

Advanced features of *Equilib*

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

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| | |
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Target phase options

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

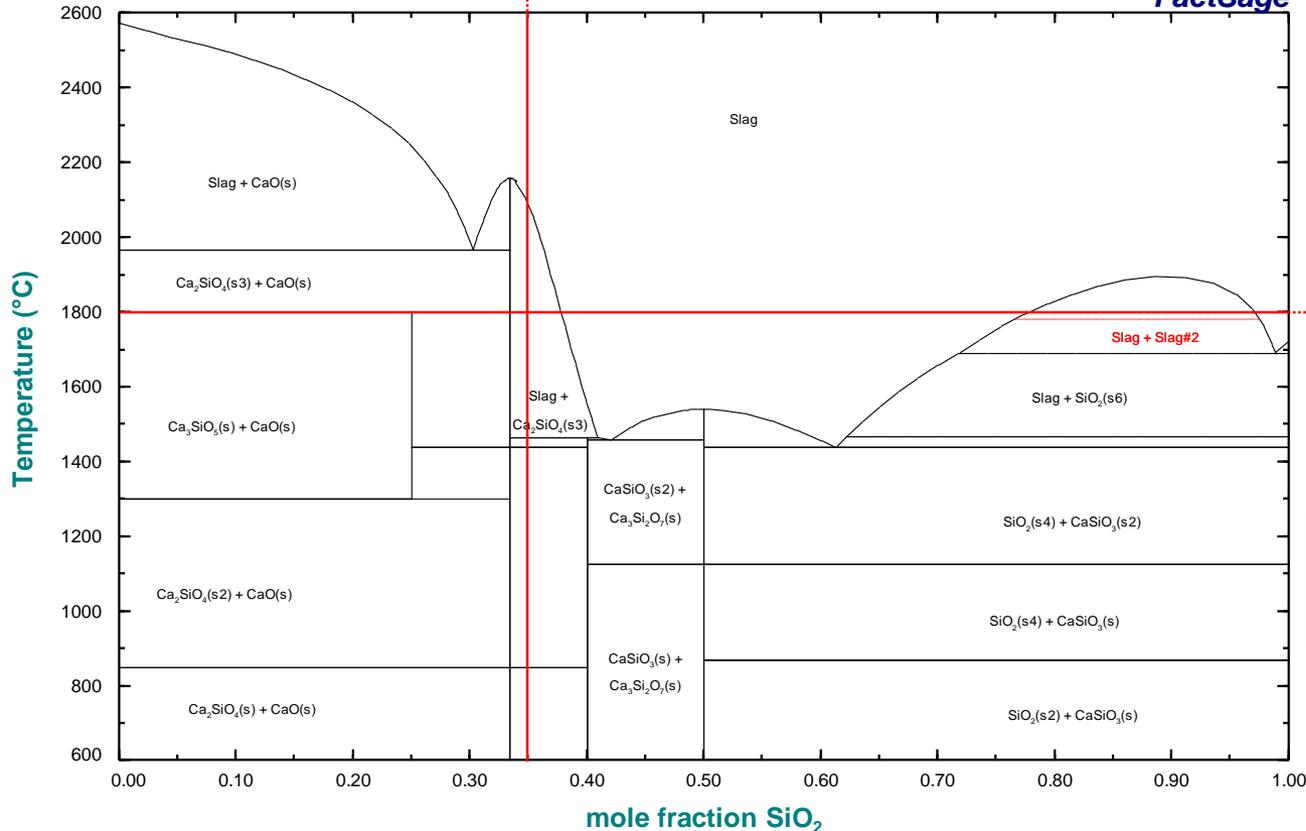
- [F] - Formation target phase:** the T (P or <A>) is calculated when the species or phase first begins to form. The final T (P, <A>) must not be specified (blank column) and an estimate of the unspecified T (P, <A>) must be entered.
- [P] - Precipitate target phase:** the T (P or <A>) is calculated 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.
- [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 - SiO₂
<A> = 0.35

FactSage



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

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

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

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

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

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

The screenshot shows the 'Equilib: Formation target phase (option F) in the CaO-SiO2 binary system' window. The 'Reactants' section contains the input '<A> CaO + <A> SiO2'. The 'Products' section is empty. The 'Solution species' table is as follows:

| * | + | Base-Phase | Full Name |
|-------------------------------------|-------------------------------------|------------|-----------------------|
| <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> | IF | FACT-SLAG Slag-liquid |

The 'Formation Target' section has 'Estimate T(C): 1000' and 'Mass(mol): 0'. The 'Final Conditions' section has '<A>' set to 0.35 and 'T(C)' set to blank. The 'Calculate' button is highlighted.

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

F Results - Equilib 1464.19 C

Output Edit Show Pages

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

```

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

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

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

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

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

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

where "A" on the reactant side is 0.35000

The cutoff concentration has been specified to 1.0000E-75

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

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

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

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

Value of <A>, $X_{\text{SiO}_2} = 0.35$

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: $X_{\text{SiO}_2} = 0.36667$

```
<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: $T = 1922.80^\circ\text{C}$

Value of <A>, $X_{\text{SiO}_2} = 0.35$

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**).

The screenshot shows the 'F Menu - Equilib: Liquid-liquid immiscibility (option I) and isothermal phase transitions in the CaO-SiO2' window. The interface is divided into several sections:

- Reactants (2):** <A> CaO + <A> SiO2
- Products:** Compound species (gas, aqueous, pure liquids, pure solids) and Solution species (Base-Phase, Full Name). The 'Solution species' table is highlighted with a red box, showing 'IF' (FACT-SLAG) and 'Slag-liquid'.
- Formation Target:** FACT-SLAG, Estimate ALPHA: 0.5, Mass(mol): 0.
- Final Conditions:** <A>, , T(C): 1800, P(atm): 1, Product H(J): [blank].
- Equilibrium:** normal, transitions, predominant, open.
- Calculate >>** button.

Red circles and arrows highlight the 'F' option in the menu, the 'IF' entry in the solution species table, the '0.5' estimate, and the '1800' temperature input.

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

```
F Results - Equilib 1800 C, A=0.3333
Output Edit Show Pages
T(C) P(atm) Energy(J) Mass(mol) Vol(litre)

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

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

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

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

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

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

+ 0.00000 mol SiO2_tridymite(1) 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.

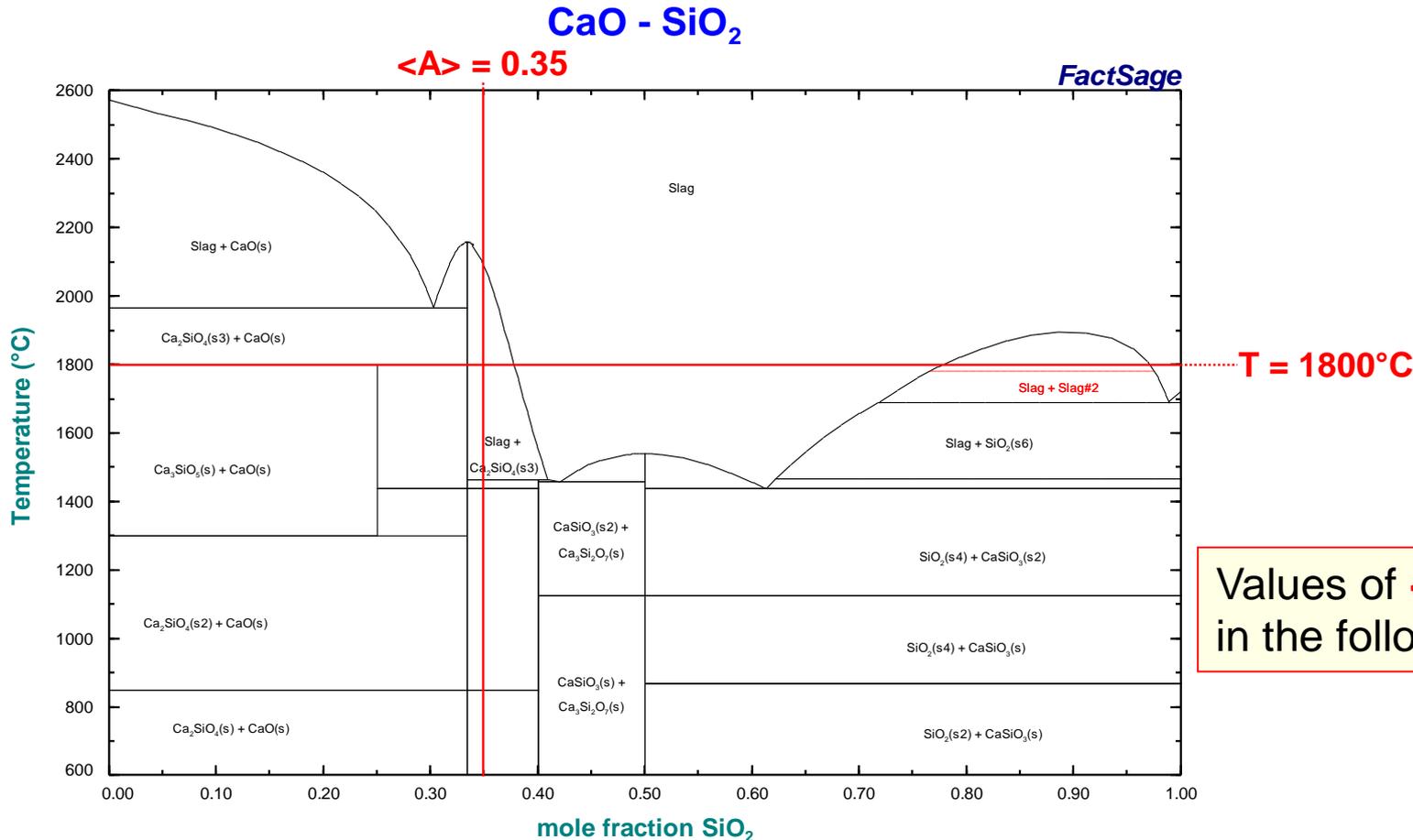
Compositions and quantities of
the solid phases in equilibrium
(activity =1) with FACT-SLAG.

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.

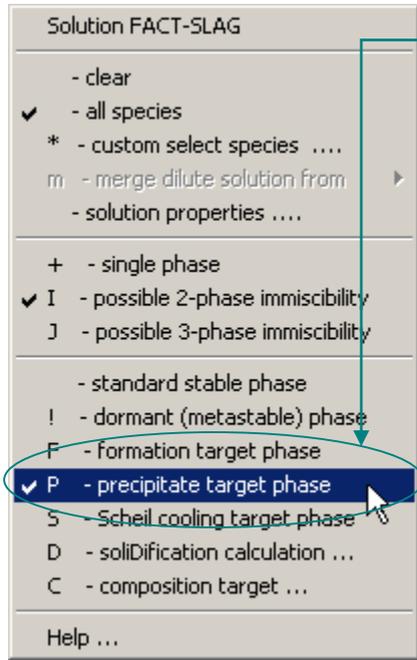


Values of **<A>** and **T** used in the following example.

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**.



Reactants [2]

<1-A> CaO + <A> SiO2

Products

Compound species

- gas ideal real 0
- aqueous 0
- pure liquids 0
- * + pure solids 17
- suppress duplicates
- * - custom selection species: 17

Precipitate Target

FACT-SLAG

Estimate T(C): 1000

Mass(mol): 0

Solution species

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

Legend

- I - immiscible
- P - precipitate target

Show all selected

species: 4 solutions: 2

Final Conditions

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

10 steps Table

Equilibrium

- normal transitions
- predominant open

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

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

F Results - Equilib 2085.37 C

Output Edit Show Pages

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

Equilibrium at 2085.37 °C

```

<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(1) T
(2085.37 C, 1 atm, S5, a=2.6429E-05)

+ 0.00000 mol SiO2_tridymite(1) 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
    
```

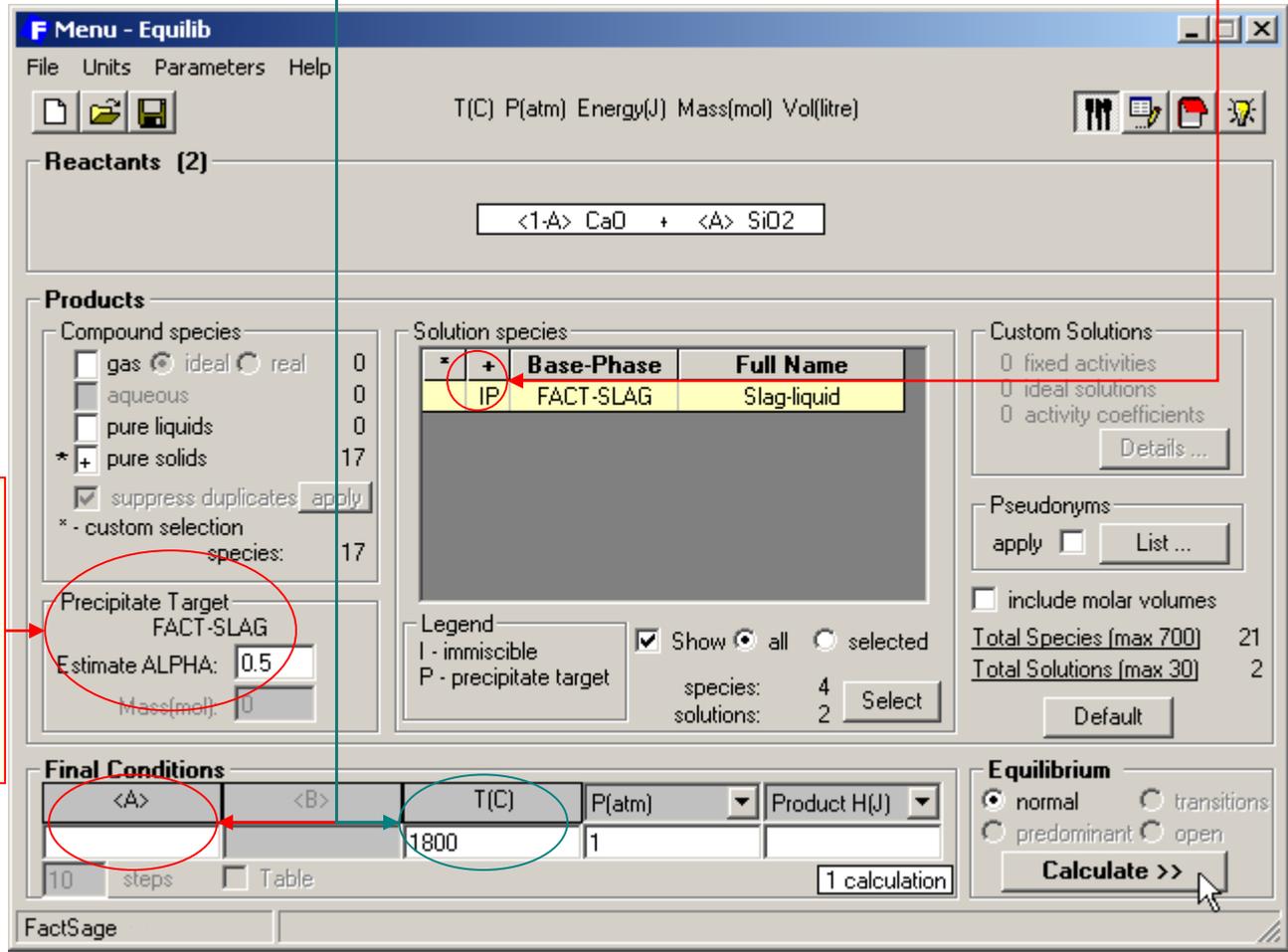
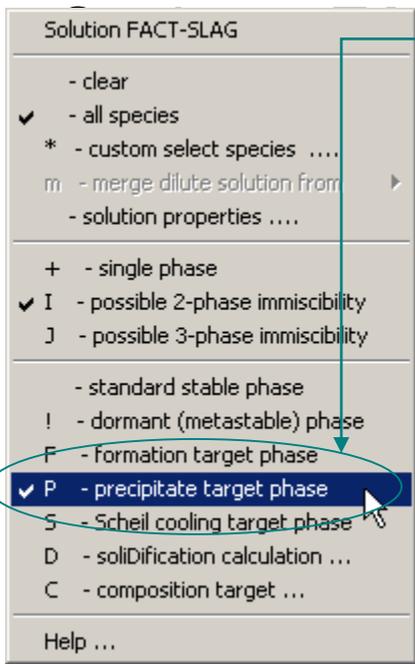
Note:
 activity = **1.0**
 number of moles = **1** (100%)
 for the first phase:
 the slag phase (liquid).

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

Value of <A>, $X_{\text{SiO}_2} = 0.35$

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.**



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

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>**, $X_{\text{SiO}_2} = 0.3767$.

```
<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(1) T
(1800.00 C, 1 atm, S5, a=2.0833E-04)

+ 0.00000 mol SiO2_tridymite(1) 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 C 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
```

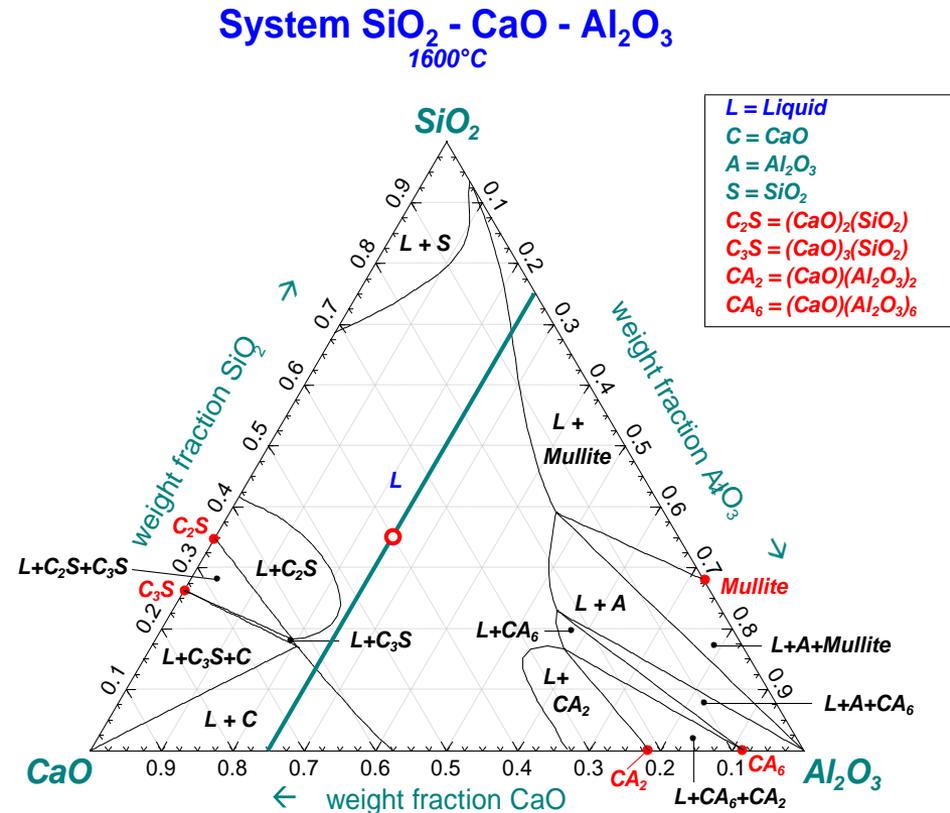
Precipitate target phase calculation for a more complex system

This is an example of a Slag-liquid precipitate target phase calculation in the **CaO-SiO₂-Al₂O₃** 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).

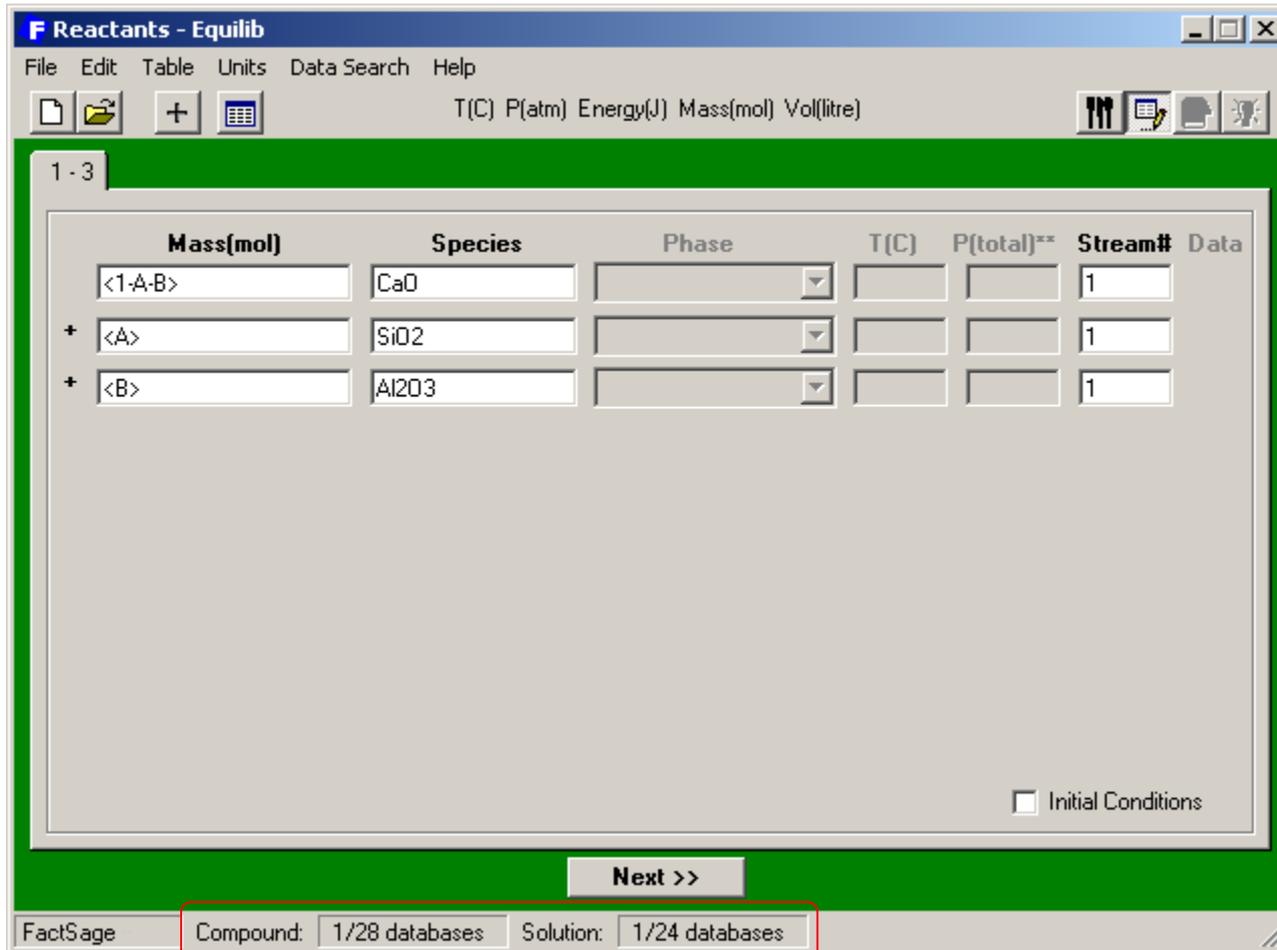
In this example that temperature is calculated when the first solid precipitate starts to deposit when Slag-liquid (FACT-SLAG) is cooled. Such a calculation is extremely important for example in the pyrometallurgy and glass industries. In principle one could select the equilibrium «**transitions**» option 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 = 25% (2nd example)



Setting a ternary system in the *Equilib* Reactants Window

In the **Reactants Window** the reactants are **<1-A-B> CaO + <A> SiO₂ + Al₂O₃**. This defines a **CaO-SiO₂-Al₂O₃** ternary system if **<A> + ** is in the range **0 to 1**. The use of unit mass (g or lb) will give the compositions in weight %.



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

Setting the FACT-SLAG precipitate target at a given composition

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

2° **Enter** values for <A> (**0.35**) and (**0.25**) (i.e. %wt CaO = **40%**, %wt SiO₂ = **35%**, %wt Al₂O₃ = **25%**) and leave **T(C) blank**.

3° The **Precipitate Target** frame is **enabled**.

Enter an estimate of the value of T(C).
Here T(C) = **2000°C**.

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

F Menu - Equilib: Precipitate target phase (option P) in the CaO-SiO₂-Al₂O₃ ternary system.

File Units Parameters Help

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

Reactants (3)

1-A-B CaO + <A> SiO₂ + Al₂O₃

Products

Compound species

gas ideal real 0

aqueous 0

pure liquids 0

* pure solids 35

suppress duplicates apply

* - custom selection species: 35

Precipitate Target

FACT-SLAG

Estimate T(C): 2000

Mass(g): 0

Final Conditions

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

10 steps Table 1 calculation

Solution species

| + | Base-Phase | Full Name |
|-------------------------------------|------------|-----------------------|
| <input checked="" type="checkbox"/> | IP | FACT-SLAG Slag-liquid |

Legend

I - immiscible Show all selected

P - precipitate target species: 6 solutions: 2 Select

Equilibrium

normal transitions

predominant open

Calculate >>

Custom Solutions

fixed activities

ideal solutions

activity coefficients

Details ...

Pseudonyms

apply List ...

include molar volumes

Total Species (max 700) 41

Total Solutions (max 30) 2

Default

FactSage

Precipitate target Results

Equilib reports the temperature (**1458.99 °C**) where the second phase (**Ca₂Al₂SiO₇(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% SiO₂ = **35%**.

Performing a **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 remains unchanged**).

The screenshot shows the 'F Menu - Equilib' window. The 'Reactants (3)' field contains '(gram) <A-B> CaO + <A> SiO2 + Al2O3'. The 'Products' section has 'Compound species' with 'pure solids' selected (35 species) and 'Solution species' with 'Slag-liquid' selected. The 'Precipitate Target' section is circled in red, showing 'FACT-SLAG' and 'Estimate ALPHA: 0.5'. The 'Final Conditions' table is circled in green, showing '<A>' as blank, '' as 0.25, and 'T(C)' as 1600. The 'Equilibrium' section has 'normal' selected. A 'Calculate >>' button is visible at the bottom right.

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

For example, if in the **Menu Window** the composition **<A>** is now unspecified (**blank**), **** 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 ($\langle A \rangle = 13.371 \text{ wt.}\%$) at 1600°C where **CaO(s1)** first starts to precipitate (**activity = 1, 0 gram**)

```
F Results - Equilib 1600 C, A=0.1337
Output Edit Show Pages
T(C) P

(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
(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 $\langle B \rangle = 25\text{wt.}\%$. 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 **SiO₂-rich side**, one can calculate the other value of <A> for which a precipitate starts to form.

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

F Results - Equilib 1600 C, A=0.683

Output Edit Show Pages

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

```
(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  
(1600.00 C, 1 atm, S1, a=2.1617E-12) T  
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
```

In the **Results Window Equilib** now reports the silica (SiO₂) composition (<A> = **68.303 wt.%**) at **1600°C** where **mullite Al₆Si₂O₁₃(s1)** first starts to precipitate (**activity = 1, 0 gram**).

Composition target phase

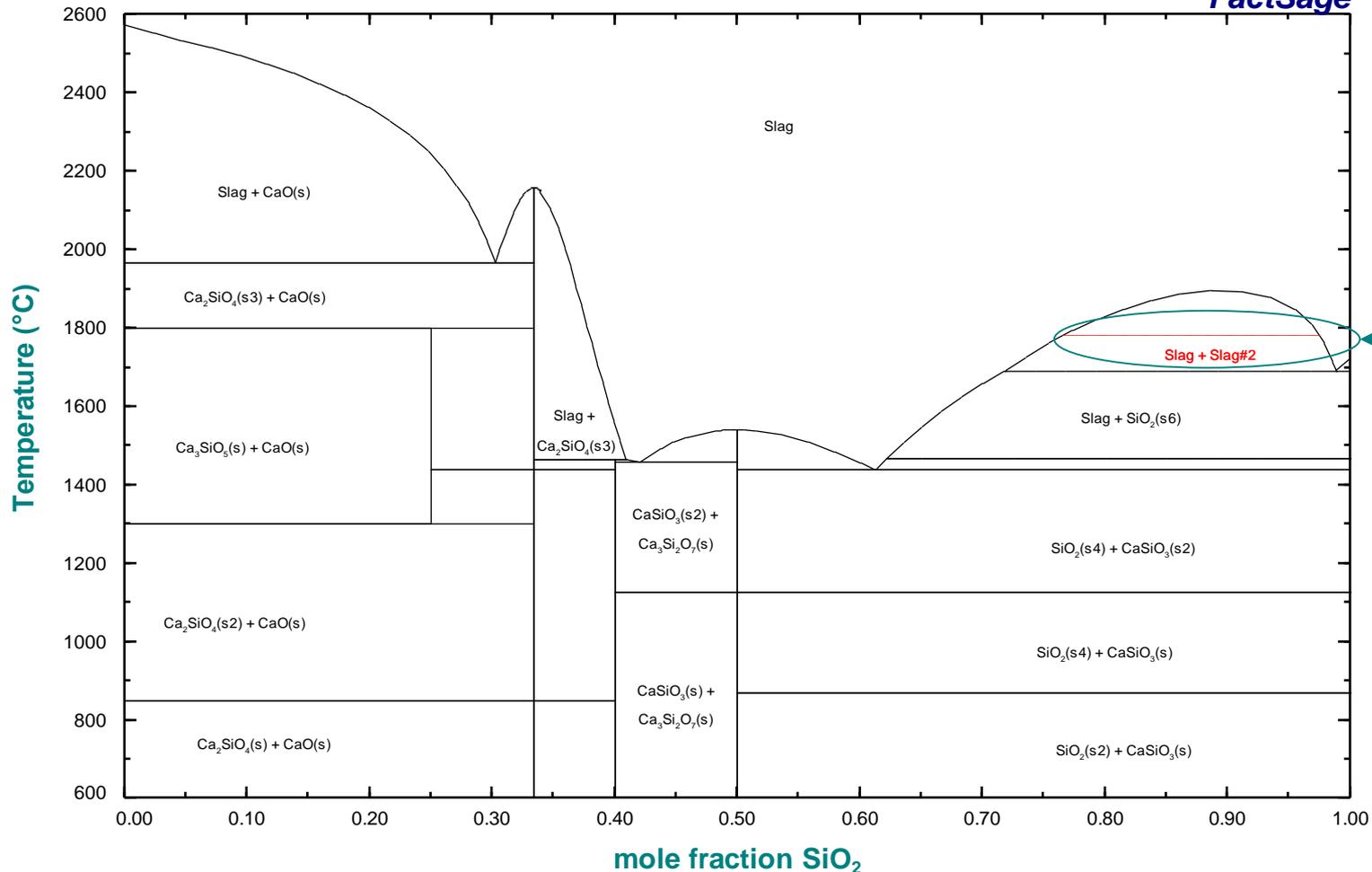
TTD

Transitions in the CaO-SiO₂ binary phase diagram

Liquid phase immiscibility – for example $X_{\text{SiO}_2} = 0.7783$ and 0.9707 at 1800°C .

CaO - SiO₂

FactSage



Isothermal phase transitions in the CaO-SiO_2 binary system

1° Binary system <1-A> CaO + <A> SiO₂.

2° Possible products:

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

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

4° Select transitions

The screenshot shows the FactSage Equilib software interface. The title bar reads "F Menu - Equilib: Liquid-liquid immiscibility (option I) and isothermal phase transitions in the CaO-Si...". The main window displays the following settings:

- Reactants (2):** <1-A> CaO + <A> SiO₂
- Products:** Under "Compound species", "pure solids" is selected with a count of 17. Under "Solution species", "I" (FACT-SLAG) is selected with a count of 2.
- Target:** Estimate T(K) is set to 1800, and Mass(mol) is 0.
- Final Conditions:** A table with columns <A>, , T(C), P(atm), and Product H(J). The first row contains values 0.7, 1.0, 0.05, 1, and an empty field. The number of steps is set to 10.
- Equilibrium:** The "transitions" radio button is selected.

Red and blue circles highlight specific elements: the reactants, the "pure solids" and "I" product options, the "transitions" radio button, and the final conditions table.

The program will calculate the equilibrium at **1800°C** for mole fractions of SiO₂ 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.

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

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

17 pure solid oxides

F Selection - Equilib
File Edit Show Sort

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 |

Show Selected Select All Select/Clear... Clear OK

Select all species containing ...
Clear all species containing ...

Ca
Si
O

Compound species

gas ideal real 0

aqueous 0

pure liquids 0

+ pure solids 17

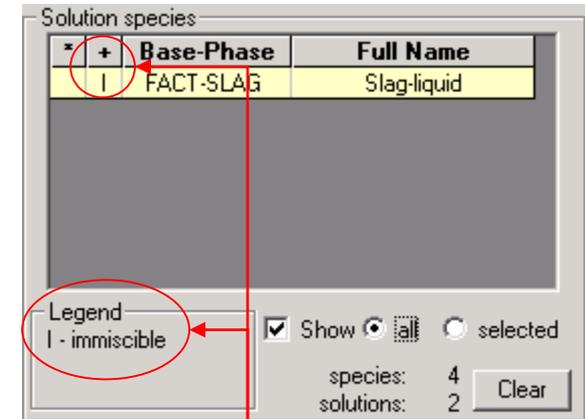
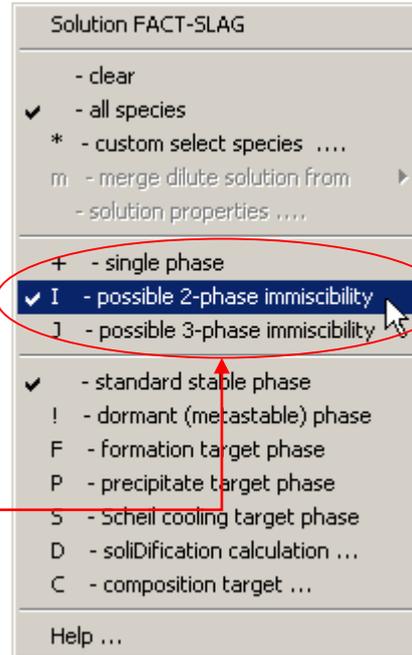
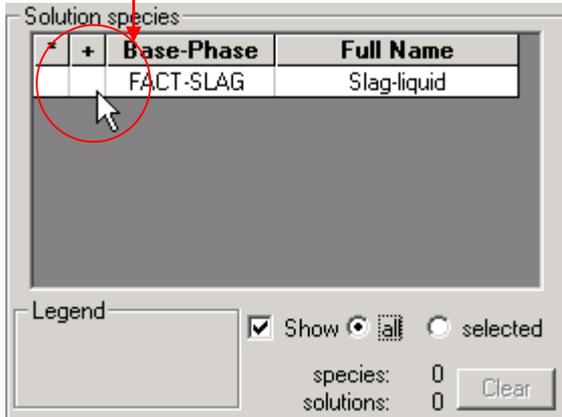
suppress duplicates

* - 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 **SiO₂ > 50%**. If the phase is not immiscible the results of the calculation will be OK - the phase will appear twice with the same composition.
Note: This option tends to slow down the speed of the calculation - you may wish to try **I!** (**immiscible** and **dormant**) to check if the phase is stable.

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

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

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

Output Edit Show Pages

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

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

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

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

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

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

Output Edit Show Pages

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

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

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

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

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

i.e. **Equilib** reports two-phase stability within the composition range:
 $0.77829 < X_{\text{SiO}_2} < 0.97074$
and one-phase stability outside this range.

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

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

Output Edit Show Pages

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

A=0.7 A=0.75 A=0.7783 A=0.8 **A=0.85** A=0.9 A=0.95 A=0.9707 A=1

<1-λ> CaO + <λ> 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 $X_{\text{SiO}_2} = 0.85$

Example of **one-phase** stability at $X_{\text{SiO}_2} = 0.75$

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

Output Edit Show Pages

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

A=0.7 **A=0.75** A=0.7783 A=0.8 A=0.85 A=0.9 A=0.95 A=0.9707 A=1

<1-λ> CaO + <λ> 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)
```

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-SiO₂ 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

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> | | T(C) | P(atm) | Product H(J) |
|------|-----|----------|--------|--------------|
| 0.35 | | 600 2600 | 1 | |

Equilibrium

- normal
- transitions
- predominant
- open

Calculate >>

2+ calculations

FactSage

$$X_{\text{SiO}_2} = 0.35$$

The program will calculate all phase transitions at $X_{\text{SiO}_2} = 0.35$ in the temperature range **600 to 2600°C**.

Transition Temperatures for $X_{\text{SiO}_2} = 0.35$ in CaO-SiO₂

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.

F Results - Equilib 1436.85 C (page 4/9)

Output Edit Show Pages

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

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

```

<1-A> CaO + <A> SiO2 =
0.00000 mol Slag-liquid#1
(1436.85 C, 1 atm, a=0.97437)
( 0.40247 SiO2
+ 0.59753 CaO)
+ 0.00000 mol Slag-liquid#2
(1436.85 C, 1 atm, a=0.97437)
( 0.40247 SiO2
+ 0.59753 CaO)
+ 0.25000 mol Ca2SiO4_alpha-prime
(43.060 gram, 0.25000 mol)
(1436.85 C, 1 atm, S2, a=1.0000)
+ 5.0000E-02 mol Ca3Si2O7_rankinite
(14.420 gram, 5.0000E-02 mol)
(1436.85 C, 1 atm, S1, a=1.0000)
+ 0.00000 mol Ca2SiO4_alpha
(1436.85 C, 1 atm, S3, a=1.0000)
+ 0.00000 mol CaSiO3_pseudowollastonite
(1436.85 C, 1 atm, S2, a=0.88453)
where "A" on the reactant side is 0.35000
The cutoff concentration has been specified to 1.0000E-75
Data on 4 product species identified with "T" have been extrapolated
*****
H G V S Cp
(J) (J) (litre) (J/K) (J/K)
*****
-6.86837E+05 -9.30583E+05 0.00000E+00 1.42541E+02 6.76591E+01
    
```

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

F Results - Equilib 1436.85 C (page 5/9)

Output Edit Show Pages

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

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

```

<1-A> CaO + <A> SiO2 =
0.00000 mol Slag-liquid#1
(1436.85 C, 1 atm, a=0.97437)
( 0.40247 SiO2
+ 0.59753 CaO)
+ 0.00000 mol Slag-liquid#2
(1436.85 C, 1 atm, a=0.97437)
( 0.40247 SiO2
+ 0.59753 CaO)
+ 0.25000 mol Ca2SiO4_alpha
(43.060 gram, 0.25000 mol)
(1436.85 C, 1 atm, S3, a=1.0000)
+ 5.0000E-02 mol Ca3Si2O7_rankinite
(14.420 gram, 5.0000E-02 mol)
(1436.85 C, 1 atm, S1, a=1.0000)
+ 0.00000 mol Ca2SiO4_alpha-prime
(1436.85 C, 1 atm, S2, a=1.0000)
+ 0.00000 mol CaSiO3_pseudowollastonite
(1436.85 C, 1 atm, S2, a=0.88453)
where "A" on the reactant side is 0.35000
The cutoff concentration has been specified to 1.0000E-75
Data on 4 product species identified with "T" have been extrapolated
*****
H G V S Cp
(J) (J) (litre) (J/K) (J/K)
*****
-6.83963E+05 -9.30583E+05 0.00000E+00 1.44222E+02 6.43721E+01
    
```

<A> = $X_{\text{SiO}_2} = 0.35$

For example at **1436.85°C**:
 α' -Ca₂SiO₄ to α -Ca₂SiO₄

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

1° The reactants are $\langle 1-A \rangle \text{NaCl} + \langle A \rangle \text{KCl}$ – i.e. the NaCl-KCl binary system where $\langle A \rangle$ 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

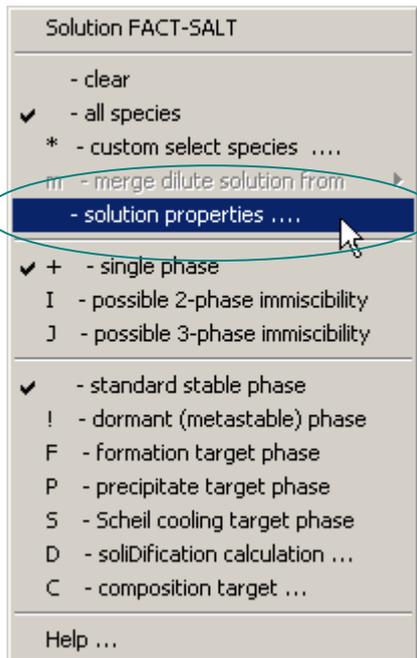
The screenshot shows the 'F Menu - Equilib' window. The 'Reactants' field contains the formula $\langle 1-A \rangle \text{NaCl} + \langle A \rangle \text{KCl}$. The 'Products' section has 'FACT-SALT' selected in the 'Solution species' table, with 'Salt-liquid' as its full name. The 'Final Conditions' table is set to calculate at $T=850$ K and $P=1$ atm, with 10 steps and 11 calculations. The 'Calculate >>' button is highlighted.

| <A> | | T(K) | P(atm) | Product H(J) |
|----------|-----|------|--------|--------------|
| 0 | 1 | 0.1 | | |
| 10 steps | | | | |

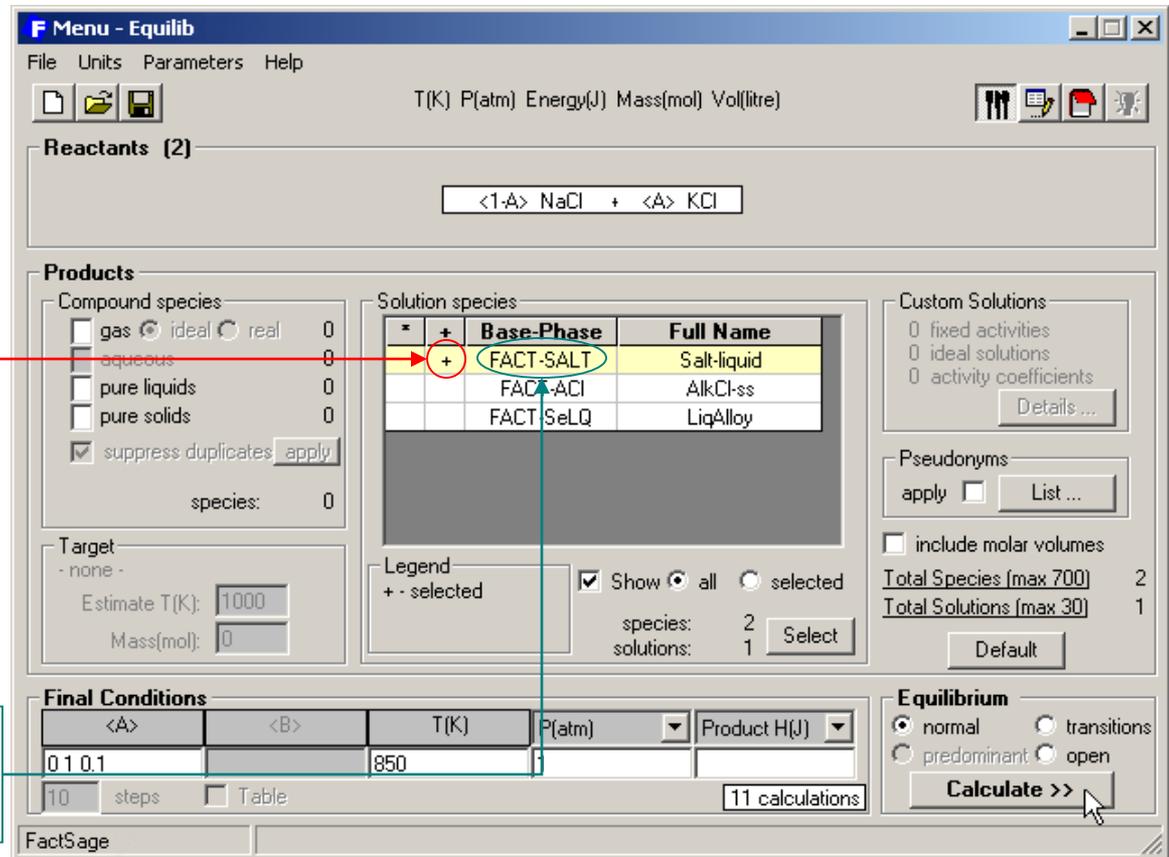
| * | + | Base-Phase | Full Name |
|---|---|------------|-------------|
| | + | FACT-SALT | Salt-liquid |
| | | FACT-ACl | AtKCl-ss |
| | | FACT-SeLQ | LiqAlloy |

Solution Properties: opening the window

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



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



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

Solution Properties Window and menus

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

Standard States

- Current Standard States ▶ NaCl
- Change Standard States ... KCl

Species

- Select all
- Clear
- ✓ 19 NaCl
- ✓ 20 KCl

F Molar Partial Properties FACT-SALT - Salt-liquid

Output Species Standard States

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

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

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

Select All Clear Close

Solution Properties: Changing Standard States

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



The 'Standard States' dialog box is shown, displaying a table of species and their standard states. The table has columns for Species, a '+' column, Data, Standard State, and Code. The table is divided into two sections for NaCl and KCl. The 'FACT-SALT' standard state is highlighted in cyan for both species.

| 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 |

Buttons at the bottom: Select Default, Close

Solution Properties: Molar Partial Properties Spreadsheet

File

- Save As
 - Text Spreadsheet ...
 - Excel Spreadsheet ...
- Print
- Print Setup ...
- Print Font ...
- Close

Edit

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

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

Swap rows and columns

| Component i | Page | <Alpha> | T(C) | P(atm) | X(NaCl) | X(KCl) | a(i) | gamma(i) | Delta_g(i) |
|-------------|------|---------|------|--------|---------|---------|-------------|-----------------|-----------------|
| NaCl_SALT | 1 | 0 | 850 | 1 | 1.0000 | 0.00000 | 1.0000 | 1.0000 | 0.00000 |
| | 2 | 0.1 | 850 | 1 | 0.90000 | 0.10000 | 0.89757 | 0.99730 | -1009.1 |
| | 3 | 0.2 | 850 | 1 | 0.80000 | 0.20000 | 0.79165 | 0.98956 | -2181.8 |
| | 4 | 0.3 | 850 | 1 | 0.70000 | 0.30000 | 0.68413 | 0.97733 | -3545.0 |
| | 5 | 0.4 | 850 | 1 | 0.60000 | 0.40000 | 0.57666 | 0.96110 | -5140.8 |
| | 6 | 0.5 | 850 | 1 | 0.50000 | 0.50000 | 0.47067 | 0.94133 | -7037.5 |
| | 7 | 0.6 | 850 | 1 | 0.40000 | 0.60000 | 0.36736 | 0.91839 | -9351.7 |
| | 8 | 0.7 | 850 | 1 | 0.30000 | 0.70000 | 0.26777 | 0.89257 | -12305. |
| | 9 | 0.8 | 850 | 1 | 0.20000 | 0.80000 | 0.17282 | 0.86408 | -16394. |
| | 10 | 0.9 | 850 | 1 | 0.10000 | 0.90000 | 8.33104E-02 | 0.83310 | -23208. |
| | 11 | 1 | 850 | 1 | 0.00000 | 1.0000 | 1.00000E-75 | <-not-calctd.-> | <-not-calctd.-> |
| 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

F Molar Integral Properties FACT-SALT - Salt-liquid

Output Species Standard States

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

partial properties integral properties 11/11 properties

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

Select All Clear

Output

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

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

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

File Edit Swap rows and columns

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

Include **dilute** solution: **Cr** in **Cu-Fe** alloy

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

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

Initial Conditions

Next >>

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

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

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

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

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

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

Menu - Equilib

File Units Parameters Help

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

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

Target

- none -

Estimate T(K): 1000

Mass(mol): 0

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 Select

Custom Solutions

fixed activities

ideal solutions

activity coefficients

Details ...

Pseudonyms

apply List ...

include molar volumes

Total Species (max 700) 9

Total Solutions (max 30) 1

Default

Final Conditions

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

10 steps Table 1 calculation

Equilibrium

normal transitions

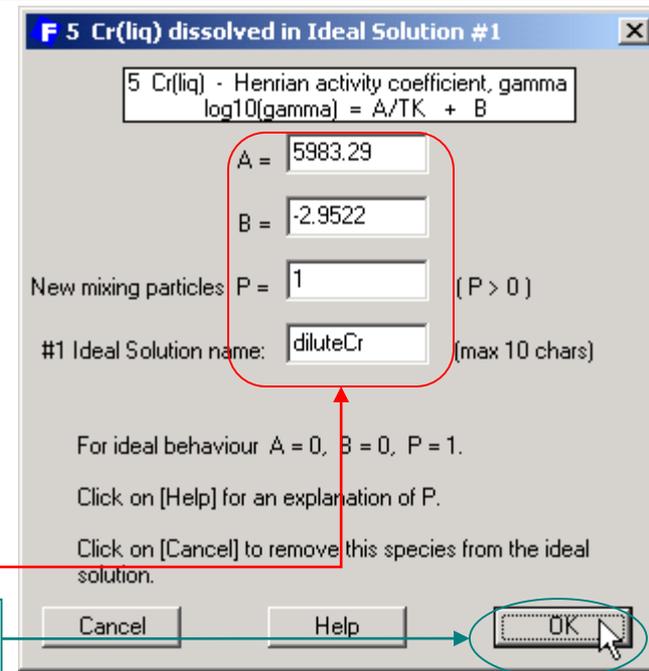
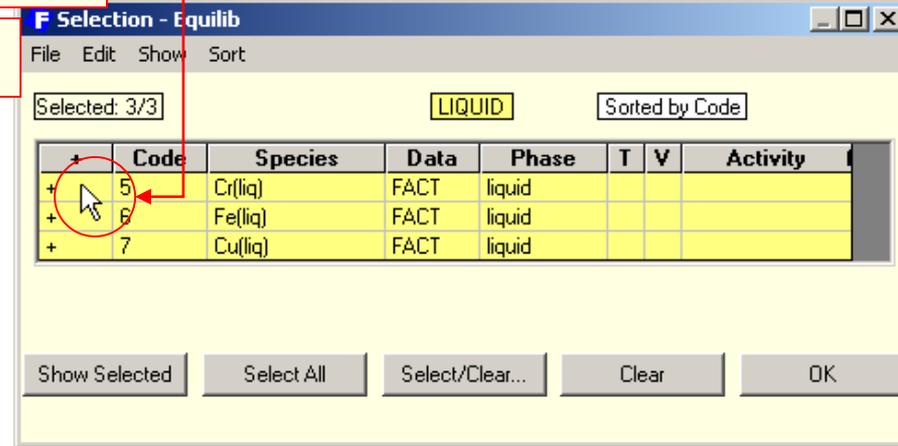
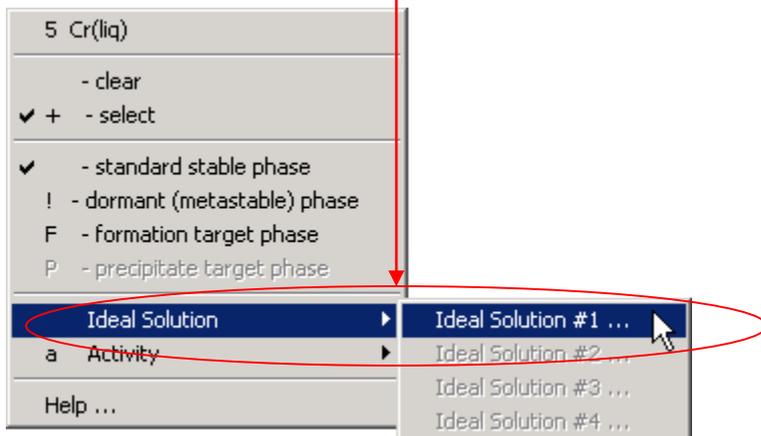
predominant open

Calculate >>

Creating an ideal Henrian solution of Cr(liq)

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

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



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

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

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

4° **Press OK**

Merging the ideal solution diluteCr and FACT-CuLQ

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

5° Press OK to return to the Menu Window

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

7° Select

m - merge dilute solution from
> Dilute Solution #1 - diluteCr

Solution FACT-CuLQ

- clear
- ✓ - all species
- * - custom select species
- m - merge dilute solution from**
 - Dilute Solution # 1 - diluteCr
 - Remove dilute components
- solution properties
- ✓ + - 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
- D - solidification calculation ...
- C - composition target ...
- Help ...

F Menu - Equilib

File Units Parameters Help

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

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

Target

- none -

Estimate T(K): 1000

Mass(mol): 0

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

Select

Final Conditions

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

10 steps Table 1 calculation

FactSage

Custom Solutions

- fixed activities
- ideal solutions
- activity coefficients

Details ...

Pseudonyms

apply List ...

include molar volumes

Total Species (max 700) 9

Total Solutions (max 30) 1

Default

Equilibrium

- normal transitions
- predominant open

Calculate >>

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:

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

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

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

Reactants (3): Cu + 0.05 Fe + 0.10 Cr

Products:

| Compound species | Count |
|---------------------|-------|
| gas | 0 |
| ideal | 0 |
| 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 |
| #1 | + | FACT-CuLQ | Cu-liq+diluteCr |
| | | FACT-FeCu | fccFe-Cu |

Legend: # - dilute components

Equilibrium: normal (selected), predominant, open, transitions

Final Conditions: T(C) = 1200, P(atm) = 1, Product H(J) = 1 calculation

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 $\gamma_{\text{Cr}(\text{liq})}$ at **1200°C**

Cr in Cu-Fe alloy – Results

```
F Results - Equilib 1200 C
Output Edit Show Page
T(C) P(atm) Energy(J) Mass(mol) Vol(litre)

Cu + 0.05 Fe + 0.1 Cr =
1.0960 mol Cu-liq+diluteCr
(68.730 gram, 1.0960 mol)
(1200.00 C, 1 atm, a=1.0000)
( 0.91242 Cu
+ 4.5621E-02 Fe
+ 4.1963E-02 Cr_liquid_diluteCr
+ 5.4009E-02 mol Cr_solid
(2.8083 gram, 5.4009E-02 mol)
(1200.00 C, 1 atm, S1, a=1.0000)
+ 0.00000 mol Cu_liquid
(1200.00 C, 1 atm, L1, a=0.92180)
+ 0.00000 mol Cu_solid
(1200.00 C, 1 atm, S1, a=0.84209)
+ 0.00000 mol Fe_fcc
(1200.00 C, 1 atm, S2, a=0.75533)
+ 0.00000 mol Fe_bcc
(1200.00 C, 1 atm, S1, a=0.75115)
+ 0.00000 mol Fe_liquid
(1200.00 C, 1 atm, L1, a=0.61312)
+ 0.00000 mol Cr_liquid
(1200.00 C, 1 atm, L1, a=0.53979)

The cutoff concentration has been specified to 1.0000E-75

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

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

T = 1200°C

$X_{Cr(liq)} = 0.041963$

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: Ti_2O and HfO_2 in **FACT-Slag**

The **FACT-SLAG** (Slag-liquid) solution does not contain the components Ti_2O and HfO_2 . This example shows how to merge Ti_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 Ti_2O dissolves as $2 Ti^+$ 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 Ti_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 $1000^\circ C$ 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 Ti_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 Ti_2O dissociates in solution to form **two** independent **Ti** ions. That is, the formula « Ti_2O » really represents **two** moles of **Ti** ions dissolved in the slag. That is, it is actually the component $TiO_{0.5}$ which follows **ideal solution behaviour**.

Ti₂O and HfO₂ in FACT-Slag – *Reactants*

The reactants are: 0.3333 CaO + 0.3333 SiO₂ + 0.3333 Al₂O₃ + 0.01 Ti₂O + 0.05 HfO₂

The system is an equimolar mixture of CaO, SiO₂ and Al₂O₃...

| Mass(mol) | Species | Phase | T(C) | P(total)** | Stream# | Data |
|-----------|---------|-------|------|------------|---------|------|
| 0.3333 | CaO | | | | 1 | |
| + 0.3333 | SiO2 | | | | 1 | |
| + 0.3333 | Al2O3 | | | | 1 | |
| + 0.01 | Ti2O | | | | 1 | |
| + 0.05 | HfO2 | | | | 1 | |

Initial Conditions

Next >>

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

...with Ti₂O and HfO₂ added as **dilute components**.

Ti₂O and HfO₂ 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

FACT-SLAG:-
90 SiO₂, 91 CaO, 92 Al₂O₃

Short description of the **FACT-Slag Solution Phase**. It does not contain **Ti₂O** nor **HfO₂**.

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

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

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

F Menu - Equilib

File Units Parameters Help

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

Reactants (5)

0.3333 CaO + 0.3333 SiO₂ + 0.3333 Al₂O₃ + 0.01 Ti₂O + 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

Legend

+ - selected

Show all selected

species: 3

solutions: 1

Clear

Custom Solutions

- fixed activities
- ideal solutions
- activity coefficients

Details ...

Pseudonyms

apply List ...

include molar volumes

Total Species (max 692) 21

Total Solutions (max 30) 1

Default

Final Conditions

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

10 steps Table 1 calculation

Equilibrium

- normal transitions
- predominant open

Calculate >>

FactSage 5.2

Creating an ideal Henrian solution of $\text{HfO}_2(\text{s})$

1° **Right-click** to open the $\text{HfO}_2(\text{s}2)$ extended menu

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

The screenshot shows the FactSage software interface with a table of species and phases. The table has columns for Code, Species, Data, Phase, T, V, and Code. The species $\text{HfO}_2(\text{s}2)$ is selected, and a mouse cursor is pointing at it. The interface also shows a 'Selected: 0/54' indicator and a 'SOLID' button.

| + Code | Species | Data | Phase | T | V | Code |
|--------|--|------|-----------------|---|---|------|
| 66 | $\text{CaSiO}_3(\text{s}2)$ | FACT | pseudowollas... | | V | |
| 67 | $\text{Ca}_2\text{SiO}_4(\text{s})$ | FACT | gamma(olivine) | | | |
| 68 | $\text{Ca}_2\text{SiO}_4(\text{s}2)$ | FACT | alpha-prime | | | |
| 69 | $\text{Ca}_2\text{SiO}_4(\text{s}3)$ | FACT | alpha | | | |
| 70 | $\text{Ca}_3\text{SiO}_5(\text{s})$ | FACT | hattrite | | o | |
| 71 | $\text{Ca}_3\text{Si}_2\text{O}_7(\text{s})$ | FACT | rankinite | | o | |
| 72 | $\text{CaAl}_2\text{SiO}_6(\text{s})$ | FACT | ca-tschermak | | V | |
| 73 | $\text{CaAl}_2\text{Si}_2\text{O}_8(\text{s})$ | FACT | hexagonal | | o | |
| 74 | $\text{CaAl}_2\text{Si}_2\text{O}_8(\text{s}2)$ | FACT | anorthite | | V | |
| 75 | $\text{Ca}_2\text{Al}_2\text{SiO}_7(\text{s})$ | FACT | gehlenite | | V | |
| 76 | $\text{Ca}_3\text{Al}_2\text{Si}_3\text{O}_{12}(\text{s})$ | FACT | grossular | | V | |
| 77 | $\text{Hf}(\text{s})$ | FACT | solid alpha | | | |
| 78 | $\text{Hf}(\text{s}2)$ | FACT | solid beta | | | |
| 79 | $\text{HfO}_2(\text{s})$ | FACT | solid-a | | | |
| 80 | $\text{HfO}_2(\text{s}2)$ | FACT | solid-b | | | |
| 81 | $(\text{CaO})(\text{HfO}_2)(\text{s})$ | FACT | solid | | o | |
| 82 | $\text{Ti}(\text{s})$ | FACT | solid-a | | | |
| 83 | $\text{Ti}(\text{s}2)$ | FACT | solid-b | | | |
| 84 | $\text{Ti}_2\text{O}(\text{s})$ | FACT | solid | | | |

The screenshot shows the context menu for $\text{HfO}_2(\text{s}2)$. The menu items are: 80 $\text{HfO}_2(\text{s}2)$, - clear, + - select, - standard stable phase, ! - dormant (metastable) phase, F - formation target phase, P - precipitate target phase, Ideal Solution, a Activity, and Help ... The 'Ideal Solution' option is selected, and a sub-menu is open showing 'Ideal Solution #1 ...', 'Ideal Solution #2 ...', 'Ideal Solution #3 ...', 'Ideal Solution #4 ...', 'Ideal Solution #5 ...', 'Ideal Solution #6 ...', 'Ideal Solution #7 ...', 'Ideal Solution #8 ...', 'Ideal Solution #9 ...', 'Ideal Solution #10 ...', and Clear.

Creating an ideal Henrian solution of $\text{HfO}_2(\text{s})$ – setting γ

3° Enter $\log_{10} [\gamma_{\text{HfO}_2(\text{s}2)}] = 1214.9/T(\text{K}) + 0$
in order that $\gamma = 9.0$ when $T = 1273.15\text{K}$ (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.

F 80 HfO2(s2) dissolved in Ideal Solution #1

80 HfO2(s2) - Henrian activity coefficient, gamma
 $\log_{10}(\text{gamma}) = A/TK + B$

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.

Cancel Help OK

Notes:

1. In general, if γ is known at only one temperature, it is better to assume that $RT \log \gamma = \text{constant}$ than to assume that $\log \gamma = \text{constant}$.
2. In this example note that γ is the activity coefficient relative to SOLID $\text{HfO}_2(\text{s}2)$ as standard state.

Adding $\text{Ti}_2\text{O}(\text{l})$ to the ideal solution

| + | 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 | |

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

7° Press OK to return in the Menu Window

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

Reactants (5)

0.3333 CaO + 0.3333 SiO2 + 0.3333 Al2O3 + 0.01 Ti2O + 0.05 HfO2

Products

Compound species

- gas ideal real 18
- aqueous 0
- pure liquids 0
- pure solids 1

suppress duplicates

* - custom selection

Species: 19

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

Clear

Final Conditions

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

10 steps Table

1 calculation

Equilibrium

- normal transitions
- predominant open

Calculate >>

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...

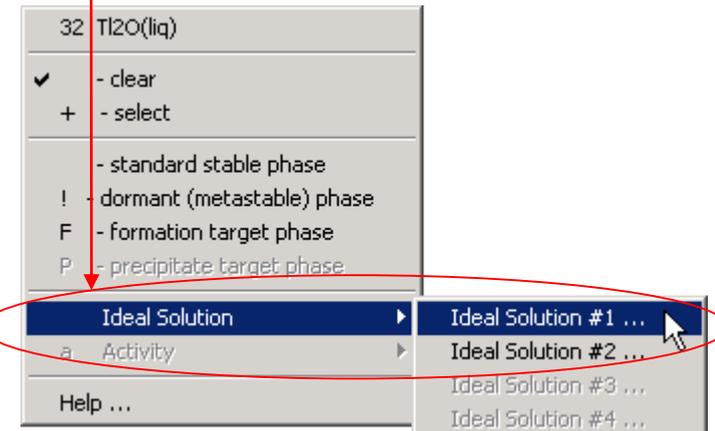
F T(C) = 200

File Edit Show Sort

Selected: 0/14

LIQUID

| + Code | Species | Data | Phase | T | V | Code |
|--------|--|------|--------|---|---|------|
| 19 | Al(liq) | FACT | liquid | | | |
| 20 | Al ₂ O ₃ (liq) | FACT | liquid | | | |
| 21 | Si(liq) | FACT | liquid | | | |
| 22 | SiO ₂ (liq) | FACT | liquid | | | |
| 23 | Ca(liq) | FACT | liquid | | | |
| 24 | CaO(liq) | FACT | liquid | | | |
| 25 | CaAl ₂ (liq) | FACT | liquid | | o | |
| 26 | CaAl ₄ (liq) | FACT | liquid | | o | |
| 27 | CaAl ₂ O ₄ (liq) | FACT | liquid | | | |
| 28 | CaAl ₄ O ₇ (liq) | FACT | liquid | | o | |
| 29 | Hf(liq) | FACT | liquid | | | |
| 30 | HfO ₂ (liq) | FACT | liquid | | | |
| 31 | Ti(liq) | FACT | liquid | | | |
| 32 | Ti ₂ O(liq) | FACT | liquid | | | |



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

F 32 Ti2O(liq) dissolved in Ideal Solution #1

32 Ti2O(liq) - Henrian activity coefficient, gamma
 $\log_{10}(\text{gamma}) = A/TK + B$

A = 0

B = 0

New mixing particles P = 2 (P > 0)

#1 Ideal Solution name: DiIOxide (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.

Cancel Help OK

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:

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

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 **S₂(liq)** dissolving in **Fe(liq)** as **S**:
P = 2.

In the present example **P = 2** because **Tl₂O** dissociates in the **slag** as:



Merging the ideal Henrian solution DiIOxide and FACT-Slag

An ideal Henrian solution (DiIOxide) of Ti_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 - DiIOxide**

F T(C) = 200

File Edit Show Sort

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 | Ti(liq) | FACT | liquid | | | |
| + | 32 #1h | Ti2O(liq) | FACT | liquid | | | |

Select All Select ... Clear **OK**

Solution FACT-SLAG

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

F Menu - Equilib

File Units Parameters Help

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

Reactants (5)

0.3333 CaO + 0.3333 SiO2 + 0.3333 Al2O3 + 0.01 Ti2O + 0.05 HfO2

Products

Compound species: 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

Pseudonyms: apply List ...

include molar volumes:

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

Final Conditions

| <A> | | T(C) | P(atm) | Product H(J) |
|-----|-----|------|--------|--------------|
| 10 | | 1000 | 1 | |

Equilibrium: normal, predominant, transitions

Calculate >>

FactSage 5.2

Calculation including a dilute solution: Ti_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,S04,P04,H2O/OH,CO3,F,Cl,I

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

Ideal Solution #1 - DiIOxide:-
 32 Ti2O(liq), 80 HfO2(s2)

Custom Solutions

Fixed Activity: 0 Species

Ideal Solution:
 #1 DiIOxide:-
 32: Ti2O(liq): $\log_{10}(\gamma) = (0/TK + 0)$, Particles = 2
 80: HfO2(s2): $\log_{10}(\gamma) = (1214.9/TK + 0)$

OK

F Menu - Equilib

File Units Parameters Help

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

Reactants (5)

0.3333 CaO + 0.3333 SiO2 + 0.3333 Al2O3 + 0.01 Ti2O + 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+DiIOxide |

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> | | 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 (**DiIOxide**) is merged into the existing **FACT-Slag** solution.

Tl₂O and HfO₂ in CaO-SiO₂-Al₂O₃ slag: Results (FACT format)

F Results

Output Edit

$$X_{\text{HfO}_2} = \frac{0.047174}{0.31446 + 0.31446 + (2 \times 0.31446) + (2 \times 0.0094349) + 0.047174} = 0.035632$$

```

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
              + 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
              (1000.00 C, 1 atm, L1, a=0.20315E-03)
    
```

...because Tl₂O dissociates into **two** Tl ions and also Al₂O₃ dissociates into **two** Al ions: **Al₂O₃ → 2 Al³⁺ + 3 O²⁻**

Note:

This information about Al₂O₃ is included in the FACT-SLAG database.

The calculated **activity** of HfO₂(s2) is:

$$a_{\text{HfO}_2} = \gamma_{\text{HfO}_2} X_{\text{HfO}_2} = (9.0)(0.035632) = 0.32070$$

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

Note:

If we increase γ_{HfO_2} , the calculated activity would increase until solid HfO₂(s) would be calculated to precipitate when its activity = 1.0. If the solubility of HfO₂ 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.

Tl₂O and HfO₂ in CaO-SiO₂-Al₂O₃ slag: Results (ChemSage format)

F Results

Output Ed



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

```

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

PHASE: gas_ideal
EQUIL AMOUNT      MOLE FRACTION      FUGACITY
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
MOLE FRACTION      ACTIVITY
mol
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      1.9199E-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
PHASE: Slag-liquid+DilOxide
ACTIVITY
mol
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 Tl₂O(liq) is:

$$a_{\text{Tl}_2\text{O}} = \gamma_{\text{Tl}_2\text{O}} X_{\text{Tl}_2\text{O}} = \gamma_{\text{Tl}_2\text{O}} (X_{\text{TlO}_{0.5}})^2$$

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

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 $\gamma_{\text{Tl}_2\text{O}}$ 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 Ti_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.

Reactants (2)

<1-A> NaCl + <A> KCl

Products

Compound species

- gas ideal real 0
- liquid 0
- aqueous 0
- solid 0
- suppress duplicates

Species: 0

Target

Estimate T(K): 1000

Mass(mol): 0

Final Conditions

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

10 steps Table 5 calculations

Equilibrium

- normal transitions
- predominant open

Calculate >>

FactSage 5.1

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

Edit a current pseudonym ▾

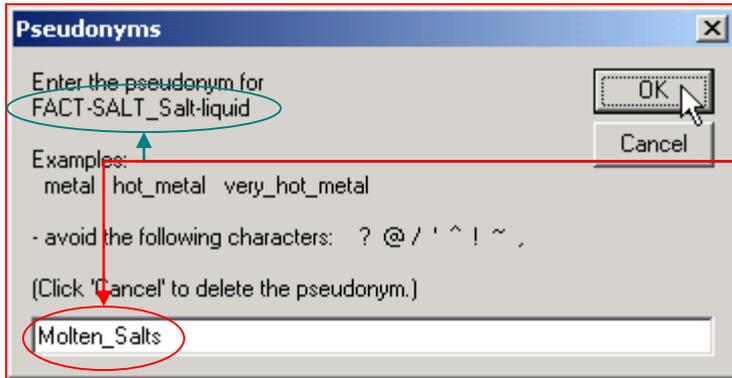
Add a new pseudonym ▾

Help ...

- FACT-SALT_Salt-liquid
- FACT-ACI_AlkCl-ss
- FACT-SeLQ_LiqAlloy

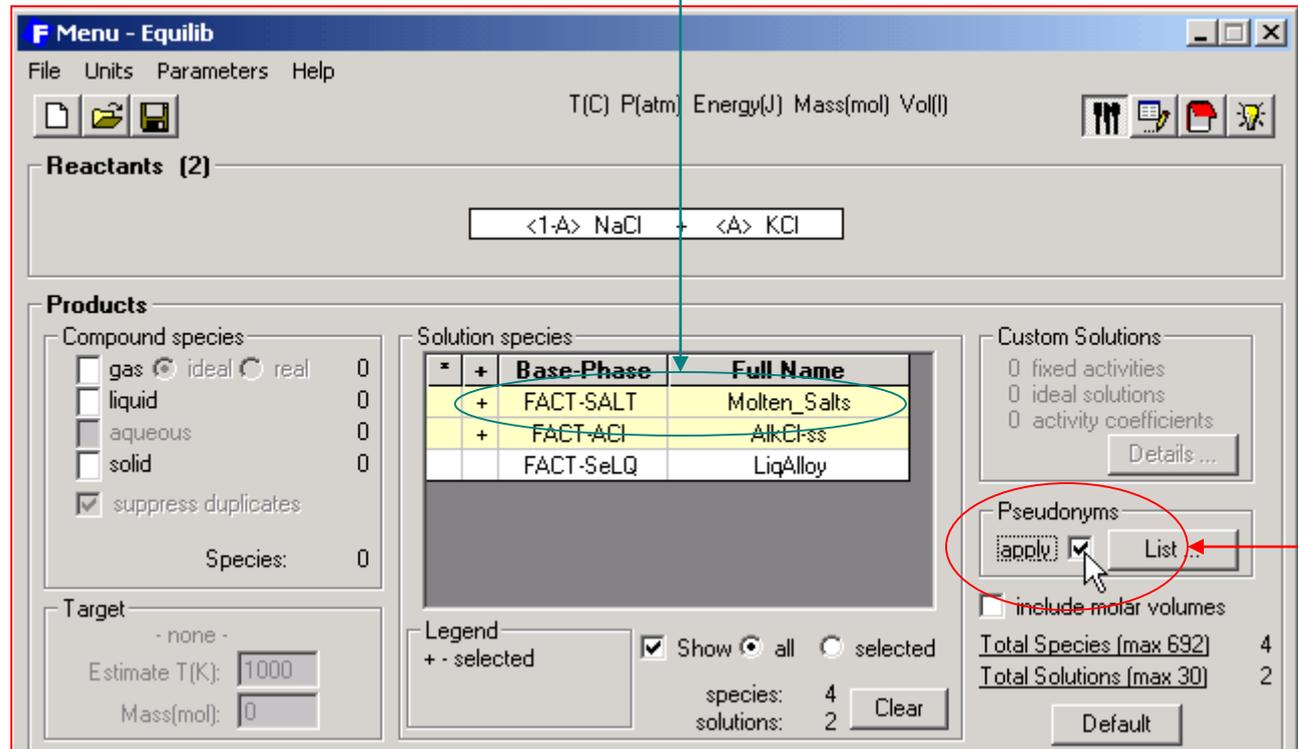
2° Select '**Edit...**' or '**Add...**' and then click on the **phase** to open the **Pseudonyms** dialog box.

Pseudonyms



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

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



Including **molar volume** data

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

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

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

Include molar volumes : graphite to diamond transition

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

1° Reactant: **C**

2° Possible products:
2 pure solids

- **Graphite**
- **Diamond**

3° T (K) = **1000 K**
P (atm) = **1×10^4 atm**,
 2×10^4 atm, ..., **1×10^5 atm**

The screenshot shows the 'Menu - Equilib' window. A red box on the right contains the text 'Include molar volumes check box is selected.' with an arrow pointing to the 'include molar volumes' checkbox in the 'Pseudonyms' section, which is checked. A blue box at the top left contains '1° Reactant: C' with an arrow pointing to the 'C' input field in the 'Reactants (1)' section. A red box in the middle left contains '2° Possible products: 2 pure solids' with an arrow pointing to the 'pure solids' option in the 'Compound species' list, which is selected with a '+' sign. A blue box at the bottom left contains '3° T (K) = 1000 K' and pressure values with an arrow pointing to the 'Estimate T(K): 1000' input field. The 'Final Conditions' table at the bottom is circled in blue. The 'Equilibrium' section at the bottom right has 'transitions' selected. The 'Calculate >>' button is visible.

| <A> | | T(K) | P(atm) | Product H(J) |
|-----|-----|------|--------------|--------------|
| | | 1000 | 1e4 10e4 1e4 | |

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.

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

Molar volume data are employed

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

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

C =
 1.0000 mol C_graphite (1000.00 K, 31488. atm, S1, a= 1.0000) V
 + 0.00000 mol C_diamond (1000.00 K, 31488. atm, S2, a= 1.0000) V

| H (J) | G (J) | V (l) | S (J/K) | Cp (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
 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 (J.K-1) | H_EQUIL (J) | S_EQUIL (J.K-1) | G_EQUIL (J) | V_EQUIL (dm3) |
|------------------|-------------|-----------------|-------------|---------------|
| 2.14886E+01 | 2.80832E+04 | 2.39695E+01 | 4.11377E+03 | 5.12697E-03 |

System density/g.cm-3 = 2.34271

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

C =
 1.0000 mol C_diamond (1000.00 K, 31488. atm, S2, a= 1.0000) V
 + 0.00000 mol C_graphite (1000.00 K, 31488. atm, S1, a=0.99999) V

| H (J) | G (J) | V (l) | S (J/K) | Cp (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
 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 (J.K-1) | H_EQUIL (J) | S_EQUIL (J.K-1) | G_EQUIL (J) | V_EQUIL (dm3) |
|------------------|-------------|-----------------|-------------|---------------|
| 2.09062E+01 | 2.39314E+04 | 1.98176E+01 | 4.11388E+03 | 3.42034E-03 |

System density/g.cm-3 = 3.51163

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.

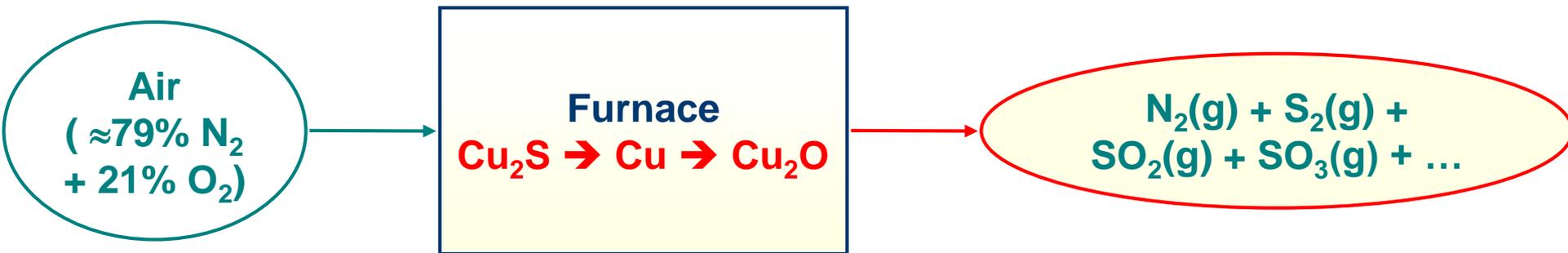
The following slide explains the **general procedure** in more detail. In sections [9.1](#) and [9.2](#) **two example applications** are shown.

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 **SO₂(g)** and **SO₃(g)** (or as **CO(g)** and **CO₂(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 **Cu₂S** converting eventually all the sulfur leaves the system and then **Cu₂O** starts to form unless the converting is stopped.

The following figures demonstrate **Cu₂S** desulphurisation by air in an **OPEN** process.



Desulphuring of Cu_2S

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

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

Desulphurisation of Cu_2S by air: setting the Reactants Window

The reactants are **one** mole of Cu_2S with a **variable amount** $\langle A \rangle$ moles of **air**.

| Mass(mol) | Species | Phase | T(C) | P(total)** | Stream# | Data |
|-------------------------|---------|--------------------|--------|------------|---------|------|
| 1 | Cu2S | solid-1 chalcocite | 298.15 | 1 | 1 | |
| $\langle 0.21A \rangle$ | O2 | gas | 298.15 | 1 | 1 | |
| $\langle 0.79A \rangle$ | N2 | gas | 298.15 | 1 | 1 | |

Initial Conditions

Next >>

FactSage 5.2 Compound: ELEM EXAM FACT SGPS SGSL Solution: FACT SGSL

In an **OPEN** system, $\langle A \rangle$ 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**, **$\text{Cu}_2\text{O}(\text{s})$**

FT(C) = 1473.15

File Edit Show Sort

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 | | | |

Select All Select ... Clear OK

F Menu - Equilib

File Units Parameters Help

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

Reactants [3]

$\text{Cu}_2\text{S} + <0.21\text{A}> \text{O}_2 + <0.79\text{A}> \text{N}_2$

Products

Compound species

- gas
- ideal
- real

30

aqueous 0

pure liquids 0

* pure solids 1

suppress duplicates

* - custom selection

Species: 31

Target

- none -

Estimate T(K): 1000

Mass(mol): 0

Legend

+- selected

Show all selected

species: 5

solutions: 2

Clear

Custom Solutions

- fixed activities
- ideal solutions
- activity coefficients

Details ...

Pseudonyms

apply List ...

include molar volumes

Total Species (max 692) 36

Total Solutions (max 30) 2

Default

Final Conditions

| <A> | | T(C) | P(atm) | Product H(J) |
|-----|-------|------|--------|--------------|
| 5 | | 1200 | 1 | |
| 10 | steps | | | |

Equilibrium

- normal
- predominant
- open

transitions

Calculate >>

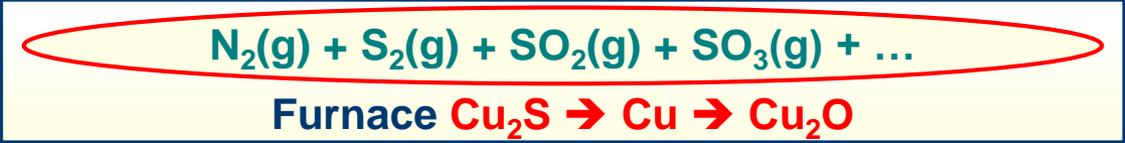
1 calculation

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
($\approx 79\% \text{ N}_2 + 21\% \text{ O}_2$)



Results - Equilib 1200 C

Output Edit Show Pages

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

```

Cu2S + <0.21A> O2 + <0.79A> N2 =
4.9501 mol ( 0.79796 N2
+ 0.20190 SO2)
(1200.00 C, 1 atm, gas_ideal)

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

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

+ 0.00000 mol Cu2O
(1200.00 C, 1 atm, 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 |

$P_{\text{SO}_2} = 0.2019$ 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**

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

Air
($\approx 79\% \text{N}_2 + 21\% \text{O}_2$)

Furnace
 $\text{Cu}_2\text{S} \rightarrow \text{Cu} \rightarrow \text{Cu}_2\text{O}$

$\text{N}_2(\text{g}) + \text{S}_2(\text{g}) + \text{SO}_2(\text{g}) + \text{SO}_3(\text{g}) + \dots$

The screenshot shows the FactSage Equilib software interface. The 'Reactants' section contains the input: $\text{Cu}_2\text{S} + \langle 0.21A \rangle \text{O}_2 + \langle 0.79A \rangle \text{N}_2$. The 'Products' section shows a list of compound species with 'gas' selected as the ideal phase. The 'Solution species' table is as follows:

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

The 'Final Conditions' section is highlighted with a red box and contains the following values:

| <A> | | T(C) | P(atm) | Product H(J) |
|-----|-------|------|--------|--------------|
| 0.1 | | 1200 | 1 | |
| 50 | steps | | | |

The 'Equilibrium' section at the bottom right has the 'open' radio button selected. A red box highlights the '50 calculations' input field. A red arrow points from the '50' in the 'Final Conditions' table to the '50 calculations' field.

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 ($\approx 79\% \text{ N}_2$
+ $21\% \text{ O}_2$)



$\text{N}_2(\text{g}) + \text{S}_2(\text{g}) + \text{SO}_2(\text{g}) +$
 $\text{SO}_3(\text{g}) + \dots$

F Results - Equilib Step 50 (page 50/50)

Output Edit Show Pages

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

Step 38 | Step 39 | Step 40 | Step 41 | Step 42 | Step 43 | Step 44 | Step 45 | Step 46 | Step 47 | Step 48 | Step 49
Step 26 | Step 27 | Step 28 | Step 29 | Step 30 | Step 31 | Step 32 | Step 33 | Step 34 | Step 35 | Step 36 | Step 37
Step 50

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

Total <A> = 5.0000

| | | | |
|-----------------|---|-------------|--|
| 0.79037E-01 mol | (| 0.99952 | N2 |
| | + | 0.39905E-03 | SO2 |
| | + | 0.53085E-04 | O2 |
| | + | 0.20787E-04 | NO |
| | + | 0.49238E-05 | Cu |
| | + | 0.12596E-06 | SO3 |
| | + | 0.20251E-07 | O |
| | + | 0.12280E-07 | SO |
| | + | 0.76342E-08 | CuO |
| | + | 0.18439E-08 | NO2 |
| | + | 0.15527E-08 | Cu2 |
| | + | 0.12770E-08 | N2O |
| | | | (1200.00 C, 1 atm, gas_ideal) |
| + 2.1004 mol | (| 0.95217 | Cu |
| | + | 0.24057E-06 | S |
| | + | 0.47829E-01 | O) |
| | | | (1200.00 C, 1 atm, Cu-liq) |
| + 0.00000 mol | (| 0.18913 | S |
| | + | 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 **Cu₂S**

$P_{\text{SO}_2} = 3.9905 \times 10^{-4}$ atm in **0.079037** mol of gas (mainly **N₂**)

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

Deleading of a copper melt

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

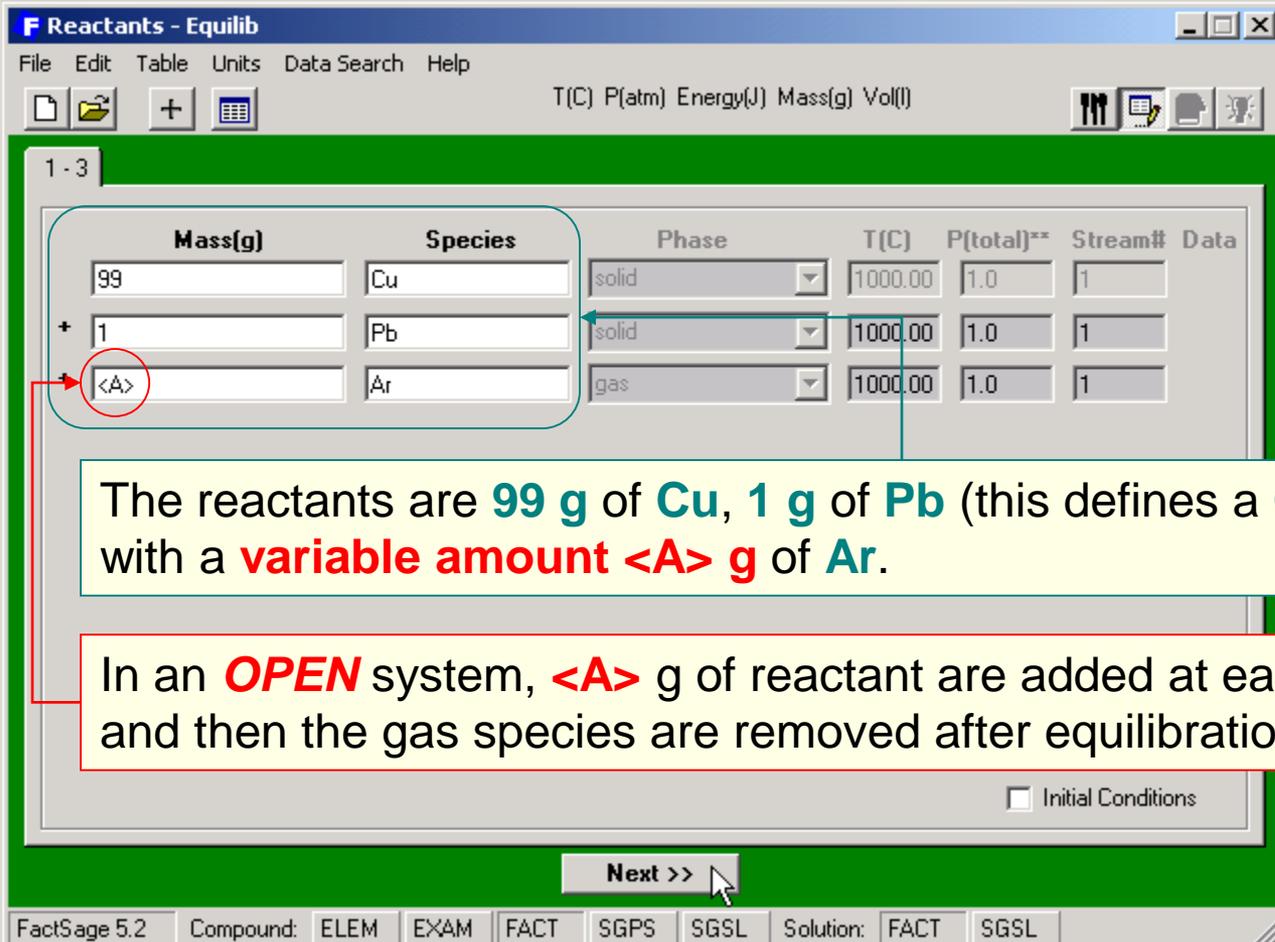
The following six slides show how the Open command can be employed to simulate the process.

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

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

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

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



The screenshot shows the 'Reactants - Equilib' window in FactSage 5.2. The interface includes a menu bar (File, Edit, Table, Units, Data Search, Help) and a toolbar with icons for file operations and calculation. The main area displays a table of reactants with columns for Mass(g), Species, Phase, T(C), P(total)**, and Stream#. The table contains three rows: Cu (99g, solid, 1000.00°C, 1.0 atm, Stream 1), Pb (1g, solid, 1000.00°C, 1.0 atm, Stream 1), and Ar (<A>g, gas, 1000.00°C, 1.0 atm, Stream 1). A red circle highlights the '<A>' input field for Ar, with a red arrow pointing to it. A yellow callout box explains that the reactants are 99 g of Cu, 1 g of Pb, and a variable amount <A> g of Ar. Another yellow callout box explains that in an OPEN system, <A> g of reactant are added at each step and then the gas species are removed after equilibration. The 'Next >>' button is visible at the bottom of the window.

| 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 | |

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**

Menu - Equilib

File Units Parameters Help

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

Target

- none -

Estimate T(K): 1000

Mass(g): 0

Solution species

| | Base-Phase | Full Name |
|-------------------------------------|------------|-----------|
| <input type="checkbox"/> | FACT-PbLQ | Pb-liq |
| <input checked="" type="checkbox"/> | FACT-CuLQ | Cu-liq |

Legend

+ - selected

Show all selected

species: 2

solutions: 1

Clear

Custom Solutions

- fixed activities
- ideal solutions
- activity coefficients

Details ...

Pseudonyms

apply List ...

include molar volumes

Total Species (max 692) 7

Total Solutions (max 30) 1

Default

Final Conditions

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

10 steps Table

Equilibrium

- normal
- predominant
- transitions
- open

1 calculation

Calculate >>

FactSage 5.2

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

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

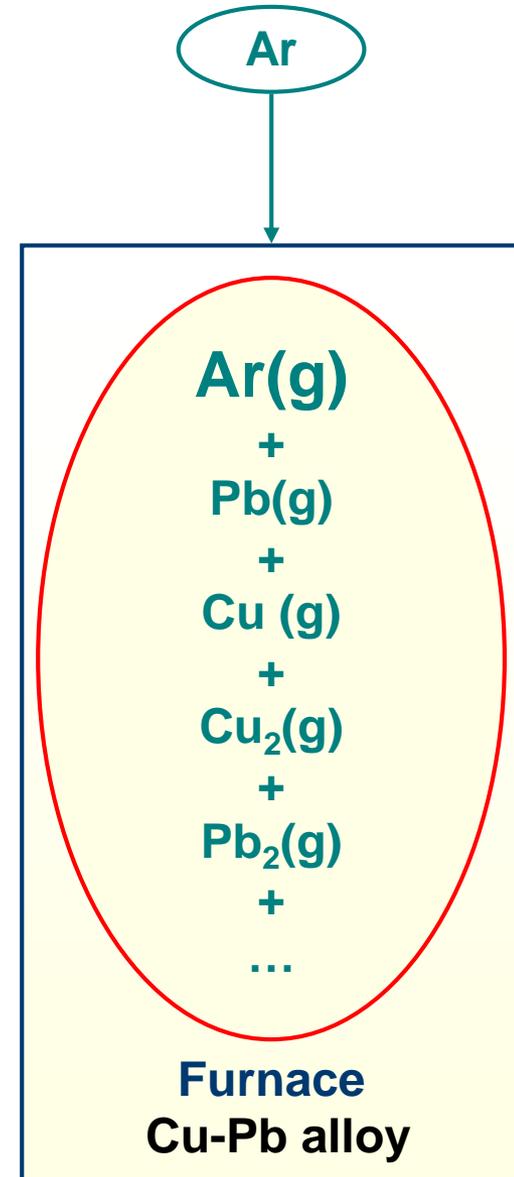
The concentration of **Pb** in **Cu(liq)** is 5.5876×10^{-2} wt.%

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

The screenshot shows the 'Results - Equilib 1200 C' window. The output is as follows:

```
(gram) 99 Cu + Pb + <A> Ar =
30970. litre ( 97.709 vol% Ar
+ 1.7796 vol% Pb
+ 0.51146 vol% Cu
+ 0.16754E-03 vol% Cu2
+ 0.59891E-06 vol% Pb2)
(1200.00 C,0.10000E-02 atm, gas_ideal)
+ 98.972 gram ( 0.55876E-01 wt.% Pb
+ 99.944 wt.% Cu)
(1200.00 C,0.10000E-02 atm, Cu-liq)
where "A" on the reactant side is 10.00
*****
H G V S Cp
(J) (J) (l) (J/K) (J/K)
*****
7.94952E+04 -2.11846E+05 3.09698E+04 1.97768E+02 5.41842E+01
```

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



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

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

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

The screenshot shows the FactSage Equilib software interface. The window title is "F Menu - Equilib". The menu bar includes "File", "Units", "Parameters", and "Help". The main area is divided into several sections:

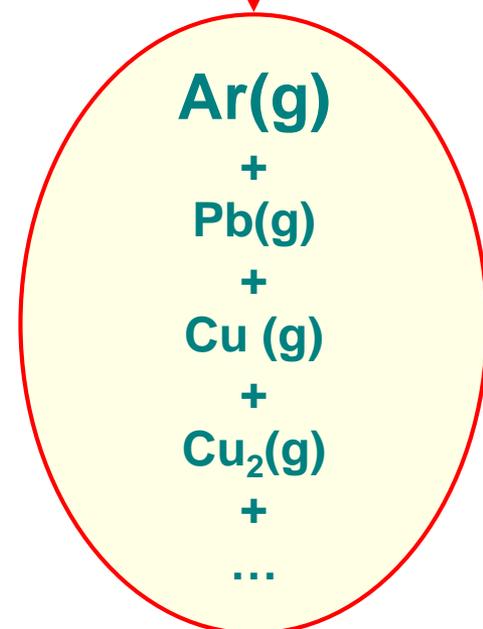
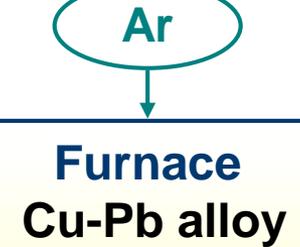
- Reactants (3):** A text box contains "(gram) 99 Cu + Pb + <A> Ar".
- Products:** Includes "Compound species" (gas, ideal, real, aqueous, pure liquids, pure solids, suppress duplicates) and "Solution species" (FACT-PbLQ, FACT-CuLQ).
- Target:** Estimate T(K): 1000, Mass(g): 0.
- Final Conditions:** A table with columns <A>, , T(C), P(atm), and Product H(J). The <A> column has "0.1" and "100 steps" below it. The T(C) column has "1200". The P(atm) column has "0.001". The Product H(J) column has a dropdown menu. A "100 calculations" box is highlighted with a red circle.
- Equilibrium:** Radio buttons for "normal", "predominant", and "open". The "open" option is selected and circled in blue. A "Calculate >>" button is also highlighted with a red circle.

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

```
Results - Equilib Step 100 (page 100/100)
Output Edit Show Pages
T(C) P(atm) Energy(J) Mass(g) Vol(l)
Step 87 Step 88 Step 89 Step 90 Step 91 Step 92 Step 93 Step 94 Step 95 Step 96 Step 97
Step 76 Step 77 Step 78 Step 79 Step 80 Step 81 Step 82 Step 83 Step 84 Step 85 Step 86
Step 98 Step 99 Step 100
(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(lig) is 1.4221×10^{-7} wt.%

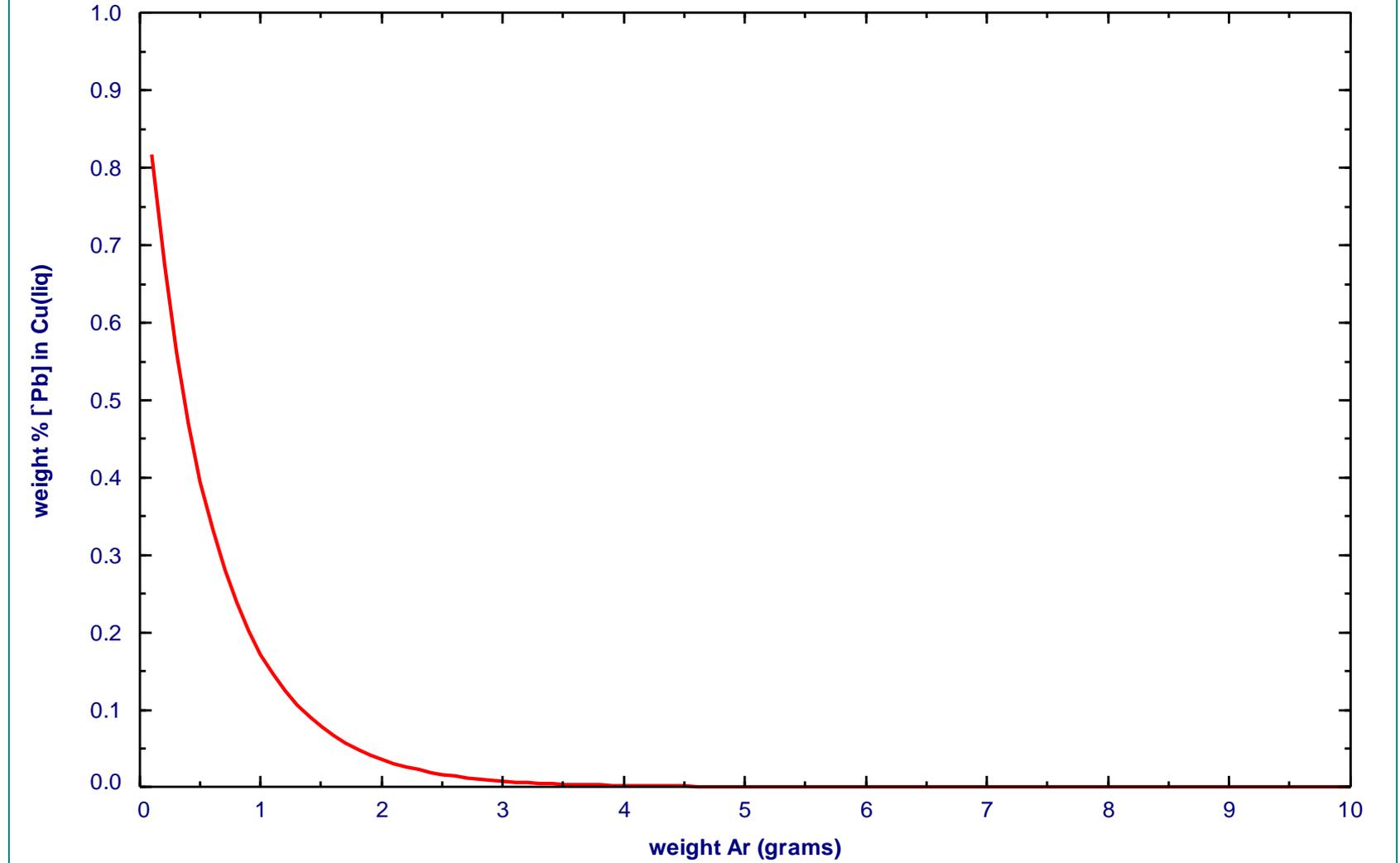
in equilibrium with 304.16 l of gas, mainly Ar.

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

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

Deleading of Cu-1wt.%Pb by Argon Vacuum Refining

Example of «Open» Equilibrium Calculation: $T=1200^{\circ}\text{C}$ and $P=0.001\text{ atm}$.



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

The screenshot shows the 'Parameters - Equilib' window with several sections highlighted by callout boxes:

- Dimensions frame:** A table with columns 'Description', 'Used', and 'Max'.

| 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 compressibility data: | | 740 |
- Target Limits frame:** Input fields for T(K), P(bar), V(l), and Alpha, with min. and max. values. A 'Default' button is also present.
- Dilute extrapolation frame:** A 'Parameter' input field set to 1.0e+6.
- Print Cut-off frame:** A 'Lower limit' input field set to 1.0E-70.
- Output Mass Units frame:** Radio buttons for 'mole', 'g', 'lb', and 'default' (selected).
- Predominant Species frame:** Input fields for 'gases (50 - 300):' and 'solids + liqs (50 - 300):', both set to 100. A 'log file' checkbox is also present.
- Stop/Kill Window frame:** A 'yes' checkbox and a 'refresh' input field set to 2 seconds.

Buttons for 'Help' and 'OK' are located at the bottom of the window.

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.

| 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 compressibility 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.

| | 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 |

Default

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

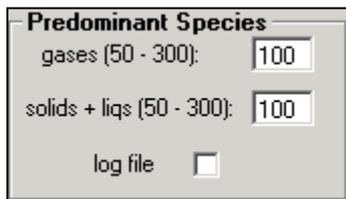
Stop and Kill Button

- 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.

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

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, **Cu₄₂Fe₂₅S₃₃**.

Likewise **0.79 N₂ + 0.21 O₂** can become **N_{1.58}O_{0.42}**.

<A> is a **variable** corresponding to the number of moles of **air**, **** is a **constant** amount of **SiO₂** defined in the **Menu Window**.

Note: N1.5800.42

Make sure you do not mix up the letter «**O**» and the integer «**0**».

The screenshot shows the 'Reactants - Equilib' window with a table of reactants. The units are T(C), P(atm), Energy(J), Mass(mol), and Vol(l). The table lists 6 reactants: Cu, Fe, S, N2, O2, and SiO2. The mass values are 42, 25, 33, <79A>, <21A>, and respectively.

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

The screenshot shows the 'Reactants - Equilib' window with a table of reactants. The units are T(C), P(total)***, Stream#, and Data. The table lists 3 reactants: Cu42Fe25S33, N1.5800.42, and SiO2. The mass values are 1, <A>, and respectively. The temperature is 11580.42 and the pressure is 1000.00.

| Mass(mol) | Species | Phase | T(C) | P(total)** | Stream# | Data |
|-----------|-------------|-------------------|----------|------------|---------|------|
| 1 | Cu42Fe25S33 | | | | | none |
| <A> | N1.5800.42 | | 11580.42 | | | none |
| | SiO2 | solid-1 quartz(l) | 1000.00 | 1.0 | 1 | |

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.

| Mass(mol) | Species | Phase | T(C) | P(total)** | Stream# |
|-----------|-------------|-------------------|---------|------------|---------|
| 1 | Cu42Fe25533 | | | | |
| <A> | N1.5800.42 | | | | |
| | SiO2 | solid-1 quartz(l) | 1000.00 | 1.0 | 1 |

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**

Cu42Fe25533: 1 mol = 5123.29 g = 11.2949 lb

- Convert this reactant amount to
 - mol
 - g**
 - lb
- Convert ALL reactant amounts to
- Set all reactant masses to 1
- Help ...

Mixing reactant mass units of mol g and lb

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

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

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

The screenshot shows the 'Reactants - Equilib' window with a table of reactants. The 'Mass(mol)' column contains '5123.285 g', '<A>', and ''. The 'Species' column contains 'Cu42Fe25S33', 'N1.5800.42', and 'SiO2'. The 'Phase' column contains '- no data -', '- no data -', and 'solid-1 quartz(l)'. The 'T(C)' column contains 'T', 'T', and '1000'.

| Mass(mol) | Species | Phase | T(C) |
|------------|-------------|-------------------|------|
| 5123.285 g | Cu42Fe25S33 | - no data - | T |
| + <A> | N1.5800.42 | - no data - | T |
| + | SiO2 | solid-1 quartz(l) | 1000 |

The screenshot shows the 'Reactants - Equilib' window with a table of reactants. The 'Mass(mol)' column contains '5123.285 g', '<A> mol', and ' mol'. The 'Species' column contains 'Cu42Fe25S33', 'N1.5800.42', and 'SiO2'. The 'Phase' column contains '- no data -', '- no data -', and 'solid-1 quartz(l)'. The 'T(C)' column contains 'T', 'T', and '1000'.

| Mass(mol) | Species | Phase | T(C) |
|------------|-------------|-------------------|------|
| 5123.285 g | Cu42Fe25S33 | - no data - | T |
| + <A> mol | N1.5800.42 | - no data - | T |
| + mol | SiO2 | solid-1 quartz(l) | 1000 |

Note:

When creating a composite species (for example $\text{Cu}_{42}\text{Fe}_{25}\text{S}_{33}$ and $\text{N}_{1.58}\text{O}_{0.42}$)

- 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 - $\text{CaCl}_2\text{-NaCl-KCl-MgCl}_2$

This example:

- **creates** and **saves** an equilibrated stream - $\text{CaCl}_2\text{-NaCl-KCl-MgCl}_2$ at 750°C .
- **imports** the stream into a new reaction
- **performs** various isothermal and adiabatic heat balances using the imported stream

The screenshot shows the FactSage Equilib software interface. The main window is titled "Reactants - Equilib" and contains a table of reactants. A secondary window, "Menu - Equilib", shows the product list and final conditions. Red boxes and arrows highlight specific elements: the units T(°C), P(atm), and Mass(g); the reactant table; the product table entry for FACT-SALT; and the final conditions table.

| Mass(g) | Species | Phase | T(C) | P(total)** | Stream# |
|---------|---------|--------------------------|---------|------------|---------|
| 40 | CaCl2 | solid | 1000.00 | 1.0 | 1 |
| 40 | NaCl | solid halite (rock salt) | 1000.00 | 1.0 | 1 |
| 5 | KCl | solid sylvite (nac_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

| Base-Phase | Full Name |
|------------|-----------------|
| FACT-SALT | Salt-liquid |
| FACT-ACI | AlkClss |
| FACT-PRVK | AMX3-Perovskite |
| FACT-AMX4 | Alk2MX4 |
| FACT-MCIL | MCI2-LT |
| FACT-SAL2 | RareEarth |
| FACT-SeLQ | LiqAlloy |

| <A> | | T(C) | P(atm) | Product H(J) |
|-----|-------|------|--------|---------------|
| 10 | steps | 750 | 1 | 1 calculation |

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

Output Edit Show Pages

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

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

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

Cl 1.0000

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

-5.78317E+05 -8.25636E+05 0.00000E+00 2.41724E+02 1.00273E+02

Equilibrated molten salt

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

Enter the stream file number (1 - 9999)

OK Cancel

12

Save File

Saving file 12

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

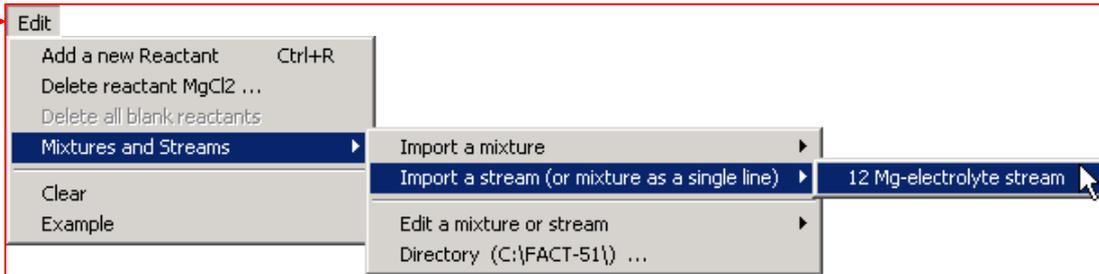
OK Cancel

Mg-electrolyte

Output

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

Importing the stream into a reaction



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

There are now **2 reactants**:
<A> **MgCl₂(s,25°C)** +
95 [Mg-electrolyte]
(stream,750°C)
i.e. <A + 95> grams total.

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.

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

Weight %:
1.0000E+02 Total
4.2105E+01 NaCl
5.2632E+00 KCl
1.0526E+01 MgCl2
4.2105E+01 CaCl2

Initial Conditions

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)

Equilibrated <0> and <5> $\text{MgCl}_2 + 95\text{g}$ [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:

Calculated $\Delta H = 4415\text{ J}$ – this is the total energy required to heat 5 g MgCl_2 from 25 to 750°C and dissolve it into the molten salt.

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

Output Edit Show Pages

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

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

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

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

where "A" on the reactant side is 0.0000
```

| DELTA H (J) | DELTA G (J) | DELTA V (l) | DELTA S (J/K) | DELTA Cp (J/K) | PROD V (l) |
|-------------|-------------|-------------|---------------|----------------|-------------|
| 0.00000E+00 | 0.00000E+00 | 0.00000E+00 | 0.00000E+00 | 0.00000E+00 | 0.00000E+00 |

A = 0

Calculated $\Delta H = 0$ – imported and equilibrated streams are the same.

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

Output Edit Show Pages

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

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

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

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

where "A" on the reactant side is 5.0000
```

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

A = 5

Adiabatic <5> MgCl₂ (solid, 25°C) + 95 g [Mg-electrolyte] stream

Menu - Equilib

File Units Parameters Help

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

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

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

Final Conditions

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

10 steps Table 1 calculation

FactSage 5.2 (Update 04Apr03)

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

Results - Equilib 708.12 C

Output Edit Show Pages

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

```
(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, 1atm, Salt-liquid)
Mole fraction of sublattice constituents in Salt-liquid:
Na 0.53915
K 0.52832E-01
Mg 0.12410
Ca 0.28391
-----
Cl 1.0000

where "A" on the reactant side is 5.000

*****
DELTA H DELTA G DELTA V DELTA S DELTA Cp PROD V
(J) (J) (1) (J/K) (J/K) (1)
*****
0.00000E+00 3.03145E+03 0.00000E+00 3.95072E+00 1.53938E+00 0.00000E+00
```

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

Adiabatic <A> MgCl₂ (solid, 25°C)+ 95 g [Mg-electrolyte] stream at 725°C

Menu - Equilib

File Units Parameters Help

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

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

Target

- none -

Estimate ALPHA: 0.5

Mass(g): 0

Solution species

| + | Base-Phase | Full Name |
|---|------------|-----------------|
| + | FACT-SALT | Salt-liquid |
| | FACT-ACI | AlkCl-ss |
| | FACT-PRVK | AMX3-Perovskite |
| | FACT-AMX4 | Alk2MX4 |
| | FACT-MCIL | MCI2-LT |
| | FACT-SAL2 | RareEarth |
| | FACT-SeLQ | LiqAlloy |

Legend

+ - selected

Show all selected

species: 4

solutions: 1

Clear

Custom Solutions

- fixed activities
- ideal solutions
- activity coefficients

Details ...

Pseudonyms

apply List ...

include molar volumes

Total Species [max 692] 4

Total Solutions [max 30] 1

Default

Equilibrium

- normal transitions
- predominant open

Calculate >>

Final Conditions

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

10 steps Table 1 calculation

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**.

The output shows:

Results - Equilib Abort

Output Edit Show Pages

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

(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

Adiabatic <100A> MgCl₂ (solid, 25°C)+ 95 g [Mg-electrolyte] stream at 725°C

Reactants - Equilib

File Edit Table Units Data Search Help

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

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

Equilib

Parameters Help

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

(2)

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

Compound species

- gas ideal real 0
- aqueous 0
- pure liquids 0
- pure solids 0
- suppress duplicates

Species: 0

Target: - none -

Estimate ALPHA: 0.5

Mass(g): 0

Final Conditions

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

10 steps Table 1 calculation

Equilibrium

- normal transitions
- predominant open

Calculate >>

This is resolved by entering <100A> MgCl₂ in the **Reactants Window**. Do not forget to check the **Initial Conditions** box.

Results - Equilib 725 C

Output Edit Show Pages

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

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

The calculation now gives <A> = 0.02939, i.e. 100 x 0.02939 = 2.939 g MgCl₂(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**.

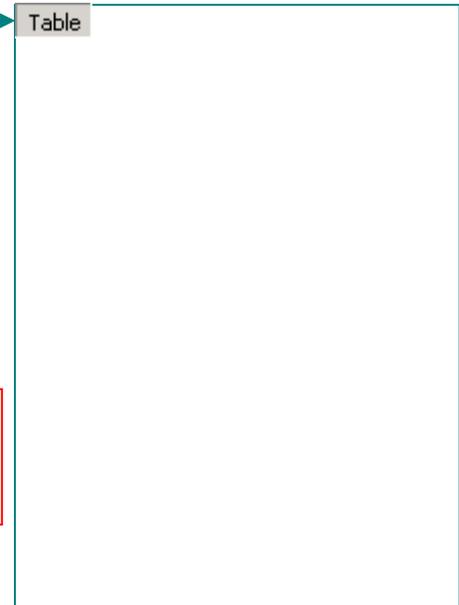
The **Page number** can also be used as an **axis variable** in the **Result module**.

Reaction Table

In the **Reactants Window** you specify a set of reactant amounts, for example: 1 mol CH₄ + 2 mol C₂H₆ + 3 mol O₂:

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.

The screenshot shows the 'Reactants - Equilib' window. The 'Table' menu is open, and the 'Close Table' option is highlighted with a red circle. The 'Reaction Table' contains the following data:

| 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 |

The 'Next >>' button is circled in red at the bottom of the window.

The 'Close Table' menu is shown, with the 'Close Table' option highlighted in blue and circled in red. The menu items are:

- Reaction Table (Ctrl+T)
- Help ...
- Add New Row 4 (Ctrl+A)
- Add Many New Row 4 ...
- Insert New Row 1 (Ctrl+I)
- Duplicate Row 1 (Ctrl+Y)
- Many Duplicates of Row 1 ...
- Delete Row 1
- Delete Rows 1 to ...
- Clear Table
- Save Table ...
- Import Table ...
- Sort Table
- Close Table**

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

Reaction Table – Results Window

Menu - Equilib

File Units Parameters Help

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

Reactants (3)

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

Products

Compound species
 gas ideal real 38
 aqueous 0
 pure liquids 0
 pure solids 5
 suppress duplicates
Species: 43

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

Final Conditions

| <A> | | T(C) | P(atm) | Delta H(J) |
|-----|-------|---------|---------|------------|
| 10 | steps | <table> | <table> | <table> |

Table 3 calculations

Equilibrium
 normal
 predomina

Calculate

Results - Equilib -3- (page 3/3)

Output Edit Show Pages

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

Total Species: 1
Total Solution: -1- -2- -3-

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

| mol | | | | |
|--------|--|-------------|--|--------|
| 15.500 | | 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)          (J)       (J/K)     (J/K)      (1)
*****
-3.49234E+06 -4.19336E+06 -6.41581E+02 2.29906E+02 1.46724E+02 8.73262E+02
*****
```

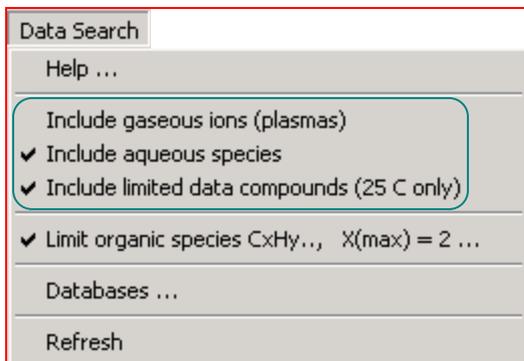
After the **Reaction Table** has been created **click** on the **Table** check box in the **Menu Window** to activate it in the calculation.

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.

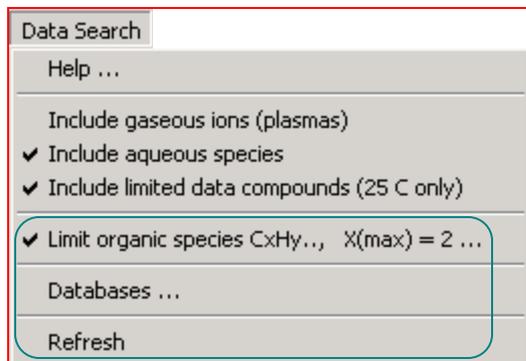
- **Include aqueous species:**

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.

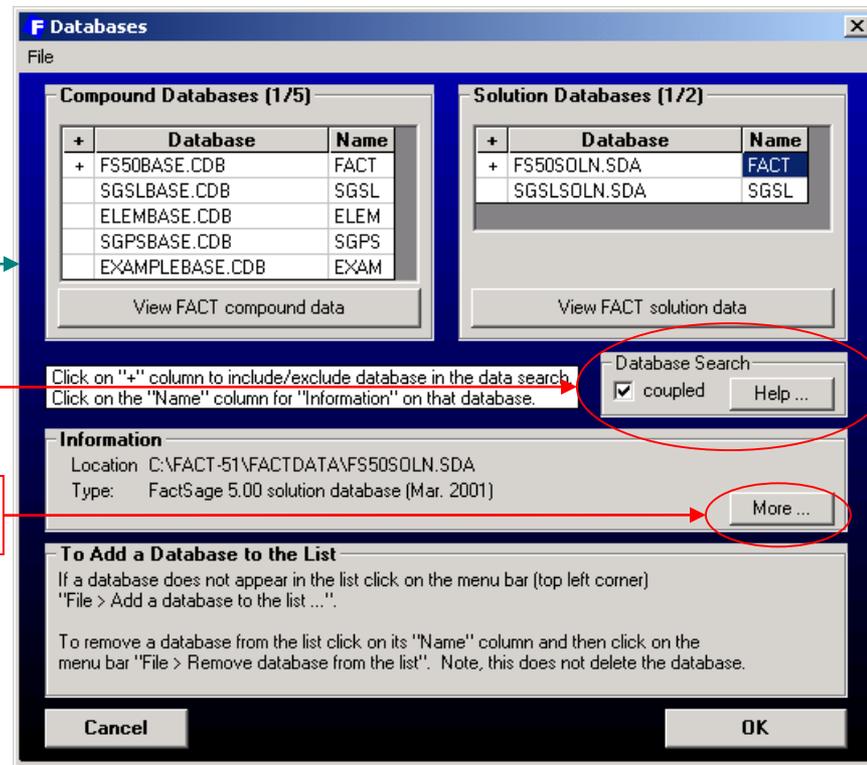
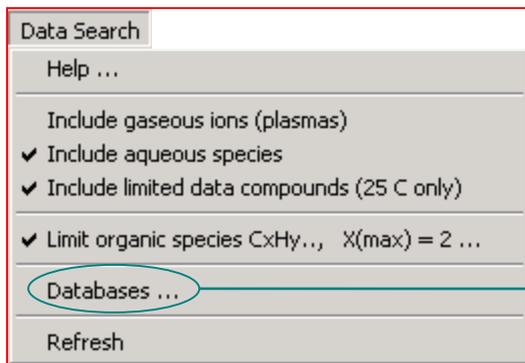
Databases may be added to or removed from the data search. For example private data entered through the Compound and Solution programs, or other commercial databases such as Thermo-Tech. If you have both FACT and SGTE databases then you use this option to tell the program to search both databases or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



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 recommended since it can lead to misleading results.

Equilib Cooling Calculations

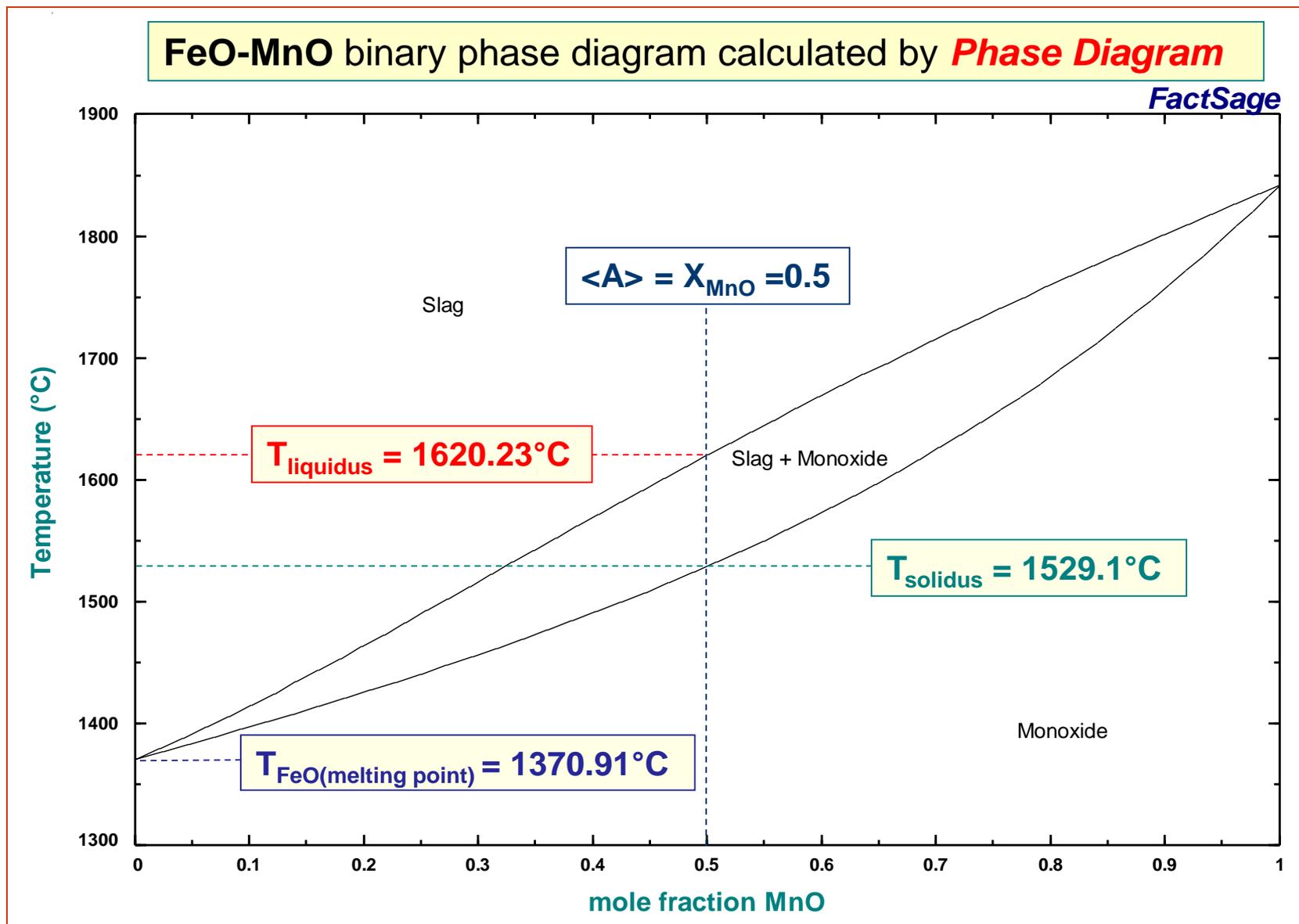
The **Equilib** module enables you to perform cooling calculations and display the phase transitions and compositions during

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

Cooling Calculations - Table of Contents

| | |
|-----------------------|--|
| Section 13.1 | <u>Table of Contents</u> |
| Section 13.2 | <u>Phase transitions : FeO-MnO</u> |
| Section 13.2.4 | <u>Simple equilibrium cooling : FeO-MnO</u> |
| Section 13.3 | <u>Simple Scheil-Gulliver cooling : FeO-MnO</u> |
| Section 13.3.6 | <u>Scheil-Gulliver cooling with back diffusion</u> |
| Section 13.4 | <u>Equilibrium cooling, plots: Al-Mg-Zn</u> |
| Section 13.5 | <u>Scheil-Gulliver cooling</u> |
| Section 13.6 | <u>Fully annealing alloy Al-Mg-Zn-Mn</u> |

FeO-MnO : Phase transitions - binary phase diagram



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

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

fixed activities

ideal solutions

activity coefficients

Details ...

Pseudonyms

apply List ...

include molar volumes

Total Species (max 1500) 5

Total Solutions (max 40) 2

Default

Transitions - temperature

Number of transitions: All

Legend

+ - selected 2

Show all selected

species: 5

solutions: 2

Select

Final Conditions

| <A> | | 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 $X_{\text{FeO}} = 0.5$ for temperatures varying from **1500°C** to **1700°C** and will search for **All** phase **transitions**.

FeO-MnO : Phase transitions showing liquidus and solidus

F Results - Equilib 1620.23 C (page 3/4)

Output Edit Show Pages

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

1500 C | 1529.11 C | **1620.23 C** | 1700 C

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

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

Equilibrium liquidus

```
+ 0.00000 mol Monoxide
(1620.23 C, 1 atm, a=1.0000)
( 0.30796 FeO
+ 0.69204 MnO)
```

where "A" on the reactant side is 0.50000

The cutoff concentration has been specified to 1.0000E-75

```
*****
H          G          V
(J)        (J)        (litre)
*****
-1.91102E+05 -5.49403E+05 0.00000E+00
```

F Results - Equilib 1529.11 C (page 2/4)

Output Edit Show Pages

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

1500 C | **1529.11 C** | 1620.23 C | 1700 C

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

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

Equilibrium solidus

```
+ 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 equilibrium 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 ...

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

2° Cooling Calculation Window

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

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

Equilibrium Cooling of **SLAG**

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

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

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

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

Menu - Equilib:

File Units Parameters Help

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

<1-A> MnO + <A> FeO

Solution species

| * | + | Base-Phase |
|---|---|-------------|
| | | FTdemo-TiSF |
| | + | FTdemo-MON |
| | L | FTdemo-SLAg |
| | | FTdemo-SPLI |
| | | FTdemo-MeO |
| | | FTdemo-FeL |
| | | FTdemo-CuL |

Legend

L - Equilibrium cooling
+ - selected T

Equilibrium cooling
FTdemo-SLAg

Cooling step : 10 T-auto:

Mass(mol): 0

Final Conditions

| <A> | | T(C) | P(atm) | Product H(J) |
|-----|-------|------|--------|--------------|
| 0.5 | | 1650 | 1 | |
| 10 | steps | | | |

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

Equilibrium

normal normal + transitions
 transitions only
 open
 para edit

Calculate >>

FeO-MnO : Equilibrium cooling – Summary and Transitions

Results - Equilib Summary (page-1/13)

Output Edit Show Pages

Summary (mol) Vol(litre)

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

CONSTITUENTS AND PHASES AT 1529.11 C
(temperature of final disappearance of Slag-liquid)

| CONS. PHASE | TOTAL AMT/mol |
|--------------|---------------|
| 1 1 Monoxide | 2.0000E+00 |

('Double-Click' on any phase listed above to view details)

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 1529.11 C
(temperature of final disappearance of Slag-liquid)

| Constituent 1 | 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 | 2.0000E+00 | 7.1391E+01 |

Results - Equilib Transitions (page 0/13)

Output Edit Show Pages

Transitions Vol(litre)

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

Temperature of transition -> 1620.23 C

EQUILIBRIUM COMPOSITION OF PHASES
Slag-liquid

| | MOLE FRACTION | MASS FRACTION |
|---------------|---------------|---------------|
| Fe | 2.5000E-01 | 3.9112E-01 |
| Mn | 2.5000E-01 | 3.8477E-01 |
| O | 5.0000E-01 | 2.2411E-01 |
| TOTAL AMT/mol | 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 | 2.0000E+00 | 7.1391E+01 |

AVERAGE COMPOSITION OF ALL PRODUCT PHASES TAKEN TOGETHER

| | MOLE FRACTION | MASS FRACTION |
|----|---------------|---------------|
| Fe | 2.5000E-01 | 3.9112E-01 |
| Mn | 2.5000E-01 | 3.8477E-01 |
| O | 5.0000E-01 | 2.2411E-01 |

FeO-MnO : Equilibrium cooling - Liquidus and Solidus

Results - Equilib 1620.23 C (page 2/13)

Output Edit Show Pages

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

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

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

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

System component Mole fraction
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 fraction
Fe 0.15398
Mn 0.34602
O 0.50000

where "A" on the reactant side is 0.50000

Liquidus

Results - Equilib 1529.11 C (page 13/13)

Output Edit Show Pages

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

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

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

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

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

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

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

where "A" on the reactant side is 0.50000

Solidus

Scheil target phase

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

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

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

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

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

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

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

F 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

| | | | |
|---------------------------------------|--|----------------------------|---|
| <input type="checkbox"/> gas | <input checked="" type="radio"/> ideal | <input type="radio"/> real | 0 |
| <input type="checkbox"/> aqueous | | | 0 |
| <input type="checkbox"/> pure liquids | | | 0 |
| <input type="checkbox"/> pure solids | | | 0 |

suppress duplicates apply

species: 0

Solution species

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

Custom Solutions

- fixed activities
- ideal solutions
- activity coefficients

Details ...

seudonyms

apply List ...

include molar volumes

al Species (max 700) 5

al Solutions (max 30) 2

Default

equilibrium

normal transitions

predominant open

Calculate >>

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

Help OK

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 \checkmark 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.

The screenshot shows the 'Menu - Equilib: last system' window. The 'Scheil cooling' section is highlighted with a blue box. The 'Options' sub-section is circled in blue. The 'Cooling step' is set to 25, 'T-auto' is checked, and 'Mass(mol)' is set to 0. The 'Final Conditions' table shows a starting temperature of 1650. The 'Equilibrium' section has 'normal' selected. A 'Calculate >>' button is visible at the bottom right.

| <A> | | T(C) | P(atm) | Product H(J) |
|-----|-------|------|--------|--------------|
| 0.5 | | 1650 | 1 | |
| 10 | steps | | | |

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

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

FeO-MnO : Scheil cooling – Summary and Transitions

Results - Equilib Summary (page-1/11)

Output Edit Show Pages

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

1425 C | 1403.47 C |

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

SCHEIL-GULLIVER COOLING

CONSTITUENTS AND PHASES AT 1403.47 C
(temperature of final disappearance of Slag-liquid)

| CONS. PHASE | TOTAL AMT/mol | TOTAL AMT |
|--------------|---------------|------------|
| 1 1 Monoxide | 2.0000E+00 | 7.1391E+01 |

('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 | MOLE FRACTION | MASS FRACTION |
|---------------|---------------|----------------|
| Monoxide | | |
| 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 |

Results - Equilib Transitions (page 0/11)

Output Edit Show Pages

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

1425 C | 1403.47 C |

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

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

AVERAGE COMPOSITION OF ALL PRODUCT PHASES TAKEN TOGETHER

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

REACTION BETWEEN 1620.23 C AND 1403.47 C

Slag-liquid -> Monoxide

Reactants

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

Products (Constituent 1)
Monoxide

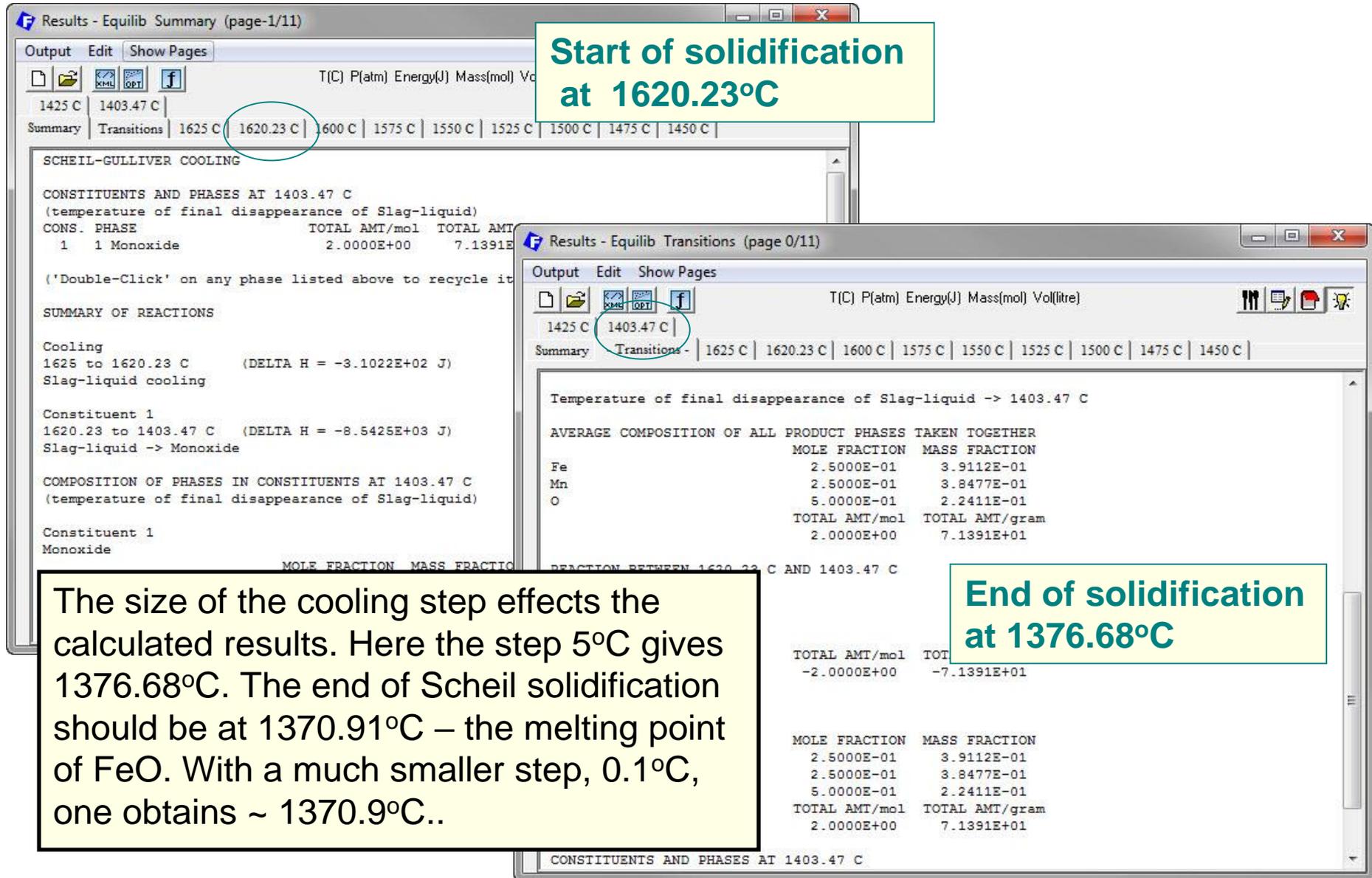
| | MOLE FRACTION | MASS FRACTION |
|----|---------------|----------------|
| Fe | 2.5000E-01 | 3.9112E-01 |
| Mn | 2.5000E-01 | 3.8477E-01 |
| O | 5.0000E-01 | 2.2411E-01 |
| | TOTAL AMT/mol | TOTAL AMT/gram |
| | 2.0000E+00 | 7.1391E+01 |

CONSTITUENTS AND PHASES AT 1403.47 C

Summary

Transitions

FeO-MnO : Scheil cooling – Start and Stop



FeO-MnO : Scheil cooling – incremental vs. accumulated

Incremental Scheil solidification at 1500°C

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

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

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

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

+ 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 fraction |
|------------------|---------------|---------------|
| Fe | 0.28734 | 0.44877 |
| Mn | 0.21266 | 0.32723 |
| 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

[Incremental Scheil]

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

Results - Equilib 1500 C (page 7/11)

Output Edit Show Pages

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

1425 C | 1403.47 C |

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

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

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

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

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

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

where "A" on the reactant side is 0.50000
The cutoff concentration has been specified to 1.0000E-70
Mass fraction precipitated according to Scheil-Gulliver = 0.77574

[Accumulated Scheil]

Accumulated Scheil solidification at 1500°C

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

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

System = Fe-Cr-C alloy

System composition: (gram) 10.84 Cr + 0.95 C + 88.21 Fe

Solution phases:

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

Legend:
I - immiscible 1
L - Scheil cooling
+ - selected 3

Final Conditions:
T(C): 1450 1200
P(atm): 1
Scheil-Gulliver cooling - T(start) = 1450, T(stop) = 1200

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

Annotations:
- Red circle around 'L' in the Solution phases table.
- Red circle around 'apply back diffusion' checkbox.
- Red circle around 'edit' button next to 'apply back diffusion'.
- Red arrow pointing from 'edit' to the 'Scheil back diffusing elements' dialog.
- Red arrow pointing from 'C' in the dialog to the text '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**

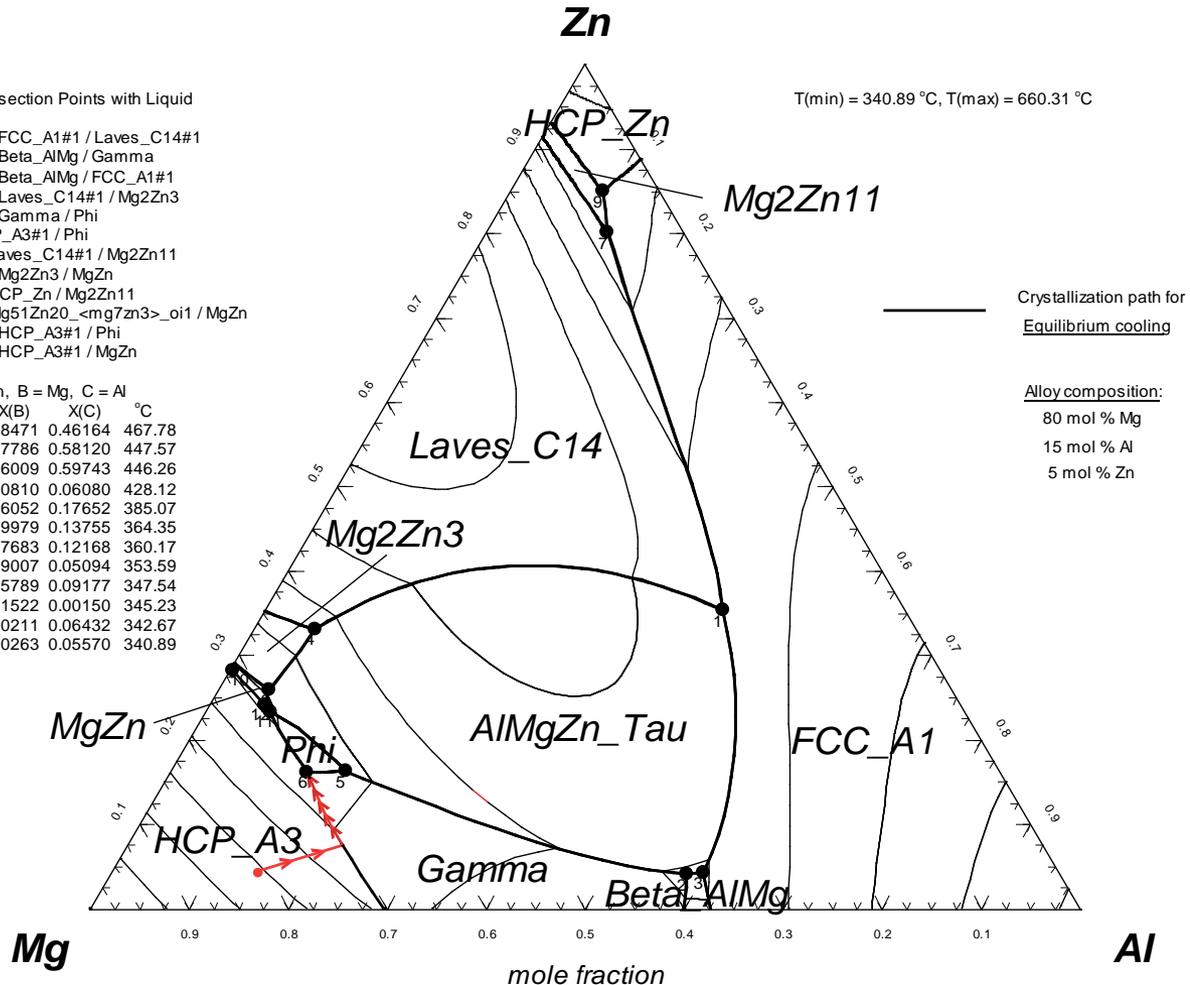


Four-Phase Intersection Points with Liquid

- 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 | °C |
|-----|---------|---------|---------|--------|
| | X(A) | X(B) | X(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



Al-Mg-Zn : Equilibrium 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

Help OK

Equilibrium cooling
FTlite-Liqu

Cooling step : 10 T-auto:

Mass(mol): 0

Equilibrium Cooling of Liquid Al-Mg-Zn

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

Parameters Help

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

80 Mg + 15 Al + 5 Zn

| * | + | 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
 fixed activities
 ideal solutions
 activity coefficients
Details ...

Pseudonyms
apply List ...

include molar volumes
Total Species (max 1500) 98
Total Solutions (max 40) 22

Default

Equilibrium
 normal normal + transitions
 transitions only
 open
 para: edit Calculate >>

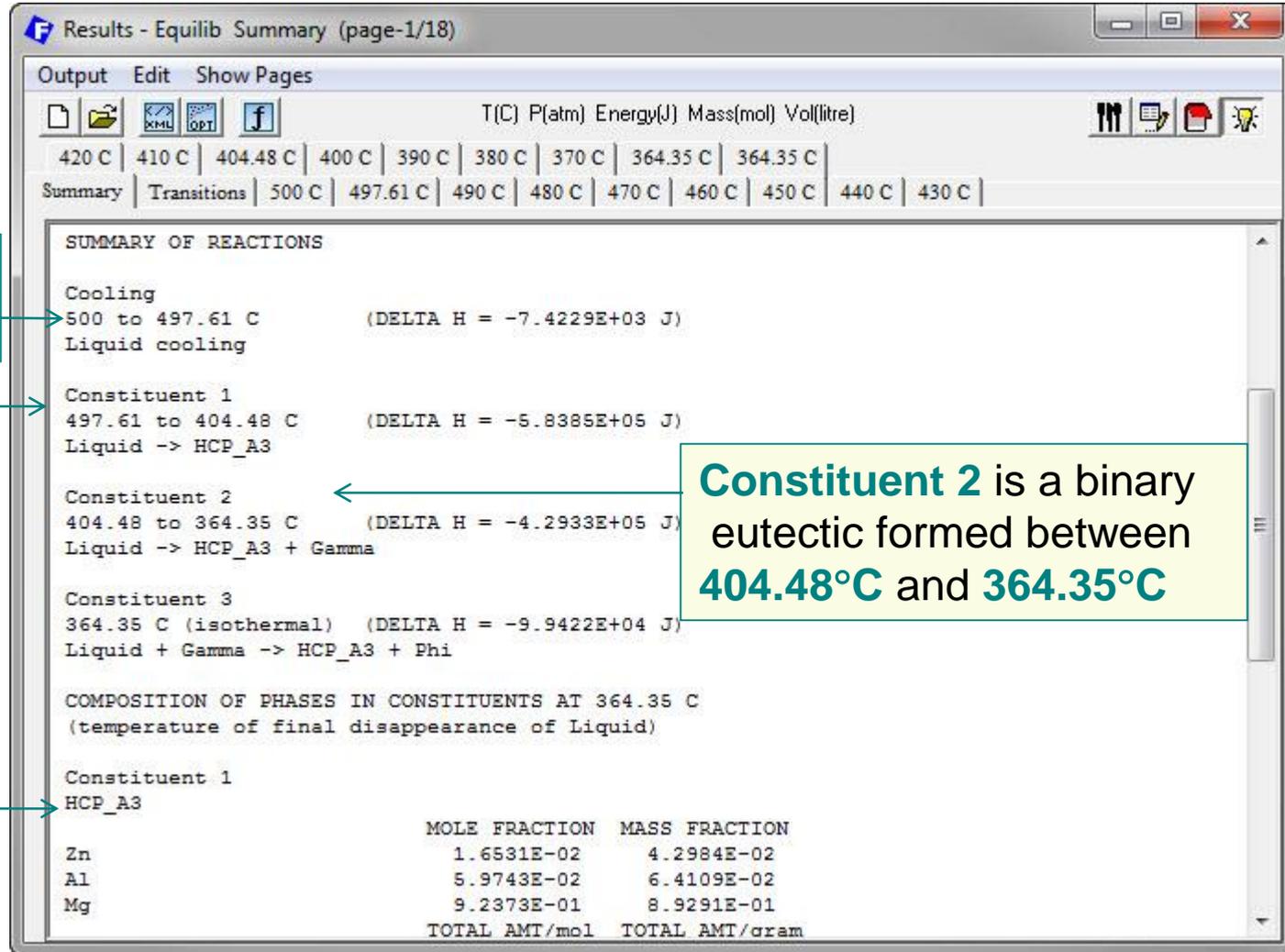
Equilibrium cooling - T(start) = T-auto, T(stop) = 0 mole

Al-Mg-Zn : Equilibrium 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



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

Al-Mg-Zn : Equilibrium cooling – Plot Results

Results - Equilib Summary (page-1/18)

Output Edit Show Pages

Save or Print ▶ T(C) P(atm) Energy(J) Mass(mol) Vol(litre)

Plot ▶ Plot Results ...

Equilib Results file ▶ Repeat Plot - gram vs T(C) ... 430 C |

Stream File ▶

Format ▶

Fact-XML ▶

Fact-Optimal ▶

Fact-Function-Builder ▶

Refresh ...

Liquid -> HCP_A3 + Gamma

Constituent 3
364.35 C (isothermal) (DELTA T)
Liquid + Gamma -> HCP_A3 + BCC54

COMPOSITION OF PHASES IN CONTACT
(temperature of final disappearance)

Constituent 1
HCP_A3

Zn
Al
Mg

Plot: gram vs T(C)

File Help

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 | |

AXES: gram vs T(C)

Y-axis: gram

X-axis: T(C)

Y-axis: maximum 2000, minimum 0, tick every 250

X-axis: maximum 500, minimum 360, tick every 10

Cancel Refresh OK

AXES: Species: 0 selected Select Repeat

Graph: Labels: size: 9 no: 9
 chemical
 integer #
 none
 color
 reactants
 file name
 full screen
 Viewer
 Figure

Plot >>

Al-Mg-Zn : Equilibrium cooling – Plot Results

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

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

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

| | + | # | Species | Gram (min) | Gram (max) | Wt.% (min) | Wt.% (max) | Act. (min) | Act. (max) |
|-----|---|-----|------------------|------------|------------|------------|------------|------------|------------|
| 600 | | 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

Clear Refresh OK

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

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

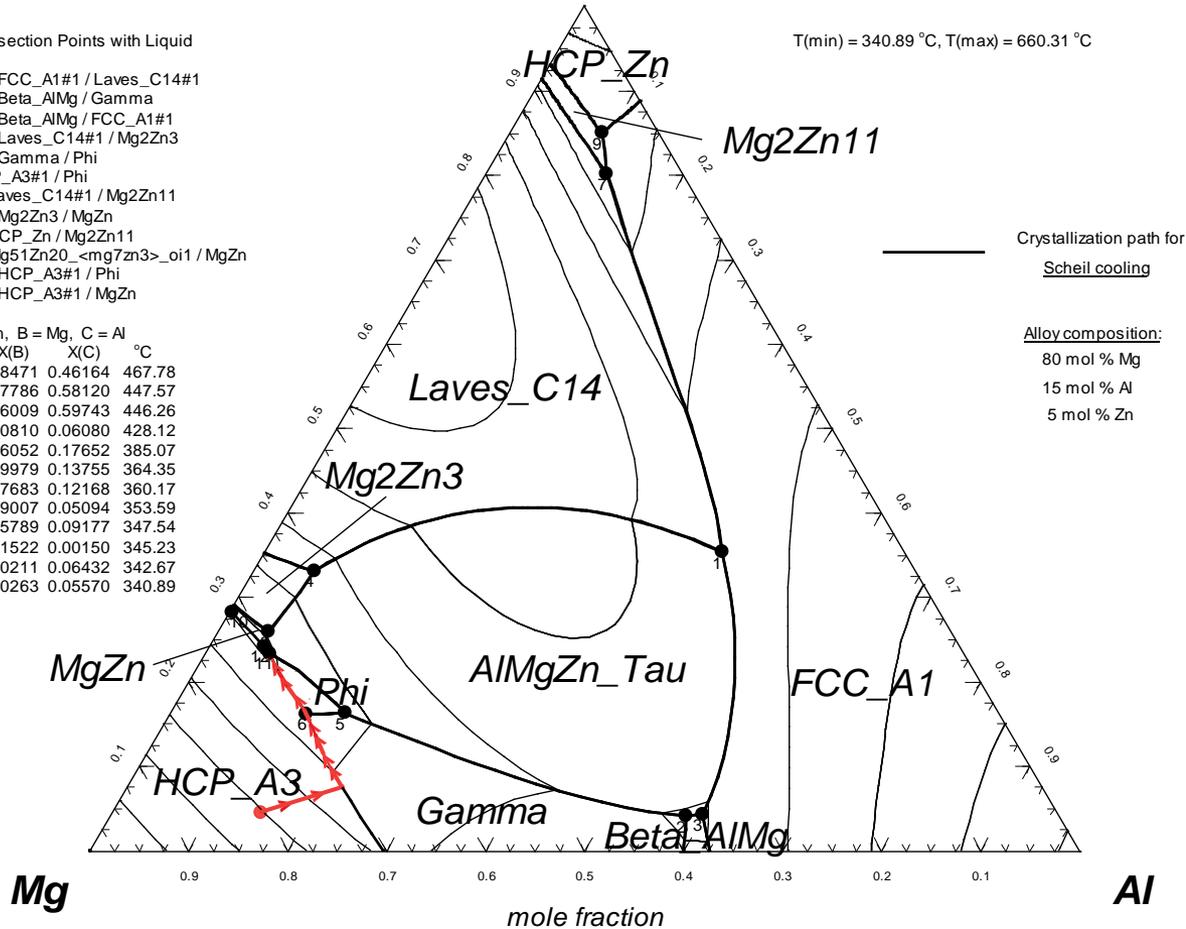
Al-Mg-Zn polythermal liquidus projection
calculated by **Phase Diagram** with data taken
from **FTlite – FACT light alloy databases**



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 | °C |
|-----|---------|---------|---------|--------|
| | X(A) | X(B) | X(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 |



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

Help OK

Menu - Equilib:

Parameters Help

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

(3)

80 Mg + 15 Al + 5 Zn

species: 28

species: 28

| * | + | 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

Select

Custom Solutions

fixed activities

ideal solutions

activity coefficients

Details ...

Pseudonyms

apply List ...

include molar volumes

Total Species (max 1500) 126

Total Solutions (max 40) 22

Default

Equilibrium

normal normal + transitions

transitions only

open

para edit

Calculate >>

Final Conditions

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

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

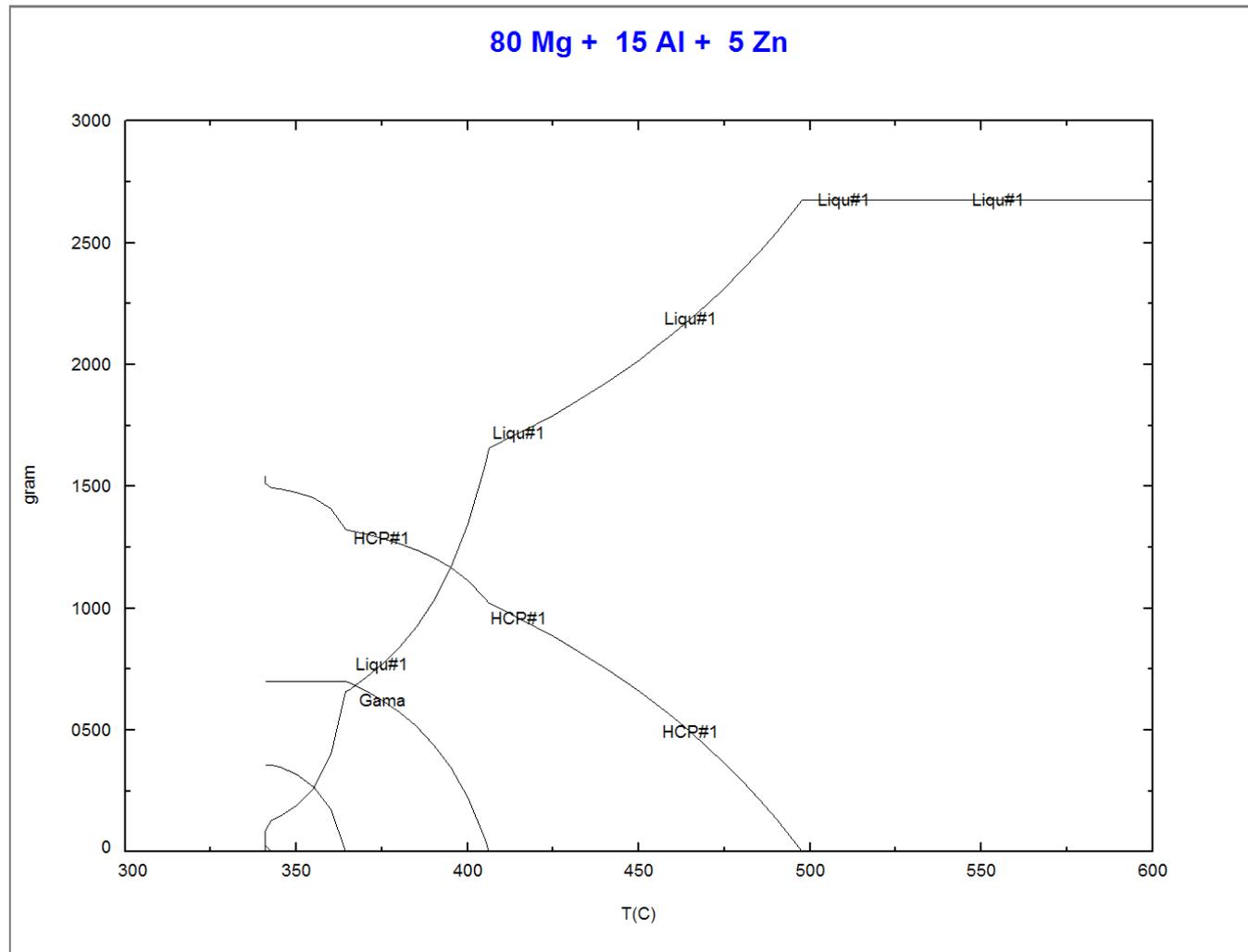
Scheil Cooling

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

Help OK

Scheil cooling

FTlite-Liqu Options

Cooling step: 5 T-auto:

Mass(g): 0

Equilib

Parameters Help

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

(4)

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

Species

Species: 42

press duplicates apply

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

L - Scheil cooling 1

+ - selected 12

Show all selected

species: 144

solutions: 26

Select

Custom Solutions

fixed activities

ideal solutions

activity coefficients

Details ...

Pseudonyms

apply List ...

include molar volumes

Total Species (max 1500) 186

Total Solutions (max 40) 26

Default

Final Conditions

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

600 1

Table

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

Equilibrium

normal normal + transitions

transitions only

open

para edit

Calculate >>

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

Results - Equilib Summary (page-1/60)

Output Edit Show Pages

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

510 C | 505 C | 500 C |
560 C | 555 C | 550 C | 545 C | 540 C | 535 C | 530 C | 525 C | 524.12 C | 520 C | 515 C |
- Summary - | Transitions | 595 C | 594.16 C | 594.07 C | 590 C | 585 C | 580 C | 575 C | 570 C | 565 C |

SCHEIL-GULLIVER COOLING

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

| CONS. | PHASE | TOTAL AMT/mol | TOTAL AMT/gram |
|-------|-----------------|---------------|----------------|
| 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 |

Summary

AZ91 + 0.25 wt.% Mn alloy:

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

Results - Equilib Transitions (page 0/60)

Output Edit Show Pages

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

510 C | 505 C | 500 C |
560 C | 555 C | 550 C | 545 C | 540 C | 535 C | 530 C | 525 C | 524.12 C | 520 C | 515 C |
Summary | - Transitions - | 595 C | 594.16 C | 594.07 C | 590 C | 585 C | 580 C | 575 C | 570 C | 565 C |

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 | 4.0461E+00 | TOTAL AMT/gram | 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 | 4.0461E+00 | TOTAL AMT/gram | 1.0000E+02 |

Temperature of transition -> 594.07 C

Transitions

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

Summary & Transitions

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

Results - Equilib Summary (page-1/60)

Output Edit Show Pages

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

510 C | 505 C | 500 C | 560 C | 555 C | 550 C | 545 C | 540 C | 535 C | 530 C | 525 C | 524.12 C | 520 C | 515 C

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

SCHEIL-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% |
| 1 | 1 HCP_A3 | 2.6553E+00 | 6.4835E+01 | 3.78% |
| 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) | 4.2238E-03 | 1.4544E-01 | 3.91% |
| 4 | 1 HCP_A3 | 6.8848E-02 | 1.6956E+00 | 9.65% |
| 4 | 2 MnAl4_s1(s) | 5.4346E-04 | 1.7702E-02 | 5.13% |
| 5 | 1 HCP_A3 | 1.9793E-01 | 4.8919E+00 | 2.78% |
| 5 | 2 Gamma | 4.5374E-01 | 1.1829E+01 | 5.85% |
| 5 | 3 MnAl4_s1(s) | 8.0662E-04 | 2.6274E-02 | 7.61% |
| 6 | 1 HCP_A3 | 7.1873E-03 | 1.8150E-01 | 1.01% |
| 6 | 2 Phi | 1.0940E-02 | 3.7598E-01 | 1.35% |
| 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 | 1.03% |

| 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

Results - Equilib Summary (page-1/60)

Output Edit Show Pages

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

510 C | 505 C | 500 C |
560 C | 555 C | 550 C | 545 C | 540 C | 535 C | 530 C | 525 C | 524.12 C | 520 C | 515 C |
- Summary - | Transitions | 595 C | 594.16 C | 594.07 C | 590 C | 585 C | 580 C | 575 C | 570 C | 565 C |

SCHEIL-GULLIVER COOLING

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

| CONS. | PHASE | TOTAL AMT/mol | TOTAL AMT/gram | TOTAL VOL/dm3 |
|-------|-----------------|---------------|----------------|---------------|
| 1 | 1 Al8Mn5_D810 | 1.3055E-05 | 5.0230E-04 | 0.0000E+00 |
| 2 | 1 HCP_A3 | 2.6553E+00 | 6.4835E+01 | 3.7348E-02 |
| 2 | 2 Al8Mn5_D810 | 7.5208E-03 | 2.8466E-01 | 0.0000E+00 |
| 3 | 1 HCP_A3 | 6.3501E-01 | 1.5580E+01 | 8.9318E-03 |
| 3 | 2 Mn4Al11_s1(s) | 4.2325E-02 | 1.4544E-01 | 3.9104E-05 |
| 3 | 3 HCP_A3 | 1.5752E-01 | 4.0519E+00 | 9.6839E-04 |
| 5 | 2 Gamma | 4.5374E-01 | 1.1829E+01 | 5.8586E-03 |
| 5 | 3 MnAl4_s1(s) | 8.0662E-04 | 2.6274E-02 | 7.6148E-06 |
| 6 | 1 HCP_A3 | 7.1873E-03 | 1.8150E-01 | 1.0109E-04 |
| 6 | 2 Phi | 1.0940E-02 | 3.7598E-01 | 1.3952E-04 |
| 6 | 3 HCP_A3 | 1.2722E-08 | 3.2228E-02 | 1.2722E-08 |
| 7 | 1 HCP_A3 | 7.1232E-01 | 1.7932E+01 | 1.0866E-05 |
| 7 | 2 AlMgZn_Tau | 6.7948E-04 | 2.9038E-02 | 7.6777E-06 |
| 7 | 3 Mn4Al11_s1(s) | 3.4950E-08 | 1.2035E-06 | 3.2358E-10 |
| 8 | 1 HCP_A3 | 1.2677E-03 | 3.2228E-02 | 1.7831E-05 |
| 8 | 2 MgZn | 9.0976E-04 | 3.9438E-02 | 1.0892E-05 |

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

2° Click OK to recycle HCP_A3

FactSage 6.3: Equilib

Do you wish to recycle Phase 1 of Constituent 2?

HCP_A3

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

OK Cancel

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

Change mass from 100% => 100 g

| Mass(g) | Species | Phase | T(C) | P(total)** | Stream# | Data |
|---------|---|-------|------|------------|---------|------|
| 100 | [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 | | | | 2 | |

List of components in HCP phase

Initial Conditions

Next >>

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

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

The screenshot shows the FactSage Equilib software interface. The window title is "Menu - Equilib". The menu bar includes "File", "Units", "Parameters", and "Help". The status bar at the top displays "T(C) P(atm) Energy(J) Mass(g) Vol(litre)".

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 |
|---|---|-------------|-----------|
| | | FTlite-Liqu | Liquid |
| | | FTlite-FCC | FCC_A1 |
| | | FTlite-HCP | HCP_A3 |
| | | FTlite-BCC | BCC_A2 |
| | + | FTlite-CBCC | CBCC_A12 |
| | + | FTlite-CUB1 | CUB_A13 |
| | | FTlite-LC14 | Laves_C14 |
| | | FTlite-LC15 | Laves_C15 |

Legend
| - immiscible 7
+ - selected 12

Show all selected
species: 144
solutions: 26

Custom Solutions
 fixed activities
 ideal solutions
 activity coefficients

Pseudonyms
apply

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

Final Conditions

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

10 steps Table

Equilibrium
 normal normal + transitions
 transitions only
 open
 para

FactSage

Anneal at 150 to 500 °C

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

Results - Equilib 150 C (page 1/71)

Output Edit Show Pages

Save or Print Plot Equilib Results file Stream File Format Fact-XML Fact-Optimal Fact-Function-Builder Refresh ...

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

260 C | 185 C | 190 C | 195 C | 200 C | 205 C

5.4908E-0
a=1.0000
Al
Mg
Mn
Zn

Mole

3.
1.
1.
0.

Mn
Al
Mg

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

Plot: log10(gram) vs T(C)

| 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) | | |

100 [Rc_C2_P1]

Y-axis X-axis Swap Axes

Y-axis X-axis

log10(gram) T(C)

maximum 2.5 500
minimum -4 150
tick every 0.5 50

Cancel Refresh OK

Labels size: 9 no: 9

color full screen
 reactants Viewer
 file name Figure

Plot >>

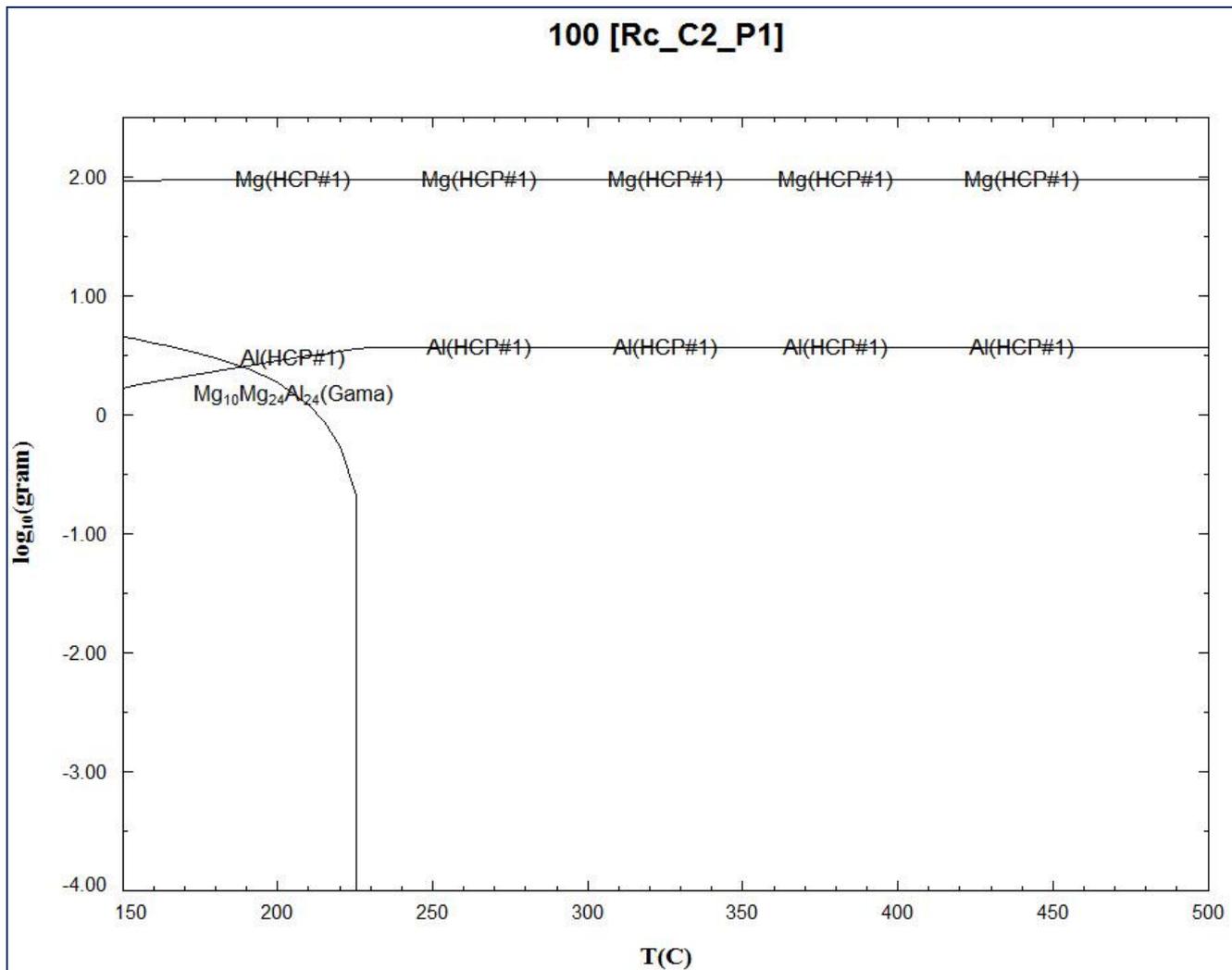
Species 3 selected

log10(gram) vs T(C)

Axes Repeat

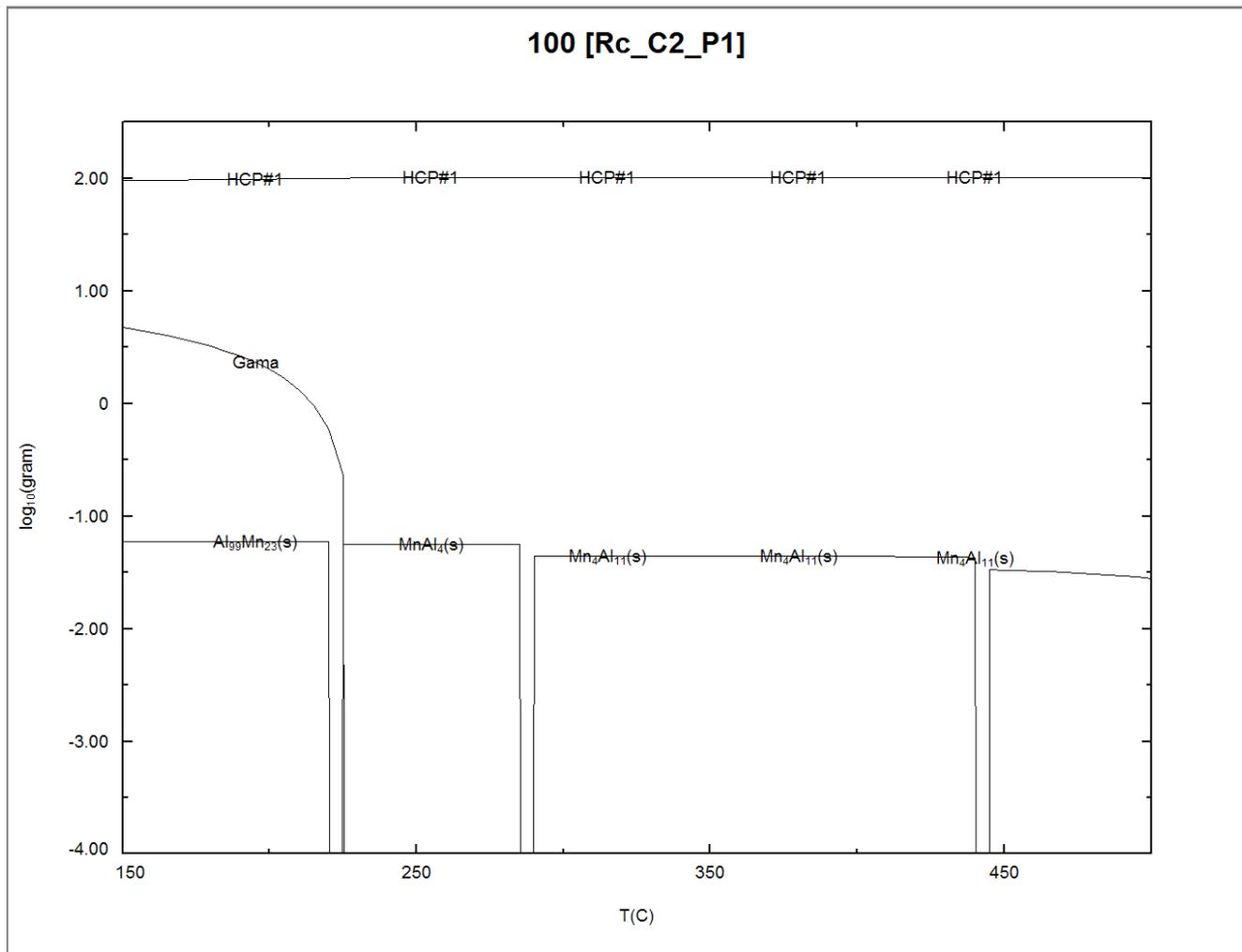
Al-Mg-Zn-Mn : Graph of fully annealed HCP phase

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

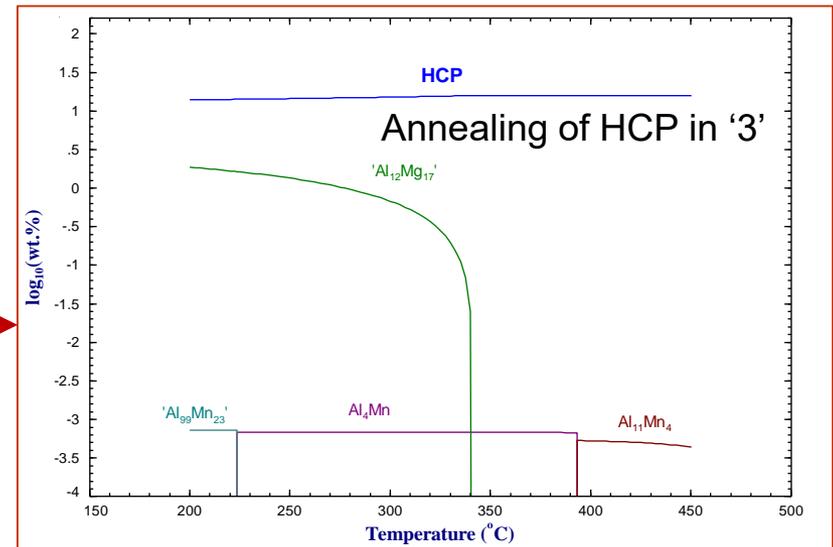
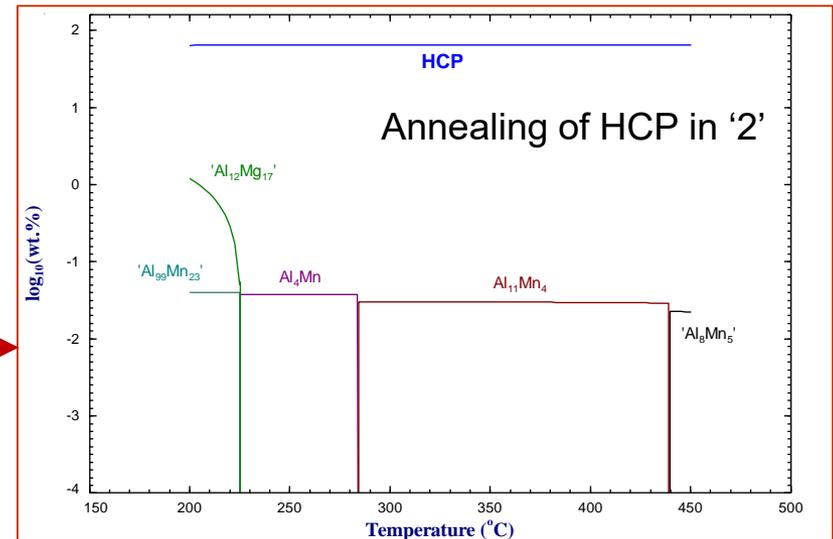
Scheil cooling and post equilibration (annealing) of Scheil microstructure: AZ91 alloy + 0.25 wt.% Mn

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

File Units Parameters Help

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

Reactants [4]

0.5 Fe + 0.5 Cr + 0.02 C + 0.02 N

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

Custom Solutions

- fixed activities
- ideal solutions
- activity coefficient

Pseudonyms

include molar volumes

paraequilibrium & Gmin

Total Species (max 3000) 82

Total Solutions (max 40) 15

Total Phases (max 1500) 30

Final Conditions

T(K) 900

P(atm) 1

Equilibrium

normal

normal + transitions

transitions only

open

Calculate >>

Equimolar Fe-Cr with $C/(Fe + Cr) = 2 \text{ mol\%}$ and $N/(Fe + Cr) = 2 \text{ mol\%}$

For comparison purposes, our first calculation is a normal (full) equilibrium calculation

Select all solids and solutions from FSstel database

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

File Units Parameters Help

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

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

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

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
 fixed activities
 ideal solutions
 activity coefficients
Details ...

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 ...

Final Conditions

| <A> | | T(K) | P(atm) | Product H(J) |
|-----|-------|------|--------|--------------|
| 10 | steps | 900 | 1 | |

Table

Equilibrium
 normal normal + transitions
 transitions only

Calculate >>

FactSage

Paraequilibrium diffusing elements

Enter the list of elements that can diffuse. OK Cancel

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

Select from: Fe Cr N C

C N

1° Click here

2° Click on « edit »

3° Click here

4° Enter elements that can diffuse

5° 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 Cr1Val
+ 0.43152 Fe1Val)

| 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 elements that can diffuse.

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

Select from: Fe Cr N C

C

OK

Cancel

Input when only **C** is permitted to diffuse

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

N

OK

Cancel

Input when only **N** is permitted to diffuse

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

OK

Cancel

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)

**2 phases are formed
at paraequilibrium**

| 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)

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

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

| 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 |

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)

**2 phases are formed
at paraequilibrium**

| 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)

**Fe/Cr molar ratio = 1/1 in
all phases**
**C/(Fe+Cr) molar ratio =
0.02 in all phases**

| 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 |

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 $\text{SO}_4[2-]$, $\text{S}[2-]$ and $\text{SO}_3[2-]$ 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 $\text{SO}_4[2-]$ in the output is equal to the amount of $\text{SO}_4[2-]$ 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

Equilib - Reactants

File Edit Macro Table Units Data Search Data Evaluation Help

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

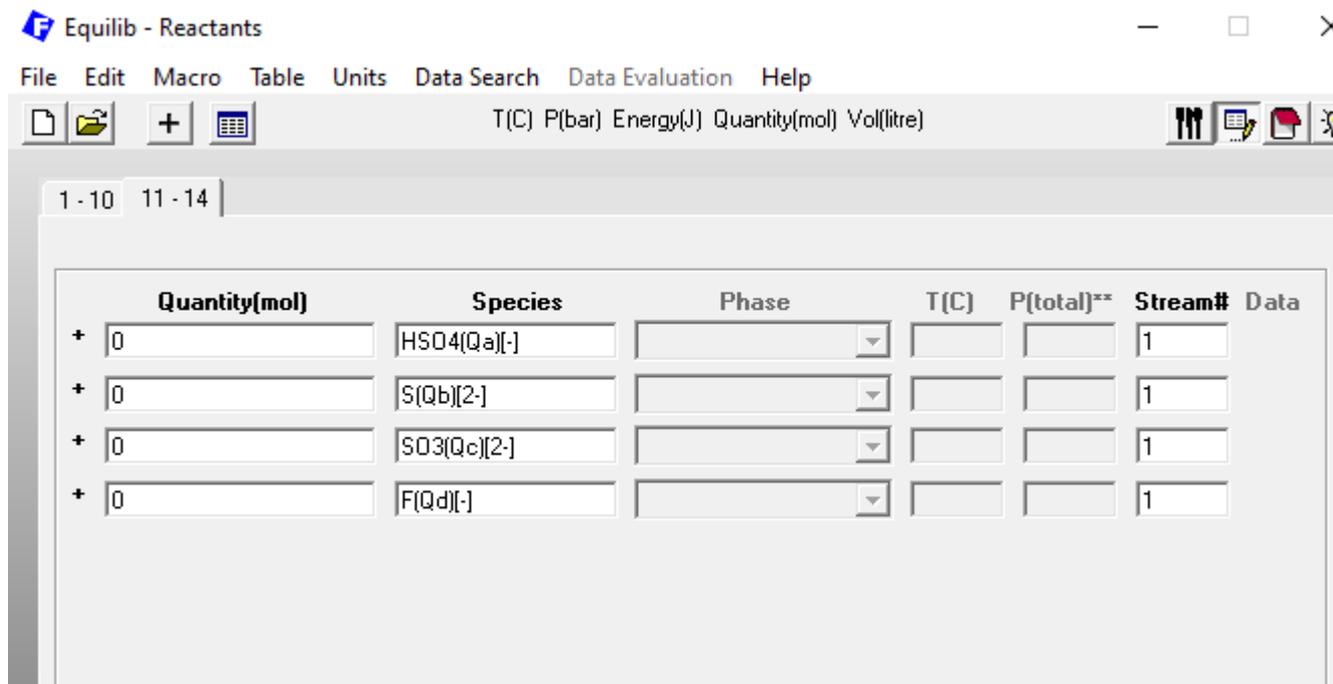
1 - 10 | 11 - 14

| 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

Next >>

In the **Input**, all $\text{SO}_4[2-]$, $\text{S}[2-]$, $\text{SO}_3[2-]$ and $\text{F}[-]$ ions are associated with equal amounts of Qa, Qb, Qc, and Qd **virtual elements** respectively



Zero amounts of $\text{SO}_4(\text{Qa})[2-]$, $\text{HSO}_4(\text{Qa})[-]$, $\text{S}(\text{Qb})[2-]$, $\text{SO}_3(\text{Qc})[2-]$ and $\text{F}(\text{Qd})[-]$ species are entered in order for them to appear in the species selection lists on the menu window. (Note, that $\text{SO}_4(\text{Qa})[2-]$ and $\text{HSO}_4(\text{Qa})[-]$ 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

File Units Parameters Help

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 |
|---|---|------------|-----------|
| | | | |

Legend

Show all selected

species: 0 solutions: 0

Target

- none -

Estimate T(K):

Quantity(mol):

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> | | T(C) | P(bar) | Product H(J) |
|-----|-----|------|--------|--------------|
| | | 25 | 1 | |

steps Table

Equilibrium

normal normal + transitions

transitions only open

- no time limit -

Aqueous species selection

File Edit Show Sort

Selected: 7/36

AQUEOUS

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 $\text{SO}_4[2-]$ to $\text{SO}_4(\text{Qa})[2-]$, the properties of $\text{HSO}_4[-]$ to $\text{HSO}_4(\text{Qa})[-]$, etc.

Solid species selection

File Edit Show Sort

Selected: 6/58

SOLID

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_Tl2SE | 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_tl36_(140) | V | | | | |
| 195 | K3F(SO4)(s2) | FactPS | alpha_cp9_(21E) | 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.

Output Edit Show Pages Final Conditions

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

```

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)

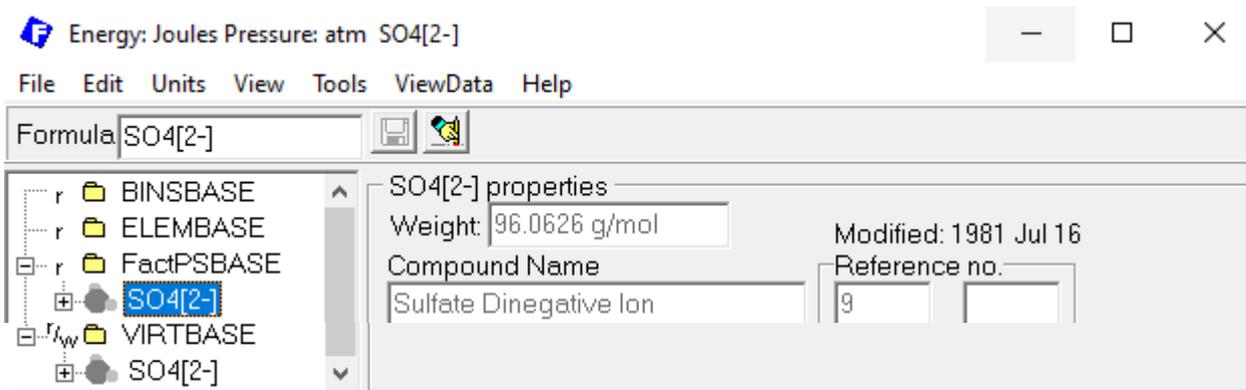
+ 1.9992     mol  K2SO4(Qa)_Solid_Alpha
(348.38 gram, 1.9992 mol)

```

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

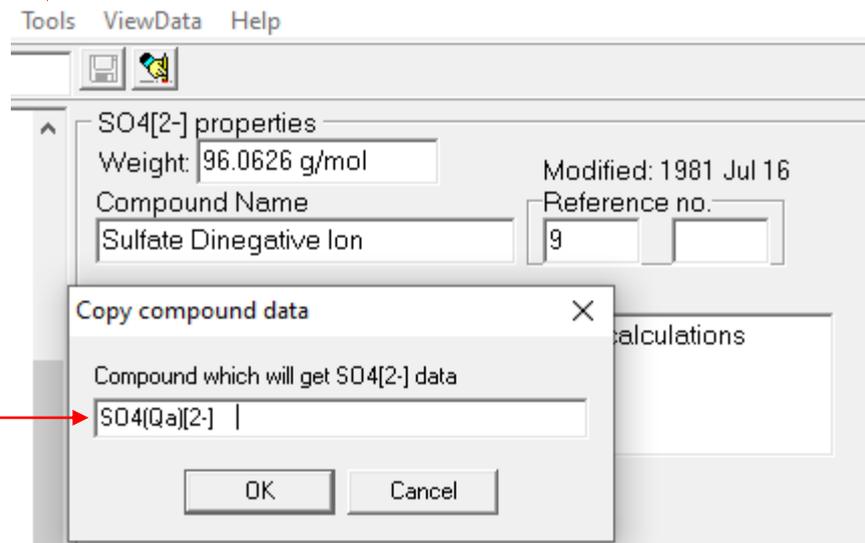
Entering data in a private **COMPOUND (cdb)** database for species containing virtual elements

- 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**.



- 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"



Enter new name

Now delete SO4[2-] from VIRTBASE

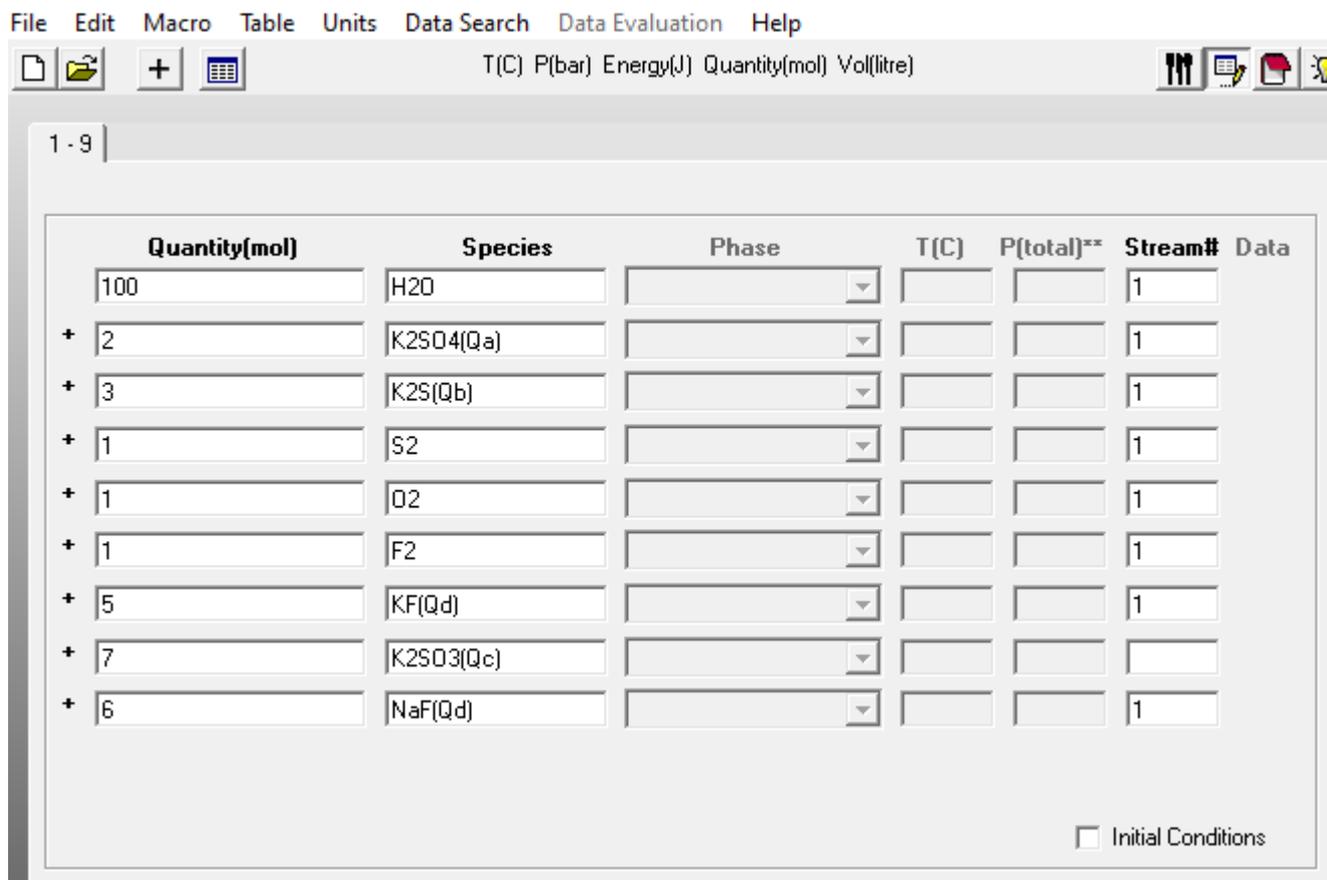


SO4(Qa)[2-] now in VIRTBASE

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



The screenshot shows the Equilib Advanced software interface. The menu bar includes File, Edit, Macro, Table, Units, Data Search, Data Evaluation, and Help. The status bar displays T(C), P(bar), Energy(J), Quantity(mol), and Vol(litre). The main window shows a list of species and their quantities, with a checkbox for "Initial Conditions" at the bottom right.

| 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 | |

Initial Conditions

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

File Units Parameters Help

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 |
|---|---|------------|-----------|
| | | | |

Legend

Show all selected

species: 0

solutions: 0

Target

- none -

Estimate T(K):

Quantity(mol):

Final Conditions

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

10 steps Table

Equilibrium

normal normal + transitions

transitions only open

- no time limit -

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

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

| | | | | | | | |
|-------|-----------------|--------|---------|--|--|--|--|
| 140 | SO3[2-](aq) | FactPS | aqueous | | | | |
| 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 Help Suppress Duplicates Edit priority list :

| | | | | | | | |
|-------|---------------|--------|------------------|---|--|--|--|
| 198 | K3F(SO4)(s) | FactPS | beta_tI36_(140) | V | | | |
| 199 | K3F(SO4)(s2) | FactPS | alpha_cP9_(21E) | 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 Help Suppress Duplicates Edit priority list :

Heating in a crucible which partially reacts with its contents

- 100 g of PbO are placed in an Al_2O_3 crucible at 25 °C and heated to 1200°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 Q_a with the Al_2O_3 which does not dissolve.

Activate **FACTDATA/VIRTBASE** in which $\text{Al}_2\text{O}_3(\text{Qa})$ 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

(Note: If an initial condition for a species containing a **virtual element** such as $\text{Al}_2\text{O}_3(\text{Qa})$ is to be selected, then the compound must first be entered in a compound (cdb) database.)

File Units Parameters Help

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

Reactants (3)

(gram) 95 PbO + 5 Al2O3 + 95 Al2O3(Qa)
 (25C,s1-FToxid,#1) (25C,s1-FToxid,#1) (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> | | T(C) | P(atm) | Delta H(J) |
|-----|-----|------|--------|------------|
| | | 1200 | 1 | |

10 steps Table

Equilibrium

normal normal + transitions

transitions only open

- no time limit -

Select only Al₂O₃(Qa)

File Edit Format View Help

```
(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)
```

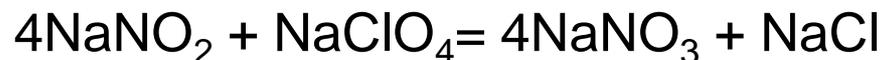
```
+ 95.000 gram Al2O3(Qa)_corundum(alpha)  
(95.000 gram, 0.93173 mol)  
(1200 C, 1 atm, S4, a=1.0000)
```

```
*****  
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:

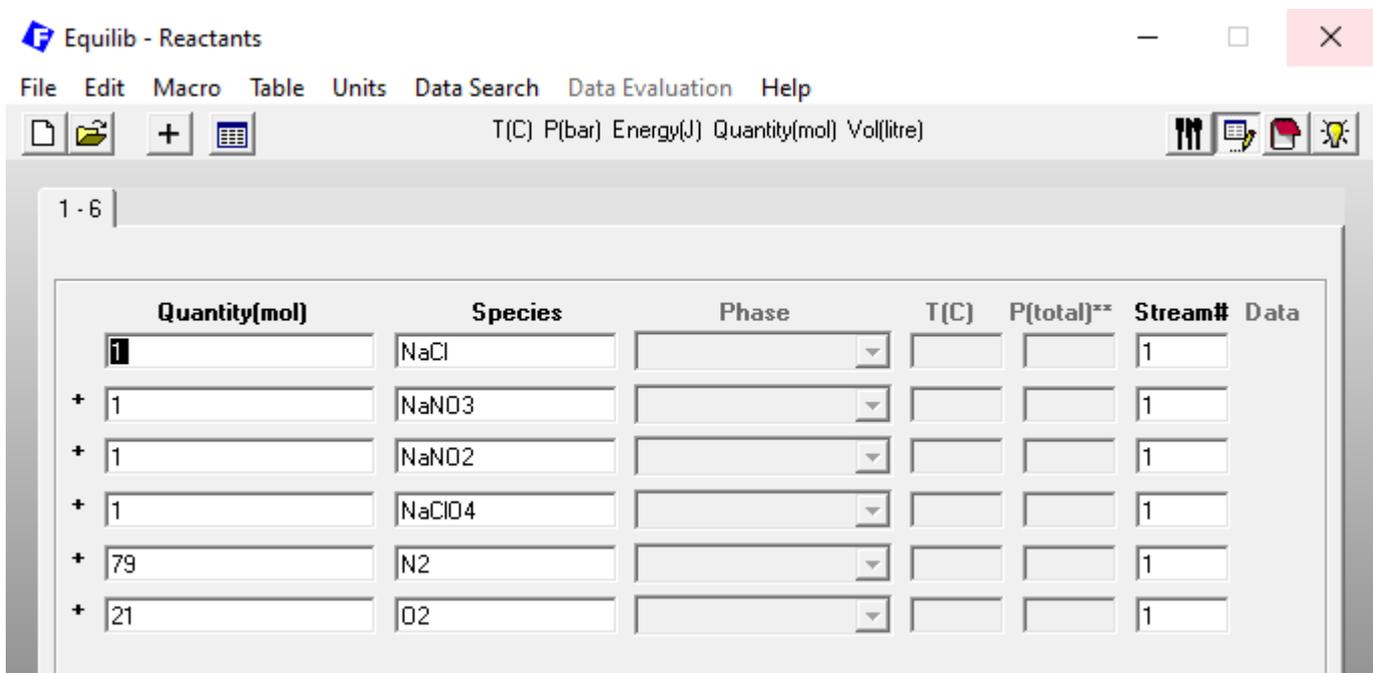


Furthermore, if air is present, the salt will react with N_2 and O_2 .

- 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



The screenshot shows the 'Equilib - Reactants' window in FactSage. The interface includes a menu bar (File, Edit, Macro, Table, Units, Data Search, Data Evaluation, Help) and a toolbar with icons for file operations and calculations. The main area displays a table of reactants with columns for Quantity(mol), Species, Phase, T(C), P(total)**, and Stream#. The table contains the following data:

| 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

File Units Parameters Help

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

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> | | T(C) | P(bar) | Product H(J) |
|-----|-----|------|--------|--------------|
| | | 550 | 1 | |

10 steps Table

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.

File Edit Macro Table Units Data Search Data Evaluation Help

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

1 - 6

| | 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_o5: | o | | | |
| | 82 | NaClO4(s2) | FTsalt | Solid_beta_(225 | o | | | |
| + | 83 | NaNO3(Qa)(s) | FTsalt | prototype_CaCO | V | | | |
| + | 84 | NaNO3(Qa)(s2) | FTsalt | prototype_NaNC | V | | | |
| + | 85 | NaNO2(Qb)(s) | FTsalt | Solid_alpha_ol8 | V | | | |
| + | 86 | NaNO2(Qb)(s2) | FTsalt | Solid_beta_ol16 | V | | | |
| + | 87 | NaClO4(Qc)(s) | FTsalt | Solid_alpha_o5: | 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**.

File Units Parameters Help

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

Target

- none -

Estimate T(K):

Quantity(mol):

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

Final Conditions

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

10 steps Table

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

Modified end-member

Using the elements

N O Na Cl

enter the modified chemical formula

(or enter a blank line to return to NaNO3)

NaNO3

OK

Cancel

3) Ready for editing

Modified end-member

Using the elements

N O Na Cl

enter the modified chemical formula

(or enter a blank line to return to NaNO3)

NaNO3(Qa)

OK

Cancel

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 550°C. No reactions within the salt or with the gas occur

Equilib - Results 550 C EQUIINTE Intel 2020-11-06

Output Edit Show Pages Final Conditions

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

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.

```
File Edit Format View Help
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

File Units Parameters Help

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

gas ideal real 0
 aqueous 0
 pure liquids 0
 pure solids 0
 species: 0

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

Legend
+- selected 1

Show all selected
species: 12 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: 0
Total Species (max 5000) 12
Total Solutions (max 200) 1
Total Phases (max 1500) 1

Final Conditions

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

10 steps Table

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

Equilibrium cation distribution at 298.15 K

Output Edit Show Pages Final Conditions

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

298.15 K | 1473 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 fraction
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 Al³⁺ ions: (Fe)[Al]₂O₄

Equilibrium cation distribution at 1473 K

Output Edit Show Pages Final Conditions

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

```

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 fraction
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
  
```

High-temperature degree of inversion = 0.265

Enthalpy at 1473 K at equilibrium

(Al)[Al]₂O₄[+]
(Al)[Fe]₂O₄[-]

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

File Edit Macro Table Units Data Search Data Evaluation Help

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

1 - 2

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

Initial Conditions

Next >>

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

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

Reactants (2)

FeAl2O4 + 0.265 Qa

Products

Compound species

gas ideal real 0
 aqueous 0
 pure liquids 0
 pure solids 0

species: 0

Target

- none -

Estimate T(K): 1000

Quantity(mol): 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) |

Legend

+ - selected 1

Show all selected

species: 12

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: 0

Total Species (max 5000) 12

Total Solutions (max 200) 1

Total Phases (max 1500) 1

Final Conditions

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

10 steps Table

Equilibrium

normal normal + transitions

transitions only open

- no time limit -

Right click to add
virtual element to
end-members

F Selection - Equilib Page 1/1 : T(K) = 550, P(bar) = 1

File Edit Show Sort

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 $(Al)[Al]_2O_4[+]$ 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

File Edit Format View Help

FeAl204 + 0.265 Qa =

1.0000 mol Spinel
 (173.81 gram, 1.0000 mol)
 (298.15 K, 1 bar, a=1.0000)
 (9.7387E-02 Fe304[2-]
 + 0.63761 Fe1Al204
 + 0.22989 Al304(Qa)[1+]
 + 3.5112E-02 Al1Fe204(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 | |

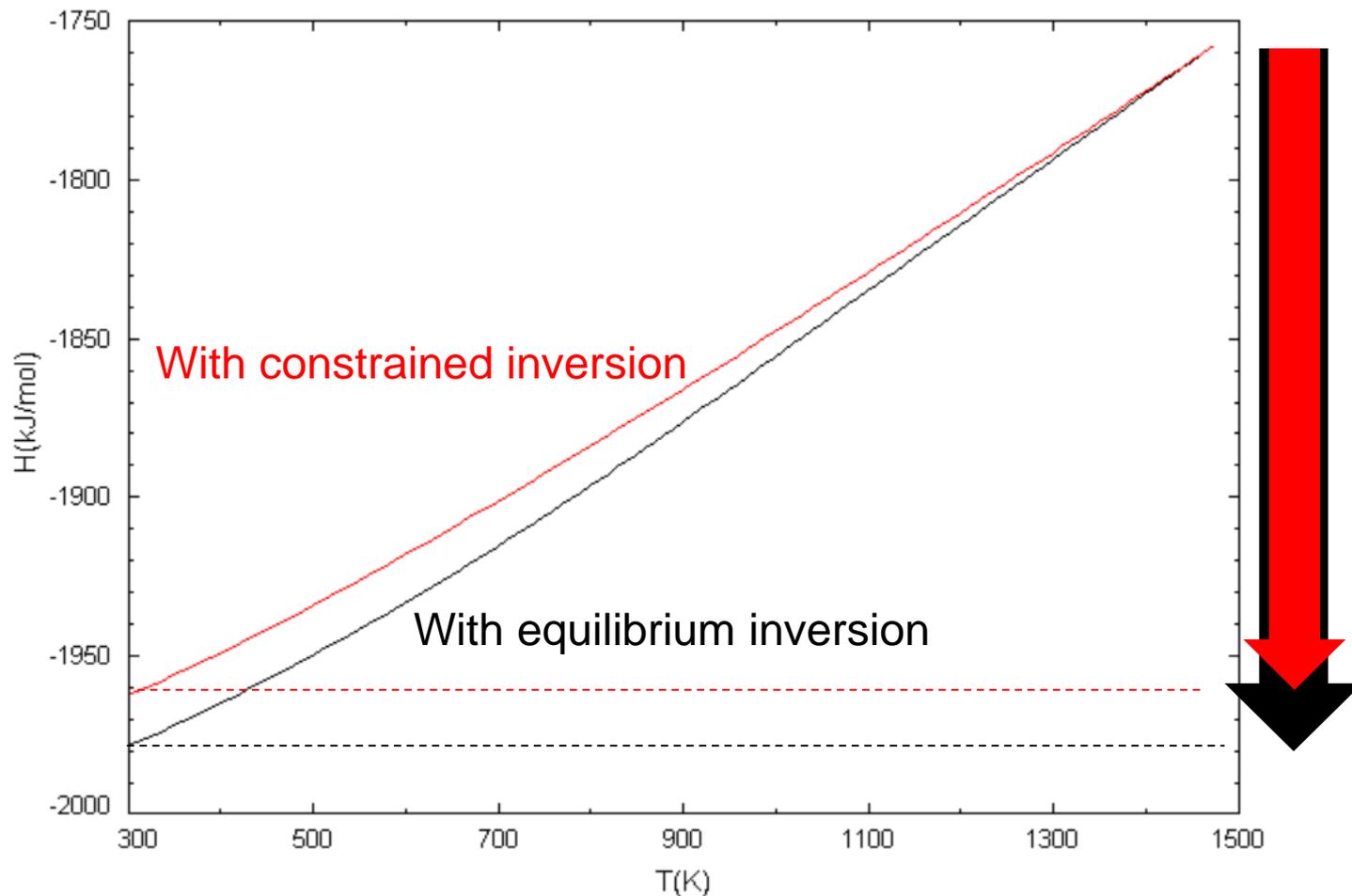
Degree of inversion = 0.265



| ***** | | | | |
|--------------|--------------|-------------|-------------|-------------|
| 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 |

Enthalpy at 298.15 K with constraint





Heat evolved during rapid cooling from 1473 K to 298.15 K

Constrained inversion: $(1.96299 - 1.75790) \times 10^6 = 205090$ Joules/mol

Equilibrium inversion: $(1.97892 - 1.75790) \times 10^6 = 221020$ 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.

File Edit Macro Table Units Data Search Data Evaluation Help

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

1 - 4

| 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

File Units Parameters Help

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> | | T(K) | P(atm) | Product V(litre) |
|-----|-----|------|--------|------------------|
| | | 1273 | | 50 |

10 steps Table

Equilibrium

normal normal + transitions

transitions only open

- no time limit -

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

Selected: 2/2

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 | | | | | |

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

$Q_a = 1.0$: 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))
```

$Q_a = 0.9$: 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))
```

$Q_a = 0.1$: 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)
```

$Q_a = 0.0$: 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 °C. Carbon diffuses between phases, but the Fe/Cr ratio remains constant in all phases.

The **FSstel** database is activated

File Edit Macro Table Units Data Search Data Evaluation Help

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

1 - 6

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

Zero amounts of three **virtual elements** are entered

File Units Parameters Help

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

Target

- none -

Estimate T(K): 1000

Quantity(mol): 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 |

Legend
+- selected 3

Show all selected

species: 10

solutions: 3

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

Final Conditions

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

10 steps Table

Equilibrium

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

Click to add virtual elements to end-members

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 700°C

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**

AxSigmaAg
= 43353

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

The screenshot displays the 'surfsoln.Func(#AxSigmaAg)' configuration window. The left pane shows a tree view where 'surfsoln' is expanded to 'Functions', and 'A (2)' is selected, with 'AxSigmaAg (1)' highlighted. The right pane shows the configuration for 'surfsoln.Func(#AxSigmaAg)' with 'AxSigmaAg' set to 43353, 'TMin (K)' at 298.15, and 'TMax (K)' at 1000. Red arrows point from the text boxes to these specific values in the interface.

Similarly, function
AxSigmaPb= 27243

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

At 1000 K: $A_{Ag} = 47329$, $\sigma_{Ag} = 0.916$. Thus $A_{Ag}\sigma_{Ag} = 43353$ J/mol (4)
 $A_{Pb} = 70215$, $\sigma_{Pb} = 0.388$. Thus, $A_{Pb}\sigma_{Pb} = 27243$ J/mol (4)

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

surface solution

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

The screenshot shows the FactSage software interface. On the left, a hierarchical tree displays the following structure:

- Ternary Interpolations (0)
 - Interactions (3)
 - (0) Ag:Pb
 - (1) Ag:Pb
 - (2) Ag:Pb
 - surff (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)

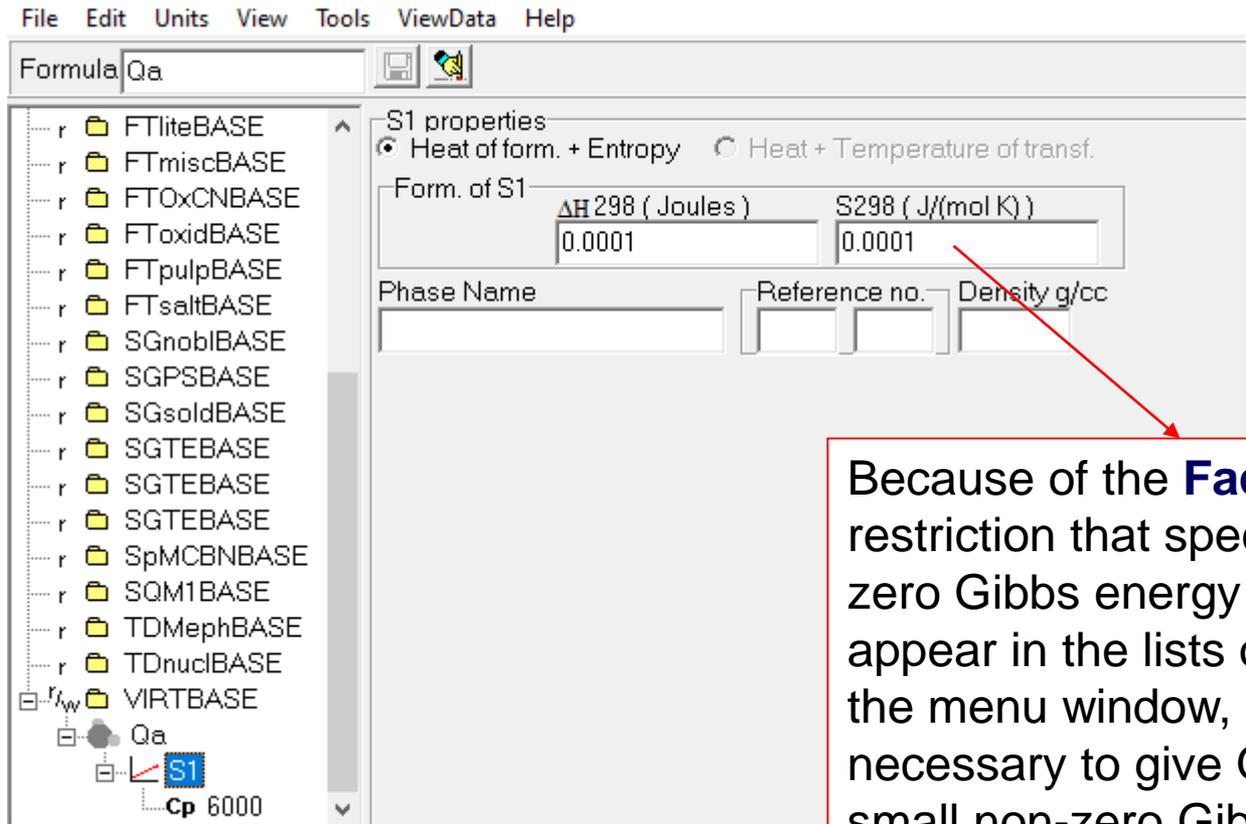
On the right, the detailed view for the selected end-member (0) Ag(Qa) is shown:

- A0: 1
- Z(Ag(Qa)): 1
- Stoic.: 1
- Name: Ag(Qa)
- Formula: Ag(Qa)
- Gibbs Energy Function: Ag#liquid + #AxSigmaAg V298;Therm. expans.;Compress.;Bulk Mod.
- Status: Normal (selected)
- X max: 1

$$g_{1000\text{K}}^{E(\text{bulk})} = X_{\text{Ag}} X_{\text{Pb}} (6741.7 - 1464.8 X_{\text{Ag}} X_{\text{Pb}} - 1978 X_{\text{Ag}}^2 X_{\text{Pb}}^2) \quad (4)$$

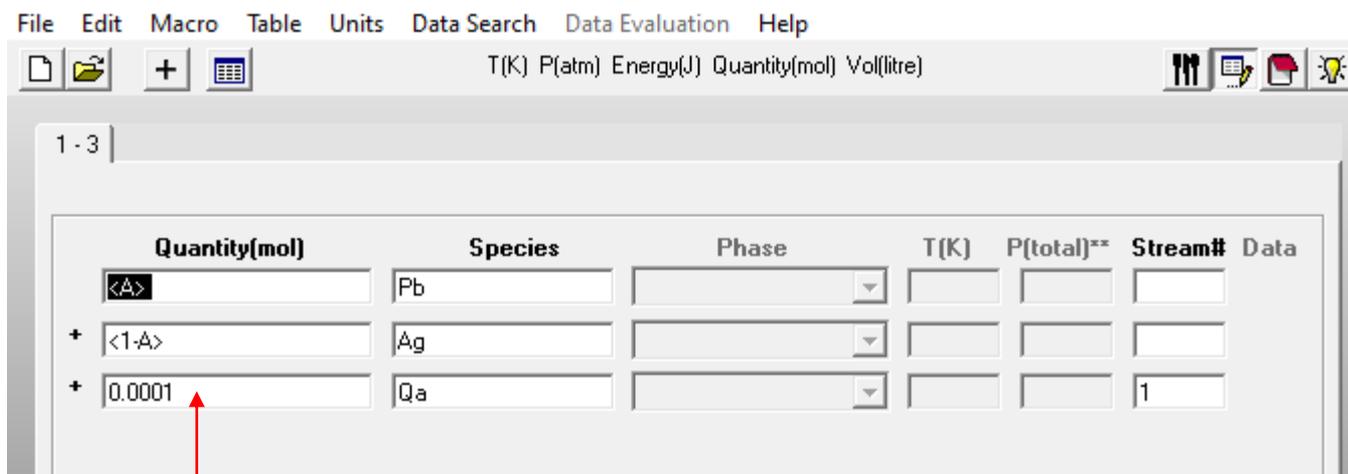
$$g_{1000\text{K}}^{E(\text{surf})} = 0.83 g^{E(\text{bulk})}$$

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



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



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

File Units Parameters Help

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

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> | | T(K) | P(atm) | Product H(J) |
|-----|-----|------|--------|--------------|
| 0.3 | | 1000 | 1 | |

10 steps Table

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

Output Edit Show Pages Final Conditions

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

FactSage 8.0

```

<A> Pb + <l-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 fraction
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 fraction
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

$$\mu(Qa) = RT \ln a(Qa) = 8.315(1000) \ln (53.978) = A\sigma$$

$$A = (0.13854)(47329) + 0.86146(70215). \text{ Therefore } \sigma = 0.495 \text{ N/m}$$