

# **FactSage Practical**

## **MSE302**

### **Practical 5. Equilib Module**

#### Advanced Applications

# Acknowledgements

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# Outline

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# Databases in FactSage for Steelmaking Applications

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In this section, we will use the Equilib Module of FactSage to solve some real-world questions regularly faced in the steel industry. While here we present you the steelmaking applications, you should be aware that FactSage has also found wide applications in the fields of alloy design/development, extraction of base metals, etc. Please review the Documentation Module to find the applications of different FACT databases. The Help Files also include a number of advanced industrial examples.

First, let us review the FactSage databases which are particularly developed for **steelmaking** applications (pyrometallurgical extraction and solidification) as well as some key phase models.

# Databases in FactSage for Steelmaking Applications

Database	Description
FactPS	All gaseous species, stoichiometric solids and liquids.
FToxid	Frequently updated <b>oxide</b> database containing (i) a large number of condensed solution phases (slag, spinel, monoxide, olivine, etc.); and (ii) pure solids and liquids, <b>but no gaseous species</b> .
FTmisc	FeLq solution which is the most reliable liquid steel database for steelmaking calculations, for example, slags/refractories/gases/ <b>molten iron</b> .
FSStel	Solid and liquid steel phases (also includes small number of gases, oxides, sulfides, nitrides, etc.) and is used for: (i) steel solidifications and alloy design; and (ii) liquid steel: reasonable calculations for steelmaking applications.

Database priority for steelmaking calculations:

(a) FToxid > FTmisc > FactPS: without FSStel for pyrometallurgical calculations.

(b) FToxid > FSStel > FactPS: with FSStel for steel solidification related calculations.

# FToxid Database: Main Solution Phases

**Main solution phases when  $T > 1550$  °C (steelmaking)**

**Note:** these phases may still exist even when  $T < 1550$  °C.

Phase	Description
Slag [I]-option	<b>Major oxide components</b> $\text{Al}_2\text{O}_3$ - $\text{CaO}$ - $\text{FeO}$ - $\text{Fe}_2\text{O}_3$ - $\text{MgO}$ - $\text{SiO}_2$ If the system contains other oxide components, for example, $\text{MnO}$ , $\text{Mn}_2\text{O}_3$ , $\text{CoO}$ , $\text{NiO}$ , $\text{PbO}$ , $\text{ZnO}$ , $\text{TiO}_2$ , $\text{Ti}_2\text{O}_3$ , etc. please consult Documentation for the limitations. Also, the gas solubility such as S ( $\text{SO}_2$ ), P, H (OH), N, C, F, ... is considered.
Spinel [I]-option	(SPIN) can be described as $(\text{Mg}, \text{Fe}, \text{Mn}, \text{Co}, \text{Ni}, \text{Zn})[\text{Al}, \text{Fe}, \text{Cr}, \text{Co}, \text{Mn}, \text{Va}]_2\text{SiO}_4$ , extensive solid solution containing $\text{MgAl}_2\text{O}_4$ , $\text{MgCr}_2\text{O}_4$ , $\text{MgFe}_2\text{O}_4$ , $\text{FeCr}_2\text{O}_4$ , $\text{Fe}_3\text{O}_4$ , $\text{FeAl}_2\text{O}_4$ , $\text{Cr}_3\text{O}_4$ , $\text{MnAl}_2\text{O}_4$ , $\text{MnCr}_2\text{O}_4$ , $\text{MnFe}_2\text{O}_4$ , etc.
Monoxide	(MeO_) can be described as $\text{CaO}$ - $\text{MgO}$ - $\text{FeO}$ - $\text{Fe}_2\text{O}_3$ - $\text{MnO}$ - $\text{NiO}$ - $\text{Al}_2\text{O}_3$ - $\text{Cr}_2\text{O}_3$ -etc. Covering most famously: lime ( $\text{CaO}$ ), periclase ( $\text{MgO}$ ) and wüstite ( $\text{FeO}$ ). [I]-option should be considered especially when $\text{CaO}$ and $\text{MgO}$ exist together.

# FToxid Database: Main Solution Phases

**Main solution phases when  $T > 1550$  °C (steelmaking)**

**Note:** these phases may still exist even when  $T < 1550$  °C.

Phase	Description
$\alpha$ -, $\alpha'$ -Ca <sub>2</sub> SiO <sub>4</sub>	(aC2S, bC2S) Ca <sub>2</sub> SiO <sub>4</sub> (CS <sub>2</sub> ) rich solution with limited solubility of Mg <sub>2</sub> SiO <sub>4</sub> , Fe <sub>2</sub> SiO <sub>4</sub> , Mn <sub>2</sub> SiO <sub>4</sub> , etc.
Olivine	(Oliv) can be described as (Mg, Fe, Ca, Mn, Ni, Zn, Co, Cr, etc.) <sub>2</sub> SiO <sub>4</sub> , covering forsterite (Mg <sub>2</sub> SiO <sub>4</sub> ), fayalite (Fe <sub>2</sub> SiO <sub>4</sub> ), $\gamma$ -Ca <sub>2</sub> SiO <sub>4</sub> , monticellite (CaMgSiO <sub>4</sub> ), tephroite (Mn <sub>2</sub> SiO <sub>4</sub> ), [I]-option is used when Ca <sub>2</sub> SiO <sub>4</sub> , exists.
Corundum [I]-option	(CORU) can be described as (Al, Cr, Fe, Mn) <sub>2</sub> O <sub>3</sub> . Solid miscibility gaps exist between the constituents.
Mullite	(Mull) non-stoichiometric Al <sub>6</sub> Si <sub>2</sub> O <sub>13</sub> with possible solubility of B. (MulF) stoichiometric Al <sub>6</sub> Si <sub>2</sub> O <sub>13</sub> with dilute Fe <sub>6</sub> Si <sub>2</sub> O <sub>13</sub> .

# FToxid Database: Main Solution Phases

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**Main solution phases when  $T > 1550$  °C (steelmaking)**

**Note:** these phases may still exist even when  $T < 1550$  °C.

Phase	Description
Mn/Ti oxides	<ul style="list-style-type: none"><li>✓ ilmenite (ILME): <math>\text{FeTiO}_3</math> (ilmenite)-<math>\text{Ti}_2\text{O}_3</math>-<math>\text{MgTiO}_3</math>-<math>\text{MnTiO}_3 + \text{Al}_2\text{O}_3</math></li><li>✓ pseudo-brookite (PSEU): <math>\text{Ti}_3\text{O}_5</math>-<math>\text{FeTi}_2\text{O}_5</math>-<math>\text{MgTi}_2\text{O}_5</math>-<math>\text{MnTi}_2\text{O}_5</math></li><li>✓ Ti-spinel (TiSp): <math>(\text{Mg, Fe, Mn})[\text{Mg, Fe, Mn, Ti, Al}]_2\text{O}_4</math></li><li>✓ Rutile (TiO2): <math>\text{TiO}_2 + \text{Ti}_2\text{O}_3</math>-<math>\text{ZrO}_2</math> solid solution</li></ul>



# FToxid Database: Main Solution Phases

## Main solution phases when $T < 1550$ °C (solidification of slag)

Phase	Description
Wollastonite	(Woll) can be described as $(\text{Ca, Mg, Mn})\text{SiO}_3$ which is a $\text{CaSiO}_3$ -rich phase stable below 1300 °C. Pseudo-wollastonite is stoichiometric $\text{CaSiO}_3$ stable below 1550 °C.
Pyroxene	(pPyr, oPyr, cPyr) $(\text{Mg, Ca, Fe}^{\text{II}})[\text{Mg, Fe}^{\text{II}}, \text{Fe}^{\text{III}}, \text{Al}]\{\text{Al, Fe}^{\text{III}}, \text{Si}\}\text{SiO}_6$ , which is a $\text{MgSiO}_3$ -rich phase stable below 1560 °C. proto-, ortho-, low-clino-pyroxene exist. Clino-pyroxene is a $\text{CaMgSi}_2\text{O}_6$ -rich phase which is stable below 1390 °C.
Rhodonite	(Rhod) $(\text{Mn, Ca})\text{SiO}_3$ which is a $\text{MnSiO}_3$ -rich solid solution stable below 1300 °C.

# FToxid Database: Main Solution Phases

**Main solution phases when  $T < 1550$  °C (mould flux, Na<sub>2</sub>O-containing system)**

Phase	Description
Nepheline	(Neph) NaAlSiO <sub>4</sub> with excess SiO <sub>2</sub> .
Carnegeite	(Carn) NaAlSiO <sub>4</sub> with excess SiO <sub>2</sub> .
NaAlO2	(NASl) low temperature-NaAlO <sub>2</sub> with excess NaAlSiO <sub>4</sub> .
NaAlO2	(NASh) high temperature-NaAlO <sub>2</sub> with excess NaAlSiO <sub>4</sub> .
Combeite	(NCSO) Na <sub>4</sub> CaSi <sub>3</sub> O <sub>9</sub> (bombeite) - Na <sub>2</sub> Ca <sub>2</sub> Si <sub>3</sub> O <sub>9</sub> solid solution.
Feldspar	(Feld) complete solution between Anorthite (CaAl <sub>2</sub> Si <sub>2</sub> O <sub>8</sub> ) and Albite (NaAlSi <sub>3</sub> O <sub>8</sub> )
NCA2	The structure can be described as (Na <sub>2</sub> , Ca)O · Na <sub>2</sub> O · 2Al <sub>2</sub> O <sub>3</sub> .
C3A1	The structure can be described as Ca <sub>3</sub> Al <sub>2</sub> O <sub>6</sub> dissolving Na <sub>2</sub> O.

# FToxid Database: Main Solution Phases

**Main solution phases in the CaO-Al<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub>-FeO-Fe<sub>2</sub>O<sub>3</sub> system with high oxygen partial pressure (e.g., Air)**

Phase	Description
CAFS	The structure can be described as $\text{Ca}_2(\text{Al}, \text{Fe}^{\text{III}})_8\text{SiO}_{16}$ .
CAF6	The structure can be described as $\text{Ca}(\text{Al}, \text{Fe}^{\text{III}})_{12}\text{O}_{19}$ .
CAF3	The structure can be described as $\text{Ca}(\text{Al}, \text{Fe}^{\text{III}})_6\text{O}_{10}$ .
CAF2	The structure can be described as $\text{Ca}(\text{Al}, \text{Fe}^{\text{III}})_4\text{O}_7$ .
CAF1	The structure can be described as $\text{Ca}(\text{Al}, \text{Fe}^{\text{III}})_2\text{O}_4$ .
C2AF	The structure can be described as $\text{Ca}_2(\text{Al}, \text{Fe}^{\text{III}})_2\text{O}_5$ .
C3AF	The structure can be described as $\text{Ca}_3(\text{Al}, \text{Fe}^{\text{III}})_2\text{O}_6$ .

# FTmisc Database

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<b>Phase</b>	<b>Description</b>
FeLQ	Liquid Fe containing Ag, Al, B, Ba, C, Ca, Ce, Co, Cr, Cu, H, Hf, La, Mg, Mn, Mo, N, Nb, Nd, Ni, O, P, Pb, Pd, S, Si, Sn, Ta, Th, Ti, U, V, W, Zr. This phase is better suited for calculations involving iron and steelmaking processes (optimized for iron-rich solutions only).

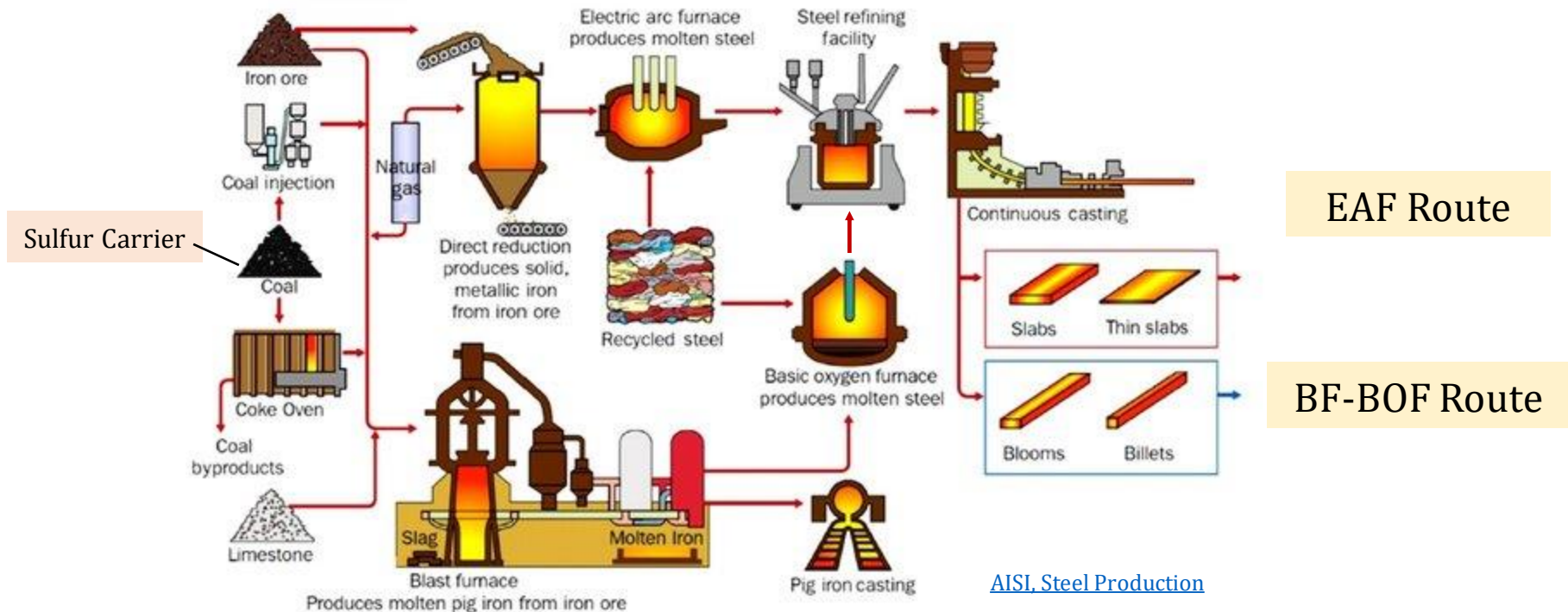
# FSStel Database

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Phase	Description
FCC/BCC	Fe, Carbide, and Nitride are all treated as FCC phases. ✓ Fe with N and C: use [J]-option (3-miscibility gaps) ✓ Fe with N or C: use [I]-option (2-miscibility gaps) For BCC phase, [I]-option is recommended.
FCC ordered phase BCC ordered phase	(FCC_L12) and (BCC_B2) normally slow down the calculations significantly. If you are not really interested in order/disorder transitions, do not select these ordered phases.
Carbon	When the C content is lower than ~1%, <b>metastable</b> Fe <sub>3</sub> C is normally formed instead of stable solid carbons. Therefore, in the selection of solid phases, “unselect” solid carbon phases to permit the appearance of <b>metastable</b> Fe <sub>3</sub> C.

# Example 1: Desulfurization (Background)

## Background: How Steel is Made

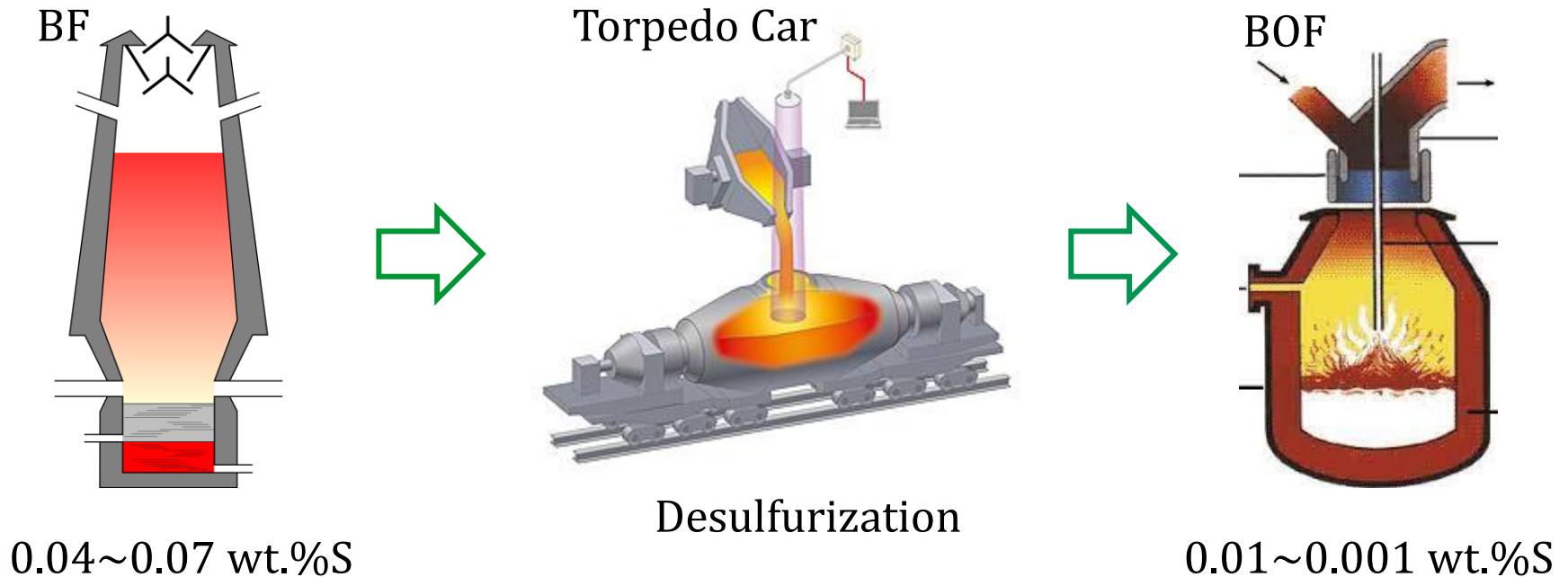


For the BF-BOF Route, there are two “spots” for desulfurization:

- (a) Hot Metal (Liquid Iron): after BF in torpedo car or desulfurization station
- (b) Liquid Steel: during ladle treatment

# Example 1: Desulfurization (Background)

## Background: Desulfurization of Hot Metal



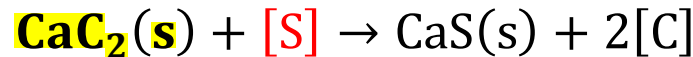
The hot metal tapped out of the BF typically contains  $0.04 \sim 0.07 \text{ wt.\%S}$ ; the BOF must be charged with de-sulfurized hot metal containing  $0.01 \sim 0.001 \text{ wt.\%S}$ . The sulfur removal is performed at a desulfurization station, e.g., torpedo car.

# Example 1: Desulfurization (Background)

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## Background: Desulfurization of Hot Metal

To remove sulfur from the hot metal, a suitable desulfurizing agent is added. The following agents are usually considered (highlighted in yellow):



**Note:** [Element] represents the element dissolved in the hot metal.

In the following pages, we will use the Equilib Module to compare the efficiency of these desulfurizing agents and to calculate the exact amount of desulfurizing agent that is required to achieve the desired sulfur content.

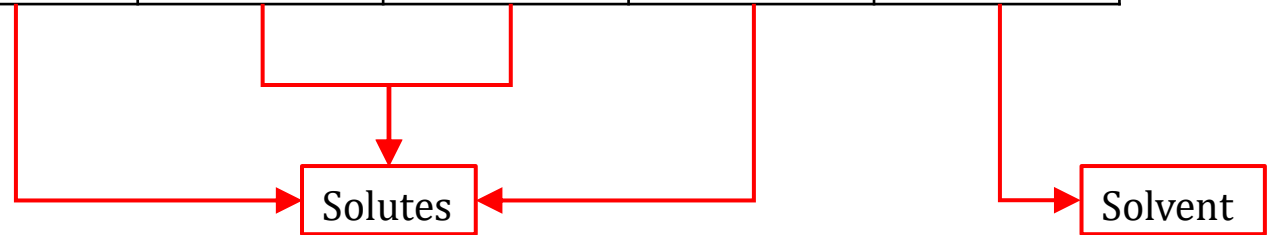


# Example 1: Desulfurization (Basic Example)

## Basic Example: Desulfurization of Hot Metal Using Mg

Let us assume the composition of hot metal (wt.%):

Element	C	Si	Mn	S	Fe
wt.%	4.50	0.50	0.60	0.065	94.335



**Note:** the main difference between hot metal and liquid steel is the content of carbon.

Now, we will add varying amounts of Mg to this hot metal to remove S as solid MgS. Our calculation will be based on 100 g hot metal.

# Example 1: Desulfurization (Basic Example)

## Basic Example: Desulfurization of Hot Metal Using Mg

The screenshot shows the 'Reactants' window in the Equilib software. The window title is 'Equilib - Reactants'. The menu bar includes File, Edit, Table, Units, Data Search, Data Evaluation, and Help. The toolbar contains icons for file operations and a 'Reactants Window' icon. The main area displays a table with the following data:

Quantity(mol)	Species	Phase	T(C)	P(total)**	Stream#	Data
1	C					
+ 1	Si					
+ 1	Mn				1	
+ 1	S				1	
+ 1	Fe				1	
+ 1	Mg				2	

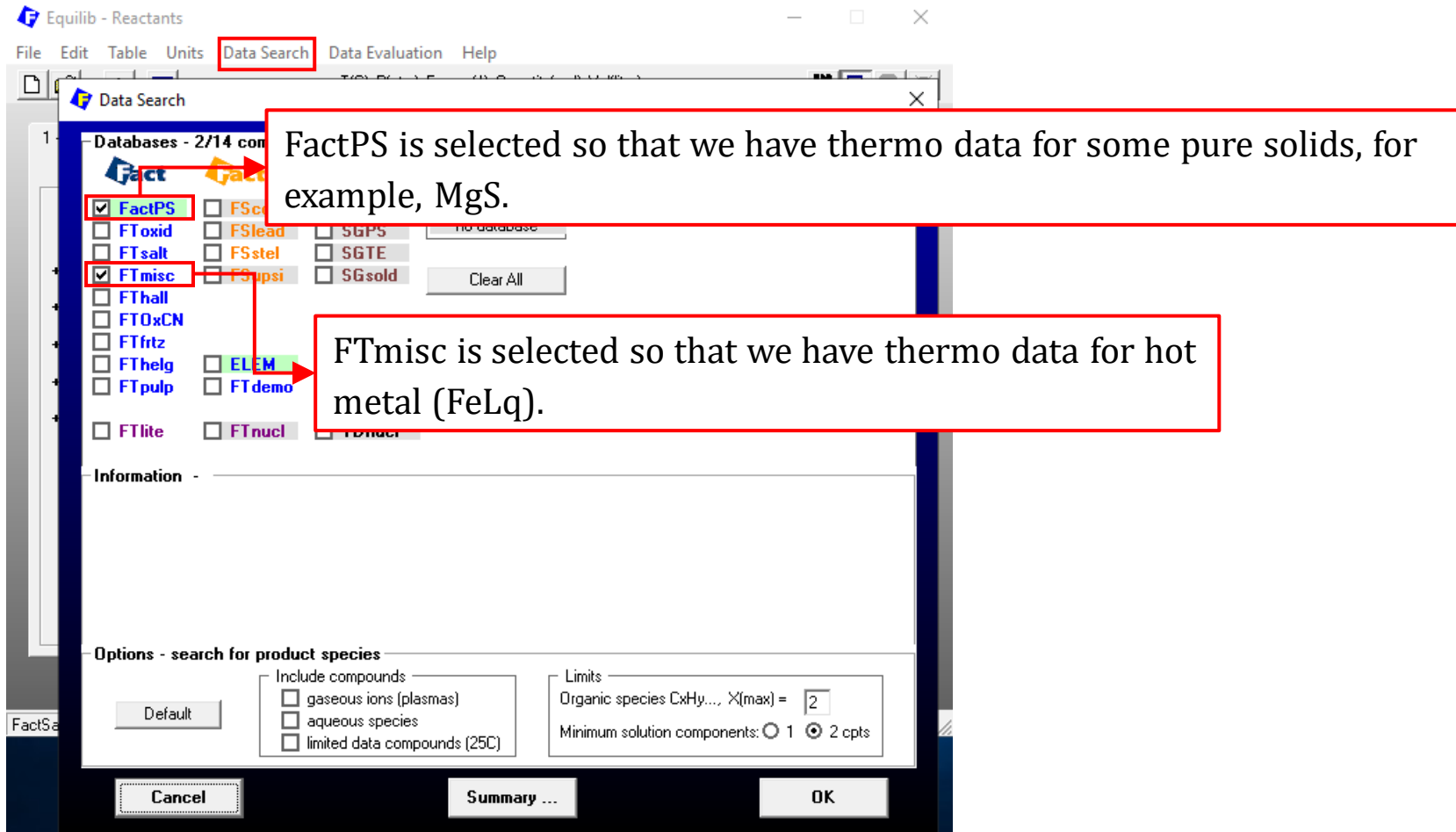
Red boxes and arrows highlight the following elements:

- The 'Reactants Window' title bar.
- The 'Species' column containing C, Si, Mn, S, Fe, and Mg.
- A box labeled 'Components of hot metal.' pointing to the Si, Mn, S, and Fe species.
- A box labeled 'Desulfurizing agent.' pointing to the Mg species.

At the bottom of the window, there is a 'Next >>' button and a status bar showing 'FactSage 7.3', 'Compound: 1/14 databases', and 'Solution: 0/15 databases'.

# Example 1: Desulfurization (Basic Example)

## Basic Example: Desulfurization of Hot Metal Using Mg



Equilib - Reactants

File Edit Table Units **Data Search** Data Evaluation Help

Databases - 2/14 con

FactPS  FSc

FToxid  FSlead  SGPS

FTsalt  FSstel  SGTE

FTmisc  FSupsi  SGsold

FTall  ELEM

FToxCN  FTdemo

FTfritz  FTnucl

FThelg  FTnucl

FTpulp  FTnucl

FTlite  FTnucl

Information -

Options - search for product species

Default

Include compounds

gaseous ions (plasmas)

aqueous species

limited data compounds (25C)

Limits

Organic species CxHy..., X(max) = 2

Minimum solution components:  1  2 cpts

Cancel Summary ... OK

FactPS is selected so that we have thermo data for some pure solids, for example, MgS.

FTmisc is selected so that we have thermo data for hot metal (FeLq).

# Example 1: Desulfurization (Basic Example)

## Basic Example: Desulfurization of Hot Metal Using Mg

The screenshot shows the 'Equilib - Reactants' window in FactSage 7.3. The interface includes a menu bar (File, Edit, Table, Units, Data Search, Data Evaluation, Help) and a toolbar. A table lists the reactants for the desulfurization process. Red boxes and arrows highlight specific features: the units 'g' for quantity, the mass values for each species, the 'Initial Conditions' checkbox, and the 'Next >>' button.

Quantity(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
4.50	C					
+ 0.50	Si					
+ 0.60	Mn				1	
+ 0.065	S				1	
+ 94.335	Fe				1	
+ <A>	Mg				2	

Annotations:

- Select Units. Use "g" for Quantity.
- Masses of components of hot metal.
- Varying amounts of Mg.
- We are **not** considering the change in thermo properties. No need to check "Initial Condition".

# Example 1: Desulfurization (Basic Example)

## Basic Example: Desulfurization of Hot Metal Using Mg

Equilib - Menu: last system  
File Units Parameters Help

Selection - Equilib - no results -  
File Edit Show Sort

Selected: 40/52 SOLID Duplicates selected.

+ Code	Species	Data	Phase
40	C(s)	FactPS	Graphite
41	C(s2)	FactPS	diamond
42	Mg(s)	FactPS	solid
43	MgC2(s)	FactPS	solid
44	Mg2C3(s)	FactPS	solid
45	Si(s)	FactPS	solid
46	SiC(s)	FactPS	Solid_Alpha
47	SiC(s2)	FactPS	Solid_Beta
48	Mg2Si(s)	FactPS	cF12-Fm(3)m
X 49	S(s)	FactPS	alpha_orthorh
X 50	S(s2)	FactPS	beta_monoclinic
+ 51	MgS(s)	FactPS	solid
+ 52	SiS(s)	FactPS	solid
+ 53	SiS2(s)	FactPS	solid
+ 54	Mn(s)	FactPS	Solid_Alpha
+ 55	Mn(s2)	FactPS	Solid_Beta
+ 56	Mn(s3)	FactPS	Solid_Gamma
+ 57	Mn(s4)	FactPS	Solid_Delta
+ 58	Mn3C(s)	FactPS	CEMENTITE
+ 59	Mn7C3(s)	FactPS	M7C3
+ 60	MnSi(s)	FactPS	cP8-P2(1)3

Reactants (6)  
(gram) 4.50 C

Products  
Compound species  
gas ideal real 0  
aqueous 0  
pure liquids 0  
+ pure solids 40  
\* - custom selection species: 40

Target  
- none -  
1000  
Quantity(g): 0

Final Conditions  
<A> <B>  
10 steps Table

permit selection of 'X' species Help Suppress Duplicates Edit priority list: FTmisc FactPS

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

Although we know the desulfurization product is MgS, we choose to select all the pure solids. This does not mean we have to do so. FactSage will determine which solid(s) should exist under the given conditions based on the “Gibbs energy minimization” principle. Of course, you can select MgS only.

You can edit the priority list. Here, we follow the sequence: FTmisc > FactPS.

# Example 1: Desulfurization (Basic Example)

## Basic Example: Desulfurization of Hot Metal Using Mg

Equilib - Menu: last system

File Units Parameters Help

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

**Reactants (6)**  
(gram) 4.50 C + 0.50 Si + 0.60 Mn + 0.05 S

**Products**

Compound species  
 gas  ideal  real 0  
 aqueous 0  
 pure liquids 0  
 pure solids 40  
\* - custom selection species: 40

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

**Solution phases**

*	+	Base-Phase	Full Name
	<input checked="" type="checkbox"/>	FTmisc-FeLQ	Fe-liq
	<input type="checkbox"/>	FTmisc-MAT	Matte
	<input type="checkbox"/>	FTmisc-FeS_	FeS-liq
	<input type="checkbox"/>	FTmisc-MAT2C	C-Liq(Matte/Metal)
	<input type="checkbox"/>	FTmisc-PYRR	C-Pyrrhotite
	<input type="checkbox"/>	FTmisc-BCCS	bcc
	<input type="checkbox"/>	FTmisc-FCCS	fcc
	<input type="checkbox"/>	FTmisc-MS-c	MeS_cubic

Legend  
+ - selected 1  
 Show  all  selected  
species: 6  
solutions: 1

Custom Solutions  
0 fixed activities

**Information...**  
Solution Phase FTmisc-FeLQ  
Fe-liq steel(I-H Jung model). Don't use with any other liq metal phase. For Iron/Steelmaking Processes, not solidification. Fe-rich(not for stainless)  
The components in FTmisc-FeLQ for the current calculation are:  
Fe, C, Mn, S, Si, Mg

**Final Conditions**

<A>	<B>	T(C)	P(atm)	Product H(J)
0.5		1000	1	

10 steps  Table

**Equilibrium**  
 normal  normal + transitions  
 transitions only  
 open

FactSage 7.3

# Example 1: Desulfurization (Basic Example)

## Basic Example: Desulfurization of Hot Metal Using Mg

Equilib - Menu: last system

File Units Parameters Help

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

**Reactants (6)**

(gram) 4.50 C + 0.50 Si + 0.60 Mn + 0.065 S + 94.335 Fe + <A> Mg

**Products**

Compound species

- gas  ideal  real 0
- aqueous 0
- pure liquids 0
- pure solids 40

\* - custom selection species: 40

Solution phases

*	+	Base-Phase	Full Name
	<input checked="" type="checkbox"/>	FTmisc-FeLQ	Fe-liq
		FTmisc-MATT	Matte
		FTmisc-FeS_	FeS-liq
		FTmisc-MAT2C	C-Liq(Matte/Metal)
		FTmisc-PYRRC	C-Pyrrhotite
		FTmisc-BCCS	bcc
		FTmisc-FCCS	fcc

Custom Solutions

- 0 fixed activities Details ...
- 0 ideal solutions

Pseudonyms

apply  Edit ...

Volume data

- assume molar volumes of solids and liquids = 0
- include molar volume data and physical properties data

paraequilibrium & Gmin edit

Total Species (max 5000) 46  
Total Solutions (max 200) 1  
Total Phases (max 1500) 41

**Final Conditions**

<A>	<B>	T(C)	P(atm)	Product H(J)
0	1	1400	1	

10 steps  Table

**Equilibrium**

- normal  normal + transitions
- transitions only
- open

Calculate >>

FactSage 7.3

The mass of desulfurization agent Mg is from 0 to 1 g in steps of 0.01 g.

# Example 1: Desulfurization (Basic Example)

## Basic Example: Desulfurization of Hot Metal Using Mg

Equilib - Results A=0 (page 1/101)

Output Edit Show Pages Final Conditions

Save or Print > T(C) P(atm) Energy(J) Quantity

Plot > Plot Results ...

Equilib Results file > Repeat Plot - ...

Stream File >

Format >

Fact-XML >

Fact-Optimal >

Fact-Function-Builder >

Refresh ...

Swap loops ...

+ 0.60 Mn + 0.065 S +

g =

1)

a=1.0000

% Fe

% C

% Mn

% S

% Si)

System component Amount/mol Amount/g

Fe 1.6892 94.335

Mn 1.0921E-02 0.60000

S 2.0271E-03 6.5000E-03

Si 1.7803E-02 0.50000

C 0.37467 4.5000

+ 0 gram C\_Graphite (1400 C, 1 atm, S1, a=0.81896)

+ 0

Final Conditions

<A>	<B>	T(C)	P(atm)
0	1	1400	1

We would like to see how the amount of sulfur in the hot metal decreases with the addition of Mg.

Results Processor: w:\MSE302\Exercise\Equi0.res

File Help

4.50 C + 0.50 Si + 0.60 Mn + 0.065 S +

Axes	Variables	Minimum	Maximum
	activity	0	12.392
	mole	0	2.1018
	mole fract. soln. species	0	0.807203
	gram	0	100.16
	weight % soln. species	0	94.394
	Alpha	0	1
	T(C)	1400	1400
	P(atm)	1	1
	Cp(J/K)	81.908	106.69
	G(J)	-1.9376E+05	-1.8936E+05
	Vol(litre)	0	0
	H(J)	1.3098E+05	1.3490E+05
	V(litre)	0	0
	S(J/K)	191.73	196.43
	-page-	1	101

0 selected

0 selected

Select

Repeat

Graph

Labels

size: 9 no: 4

chemical

integer #

none

offset

Display

color

colors ...

full screen

Viewer

Figure

Plot >>

FactSage 7.3 w:\MSE302\Exercise\Equi0.res 05Aug22 101 sets



# Example 1: Desulfurization (Basic Example)

## Basic Example: Desulfurization of Hot Metal Using Mg

Equilib - Results A=0 (page 1/101)

Output Edit Show Pages Final Conditions

Save or Print > T(C) P(atm) Energy(J) Quantity

Plot > Plot Results ...

Equilib Results file > Repeat Plot - ...

Stream File >

Format >

Fact-XML >

Fact-Optimal >

Fact-Function-Builder >

Refresh ...

Swap loops ...

4.50 C + 0.50 Si + 0.60 Mn + 0.065 S +

a=1.0000

% Fe

% C

% Mn

% S

% Si

System component	Amount/mol	Amount/g
Fe	1.6892	94.335
Mn	1.0921E-02	0.60000
S	2.0271E-03	6.5000E-02
Si	1.7803E-02	0.50000
C	0.37467	4.5000

gram C\_Graphite  
(1400 C, 1 atm, S1, a=0.81896)

Final Conditions			
<A>	<B>	T(C)	P(atm)
0	1	1400	1

Results Processor: w:\MSE302\Exercise\Equi0.res

Axes	Variables	Minimum	Maximum
	activity	0	12.392
	mole	0	2.1018
	mole fract. soln. species	0	0.807203
	gram	0	100.16
	weight % soln. species	0	94.394
	Alpha	0	1
	T(C)	1400	1400
	P(atm)	1	1
	Cp(J/K)	81.908	106.69
	G(J)	-1.9376E+05	-1.8936E+05
	Vol(litre)	0	0
	H(J)	1.3098E+05	1.3490E+05
	V(litre)		
	S(J/K)		
	-page-		

Choose S in the hot metal.

wt. %S ~ < A > graph.

# Example 1: Desulfurization (Basic Example)

## Basic Example: Desulfurization of Hot Metal Using Mg

Plot Species Selection - Equilib Results: vs

File Show Select

+	#	Species	Mole (min)	Mole (max)	Fraction (mi)
	45	Fe10S11	0	0	0
	46	Fe11S12	0	0	0
		<b>SOLUTIONS</b>			
	47	GAS	0	0	0
	48	FeLQ	2.0927	2.1018	0
		<b>ELEMENTS</b>			
	49	Fe_GAS	0	0	0
	50	Mn_GAS	0	0	0
	51	S_GAS	0	0	0
	52	Si_GAS	0	0	0
	53	Mg_GAS	0	0	0
	54	C_GAS	0	0	0
	55	Fe_FeLQ	1.6892	1.6892	0.803704
	56	Mn_FeLQ	1.0921E-02	1.0921E-02	5.1962E-03
	+ 57	S_FeLQ	1.2586E-07	2.0271E-03	5.9881E-08
	58	Si_FeLQ	1.7803E-02	1.7803E-02	8.4702E-03
	59	Mg_FeLQ	0	9.1863E-03	0
	60	C_FeLQ	0.374666	0.374666	0.178259

Display

source  phase  name  [page]

Clear

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

101 p

Choose wt.%S.

The amount of Mg.

Axes: weight % soln. species vs Alpha

Y-variable X-variable Swap Axes

Y-axis: weight % soln. species

X-axis: Alpha

maximum 0.1

minimum 0

tick every 0.02

maximum 1

minimum 0

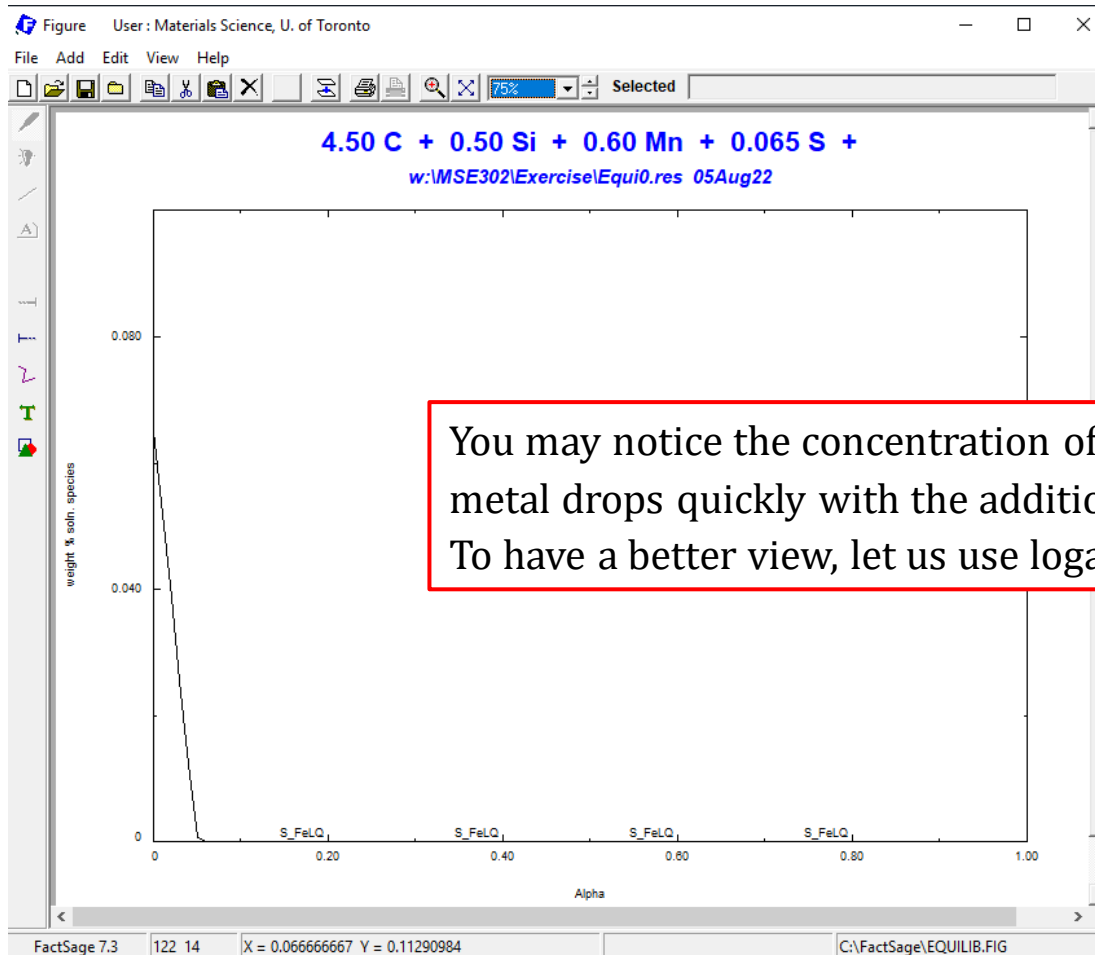
tick every 0.1

Cancel Refresh OK

You may need to manually adjust the maximum and minimum values.

# Example 1: Desulfurization (Basic Example)

## Basic Example: Desulfurization of Hot Metal Using Mg



You may notice the concentration of sulfur in the hot metal drops quickly with the addition of Mg. To have a better view, let us use logarithm for Y-axis.

# Example 1: Desulfurization (Basic Example)

## Basic Example: Desulfurization of Hot Metal Using Mg

activity  
mole  
mole fract. soln. species  
gram  
✓ weight % soln. species  
Alpha  
T(C)  
P(atm)  
Cp(J/K)  
G(J)  
Vol(litre)  
H(J)  
V(litre)  
S(J/K)  
- page -  
Y  
✓ log10(Y)  
ln(Y)  
exp(Y)  
1/Y  
phase distribution

Y-axis: log10(weight % soln. species)  
X-axis: Alpha

maximum 0  
minimum -10  
tick every 1

maximum 1  
minimum 0  
tick every 0.1

Cancel Refresh OK

Plot: log10(weight % soln. species) vs Alpha

4.50 C + 0.50 Si + 0.60 Mn + 0.065 S +

Axis	Variables	Minimum	Maximum
	activity	0	12.392
	mole	0	2.1018
	mole fract. soln. species	0	0.807203
	gram	0	100.16
Y-axis	weight % soln. species	0	94.394
X-axis	Alpha	0	1
	T(C)	1400	1400
	P(atm)	1	1
	Cp(J/K)	81.908	106.69
	G(J)	-1.9376E+05	-1.8936E+05
	Vol(litre)	0	0
	H(J)	1.3098E+05	1.3490E+05
	V(litre)	0	0
	S(J/K)	191.73	196.43
	- page -	1	101

Species: 1 selected

Graph: size: 9 no: 4

Display: color, reactants, file name

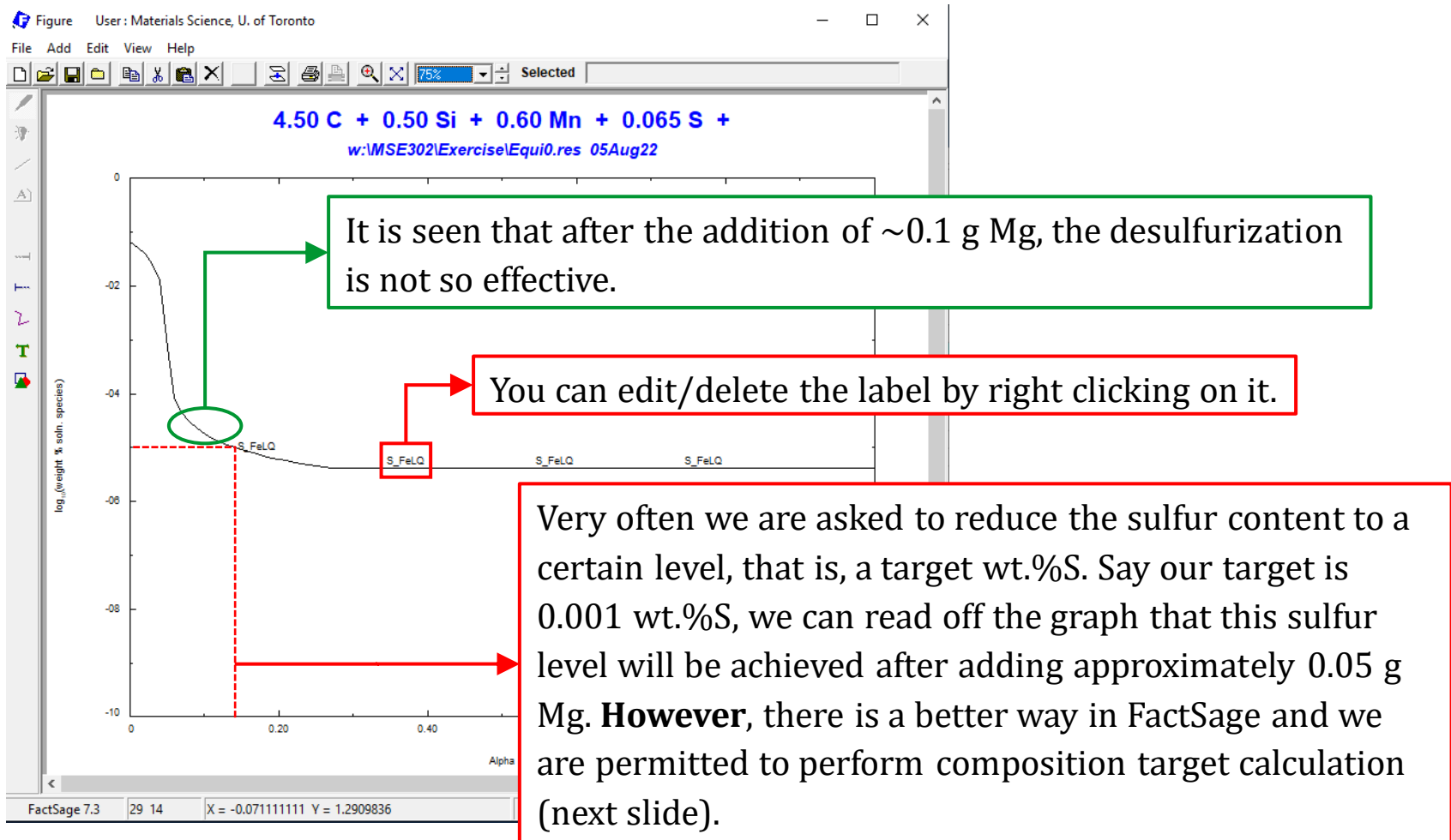
Plot >>

FactSage 7.3 w:\MSE302\Exercise\Equi0.res 05Aug22 101 sets

Back to the Plot window. Click on "Axes".

# Example 1: Desulfurization (Basic Example)

## Basic Example: Desulfurization of Hot Metal Using Mg



# Example 1: Desulfurization (Basic Example)

## Basic Example: Desulfurization of Hot Metal Using Mg

Equilib - Menu: last system  
File Units Parameters Help

Composition Target Calculation

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

Reactants (S)

Products

Compound species

Solution phases

*	+	Base-Phase	Full Name
	+	FTmisc-FeLQ	Fe-liq
		FTmisc-MATT	Matte
		FTmisc-FeS_	FeS-liq
			liq(Matte/Metal)
			C-Pyrrhotite
			bcc
		FTmisc-FCCS	fcc
		FTmisc-MS-c	MeS_cubic

Legend

+ selected 1

Show  all  selected

species: 6

solutions: 1

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

400 1

101 calculations

Composition Target

Solution MI53-FeLQ

Variable

species composition

log10 (species composition)

element composition

log10 (element composition)

species activity

log10(species activity)

- none (removes targets) -

Species

Code numbers (92-97)

Fe, C, Mn, ...

92

Element

Elements C Mg Si S Mn Fe

Element:

Values

Enter a single value - or enter a range of values 'first last step'

Element S

mass fraction: (0.001%)

Set the target sulfur content.

Cancel Help OK

This will change to "C" after setting the target.

Right click

# Example 1: Desulfurization (Basic Example)

## Basic Example: Desulfurization of Hot Metal Using Mg

The screenshot shows the FactSage 7.3 software interface. The title bar reads "Equilib - Menu: last system". The menu bar includes "File", "Units", "Parameters", and "Help". The main window displays the "Composition Target Calculation" dialog. The "Reactants (6)" field contains "(gram) 4.50 C + 0.50 Si + 0.60 Mn + 0.065 S + 94.335 Fe + <A> Mg". The "Products" section is set to "pure solids" with a quantity of 40. The "Solution phases" table is highlighted, showing the following data:

*	Base-Phase	Full Name
C	FTmisc-FeLQ	Fe-liq
	FTmisc-MATT	Matte
	FTmisc-FeS_	FeS-liq
	FTmisc-MAT2C	C-Liq(Matte/Metal)
	FTmisc-PYRRC	C-Pyrrhotite
	FTmisc-BCCS	bcc
	FTmisc-FCCS	fcc

The "Target" section is set to "none". The "Final Conditions" section shows "T(C)" set to 1400 and "P(atm)" set to 1. The "Equilibrium" section has "normal" selected. A "Calculate >>" button is visible at the bottom right. Red boxes and arrows highlight the "Composition Target Calculation" title, the "C" in the solution phases table, and the "Final Conditions" section.

Composition Target Calculation

Now we are performing composition target calculation.

We must leave this blank because we are calculating the required amount of Mg which gives the target sulfur content in hot metal.

Final Conditions

Equilibrium

# Example 1: Desulfurization (Basic Example)

## Basic Example: Desulfurization of Hot Metal Using Mg

Equilib - Results 1400 C, **A=0.0494**

Output Edit Show Pages Final Conditions

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

FactSage 7.3

T = 1400 C  
P = 1 atm  
V = 0 dm<sup>3</sup>

STREAM CONSTITUENTS

STREAM CONSTITUENTS	AMOUNT/gram
C	4.5000E+00
Si	5.0000E-01
Mn	6.0000E-01
S	6.5000E-02
Fe	9.4335E+01
*Mg	4.9405E-02

PHASE: Fe-liq

	EQUIL AMOUNT gram	MASS FRACTION	ACTIVITY
Fe	9.4335E+01	9.4395E-01	6.6655E-01
C	4.5000E+00	4.5028E-02	8.2029E-01
Mn	6.0000E-01	6.0038E-03	2.8711E-03
<b>S</b>	<b>9.9937E-04</b>	<b>1.0000E-05</b>	<b>3.0200E-06</b>
Si	5.0000E-01	5.0032E-03	4.6699E-05
Mg	8.9328E-04	8.9384E-06	4.9659E-02
TOTAL:	9.9937E+01	1.0000E+00	1.0000E+00

System component

System component	Amount/mol	Amount/gram	Mole fraction	Mass fraction
Fe	1.6892	94.335	0.80721	0.94395
Mn	1.0000E-01	6.0000	5.0100E-02	6.0000E-02
S	1.0000E-05	9.9937E-04	1.0000E-05	1.0000E-05
Si	1.0000E-01	5.0000	5.0032E-03	5.0032E-03
Mg	1.0000E-05	8.9328E-04	8.9384E-06	8.9384E-06

Final Conditions

<A>	<B>	T(C)	P(atm)	Product H(J)
		1400	1	

1 calculation

Calculate >>

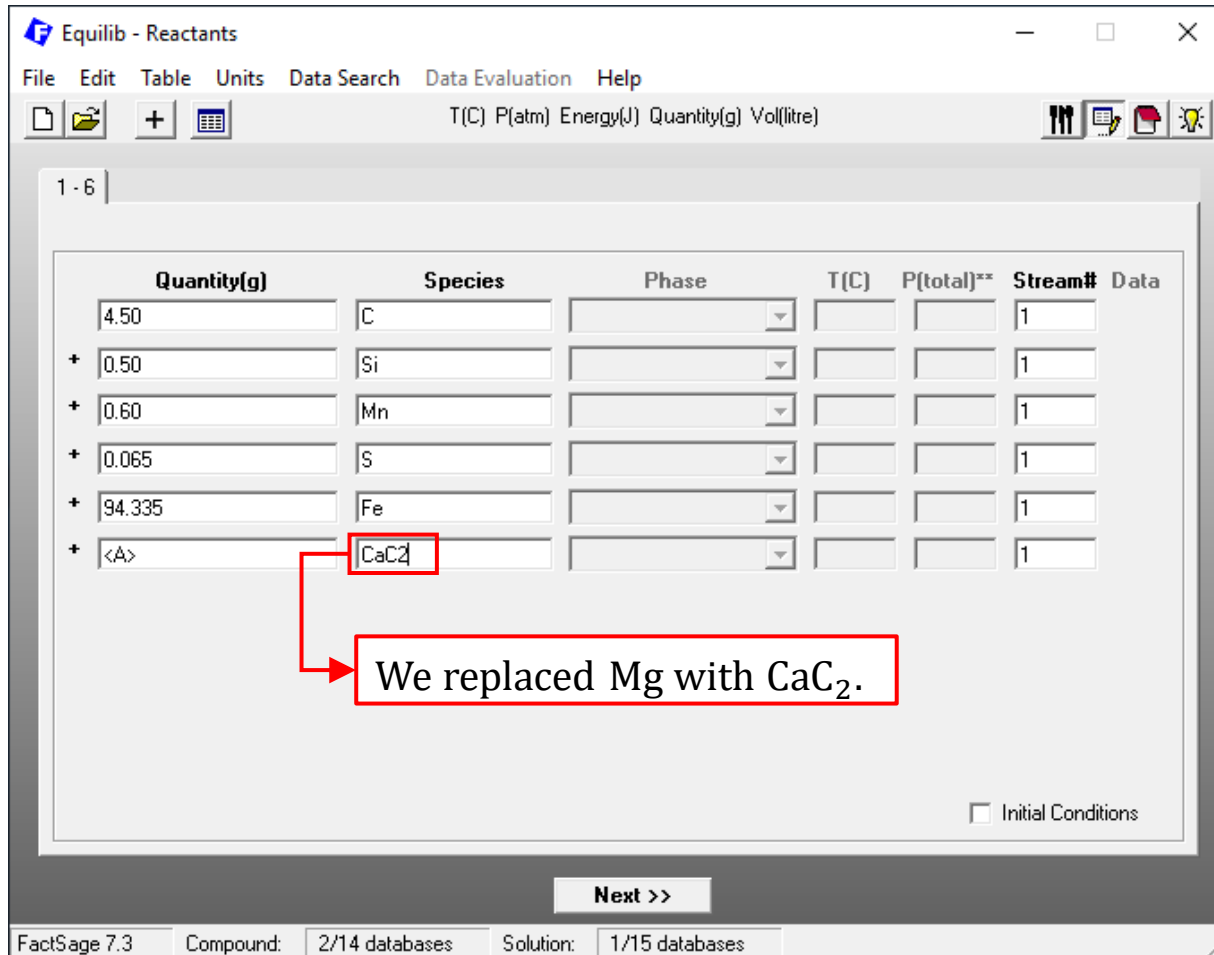
Composition Target Calculation

This is the mass of Mg required to achieve the desired sulfur content in the hot metal.



# Example 1: Desulfurization (Basic Example)

## Basic Example: Desulfurization of Hot Metal Using $\text{CaC}_2$



The screenshot shows the 'Equilib - Reactants' window in FactSage 7.3. The window contains a table with the following data:

Quantity(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
4.50	C				1	
+ 0.50	Si				1	
+ 0.60	Mn				1	
+ 0.065	S				1	
+ 94.335	Fe				1	
+ <A>	CaC <sub>2</sub>				1	

A red box highlights the 'CaC<sub>2</sub>' entry in the 'Species' column. A red arrow points from this box to a text box containing the text: "We replaced Mg with CaC<sub>2</sub>."

At the bottom of the window, there is a 'Next >>' button and a status bar showing 'FactSage 7.3', 'Compound: 2/14 databases', and 'Solution: 1/15 databases'.

# Example 1: Desulfurization (Basic Example)

## Basic Example: Desulfurization of Hot Metal Using $\text{CaC}_2$

Equilib - Menu: last system

File Units Parameters Help

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

**Reactants (6)**

(gram) 4.50 C + 0.50 Si + 0.60 Mn + 0.065 S + 94.335 Fe + <A> CaC2

**Products**

Compound species

- gas
- ideal
- real
- 0
- aqueous
- 0
- pure liquids
- 0
- pure solids
- 43

\* - custom selection  
species: 43

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

**Solution phases**

*	+	Base-Phase	Full Name
	<input checked="" type="checkbox"/>	FTmisc-FeLQ	Fe-liq
	<input type="checkbox"/>	FTmisc-MAT	Matte
	<input type="checkbox"/>	FTmisc-FeS_	FeS-liq
	<input type="checkbox"/>	FTmisc-MAT2C	C-Liq(Matte/Metal)
	<input type="checkbox"/>	FTmisc-PYRRC	C-Pyrrhotite
	<input type="checkbox"/>	FTmisc-BCCS	bcc
	<input type="checkbox"/>	FTmisc-FCCS	
	<input type="checkbox"/>	FTmisc-MS-c	

Legend  
+ - selected 1

species: 1  
solutions: 1

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

Pseudonyms  
apply   
Edit ...

Volume data  
 assume molar volumes of solids and liquids = 0  
 include molar volume data

**Final Conditions**

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

0 1 0.01 1400 1

10 steps  Table 101 calculations

**Equilibrium**

- normal
- normal + transitions
- transitions only
- open

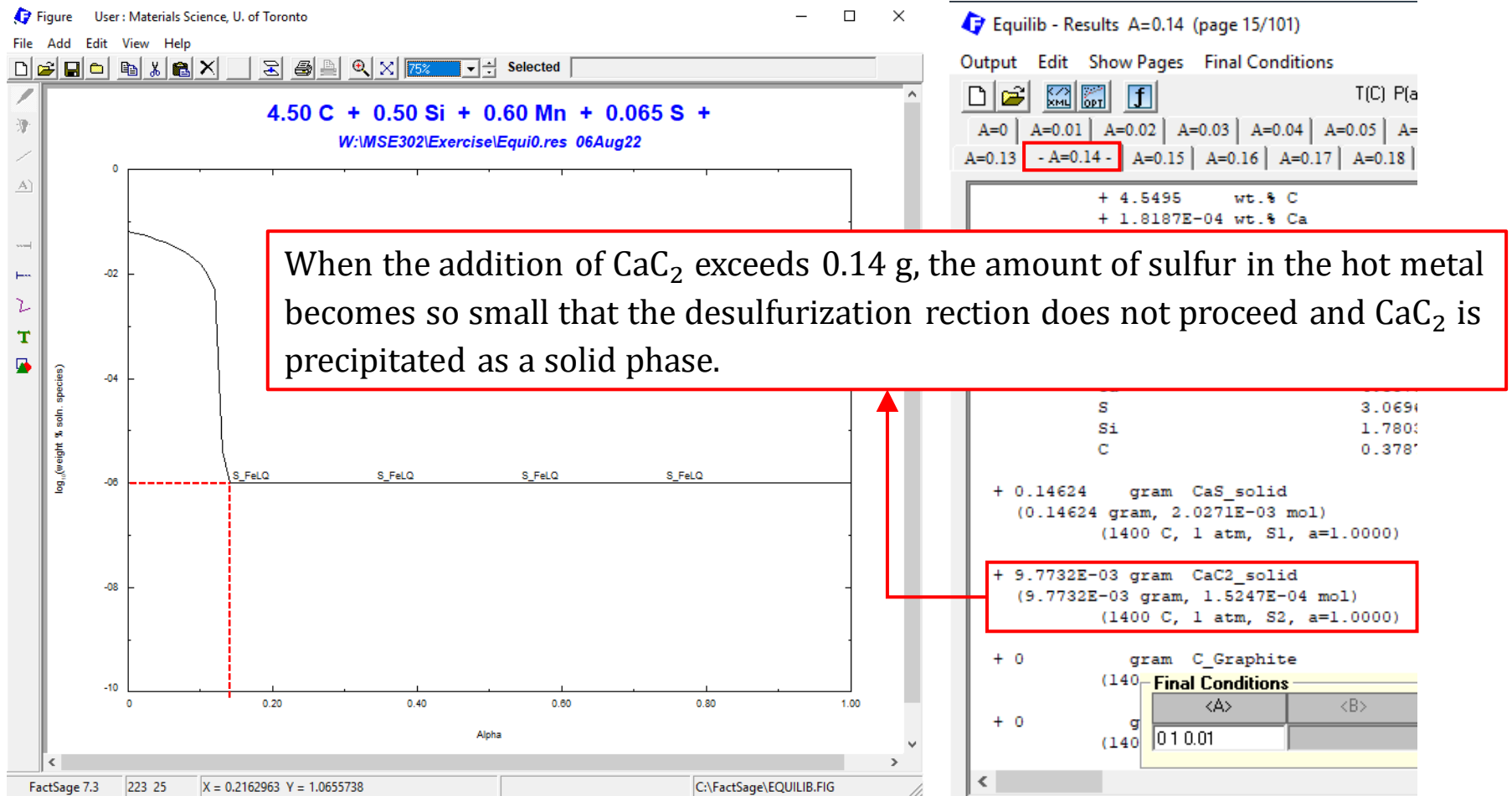
Calculate >>

FactSage 7.3

We keep all the settings, i.e., phase selection and final conditions same to the case where Mg was used.

# Example 1: Desulfurization (Basic Example)

## Basic Example: Desulfurization of Hot Metal Using $\text{CaC}_2$



# Example 1: Desulfurization (Basic Example)

## Basic Example: Desulfurization of Hot Metal Using $\text{CaC}_2$

**Composition Target Calculation**

Reactants (6): (gram) 4.50 C + 0.50 Si + 0.60 Mn + 0.065 S + 94.335 Fe + <A> CaC2

Products: pure solids 43

*	+	Base-Phase	Full Name
	C	FTmisc-FeLQ	Fe-liq
		FTmisc-MATT	Matte
		FTmisc-FeS_	FeS-liq
		FTmisc-MAT2C	C-Liq(Matte/Metal)
		FTmisc-PYRRC	C-Pyrrhotite
		FTmisc-BCCS	bcc
		FTmisc-FCCS	fcc
		FTmisc-MS-c	MeS_cubic

Composition target: Element S - FTmisc-FeLQ

Estimate ALPHA: **Leave it Blank.**

Final Conditions: T(C) 1400, P(atm) 1

**Composition Target** dialog:

- Variable: **element composition**
- Species: 95 Fe
- Element: S
- Values: Element S mass fraction: 0.00001 (0.001%)

Equilibrium: normal

Calculate >>

# Example 1: Desulfurization (Basic Example)

## Basic Example: Desulfurization of Hot Metal Using $\text{CaC}_2$

Equilib - Results 1400 C, A=0.1279

Composition Target Calculation

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

FactSage 7.3

T = 1400 C  
P = 1 atm  
V = 0 dm<sup>3</sup>

STREAM CONSTITUENTS	AMOUNT/gram
C	4.5000E+00
Si	5.0000E-01
Mn	6.0000E-01
S	6.5000E-02
Fe	9.4335E+01
*CaC <sub>2</sub>	1.2794E-01

PHASE: Fe-liq	EQUIL AMOUNT gram	MASS FRACTION	ACTIVITY
Fe	9.4335E+01	9.4350E-01	6.6285E-01
C	4.5479E+00	4.5487E-02	8.4085E-01
Ca	1.7895E-07	1.7898E-09	4.6917E-07
Mn	6.0000E-01	6.0010E-03	2.8460E-03
S	9.9984E-04	1.0000E-05	3.0379E-06
Si	5.0000E-01	5.0008E-03	4.7231E-05
TOTAL:	9.9984E+01	1.0000E+00	1.0000E+00

System component	Amount/mol	Amount/gram	Mole fraction	Mass fraction
Fe	1.6892	94.335	0.80568	0.94350
Mn	1.0000E-01	6.0000	5.0000E-02	6.0000E-02
Ca				
S				
Si				
C				

Final Conditions

<A>	<B>	T(C)	P(atm)	Product H(J)
		1400	1	

1 calculation

Calculate >>

# Example 1: Desulfurization (Basic Example)

## Basic Example: Desulfurization of Hot Metal Using CaO + Mg

Equilib - Reactants

File Edit Table Units Data Search Data Evaluation Help

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

1 - 7

Quantity(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
4.50	C				1	
+ 0.50	Si				1	
+ 0.60	Mn				1	
+ 0.065	S				1	
+ 94.335	Fe				1	
+ <A>	Mg				2	
+ <A>	CaO				2	

Initial Conditions

Next >>

FactSage 7.3 Compound: 2/14 databases Solution: 1/15 databases

This time, we are adding varying amount of CaO and Mg to remove the sulfur in the hot metal.

# Example 1: Desulfurization (Basic Example)

## Basic Example: Desulfurization of Hot Metal Using CaO + Mg

The screenshot shows the FactSage Equilib software interface. The main window is titled "Selection - Equilib - no results -". The "Reactants" section shows 7 species, and the "Products" section shows 130 pure solids selected. A table of selected species is displayed, listing their codes, species names, data sources, phases, and activities. A red box highlights the "pure solids" selection in the products list, and a text box explains that all pure solids are selected to determine stable pure solids after reaction. The "Edit priority list" field is set to "FTmisc FactPS".

Selected: 130/142    SOLID    Duplicates    selected    X denotes species excluded by default

- no results -

	+	Code	Species	Data	Phase	T	V	Activity	Minimum	Maximum
	+	74	C(s)	FactPS	Graphite		V			
	+	75	C(s2)	FactPS	diamond		V			
	+	76	Mg(s)	FactPS	solid		V			
	+	77	MgC2(s)	FactPS	solid		o			
	+	78	Mg2C3(s)	FactPS	solid		o			
	+	79	MgO(s)	FactPS	Periclase		V			
	+	80	MgCO3(s)	FactPS	magnesite_CaC		V			
	+	81	Si(s)	FactPS	solid		V			
	+	88	SiO2(s5)	FactPS	Cristobalite(l)		V			
	+	89	SiO2(s6)	FactPS	Cristobalite(h)		V			
	+	90	SiO2(s7)	FactPS	coesite		V			
	+	91	SiO2(s8)	FactPS	stishovite		V			
	+	92	Mg2Si(s)	FactPS	cf12-Fm(3)m		V			
	+	93	MgSiO3(s)	FactPS	low-clinoenstatit		V			
	+	94	MgSiO3(s2)	FactPS	ortho-enstatite		V			

permit selection of 'X' species    Help    Suppress Duplicates    Edit priority list: FTmisc FactPS

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

FactSage 7.3    w:\MSE3

We select all the pure solids and ask FactSage to determine the stable pure solids after reaction. Again, you don't have to do so because you probably already know what pure solids will form.

# Example 1: Desulfurization (Basic Example)

## Basic Example: Desulfurization of Hot Metal Using CaO + Mg

Equilib - Menu: last system

File Units Parameters Help

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

Reactants (7)

[gram] 4.50 C + 0.50 Si + 0.60 Mn + 0.065 S + 94.335 Fe + <A> Mg + <A> CaO

Products

Compound species

- gas
- ideal
- real
- 0
- aqueous
- 0
- pure liquids
- 0
- pure solids
- 130

\* - custom selection  
species: 130

Target

- none -

Estimate P(atm): 1.0

Quantity(g): 0

Solution phases

*	+	Base-Phase	Full Name
	<input checked="" type="checkbox"/>	FTmisc-FeLQ	Fe-liq
	<input type="checkbox"/>	FTmisc-MAT	Matte
	<input type="checkbox"/>	FTmisc-FeS_	FeS-liq
	<input type="checkbox"/>	FTmisc-MAT2C	C-Liq(Matte/Metal)
	<input type="checkbox"/>	FTmisc-PYRRC	C-Pyrrhotite
	<input type="checkbox"/>	FTmisc-BCCS	bcc
	<input type="checkbox"/>	FTmisc-FCCS	fcc
	<input type="checkbox"/>	FTmisc-MS-c	MeS_cubic

Legend

+ - selected 1

Show  all  selected

Custom Solutions

fixed activities Details ...

ideal solutions

Pseudonyms

apply  Edit ...

Volume data

assume molar volumes of solids and liquids = 0

include molar volume data and physical properties data

paraequilibrium & Gmin edit

Final Conditions

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

0 1 0.01 1400 1

10 steps  Table 101 calculations

normal  normal + transitions

transitions only

open Calculate >>

FactSage 7.3 w:\MSE302\Exercise\EquiDe-S\_Using\_Mg.DAT

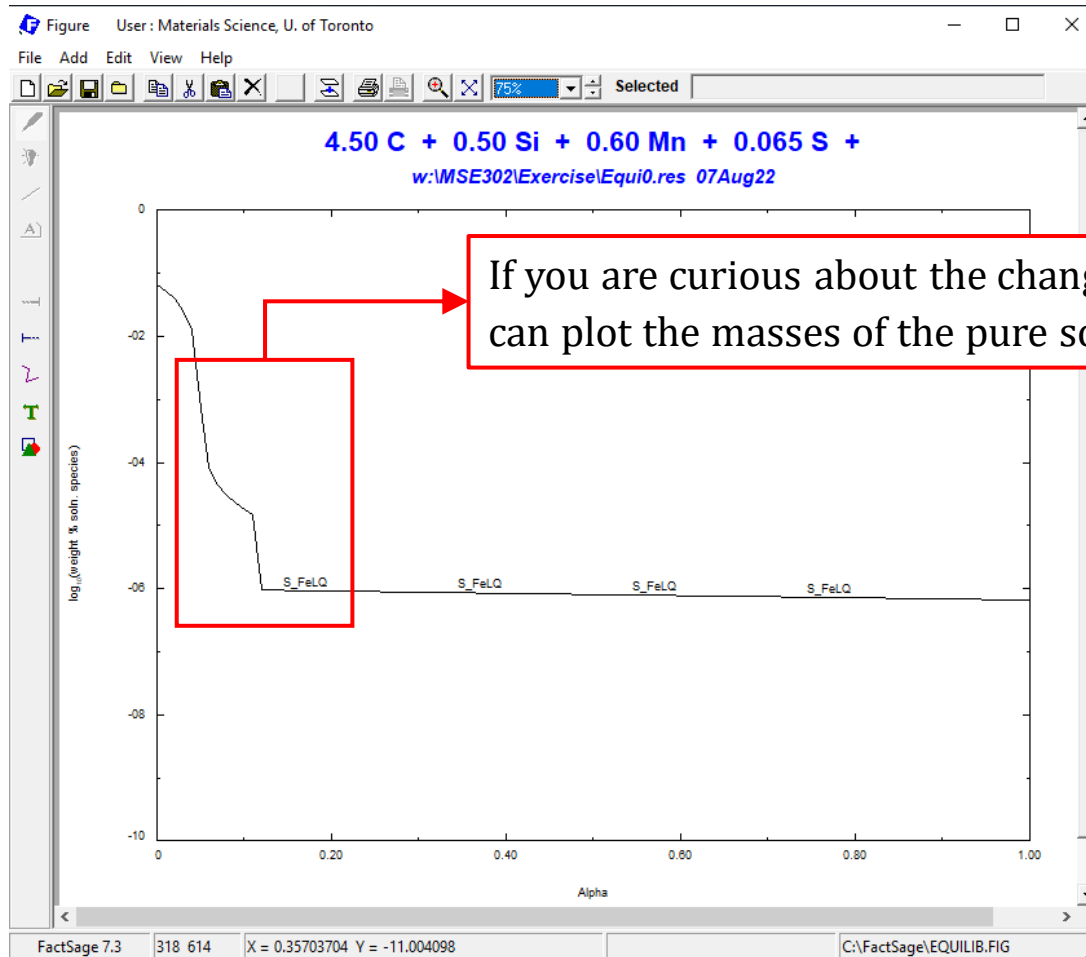
Select FeLQ for the hot metal.

The mass of both CaO and Mg are varied from 0 to 1.0 g, and the temperature is 1400 °C



# Example 1: Desulfurization (Basic Example)

## Basic Example: Desulfurization of Hot Metal Using CaO + Mg



If you are curious about the change in the slope of wt. %S~<A>, you can plot the masses of the pure solids against <A>.

# Example 1: Desulfurization (Basic Example)

## Basic Example: Desulfurization of Hot Metal Using CaO + Mg

Plot Species Selection - Equilib Results: gram vs Alpha

File Show Select

#	Species	Mole (min)	Mole (max)	Fraction (min)	Fraction (max)	Activity (min)	Activity (max)
153	Fe_FeLQ	1.6892	1.6892	0.806235	0.816116	0	0
160	C_FeLQ	0.343066	0.374666	0.165745	0.179035	0	0
2	C	0.343066	0.374666	0.165745	0.179035	0.663144	0.82257
+ 18	MgO	0	1.7832E-02	0	0	0	1
7	Si	1.7803E-02	1.7803E-02	8.4969E-03	8.6011E-03	4.0261E-05	4.6983E-
157	Si_FeLQ	1.7803E-02	1.7803E-02	8.4969E-03	8.6010E-03	0	0
+ 51	CaC2	0	1.5995E-02	0	0	0	1
+ 15	Mg	0	1.7832E-02	0	0	0	1
154	Mn_FeLQ	0	5.3789E-06	0	2.5987E-06	0	0
4	Mn	0	5.3789E-06	0	2.5987E-06	0	0
8	Mg	0	1.7832E-02	0	0	0	1
158	Mg_FeLQ	0	5.3789E-06	0	2.5987E-06	0	0
+ 75	CaS	0	1.1135E-03	0	0	0	1
156	S_FeLQ	2.0221E-08	2.0271E-03	9.7692E-09	9.6777E-04	0	0
6	S	2.0221E-08	2.0271E-03	9.7692E-09	9.6777E-04	1.8592E-09	1.9459E-
+ 43	MgS	0	1.1135E-03	0	0	0	1
155	Ca_FeLQ	0	5.3789E-06	0	2.5987E-06	0	0
3	Ca	0	5.3628E-06	0	2.5909E-06	0	7.6662E-

Double click on "Mole (max)" to sort the pure solids (highlighted in green) and choose the pure solids that are present, i.e., number of moles greater than 0.

Plot Species Selection - Equilib Result

File Show Select

- gas phase
- aqueous species
- pure liquids
- + pure solids
- FeLQ
- SOLUTIONS
- ELEMENTS
- 
- All
- Clear

Display:  source,  phase,  name,  [page]

Mass:  mole,  gram

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

Select Top: 15, 5 species selected

ignore species and phases with zero mass

Clear, Select..., OK

Click on the '+' column to add or remove species. 101 pages

# Example 1: Desulfurization (Basic Example)

## Basic Example: Desulfurization of Hot Metal Using CaO + Mg

Plot: gram vs Alpha

File Help

4.50 C + 0.50 Si + 0.60 Mn + 0.065 S +

Axes	Variables	Minimum	Maximum
	activity	0	12.392
	mole	0	2.0952
			6117
Y-axis			0.04
			0.553
X-axis			1
			400
			1
			06.
			36E+05
			0
			8E+05
			0
			8.43
			01

Y-axis: gram

X-axis: Alpha

maximum: 1.2, minimum: 0, tick every: 0.2

maximum: 1, minimum: 0, tick every: 0.1

Cancel Refresh OK

size: 9 no: 4

color  full screen

reactants  Viewer

file name  Figure

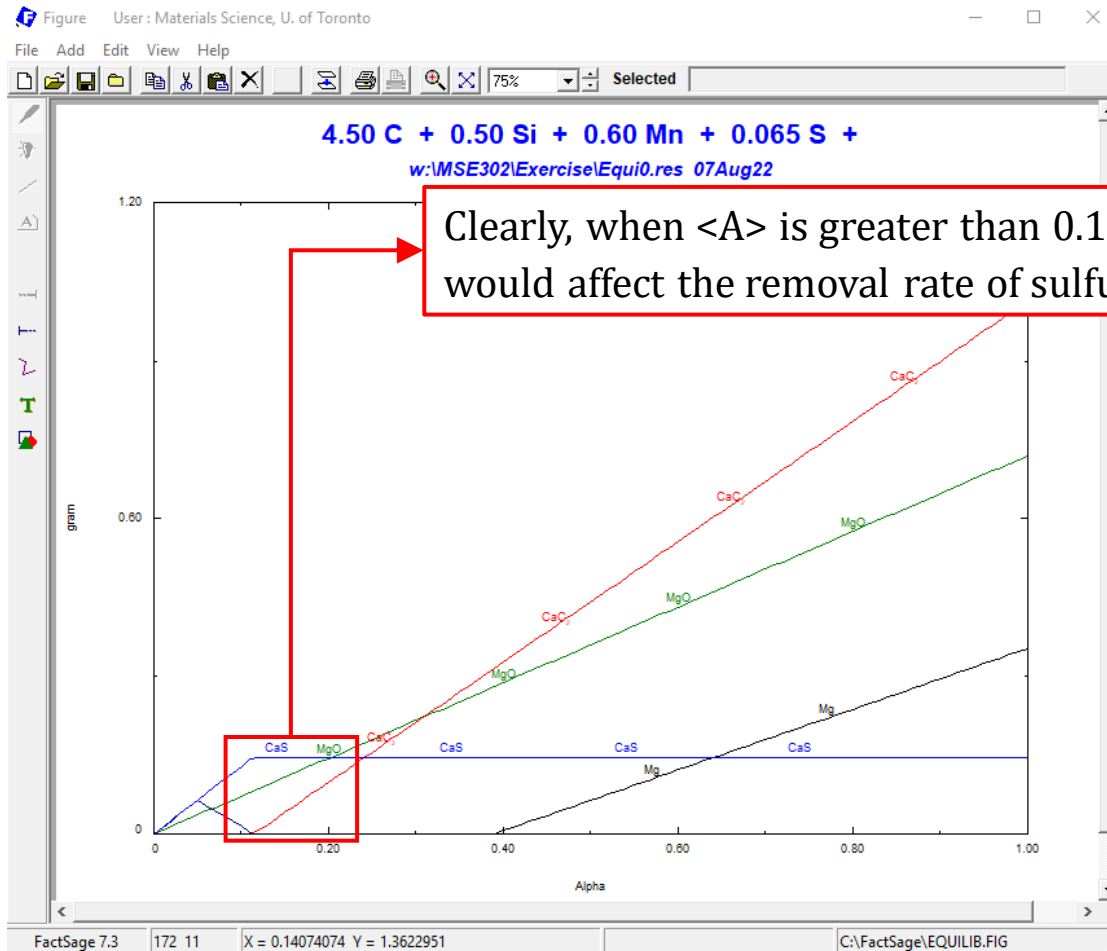
Plot >>

FactSage 7.3 w:\MSE302\Exercise\Equi0.res 07Aug22 101 sets

Select gram for Y-axis and <A> for X-axis.

# Example 1: Desulfurization (Basic Example)

## Basic Example: Desulfurization of Hot Metal Using CaO + Mg



# Example 1: Desulfurization (Basic Example)

## Basic Example: Desulfurization of Hot Metal Using CaO + Mg

Equilib - Menu: last system

File Units Parameters Help

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

**Reactants (7)**

[gram] 4.50 C + 0.50 Si + 0.60 Mn + 0.065 S + 94.335 Fe + <A> Mg + <A> CaO

**Products**

Compound species

gas ideal real 0

aqueous 0

pure liquids 0

\* + pure solids 130

\* - custom selection species: 130

Composition target

Element S - FTmisc-FeLQ

Estimate ALPHA: [ ]

Quantity(g)

**Final Conditions**

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

1400 1

10 steps Table 1 calculation

**Composition Target**

Solution MI53-FeLQ

**Variable**

species composition

log10 (species composition)

element composition

log10 (element composition)

species activity

log10(species activity)

- none (removes targets) -

**Species**

Code numbers (216-227)

Fe, C, Ca, ...

216 [Fe]

**Element**

Elements C O Mg Si S Ca Mn Fe

Element: [S]

**Values**

Enter a single value - or enter a range of values 'first last step'

Element S mass fraction: [0.00001] (0.001%)

Cancel Help OK

**Table: Solution Phases**

*	+	Base-Phase	Full Name
	C	FTmisc-FeLQ	Fe-liq
		FTmisc-MATT	Matte
		FTmisc-FeS_	FeS-liq
		FTmisc-MAT2C	C-Liq(Matte/Metal)
		FTmisc-PYRRC	C-Pyrrhotite
		FTmisc-BCCS	bcc
		FTmisc-FCCS	fcc
		FTmisc-MS-c	MeS_cubic

Legend

Show  all  selected

species: 12

solutions: 1 [Select]

Equilibrium

normal  normal -

transitions only

open

Calculate >>

FactSage 7.3 w:\MSE302\Exercise\EquiDe-S\_Using\_Mg.DAT

Leave it Blank.

# Example 1: Desulfurization (Basic Example)

## Basic Example: Desulfurization of Hot Metal Using CaO + Mg

Equilib - Results 1400 C, A=0.0494

Composition Target Calculation

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

C	4.5000E+00			
Si	5.0000E-01			
Mn	6.0000E-01			
S	6.5000E-02			
Fe	9.4335E+01			
*Mg	4.9405E-02			
*CaO	4.9405E-02			

EQUIL AMOUNT

	gram		
Fe	9.4335E+01	9.4395E-01	6.6655E-01
C	4.5000E+00	4.5028E-02	8.2029E-01
Ca	1.7416E-07	1.7427E-09	4.7195E-07
Mn	6.0000E-01	6.0038E-03	2.8711E-03
O	1.8292E-07	1.8304E-09	1.6145E-11
S	9.9937E-04	1.0000E-05	3.0200E-06
Si	5.0000E-01	5.0032E-03	4.6699E-05
Mg	8.9328E-04	8.9384E-06	4.9659E-02
MgO	3.9633E-05	3.9658E-07	3.8801E-07
CaO	1.4522E-07	1.4531E-09	1.0218E-09
SiO	2.6569E-08	2.6586E-10	2.3781E-10
MnO	1.0473E-08	1.0479E-10	5.8253E-11
TOTAL:	9.9937E+01	1.0000E+00	1.0000E+00

PHASE: Fe-liq

System component	Amount/mol	Amount/gram	Mole fraction	Mass fraction
Fe	1.0000	64.235	0.0000	0.0000
Mn				
Ca				
S				
Si				

Final Conditions

<A>	<B>	T(C)	P(atm)	Product H(J)
		1400	1	

1 calculation

Calculate >>

This is the mass of CaO and Mg required to achieve the desired sulfur content in the hot metal.

# Example 1: Desulfurization (Basic Example)

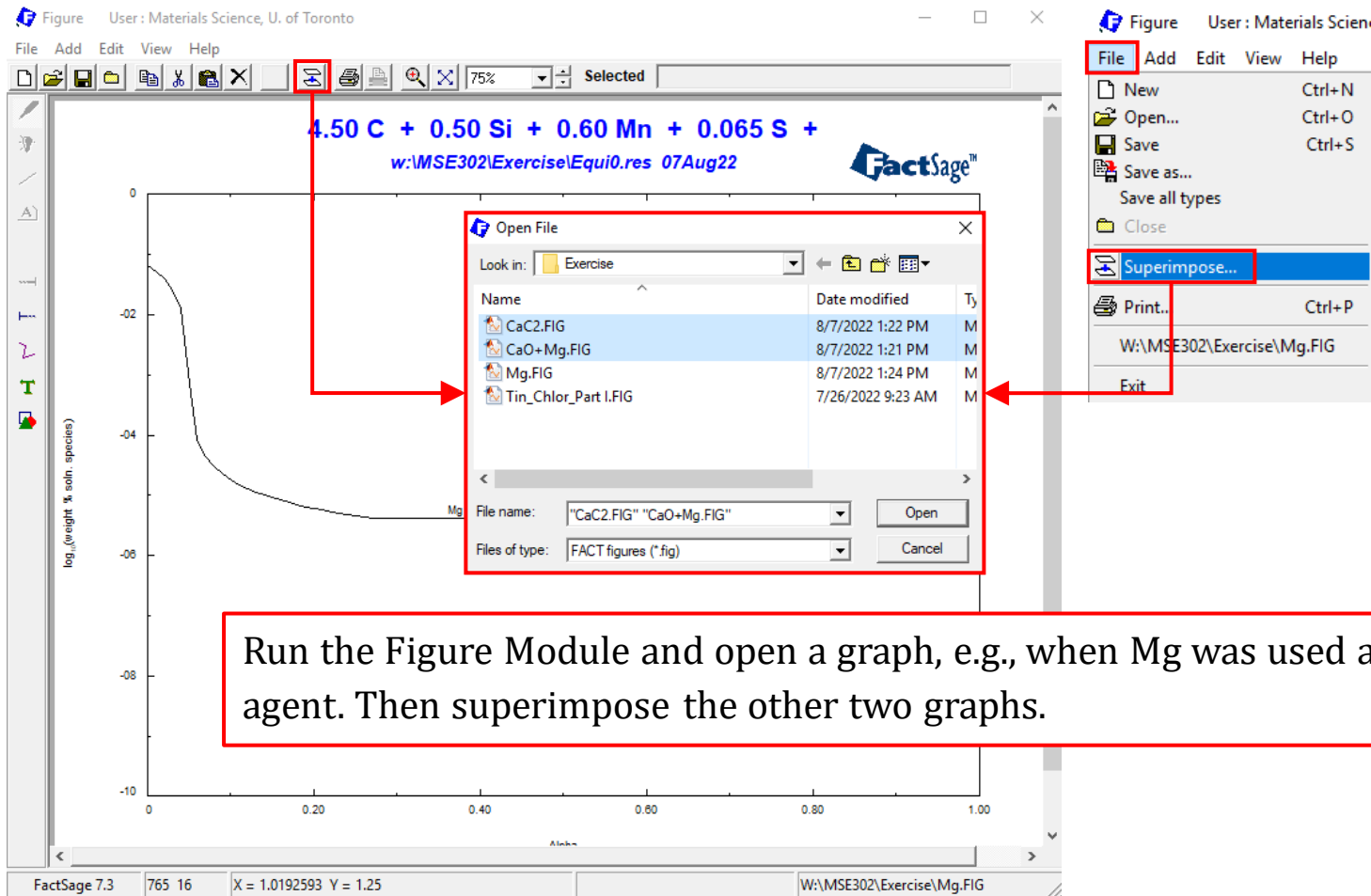
---

## **Basic Example: Comparison of Desulfurizing Agents**

To compare the efficiency of different desulfurizing agents, we can superimpose all the graphs, wt. %S~<A>, using the Figure Module.

# Example 1: Desulfurization (Basic Example)

## Basic Example: Comparison of Desulfurizing Agents

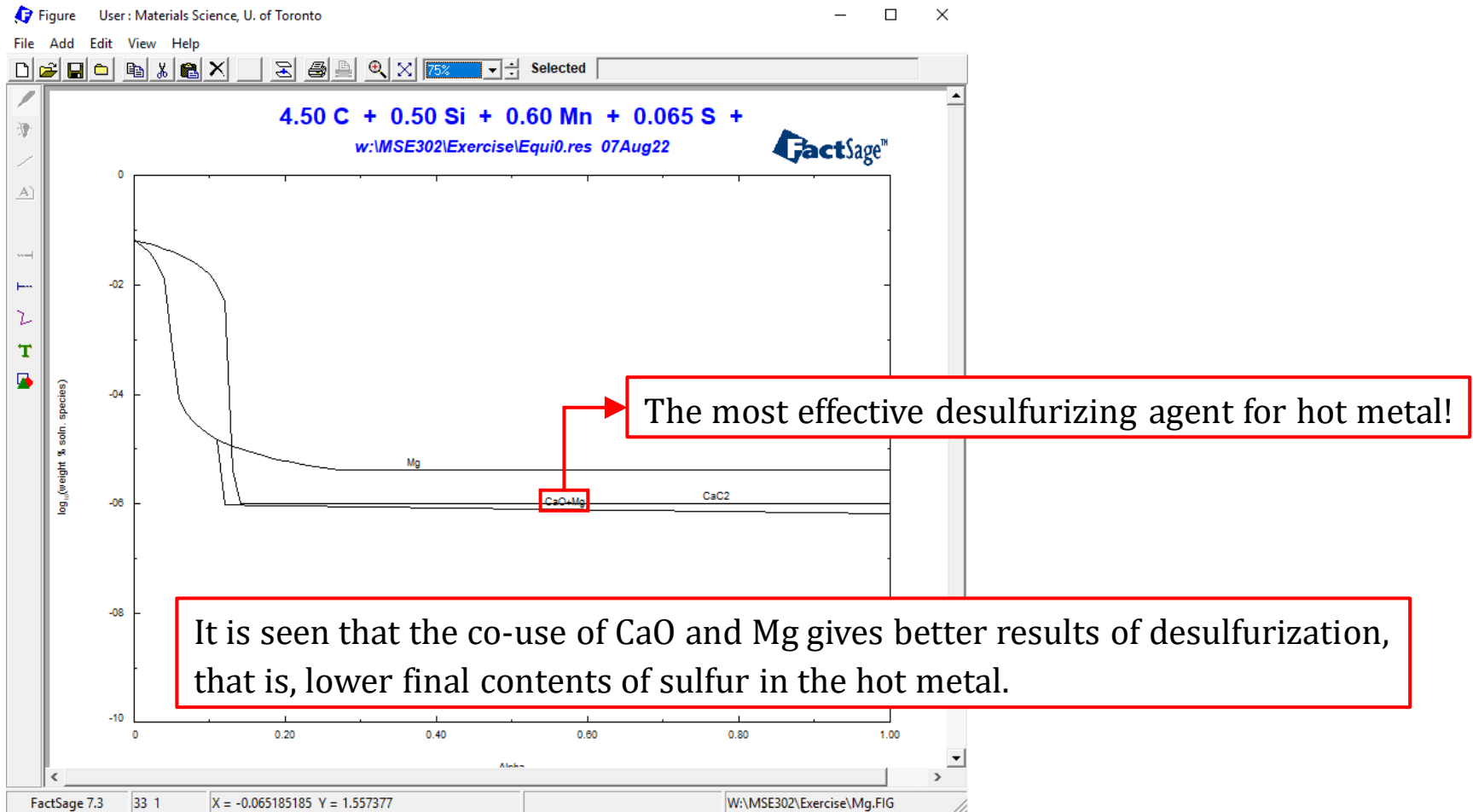


Run the Figure Module and open a graph, e.g., when Mg was used as desulfurizing agent. Then superimpose the other two graphs.



# Example 1: Desulfurization (Basic Example)

## Basic Example: Comparison of Desulfurizing Agents



# Example 1: Desulfurization (Advanced Example)

---

Now, we know the “CaO + Mg” mixture can be used as an effective desulfurizing agent, and we would like to use this mixture for hot metal desulfurization in a torpedo car. It should be noted that **the commercial grade** “CaO + Mg” agent typically assaying 70 wt.% CaO and 30 wt.% Mg.

**Background data:** in a torpedo car, we assume the blast furnace slag carry over is 10 kg/tHM and the temperature is 1427 °C. The compositions of hot metal and slag are as follows:

Hot metal composition:

Element	C	Si	Mn	Ti	S	Fe
wt.%	4.50	0.80	1.00	0.05	0.06	93.59

Slag composition:

Component	CaO	SiO <sub>2</sub>	MgO	Al <sub>2</sub> O <sub>3</sub>	MnO	TiO <sub>2</sub>	CaS
wt.%	34.5	34.0	14.0	9.00	2.00	2.00	4.50

# Example 1: Desulfurization (Advanced Example)

---

Also, the “CaO + Mg” agent is carried by the carrier argon gas at a rate of roughly 0.125 Nm<sup>3</sup>/kg Mg.

For 1 Nm<sup>3</sup> argon (Nm<sup>3</sup> means normal cubic meter), the equivalent mass is calculated as follows:

$$\frac{1000 \text{ liter}}{1 \text{ Nm}^3} \times \frac{1}{22.4} \frac{\text{mol}}{\text{liter}} \times \frac{40 \text{ g}}{1 \text{ mol}} \times \frac{10^{-3} \text{ kg}}{1 \text{ g}} = 1.79 \text{ kg/Nm}^3 \text{ Ar}$$

**Note:** at standard temperature and pressure, i.e., 0 °C and 1 atm, 1 mole of any gas will occupy a volume of 22.4 liter.

Now, let us simulate the system consisting hot metal / slag / CaO-Mg agent / Ar using the Equilib Module.

# Example 1: Desulfurization (Advanced Example)

---

## Step 1. Define the Reactants (Type and Quantity)

Since there are a quite number of species in this advanced example, we could either (a) calculate the quantities of all species and then enter all at once in the Reactants Window, or (b) define **2 separate** streams for hot metal and slag which contain many species and then input these 2 streams together with the CaO-Mg agent and Ar in the Reactants Window.

We will choose the second approach because it avoids entering many species at the same time, and the input species will be more organized.

**Note:** our calculation will be based on 1 tonne (= 1000 kg) hot metal.

# Example 1: Desulfurization (Advanced Example)

## What is a Stream?

FactSage 7.3

Information Programs Tools About

Materials Science, U. of Toronto

FactSage 7.3

Info

- Information

Databases

- Documentation
- View Data
- Compound
- Solution

Calculate

- Reaction
- Predom
- EpH
- Equilib
- Phase Diagram
- OptiSage

Manipulate

- Results
- Mixture

Run the Mixture Module.

Mixtures and Streams

File Edit Table Units Data Search Help Mixture or Stream?

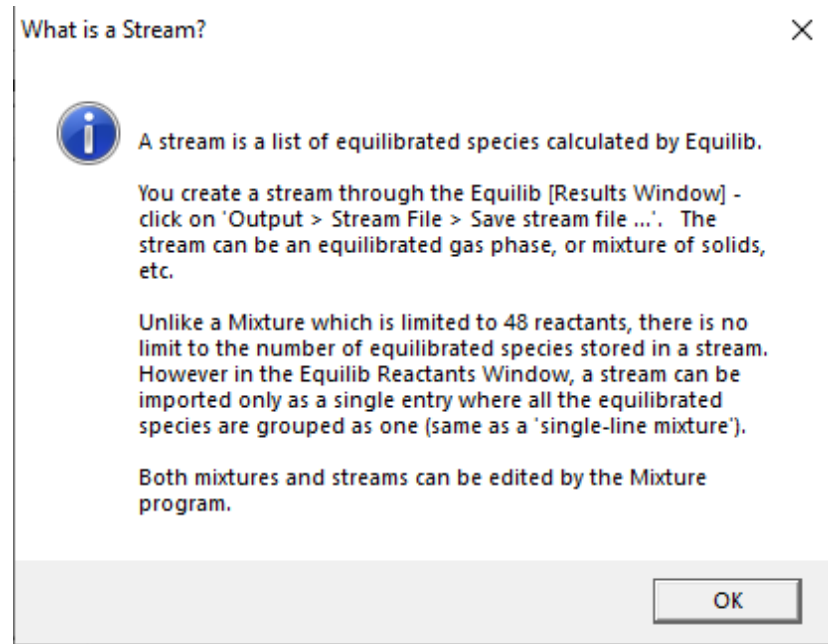
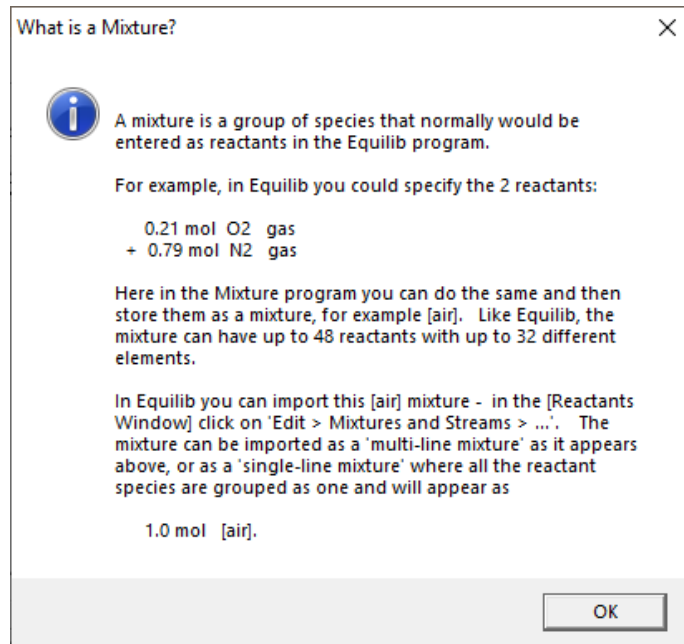
- What is a mixture? ...
- What is a stream? ...
- About ...

Quantity(mol)	Species	Phase	T(K)	P(total)
0.79	N2	gas	298.15	1
+ 0.21	O2	gas	298.15	1

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# Example 1: Desulfurization (Advanced Example)

## What is a Stream?



We will use the Equilib Module to define the streams, each of which simulate one of the following: hot metal / slag / CaO-Mg agent / Ar.

**Note:** defining a stream is a simple equilibrium calculation

# Example 1: Desulfurization (Advanced Example)

## Stream 1: Hot Metal (FTmisc-FeLQ)

Equilib - Reactants

File Edit Table Units **Data Search** Data Evaluation Help

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

Select the Units.

Quantity(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
4.50	C				1	
+ 0.80	Si					
+ 1.00	Mn					
+ 0.05	Ti					
+ 0.06	S					
+ 93.59	Fe					

100 gram hot metal.

FTmisc contains a model for liquid iron solution, FeLQ.

Data Search

Databases - 1/14 compound databases, 1/15 solution databa

**Fact** **FactSage™** **SGTE**

FactPS  FSopp  BINS  compounds only

FToxid  FSlead  SGPS  solutions only

FTsalt  FSstel  SGTE  no database

**FTmisc**  FSupsi  SGsold

FTHall  ELEM  SGnobl

FTDxCN  FTdemo  SpMCBN

FTfrtz  TDmeph

FTThelg  TDnucl

FTpulp  FTlite  FTnucl

Information -

FactSage 7.3 Compound: 1/14 databases Solution: 1/15 databases

# Example 1: Desulfurization (Advanced Example)

## Stream 1: Hot Metal (FTmisc-FeLQ)

Equilib - Menu: last system

File Units Parameters Help

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

**Reactants (6)**

(gram) 4.50 C + 0.80 Si + 1.00 Mn + 0.05 Ti + 0.06 S + 93.59 Fe

**Products**

Compound species

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

species: 0

Target

- none -

Estimate T(K): 1000

Quantity(g): 0

**Solution phases**

*	+	Base-Phase	Full Name
	<input checked="" type="checkbox"/>	FTmisc-FeLQ	Fe-liq
	<input type="checkbox"/>	FTmisc-MATT	Matte
	<input type="checkbox"/>	FTmisc-FeS_	FeS-liq
	<input type="checkbox"/>	FTmisc-MAT2C	C-Liq(Matte/Metal)
	<input type="checkbox"/>	FTmisc-PYRRC	C-Pyrrhotite
	<input type="checkbox"/>	FTmisc-BCCS	bcc
	<input type="checkbox"/>	FTmisc-FCCS	fcc
	<input type="checkbox"/>	FTmisc-MS-c	MeS_cubic

Legend

+ · selected 1  Show  all  selected

**Final Conditions**

<A>	<B>	T(C)	P(atm)	Product H(J)
		1427	1	

10 steps  Table

**Equilibrium**

- normal  normal + transitions
- transitions only
- open

**Calculate >>**

FactSage 7.3

Select FTmisc-FeLQ only.

We need a hot metal stream at 1427 °C.



# Example 1: Desulfurization (Advanced Example)

## Stream 1: Hot Metal (FTmisc-FeLQ)

Equilib - Results 1427 C

Output Edit Show Pages Final Conditions

Save or Print > T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

Plot >

Equilib Results file >

Stream File > Recycle all streams ...

Format > Save stream file > Save gas phase ...

Fact-XML > Stream file properties ...

Fact-Optimal > Summary of streams > Save pure liquids ...

Fact-Function-Builder > Directory (w:\MSE302\Exercise\) ... Save aqueous ...

Refresh ... Save pure solids ...

Swap loops ...

Save solutions > ALL solutions

FTmisc-FeLQ Fe-liq

Save File w:\MSE302\Exercise\MixtHM\_1427\_°C.DAT

Saving file HM\_1427\_°C

Enter one line of comments

Enter some description.

FTmisc-FeLQ Fe-liq, 100 g HM

Save File in w:\MSE302\Exercise\Mixt\*.dat

FTmisc-FeLQ Fe-liq

Enter a stream file number (1 - 9999)

or enter a stream file name (up to 26 characters), for example

My Give a name for the stream

HM\_1427 °C

	EQUIL AMOUNT	MASS FRACTION	ACTIVITY
PHASE: Fe-liq	gram		
Fe	9.3590E+01	9.3590E-01	6.5668E-01
C	4.5000E+00	4.5000E-02	8.0822E-01
Mn	1.0000E+00	1.0000E-02	4.6513E-03
			2.0310E-04
			8.4768E-05
			2.3458E-08
			1.0000E+00
Mole fraction			0.79798
Mass			0.6618

# Example 1: Desulfurization (Advanced Example)

## Stream 2: Slag (FToxid-Slag)

The screenshot shows the FactSage software interface. The main window is titled "Equilib - Reactants" and has a menu bar with "File", "Edit", "Table", "Units", "Data Search", "Data Evaluation", and "Help". Below the menu bar is a toolbar with icons for file operations and a unit selection dropdown. The unit selection dropdown is highlighted with a red box and labeled "Select the Units." The unit selection dropdown shows "T(C)", "P(atm)", "Energy(J)", "Quantity(g)", and "Vol(litre)".

The main window displays a table with the following columns: "Quantity(g)", "Species", "Phase", "T(C)", "P(total)\*\*", and "Stream#". The table contains the following data:

Quantity(g)	Species	Phase	T(C)	P(total)**	Stream#
34.5	CaO				2
+ 34.0	SiO2				2
+ 14.0	MgO				2
+ 9.00	Al2O3				2
+ 2.00	MnO				2
+ 2.00	TiO2				2
+ 4.50	CaS				2

The "Data Search" dialog is open, showing a list of databases. The "FToxid" database is selected, indicated by a red box and a red arrow pointing to it. The "Data Search" dialog also shows a list of databases, including "FactPS", "FactSage", "SGTE", "FToxid", "FTsalt", "FTmisc", "FThall", "FToxCN", "FTfrtz", "FThelg", "FTpulp", "FTlite", "FScope", "FSlead", "FSstel", "FSupsi", "ELEM", "FTdemo", "FTnucl", "BINS", "SGPS", "SGTE", "SGsold", "SGnobl", "SpMCBN", "TDmeph", and "TDnucl". The "Data Search" dialog also has a "Clear All" button and an "Add/Remove Data" button.

Annotations in the image include:

- "100 gram slag." pointing to the "Quantity(g)" column.
- "FToxid contains a model for liquid slag, SLAGA." pointing to the "FToxid" database in the "Data Search" dialog.

# Example 1: Desulfurization (Advanced Example)

## Stream 2: Slag (FToxid-Slag)

Equilib - Menu: last system  
File Units Parameters Help

Reactants (7)  
(gram) 34.5 CaO + 34.0 SiO2 + 14.0 MgO + 9.00 Al2O3

Products

*	+	Base-Phase	Full Name
1		FToxid-SLAGA	A-Slag-liq all oxides + S
		FToxid-SLAGB	B-Slag-liq with SO4
		FToxid-SLAG?	?
		FToxid-SPINB	
		FToxid-MeO_A	
		FToxid-MeO_B	
		FToxid-MeO_?	
		FToxid-cPyrA	

Legend  
I - immiscible 1

Final Conditions

<A>	<B>	T(C)	P(atm)
		1427	1

We need a slag stream at 1427 °C.

Select FTmisc-SLAGA only. Please click on the phase to see the information for SLAGA and SLAGB. To simply put, SLAGA considers all sulfur as sulfide (under the reducing conditions), whereas SLAGB considers all sulfur as sulfate (under oxidizing conditions).

(12) Solubility of Sulfide:  
The model used, and most of the optimizations, are described in the references below. Sulfur contents as sulfide will be calculated.  
References: 2039, 2060, 2061, 2115, 2116

Complete list of references for FToxid-SLAGA:-  
References: 2002, 2003, 2004, 2005, 2006, 2007, 2008, 2009, 2010, 2011, 2012, 2013  
References: 2014, 2015, 2017, 2018, 2019, 2020, 2031, 2032, 2035, 2036, 2037, 2038, 2039, 2040, 2042, 2043  
References: 2044, 2045, 2046, 2047, 2048, 2049, 2050, 2051, 2052, 2053, 2054, 2055, 2056, 2057, 2058, 2059, 2060, 2061, 2062, 2063, 2064, 2065, 2066, 2067, 2068, 2069, 2070, 2071, 2072, 2073, 2074, 2075, 2076, 2077, 2078, 2079, 2080, 2081, 2082, 2083, 2084, 2085, 2086, 2087, 2088, 2089, 2090, 2091, 2092, 2093, 2094, 2095, 2096, 2097, 2098, 2099, 2100, 2101, 2102, 2103, 2104, 2105, 2106, 2107, 2108, 2109, 2110, 2111, 2112, 2113, 2114, 2115, 2116, 2117, 2118, 2119, 2120, 2121, 2122, 2123, 2124, 2125, 2126, 2127, 2128, 2129, 2130, 2131, 2132, 2133, 2134, 2135, 2136, 2137, 2138, 2139, 2140, 2141, 2142, 2143, 2144, 2145, 2146, 2147, 2148, 2149, 2150, 2151, 2152, 2153, 2154, 2155, 2156, 2157, 2158, 2159, 2160, 2161, 2162, 2163, 2164, 2165, 2166, 2167, 2168, 2169, 2170, 2171, 2172, 2173, 2174, 2175, 2176, 2177, 2178, 2179, 2180, 2181, 2182, 2183, 2184, 2185, 2186, 2187, 2188, 2189, 2190, 2191, 2192, 2193, 2194, 2195, 2196, 2197, 2198, 2199, 2200, 2201, 2202, 2203, 2204, 2205, 2206, 2207, 2208, 2209, 2210, 2211, 2212, 2213, 2214, 2215, 2216, 2217, 2218, 2219, 2220, 2221, 2222, 2223, 2224, 2225, 2226, 2227, 2228, 2229, 2230, 2231, 2232, 2233, 2234, 2235, 2236, 2237, 2238, 2239, 2240, 2241, 2242, 2243, 2244, 2245, 2246, 2247, 2248, 2249, 2250, 2251, 2252, 2253, 2254, 2255, 2256, 2257, 2258, 2259, 2260, 2261, 2262, 2263, 2264, 2265, 2266, 2267, 2268, 2269, 2270, 2271, 2272, 2273, 2274, 2275, 2276, 2277, 2278, 2279, 2280, 2281, 2282, 2283, 2284, 2285, 2286, 2287, 2288, 2289, 2290, 2291, 2292, 2293, 2294, 2295, 2296, 2297, 2298, 2299, 2300, 2301, 2302, 2303, 2304, 2305, 2306, 2307, 2308, 2309, 2310, 2311, 2312, 2313, 2314, 2315, 2316, 2317, 2318, 2319, 2320, 2321, 2322, 2323, 2324, 2325, 2326, 2327, 2328, 2329, 2330, 2331, 2332, 2333, 2334, 2335, 2336, 2337, 2338, 2339, 2340, 2341, 2342, 2343, 2344, 2345, 2346, 2347, 2348, 2349, 2350, 2351, 2352, 2353, 2354, 2355, 2356, 2357, 2358, 2359, 2360, 2361, 2362, 2363, 2364, 2365, 2366, 2367, 2368, 2369, 2370, 2371, 2372, 2373, 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2540, 2541, 2542, 2543, 2544, 2545, 2546, 2547, 2548, 2549, 2550, 2551, 2552, 2553, 2554, 2555, 2556, 2557, 2558, 2559, 2560, 2561, 2562, 2563, 2564, 2565, 2566, 2567, 2568, 2569, 2570, 2571, 2572, 2573, 2574, 2575, 2576, 2577, 2578, 2579, 2580, 2581, 2582, 2583, 2584, 2585, 2586, 2587, 2588, 2589, 2590, 2591, 2592, 2593, 2594, 2595, 2596, 2597, 2598, 2599, 2600, 2601, 2602, 2603, 2604, 2605, 2606, 2607, 2608, 2609, 2610, 2611, 2612, 2613, 2614, 2615, 2616, 2617, 2618, 2619, 2620, 2621, 2622, 2623, 2624, 2625, 2626, 2627, 2628, 2629, 2630, 2631, 2632, 2633, 2634, 2635, 2636, 2637, 2638, 2639, 2640, 2641, 2642, 2643, 2644, 2645, 2646, 2647, 2648, 2649, 2650, 2651, 2652, 2653, 2654, 2655, 2656, 2657, 2658, 2659, 2660, 2661, 2662, 2663, 2664, 2665, 2666, 2667, 2668, 2669, 2670, 2671, 2672, 2673, 2674, 2675, 2676, 2677, 2678, 2679, 2680, 2681, 2682, 2683, 2684, 2685, 2686, 2687, 2688, 2689, 2690, 2691, 2692, 2693, 2694, 2695, 2696, 2697, 2698, 2699, 2700, 2701, 2702, 2703, 2704, 2705, 2706, 2707, 2708, 2709, 2710, 2711, 2712, 2713, 2714, 2715, 2716, 2717, 2718, 2719, 2720, 2721, 2722, 2723, 2724, 2725, 2726, 2727, 2728, 2729, 2730, 2731, 2732, 2733, 2734, 2735, 2736, 2737, 2738, 2739, 2740, 2741, 2742, 2743, 2744, 2745, 2746, 2747, 2748, 2749, 2750, 2751, 2752, 2753, 2754, 2755, 2756, 2757, 2758, 2759, 2760, 2761, 2762, 2763, 2764, 2765, 2766, 2767, 2768, 2769, 2770, 2771, 2772, 2773, 2774, 2775, 2776, 2777, 2778, 2779, 2780, 2781, 2782, 2783, 2784, 2785, 2786, 2787, 2788, 2789, 2790, 2791, 2792, 2793, 2794, 2795, 2796, 2797, 2798, 2799, 2800, 2801, 2802, 2803, 2804, 2805, 2806, 2807, 2808, 2809, 2810, 2811, 2812, 2813, 2814, 2815, 2816, 2817, 2818, 2819, 2820, 2821, 2822, 2823, 2824, 2825, 2826, 2827, 2828, 2829, 2830, 2831, 2832, 2833, 2834, 2835, 2836, 2837, 2838, 2839, 2840, 2841, 2842, 2843, 2844, 2845, 2846, 2847, 2848, 2849, 2850, 2851, 2852, 2853, 2854, 2855, 2856, 2857, 2858, 2859, 2860, 2861, 2862, 2863, 2864, 2865, 2866, 2867, 2868, 2869, 2870, 2871, 2872, 2873, 2874, 2875, 2876, 2877, 2878, 2879, 2880, 2881, 2882, 2883, 2884, 2885, 2886, 2887, 2888, 2889, 2890, 2891, 2892, 2893, 2894, 2895, 2896, 2897, 2898, 2899, 2900, 2901, 2902, 2903, 2904, 2905, 2906, 2907, 2908, 2909, 2910, 2911, 2912, 2913, 2914, 2915, 2916, 2917, 2918, 2919, 2920, 2921, 2922, 2923, 2924, 2925, 2926, 2927, 2928, 2929, 2930, 2931, 2932, 2933, 2934, 2935, 2936, 2937, 2938, 2939, 2940, 2941, 2942, 2943, 2944, 2945, 2946, 2947, 2948, 2949, 2950, 2951, 2952, 2953, 2954, 2955, 2956, 2957, 2958, 2959, 2960, 2961, 2962, 2963, 2964, 2965, 2966, 2967, 2968, 2969, 2970, 2971, 2972, 2973, 2974, 2975, 2976, 2977, 2978, 2979, 2980, 2981, 2982, 2983, 2984, 2985, 2986, 2987, 2988, 2989, 2990, 2991, 2992, 2993, 2994, 2995, 2996, 2997, 2998, 2999, 3000, 3001, 3002, 3003, 3004, 3005, 3006, 3007, 3008, 3009, 3010, 3011, 3012, 3013, 3014, 3015, 3016, 3017, 3018, 3019, 3020, 3021, 3022, 3023, 3024, 3025, 3026, 3027, 3028, 3029, 3030, 3031, 3032, 3033, 3034, 3035, 3036, 3037, 3038, 3039, 3040, 3041, 3042, 3043, 3044, 3045, 3046, 3047, 3048, 3049, 3050, 3051, 3052, 3053, 3054, 3055, 3056, 3057, 3058, 3059, 3060, 3061, 3062, 3063, 3064, 3065, 3066, 3067, 3068, 3069, 3070, 3071, 3072, 3073, 3074, 3075, 3076, 3077, 3078, 3079, 3080, 3081, 3082, 3083, 3084, 3085, 3086, 3087, 3088, 3089, 3090, 3091, 3092, 3093, 3094, 3095, 3096, 3097, 3098, 3099, 3100, 3101, 3102, 3103, 3104, 3105, 3106, 3107, 3108, 3109, 3110, 3111, 3112, 3113, 3114, 3115, 3116, 3117, 3118, 3119, 3120, 3121, 3122, 3123, 3124, 3125, 3126, 3127, 3128, 3129, 3130, 3131, 3132, 3133, 3134, 3135, 3136, 3137, 3138, 3139, 3140, 3141, 3142, 3143, 3144, 3145, 3146, 3147, 3148, 3149, 3150, 3151, 3152, 3153, 3154, 3155, 3156, 3157, 3158, 3159, 3160, 3161, 3162, 3163, 3164, 3165, 3166, 3167, 3168, 3169, 3170, 3171, 3172, 3173, 3174, 3175, 3176, 3177, 3178, 3179, 3180, 3181, 3182, 3183, 3184, 3185, 3186, 3187, 3188, 3189, 3190, 3191, 3192, 3193, 3194, 3195, 3196, 3197, 3198, 3199, 3200, 3201, 3202, 3203, 3204, 3205, 3206, 3207, 3208, 3209, 3210, 3211, 3212, 3213, 3214, 3215, 3216, 3217, 3218, 3219, 3220, 3221, 3222, 3223, 3224, 3225, 3226, 3227, 3228, 3229, 3230, 3231, 3232, 3233, 3234, 3235, 3236, 3237, 3238, 3239, 3240, 3241, 3242, 3243, 3244, 3245, 3246, 3247, 3248, 3249, 3250, 3251, 3252, 3253, 3254, 3255, 3256, 3257, 3258, 3259, 3260, 3261, 3262, 3263, 3264, 3265, 3266, 3267, 3268, 3269, 3270, 3271, 3272, 3273, 3274, 3275, 3276, 3277, 3278, 3279, 3280, 3281, 3282, 3283, 3284, 3285, 3286, 3287, 3288, 3289, 3290, 3291, 3292, 3293, 3294, 3295, 3296, 3297, 3298, 3299, 3300, 3301, 3302, 3303, 3304, 3305, 3306, 3307, 3308, 3309, 3310, 3311, 3312, 3313, 3314, 3315, 3316, 3317, 3318, 3319, 3320, 3321, 3322, 3323, 3324, 3325, 3326, 3327, 3328, 3329, 3330, 3331, 3332, 3333, 3334, 3335, 3336, 3337, 3338, 3339, 3340, 3341, 3342, 3343, 3344, 3345, 3346, 3347, 3348, 3349, 3350, 3351, 3352, 3353, 3354, 3355, 3356, 3357, 3358, 3359, 3360, 3361, 3362, 3363, 3364, 3365, 3366, 3367, 3368, 3369, 3370, 3371, 3372, 3373, 3374, 3375, 3376, 3377, 3378, 3379, 3380, 3381, 3382, 3383, 3384, 3385, 3386, 3387, 3388, 3389, 3390, 3391, 3392, 3393, 3394, 3395, 3396, 3397, 3398, 3399, 3400, 3401, 3402, 3403, 3404, 3405, 3406, 3407, 3408, 3409, 3410, 3411, 3412, 3413, 3414, 3415, 3416, 3417, 3418, 3419, 3420, 3421, 3422, 3423, 3424, 3425, 3426, 3427, 3428, 3429, 3430, 3431, 3432, 3433, 3434, 3435, 3436, 3437, 3438, 3439, 3440, 3441, 3442, 3443, 3444, 3445, 3446, 3447, 3448, 3449, 3450, 3451, 3452, 3453, 3454, 3455, 3456, 3457, 3458, 3459, 3460, 3461, 3462, 3463, 3464, 3465, 3466, 3467, 3468, 3469, 3470, 3471, 3472, 3473, 3474, 3475, 3476, 3477, 3478, 3479, 3480, 3481, 3482, 3483, 3484, 3485, 3486, 3487, 3488, 3489, 3490, 3491, 3492, 3493, 3494, 3495, 3496, 3497, 3498, 3499, 3500, 3501, 3502, 3503, 3504, 3505, 3506, 3507, 3508, 3509, 3510, 3511, 3512, 3513, 3514, 3515, 3516, 3517, 3518, 3519, 3520, 3521, 3522, 3523, 3524, 3525, 3526, 3527, 3528, 3529, 3530, 3531, 3532, 3533, 3534, 3535, 3536, 3537, 3538, 3539, 3540, 3541, 3542, 3543, 3544, 3545, 3546, 3547, 3548, 3549, 3550, 3551, 3552, 3553, 3554, 3555, 3556, 3557, 3558, 3559, 3560, 3561, 3562, 3563, 3564, 3565, 3566, 3567, 3568, 3569, 3570, 3571, 3572, 3573, 3574, 3575, 3576, 3577, 3578, 3579, 3580, 3581, 3582, 3583, 3584, 3585, 3586, 3587, 3588, 3589, 3590, 3591, 3592, 3593, 3594, 3595, 3596, 3597, 3598, 3599, 3600, 3601, 3602, 3603, 3604, 3605, 3606, 3607, 3608, 3609, 3610, 3611, 3612, 3613, 3614, 3615, 3616, 3617, 3618, 3619, 3620, 3621, 3622, 3623, 3624, 3625, 3626, 3627, 3628, 3629, 3630, 3631, 3632, 3633, 3634, 3635, 3636, 3637, 3638, 3639, 3640, 3641, 3642, 3643, 3644, 3645, 3646, 3647, 3648, 3649, 3650, 3651, 3652, 3653, 3654, 3655, 3656, 3657, 3658, 3659, 3660, 3661, 3662, 3663, 3664, 3665, 3666, 3667, 3668, 3669, 3670, 3671, 3672, 3673, 3674, 3675, 3676, 3677, 3678, 3679, 3680, 3681, 3682, 3683, 3684, 3685, 3686, 3687, 3688, 3689, 3690, 3691, 3692, 3693, 3694, 3695, 3696, 3697, 3698, 3699, 3700, 3701, 3702, 3703, 3704, 3705, 3706, 3707, 3708, 3709, 3710, 3711, 3712, 3713, 3714, 3715, 3716, 3717, 3718, 3719, 3720, 3721, 3722, 3723, 3724, 3725, 3726, 3727, 3728, 3729, 3730, 3731, 3732, 3733, 3734, 3735, 3736, 3737, 3738, 3739, 3740, 3741, 3742, 3743, 3744, 3745, 3746, 3747, 3748, 3749, 3750, 3751, 3752, 3753, 3754, 3755, 3756, 3757, 3758, 3759, 3760, 3761, 3762, 3763, 3764, 3765, 3766, 3767, 3768, 3769, 3770, 3771, 3772, 3773, 3774, 3775, 3776, 3777, 3778, 3779, 3780, 3781, 3782, 3783, 3784, 3785, 3786, 3787, 3788, 3789, 3790, 3791, 3792, 3793, 3794, 3795, 3796, 3797, 3798, 3799, 3800, 3801, 3802, 3803, 3804, 3805, 3806, 3807, 3808, 3809, 3810, 3811, 3812, 3813, 3814, 3815, 3816, 3817, 3818, 3819, 3820, 3821, 3822, 3823, 3824, 3825, 3826, 3827, 3828, 3829, 3830, 3831, 3832, 3833, 3834, 3835, 3836, 3837, 3838, 3839, 3840, 3841, 3842, 3843, 3844, 3845, 3846, 3847, 3848, 3849, 3850, 3851, 3852, 3853, 3854, 3855, 3856, 3857, 3858, 3859, 3860, 3861, 3862, 3863, 3864, 3865, 3866, 3867, 3868, 3869, 3870, 3871, 3872, 3873, 3874, 3875, 3876, 3877, 3878, 3879, 3880, 3881, 3882, 3883, 3884, 3885, 3886, 3887, 3888, 3889, 3890, 3891, 3892, 3893, 3894, 3895, 3896, 3897, 3898, 3899, 3900, 3901, 3902, 3903, 3904, 3905, 3906, 3907, 3908, 3909, 3910, 3911, 3912, 3913, 3914, 3915, 3916, 3917, 3918, 3919, 3920, 3921, 3922, 3923, 3924, 3925, 3926, 3927, 3928, 3

# Example 1: Desulfurization (Advanced Example)

## Stream 2: Slag (FToxid-Slag)

Equilib - Results 1427 C

Output Edit Show Pages Final Conditions

Save or Print > T(C) P(atm) Energy(J) Quantity(g)

Plot >

Equilib Results file >

Stream File > Recycle all streams ...

Format > Save stream file > Save gas phase ...

Fact-XML > Stream file properties ...

Fact-Optimal > Summary of streams > Save pure liquids ...

Fact-Function-Builder > Directory (w:\MSE302\Exercise\) ... Save aqueous ...

Refresh ... Save pure solids ...

Swap loops ...

Save solutions > ALL solutions

FToxid-SLAGA#1 A-Slag-liq

FToxid-SLAGA#2 A-Slag-liq

PHASE: Slag-liq#1 (;#2)

	EQUIL AMOUNT	MASS FRACTION	ACTIVITY
Al2O3	8.7754E+00	8.7754E-02	3.3013E-03
SiO2	3.3152E+01	3.3152E-01	1.4207E-02
			3.5767E-03
			5.1190E-02
			7.2150E-03
			1.1799E-07
			5.4045E-03
			1.6061E-08
			2.4000E-10

Save File w:\MSE302\Exercise\MixtSLAG\_1427\_°C.DAT

Saving file SLAG\_1427\_°C

Enter one line of comments

Enter some description.

FToxid-SLAGA#1 A-Slag-liq 100 g Slag

Save File in w:\MSE302\Exercise\Mixt\*.dat

FToxid-SLAGA#1 A-Slag-liq

Enter a stream file number (1 - 9999)

or enter a stream file name (up to 26 characters), for example

My Give a name for the stream

SLAG\_1427 °C

We only need to select SLAGA#1, because immiscibility doesn't occur.

# Example 1: Desulfurization (Advanced Example)

## Import the streams: hot metal and slag

Click on "New Reaction", and then import the streams.

The screenshot shows the FactSage 7.3 software interface. The 'Edit' menu is open, and the 'Mixtures and Streams' option is selected. The 'Import a stream (or single-line mixture)' option is highlighted. The 'Data Search' dialog box is open, showing a list of databases. The 'FactPS', 'FToxid', and 'FTmisc' databases are checked. The 'Data Search' dialog box also shows a list of databases with checkboxes for selection. The 'FactPS', 'FToxid', and 'FTmisc' databases are checked. The 'Data Search' dialog box also shows a list of databases with checkboxes for selection. The 'FactPS', 'FToxid', and 'FTmisc' databases are checked.

Make sure these three databases are selected.

HM\_1427\_°C FTmisc-FeLQ Fe-liq, 100 g ... stream  
SLAG\_1427\_°C FToxid-SLAGA#1 A-Slag-li ... stream

# Example 1: Desulfurization (Advanced Example)

## Import the streams, add desulfurizing agent and Ar

The screenshot shows the 'Equilib - Reactants' software interface. A table lists reactants with columns for Quantity(g), Species, Phase, T(C), P(total)\*\*, and Stream#. The table contains five rows: 1.0E6 g of [HM\_1427\_°C], <B> g of [SLAG\_1427\_°C], <0.7A> g of CaO, <0.3A> g of Mg, and <0.067A> g of Ar. Red boxes highlight the quantity input fields and the Ar row. Red arrows point from text boxes to these fields and the Ar row.

Quantity(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
1.0E6	[HM_1427_°C]				1	
<B>	[SLAG_1427_°C]				2	
<0.7A>	CaO				3	
<0.3A>	Mg					
<0.067A>	Ar					

You can input gram or percentage. Let us use the hot metal stream. When defining the hot metal stream, we use 100 gram. Therefore, if we use percentage, e.g., 100%, the total mass would be 100 gram. If we use gram, e.g., 1 gram, the total mass would be 1 gram.

It was calculated that for 1 kg Mg, the mass of Ar was calculated as:  $0.125 \times 1.79$  kg Ar.

The total mass of desulfurizing agent is <A> gram, the mass of CaO and Mg can be determined based on the composition: 70 wt. % CaO + 30 wt. % Mg.

The variable <B> permits us to change the amount of slag carry-over. Here, we will set 10 kg per 1tonne hot metal.

1 tonne hot metal.

Next >>

FactSage Solution: 2/15 databases

# Example 1: Desulfurization (Advanced Example)

## Selection of Compound Species

Equilib - Menu: comments

Selection - Equilib Page 101/101 : T(C) = 1427, P(atm) = 1, Alpha = 10000

File Units Parameters Help

File Edit Show Sort

Selected: 216/360 SOLID Duplicates selected X denc 101 Pages: 1 - 101 [page]

Page 101/101 : T(C) = 1427, P(atm) = 1, Alpha = 10000 [min = 0 at p. 1; max = 0 at p. 101]

	Code	Species	Data	Phase	T	V	Activity	Minimum	Maximum
	112	C(s)	FactPS	Graphite		V	0.8078	0.7968 [3]	0.8078 [101]
						V	0.4250	0.4193 [3]	0.4250 [101]
					T	V	4.9142E-04	4.0271E-06 [1]	4.9142E-04 [101]
+	116	MgC2(s)	FactPS	solid		o	5.7757E-06	4.6149E-08 [1]	5.7757E-06 [101]
+	117	Mg2C3(s)	FactPS	solid		o	1.2392E-08	8.0119E-13 [1]	1.2392E-08 [101]
X	118	MgO(s)	FactPS	Periclase		V	0.9978		
+	119	MgCO3(s)	FactPS	magnesite_CaC	T	V	1.0026E-12	1.0026E-12 [101]	8.5503E-10 [2]
+	120	Al(s)	FactPS	solid	T	V	4.1346E-05	6.3549E-07 [2]	4.2540E-05 [50]
+	121	Al4C3(s)	FactPS	solid		V	2.0063E-14	1.0790E-21 [2]	2.1920E-14 [50]
X	122	Al2O3(s)	FactPS	gamma		V	3.0863E-03		
X	123	Al2O3(s2)	FactPS	delta		V	4.0740E-03		
V	124	Al2O3(s3)	FactPS	kappa		V	3.8145E-03		
+	129	SiC(s2)	FactPS	Solid_Beta		V	5.2905E-03	4.5706E-03 [17]	5.2905E-03 [101]
X	130	SiO2(s)	FactPS	Quartz(l)	T	V	6.5008E-06		
X	131	SiO2(s2)	FactPS	Quartz(h)		V	3.4510E-05		
X	132	SiO2(s3)	FactPS	Tridymite(l)	T	V	1.5253E-07		
X	133	SiO2(s4)	FactPS	Tridymite(h)		V	3.7342E-05		

Choose all gas species (ideal).

Choose all pure solids. We ask FactSage to determine which pure solids will exist at equilibrium. It is recommended to edit the priority list when suppressing duplicates.

permit selection of 'X' species Help Suppress Duplicates Edit priority list : FToxid FTmisc FactPS

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

# Example 1: Desulfurization (Advanced Example)

## Selection of Compound Species

Equilib - Menu: comments

File Units Parameters Help

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

Reactants (5)

[gram] 1.0E6 [HM\_1427\_°C] + <B> [SLAG\_1427\_°C] + <0.7A> CaO + <0.3A> Mg + <0.067A> Ar

Products

Compound species

gas ideal real 69

aqueous 0

pure liquids 0

pure solids 216

\* - custom selection species: 285

Target

- none -

Estimate T(K): 1000

Legend

- immiscible 7

+ selected 7

species: 272

Select

101 calculations

FactSage 7.3 w:\MSE302\Exercise\EquiDe-S\_Advanced\_Example.DAT

This is slag.

This is hot metal.

The 12 solid solutions are selected based on the suggestions mentioned slides (1, 2, 3, 4). However, you should be aware that for most of these solid solutions in the current system, their amounts are only a small fraction and thus do not have a significant influence on the equilibrium state. For primary calculations, you don't need to select these solid solutions.



# Example 1: Desulfurization (Advanced Example)

## Setting Final Conditions

The screenshot displays the FactSage 7.3 software interface. The window title is "Equilib - Menu: comments". The menu bar includes "File", "Units", "Parameters", and "Help". The main window shows a list of reactants and products, a table of species, and a "Final Conditions" section. The "Final Conditions" section has the following values: <A> = 0, <B> = 1E4, T(C) = 1427, P(atm) = 1, and Product H(J) = 1. The "Equilibrium" section has "normal" selected. The "Calculate" button is visible.

**Reactants (5)**  
(gram) 1.0

**Products**  
Compound spec  
+ gas (idea)  
- aqueous 0  
- pure liquids 0  
\* + pure solids 216  
\* - custom selection species: 285

Species	Quantity
FToxid-SLAGA	A-Slag-liq all oxides + S
FToxid-SPINB	B-Spinel

**Final Conditions**  
<A> 0 10000 100  
<B> 1E4  
T(C) 1427  
P(atm) 1  
Product H(J) 1  
10 steps  
Table  
101 calculations

**Equilibrium**  
 normal  
 normal + transitions  
 transitions only  
 open  
Calculate >>

This is the mass range and step of the desulfurizing agent.

For 1 tonne hot metal which contains 0.06 wt.% S, the maximum mass of the desulfurization agent “70 wt.% CaO + 30 wt.% Mg” is 10 kg. When  $\langle A \rangle = 0$ , we consider only the slag/hot metal interaction.

Here, we consider the slag carry-over is 10 kg per 1 tonne hot metal. If you would like to study the effect of slag carry-over, you can repeat the calculations by changing the values of  $\langle B \rangle$ .

The temperature is 1427 °C.

# Example 1: Desulfurization (Advanced Example)

The screenshot displays the FactSage 7.3 interface for setting up a plot. The main window shows the plot title "Plot: log10(weight % soln. species) vs Alpha". The "Plot Species Selection" dialog is open, showing a list of species and their mole fractions. The "Axes" dialog is also open, showing the Y-axis variable as "log10(weight % soln. species)" and the X-axis variable as "Alpha".

**Plot Species Selection - Equilib Results: log10(weight % soln. species) vs Alpha**

#	Species	Mole (min)
585	S_GAS	0
586	Si_GAS	0
587	Al_GAS	0
588	Mg_GAS	0
589	O_GAS	0
590	C_GAS	0
591	Fe_FeLQ	1.6759E+04
592	Mn_FeLQ	183.98
593	Ti_FeLQ	12.922
594	Ca_FeLQ	3.8620E-04
595	Ar_FeLQ	0
596	S_FeLQ	9.8311E-03
597	Si_FeLQ	279.91
598	Al_FeLQ	0.182549
599	Mg_FeLQ	7.4458E-03
600	O_FeLQ	4.0295E-02
601	C_FeLQ	3745.1

**Axes: log10(weight % soln. species) vs Alpha**

Y-axis: log10(weight % soln. species)  
X-axis: Alpha

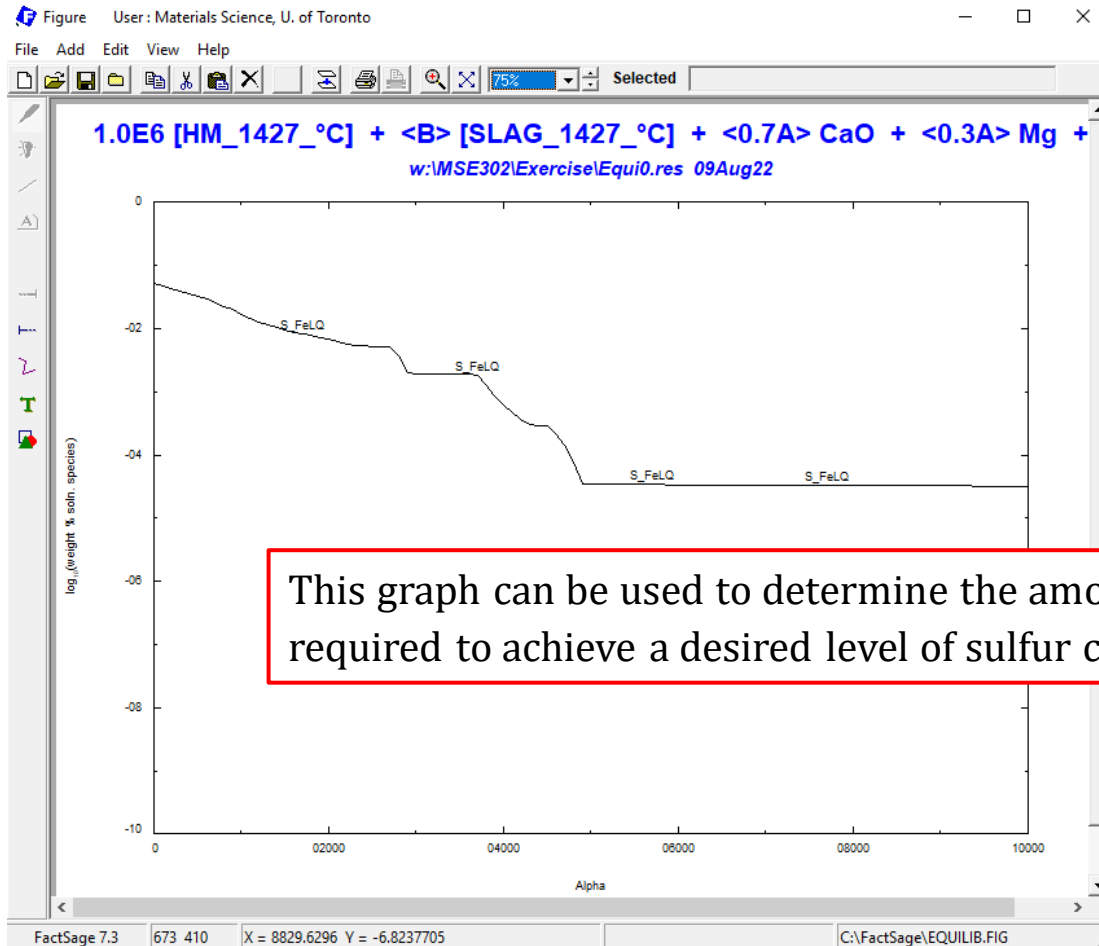
Y-axis settings: maximum 0, minimum -10, tick every 1  
X-axis settings: maximum 10000, minimum 0, tick every 1000

**Species Selection**  
1 selected  
Select  
Repeat

**Graph**  
Labels: size: 9, no: 4  
Display:  color,  full screen,  reactants,  file name,  Viewer,  Figure  
Plot >>

# Example 1: Desulfurization (Advanced Example)

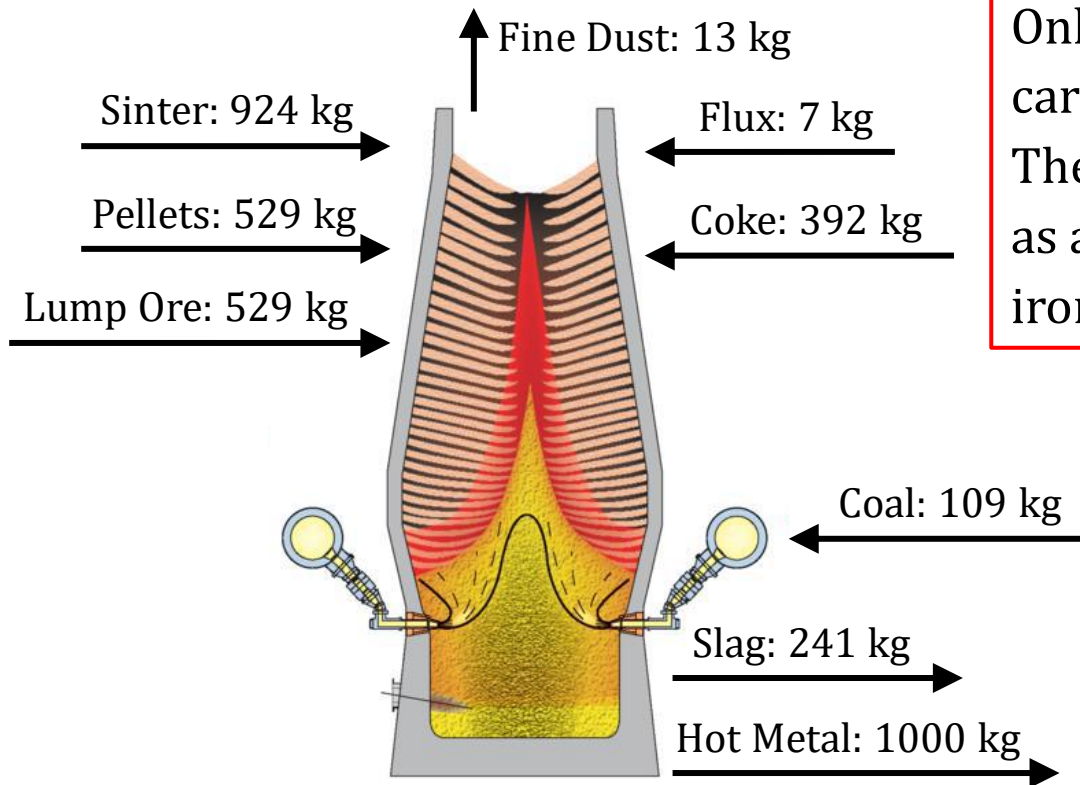
## Plot: wt. %S~<A>



# Example 2: Slag: Enthalpy, Melting Temperature

## Background: Blast Furnace Slag

The following graph shows the mass balance for a typical ironmaking blast furnace.



Only a small fraction of slag is carried over to the torpedo car. The majority of slag will be tapped as a separate by-product of the ironmaking blast furnace process.

# Example 2: Slag: Enthalpy, Melting Temperature

---

## Background: Blast Furnace Slag

Each year, over 300 million tonnes of blast furnace slag are generated all over the world. The molten blast furnace slag, when tapped, has a temperature  $\sim 1500$  °C, and thus the thermal energy contained is quite substantial. For the purpose of heat recovery from the molten blast furnace slag, its enthalpy and melting temperature data are required. We can use the Equilib Module in FactSage to calculate these data.

We will assume the molten blast furnace slag (1500 °C) has the following composition:

<b>Oxide</b>	CaO	SiO <sub>2</sub>	Al <sub>2</sub> O <sub>3</sub>
<b>wt.%</b>	40.0	40.0	20.0

# Example 2: Slag: Enthalpy, Melting Temperature

---

## Task 1: Calculating the Enthalpy of Slag and Recoverable Heat

The Enthalpy of molten slag at 1500 °C based on [the SER state](#) can be directly calculated in the Equilib Module.

The maximum amount of heat (strictly speaking, the amount of thermal energy) that can be recovered corresponds to the Enthalpy change when the molten slag is cooled to room temperature. That is,

$$\left| H_{\text{slag},1500\text{ °C}} - \sum n_i h_{i(\text{solid}),25\text{ °C}}^{\circ} \right|$$

Therefore, two equilibrium states are required: 25 °C and 1500 °C. The following slides present **one** approach to calculate the difference in the Enthalpy at these two temperatures.

# Example 2: Slag: Enthalpy, Melting Temperature

## Task 1: Calculating the Enthalpy of Slag and Recoverable Heat

The screenshot shows the FactSage 7.3 Equilib - Reactants interface. The main window displays a table of reactants with the following data:

Quantity(g)	Species	Phase	T(C)	P(total)**	Stream#
40	CaO				1
+ 40	SiO2				1
+ 20	Al2O3				1

A red box highlights the reactant table. A callout box points to it with the text: "100 g blast furnace slag." Another red box highlights the "FToxid" checkbox in the "Data Search" panel, with a callout box stating: "The slag is an oxide system and we are not considering the gas phase. Only FToxid is needed."

The "Data Search" panel on the right shows the following databases selected:

- FactPS
- FToxid
- FTsalt
- FTmisc
- FTball
- FTOxCN
- FTfrtz
- FThelg
- FTpulp
- FTlite

The "Other" section includes:

- ELEM
- FTdemo
- FTnucl

The "Information" section shows:

- SGTE
- SGPS
- SGTE
- SGsold
- SGnobl
- SpMCBN
- TDmeph
- TDnucl

The status bar at the bottom indicates: FactSage 7.3, Compound: 1/14 databases, Solution: 1/15 databases.

# Example 2: Slag: Enthalpy, Melting Temperature

## Task 1: Calculating the Enthalpy of Slag and Recoverable Heat

Equilib - Menu: last system

File Units Parameters Help

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

Reactants (3)

(gram) 40 CaO + 40 SiO2 + 20 Al2O3

Products

Compound species

gas  ideal  real 0

aqueous 0

pure liquids 0

pure solids 0

species: 0

Target

- none -

Estimate T(K): 1000

Quantity(g): 0

Solution phases

*	+	Base-Phase	Full Name
	I	FToxid-SLAGA	A-Slag-liq all oxides + S
		FToxid-MeO_A	A-Monoxide
		FToxid-Mel_A	A-Melilite

Custom Solutions

fixed activities

ideal solutions

Details ...

Pseudonyms

apply  Edit ...

Assume we know at 1500 °C, the oxide system of interest is fully molten. Therefore, only FToxid-SLAGA is selected.

However, say we are unsure if the molten slag is the only phase at 1500 °C. You could select other solid solutions and pure solids and perform the calculation. You should find from the result that SLAGA is the only phase.

Final Conditions

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

Equilibrium

normal  normal + transitions

transitions only

We would like to calculate the Enthalpy (relative to SER) of the molten slag at 1500 °C.

FactSage 7.3



# Example 2: Slag: Enthalpy, Melting Temperature

## Task 1: Calculating the Enthalpy of Slag and Recoverable Heat

Equilib - Results 1500 C

Output Edit Show Pages Final Conditions

T(C) P(atm)

Output Edit Show Pages Final Conditions

Save or Print > T(C) P(atm) Energy(J) Quantity(g) Vol(m)

Plot >

Equilib Results file >

Stream File > 1.0000E+02 1.0000E+00

Format > FACT Format

Fact-XML >  ChemSage Format

Fact-Optimal > FACT + ChemSage

Fact-Function-Builder > ChemSage + FACT

Append list of input streams

Refresh ... 2.6332 42.130

Swap loops ... S G

TOTAL: 1.0000E+02 1.0000E+00 1.0000E+00

Site fraction of sublattice constituents:

Al 0.22147 Stoichiometry calculated

Si 0.37584

Ca 0.40269

-----

O 1.0000 Stoichiometry calculated

System component Amount/mol Amount/gram Mole fraction Mass fraction

Ca 0.71330 28.588 0.16195 0.28588

Si 0.66573 18.667 0.15115 0.18667

Al 0.39231 13.503 0.09115 0.13503

O 2.6332 106.697 0.59575 1.06697

\*\*\*\*\*

Cp H S

J.K-1 J J.K-1

\*\*\*\*\*

1.18482E+02 -1.24063E+06 2.82653E+02 -1.74181E+06 0.00000E+00

\*\*\*\*\*

Cp H S G

J.K-1 J J.K-1 J

Slag-liq#1 1.18482E+02 -1.24063E+06 2.82653E+02 -1.74181E+06

Cut-off limit for phase activities = 1.00E-75

Database: TTP-1500-75

Data Set: Final Conditions

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

Calculate >>

We are using the ChemSage Format to view the result.

This is the Enthalpy (relative to SER) of the molten slag at 1500 °C. Note the system consists of slag only.

# Example 2: Slag: Enthalpy, Melting Temperature

## Task 1: Calculating the Enthalpy of Slag and Recoverable Heat

Equilib - Menu: last system

File Units Parameters Help

Reactants (3)  
(gram) 40 CaO + 40 SiO2 + 20 Al2O3

Products

Compound species

Solution phases

Right Click

Molar Partial Properties FToxid-SLAGA - A-Slag-liq

Output Species Standard States

Open Spreadsheet

Save Excel Spreadsheet ...

Save Text Spreadsheet ...

Show Columns

Quantity(g), Vol(litre)

integral properties 17/17 properties

Table of Partial Property

+ 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_exc	= s(i) - s_ideal(i)
+ cp(i)	heat capacity of species i = d(h(i))/dT

Select All Clear Close

74

# Example 2: Slag: Enthalpy, Melting Temperature

## Task 1: Calculating the Enthalpy of Slag and Recoverable Heat

The screenshot shows the FactSage Equilib software interface. The main window displays a table of results for a 1500 °C calculation. The table has columns for T(C), P(atm), Energy(J), Quantity(g), and Vol(litre). The first row shows values: 1.0000E+02, 1.0000E+00, 1.0000E+00. Below this, there are several rows of data, including a row with values: 0.66573, 16.697, 0.11, 0.39231, 10.585, 8.966E-02, 0.16363, 2.6332, 42.130, 0.59784, 0.42130. A red box highlights the 'Save solutions' menu item, which has opened a sub-menu with options: 'ALL solutions', 'FToxid-SLAGA#1 A-Slag-liq', and 'FToxid-SLAGA#2 A-Slag-liq'. Another red box highlights the 'Save File' dialog box, which is open to save a file named 'FToxid-SLAGA#1 A-Slag-liq'. The dialog box has a text field containing 'SCA Slag\_1500 °C' and buttons for 'OK' and 'Cancel'. A red arrow points from the 'Save solutions' menu to the dialog box. A large red box contains the following text:

We save the 1500 °C molten slag as a stream. Then this slag stream will be cooled to room temperature. In doing so, the maximum amount of thermal energy that can be recovered is calculated.

# Example 2: Slag: Enthalpy, Melting Temperature

## Task 1: Calculating the Enthalpy of Slag and Recoverable Heat

Equilib - Reactants

File Edit Table Units Data Search Data Evaluation Help

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

1 - 1

The calculation is based on 100 g blast furnace slag.

Quantity(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
100%	[SCA_Slag_1500_°C]	[Stream]	1500	1	1	

( [SCA\_Slag\_1500\_°C]: 100 g = 1.57518 mol = 0.220462 lb ) X 100% = 100 g = 1.57518 mol = 0.220462 lb

“Initial Conditions” is checked because we are looking for the change in the Enthalpy when the temperature is reduced from 1500 to 25 °C.

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

Initial Conditions

Next >>

FactSage 7.3 Compound: 1/14 databases Solution: 1/15 databases

# Example 2: Slag: Enthalpy, Melting Temperature

## Task 1: Calculating the Enthalpy of Slag and Recoverable Heat

Equilib - Menu: last system

File Units Parameters Help

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

**Reactants (1)**

(gram) 100% [SCA\_Slag\_1500\_°C (1500C\_#1)]

**Products**

Compound species

gas  ideal  real 0

aqueous 0

pure liquids 0

pure solids 30

species: 30

**Solution phases**

*	+	Base-Phase	Full Name
		FToxid-SLAGA	A-Slag-liq all oxides + S
		FToxid-MeO_A	A-Monoxide
	+	FToxid-Mel_A	A-Mellite
		FToxid-Mull	Mullite

**Final Conditions**

T(C) 25

P(atm) 1

Delta H(J)

**Equilibrium**

normal  normal + transitions

Annotations:

- No need to select SLAGA because at 25 °C we are sure this is no liquid phase.
- We select all other solid phases (pure solids and solid solutions).
- We cool the slag to room temperature, which is the final temperature.

# Example 2: Slag: Enthalpy, Melting Temperature

## Task 1: Calculating the Enthalpy of Slag and Recoverable Heat

Equilib - Results 25 C

Output Edit Show Pages Final

PHASE: Melilite  
Ca2Al3O7 [1-]  
Ca2Al1Si2O7 [1+]  
TOTAL:  
PHASE: Monoxide#1;#2  
gram MASS FRACTION ACTIVITY  
CaO 0.0000E+00 9.9920E-01 1.0943E-05  
Al2O3 0.0000E+00 8.0460E-04 9.3946E-17  
TOTAL: 0.0000E+00 1.0000E+00 1.0952E-05  
PHASE: Mullite#1;#2  
gram MASS FRACTION ACTIVITY  
Al2Al1O5 [-1] 0.0000E+00 4.2539E-01  
Al2Al1Va5 [+9] 0.0000E+00 9.7732E-05  
Al2Si1O5 [0] 0.0000E+00 5.5207E-01  
Al2Si1Va5 [+10] 0.0000E+00 1.2769E-02  
TOTAL: 0.0000E+00 1.0000E+00 2.5519E-13  
gram ACTIVITY  
Ca3Al2Si3O12\_Grossula (s) 8.8356E+01 1.0000E+00  
Ca3Si2O7\_Rankinite (s) 8.5667E+00 1.0000E+00  
Ca2SiO4\_Gamma (olivine) (s) 3.0770E+00 1.0000E+00  
Ca2Al2SiO7\_Gehlenite (s) 0.0000E+00 2.9212E-01  
CaSiO3\_Wollastonite (s) 0.0000E+00 1.7315E-02  
Al2O3\_corundum (alpha) (s4) 0.0000E+00 3.4150E-03  
CaSiO3\_Ps-wollastoni (s2) 0.0000E+00 1.0091E-03  
CaAl2O4 0.0000E+00 1.0000E+00  
Al2O3\_d 0.0000E+00 1.0000E+00  
Ca2SiO4 0.0000E+00 1.0000E+00  
Al2O3\_k 0.0000E+00 1.0000E+00  
CaO\_Lim 0.0000E+00 1.0000E+00

Final Conditions

<A>	<B>	T(C)	P(atm)	Delta H(J)
		25	1	

1 calculation X

Calculate >>

However, you should be aware we are performing equilibrium cooling calculations. In the real world, the equilibrium cooling of molten slag is never the case. As a result, the cooled slag usually contain a fraction of glass phase (meta-stable), and thus the recovered thermal energy is less than if the equilibrium cooling is achieved.

Only those solids with unity activity are stable.

# Example 2: Slag: Enthalpy, Melting Temperature

## Task 1: Calculating the Enthalpy of Slag and Recoverable Heat

The screenshot displays the FactSage software interface. The main window shows a list of components and their thermodynamic properties. A red box highlights the 'DELTA H' value for the slag components, which is  $-2.19303E+05$  J. A red arrow points from this value to a text box. Below the main window, a 'Final Conditions' dialog box is open, showing a table with columns for 'T(C)', 'P(atm)', and 'Delta H(J)'. The 'T(C)' column has the value '25' and the 'P(atm)' column has the value '1'. A 'Calculate >>' button is visible at the bottom right of the dialog box.

Component	T(C)	P(atm)	Energy(J)	Quantity(g)	Vol(litre)
Ca3Al2O6_solid(s)	0.000				
CaAl12O19_solid(s)	0.000				
Ca3SiO5_Hatrurite(s)	0.000				
CaAl2Si2O8_Hexagonal(s)	0.0000E+00				1.1069E-19
SiO2_stishovite(s8)	0.0000E+00				6.1583E-22

DELTA Cp	DELTA H	DELTA S	DELTA G	DELTA V
J.K-1	J	J.K-1	J	dm3
-4.55498E+01	-2.19303E+05	-2.24361E+02	2.64503E+05	0.00000E+00

Cp	H	S	G	V
7.23				

Final Conditions dialog box:

<A>	<B>	T(C)	P(atm)	Delta H(J)
		25	1	

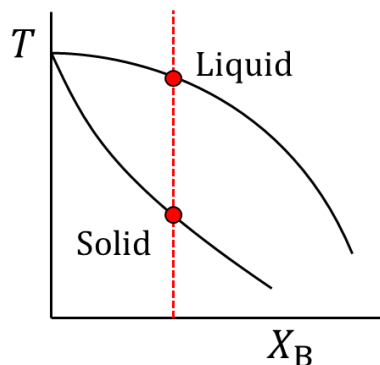
This is the maximum amount of thermal energy we can recover from 100 g molten blast furnace slag (at 1500 °C) that is considered.

You can carry out a quick calculation for the amount of thermal energy that can be recovered from 300 million tonnes of blast furnace slag. Unfortunately, the majority of these energy is currently wasted, and many attempts are made to develop a sustainable technology for its recovery.

# Example 2: Slag: Enthalpy, Melting Temperature

## Task 2: Calculating the Melting Temperature of Slag

First of all, you need to be aware that for pure substances, the melting or solidification process occurs at a fixed temperature (determined by the Gibbs phase rule). On the contrast, for solution phases, the melting or solidification process occurs within a certain temperature range, bounded by the liquidus temperature and solidus temperature. **The melting temperature of slag** refers to the liquidus temperature, that is, the temperature above which the system exists as 100% liquid. There are generally two approaches to calculating the melting temperature:



**(a) Cooling Approach.** Start with a temperature which is high enough so that the system is 100% liquid. Then cool the system to find the temperature when the first solid forms

**(b) Heating Approach.** Heat up the solid mixture and find the temperature when the last solid disappears.



# Example 2: Slag: Enthalpy, Melting Temperature

## Task 2: Calculating the Melting Temperature of Slag (Cooling Approach)

We have already defined a molten CSA slag stream at 1500 °C. Import this slag stream. Of course, you can also manually input the three oxides. We will cool this molten slag and find the temperature at which the first solid appears.

Check the option of “Initial Conditions” to indicate the slag is fully molten at 1500 °C. However, you don’t have to do so.

Quantity(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
100%	[SCA_Slag_1500_°]	[Stream]	1500	1	1	

FactSage 7.3    Compound: 1/14 databases    Solution: 1/15 databases

# Example 2: Slag: Enthalpy, Melting Temperature

## Task 2: Calculating the Melting Temperature of Slag (**Cooling Approach**)

Equilib - Menu: last system

File Units Parameters Help

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

Reactants (1)

(gram) 100% [SCA\_Slag\_1500\_°C]  
(1500C,#1)

Products

Compound Species Solution phases

*	+	Base-Phase	Full Name
IL		FToxid-SLAGA	A-Slag-liq all oxides + S
I		FToxid-MeO_A	A-Monoxide

Custom Solutions  
0 fixed activities  
0 ideal solutions

Pseudonyms

Help

Help ...

Right Click

Not cooling calculation!

In the Equilib Module, "Cooling Calculation" is permitted. We could perform either equilibrium cooling or non-equilibrium cooling (Scheil-Gulliver cooling). The equilibrium cooling mode will calculate all the characteristic temperatures when new solids precipitate.

Equilibrium cooling - T(start) = 1500, T(stop) = 0

Calculate >>

# Example 2: Slag: Enthalpy, Melting Temperature

## Task 2: Calculating the Melting Temperature of Slag (**Cooling Approach**)

Equilib - Menu: last system

File Units Parameters Help

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

Reactants (1)

(gram) 100% [SCA\_Slag\_1500\_°C]  
(1500C,#1)

Select all the pure solids.

Select all the solid solutions.

*	+	Base-Phase	Full Name
		IL	FToxid-SLAGA
		I	FToxid-MeO_A
		+	FToxid-Mel_A
		I	FToxid-Mull

Custom Solutions  
0 fixed activities  
0 ideal solutions

Pseudonyms  
apply  Edit ...

Volume data  
assume molar volumes of

Equilibrium cooling  
FToxid-SLAGA  
Cooling step: 25 T-auto:   
Quantity(g): 0

We will use the default cooling step 25 °C. However, this does not affect the calculation of characteristic temperatures.

Cooling starts at 1500 °C. That's why we don't have to check the option of "Initial Conditions".

Final Conditions

<A>	<B>	T(C)	P(atm)	Delta H(J)
		1500	1	

10 steps  Table

Equilibrium cooling - T(start) = 1500, T(stop) = 0

normal  normal + transitions  
 transitions only  
 open

Calculate >>

FactSage 7.3

# Example 2: Slag: Enthalpy, Melting Temperature

## Task 2: Calculating the Melting Temperature of Slag (**Cooling Approach**)

Select all the pure solids.

Equilib

Output Edit Show Pages Final Conditions

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

- Summary - Transitions 1325 C | 1321.49 C | 1300 C | 1275 C | 1265.79 C | 1257.43 C | 1257.43 C

(Double-Click on any phase listed above to recycle

**SUMMARY OF REACTIONS**

Cooling  
1325 to 1321.49 C (DELTA H = -4.1481E+02 J)  
Slag-liq cooling

Constituent 1  
1321.49 to 1265.79 C (DELTA H = -1...)  
Slag-liq -> Melilite

Constituent 2  
1265.79 to 1257.43 C (DELTA H = -2...)  
Slag-liq -> Melilite + CaAl2Si2O8 Anorthite(s2)

Constituent 3  
1257.43 C (isothermal) (DELTA H = -3.9243E+04 J)  
Slag-liq -> Melilite + CaSiO3\_Ps-wollastonite(s2) + CaAl2Si2O8 Anorthite(s2)

COMPOSITION OF PHASES IN CONSTITUENTS AT (temperature of final disappearance of S

**Final Conditions**

	<A>	<B>	T(C)	P(atm)	Delta H(J)
Melilite			1500	1	
Ca					
Si					

Deactivated for Scheil cooling

All the equilibrium calculations. The temperatures of 1321.49, 1265.79, and 1257.43 °C are when new solids start to precipitate.

The first solid – Melilite forms at 1321.49 °C. Clearly, this temperature is the melting temperature.

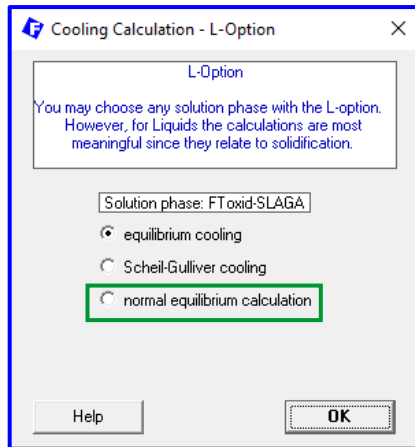
Please view other tabs and see if you can comprehend the calculation results (use the ChemSage format)

# Example 2: Slag: Enthalpy, Melting Temperature

## Task 2: Calculating the Melting Temperature of Slag (**Cooling Approach**)

A Note on “Normal Equilibrium Calculation”:

You can also use the mode of “normal equilibrium calculation” to calculate the melting temperature (Next Page).



# Example 2: Slag: Enthalpy, Melting Temperature

## Task 2: Calculating the Melting Temperature of Slag (Cooling Approach)

Equilib - Menu: last system

File Units Parameters Help

Reactants (1)

(gram) 100% [SCA\_Slag\_1500\_°C]  
(1500C,#1)

Products

Compound species

gas  ideal  real 0  
aqueous 0  
pure liquids 0  
pure solids 30

species: 30

Transitions - temperature

Number of transitions: All

Final Conditions

<A>	<B>	T(°C)	P(atm)	Delta H(J)
1500	1000	1		

Equilibrium

normal  normal  
 transitions only

Calculate >>

Normal equilibrium calculation.

We estimate the melting temperature in this temperature range, and we perform an equilibrium calculation at every 1 °C.

We will look at the characteristic temperatures (transitions).

# Example 2: Slag: Enthalpy, Melting Temperature

## Task 2: Calculating the Melting Temperature of Slag (Cooling Approach)

Equilib - Results 1321.49 C

Output Edit Show Pa

This is the first transition when temperature is reduced from 1500 °C.

1321.49 C | 1265.79 C | 1257.43 C | 1257.43 C | 1125.31 C | 1125.31 C

PHASE: Slag-liq#1(;;#2)	EQUIL AMOUNT	MASS FRACTION	ACTIVITY
Al2O3	2.0000E+01	2.0000E-01	1.2609E-02
SiO2	4.0000E+01	4.0000E-01	8.4424E-02
CaO	4.0000E+01	4.0000E-01	7.6344E-04
TOTAL:	1.0000E+02	1.0000E+00	1.0000E+00

Site fraction of sublattice constituents:  
Al 0.22147  
Si 0.37584  
Ca

Stoichiometry calculated

Slag is a stable phase because its activity (activity of phase, not constituents) is unity.

PHASE: Melilite	EQUIL AMOUNT	MASS FRACTION	ACTIVITY
Ca2Al3O7[1-]	0.0000E+00	4.9799E-01	2.5000E-01
Ca2Al1Si2O7[1+]	0.0000E+00	5.0201E-01	2.5000E-01
TOTAL:	0.0000E+00	1.0000E+00	1.0000E+00

PHASE: Mullite#1;#2

PHASE: Mullite#1;#2	EQUIL AMOUNT	MASS FRACTION	ACTIVITY
Al2Al1O5[1-]	0.0000E+00	3.2437E-01	7.2660E-04

Melilite is the only stable solid. This transition temperature (1321.49 °C) is when melilite first forms.

# Example 2: Slag: Enthalpy, Melting Temperature

---

## Task 2: Calculating the Melting Temperature of Slag (**Heating Approach**)

In the heating approach, we will manually input the oxides at 25 °C, and then perform higher-temperature calculations. The following slides show the calculation details.



# Example 2: Slag: Enthalpy, Melting Temperature

## Task 2: Calculating the Melting Temperature of Slag (**Heating Approach**)

Equilib - Reactants

File Edit Table Units Data Search Data Evaluation Help

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

1 - 3

Right Click

CaO

Compound data on CaO ...

Help

Quantity(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
40	CaO	solid Lime	25	1.0	1	
+ 40	SiO2	solid-1 Quartz(l)	25			
+ 20	Al2O3	solid-4 corundum(alpha)	25			

We can use the View Data Module to determine the phase type at 25 °C.

View Data CaO Units: T(K) P(atm) Energy(J) Quantity(mol)

File Edit Sort Compounds Summary Databases Units Atomic Wts. Table Graph Help << Back

2 Phases FToxid - FACT oxide compounds (2019)

Phases Cp(T) H(T) G(T) S(T) Volume Magnetic Refs. **Trans.** Mol Wt.%

Name: Calcium

Clearly, S1 is the stable CaO at 25 °C.

Transition	T(K)	T(C)	Delta H J/mol	Delta S J/mol-K	Delta Cp J/mol-K
S1 -> L1	2845.16	2572.01	79496.0	27.941	0.000

Check the option of "Initial Conditions" to indicate the oxide mixture is initially at 25 °C. However, you don't have to do so.

Initial Conditions

Next >>

FactSage 7.3 Compound: 1/14 databases Solution: 1/15 databases

# Example 2: Slag: Enthalpy, Melting Temperature

## Task 2: Calculating the Melting Temperature of Slag (**Heating Approach**)

Equilib - Reactants

File Edit Table Units Data Search Data Evaluation Help

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

1 - 3

Right Click

CaO

Compound data on CaO ...

Help

Quantity(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
40	CaO	solid Lime	25	1.0	1	
+ 40	SiO2	solid-1 Quartz(l)	25			
+ 20	Al2O3	solid-4 corundum(alpha)	25			

We can use the View Data Module to determine the phase type at 25 °C.

View Data CaO Units: T(K) P(atm) Energy(J) Quantity(mol)

File Edit Sort Compounds Summary Databases Units Atomic Wts. Table Graph Help << Back

2 Phases FToxid - FACT oxide compounds (2019)

Phases Cp(T) H(T) G(T) S(T) Volume Magnetic Refs. **Trans.** Mol Wt.%

Name: Calcium

Clearly, S1 is the stable CaO at 25 °C.

Transition	T(K)	T(C)	Delta H J/mol	Delta S J/mol-K	Delta Cp J/mol-K
S1 -> L1	2845.16	2572.01	79496.0	27.941	0.000

Check the option of "Initial Conditions" to indicate the oxide mixture is initially at 25 °C. However, you don't have to do so.

Initial Conditions

Next >>

FactSage 7.3 Compound: 1/14 databases Solution: 1/15 databases

# Example 2: Slag: Enthalpy, Melting Temperature

## Task 2: Calculating the Melting Temperature of Slag (**Heating Approach**)

The screenshot shows the FactSage Equilib software interface. The reactants are (gram) 40 CaO + 40 SiO2 + 20 Al2O3. The products list includes pure solids (30 species). The solution phases table is highlighted, showing phases like FToxid-SLAGA (A-Slag-liq all oxides + S), FToxid-MeO\_A (A-Monoxide), FToxid-Mel\_A (A-Mellite), and FToxid-Mull (Mullite). The final conditions are set to T(C) 25 1500 25. The equilibrium options are set to 'transitions only'. Red boxes and arrows highlight these key settings.

Choose all the pure solids.

Choose all the solution phases.

We are heating up the oxide mixture from 25 °C up to 1500 °C.

We will look at the characteristic temperatures (transitions).

*	+	Base-Phase	Full Name
		FToxid-SLAGA	A-Slag-liq all oxides + S
		FToxid-MeO_A	A-Monoxide
	+	FToxid-Mel_A	A-Mellite
		FToxid-Mull	Mullite

<A>	<B>	T(C)	P(atm)	Delta H(J)
		25 1500 25	1	

# Example 2: Slag: Enthalpy, Melting Temperature

## Task 2: Calculating the Melting Temperature of Slag (**Heating Approach**)

Equilib - Results 1257.43 C (page 9/12)

Output Edit Show Pages Final Conditions

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

1321.49 C

63.49 C | 63.49 C | 749.2 C | 749.2 C | 859.36 C | 859.36 C | 1125.31 C | 1125.31 C | **- 1257.43 C** | 1257.43 C | 1265.79 C

System component	Amount/mol	Amount/gram	Mole fraction
Al	1.0000		
Si	0.50000		
Al	0.50000		
Ca	0.24372	9.7679	0.16667
Si	0.12186	3.4225	8.3333E-02
Al	0.24372	6.5760	0.16667
O	0.85302	13.648	0.58333
TOTAL:	0.0000E+00	1.0000E+00	<b>1.0000E+00</b>
PHASE: Slag-liq#1;#2	gram	MASS FRACTION	ACTIVITY
Al2O3	0.0000E+00	1.8049E-01	7.5821E-03
SiO2	0.0000E+00	4.1696E-01	1.0318E-01
CaO	0.0000E+00	4.0255E-01	4.6771E-04
PHASE: Mullite#1;#2	gram	MASS FRACTION	ACTIVITY
Al2Al10S[-1]	0.0000E+00	3.0242E-01	4.5553E-04
Al2Al1VaS[+9]	0.0000E+00	4.8452E-03	1.4948E-11
Al2Si10S[0]	0.0000E+00	6.8174E-01	1.6224E-02
Al2Si1VaS[+10]	0.0000E+00	1.0996E-02	5.3239E-10
TOTAL:	0.0000E+00	1.0000E+00	5.4708E-02
PHASE: Monoxide#1;#2	gram	MASS FRACTION	ACTIVITY
CaO	0.0000E+00	3.1974E-01	8.3843E-03
Al2O3			
TOTAL:			

Final Conditions

<A>	<B>	T(C)	P(atm)	Delta H(J)
CaSiO3		25 1500 25	1	
CaAl2Si				

60+ calculations

Calculate >>

At 1257.43 °C, the liquid slag starts to form (solidus temperature or first melting temperature).

# Example 2: Slag: Enthalpy, Melting Temperature

## Task 2: Calculating the Melting Temperature of Slag (**Heating Approach**)

Equilib - Results 1321.49 C (page 12/12)

Output Edit Show Pages Final Conditions

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

63.49 C | 63.49 C | 749.2 C | 749.2 C | 859.36 C | 859.36 C | 1125.31 C | 1125.31 C | 1257.43 C | 1257.43 C | 1265.79 C

-1321.49 C-

System component	Amount/mol	Amount/gram	Mole fraction
Ca	0.71330	28.588	0.16195
Si	0.66573	18.697	0.15115
Al	0.39231	10.585	8.9068E-02
O	2.6332	42.130	0.59784

PHASE: Melilite

System component	Amount/mol	Amount/gram	Mole fraction	ACTIVITY
Ca <sub>2</sub> Al <sub>3</sub> O <sub>7</sub> [1-]	0.0000E+00	4.9799E-01	2.5000E-01	2.5000E-01
Ca <sub>2</sub> Al <sub>1</sub> Si <sub>2</sub> O <sub>7</sub> [1+]	0.0000E+00	5.0201E-01	2.5000E-01	2.5000E-01
TOTAL:	0.0000E+00	1.0000E+00	1.0000E+00	1.0000E+00

Site fraction of sublattice constituents:

System component	Amount/mol	Amount/gram	Mole fraction	Mass fraction
Ca	0	0	0.16667	0.29233
Si	0	0	8.3333E-02	0.10243
Al	0	0	0.16667	0.19680

Final Conditions

PHASE:	<A>	<B>	T(C)	P(atm)	Delta H(J)
Al2Al10			25 1500 25	1	
Al2Al1V					
Al2Si10					

60+ calculations X

Calculate >>

At 1321.49 °C, only melilite is present, but this is the last solid before the system becomes 100% liquid.

# In-Class Exercise

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**Question 1.** The typical composition of copper slag is shown below.

<b>Oxide</b>	FeO	SiO <sub>2</sub>	CaO	Al <sub>2</sub> O <sub>3</sub>
<b>wt.%</b>	40.0	40.0	10.0	10.0

Calculate the equilibrium when this copper slag is heated between 1000 and 1800 °C in air (i.e.,  $P_{O_2} = 0.21$  atm).

Tip: (1) perform the calculation based on 100 gram of copper slag; (2) plot the masses of all stable phases against temperature.

# In-Class Exercise

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## Question 2. Desulfurization of Liquid Steel

We have studied the desulfurization of hot metal using different desulfurizing agents. The hot metal after desulfurization is transferred to a basic oxygen furnace (BOF) for decarbonation. The resulting metal product is referred to as liquid steel.

[Another spot](#) of desulfurization is during ladle refining of liquid steel. Say we choose Mg as the desulfurization agent. Use the Equilib Module to find the required Mg if the sulfur content is reduced from 0.01 to 0.001 wt.%S. You may need the data shown on the next slide.

# In-Class Exercise

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## Question 2. Desulfurization of Liquid Steel

Liquid Steel Composition.

<b>Element</b>	C	Mn	S	Fe
<b>wt.%</b>	0.05	0.10	0.01	99.84

Ladle Furnace Slag Composition.

<b>Component</b>	CaO	SiO <sub>2</sub>	MgO	Al <sub>2</sub> O <sub>3</sub>
<b>wt.%</b>	40.0	10.0	10.0	40.0

The slag carry-over is 100 kg/tonne steel, and the temperature is 1600 °C.

**Note:** you don't have to consider the gas phase.



# In-Class Exercise

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## Question 3. Preparation of Synthetic Slags

Use the Equilib Module to solve the following questions

As a summer student, your professor asked you to prepare a synthetic blast furnace slag. You have the following available chemical reagents, including solid quartz (low-temperature,  $\text{SiO}_2$ ), solid lime ( $\text{CaO}$ ), solid alpha corundum ( $\text{Al}_2\text{O}_3$ ), and solid periclase ( $\text{MgO}$ ).

(1) If the composition of the blast furnace slag is 32 wt.%  $\text{SiO}_2$ , 40 wt.%  $\text{CaO}$ , 17 wt.%  $\text{Al}_2\text{O}_3$  and 11 wt.%  $\text{MgO}$ , what is the melting temperature?

(2) If all the chemical reagents which are initially at room temperature ( $25\text{ }^\circ\text{C}$ ) are fed into the furnace, calculate the minimum energy requirement when forming 100 g slag with the temperature determined in (1).