

# **Ilmenite Smelting & Drying**

## Process Simulation

Computational Thermodynamics  
MIME 572

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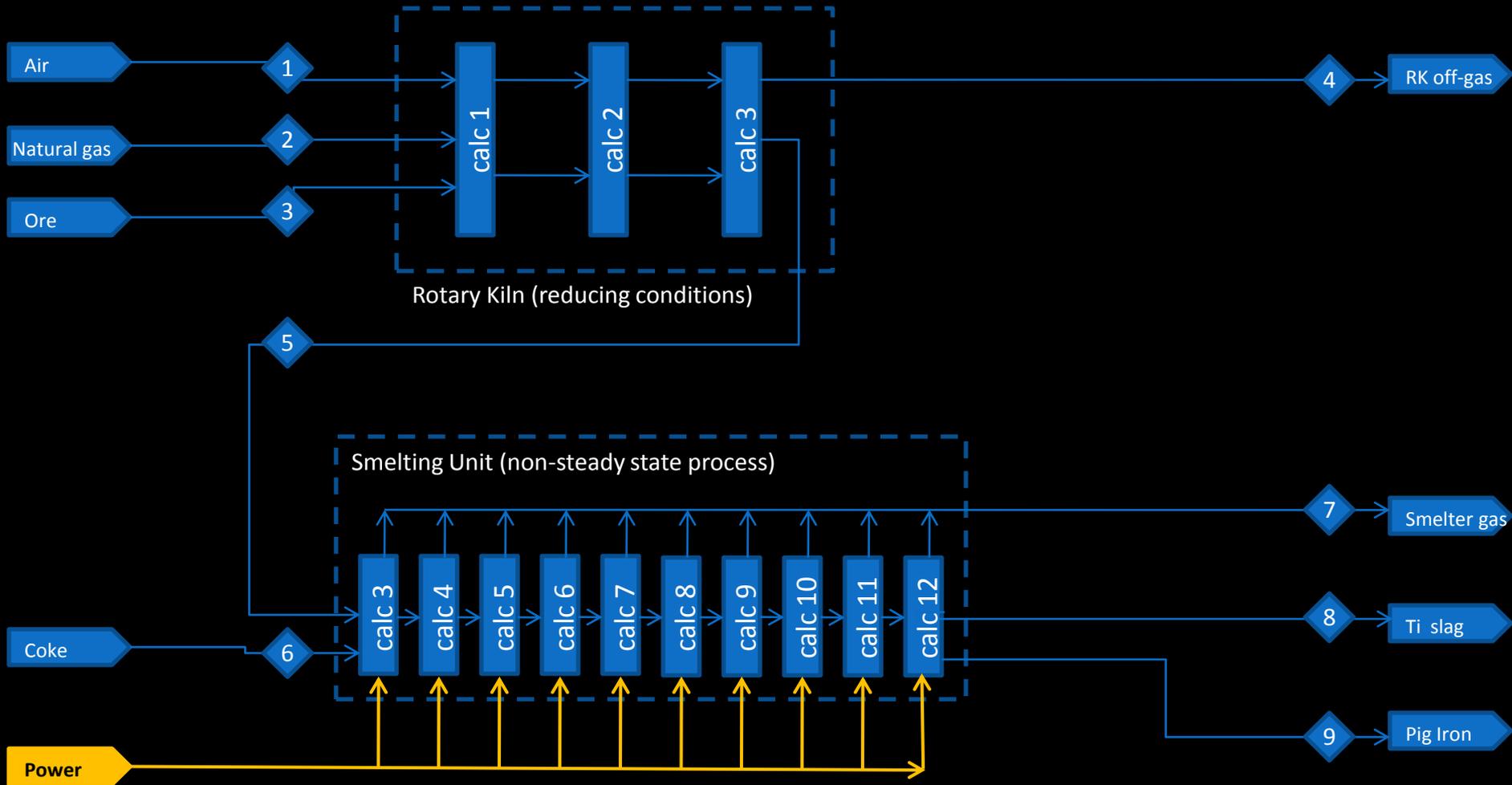
# OUTLINE

- Process Flow Diagrams
- Smelter Simulation
  - Ore Feed
  - Metallurgical Coke Feed
  - Ore to Coke ratio
  - Equilibrium Calculations
- Rotary Kiln
  - CO Flame Calibration
  - Rotary Kiln Input
  - Rotary Kiln dynamic simulation
  - Rotary Kiln calculations
- Assumptions vs Results
- Discussion
- Conclusion

# Process Flow Diagrams

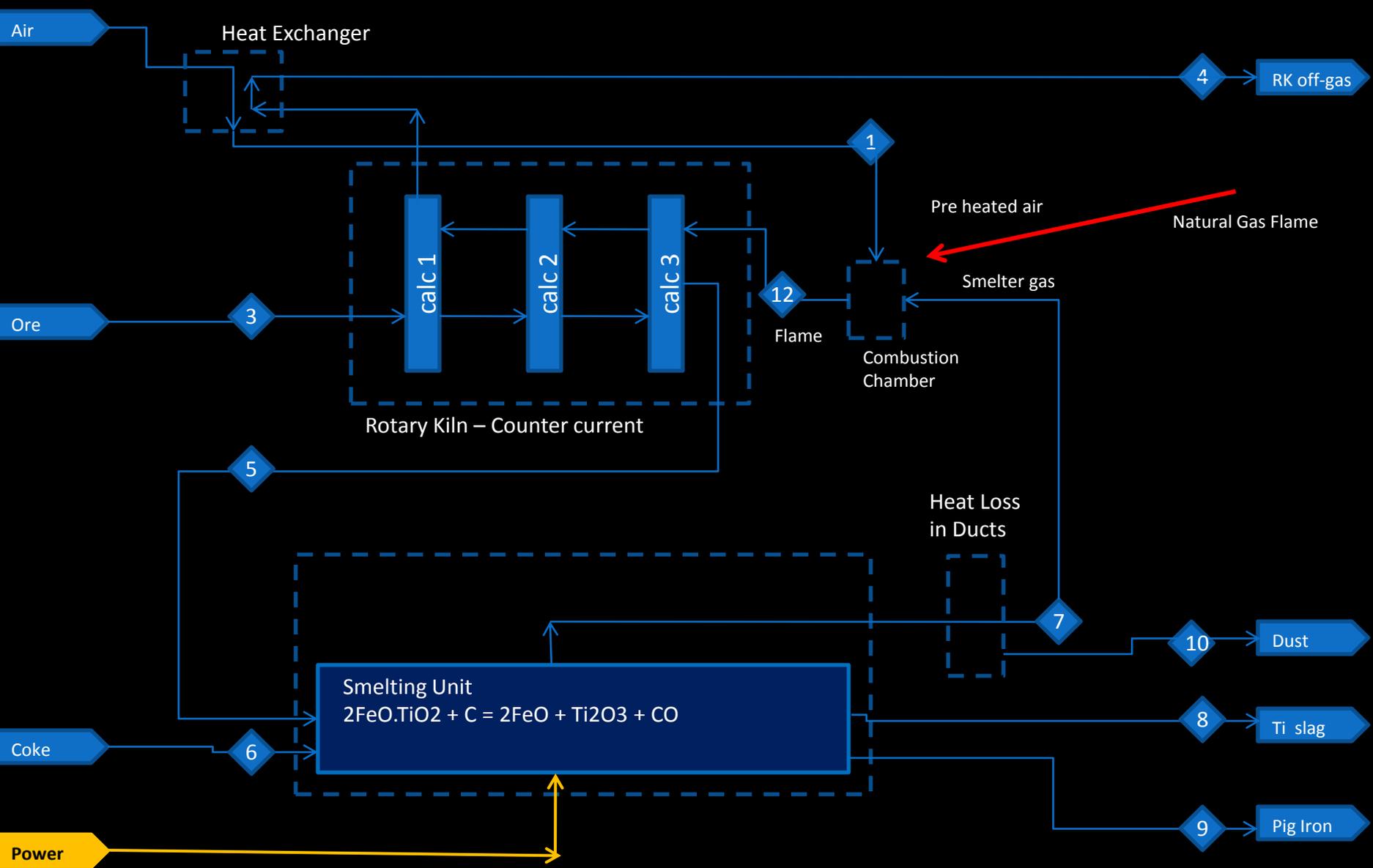
# Process Flow Diagram

## FIRST CONCEPT :



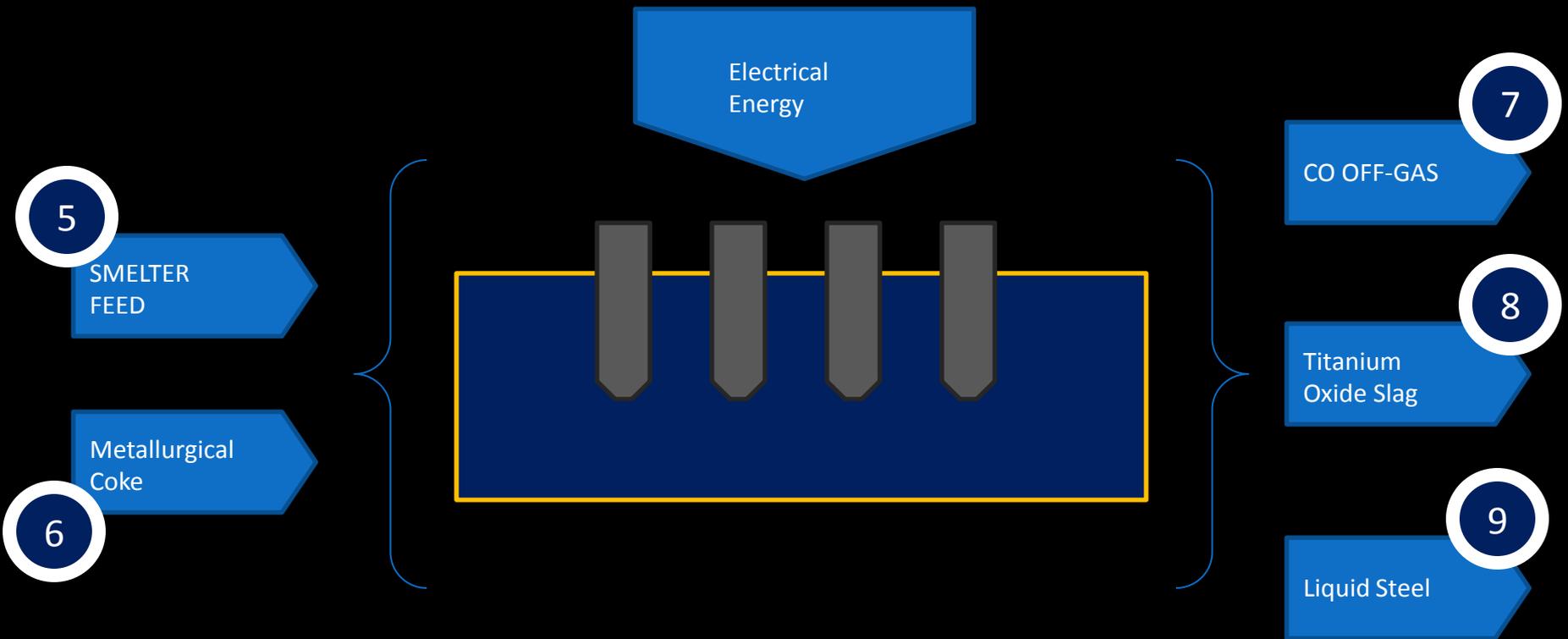
# Process Flow Diagram

## REVISED CONCEPT



# SMELTER SIMULATION

# SMELTER SIMULATION



The Smelting Process is Continuous:  
A single calculation is thus required.

# SMELTER SIMULATION

## Ore Feed

**F Reactants - Equilib**

File Edit Table Units Data Search Help

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

1 - 5

Mass(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
50000	TiO <sub>2</sub>	solid-1-FACT53 rutile	1000.00	1.0	1	FACT53
+ 26700	FeO	solid-FACT53 wustit	1000.00	1.0	1	FACT53
+ 22000	Fe <sub>2</sub> O <sub>3</sub>	solid-1-FACT53 hem	1000.00	1.0	1	FACT53
+ 1260	MnO	solid-FACT53	1000.00	1.0	1	FACT53
+ 40	C	solid-1-FACT53 grap	1000.00	1.0	1	FACT53

Initial Conditions

**Next >>**

FactSage 6.1 Compound: 3/19 databases Solution: 2/19 databases

**F Menu - Equilib:**

File Units Parameters Help

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

**Reactants (5)**

(gram) 50000 TiO<sub>2</sub> + 26700 FeO + 22000 Fe<sub>2</sub>O<sub>3</sub> + 1260 MnO  
(1000.00C,s1-FACT53,#1) (1000.00C,s-FACT53,#1) (1000.00C,s1-FACT53,#1) (1000.00C,s-FACT53,#1)

**Products**

Compound species:  gas  ideal  real 18  
 aqueous 0  
 pure liquids 0  
 pure solids 124  
 suppress duplicates **apply**  
species: 142

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

Solution species

	+	Base-Phase	Full Name
	+	FSstel-MONO	Monoxide
	+	FSstel-FE-L	Fe-LIQUID
	+	FSstel-CBCC	CBCC_A12
	+	FSstel-CUB	CUB_A13
	+	FSstel-LAV1	LAVES_C14
	+	FSstel-HCP	HCP_A3:Me2[C,N]
		FToxid-SLAGA	ASlag-liq

Legend: | - immiscible 1, + - selected 7  
 Show  all  selected  
species: 53, solutions: 9 **Select**

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

Pseudonyms: **apply**  **List ...**

include molar volumes  
Total Species (max 1500) 195  
Total Solutions (max 40) 9  
**Default**

**Final Conditions**

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

10 steps  Table **1 calculation**

Equilibrium:  normal  transitions,  predominant  open  
**Calculate >>**

FactSage 6.1

Ore feed was assumed to come from the Rotary Kiln at 1000 °C. The composition was reacted at the same temperature in order to identify the stable phases.

# SMELTER SIMULATION

## Ore Feed

**F Data Search** ✕

Databases - 3/19 compound databases, 2/19 solution databases

		<b>SGTE</b>	<input type="checkbox"/> compounds only	<b>Miscellaneous</b>		
<input type="checkbox"/> ELEM	<input type="checkbox"/> FS <sub>copp</sub>	<input type="checkbox"/> BINS	<input type="checkbox"/> solutions only	<input type="checkbox"/> ASS2	<input type="checkbox"/> ASS1	<input type="checkbox"/> CUBH
<input type="checkbox"/> FACT	<input type="checkbox"/> FS <sub>lead</sub>	<input type="checkbox"/> SGPS	<input type="checkbox"/> no data	<input type="checkbox"/> CUS0	<input type="checkbox"/> EXAM	<input type="checkbox"/> MPGA
<input checked="" type="checkbox"/> Fact53	<input type="checkbox"/> FS <sub>lite</sub>	<input type="checkbox"/> SGTE	Clear All	<input type="checkbox"/> P205	<input type="checkbox"/> PIER	<input type="checkbox"/> PINH
<input checked="" type="checkbox"/> FT <sub>oxid</sub>	<input checked="" type="checkbox"/> FS <sub>stel</sub>	<input type="checkbox"/> SG <sub>nobl</sub>	Select All	<input type="checkbox"/> PS2	<input type="checkbox"/> PS3F	<input type="checkbox"/> PSOL
<input type="checkbox"/> FT <sub>salt</sub>	<input type="checkbox"/> FS <sub>upsi</sub>	<input type="checkbox"/> SG <sub>sold</sub>	Add/Remove Data	<input type="checkbox"/> SLAG		
<input type="checkbox"/> FT <sub>misc</sub>	<input type="checkbox"/> FS <sub>nobl</sub>	<input type="checkbox"/> SG <sub>nucl</sub>	RefreshDatabases			
<input type="checkbox"/> FT <sub>hall</sub>						
<input type="checkbox"/> FT <sub>helg</sub>	<b>Other</b>	<input type="checkbox"/> TD <sub>nucl</sub>				
<input type="checkbox"/> FT <sub>pulp</sub>	<input type="checkbox"/> OLIP	<input type="checkbox"/> OLIC				
<input type="checkbox"/> FT <sub>lite</sub>	<input type="checkbox"/> OLIG	<input type="checkbox"/> OLIL				

**Information** -  
Click on a box to include (or exclude) a database in the data search. Normally databases are 'coupled' - that is both the compound and solution database (when available) will be selected. To 'uncouple' a databases click-mouse-right-button (note, this is NOT recommended).  
If database is stored on your PC but not listed here then you must 'add the database to the list' - click on 'Add/Remove ...'!

**Options**

<input type="button" value="Default"/>	<b>Include</b> <input type="checkbox"/> gaseous ions (plasmas) <input type="checkbox"/> aqueous species <input checked="" type="checkbox"/> limited data compounds (25C)	<b>Limits</b> Organic species C <sub>x</sub> H <sub>y</sub> ..., X(max) = <input type="text" value="2"/> Minimum solution components: <input type="radio"/> 1 <input checked="" type="radio"/> 2 cpts
--	---	---

# SMELTER SIMULATION

## Ore Feed

5

SMELTER  
FEED

```
F Results - Equilib 1000 C
Output Edit Show Pages
T(C) P(atm) Energy(J) Mass(g) Vol(litre)

+ 38512. gram (FeO)(TiO2)_ilmenite FACT53
(38512. gram, 253.83 mol)
(1000.00 C, 1 atm, S1, a=1.0000)

+ 30357. gram Fe3O4_magnetite FSstel
(30357. gram, 131.11 mol)
(1000.00 C, 1 atm, S2, a=1.0000)

+ 28306. gram TiO2_rutile FACT53
(28306. gram, 354.36 mol)
(1000.00 C, 1 atm, S1, a=1.0000)

+ 2678.8 gram (MnO)(TiO2)_solid FACT53
(2678.8 gram, 17.762 mol)
(1000.00 C, 1 atm, S1, a=1.0000)

+ 0.00000 gram TiO2_rutile FToxid
(1000.00 C, 1 atm, S1, a=1.0000)

+ 0.00000 gram (FeO)(TiO2)_ilmenite FToxid
(1000.00 C, 1 atm, S1, a=1.0000)

+ 0.00000 gram Fe3O4_magnetite FACT53
(1000.00 C, 1 atm, S2, a=1.0000)

+ 0.00000 gram MnTiO3_pyrophanite FToxid
(1000.00 C, 1 atm, S1, a=0.95957)

+ 0.00000 gram Fe3O4_magnetite FSstel
```

```
F Results - Equilib 1000 C
Output Edit Show Pages
T(C) P(atm) Energy(J) Mass(g) Vol(litre)

(gram) 50000 TiO2 + 26700 FeO + 22000 Fe2O3 + 1260 MnO +
(1000.00,1,s1-FACT53,#1) (1000.00,1,s-FACT53,#1) (1000.00,1,s1-FACT53,#1) (1
(gram) 40 C =
(1000.00,1,s1-FACT53,#1)

3.3303 mol gas_ideal
(146.47 gram, 3.3303 mol, 347.92 litre, 4.2099E-04 g/ml)
(1000.00 C, 1 atm, a=1.0000)
( 0.99823 CO2 FACT53
+ 1.7708E-03 CO FACT53
+ 2.3627E-09 O2 FACT53
+ 5.2112E-12 O FACT53
+ 6.8764E-14 Fe FACT53
+ 6.7002E-14 FeO FACT53
+ 4.5139E-14 Mn FACT53
+ 4.6848E-23 TiO FACT53
+ 4.1067E-23 O3 FACT53
+ 2.1177E-25 C3O2 FACT53
+ 1.0688E-25 C2O FACT53
+ 1.3900E-29 C FACT53
+ 2.9734E-33 Ti FACT53
+ 3.1112E-40 C2 FACT53
+ 1.1152E-40 Fe(CO)5 FACT53
+ 5.9994E-46 C3 FACT53
+ 3.3167E-60 C4 FACT53
+ 1.0294E-67 C5 FACT53)

+ 0.00000 gram ASlag-liq#1
(1000.00 C, 1 atm, a=0.59427)
( 19.930 wt.% FeO FToxid
+ 25.397 wt.% Fe2O3 FToxid
+ 7.3275 wt.% MnO FToxid
+ 2.2126E-02 wt.% Ti2O3 FToxid
+ 47.198 wt.% TiO2 FToxid
+ 0.12493 wt.% Mn2O3 FToxid)

+ 0.00000 gram ASlag-liq#2
(1000.00 C, 1 atm, a=0.59427)
( 19.930 wt.% FeO FToxid
+ 25.397 wt.% Fe2O3 FToxid
```

On a 100 kg basis. Gases are generated and not considered in the calculations. Solids are saved as a stream and their composition serve to create a 100 kg ore feed into the smelter.

# SMELTER SIMULATION

## Metallurgical Coke Feed

A simplified metallurgical coke composition was used.

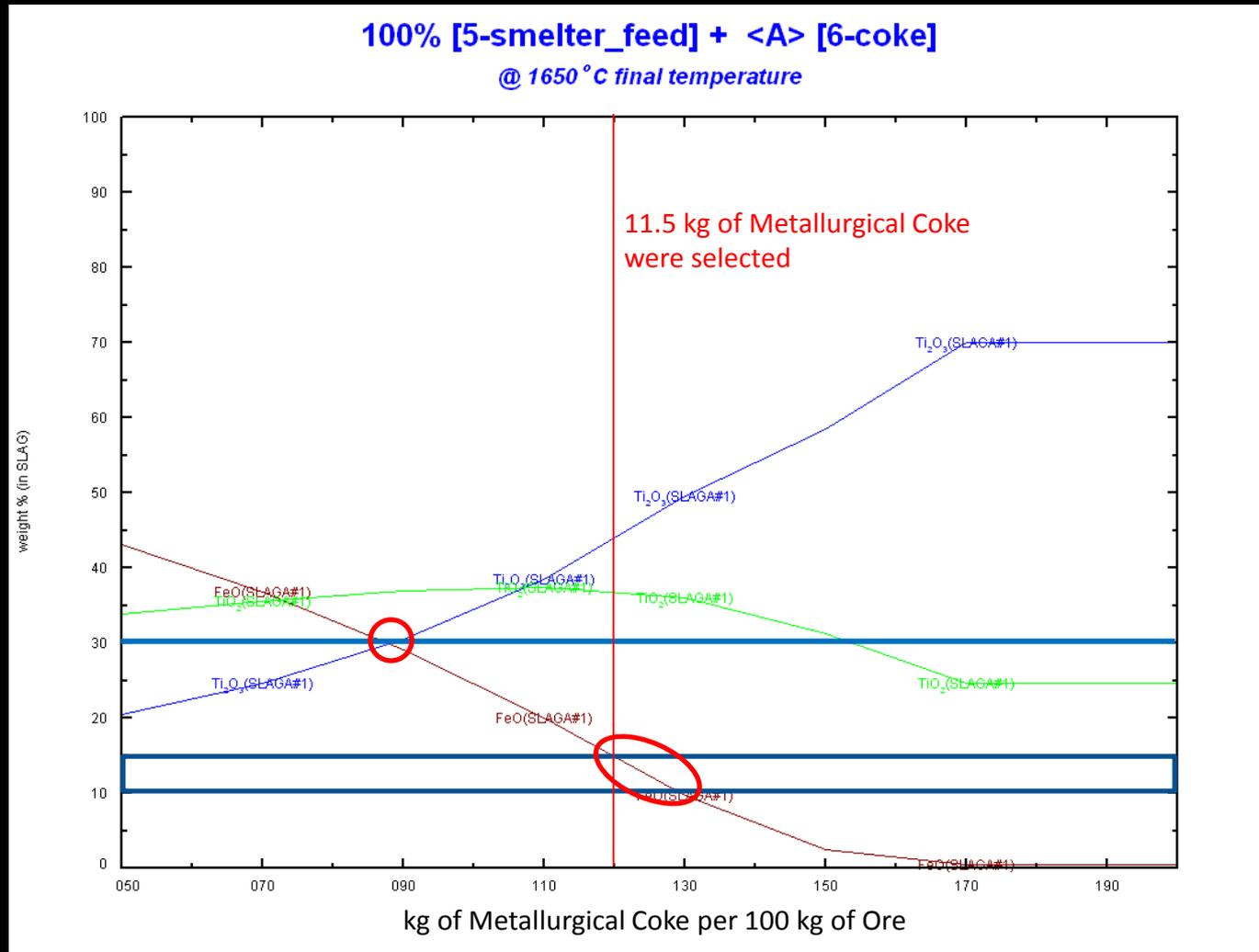
Met COKE	wt%	Ash	wt%
C	85	Al <sub>2</sub> O <sub>3</sub>	36
Ash	11	SiO <sub>2</sub>	59
S	1	Fe <sub>2</sub> O <sub>3</sub>	5
H <sub>2</sub> O	3	total	100
total	100		

STREAM 6	wt%
C	85
Al <sub>2</sub> O <sub>3</sub>	3.96
SiO <sub>2</sub>	6.49
Fe <sub>2</sub> O <sub>3</sub>	0.55
S	1
H <sub>2</sub> O	3
total	100

# SMELTER SIMULATION: ORE to COKE ratio

**ASSUMPTION:** In Titanium Slag =>  $\text{FeO} \approx 10\text{-}15\%$ ,  $\text{Ti}_2\text{O}_3 \approx 30\%$ , Final Temp. is  $1650^\circ\text{C}$

For 100 kg of Ore, what is the quantity of Metallurgical Coke that will fulfill these conditions?



# SMELTER SIMULATION

## Metallurgical Coke Feed

Thermodynamically stable compounds for metallurgical coke were determined by bringing to equilibrium the chemical composition at 25 °C.

The screenshot shows the 'F Reactants - Equilib' window. It contains a table with the following data:

Mass(g)	Species	Phase	T[C]	P[total]**	Stream#	Data
9775	C	solid-1-FACT53 grap	25	1.0	1	FACT53
+ 455.4	Al2O3	solid-1-FACT53 gam	25	1.0	1	FACT53
+ 746.35	SiO2	solid-1-FACT53 quai	25	1.0	1	FACT53
+ 63.25	Fe2O3	solid-1-FACT53 hem	25	1.0	1	FACT53
+ 115	S	solid-1-FACT53 orth	25	1.0	1	FACT53
+ 345	H2O	liquid-FACT53	25	1.0	1	FACT53

At the bottom of the window, there is a 'Next >>' button and a checked 'Initial Conditions' option.

The screenshot shows the 'F Menu - Equilib' window. It displays the following information:

**Reactants (6):** (gram) 9775 C + 455.4 Al2O3 + 746.35 SiO2 + 63.25 Fe2O3 + 115 S

**Products:** A list of species types with counts: gas (0), aqueous (0), pure liquids (47), pure solids (154). Total species: 201.

**Final Conditions:** T(C) = 25, P(atm) = 1, Delta H(J) = [dropdown]. 1 calculation.

**Equilibrium:** Radio buttons for 'normal', 'transitions', 'predominant', and 'open'. A 'Calculate >>' button is present.

Contents total 11.5 kg. No gases were allowed to evolve.

# SMELTER SIMULATION

## Metallurgical Coke Feed

```
F Results - Equilib 25 C
Output Edit Show Pages
T(C) P(atm) Energy(J) Mass(g) Vol(litre)

(grammar) 9775 C + 455.4 Al2O3 + 746.35 SiO2 + 63.25 Fe2O3 +
(25,l,s1-FACT53,#1) (25,l,s1-FACT53,#1) (25,l,s1-FACT53,#1) (25,l,s1-FACT53,
(grammar) 115 S + 345 H2O =
(25,l,s1-FACT53,#1) (25,l,liq-FACT53,#1)

9775.0      gram C_c<graphite>                FSstel
(9775.0 gram, 313.84 mol)
(25.00 C, 1 atm, S1, a=1.0000)

+ 572.44    gram H4SiO4_solid                 FACT53
(572.44 gram, 5.9557 mol)
(25.00 C, 1 atm, S1, a=1.0000)

+ 535.86    gram Al2O3(H2O)_diaspore          FACT53
(535.86 gram, 4.4664 mol)
(25.00 C, 1 atm, S1, a=1.0000)

+ 388.50    gram SiO2_quartz(1)              FACT53
(388.50 gram, 6.4660 mol)
(25.00 C, 1 atm, S1, a=1.0000)

+ 95.041    gram FeS2_pyrite                 FACT53
(95.041 gram, 0.79215 mol)
(25.00 C, 1 atm, S1, a=1.0000)

+ 81.659    gram H2SO4(H2O)6_liquid          FACT53
(81.659 gram, 0.39607 mol)
(25.00 C, 1 atm, L1, a=1.0000)

+ 51.497    gram S_s<fc_orthorhombic>        FSstel
(51.497 gram, 1.6060 mol)
(25.00 C, 1 atm, S1, a=1.0000)

+ 0.00000   gram FeS2_fes2_pyrite(s1)       FSstel
(25.00 C, 1 atm, S1, a=1.0000)

+ 0.00000   gram SiO2_quartz(1)             FSstel
(25.00 C, 1 atm, S1, a=1.0000)
```

Metallurgical  
Coke

6

Metallurgical Coke stream was saved as 2 streams, solids + liquids

# SMELTER SIMULATION EQUILIBRIUM CALCULATIONS

**F Reactants - Equilib**

File Edit Table Units Data Search Help

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

1 - 3

Mass(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
100000	[DREFEED100]	[Stream]	1000	1	1	
+ 100%	[CokeSolids25]	[Stream]	25	1	2	
+ 100%	[CokeLiquids2]	[Stream]	25	1	3	

\*\* 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 6.1 Compound: 3/19 databases Solution: 2/19 databases

**F Menu - Equilib: last system**

File Units Parameters Help

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

Reactants [3]

(gram) 100000 [DREFEED100] + 100% [CokeSolids25] + 100% [CokeLiquids25]  
(1000C,#1) (25C,s,#2) (25C,liq,#3)

Products

Compound species:  gas  ideal  real 101  
 aqueous 0  
 pure liquids 0  
 pure solids 308  
 suppress duplicates apply  
 species: 409

Solution species

*	+	Base-Phase	Full Name
	+	FSstel-ALTI	ALTI
	+	FSstel-SI3T	SI3TI5
	+	FSstel-ALM	ALM_D019
	+	FSstel-HCP	HCP_A3:Me2(C,N)
	+	FSstel-AL21	Al2Fe
	+	FSstel-BCC2	BCC_B2 BCC_A2
		FToxid-SLAGA	ASlag-liq

Legend  
 | - immiscible 1  
 + - selected 35  
 species: 219  
 solutions: 37

Final Conditions

<A>	<B>	T(C)	P(atm)	Delta H(J)
10	steps	1650	1	1 calculation

Equilibrium  
 normal  transitions  
 predominant  open  
 Calculate >>

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

Pseudonyms  
 apply  List ...

include molar volumes  
 Total Species [max 1500] 628  
 Total Solutions [max 40] 37  
 Default

FactSage 6.1

1700 °C is a typical temperature for slag while 1600 °C is a typical temperature for liquid steel.  
1650 °C was fixed as the final temperature. All solution phases from the Fstel database

# SMELTER SIMULATION EQUILIBRIUM CALCULATIONS

## RESULTS

```
F Results - Equilib 1650 C
Output Edit Show Pages
T(C) P(atm) Energy(J) Mass(g) Vol(litre)

(gram) 100000 [XCOREFEED1000] + 100% [XCCokeSolids25] + 100% [XCCokeLiquid...
(1000,1,stream,#1) (25,1,s,#2) (25,1,liq,#3)

831.12 mol gas_ideal
(22958. gram, 831.12 mol, 1.3116E+05 litre, 1.7504E-04 g/ml)
(1650.00 C, 1 atm, a=1.0000)
( 0.96485 CO FACT53
+ 2.1835E-02 H2 FACT53
+ 1.1785E-02 CO2 FACT53
+ 1.1258E-03 H2O FACT53
+ 1.5354E-04 Fe FACT53
+ 1.3863E-04 H FACT53
+ 5.5835E-05 SiO FACT53
+ 2.9806E-05 Mn FACT53
+ 1.4066E-05 CO8 FACT53
+ 8.8985E-06 H2S FACT53
+ 4.8692E-06 HS FACT53
+ 1.0274E-06 S FACT53
+ 6.2864E-07 OH FACT53
+ 5.9726E-07 SiS FACT53
+ 3.2742E-07 SO FACT53
+ 2.9654E-07 S2 FACT53
+ 2.3435E-07 FeS FACT53
+ 1.2693E-07 FeO FACT53
+ 1.0933E-07 CS FACT53
+ 5.5702E-08 HCO FACT53
+ 3.7049E-08 SO2 FACT53
+ 3.5359E-08 Fe(OH)2 FACT53
+ 1.4434E-08 H2CO FACT53
```

8

Titanium  
Oxide Slag

```
F Results - Equilib 1650 C
Output Edit Show Pages
T(C) P(atm) Energy(J) Mass(g) Vol(litre)

+ 27882. gram Fe-LIQUID
(27882. gram, 500.50 mol)
(1650.00 C, 1 atm, a=1.0000)
( 99.415 wt.% Fe FSstel
+ 9.1626E-02 wt.% C FSstel
+ 1.0725E-05 wt.% Al FSstel
+ 4.5449E-02 wt.% Mn FSstel
+ 8.8830E-04 wt.% S T FSstel
+ 1.3948E-02 wt.% Si FSstel
+ 5.6978E-04 wt.% Ti FSstel
+ 1.9353E-02 wt.% O FSstel
+ 6.1285E-06 wt.% AlO FSstel
+ 1.1404E-10 wt.% Al2O FSstel
+ 1.2070E-04 wt.% MnO FSstel
+ 5.7776E-05 wt.% SiO FSstel
+ 2.5262E-04 wt.% TiO FSstel
+ 6.3228E-08 wt.% Ti2O FSstel
+ 0.41228 wt.% FeS FSstel
+ 4.9081E-04 wt.% MnS FSstel
+ 6.4429E-07 wt.% TiS FSstel)
```

All 3 streams were saved.

```
F Results - Equilib 1650 C
Output Edit Show Pages
T(C) P(atm) Energy(J) Mass(g) Vol(litre)

+ 60660. gram ASlag-liq#1
(60660. gram, 640.33 mol)
(1650.00 C, 1 atm, a=1.0000)
( 0.74943 wt.% Al2O3 FToxid
+ 1.2099 wt.% SiO2 FToxid
+ 17.804 wt.% FeO FToxid
+ 7.0905E-02 wt.% Fe2O3 FToxid
+ 2.0438 wt.% MnO FToxid
+ 40.596 wt.% Ti2O3 FToxid
+ 37.289 wt.% TiO2 FToxid
+ 3.0058E-03 wt.% Mn2O3 FToxid
+ 1.9248E-03 wt.% Al2S3 FToxid
+ 3.2384E-03 wt.% SiS2 FToxid
+ 3.7992E-02 wt.% FeS FToxid
+ 1.6098E-04 wt.% Fe2S3 FToxid
+ 4.3716E-03 wt.% MnS FToxid
+ 9.4535E-02 wt.% Ti2S3 T FToxid
+ 9.1190E-02 wt.% TiS2 T FToxid
+ 6.8422E-06 wt.% Mn2S3 FToxid)

Mole fraction of sublattice constituents:
Al 1.0938E-02
Si 1.4983E-02
Fe2+ 0.18438
Fe3+ 6.6073E-04
Mn2+ 2.1437E-02
Ti3+ 0.42023
Ti4+ 0.34734
Mn3+ 2.8332E-05
```

9

Liquid Steel

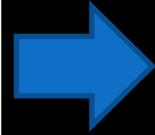
# SMELTER SIMULATION EQUILIBRIUM CALCULATIONS

## RESULTS

CO gas stream was cooled down to 1000 °C to simulate heat losses in ducts.

```
F Results - Equilib 1650 C
Output Edit Show Pages
T(C) P(atm) Energy(J) Mass(g) Vol(litre)

+ 27882. gram Fe-LIQUID
(27882. gram, 500.50 mol)
(1650.00 C, 1 atm, a=1.0000)
( 99.415 wt.% Fe FSstel
+ 9.1626E-02 wt.% C FSstel
+ 1.0725E-05 wt.% Al FSstel
+ 4.5449E-02 wt.% Mn FSstel
+ 8.8830E-04 wt.% S T FSstel
+ 1.3948E-02 wt.% Si FSstel
+ 5.6978E-04 wt.% Ti FSstel
+ 1.9353E-02 wt.% O FSstel
+ 6.1285E-06 wt.% AlO FSstel
+ 1.1404E-10 wt.% Al2O FSstel
+ 1.2070E-04 wt.% MnO FSstel
+ 5.7776E-05 wt.% SiO FSstel
+ 2.5262E-04 wt.% TiO FSstel
+ 6.3228E-08 wt.% Ti2O FSstel
+ 0.41228 wt.% FeS FSstel
+ 4.9081E-04 wt.% MnS FSstel
+ 6.4429E-07 wt.% TiS FSstel)
```



```
F Results - Equilib 1000 C
Output Edit Show Pages
T(C) P(atm) Energy(J) Mass(g) Vol(litre)

(1650,1,g,#1)

830.86 mol gas_ideal
(22946. gram, 830.86 mol, 86801. litre, 2.6435E-04 g/ml)
(1000.00 C, 1 atm, a=1.0000)
( 0.96458 CO FACT53
+ 2.2559E-02 H2 FACT53
+ 1.2360E-02 CO2 FACT53
+ 4.7173E-04 H2O FACT53
+ 1.7794E-05 COS FACT53
+ 1.2935E-05 H2S FACT53
+ 2.6445E-06 CH4 FACT53
+ 1.0674E-07 H FACT53
+ 3.6180E-08 HS FACT53
+ 2.1752E-08 H2CO FACT53
+ 6.5091E-09 CS2 FACT53
+ 3.0749E-09 C2H2 FACT53
+ 2.1486E-09 Mn FACT53
+ 1.7952E-09 S2 FACT53
+ 1.7901E-09 CS FACT53
+ 5.9995E-10 Fe FACT53)
```



```
F Results - Equilib 1000 C
Output Edit Show Pages
T(C) P(atm) Energy(J) Mass(g) Vol(litre)

+ 7.1452 gram Fe_fcc_al FSstel
(7.1452 gram, 0.12794 mol)
(1000.00 C, 1 atm, S2, a=1.0000)

+ 3.2453 gram MnSiO3_rhodonite FACT53
(3.2453 gram, 2.4769E-02 mol)
(1000.00 C, 1 atm, S1, a=1.0000)

+ 1.3298 gram SiO2_tridymite(h) FACT53
(1.3298 gram, 2.2132E-02 mol)
(1000.00 C, 1 atm, S4, a=1.0000)

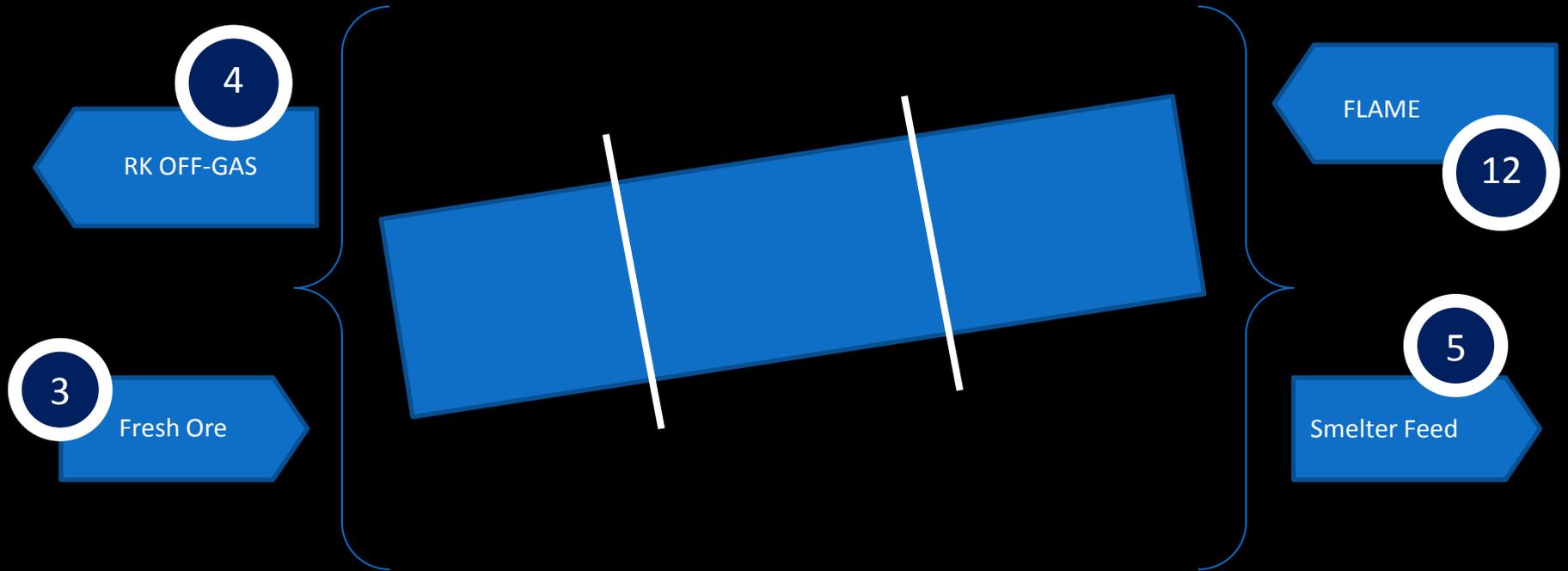
+ 6.1166E-04 gram (MnO)(TiO2)_solid FACT53
(6.1166E-04 gram, 4.0557E-06 mol)
(1000.00 C, 1 atm, S1, a=1.0000)

+ 1.4381E-04 gram Mn3Al2Si3O12_mn-pyrope(garnet) FACT53
(1.4381E-04 gram, 2.9052E-07 mol)
(1000.00 C, 1 atm, S1, a=1.0000)
```

At 1000 °C, solids were precipitated (dust).  
Only the Gas components were saved as a stream

# ROTARY KILN MODELLING

# ROTARY KILN



# CO FLAME CALIBRATION

CO gas is used as a fuel for the Rotary Kiln. Optimal air mixtures were found by varying the Air content as variable <A> from 10,000 to 80,000 g by steps of 1000g. The air is assumed to have been pre-heated to a temperature of 200 °C (saved as a stream previously) by means of a heat exchange with the Rotary Kiln off-gas.

**F Reactants - Equilib**

File Edit Table Units Data Search Help

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

Mass(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
100%	[CO]gas	[Stream]	1650	1	1	
+ <A>	[1-PreheatedAir]	[Stream]	200	1	2	

Initial Conditions

**Next >>**

FactSage 6.1 Compound: 3/19 databases Solution: 2/19 databases

**F Menu - Equilib: last system**

File Units Parameters Help

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

**Reactants (2)**

(gram) 100% [CO]gas + <A> [1-PreheatedAir]  
(1650C,g,#1) (200C,#2)

**Products**

Compound species: gas (ideal/real), aqueous, pure liquids, pure solids, suppress duplicates, species: 488

Solution species: Base-Phase, Full Name

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

Final Conditions:

<A>	<B>	T(C)	P(atm)	Delta H(J)
10000	80000	100	1	0

Equilibrium: normal, transitions, predominant, open

**Calculate >>**

71 calculations

FactSage 6.1

# CO FLAME CALIBRATION

## RESULTS

The highest temperature ( $\approx 2371$  °C) is reached at around  $\langle A \rangle = 35,000$  g of Air

```
F Results - Equilib 2370.6 C, A=0 (page 26/71)
Output Edit Show Pages
T(C) P(atm) Energy(J) Mass(g) Vol(litre)
2314.76 C, A=0 | 2309.74 C, A=0 | 2304.58 C, A=0 | 2299.27 C, A=0 | 2293.83 C, A=0 | 2288.25 C, A=0 | 2282.53 C, A=0 |
2352.33 C, A=0 | 2348.93 C, A=0 | 2345.3 C, A=0 | 2341.48 C, A=0 | 2337.46 C, A=0 | 2333.25 C, A=0 | 2328.88 C, A=0 | 2324.33 C, A=0 | 2319.62 C, A=0 |
-2370.6 C, A=0 | 2369.94 C, A=0 | 2368.88 C, A=0 | 2367.43 C, A=0 | 2365.65 C, A=0 | 2363.54 C, A=0 | 2361.14 C, A=0 | 2358.46 C, A=0 | 2355.52 C, A=0 |

+ 0.00000 gram Fe3S17_fe3si7<fesi2_h> FSstel
(2370.60 C, 1 atm, 51 a=2.7099E-74)

where "A" on the reactant side is 35000.

The cutoff concentration has been specified to 1.0000E-75

Data on 6 product species identified with "X" have not been extrapolated in
computing the phase assemblage

Data on 245 product species identified with "T" have been extrapolated

*****
DELTA H DELTA G DELTA V DELTA S DELTA Cp
(J) (J) (litre) (J/K) (J/K)
*****
0.00000E+00 -8.64813E+08 3.98899E+05 5.73142E+04 9.67961E+04

*****
H G V S Cp
(J) (J) (litre) (J/K) (J/K)
*****
-4.12657E+07 -1.43987E+09 3.98899E+05 5.29023E+05 1.64409E+05

Total mass/gram = 57958.

*****

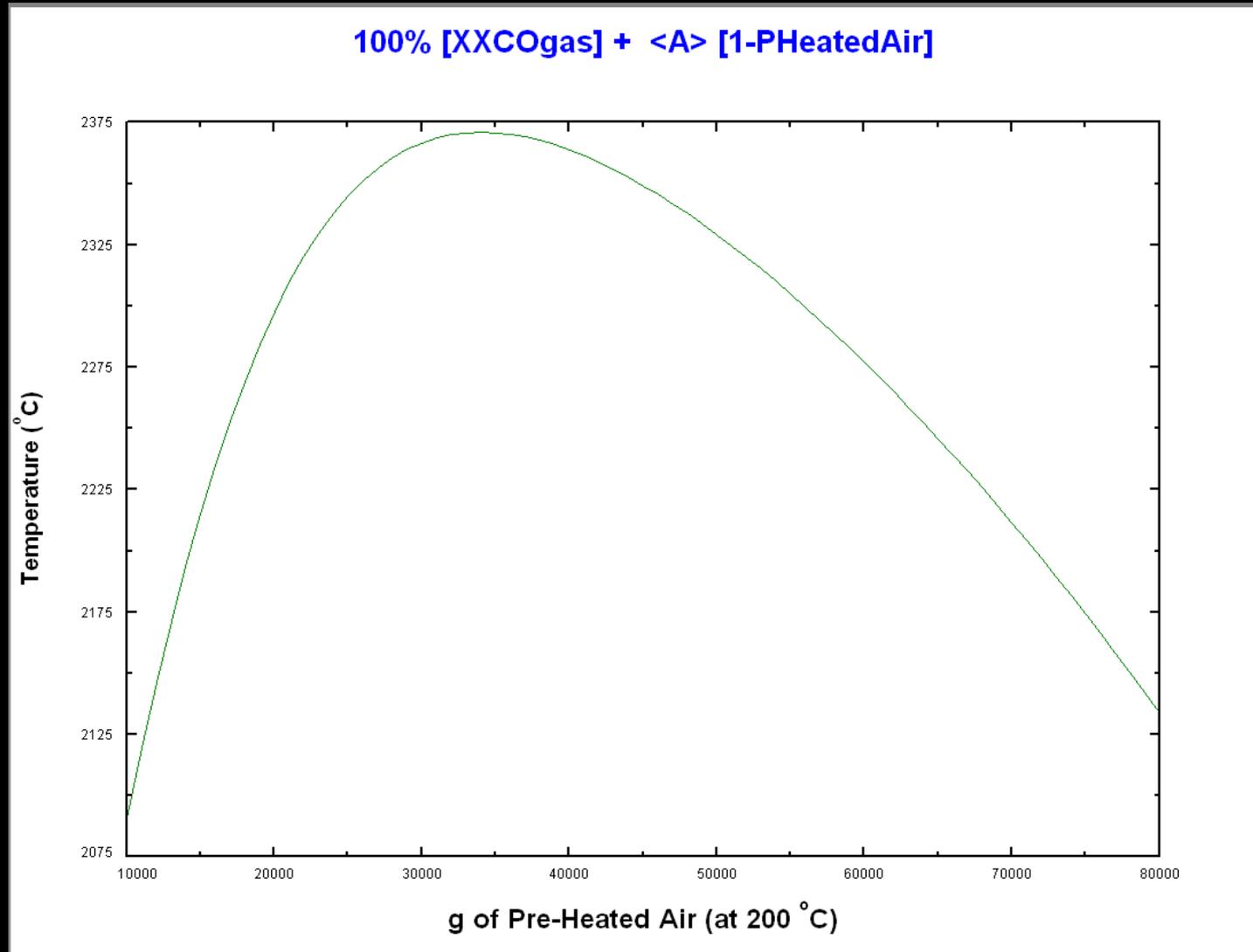
*T = 2370.60 C
P = 1.00000E+00 atm
V = 3.98899E+05 dm3

STREAM CONSTITUENTS AMOUNT/gram TEMPERATURE/C PRESSURE/atm STREAM
```

# CO FLAME CALIBRATION

## RESULTS

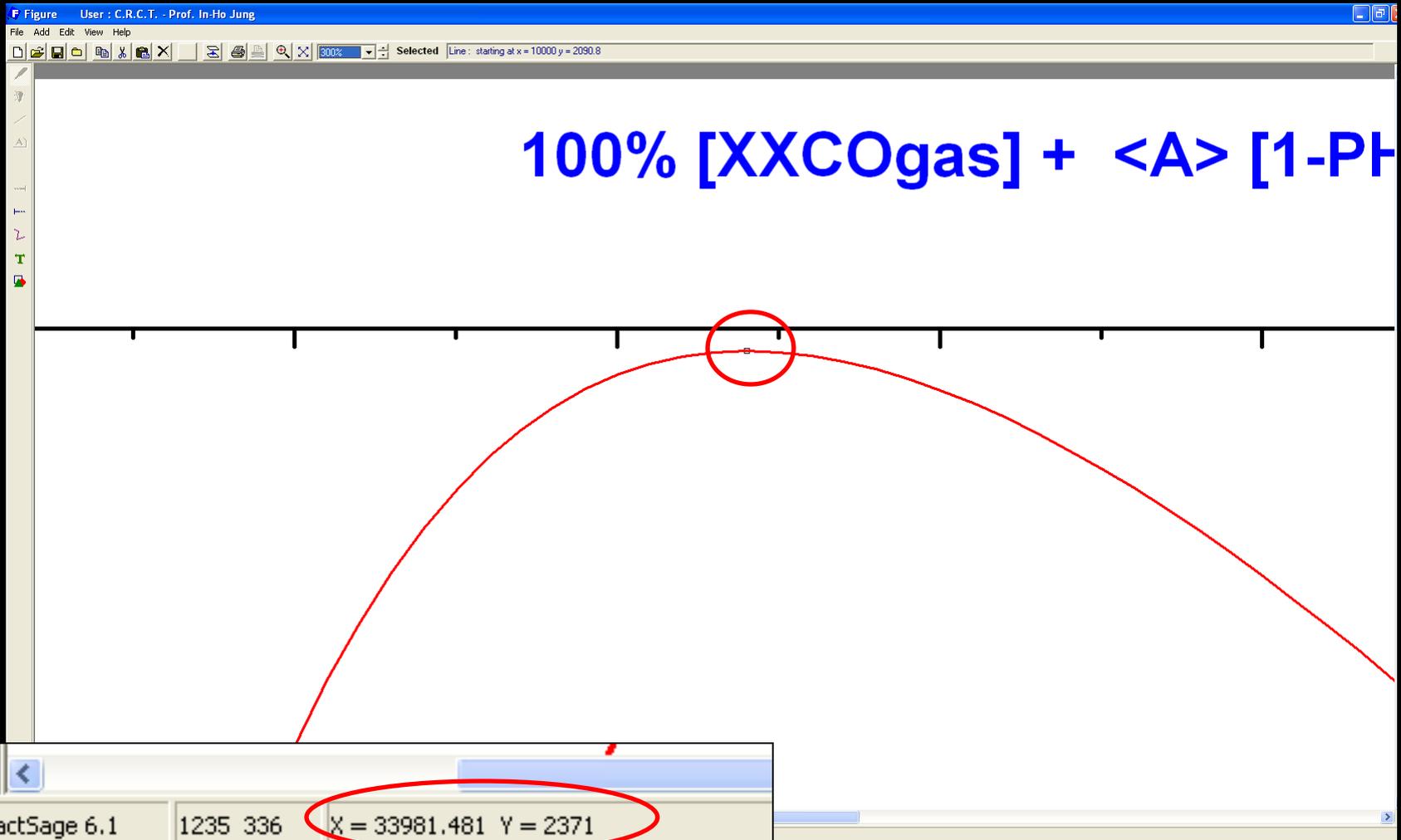
A plot of equilibrium temperature vs. g of air was generated.



# CO FLAME CALIBRATION

## RESULTS

A plot of equilibrium temperature vs. g of air was generated. A peak was found at: 33,981 g of air, generating an adiabatic flame temperature of 2371 °C.



# CO FLAME CALIBRATION

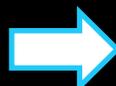
## “CO FLAME”

The resultant equilibrium of 100% of the CO gas stream and 33,981 g of air were combined as a single “CO FLAME” stream.

Mass(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
100%	[CO]gas	[Stream]	1650	1	1	
+ 33981	[1-PHeatedAir]	[Stream]	200	1	2	

Initial Conditions

Next >>



## “CO FLAME” stream

```
(gram) 100% [CO]gas + 33981 [1-PHeatedAir] =
(1650,1,g,#1) (200,1,stream,#2)

1808.3 mol gas_ideal
(56939. gram, 1808.3 mol, 3.9232E+05 litre, 1.4514E-04 g/ml)
(2370.82 C, 1 atm, a=1.0000)

0.52634 N2 FACTS3
+ 0.22749 CO2 FACTS3
+ 0.22140 CO FACTS3
+ 7.4482E-03 H2O FACTS3
+ 5.7645E-03 O2 FACTS3
+ 4.1394E-03 NO FACTS3
+ 2.4966E-03 OH FACTS3
+ 2.1387E-03 O FACTS3
+ 1.5298E-03 H FACTS3
+ 1.1286E-03 H2 FACTS3
+ 4.9574E-05 Fe FACTS3
+ 2.5938E-05 SiO FACTS3
+ 2.0966E-05 FeO FACTS3
+ 1.3702E-05 Mn FACTS3
+ 1.2120E-05 SO2 FACTS3
+ 1.9405E-06 SO FACTS3
+ 7.4267E-07 N FACTS3
+ 6.1035E-07 H2O FACTS3
+ 4.7898E-07 NO2 FACTS3
+ 2.1509E-07 Fe(OH)2 FACTS3
+ 1.7008E-07 N2O FACTS3
+ 7.3622E-08 S T FACTS3
+ 6.2130E-08 HMO FACTS3
```

# ROTARY KILN ENERGY INPUT

## ASSUMPTIONS & SIMPLIFICATIONS

To determine the necessary energy input of the rotary kiln (RK), we need to make some assumptions and simplifications:

- The RK is divided in 3 zones;
- Each zone is assumed to reach equilibrium (i.e. have uniform composition and temperature);
- At steady state, the temperature in zone 2 (at the center) is 400 °C;
- At steady state, the temperature in zone 3 (at the flame and RK discharge) should be 1000 °C;



# ROTARY KILN ENERGY INPUT

## FIRST TEST

At first, Rotary Kiln (RKF) material at 400 °C (to simulate material coming from zone 2) is reacted with 100% of the "CO FLAME". Solution and Slag phases were allowed to be created.

**F Reactants - Equilib**

File Edit Table Units Data Search Help

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

1 - 2

Mass(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
100%	[COFLAME]	[Stream]	2370.82	1	3	
+ 100%	[RKMAT400]	[Stream]	400	1	4	

Initial Conditions

**Next >>**

FactSage 6.1 Compound: 3/19 databases Solution: 2/19 databases

**F Menu - Equilib: last system**

File Units Parameters Help

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

**Reactants (2)**

(gram) 100% [COFLAME] + 100% [RKMAT400]  
(2370.82C.#3) (400C.#4)

**Products**

Compound species: 146 (gas ideal), 0 (aqueous), 0 (pure liquids), 342 (pure solids), 488 (total).  
Legend: 1 (immiscible), 37 (selected).

Base-Phase	Full Name
FSstel-AL8M	AL8MN5D810
FSstel-D022	AL3MD022
FSstel-CBCC	CBCC_A12
FSstel-CUB	CUB_A13
FSstel-LAV1	LAVES_C14
FSstel-ALTI	ALTI
FSstel-SI3T	SI3TI5

species: 254, solutions: 39

**Final Conditions**

T(C): 400, P(atm): 1, Delta H(J): 0

10 steps, Table, 1 calculation

**Equilibrium**

normal, predominant, transitions, open

**Calculate >>**

FactSage 6.1

# ROTARY KILN ENERGY INPUT

## FIRST TEST: RESULTS

The final equilibrium temperature was 1321 °C and a slag phase was formed. This means that the energy from the CO flame, if our assumptions are more or less accurate, is too high.

```
F Results - Equilib 1320.94 C
Output Edit Show Pages
T(C) P(atm) Energy(J) Mass(g) Vol(litre)

(g) 100% [COCOFLAME] + 100% [PKMAT400] =
(2370.82,1,stream,#3) (400,1,stream,#4)

1786.4 mol gas_ideal
(58901. gram, 1786.4 mol, 2.3367E+05 litre, 2.5207E-04 g/ml)
(1320.94 C, 1 atm, a=1.0000)
( 0.53488 N2 FACTS3
+ 0.31808 CO2 FACTS3
+ 0.13631 CO FACTS3
+ 9.3527E-03 H2O FACTS3
+ 1.3660E-03 H2 FACTS3
+ 6.6048E-06 SO2 FACTS3
+ 1.8767E-06 H FACTS3
+ 5.0681E-07 OH FACTS3
+ 3.7707E-07 COS FACTS3
+ 2.5472E-07 Fe(OH)2 FACTS3
+ 2.2875E-07 SO FACTS3
+ 1.5354E-07 NO FACTS3
+ 1.1184E-07 H2S FACTS3
+ 5.2353E-08 Fe FACTS3
+ 2.9216E-08 HS FACTS3
+ 8.6171E-09 Mn FACTS3
+ 3.8693E-09 S FACTS3
+ 1.9385E-09 Fe0 FACTS3
+ 1.7994E-09 NH3 FACTS3
+ 1.7633E-09 O2 FACTS3
+ 1.1512E-09 S2 FACTS3
+ 9.7270E-10 HCN FACTS3
+ 6.5582E-10 HNCO FACTS3
```

```
F Results - Equilib 1320.94 C
Output Edit Show Pages
T(C) P(atm) Energy(J) Mass(g) Vol(litre)

+ 23579. gram ASlag-liq#1
(23579. gram, 303.95 mol)
(1320.94 C, 1 atm, a=1.0000)
( 1.2352E-07 wt.% Al2O3 FToxid
+ 1.1951E-02 wt.% SiO2 FToxid
+ 44.903 wt.% FeO FToxid
+ 4.4565 wt.% Fe2O3 FToxid
+ 5.9189 wt.% MnO FToxid
+ 1.2563 wt.% Ti2O3 FToxid
+ 43.421 wt.% TiO2 FToxid
+ 2.8845E-02 wt.% Mn2O3 FToxid
+ 5.1166E-12 wt.% Al2S3 FToxid
+ 5.0730E-07 wt.% SiS2 FToxid
+ 1.5195E-03 wt.% FeS FToxid
+ 1.6045E-04 wt.% Fe2S3 FToxid
+ 2.0077E-04 wt.% MnS FToxid
+ 4.6392E-05 wt.% Ti2S3 T FToxid
+ 1.6840E-03 wt.% TiS2 T FToxid
+ 1.0413E-06 wt.% Mn2S3 FToxid)

Mole fraction of sublattice constituents:
Al 1.8585E-09
Si 1.5002E-04
Fe2+ 0.47137
Fe3+ 4.2096E-02
Mn2+ 6.2932E-02
Ti3+ 1.3182E-02
```

# ROTARY KILN ENERGY INPUT

## HOW MUCH CO FLAME SHOULD BE ADDED?

The total flame quantity is 56,939 g. "CO FLAME" was reacted with Rotary Kiln material at 400 °C in varying amounts. The quantity of "CO FLAME" was varied from 20,000g to 56,000g in steps of 1000g. Slag and solutions phases were allowed to be formed.

Mass(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
<A>	[COFLAME]	[Stream]	2370.82	1	3	
+ 100%	[RKMAT400]	[Stream]	400	1	4	

Initial Conditions

Next >>

Reactants (2)

(gram) <A> [COFLAME] + 100% [RKMAT400]  
(2370.82C,#3) (400C,#4)

Products

+	Base-Phase	Full Name
+	FSstel-AL8M	AL8MN5D810
+	FSstel-DO22	AL3MD022
+	FSstel-CBCC	CBCC_A12
+	FSstel-CUB	CUB_A13
+	FSstel-LAV1	LAVES_C14
+	FSstel-ALTI	ALTI
+	FSstel-SI3T	SI3TI5

Final Conditions

<A>	<B>	T(C)	P(atm)	Delta H(J)
20000	56000	100	1	0

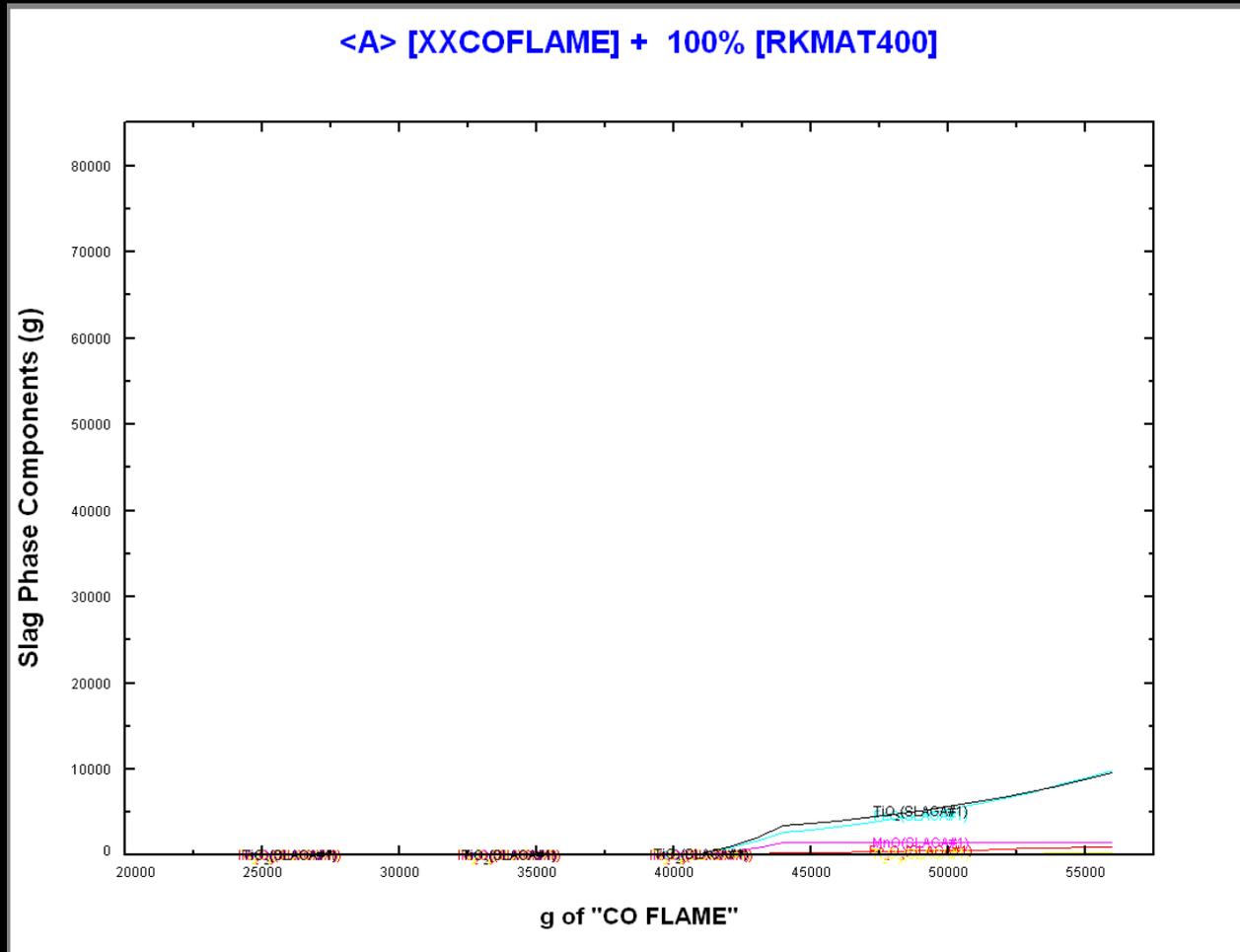
37 calculations

Calculate >>

# ROTARY KILN ENERGY INPUT

## HOW MUCH CO FLAME SHOULD BE ADDED? RESULTS

A graph was generated representing the quantity of slag present at equilibrium as a function of grams of "CO FLAME". This graph shows slag products being created slightly after 40,000 grams of "CO FLAME" have been added.



# ROTARY KILN ENERGY INPUT

## SECOND TEST

A second test was run with material at 400 °C and a 35,000 g of "CO FLAME". The value of 35,000 g was chosen arbitrarily to pick a value below 40,000 g.

**F Reactants - Equilib**

File Edit Table Units Data Search Help

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

Mass(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
35000	[COFLAME]	[Stream]	2370.82	1	3	
+ 100%	[RKMAT400]	[Stream]	400	1	4	

Initial Conditions

**Next >>**

FactSage 6.1 Compound: 3/19 databases Solution: 2/19 databases

**F Menu - Equilib: last system**

File Units Parameters Help

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

**Reactants (2)**

(gram) 35000 [COFLAME] + 100% [RKMAT400]  
(2370.82C,#3) (400C,#4)

**Products**

Compound species: 146 (gas ideal real), 0 (aqueous), 0 (pure liquids), 342 (pure solids), 488 (total).  suppress duplicates apply

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

**Solution species**

*	+	Base-Phase	Full Name
	+	FSstel-AL8M	AL8MN5D810
	+	FSstel-DO22	AL3MD022
	+	FSstel-CBCC	CBCC_A12
	+	FSstel-CUB	CUB_A13
	+	FSstel-LAW1	LAVES_C14
	+	FSstel-ALTI	ALTI
	+	FSstel-SI3T	SI3TI5

Legend: I - immiscible 1, + - selected 37. Show all selected. species: 254, solutions: 39.

**Final Conditions**

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

10 steps  Table 1 calculation

**Equilibrium**

normal  transitions  
 predominant  open

**Calculate >>**

FactSage 6.1



# ROTARY KILN DYNAMIC SIMULATION

# ROTARY KILN DYNAMIC SIMULATION: Principle

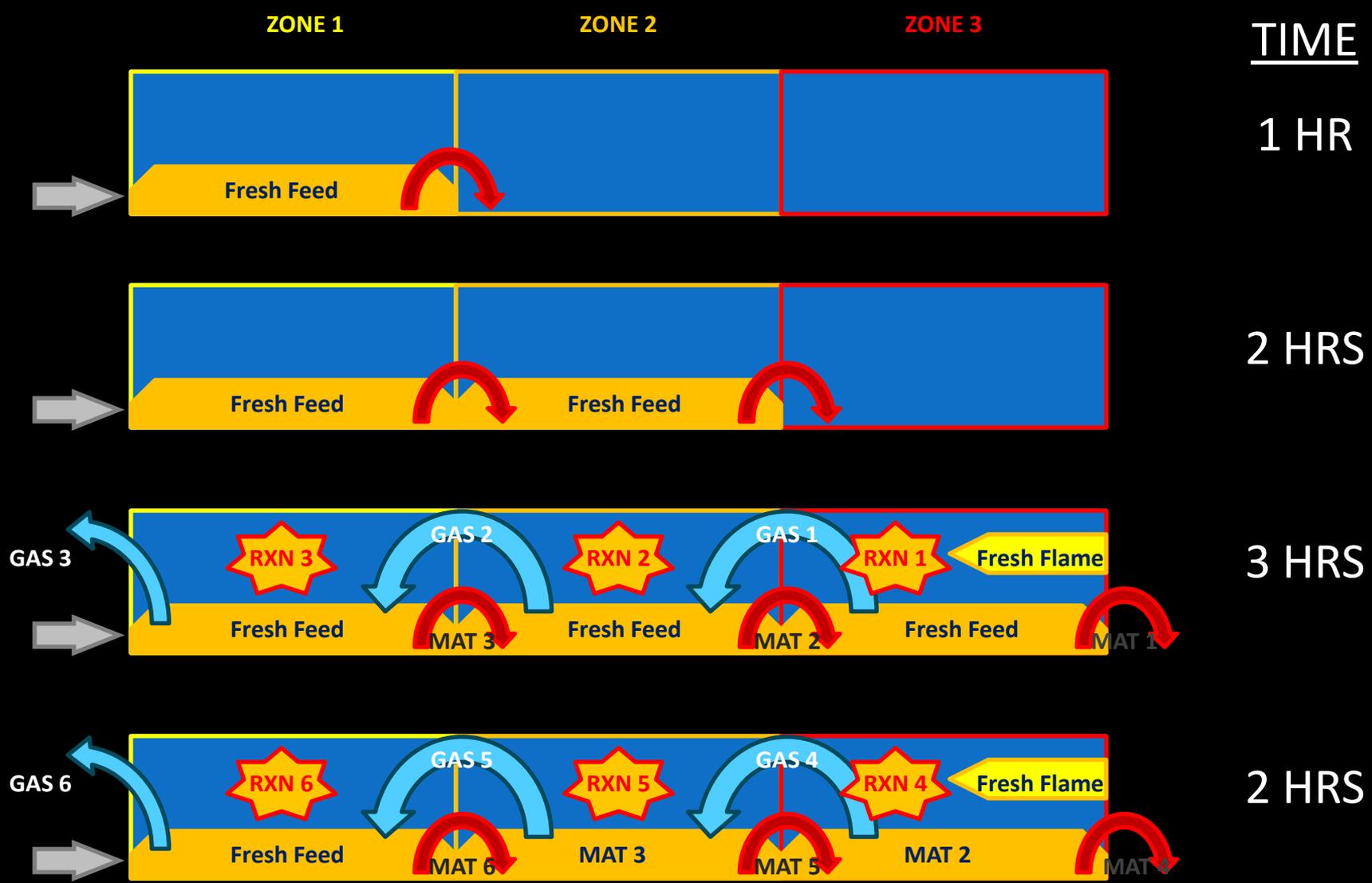
TIME



# Rotary Kiln Calculations

# THE ROTARY KILN START-UP: 1 to 4 hrs

Material flows in to fill the empty RK and the flame is ignited once material has reached zone 3.



# THE ROTARY KILN START-UP: 5 to 8 hrs

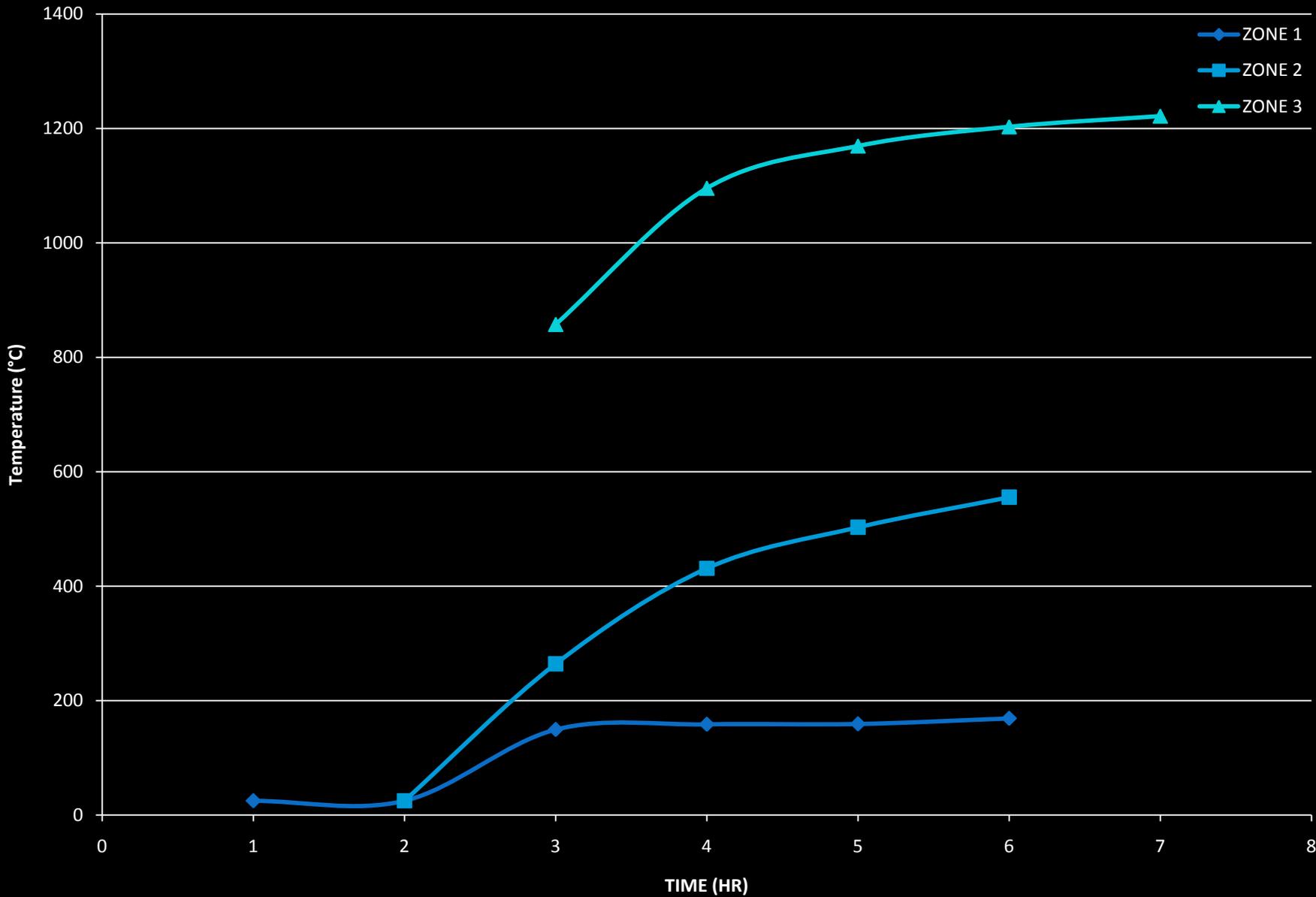
RK is filled and approaches Steady State



Rotary Kiln Calculations  
FIRST RUN (13 reactions)

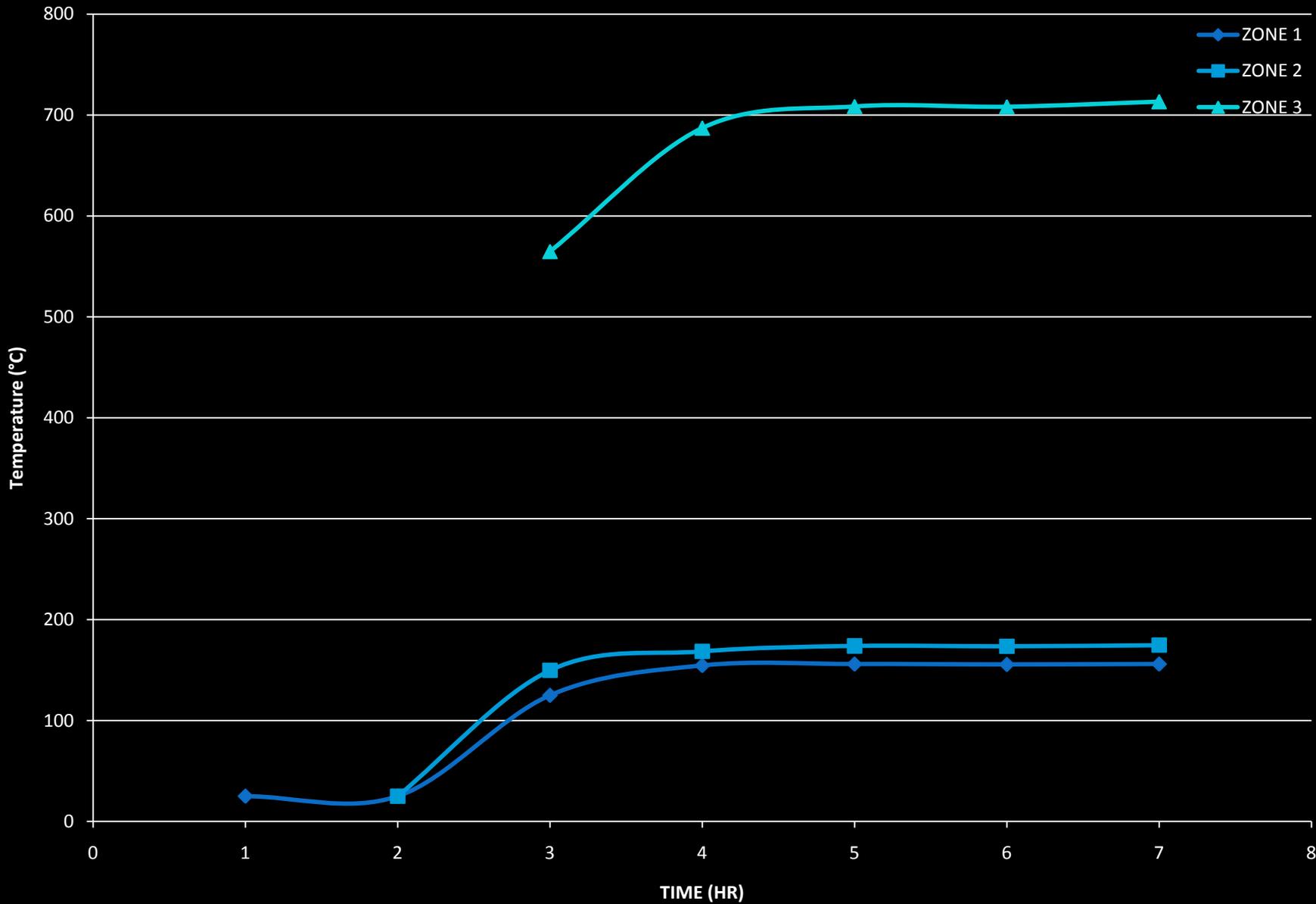
Aborted after 7 hrs of simulation because zone 3 reached slag making temperature.

# ROTARY KILN TEMPERATURE PROFILES FROM START UP



Rotary Kiln Calculations  
SECOND RUN (15 reactions)  
Use 20,000 g of "CO FLAME"

# ROTARY KILN TEMPERATURE PROFILES FROM START UP



# ASSUMPTIONS vs. RESULTS

## Smelter Feed (ASSUMPTION)

	wt%
$\text{FeTiO}_3$	38.57
$\text{Fe}_3\text{O}_4$	30.40
$\text{TiO}_2$	28.35
$\text{MnTiO}_3$	2.68
	100.00

## Smelter Feed/RK discharge (RESULT)

	wt%
$\text{FeTiO}_3$	62.01
$\text{Fe}_3\text{O}_4$	2.25
$\text{TiO}_2$	33.72
$\text{MnTiO}_3$	2.02
	100.00

## Rotary Kiln (ASSUMPTION)

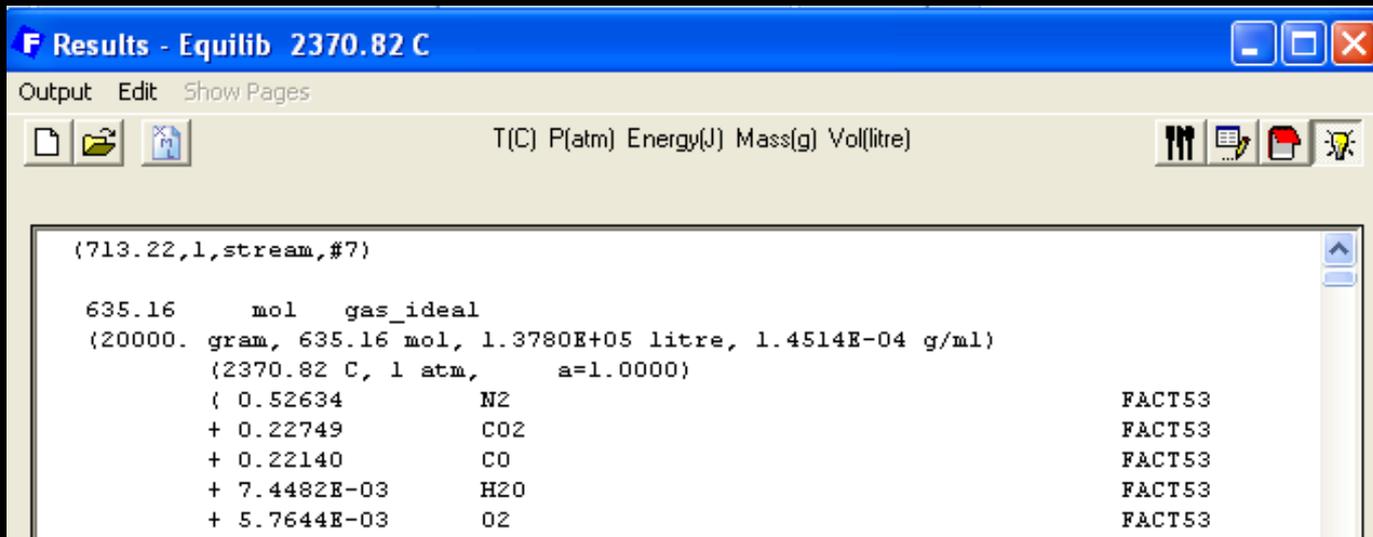
	ZONE 1	ZONE 2	ZONE 3
T (°C)	?	400	1000

## Rotary Kiln (RESULT)

	ZONE 1	ZONE 2	ZONE 3
T (°C)	155	175	710

# DISCUSSION

Significant difference exist between the assumptions and the RK discharge. Discrepancies in chemistries are explained by the atmosphere created by the burning of the CO gas. At peak temperature, the composition of the "CO FLAME" retains a significant amount of CO gas, almost equivalent to that of CO<sub>2</sub>. The reducing conditions explain a higher content of FeTiO<sub>3</sub>.



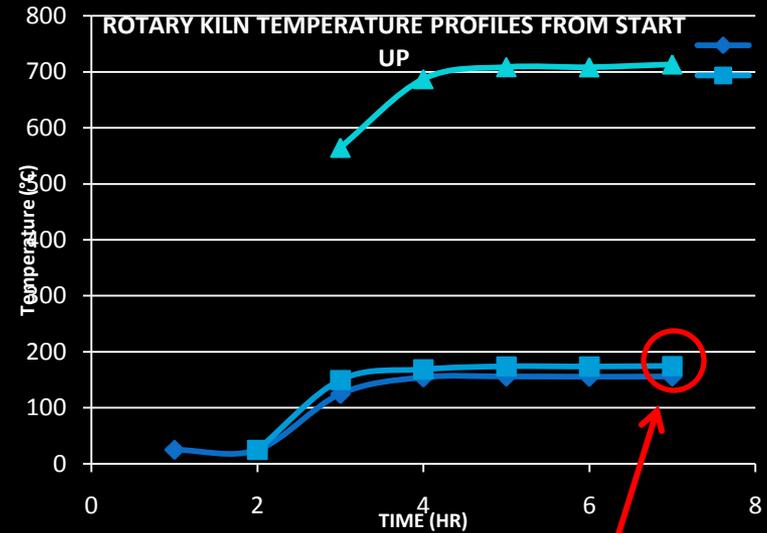
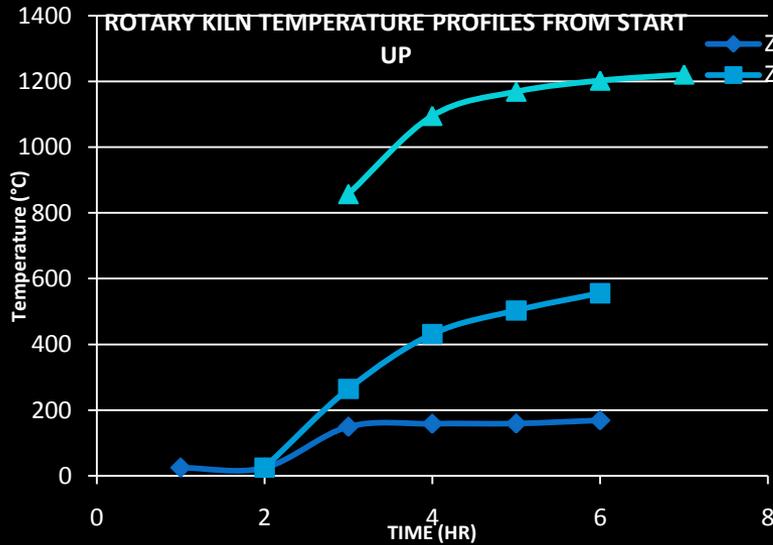
The screenshot shows a software window titled "Results - Equilib 2370.82 C". The window contains a table of equilibrium data for a gas mixture. The data is as follows:

T(C)	P(atm)	Energy(J)	Mass(g)	Vol(litre)
635.16				
mol gas_ideal				
(20000. gram, 635.16 mol, 1.3780E+05 litre, 1.4514E-04 g/ml)				
(2370.82 C, 1 atm, a=1.0000)				
0.52634				
		N2		FACT53
+ 0.22749				
		CO2		FACT53
+ 0.22140				
		CO		FACT53
+ 7.4482E-03				
		H2O		FACT53
+ 5.7644E-03				
		O2		FACT53

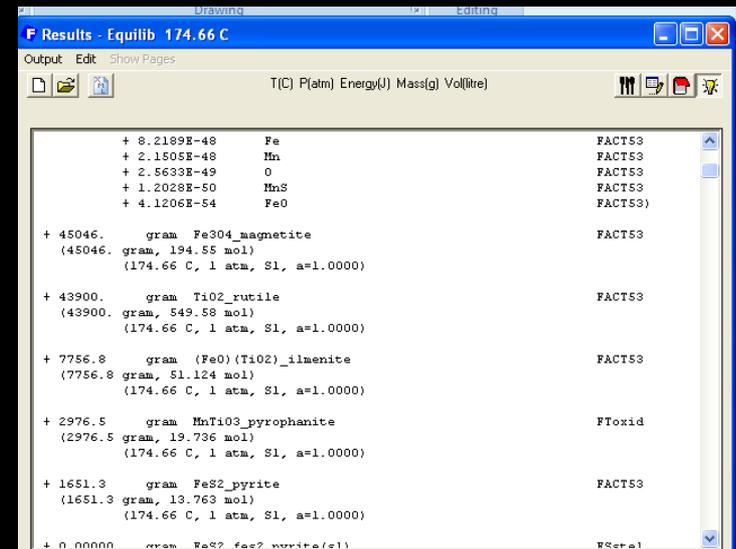
The original strategy used to determine the CO gas/air ratio was to choose a composition at which peak temperature would be achieved. This strategy should be revised as it does not consider the differences in heat capacity between CO and CO<sub>2</sub>. Heat content should be used to determine a proper CO gas/air ratio.

# DISCUSSION

The first and second run produced very different heat patterns across the 3 zones of the rotary kiln.



The change in pattern is explained by the energy necessary for  $\text{SO}_2$  gas evolution from pyrite. In the second run, insufficient energy is present in the second zone for this reaction to occur.



# CONCLUSION

- Results and assumptions were dissimilar due to the presence of a reducing gas
- Calibrating the flame should be done on a heat content basis
- Heat patterns across the RK are not strictly linear due to reactions occurring at specific temperatures
- FactSage is a powerful tool
- The Macro Tool should be used to minimize calculations (More than 100 calculations were performed during this project)