20

 ********************************************************************
       H             G             V             S             Cp
      (J)           (J)         (litre)        (J/K)         (J/K)
 ********************************************************************
-1.75790E+06  -2.31351E+06   0.00000E+00   3.77192E+02   2.04723E+02
```

(Al)[Al]$_2$O$_4$[+]
(Al)[Fe]$_2$O$_4$[-]

High-temperature degree of inversion = 0.265

Enthalpy at 1473 K at equilibrium

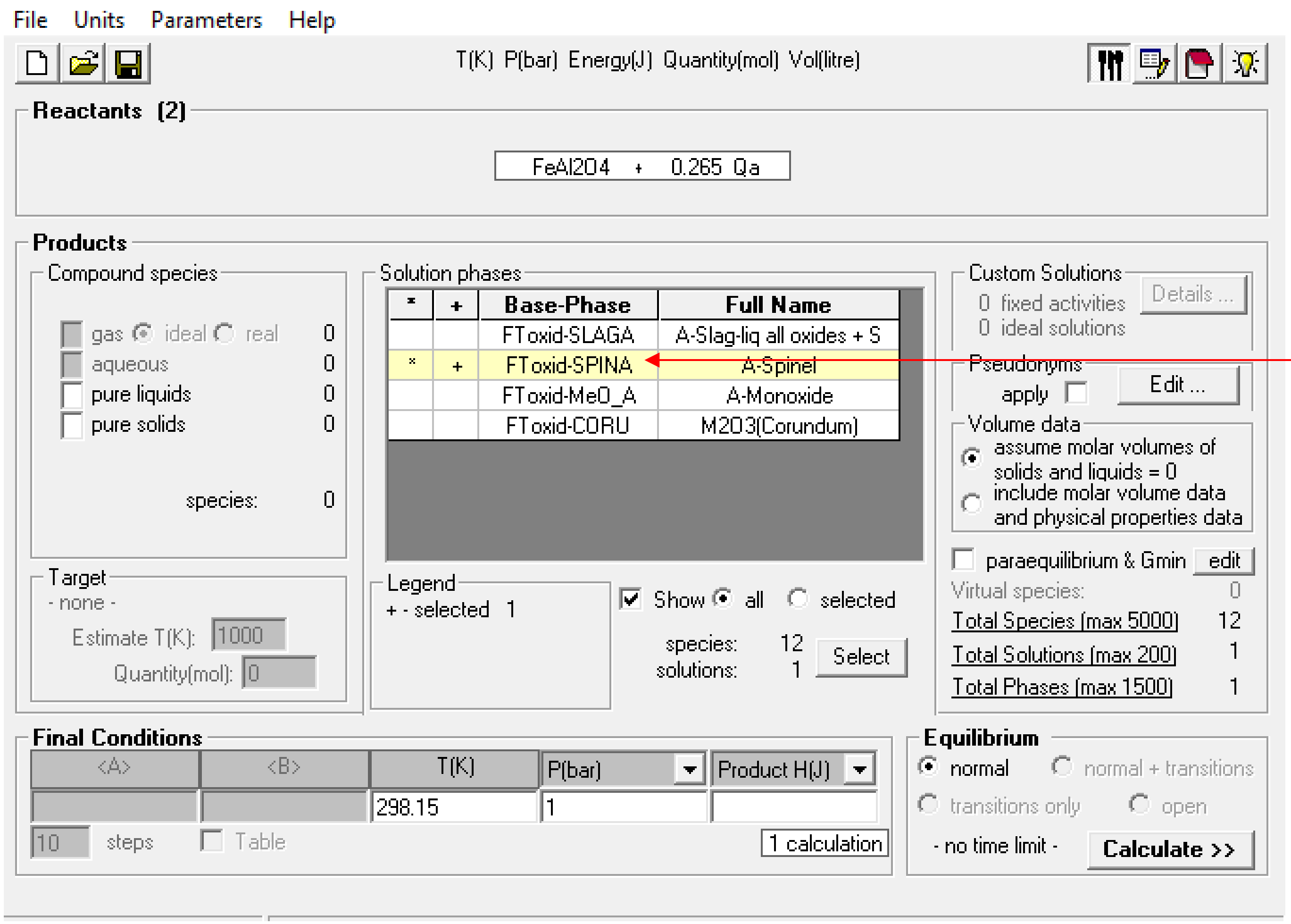
Input to calculate enthalpy at 298.15 K when degree of inversion is constrained to be 0.265



	Quantity(mol)	Species	Phase	T(K)	P(total)**	Stream#	Data
	1	FeAl2O4				1	
+	0.265	Qa					

☐ Initial Conditions

Enter 0.265 moles of a virtual element to be linked to the end-members related to Al[3+]T



Reactants (2)

FeAl2O4 + 0.265 Qa

Products

Compound species

☐ gas ● ideal ○ real	0
☐ aqueous	0
☐ pure liquids	0
☐ pure solids	0
species:	0

Solution phases

*	+	Base-Phase	Full Name
		FToxid-SLAGA	A-Slag-liq all oxides + S
*	+	FToxid-SPINA	A-Spinel
		FToxid-MeO_A	A-Monoxide
		FToxid-CORU	M2O3(Corundum)

Custom Solutions
0 fixed activities
0 ideal solutions

Pseudonyms
apply ☐

Volume data
● assume molar volumes of solids and liquids = 0
○ include molar volume data and physical properties data

☐ paraequilibrium & Gmin

Virtual species: 0
Total Species (max 5000) 12
Total Solutions (max 200) 1
Total Phases (max 1500) 1

Target
- none -
Estimate T(K): 1000
Quantity(mol): 0

Legend
+ - selected 1

☑ Show ● all ○ selected
species: 12
solutions: 1

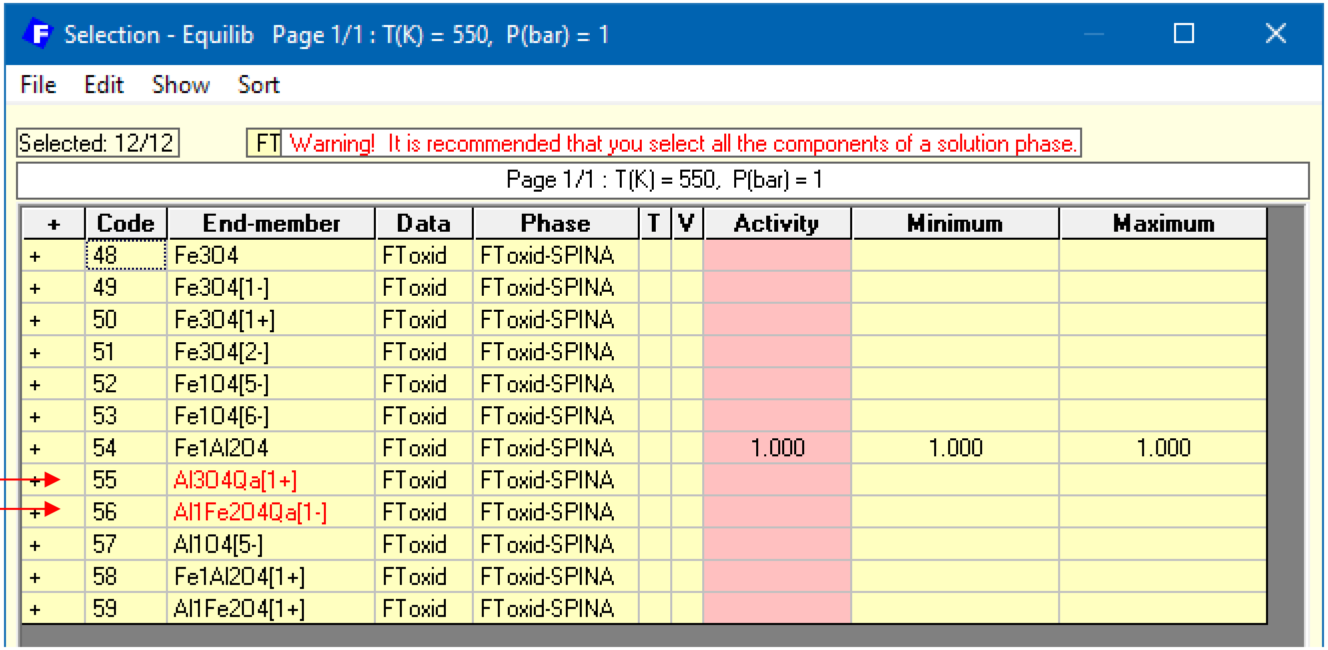
Final Conditions

<A>	<B>	T(K)	P(bar)	Product H(J)
		298.15	1	

10 steps ☐ Table
1 calculation

Equilibrium
● normal ○ normal + transitions
○ transitions only ○ open
- no time limit -

Right click to add virtual element to end-members



Selected: 12/12

FT Warning! It is recommended that you select all the components of a solution phase.

Page 1/1 : T(K) = 550, P(bar) = 1

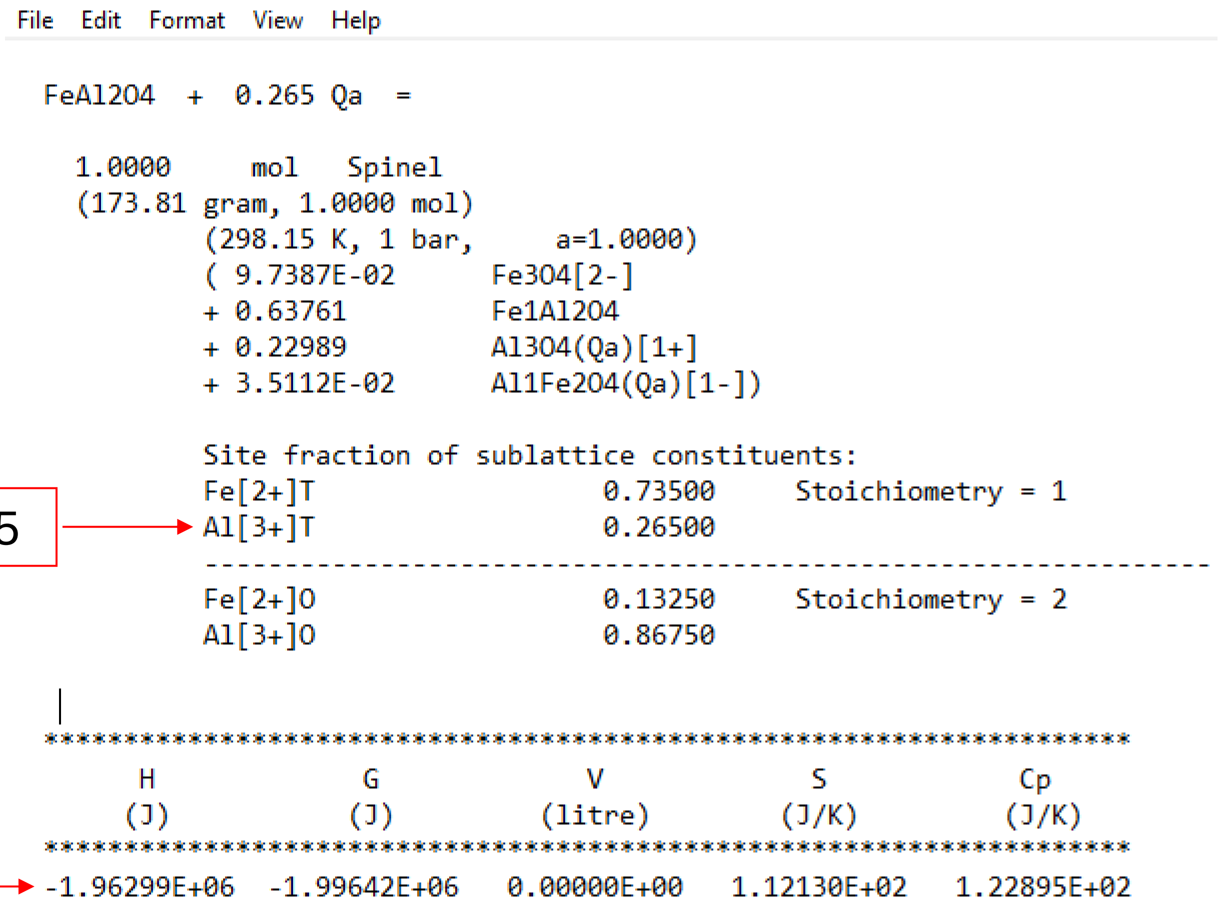
+	Code	End-member	Data	Phase	T	V	Activity	Minimum	Maximum
+	48	Fe3O4	FToxid	FToxid-SPINA					
+	49	Fe3O4[1-]	FToxid	FToxid-SPINA					
+	50	Fe3O4[1+]	FToxid	FToxid-SPINA					
+	51	Fe3O4[2-]	FToxid	FToxid-SPINA					
+	52	Fe1O4[5-]	FToxid	FToxid-SPINA					
+	53	Fe1O4[6-]	FToxid	FToxid-SPINA					
+	54	Fe1Al2O4	FToxid	FToxid-SPINA			1.000	1.000	1.000
+	55	Al3O4Qa[1+]	FToxid	FToxid-SPINA					
+	56	Al1Fe2O4Qa[1-]	FToxid	FToxid-SPINA					
+	57	Al1O4[5-]	FToxid	FToxid-SPINA					
+	58	Fe1Al2O4[1+]	FToxid	FToxid-SPINA					
+	59	Al1Fe2O4[1+]	FToxid	FToxid-SPINA					

Add Qa to formulae
(see slide 15.6.7)

```
FeAl2O4  =

  1.0000     mol   Spinel
  (173.81 gram, 1.0000 mol)
          (1473 K, 1 bar,     a=1.0000)
          ( 9.7426E-02        Fe3O4[2-]
          + 0.63741           Fe1Al2O4
          + 0.23001           Al3O4[1+]
          + 3.5156E-02        Al1Fe2O4[1-])

          Site fraction of sublattice constituents:
          Fe[2+]T                  0.73484     Stoichiometry = 1
          Al[3+]T                  0.26516
          --------------------------------------------------------
          Fe[2+]O                  0.13258     Stoichiometry = 2
          Al[3+]O                  0.86742
```

The degree of inversion is equal to Al[3+]T which is the sum of the amounts of end-members (Al)[Al]$_2$O$_4$[+] and (Al)[Fe]O$_4$[-]. By adding Qa to these formulae, we constrain the degree of inversion to be equal to Qa.

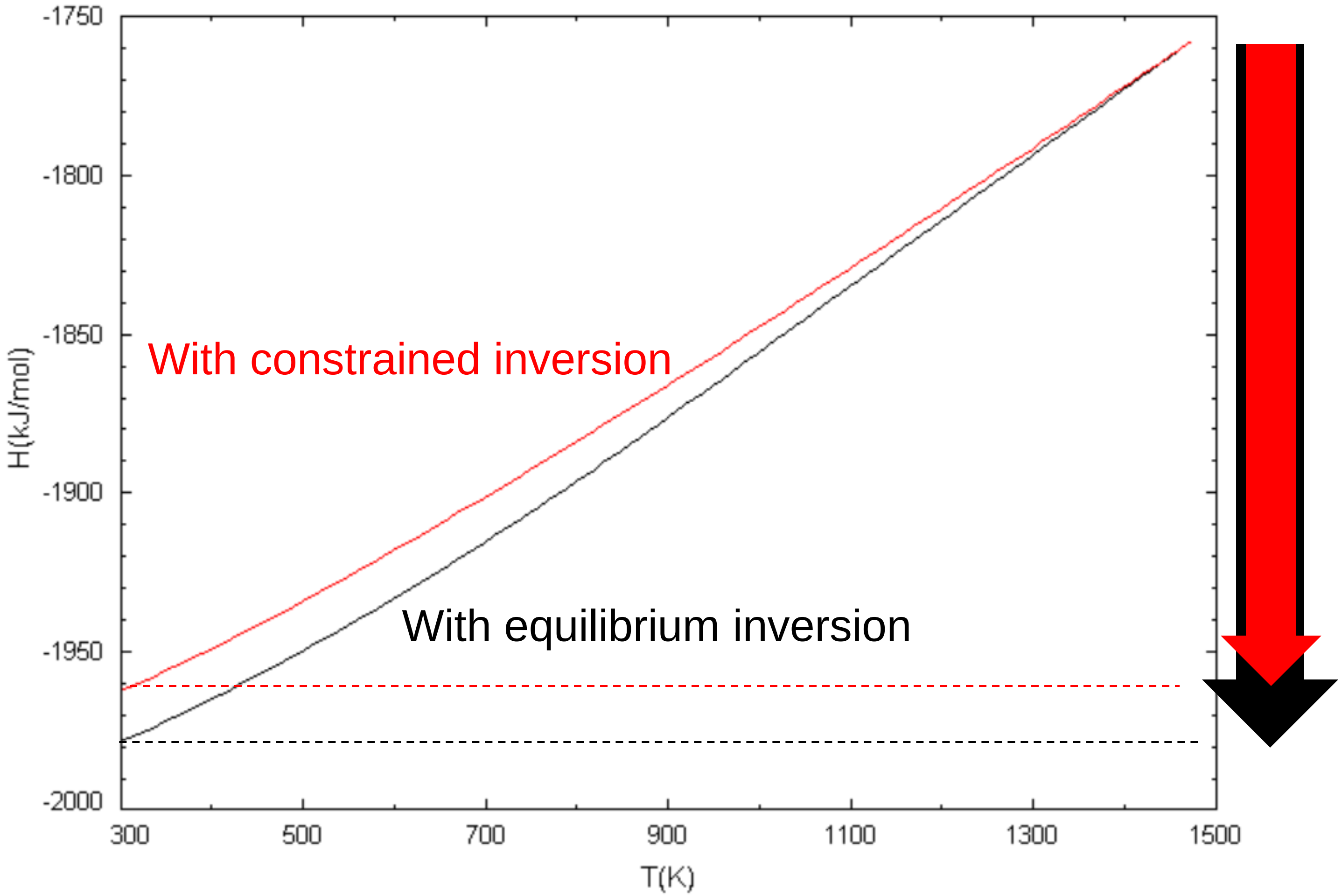
Output at 298.15 K with degree of inversion constrained to be 0.265



```
 FeAl2O4  +  0.265 Qa  =

   1.0000     mol   Spinel
   (173.81 gram, 1.0000 mol)
           (298.15 K, 1 bar,     a=1.0000)
           ( 9.7387E-02       Fe3O4[2-]
           + 0.63761          Fe1Al2O4
           + 0.22989          Al3O4(Qa)[1+]
           + 3.5112E-02       Al1Fe2O4(Qa)[1-])

           Site fraction of sublattice constituents:
           Fe[2+]T                  0.73500     Stoichiometry = 1
           Al[3+]T                  0.26500
           ---------------------------------------------------------------
           Fe[2+]O                  0.13250     Stoichiometry = 2
           Al[3+]O                  0.86750

 ********************************************************************
       H              G              V              S              Cp
      (J)            (J)          (litre)         (J/K)          (J/K)
 ********************************************************************
 -1.96299E+06  -1.99642E+06   0.00000E+00   1.12130E+02   1.22895E+02
```

Degree of inversion = 0.265

Enthalpy at 298.15 K
with constraint



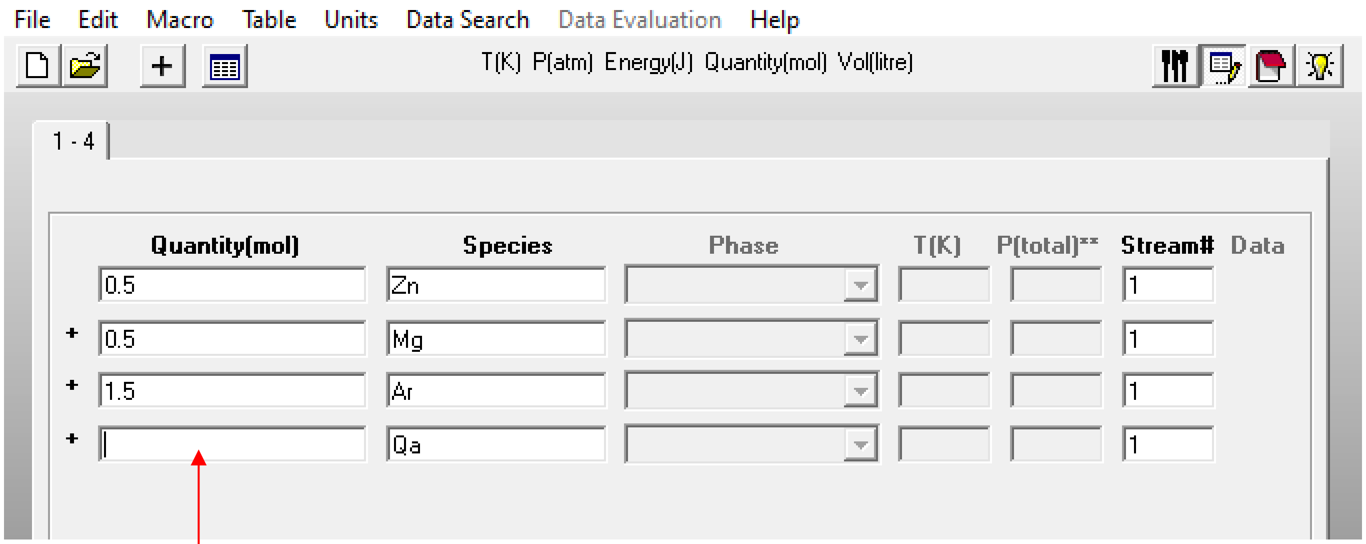
Heat evolved during rapid cooling from 1473 K to 298.15 K

Constrained inversion: (1.96299 – 1.75790) x 10^6 = 205090 Joules/mol

Equilibrium inversion: (1.97892 – 1.75790) x 10^6 = 221020 Joules/mol

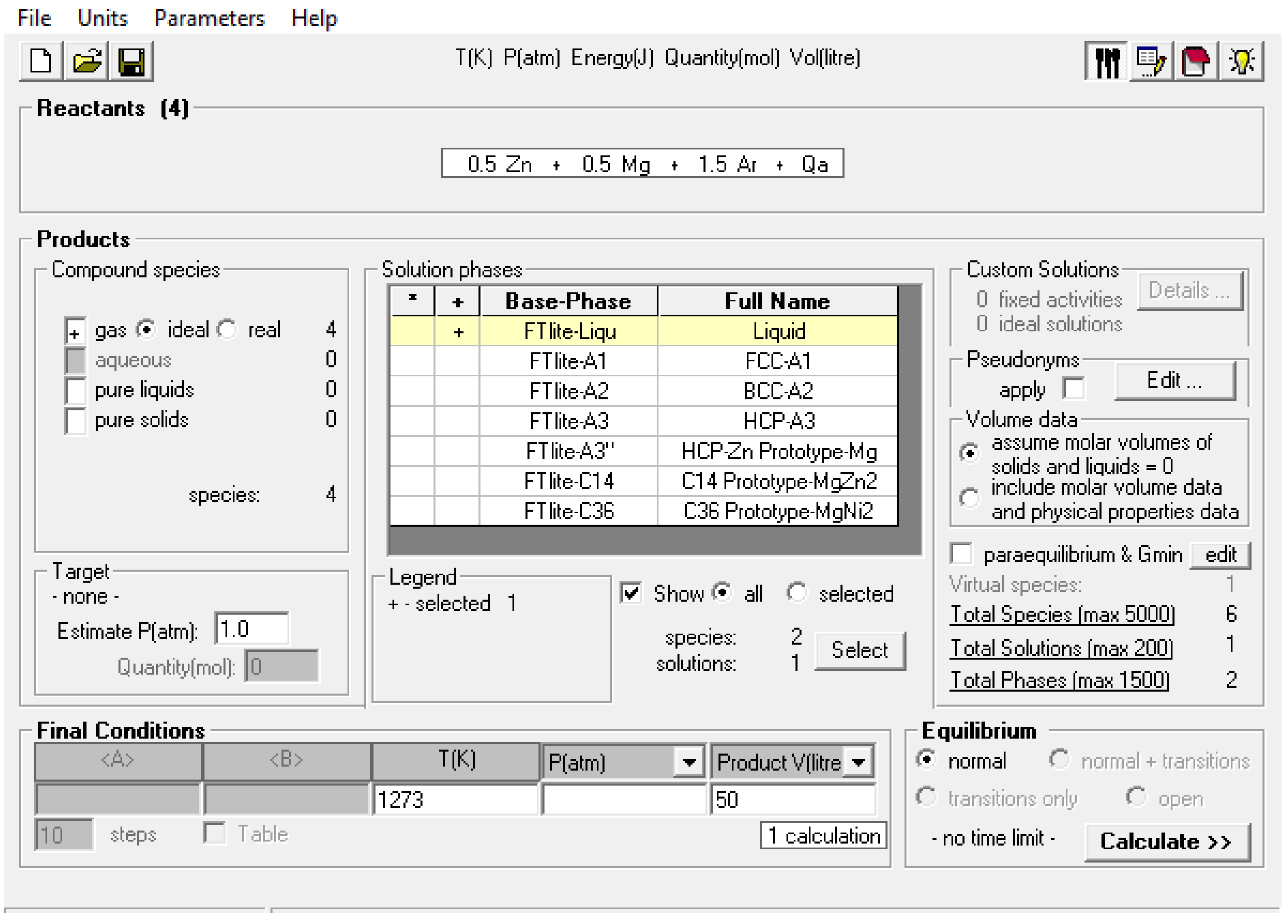
Following the course of a reaction with time

- 1.0 mol of an equimolar Zn-Mg solution is placed in a 50 litre container with 1.5 mol Ar at 1273 K.
- Follow the compositions of the liquid and gaseous phases with time as evaporation occurs, assuming gas/liquid equilibrium with constraint on the total amount of remaining liquid.



	Quantity(mol)	Species	Phase	T(K)	P(total)**	Stream#	Data
	0.5	Zn				1	
+	0.5	Mg				1	
+	1.5	Ar				1	
+		Qa				1	

The amount of Qa will vary with time



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

Reactants (4)

0.5 Zn + 0.5 Mg + 1.5 Ar + Qa

Products

Compound species

☑	gas ● ideal ○ real	4
☐	aqueous	0
☐	pure liquids	0
☐	pure solids	0
	species:	4

Target
- none -
Estimate P(atm): 1.0
Quantity(mol): 0

Solution phases

*	+	Base-Phase	Full Name
	+	FTlite-Liqu	Liquid
		FTlite-A1	FCC-A1
		FTlite-A2	BCC-A2
		FTlite-A3	HCP-A3
		FTlite-A3''	HCP-Zn Prototype-Mg
		FTlite-C14	C14 Prototype-MgZn2
		FTlite-C36	C36 Prototype-MgNi2

Legend
+ - selected 1

☑ Show ● all ○ selected
species: 2
solutions: 1

Custom Solutions
0 fixed activities
0 ideal solutions

Pseudonyms
apply ☐

Volume data
● assume molar volumes of solids and liquids = 0
○ include molar volume data and physical properties data

☐ paraequilibrium & Gmin

Virtual species:	1
Total Species (max 5000)	6
Total Solutions (max 200)	1
Total Phases (max 1500)	2

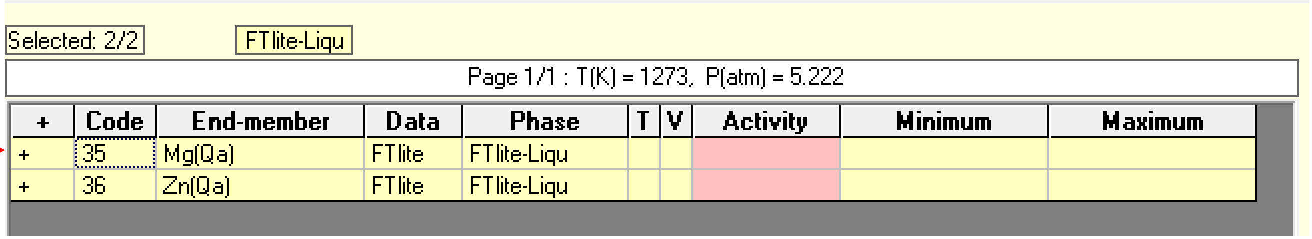
Final Conditions

<A>	<B>	T(K)	P(atm)	Product V(litre
		1273		50

10 steps ☐ Table
1 calculation

Equilibrium

● normal ○ normal + transitions
○ transitions only ○ open
- no time limit -



Selected: 2/2 FTlite-Liqu

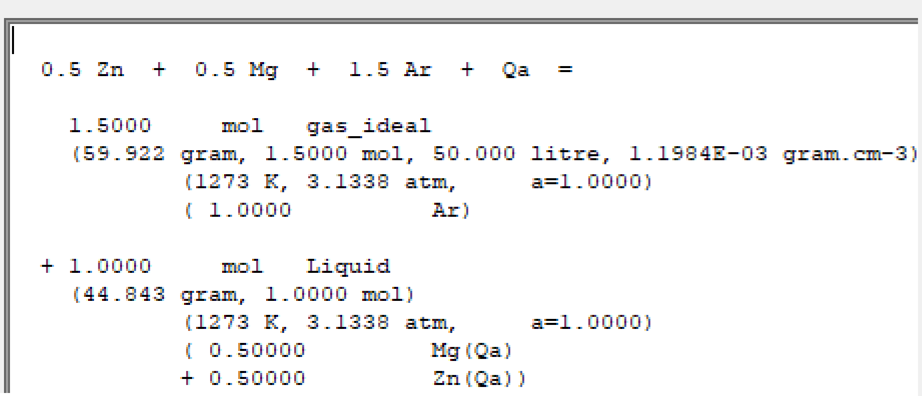
Page 1/1 : T(K) = 1273, P(atm) = 5.222

+	Code	End-member	Data	Phase	T	V	Activity	Minimum	Maximum
+	35	Mg(Qa)	FTlite	FTlite-Liqu					
+	36	Zn(Qa)	FTlite	FTlite-Liqu					

Associate Qa with each end-member of the liquid. There are thus Qa moles of liquid in total

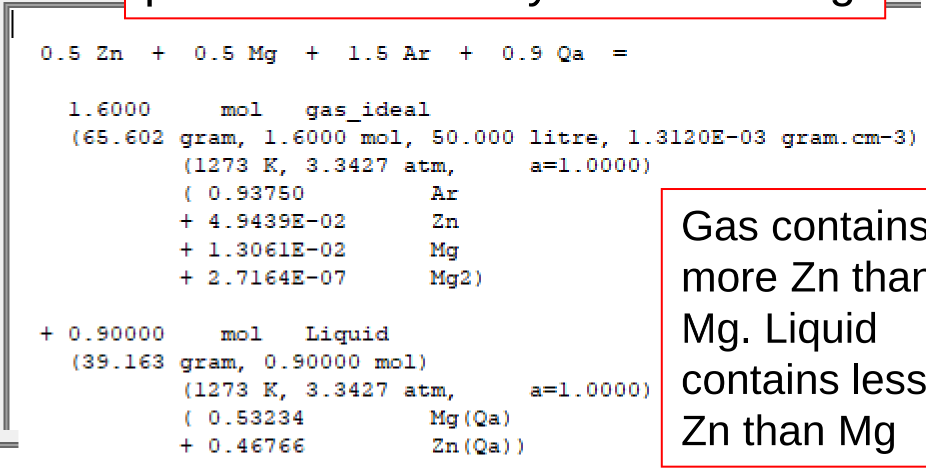
Outputs as amount of liquid decreases from Qa=1.0 (only liquid) to Qa = 0.0 (only vapour)

Qa = 1.0 : All Mg and Cr in liquid



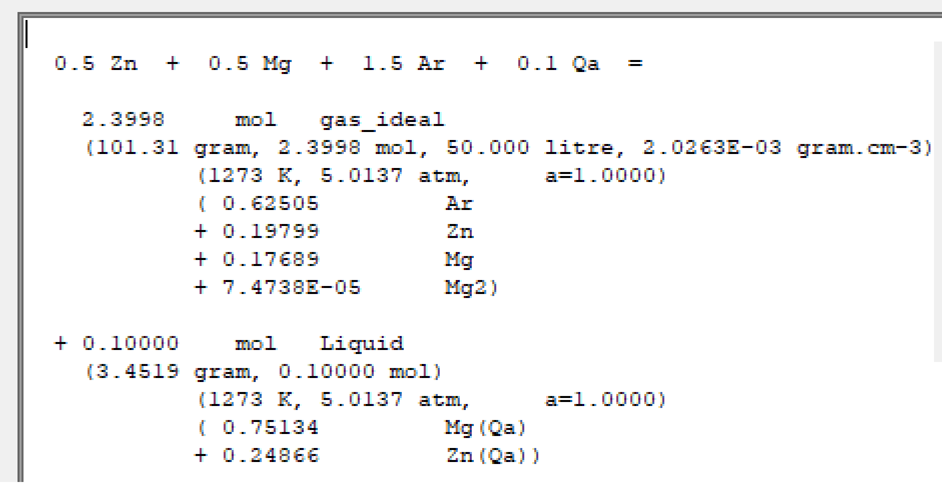
```
 0.5 Zn  +  0.5 Mg  +  1.5 Ar  +  Qa  =

   1.5000     mol   gas_ideal
   (59.922 gram, 1.5000 mol, 50.000 litre, 1.1984E-03 gram.cm-3)
           (1273 K, 3.1338 atm,     a=1.0000)
           ( 1.0000          Ar)

 + 1.0000     mol   Liquid
   (44.843 gram, 1.0000 mol)
           (1273 K, 3.1338 atm,     a=1.0000)
           ( 0.50000          Mg(Qa)
           + 0.50000          Zn(Qa))
```

Qa = 0.9 : Zn passes into gas phase more readily than does Mg



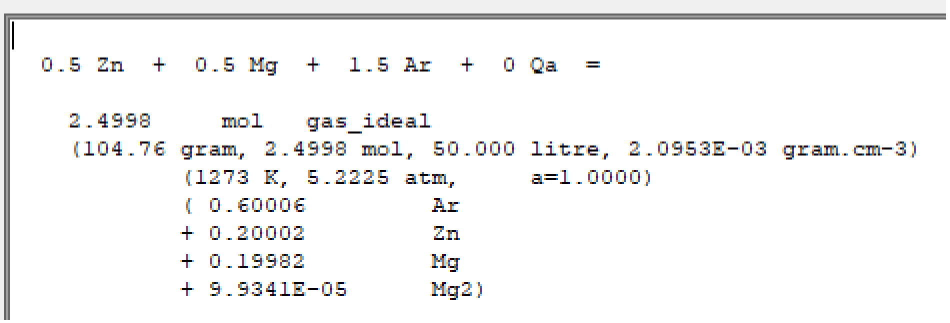
```
 0.5 Zn  +  0.5 Mg  +  1.5 Ar  +  0.9 Qa  =

   1.6000     mol   gas_ideal
   (65.602 gram, 1.6000 mol, 50.000 litre, 1.3120E-03 gram.cm-3)
           (1273 K, 3.3427 atm,     a=1.0000)
           ( 0.93750          Ar
           + 4.9439E-02       Zn
           + 1.3061E-02       Mg
           + 2.7164E-07       Mg2)

 + 0.90000    mol   Liquid
   (39.163 gram, 0.90000 mol)
           (1273 K, 3.3427 atm,     a=1.0000)
           ( 0.53234          Mg(Qa)
           + 0.46766          Zn(Qa))
```

Gas contains more Zn than Mg. Liquid contains less Zn than Mg



```
 0.5 Zn  +  0.5 Mg  +  1.5 Ar  +  0.1 Qa  =

   2.3998     mol   gas_ideal
   (101.31 gram, 2.3998 mol, 50.000 litre, 2.0263E-03 gram.cm-3)
           (1273 K, 5.0137 atm,     a=1.0000)
           ( 0.62505          Ar
           + 0.19799          Zn
           + 0.17689          Mg
           + 7.4738E-05       Mg2)

 + 0.10000    mol   Liquid
   (3.4519 gram, 0.10000 mol)
           (1273 K, 5.0137 atm,     a=1.0000)
           ( 0.75134          Mg(Qa)
           + 0.24866          Zn(Qa))
```

Qa =0.1 : Zn/Mg ratio in gas now close to 0.5



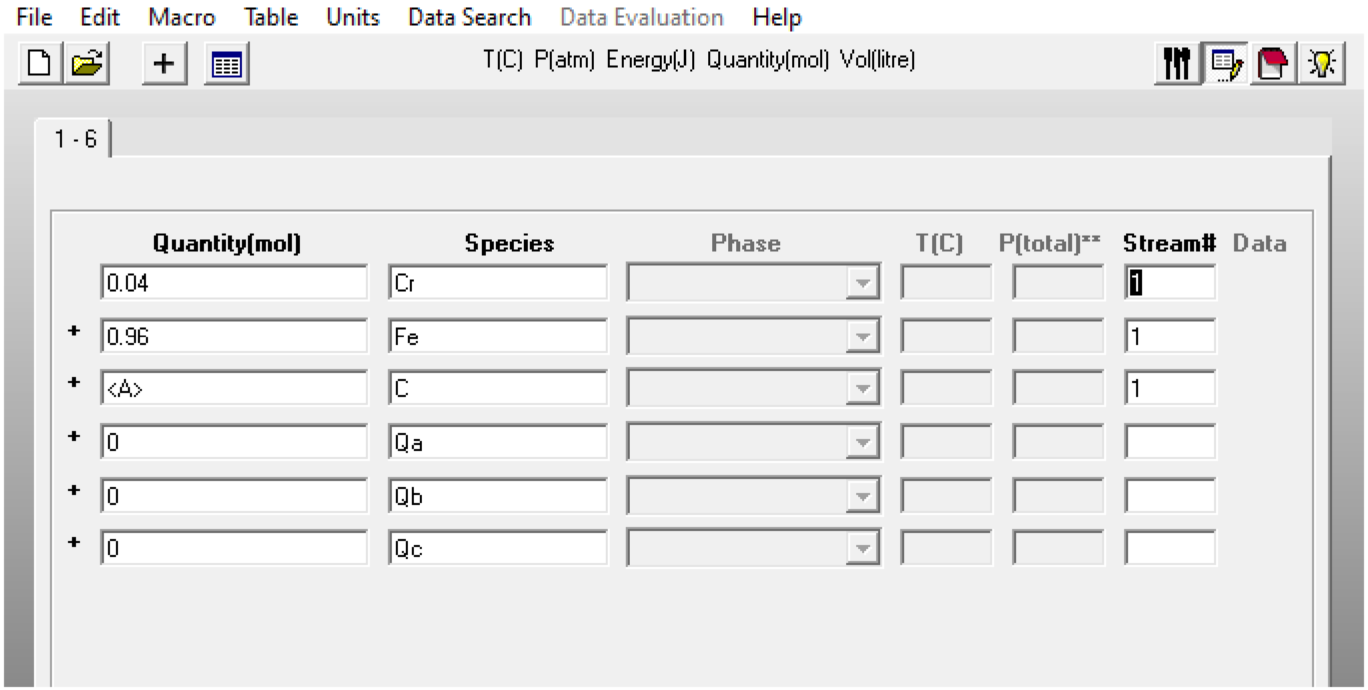
```
 0.5 Zn  +  0.5 Mg  +  1.5 Ar  +  0 Qa  =

   2.4998     mol   gas_ideal
   (104.76 gram, 2.4998 mol, 50.000 litre, 2.0953E-03 gram.cm-3)
           (1273 K, 5.2225 atm,     a=1.0000)
           ( 0.60006          Ar
           + 0.20002          Zn
           + 0.19982          Mg
           + 9.9341E-05       Mg2)
```

Qa = 0.0 : All liquid has evaporated. Gas is now equimolar in Zn and Mg

Paraequilibrium calculation

- For a description of paraequilibrium, see Section 14 where the **FactSage** software for calculating paraequilibrium is described.
- The present example illustrates the principle behind these calculations.
- An Fe(0.96)Cr(0.04)C(0.01) alloy is rapidly cooled from the γ-austenite (fcc) range to 700 ^{o}C. Carbon diffuses between phases, but the Fe/Cr ratio remains constant in all phases.

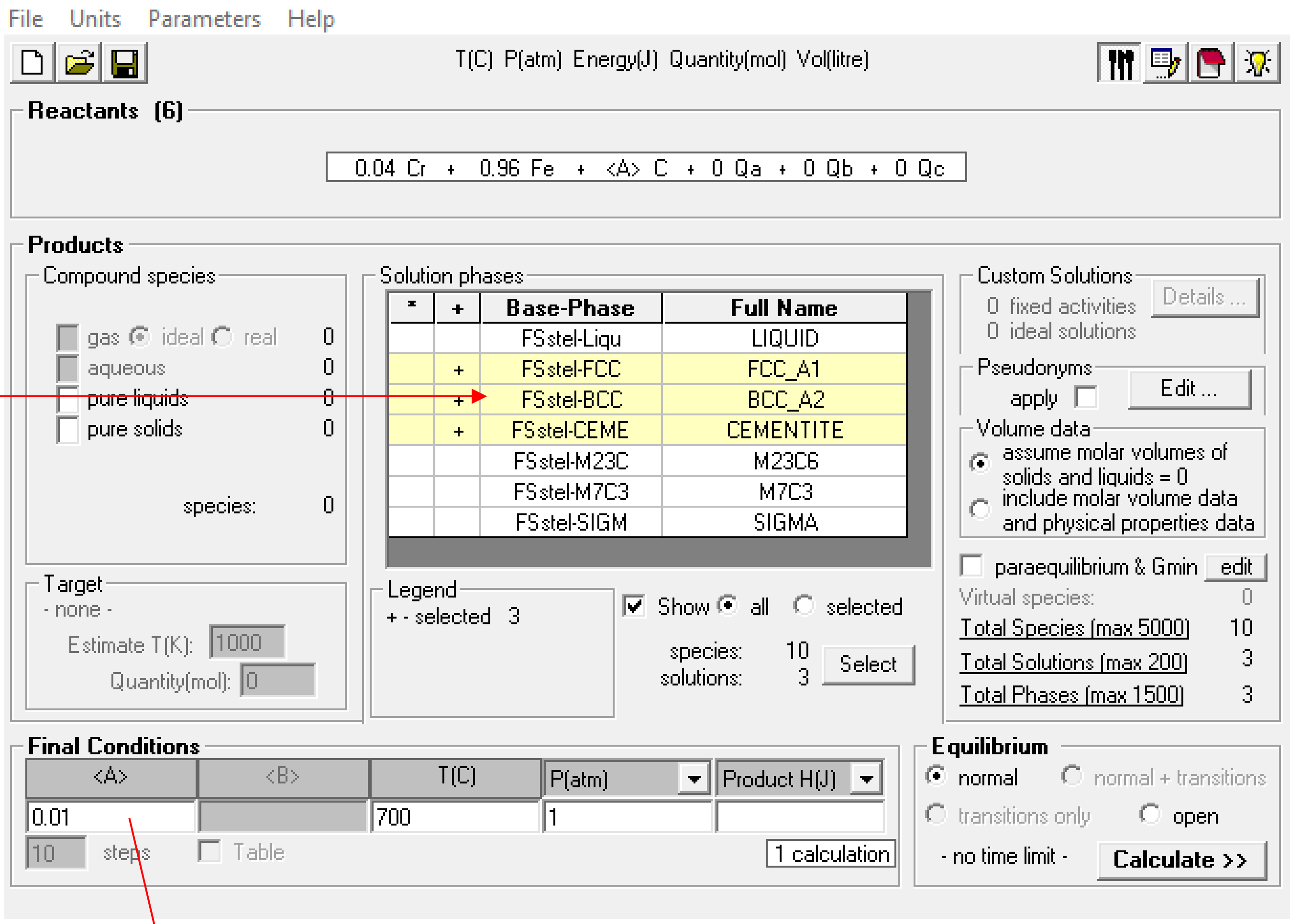
The **FSstel** database is activated



	Quantity(mol)	Species	Phase	T(C)	P(total)**	Stream#	Data
	0.04	Cr				1	
+	0.96	Fe				1	
+	<A>	C				1	
+	0	Qa					
+	0	Qb					
+	0	Qc					

Zero amounts of three virtual elements are entered

Click to add virtual elements to end-members



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

Reactants (6)

0.04 Cr + 0.96 Fe + <A> C + 0 Qa + 0 Qb + 0 Qc

Products

Compound species

☐	gas ● ideal ○ real	0
☐	aqueous	0
☐	pure liquids	0
☐	pure solids	0
	species:	0

Solution phases

*	+	Base-Phase	Full Name
		FSstel-Liqu	LIQUID
	+	FSstel-FCC	FCC_A1
	+	FSstel-BCC	BCC_A2
	+	FSstel-CEME	CEMENTITE
		FSstel-M23C	M23C6
		FSstel-M7C3	M7C3
		FSstel-SIGM	SIGMA

Custom Solutions
0 fixed activities
0 ideal solutions

Pseudonyms
apply ☐

Volume data
● assume molar volumes of solids and liquids = 0
○ include molar volume data and physical properties data

☐ paraequilibrium & Gmin

Virtual species:	0
Total Species (max 5000)	10
Total Solutions (max 200)	3
Total Phases (max 1500)	3

Target
- none -
Estimate T(K): 1000
Quantity(mol): 0

Legend
+ - selected 3

☑ Show ● all ○ selected

species: 10
solutions: 3

Final Conditions

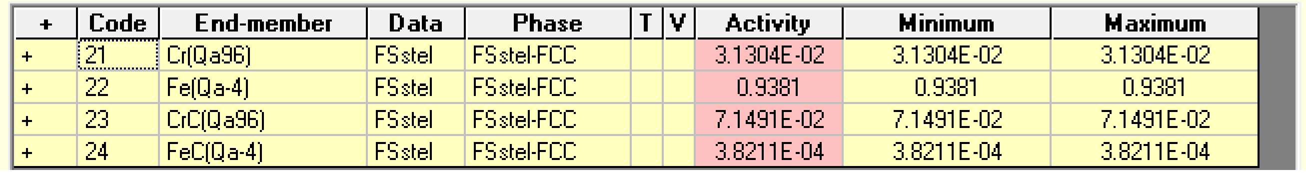
<A>	<B>	T(C)	P(atm)	Product H(J)
0.01		700	1	

10 steps ☐ Table

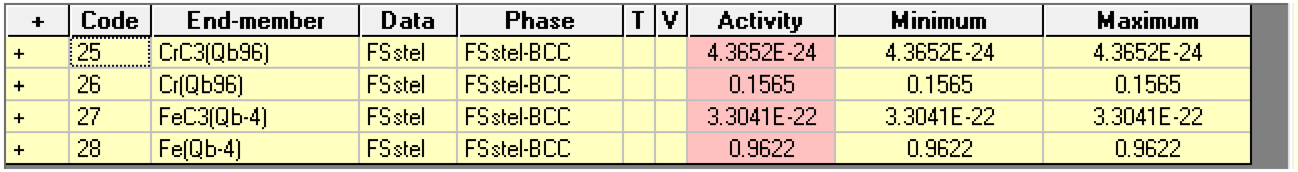
1 calculation

Equilibrium
● normal ○ normal + transitions
○ transitions only ○ open
- no time limit -

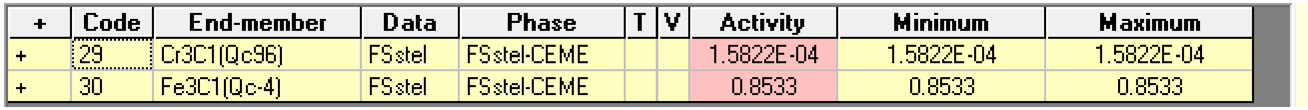
A = 0.01 (1% C)



+	Code	End-member	Data	Phase	T	V	Activity	Minimum	Maximum
+	21	Cr(Qa96)	FSstel	FSstel-FCC			3.1304E-02	3.1304E-02	3.1304E-02
+	22	Fe(Qa-4)	FSstel	FSstel-FCC			0.9381	0.9381	0.9381
+	23	CrC(Qa96)	FSstel	FSstel-FCC			7.1491E-02	7.1491E-02	7.1491E-02
+	24	FeC(Qa-4)	FSstel	FSstel-FCC			3.8211E-04	3.8211E-04	3.8211E-04



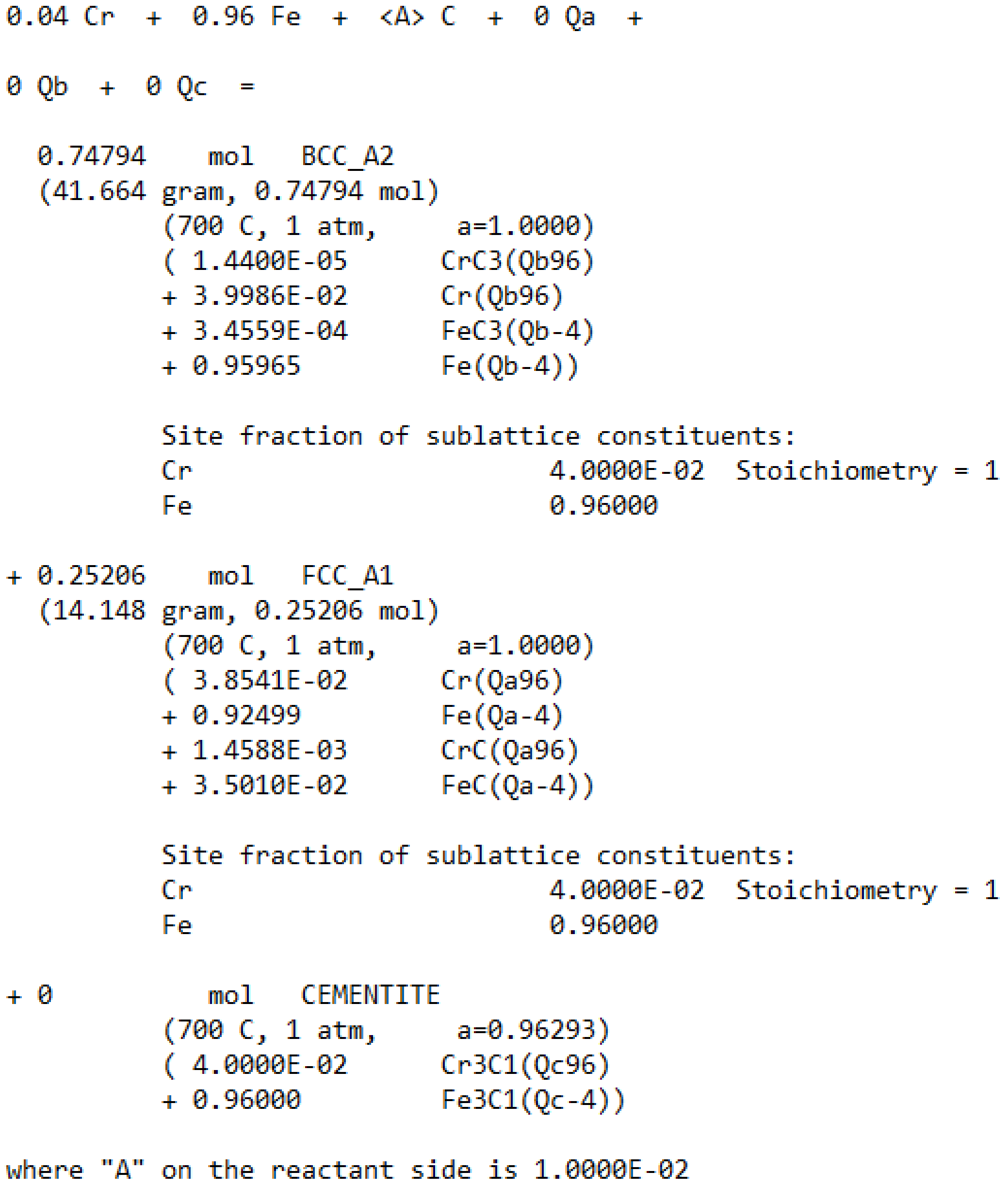
+	Code	End-member	Data	Phase	T	V	Activity	Minimum	Maximum
+	25	CrC3(Qb96)	FSstel	FSstel-BCC			4.3652E-24	4.3652E-24	4.3652E-24
+	26	Cr(Qb96)	FSstel	FSstel-BCC			0.1565	0.1565	0.1565
+	27	FeC3(Qb-4)	FSstel	FSstel-BCC			3.3041E-22	3.3041E-22	3.3041E-22
+	28	Fe(Qb-4)	FSstel	FSstel-BCC			0.9622	0.9622	0.9622



+	Code	End-member	Data	Phase	T	V	Activity	Minimum	Maximum
+	29	Cr3C1(Qc96)	FSstel	FSstel-CEME			1.5822E-04	1.5822E-04	1.5822E-04
+	30	Fe3C1(Qc-4)	FSstel	FSstel-CEME			0.8533	0.8533	0.8533

In each phase, 96 moles of Qi are associated with each mole of Cr and (-4) moles of Qi are associated with each mole of Fe. Since the total amount of Qi = 0.0, this constrains the Cr/Fe ratio in every phase to be equal to 4/96

Output at paraequilibrium at 700ºC



```
0.04 Cr  +  0.96 Fe  +  <A> C  +  0 Qa  +

0 Qb  +  0 Qc  =

  0.74794    mol   BCC_A2
  (41.664 gram, 0.74794 mol)
          (700 C, 1 atm,     a=1.0000)
          ( 1.4400E-05      CrC3(Qb96)
          + 3.9986E-02      Cr(Qb96)
          + 3.4559E-04      FeC3(Qb-4)
          + 0.95965         Fe(Qb-4))

          Site fraction of sublattice constituents:
          Cr                       4.0000E-02  Stoichiometry = 1
          Fe                       0.96000

+ 0.25206    mol   FCC_A1
  (14.148 gram, 0.25206 mol)
          (700 C, 1 atm,     a=1.0000)
          ( 3.8541E-02      Cr(Qa96)
          + 0.92499         Fe(Qa-4)
          + 1.4588E-03      CrC(Qa96)
          + 3.5010E-02      FeC(Qa-4))

          Site fraction of sublattice constituents:
          Cr                       4.0000E-02  Stoichiometry = 1
          Fe                       0.96000

+ 0          mol   CEMENTITE
          (700 C, 1 atm,     a=0.96293)
          ( 4.0000E-02      Cr3C1(Qc96)
          + 0.96000         Fe3C1(Qc-4))

where "A" on the reactant side is 1.0000E-02
```

In each phase,

(total Cr/total Fe) = 4/96

Surface tension of a solution

- According to Butler (1), the surface of a solution may be considered as a separate phase consisting of a monolayer of atoms.
- For a solution with components M-N, Pajarre et al (2) proposed treating the surface phase as a solution M(Qa)-N(Qa) containing the virtual element Qa. (See also Kang (3) and Koukkari (4).)
- The Gibbs energy difference between M and M(Qa) is the molar surface energy $A_{(M)}\sigma_{(M)}$ (J/mol), where $A_{(M)}$ is the molar surface area (m^2/mol) and $\sigma_{(M)}$ is the surface tension of pure M (N/m). $A_{(M)}$ can be calculated from lattice parameters, and $\sigma_{(M)}$ is determined experimentally.
- It can be shown (2) that the surface energy $A\sigma$ of the binary solution is equal to the chemical potential of Qa (where the molar surface area A of the solution is estimated as varying linearly with the surface mole fractions between the molar surface areas of pure M and N.)
- It may be noted that this situation is formally analogous to an equilibrium between a solution M-N and a very small amount of an oxide solution MO-NO.
-
- The present example calculates the surface energy of a liquid Ag-Pb solution containing 30 mol% Pb at 1000 K.
-

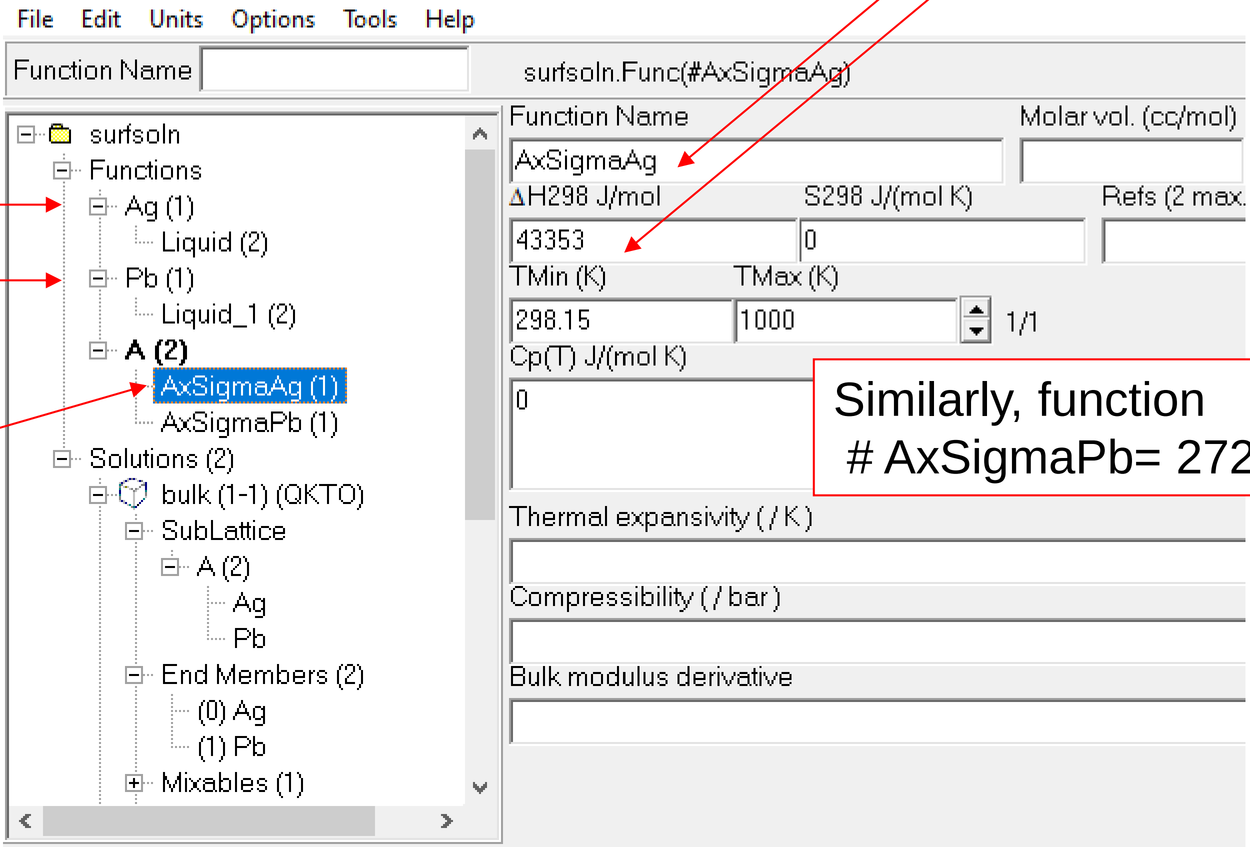
- (1) J.A.V. Butler, Proc. R. Soc. London A: Math. Phys. Eng. Sci., 135 (1932) 348.
- (2) R. Pajarre, P. Koukkari, T. Tanaka and J. Lee, Calphad, 30 (2006) 196.
- (3) Y.-B. Kang, Calphad, 50 (2015) 23-31.
- (4) P. Koukkari, VTT Bulletin 160 (2014) VTT Tech. Res. Ctr. of Finland, Espoo, Finland
- (5) T. Tanaka, K. Hack, T. Ida, S. Hara, Z. Metallkd., 87 (1996) 389-389.

The **SOLUTION** module is used to create a bulk solution phase, and surface solution phase.

- Data are stored in **FACTDATA/surf**

Functions Ag#liquid and Pb#liquid are Gibbs energies of pure Ag(liq) and pure Pb(liq) taken from **FactPS**

AxSigmaAg = 43353



Function Name

surfsoln.Func(#AxSigmaAg)

Function Name: AxSigmaAg

ΔH298 J/mol: 43353

S298 J/(mol K): 0

TMin (K): 298.15

TMax (K): 1000

Cp(T) J/(mol K): 0

Similarly, function # AxSigmaPb= 27243

Functions #AxSigmaAg and #AxSigmaPb are surface energies of pure Ag and Pb at 1000 K

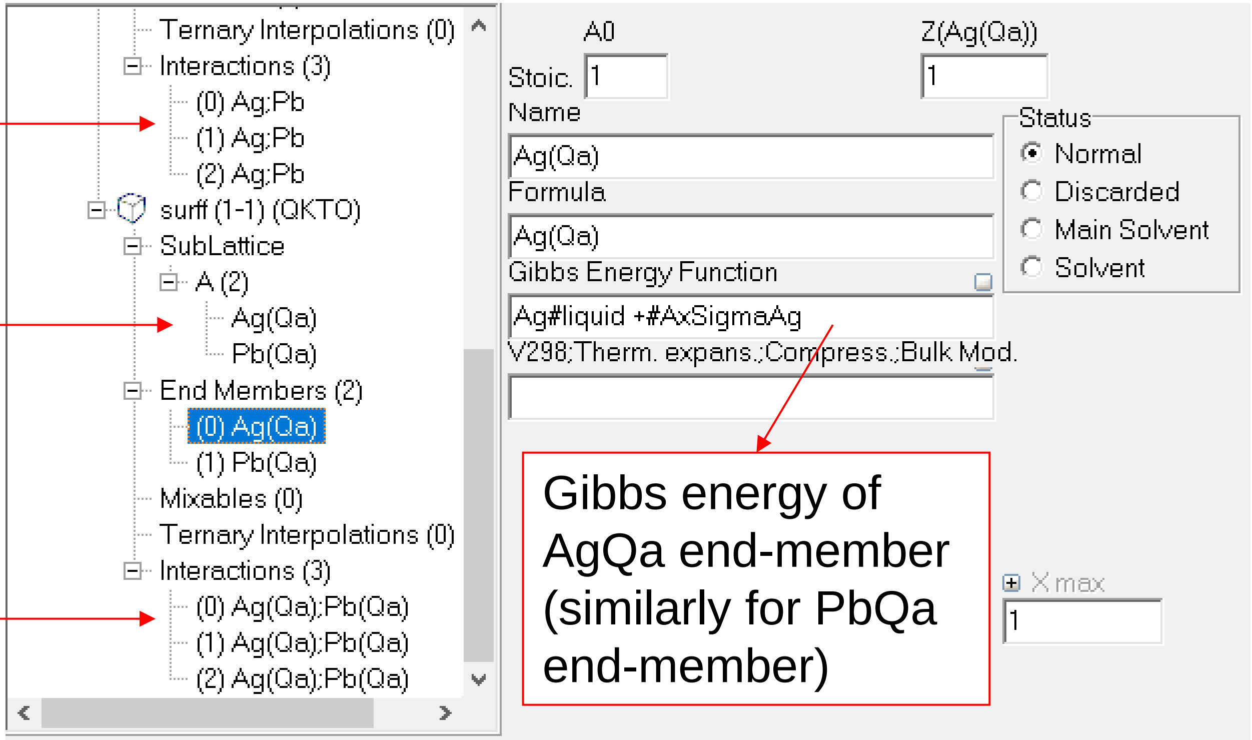
At 1000 K: A_{Ag} = 47329, σ_{Ag} = 0.916. Thus $A_{Ag}\sigma_{Ag}$= 43353 J/mol (4)

A_{Pb} = 70215, σ_{Pb} = 0.388. Thus, $A_{Pb}\sigma_{Pb}$ = 27243 J/mol (4)

$g^{E(bulk)}$ parameters for bulk solution at 1000 K (see below)

surface solution

$g^{E(surf)}$ parameters for surface solution at 1000 K (see below)



- Ternary Interpolations (0)
- Interactions (3)
  - (0) Ag:Pb
  - (1) Ag:Pb
  - (2) Ag:Pb
- surf (1-1) (QKTO)
  - SubLattice
    - A (2)
      - Ag(Qa)
      - Pb(Qa)
  - End Members (2)
    - (0) Ag(Qa)
    - (1) Pb(Qa)
  - Mixables (0)
  - Ternary Interpolations (0)
  - Interactions (3)
    - (0) Ag(Qa):Pb(Qa)
    - (1) Ag(Qa):Pb(Qa)
    - (2) Ag(Qa):Pb(Qa)

A0 Stoic. 1

Z(Ag(Qa)) 1

Name: Ag(Qa)

Formula: Ag(Qa)

Gibbs Energy Function: Ag#liquid +#AxSigmaAg

V298;Therm. expans.;Compress.;Bulk Mod.

Status: ● Normal ○ Discarded ○ Main Solvent ○ Solvent

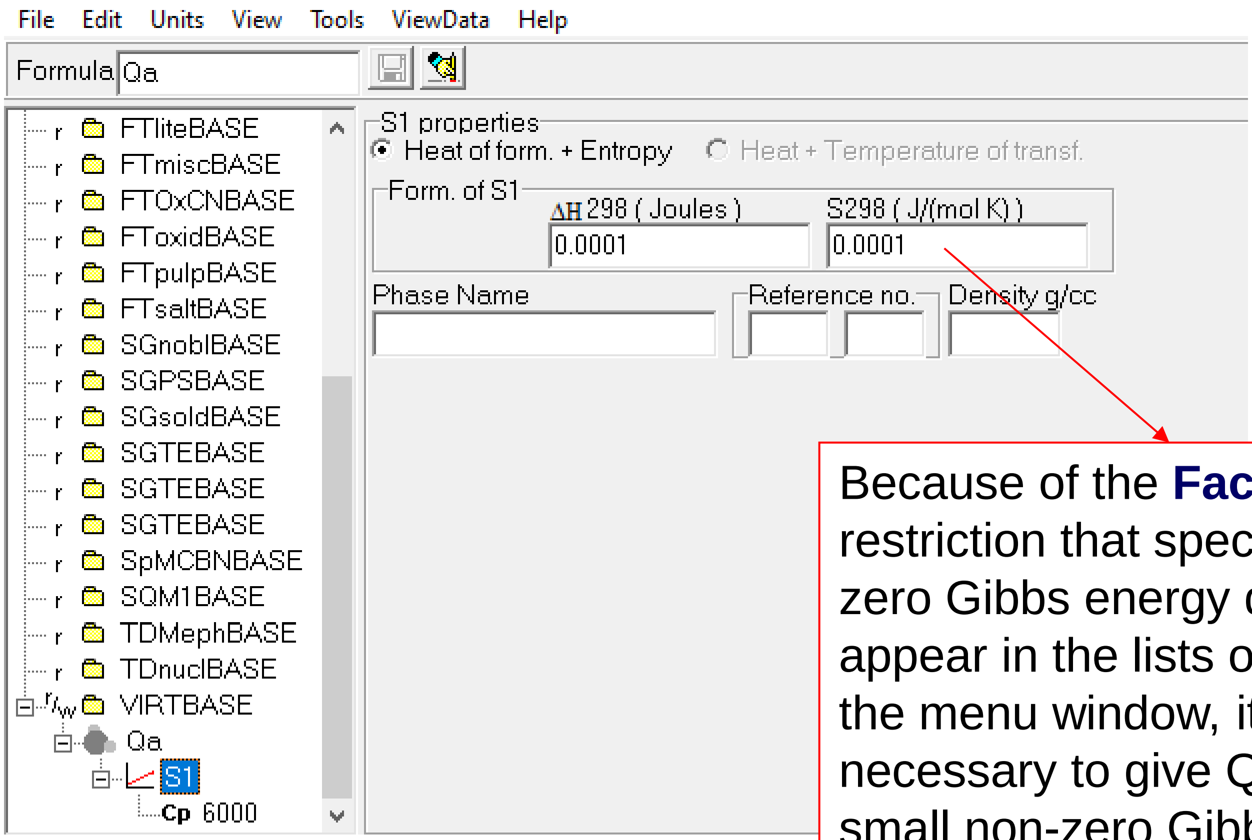
X max: 1

Gibbs energy of AgQa end-member (similarly for PbQa end-member)

$$g^{E(bulk)}_{1000K} = X_{Ag}X_{Pb}(6741.7 - 1464.8X_{Ag}X_{Pb} - 1978X^2_{Ag}X^2_{Pb})\ (4)$$

$$g^{E(surf)}_{1000K} = 0.83g^{E(bulk)}$$

(as proposed by Tanaka et al. (5) due to the effect of the reduced coordination number of surface atoms)



Formula: Qa

S1 properties

● Heat of form. + Entropy ○ Heat + Temperature of transf.

Form. of S1

ΔH 298 (Joules): 0.0001

S298 (J/(mol K)): 0.0001

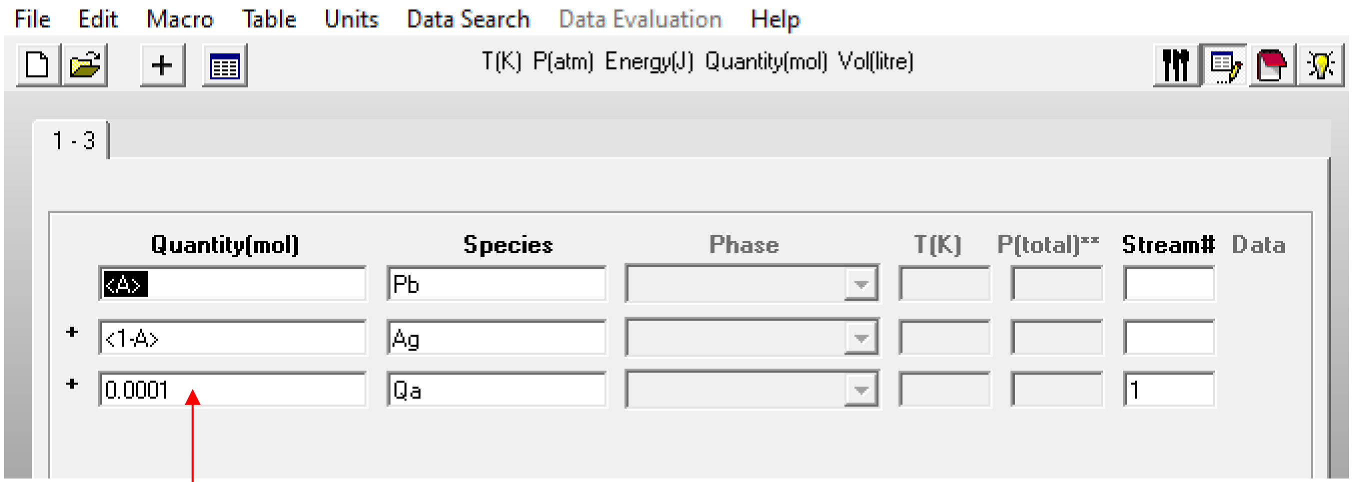
Phase Name:

Reference no.:

Density g/cc:

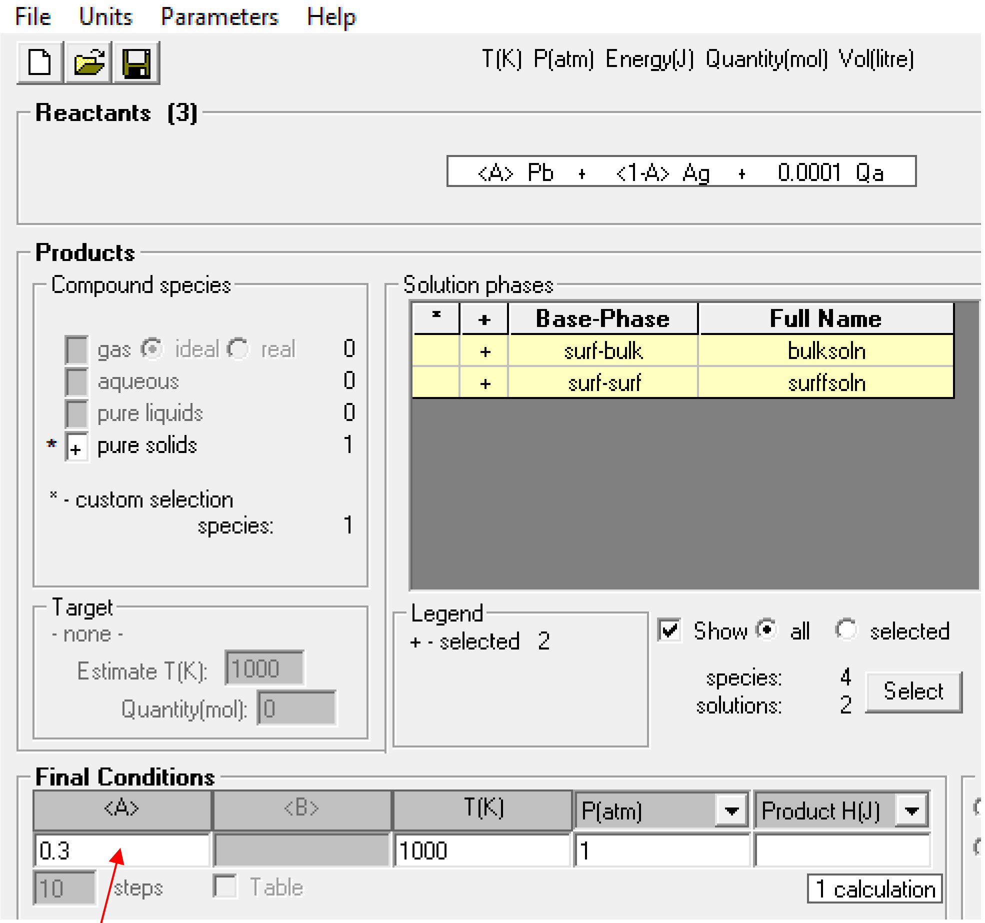
Because of the **FactSage** restriction that species with zero Gibbs energy do not appear in the lists of species in the menu window, it is necessary to give Qa a very small non-zero Gibbs energy

Use the **COMPOUND** module to enter the species Qa into the private **VIRTBASE.cdb** database with Gibbs energy = 0.0



	Quantity(mol)	Species	Phase	T(K)	P(total)**	Stream#	Data
	<A>	Pb					
+	<1-A>	Ag					
+	0.0001	Qa				1	

A very small value of Qa is entered in order that the amount of the surface phase is very small. (As long as Qa is very small, the result will be independent of Qa.)



Reactants (3)

<A> Pb + <1-A> Ag + 0.0001 Qa

Products

Compound species

☐	gas ● ideal ○ real	0
☐	aqueous	0
☐	pure liquids	0
* +	pure solids	1

* - custom selection
species: 1

Solution phases

*	+	Base-Phase	Full Name
	+	surf-bulk	bulksoln
	+	surf-surf	surffsoln

Target
- none -
Estimate T(K): 1000
Quantity(mol): 0

Legend
+ - selected 2

☑ Show ● all ○ selected

species: 4
solutions: 2

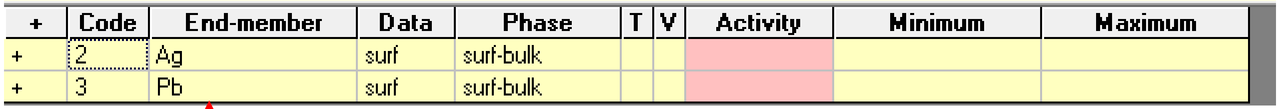
Final Conditions

<A>	<B>	T(K)	P(atm)	Product H(J)
0.3		1000	1	

10 steps ☐ Table

1 calculation

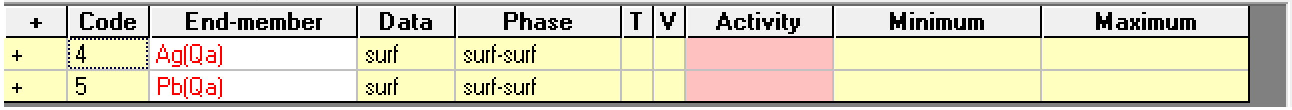
Bulk phase to contain 30 mol% Pb



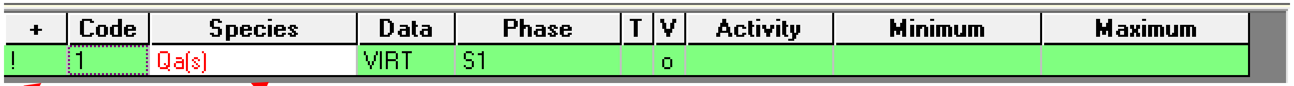
+	Code	End-member	Data	Phase	T	V	Activity	Minimum	Maximum
+	2	Ag	surf	surf-bulk					
+	3	Pb	surf	surf-bulk					

Bulk phase

Surface phase



+	Code	End-member	Data	Phase	T	V	Activity	Minimum	Maximum
+	4	Ag(Qa)	surf	surf-surf					
+	5	Pb(Qa)	surf	surf-surf					

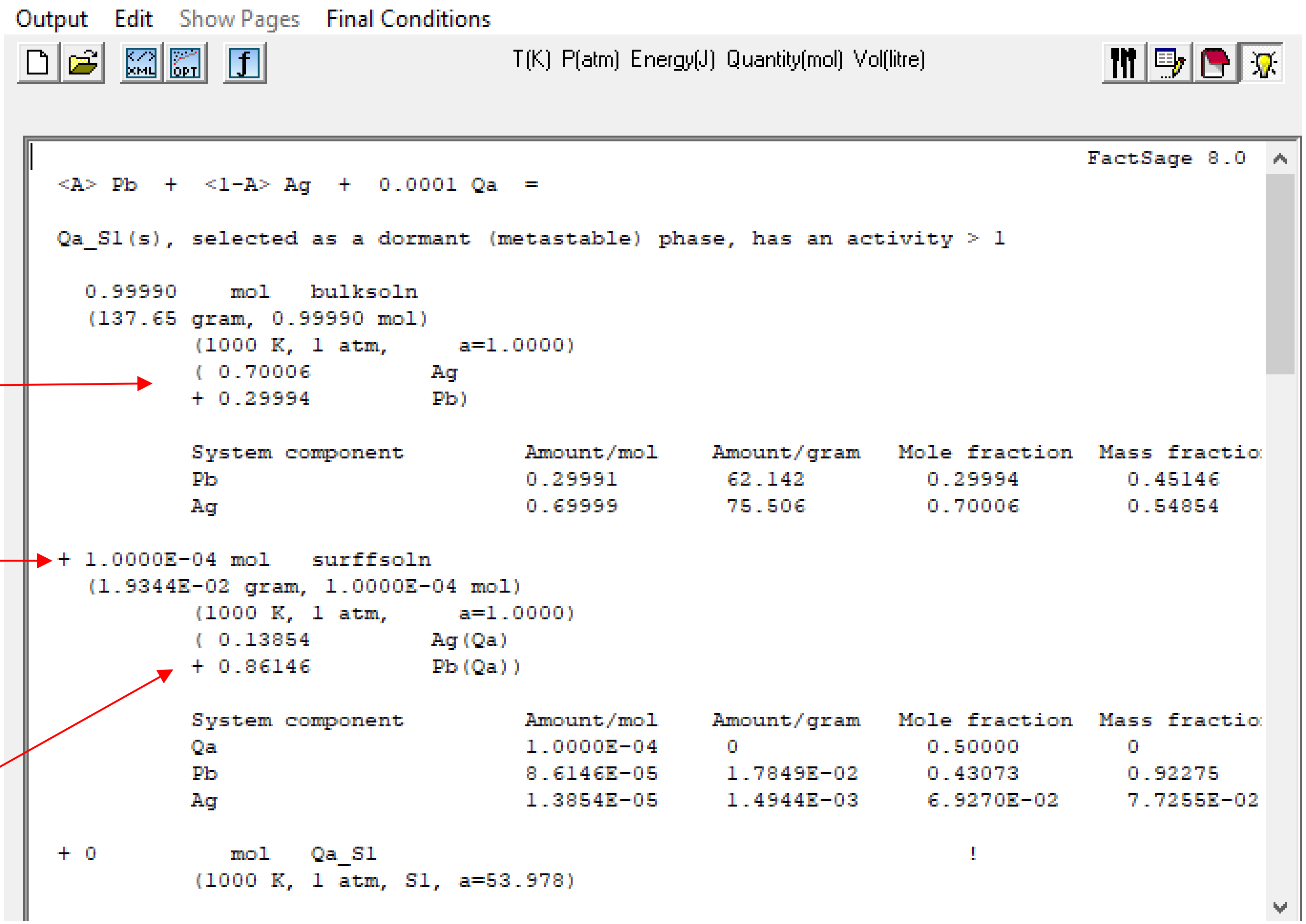


+	Code	Species	Data	Phase	T	V	Activity	Minimum	Maximum
!	1	Qa(s)	VIRT	S1		o			

Set Qa to be “dormant (metastable)”

Select Qa from **VIRTBASE**

Equilibrium at 1000 K



```
                                                                   FactSage 8.0
 <A> Pb  +  <1-A> Ag  +  0.0001 Qa  =

 Qa_S1(s), selected as a dormant (metastable) phase, has an activity > 1

   0.99990    mol   bulksoln
   (137.65 gram, 0.99990 mol)
           (1000 K, 1 atm,     a=1.0000)
           ( 0.70006         Ag
           + 0.29994         Pb)

           System component          Amount/mol    Amount/gram   Mole fraction   Mass fractio
           Pb                        0.29991        62.142        0.29994         0.45146
           Ag                        0.69999        75.506        0.70006         0.54854

 + 1.0000E-04 mol   surffsoln
   (1.9344E-02 gram, 1.0000E-04 mol)
           (1000 K, 1 atm,     a=1.0000)
           ( 0.13854         Ag(Qa)
           + 0.86146         Pb(Qa))

           System component          Amount/mol    Amount/gram   Mole fraction   Mass fractio
           Qa                        1.0000E-04     0             0.50000         0
           Pb                        8.6146E-05     1.7849E-02    0.43073         0.92275
           Ag                        1.3854E-05     1.4944E-03    6.9270E-02      7.7255E-02

 + 0          mol   Qa_S1                                       !
           (1000 K, 1 atm, S1, a=53.978)
```

Bulk phase composition

Amount of surface phase is negligibly small

Surface phase composition

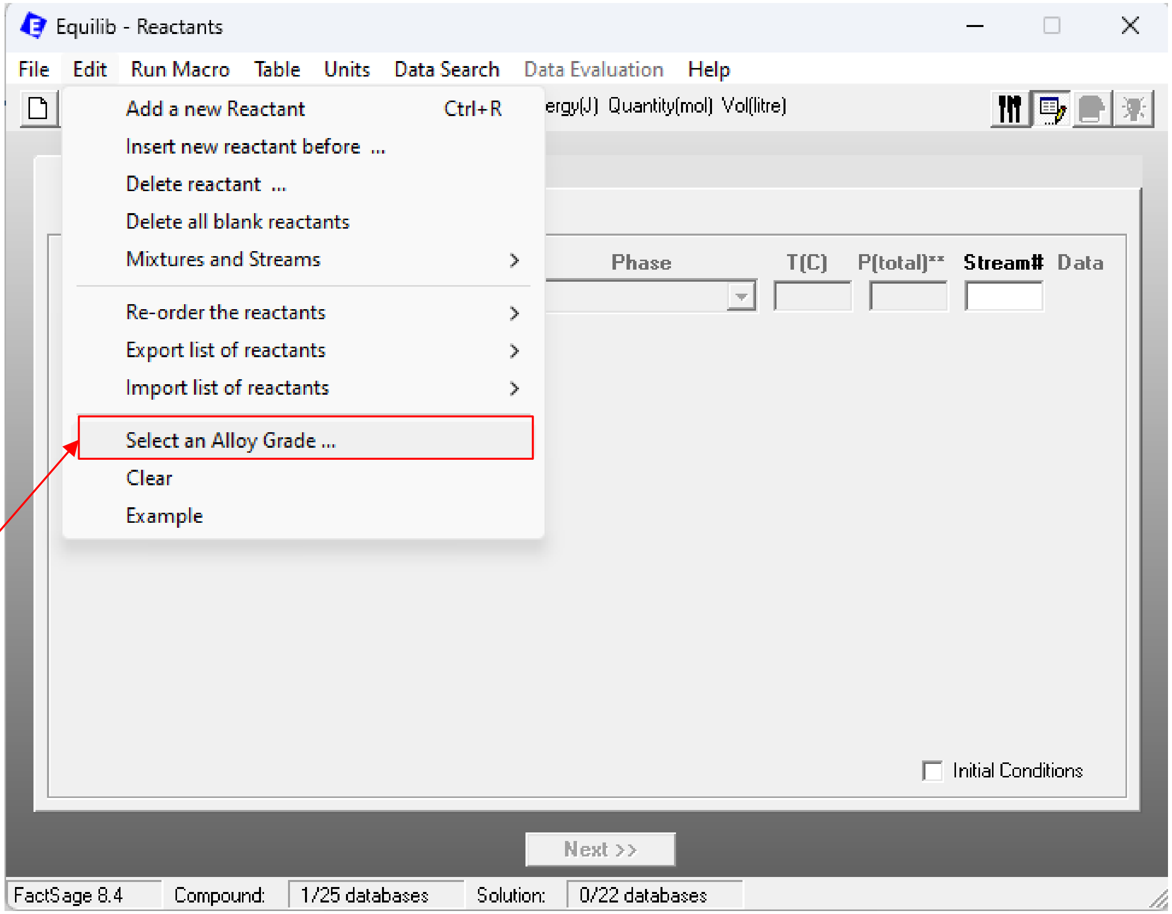
μ(Qa) = RT ln a(Qa) = 8.315(1000) ln (53.978) = Aσ

A = (0.13854)(47329) + 0.86146(70215). Therefore σ = 0.495 N/m

Selection of an Industrial Grade Alloy

Several hundreds of standard alloys grade compositions were introduced in the new FactSage **“Alloy Grades” Form**. They presently consist in aluminum (wrought & cast), magnesium, copper (brass, bronze & casting) and titanium (α/β, α-near α, β) alloys compositions. Fe-based alloys will be introduced soon.

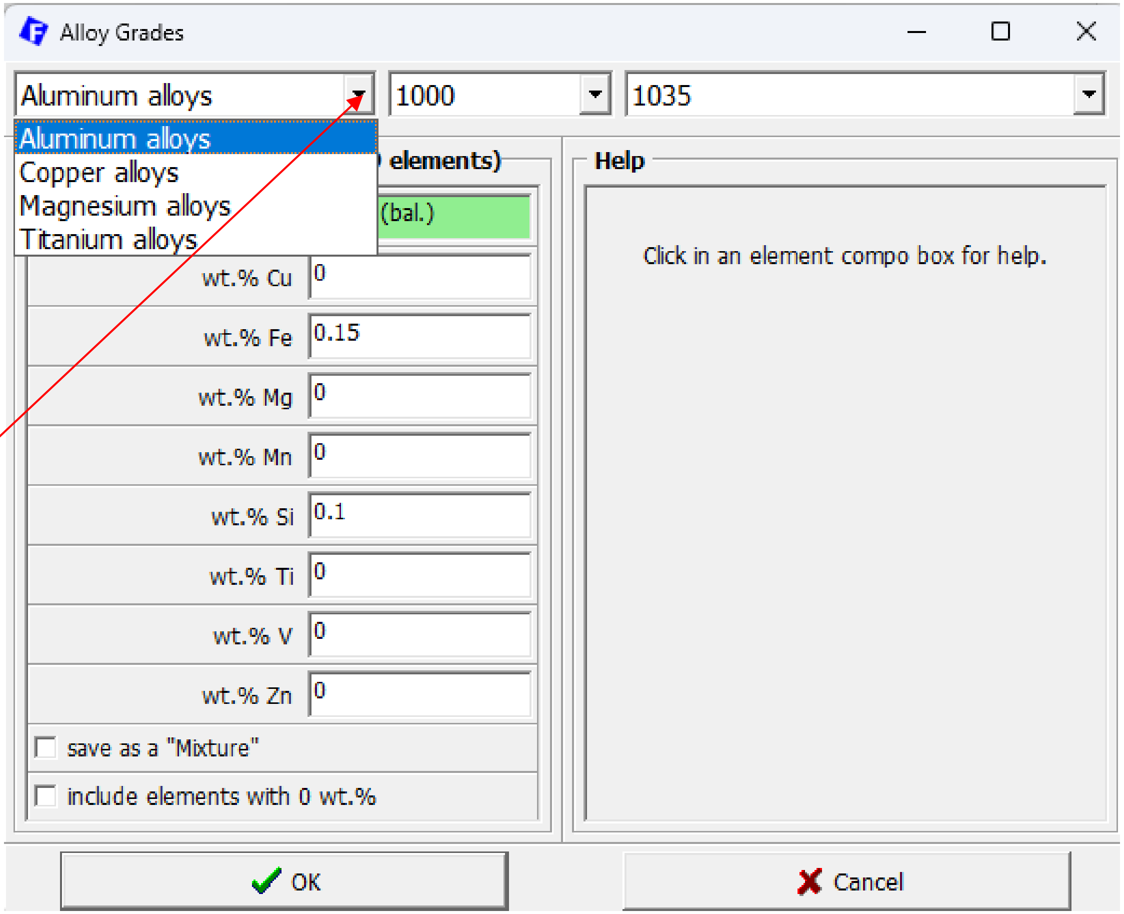
The **user selected alloy grade composition** can then be introduced as a **multi-line mixture** or as a **single-line mixture** in EQUILIB Reactants.



Click on “Edit | Select an Alloy Grade…” to open the “Alloy Grades” Form in “EQUILIB – Reactants”

Selection of Alloy Type

FactSage **“Alloy Grades” Form**.



Alloy Grades

Aluminum alloys | 1000 | 1035

- Aluminum alloys
- Copper alloys
- Magnesium alloys
- Titanium alloys

elements)

(bal.)

wt.% Cu	0
wt.% Fe	0.15
wt.% Mg	0
wt.% Mn	0
wt.% Si	0.1
wt.% Ti	0
wt.% V	0
wt.% Zn	0

☐ save as a "Mixture"

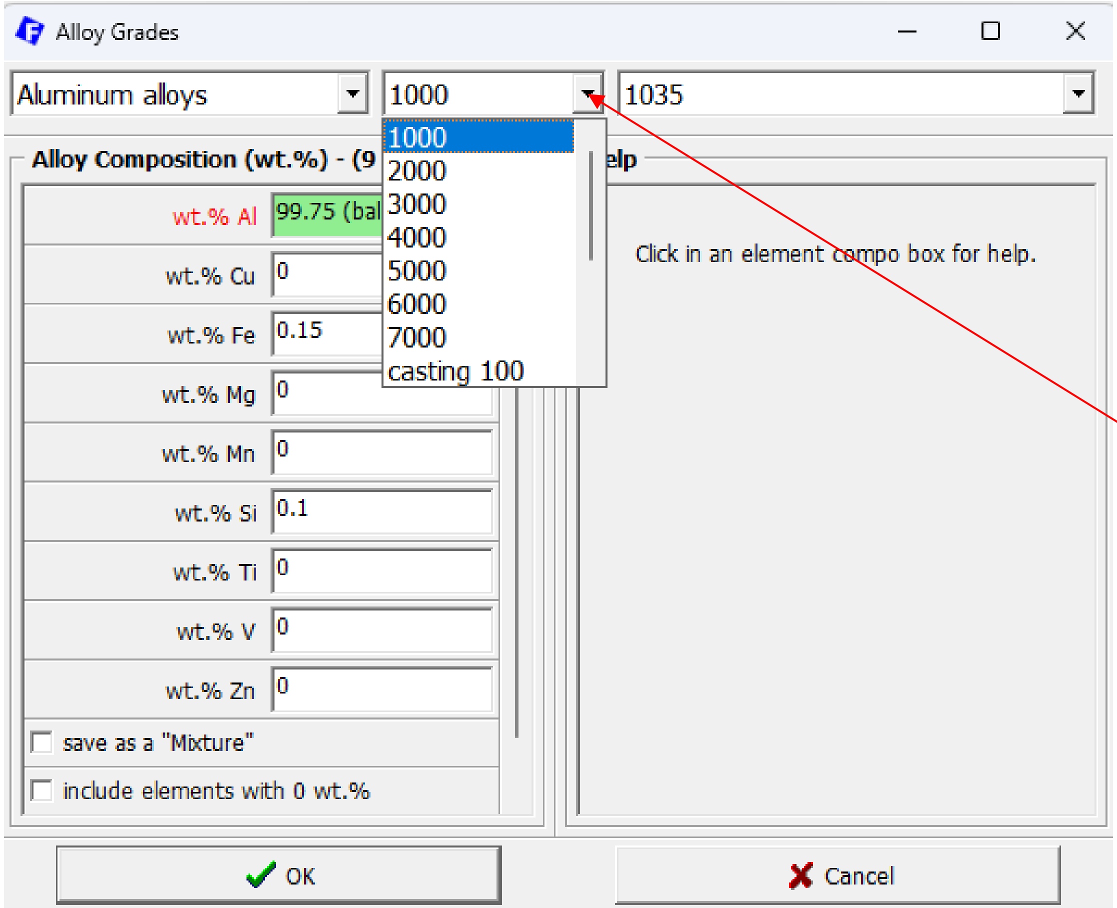
☐ include elements with 0 wt.%

Help

Click in an element compo box for help.

Click to choose among Al-, Cu-, Mg- or Ti- alloys

Selection of Aluminum Alloy Series 1000-7000



wt.% Al: 99.75 (bal
wt.% Cu: 0
wt.% Fe: 0.15
wt.% Mg: 0
wt.% Mn: 0
wt.% Si: 0.1
wt.% Ti: 0
wt.% V: 0
wt.% Zn: 0

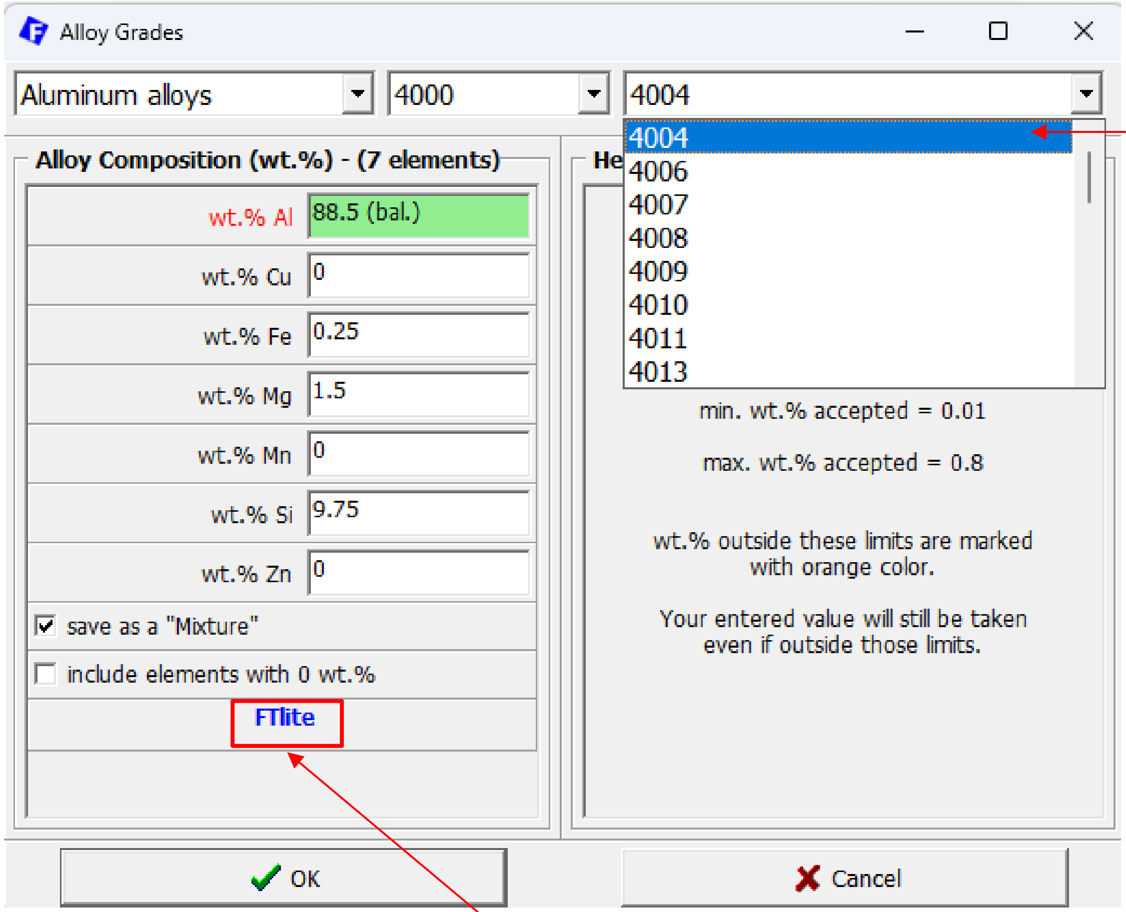
☐ save as a "Mixture"

☐ include elements with 0 wt.%

Click in an element compo box for help.

Click to choose Aluminum series 1000-7000 (wrought alloys)

Selection of Aluminum Alloy in the Series 1000-7000



Aluminum alloys | 4000 | 4004

4004
4006
4007
4008
4009
4010
4011
4013

Alloy Composition (wt.%) - (7 elements)

wt.% Al	88.5 (bal.)
wt.% Cu	0
wt.% Fe	0.25
wt.% Mg	1.5
wt.% Mn	0
wt.% Si	9.75
wt.% Zn	0

☑ save as a "Mixture"

☐ include elements with 0 wt.%

min. wt.% accepted = 0.01

max. wt.% accepted = 0.8

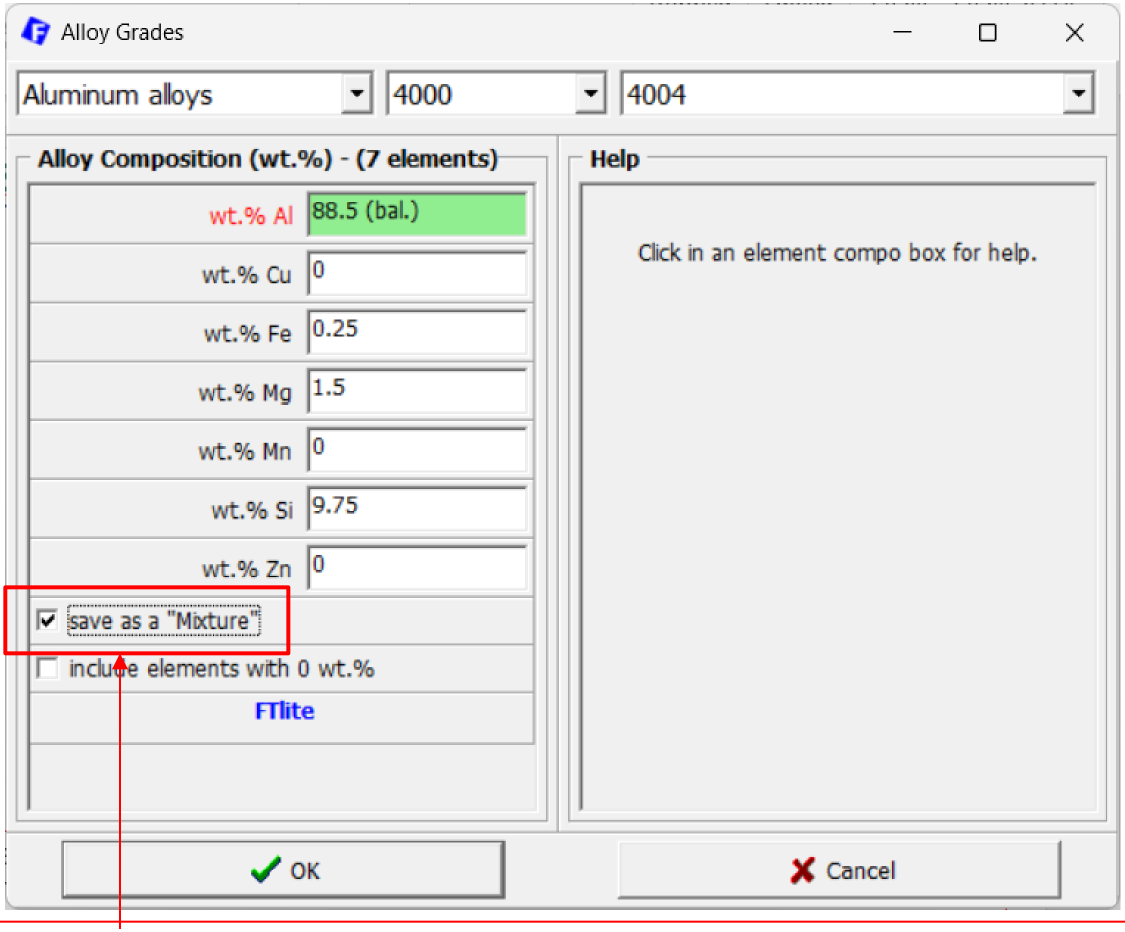
wt.% outside these limits are marked with orange color.

Your entered value will still be taken even if outside those limits.

Click to choose a specific Al-4000 alloy in the selected series.

Recommended FactSage Database for the selected alloy composition.

Selection of Aluminum Alloy in the Series 1000-7000



Aluminum alloys | 4000 | 4004

Alloy Composition (wt.%) - (7 elements)

wt.% Al	88.5 (bal.)
wt.% Cu	0
wt.% Fe	0.25
wt.% Mg	1.5
wt.% Mn	0
wt.% Si	9.75
wt.% Zn	0

☑ save as a "Mixture"

☐ include elements with 0 wt.%

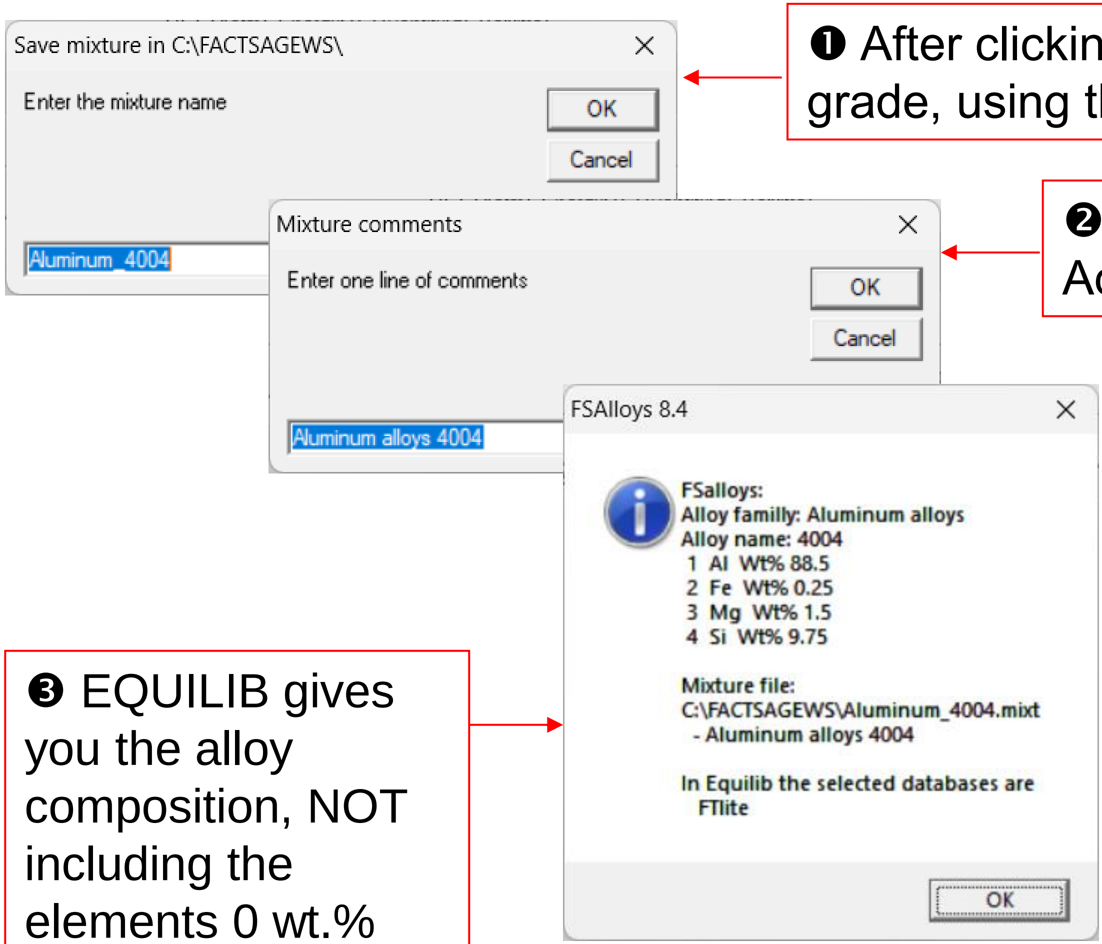
Help

Click in an element compo box for help.

Check “save as a “Mixture””, if you want to create an input stream in EQUILIB with this alloy composition.
Otherwise, a multi-line input will be entered in EQUILIB.

Selection of Aluminum Alloy in the Series 1000-7000

❶ After clicking “OK” to accept the AA4004 grade, using the “save as “Mixture””, you get…



Aluminum_4004

Aluminum alloys 4004

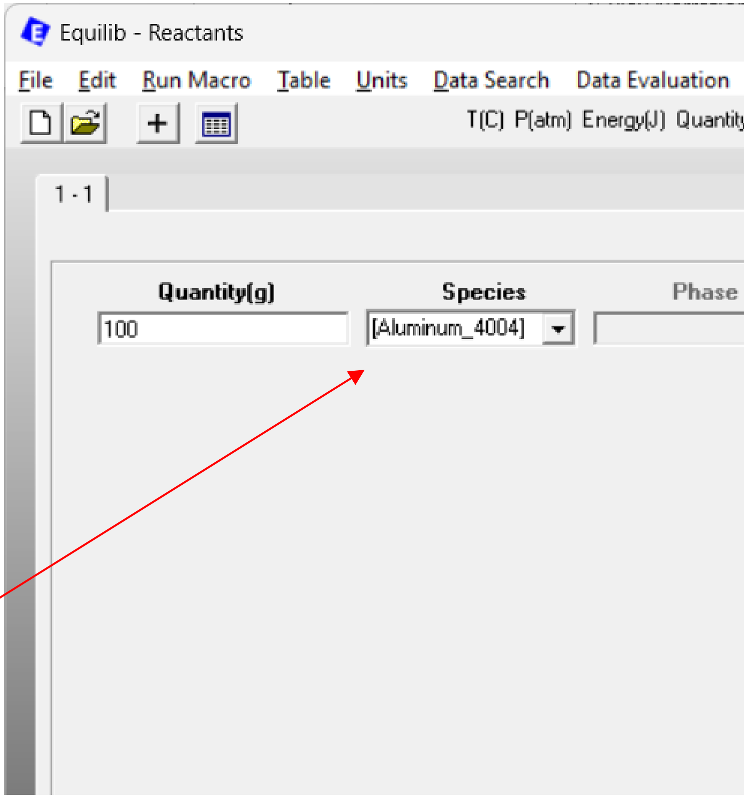
FSalloys:
Alloy familly: Aluminum alloys
Alloy name: 4004
1 Al Wt% 88.5
2 Fe Wt% 0.25
3 Mg Wt% 1.5
4 Si Wt% 9.75

Mixture file:
C:\FACTSAGEWS\Aluminum_4004.mixt
- Aluminum alloys 4004

In Equilib the selected databases are
FTlite

❷ A **single-line mixture** is created. Add a comment if you wish…

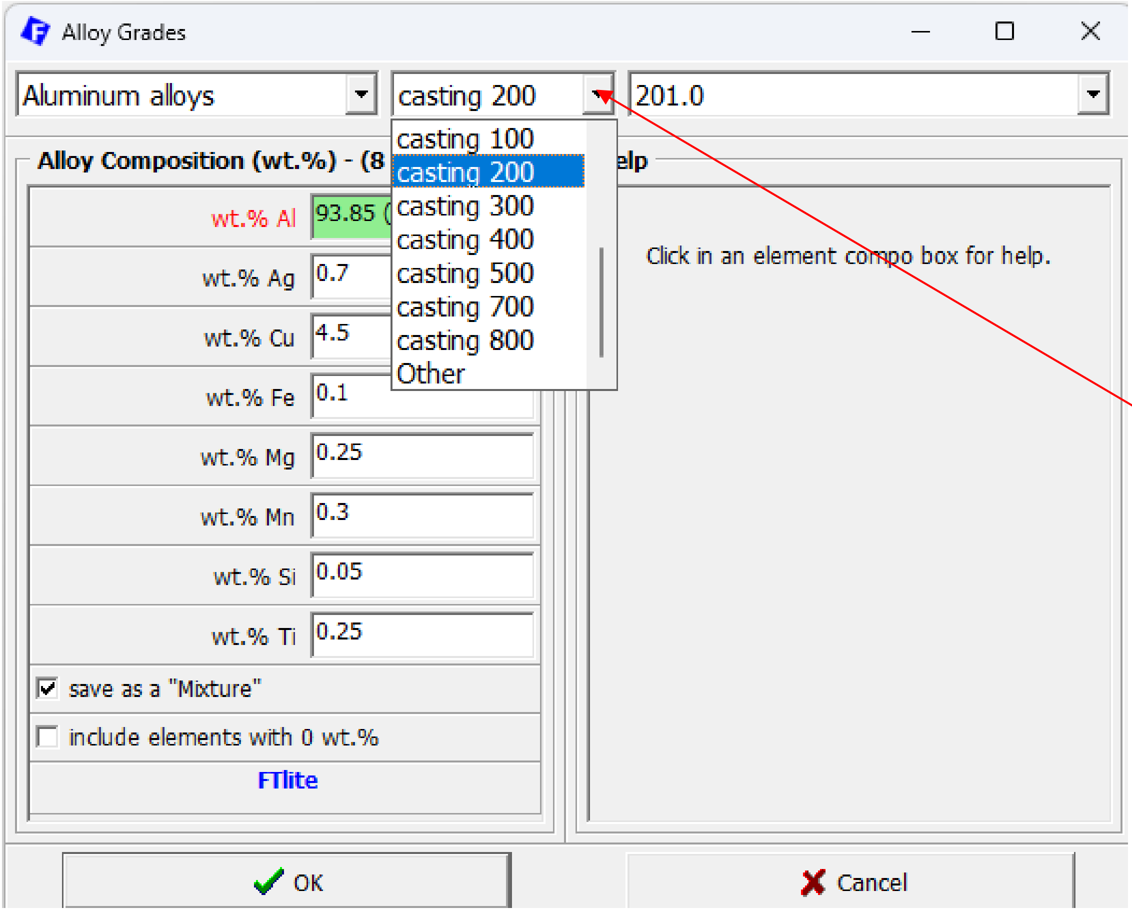
❸ EQUILIB gives you the alloy composition, NOT including the elements 0 wt.% (see previous slide)



Quantity(g)	Species
100	[Aluminum_4004]

❹ Finally, the single-line mixture is entered in EQUILIB, with a default mass of 100 grams.

Selection of Aluminum Alloy Series casting 100-800



Aluminum alloys | casting 200 | 201.0

wt.% Al	93.85 (
wt.% Ag	0.7
wt.% Cu	4.5
wt.% Fe	0.1
wt.% Mg	0.25
wt.% Mn	0.3
wt.% Si	0.05
wt.% Ti	0.25

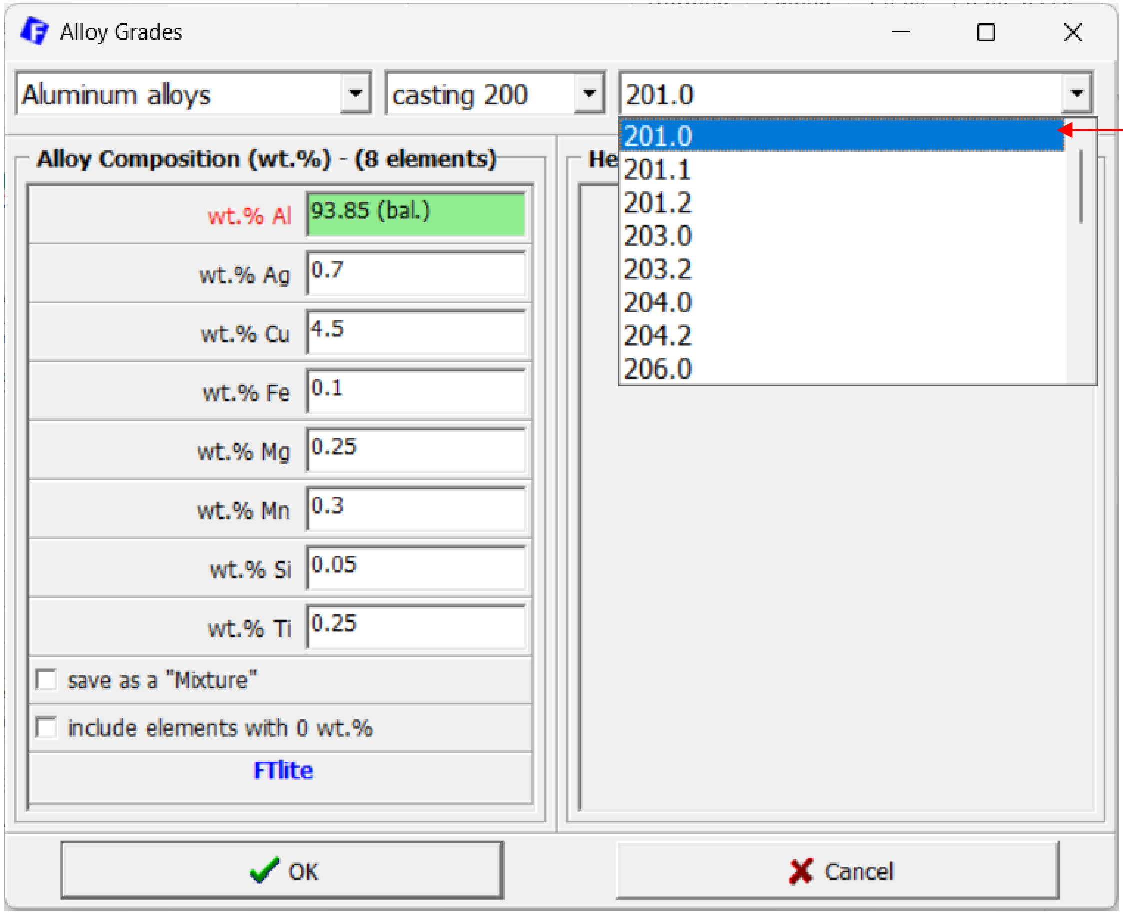
☑ save as a "Mixture"

☐ include elements with 0 wt.%

Click in an element compo box for help.

Click to choose Aluminum series casting 100-800

Selection of Aluminum Alloy in the Series casting 100-800



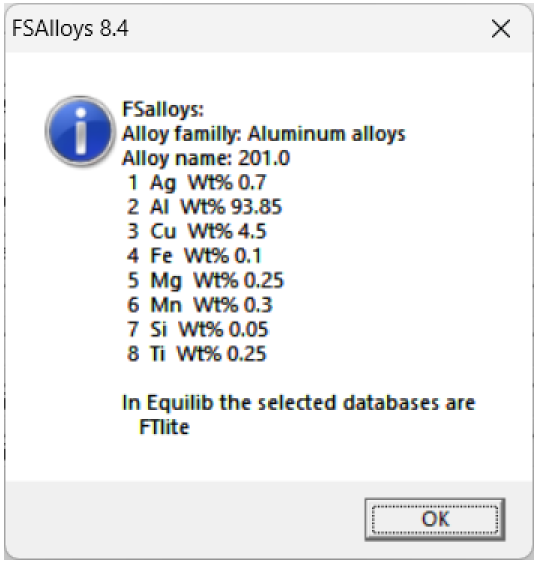
Alloy Composition (wt.%) - (8 elements)

wt.% Al: 93.85 (bal.)
wt.% Ag: 0.7
wt.% Cu: 4.5
wt.% Fe: 0.1
wt.% Mg: 0.25
wt.% Mn: 0.3
wt.% Si: 0.05
wt.% Ti: 0.25

☐ save as a "Mixture"
☐ include elements with 0 wt.%

Click to choose the alloy in the selected series

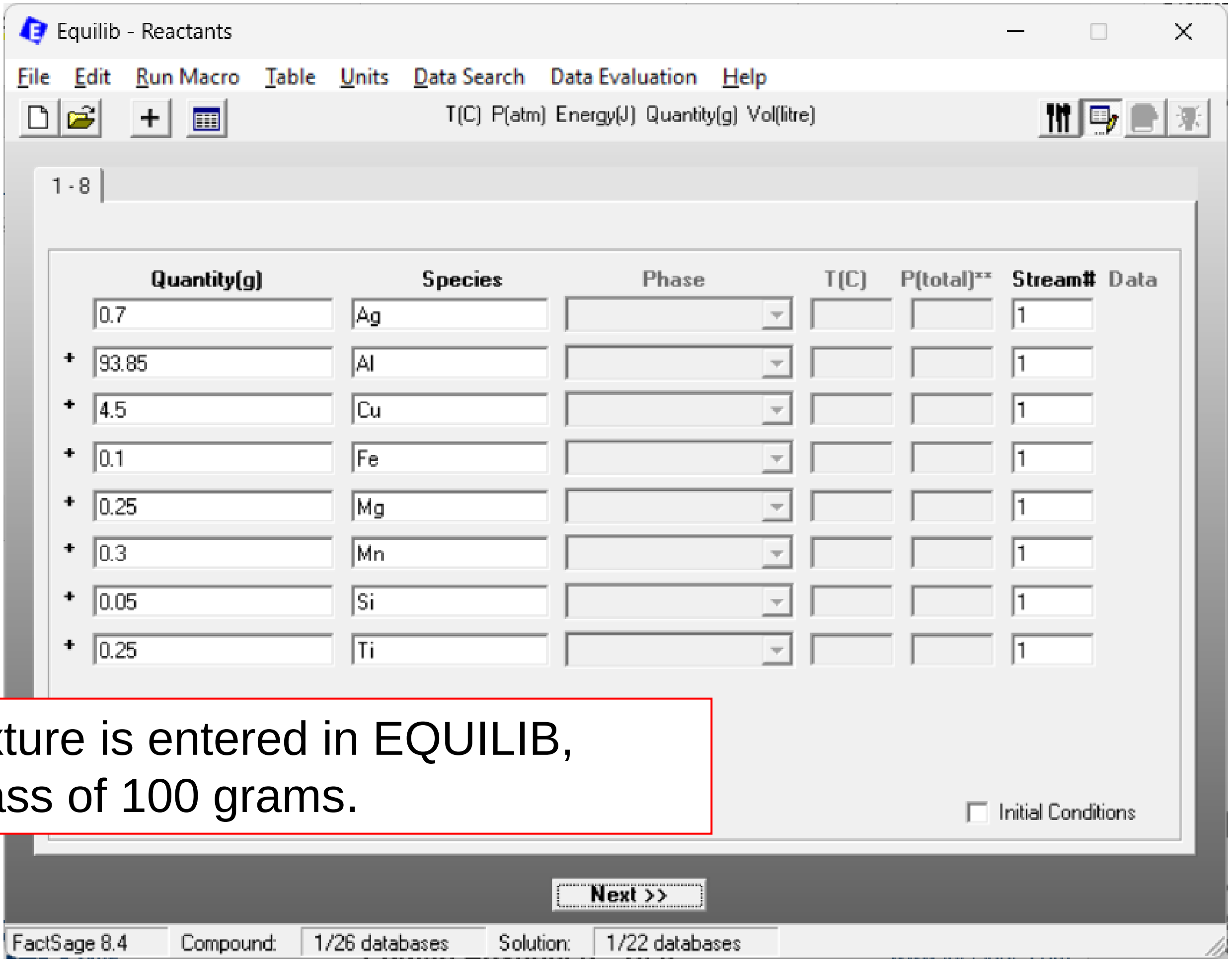
Selection of Aluminum Alloy in the Series casting 100-800



FSalloys:
Alloy familly: Aluminum alloys
Alloy name: 201.0
1 Ag Wt% 0.7
2 Al Wt% 93.85
3 Cu Wt% 4.5
4 Fe Wt% 0.1
5 Mg Wt% 0.25
6 Mn Wt% 0.3
7 Si Wt% 0.05
8 Ti Wt% 0.25

In Equilib the selected databases are
FTlite

❶ After clicking "OK" to accept the AA201.0 grade, with "save as "Mixture"" NOT checked, you get the information about the alloy.

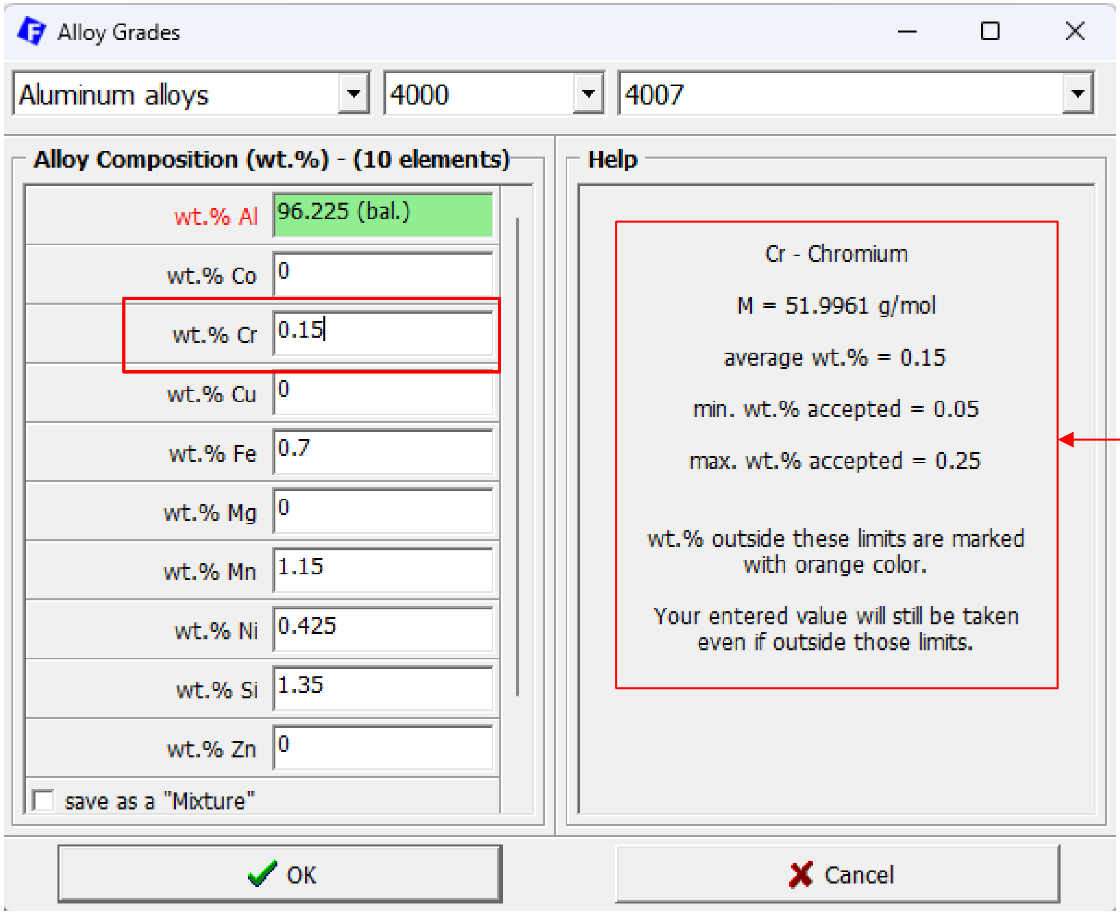


Quantity(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
0.7	Ag				1	
+ 93.85	Al				1	
+ 4.5	Cu				1	
+ 0.1	Fe				1	
+ 0.25	Mg				1	
+ 0.3	Mn				1	
+ 0.05	Si				1	
+ 0.25	Ti				1	

☐ Initial Conditions

❷ Finally, the multi-line mixture is entered in EQUILIB, based on a total default mass of 100 grams.

Min., Max and Average of Each Element



Aluminum alloys | 4000 | 4007

Alloy Composition (wt.%) - (10 elements)

wt.% Al	96.225 (bal.)
wt.% Co	0
wt.% Cr	0.15
wt.% Cu	0
wt.% Fe	0.7
wt.% Mg	0
wt.% Mn	1.15
wt.% Ni	0.425
wt.% Si	1.35
wt.% Zn	0

☐ save as a "Mixture"

Help

Cr - Chromium

M = 51.9961 g/mol

average wt.% = 0.15

min. wt.% accepted = 0.05

max. wt.% accepted = 0.25

wt.% outside these limits are marked with orange color.

Your entered value will still be taken even if outside those limits.

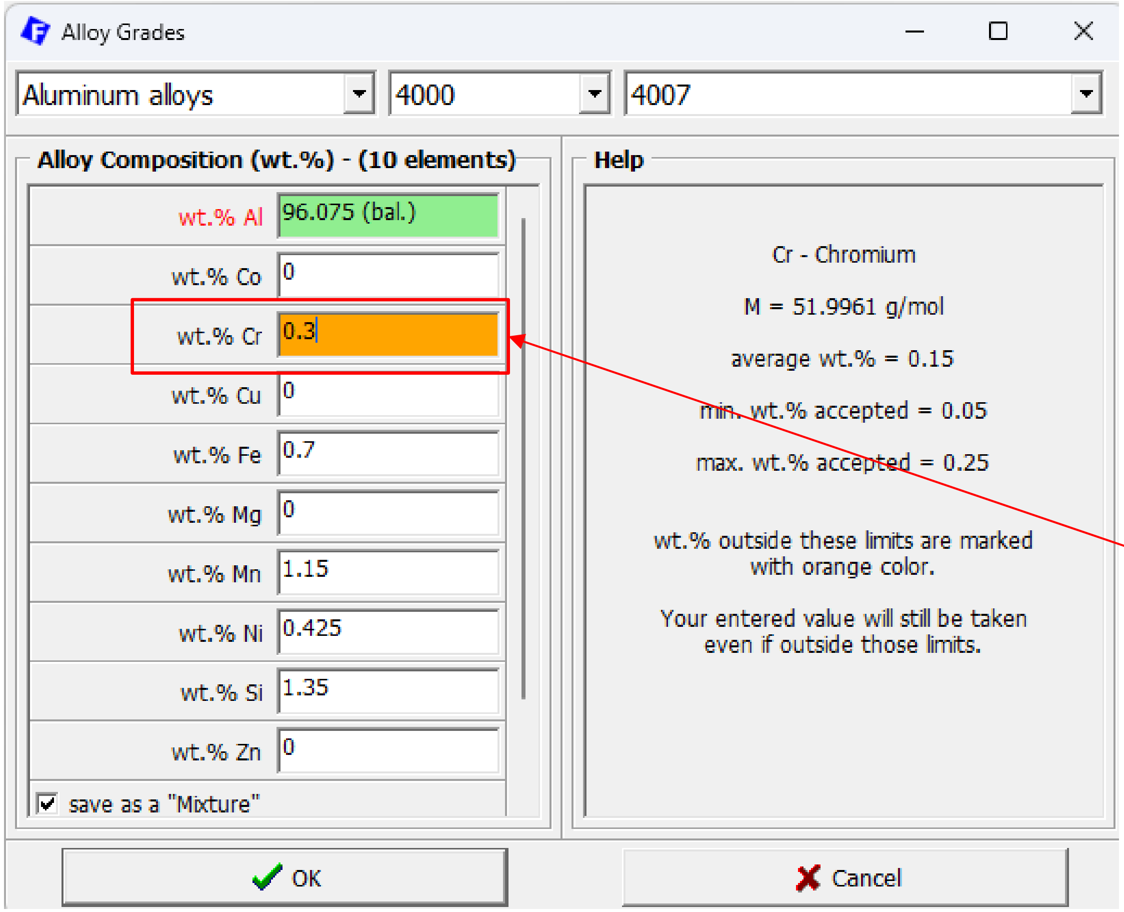
In this example, the **AA4007** aluminum wrought alloy (UNS A94007; Aluminium 4007; Al4007) is selected.

The user may want to adjust the chromium content.

Min., max and average wt.% of a selected alloying element are displayed for information.

You can edit that composition (in wt.%) modifying the major element composition accordingly.

Min., Max and Average of Each Element



Aluminum alloys | 4000 | 4007

Alloy Composition (wt.%) - (10 elements)

wt.% Al	96.075 (bal.)
wt.% Co	0
wt.% Cr	0.3
wt.% Cu	0
wt.% Fe	0.7
wt.% Mg	0
wt.% Mn	1.15
wt.% Ni	0.425
wt.% Si	1.35
wt.% Zn	0

☑ save as a "Mixture"

Help

Cr - Chromium

M = 51.9961 g/mol

average wt.% = 0.15

min. wt.% accepted = 0.05

max. wt.% accepted = 0.25

wt.% outside these limits are marked with orange color.

Your entered value will still be taken even if outside those limits.

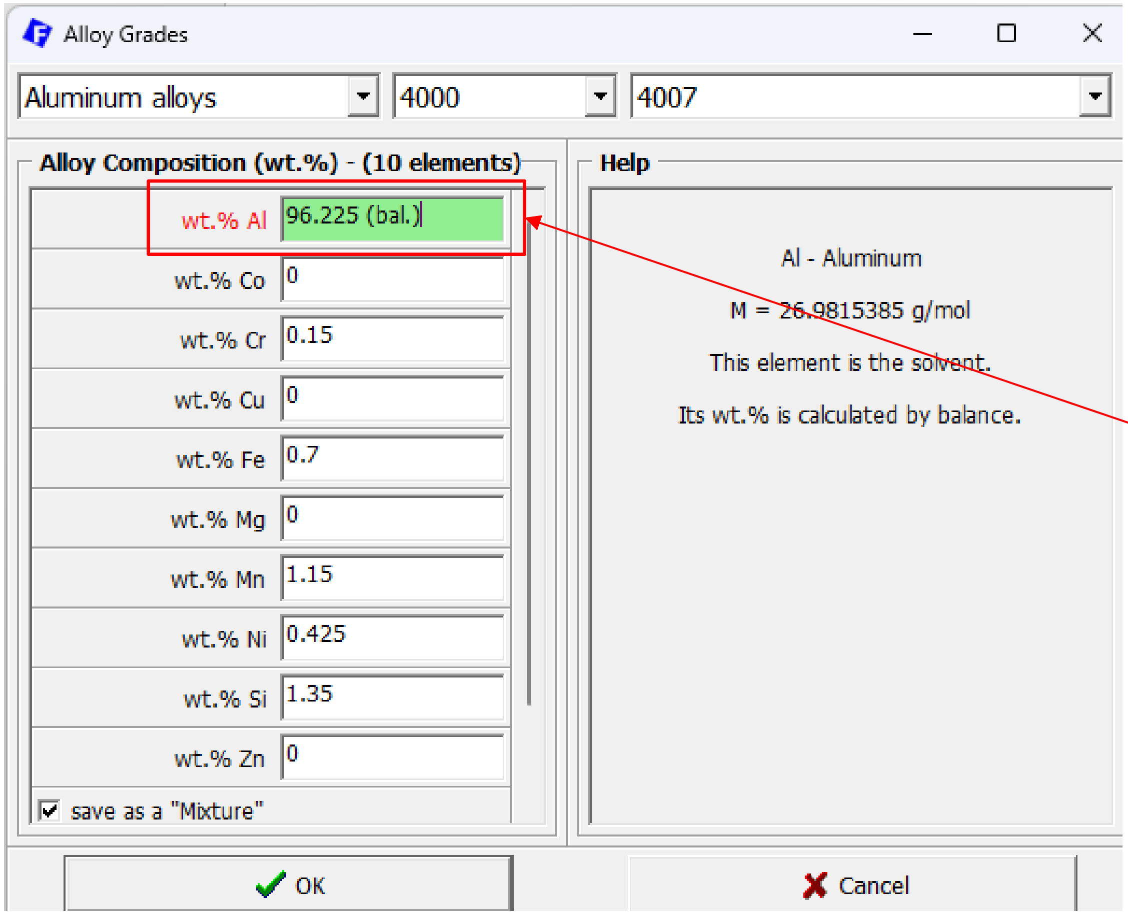
In this example, the **AA4007** aluminum wrought alloy (UNS A94007; Aluminium 4007; Al4007) is selected.

The user may want to adjust the chromium content.

wt.% outside the min.-max limits are marked with orange color, but the value you entered will still be taken even of outside those limits.

Min., Max and Average of Each Element

In this example, the **AA4007** aluminum wrought alloy (UNS A94007; Aluminium 4007; Al4007) is selected.



Aluminum alloys | 4000 | 4007

Alloy Composition (wt.%) - (10 elements)

wt.% Al: 96.225 (bal.)
wt.% Co: 0
wt.% Cr: 0.15
wt.% Cu: 0
wt.% Fe: 0.7
wt.% Mg: 0
wt.% Mn: 1.15
wt.% Ni: 0.425
wt.% Si: 1.35
wt.% Zn: 0

☑ save as a "Mixture"

Help

Al - Aluminum

M = 26.9815385 g/mol

This element is the solvent.

Its wt.% is calculated by balance.

This element is the solvent.

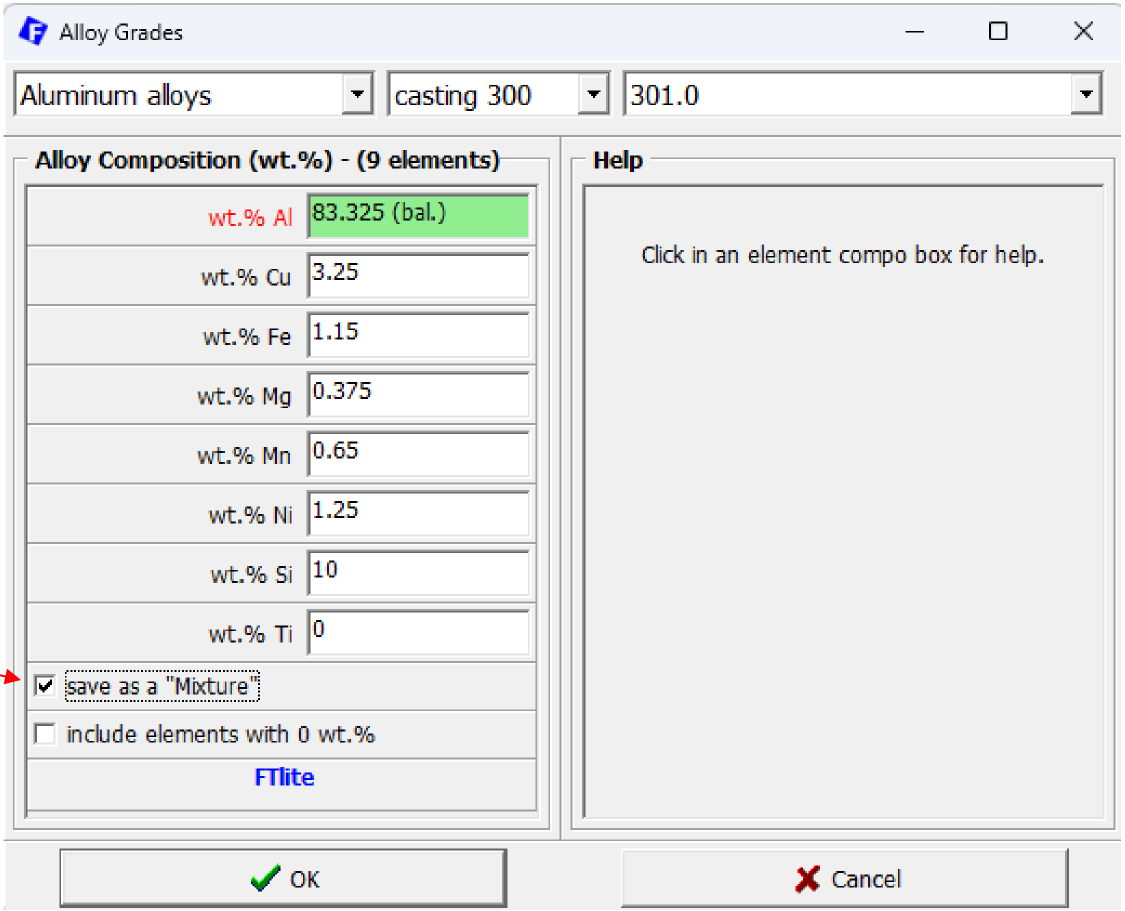
Its wt.% is calculated by balance from 100% and you can't change it by itself, you must change another alloying element…

Creating an Input Stream in EQUILIB

In this example, the **AA301.0** aluminum cast alloy (UNS A03010; Aluminium 301.0; Al301) is selected.

Check “save as a “Mixture””, if you want to create an input stream in EQUILIB with this alloy composition.

Otherwise, a multi-line input will be entered in EQUILIB.



Aluminum alloys | casting 300 | 301.0

Alloy Composition (wt.%) - (9 elements)

wt.% Al	83.325 (bal.)
wt.% Cu	3.25
wt.% Fe	1.15
wt.% Mg	0.375
wt.% Mn	0.65
wt.% Ni	1.25
wt.% Si	10
wt.% Ti	0

☑ save as a "Mixture"

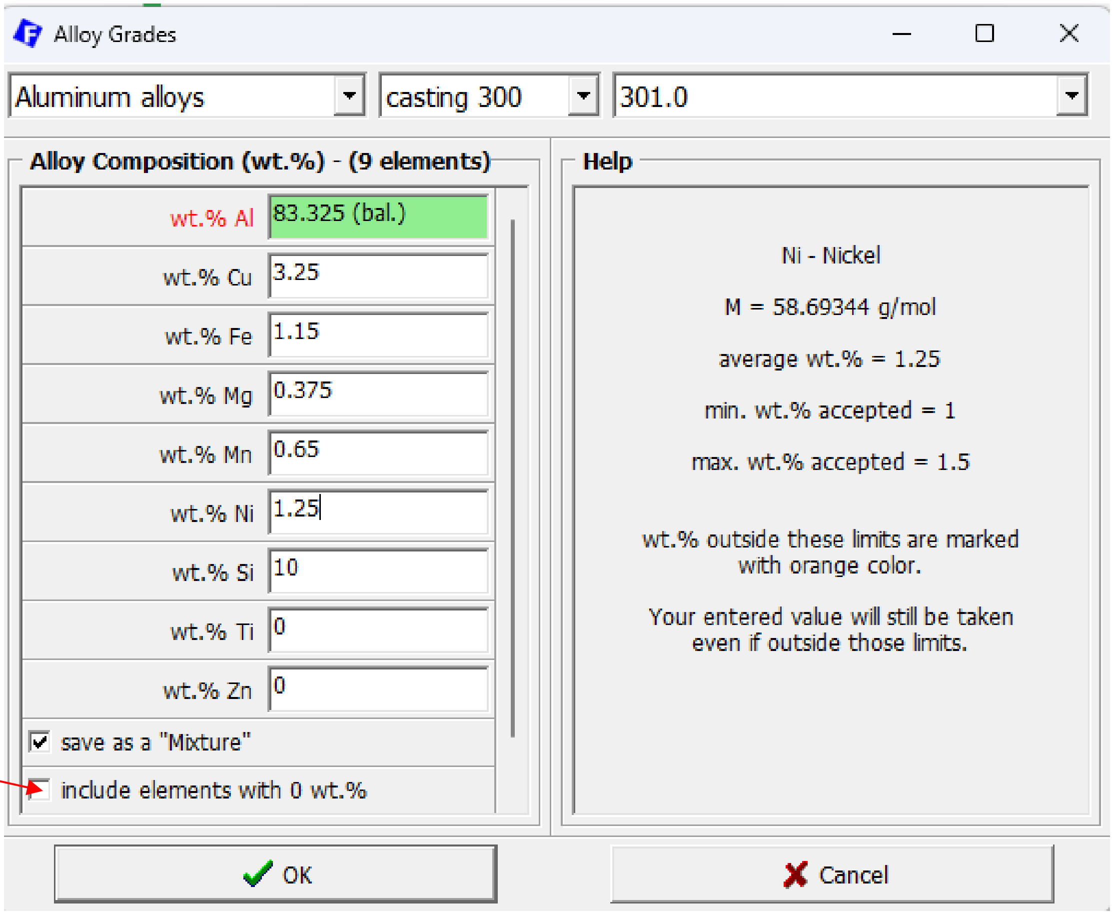
☐ include elements with 0 wt.%

Help

Click in an element compo box for help.

Creating an Input Stream in EQUILIB

In this example, the **AA301.0** aluminum cast alloy (UNS A03010; Aluminium 301.0; Al301) is selected.



Alloy Grades

Aluminum alloys | casting 300 | 301.0

Alloy Composition (wt.%) - (9 elements)

wt.% Al	83.325 (bal.)
wt.% Cu	3.25
wt.% Fe	1.15
wt.% Mg	0.375
wt.% Mn	0.65
wt.% Ni	1.25
wt.% Si	10
wt.% Ti	0
wt.% Zn	0

☑ save as a "Mixture"

☐ include elements with 0 wt.%

Help

Ni - Nickel

M = 58.69344 g/mol

average wt.% = 1.25

min. wt.% accepted = 1

max. wt.% accepted = 1.5

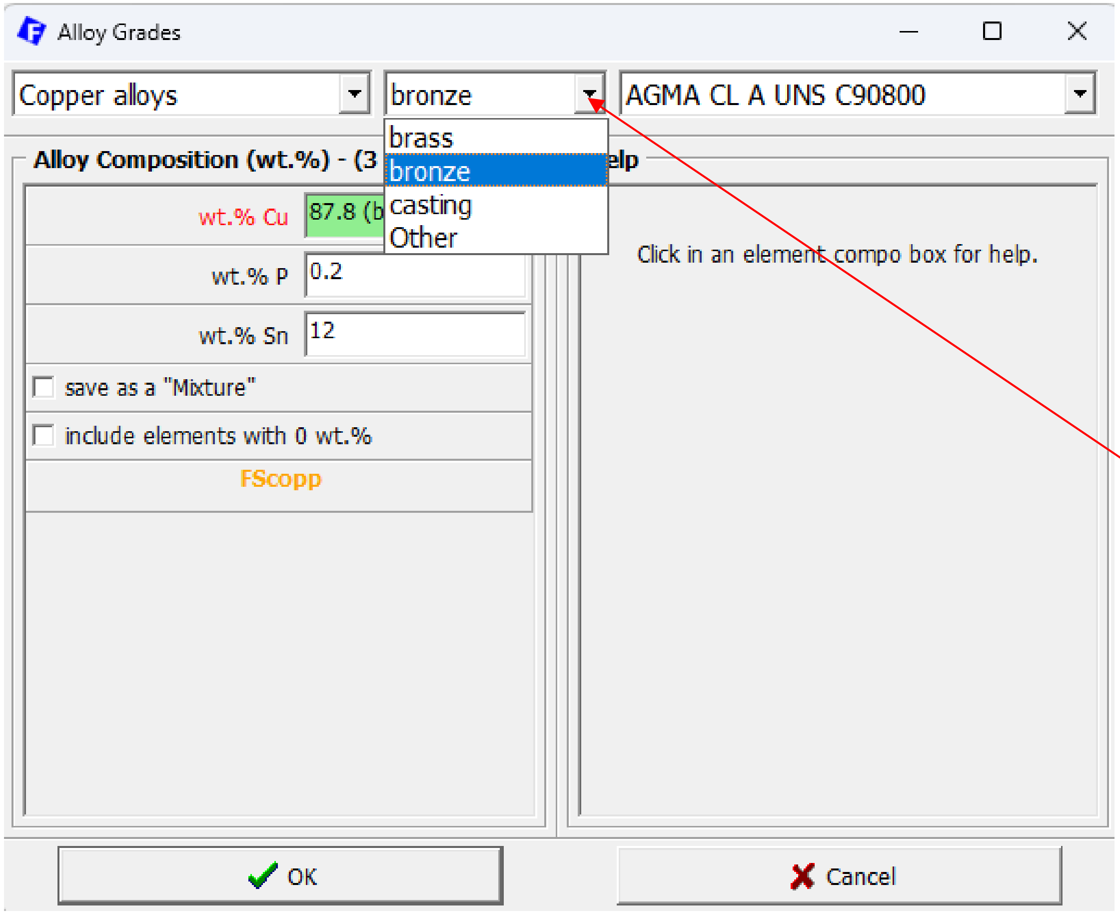
wt.% outside these limits are marked with orange color.

Your entered value will still be taken even if outside those limits.

Check “include elements with 0 wt.%”, if you want to have alloying elements with 0 wt.% included in the MIXTURE or the multi-line input in EQUILIB.

This will generate a longer list of possible products including these elements in the COMPOUNDS and SOLUTIONS.

Selection of Copper Alloy Series



Alloy Grades

Copper alloys | bronze | AGMA CL A UNS C90800

Alloy Composition (wt.%) - (3

wt.% Cu: 87.8 (b

wt.% P: 0.2

wt.% Sn: 12

☐ save as a "Mixture"

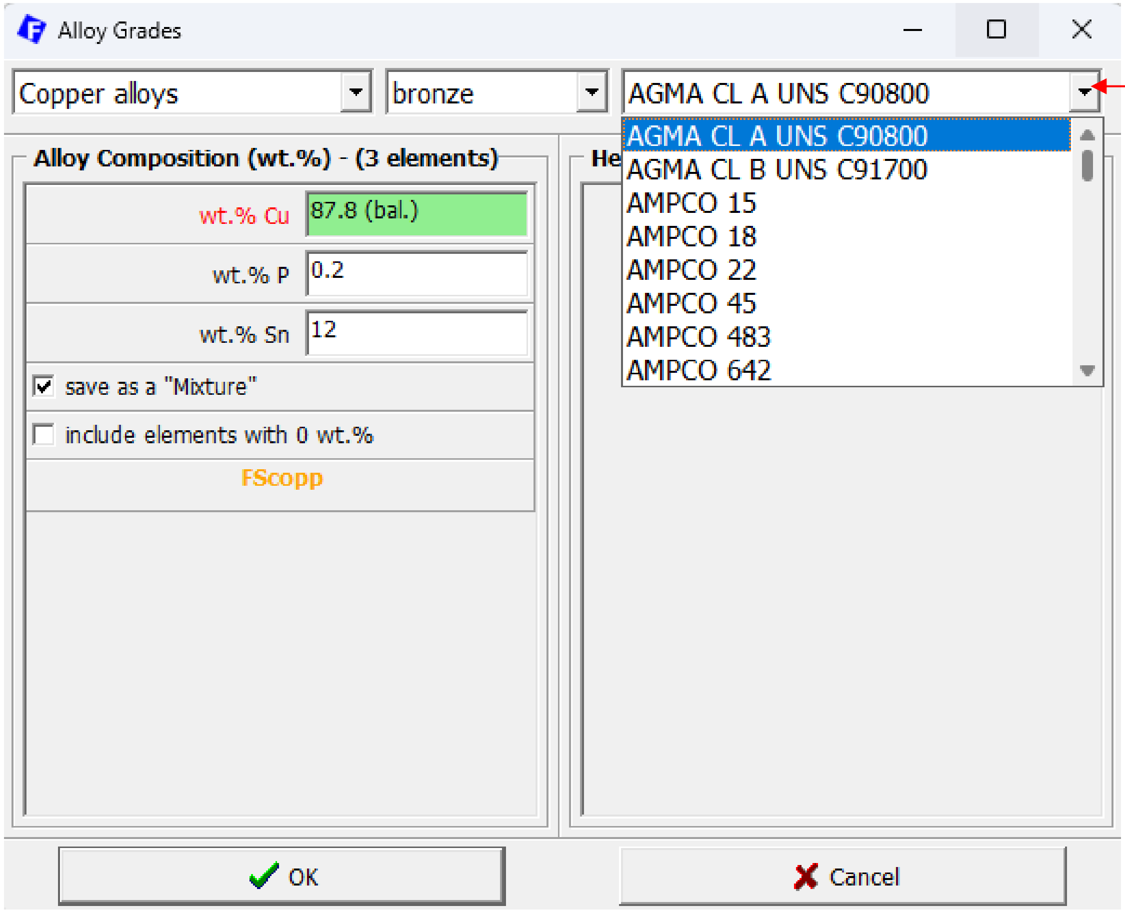
☐ include elements with 0 wt.%

Click in an element compo box for help.

In this example, the **UNS C90800** bronze alloy (Cast UNS C90800; Cast Grade C90800; Cast ASTM B427, B505) is selected.

Click to choose Copper series

Selection of Copper Alloy in the Selected Series



Copper alloys | bronze | AGMA CL A UNS C90800

AGMA CL A UNS C90800
AGMA CL B UNS C91700
AMPCO 15
AMPCO 18
AMPCO 22
AMPCO 45
AMPCO 483
AMPCO 642

Alloy Composition (wt.%) - (3 elements)

wt.% Cu	87.8 (bal.)
wt.% P	0.2
wt.% Sn	12

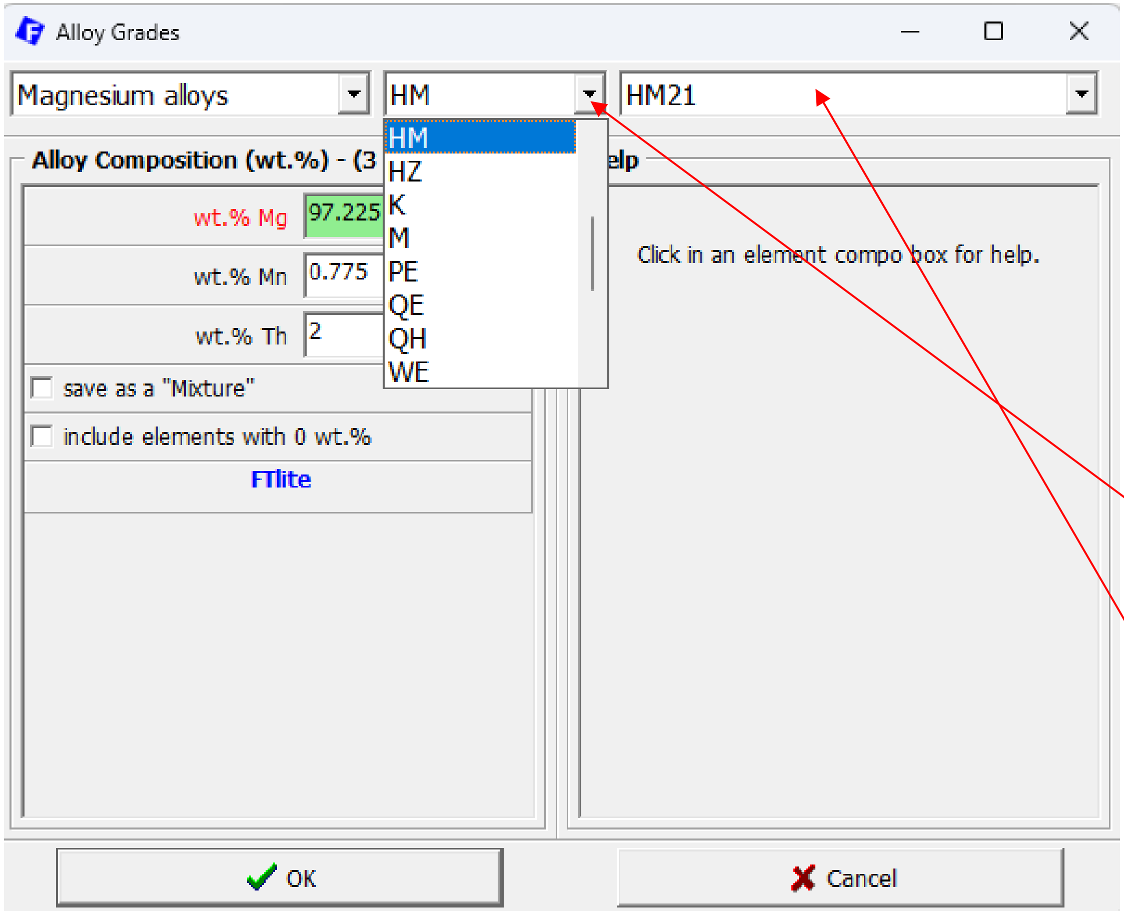
☑ save as a "Mixture"

☐ include elements with 0 wt.%

FScopp

Click to choose the **AGMA CL A UNS C90800** Cu-bronze alloy in the selected series

Selection of Magnesium Alloy Series



wt.% Mg 97.225
wt.% Mn 0.775
wt.% Th 2

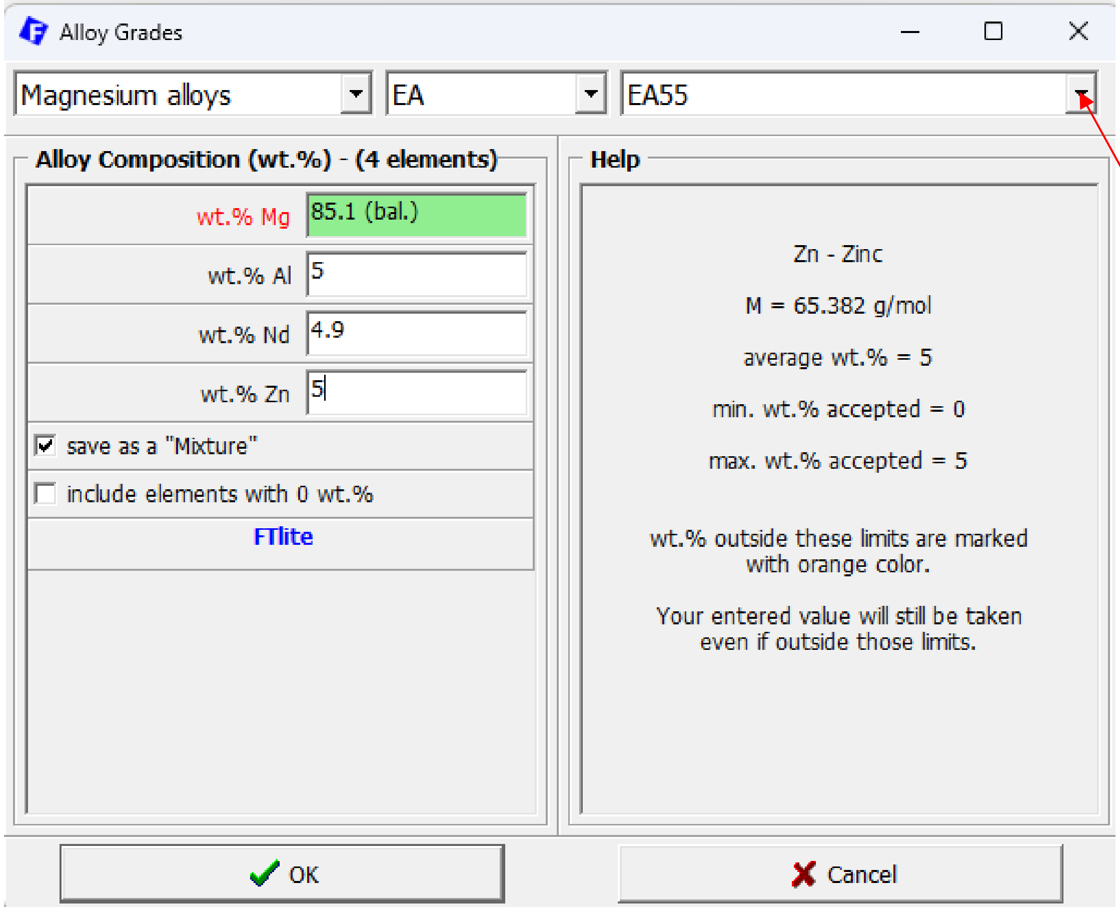
Click in an element compo box for help.

In this example, the **HM21** magnesium alloy is selected.

Click to choose the magnesium HM-series.

Then click to select the HM21 alloy.

Selection of Magnesium Alloy in the Selected Series



Magnesium alloys | EA | EA55

Alloy Composition (wt.%) - (4 elements)

wt.% Mg	85.1 (bal.)
wt.% Al	5
wt.% Nd	4.9
wt.% Zn	5

☑ save as a "Mixture"

☐ include elements with 0 wt.%

Help

Zn - Zinc

M = 65.382 g/mol

average wt.% = 5

min. wt.% accepted = 0

max. wt.% accepted = 5

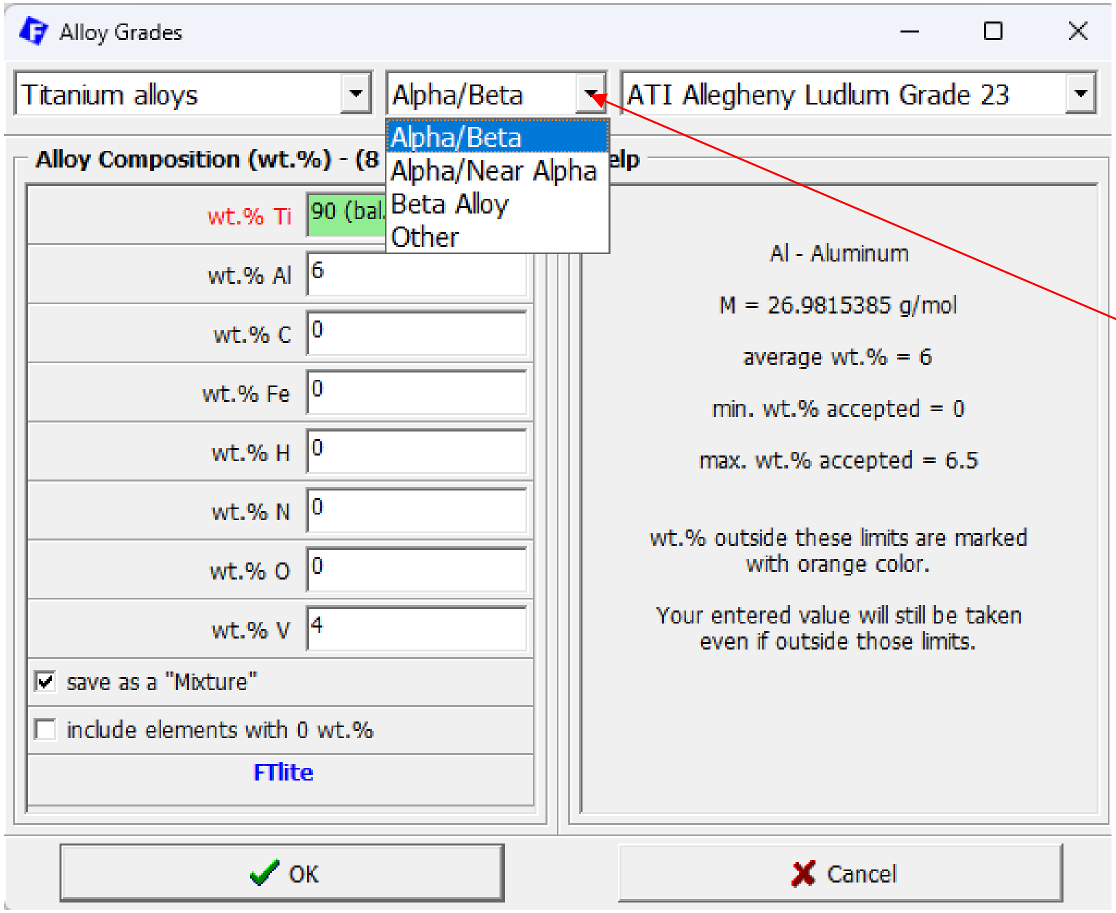
wt.% outside these limits are marked with orange color.

Your entered value will still be taken even if outside those limits.

In this example, the **EA55** magnesium alloy is selected.

Click to choose the **Mg EA55 alloy** in the selected EA series.

Selection of Titanium Alloy Series



Alloy Composition (wt.%) - (8 … **elp**

wt.% Ti 90 (bal.
wt.% Al 6
wt.% C 0
wt.% Fe 0
wt.% H 0
wt.% N 0
wt.% O 0
wt.% V 4

☑ save as a "Mixture"
☐ include elements with 0 wt.%

Al - Aluminum

M = 26.9815385 g/mol

average wt.% = 6

min. wt.% accepted = 0

max. wt.% accepted = 6.5

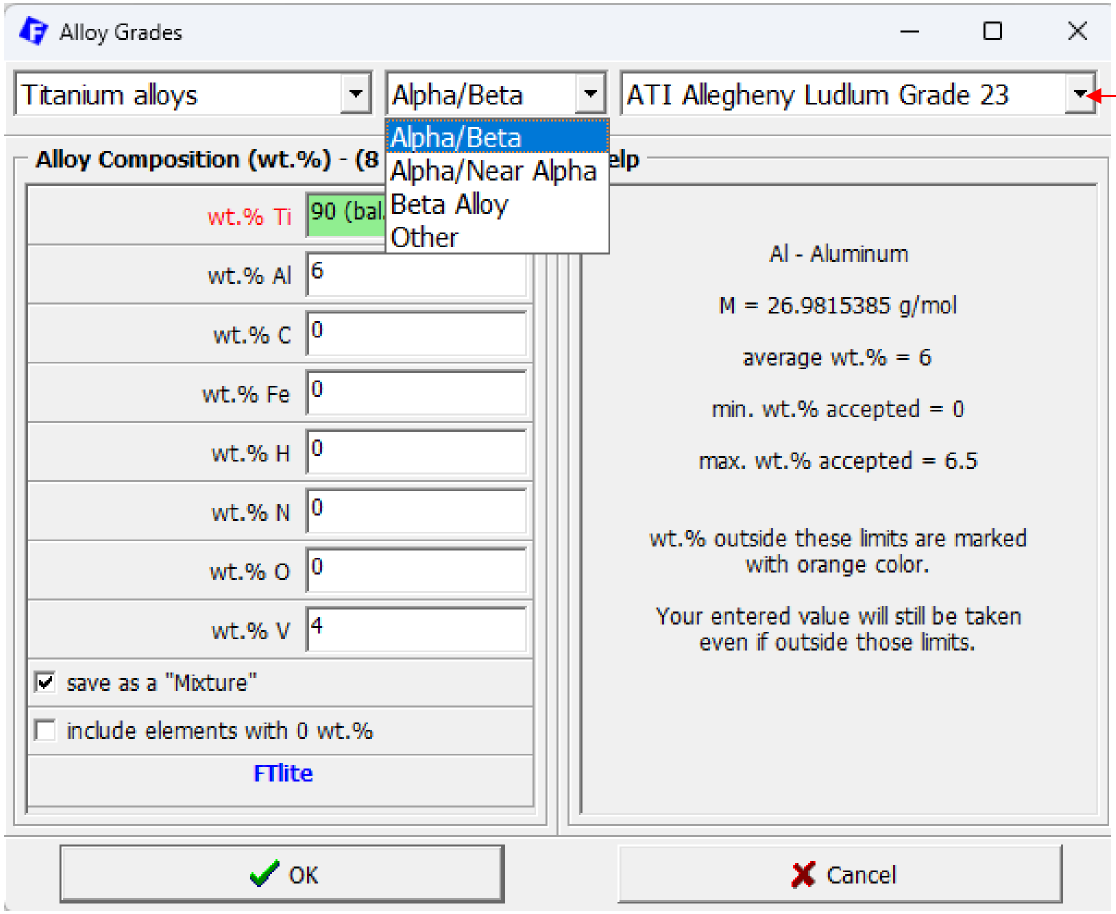
wt.% outside these limits are marked with orange color.

Your entered value will still be taken even if outside those limits.

In this example, the **ATI Allegheny Ludlum Grade 23** α/β titanium alloy is selected.

Click to choose Titanium series

Selection of Titanium Alloy in the Selected Series



wt.% Ti: 90 (bal.
wt.% Al: 6
wt.% C: 0
wt.% Fe: 0
wt.% H: 0
wt.% N: 0
wt.% O: 0
wt.% V: 4

☑ save as a "Mixture"
☐ include elements with 0 wt.%

Al - Aluminum

M = 26.9815385 g/mol

average wt.% = 6

min. wt.% accepted = 0

max. wt.% accepted = 6.5

wt.% outside these limits are marked with orange color.

Your entered value will still be taken even if outside those limits.

Click to choose the Alloy in the selected series