Ilmenite Smelting & Drying

Process Simulation

Computational Thermodynamics
MIME 572

Gabriel Garcia Curiel

OUTLINE

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- Smelter Simulation
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  - Ore to Coke ratio
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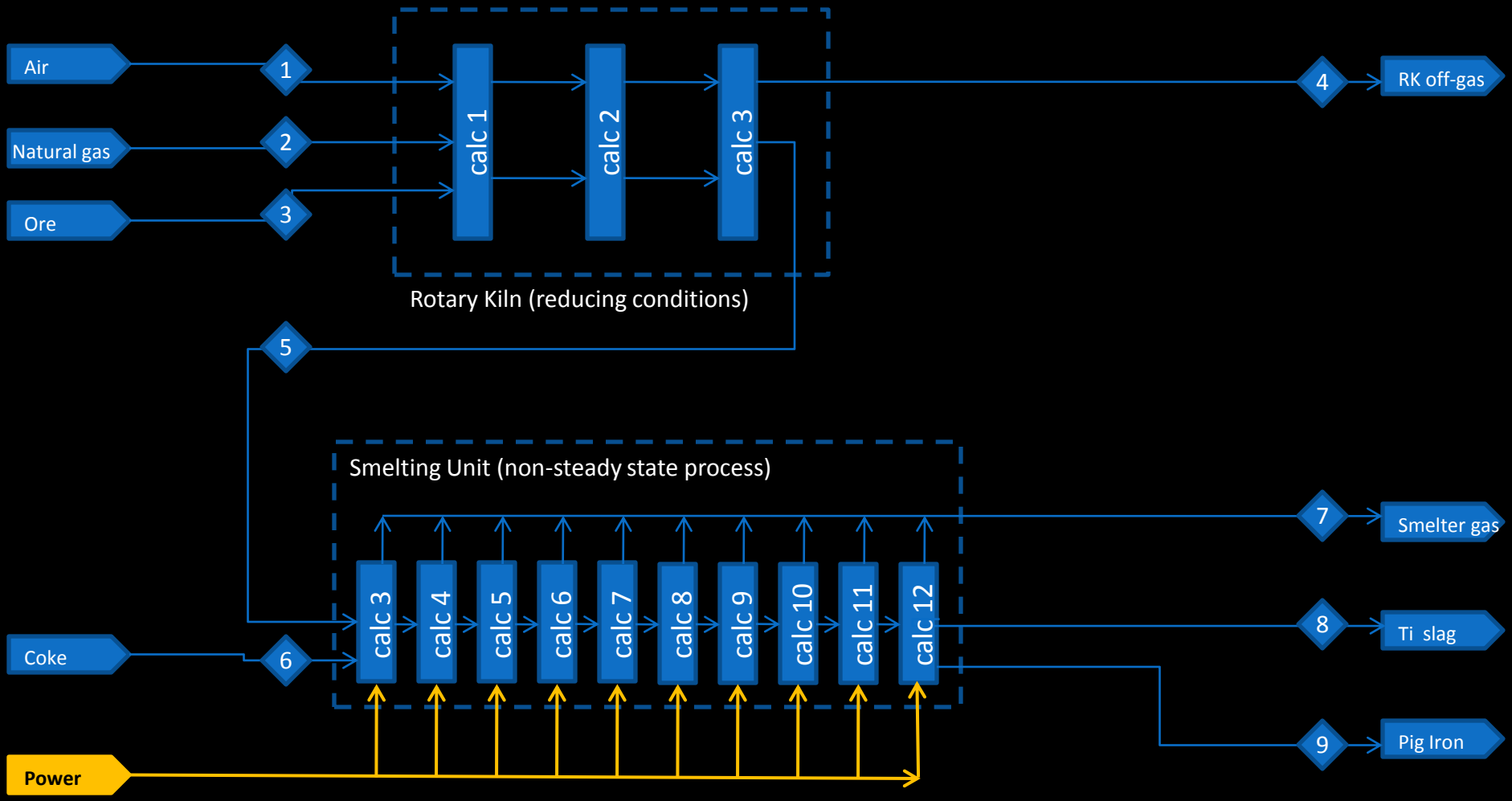
  - Rotary Kiln Input
  - Rotary Kiln dynamic simulation
  - Rotary Kiln calculations
- Assumptions vs Results
- Discussion
- Conclusion

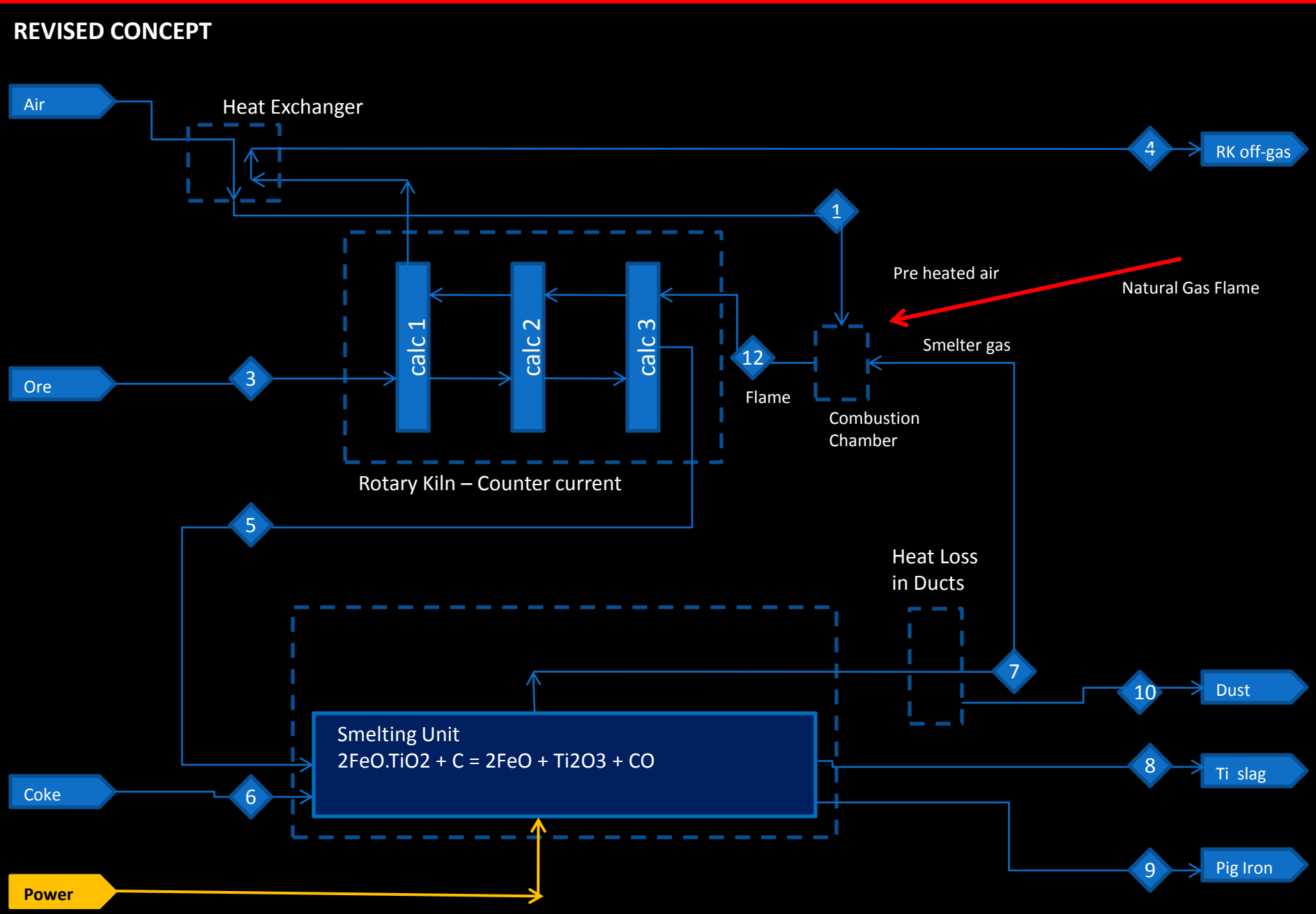
Process Flow Diagrams

Process Flow Diagram

FIRST CONCEPT :

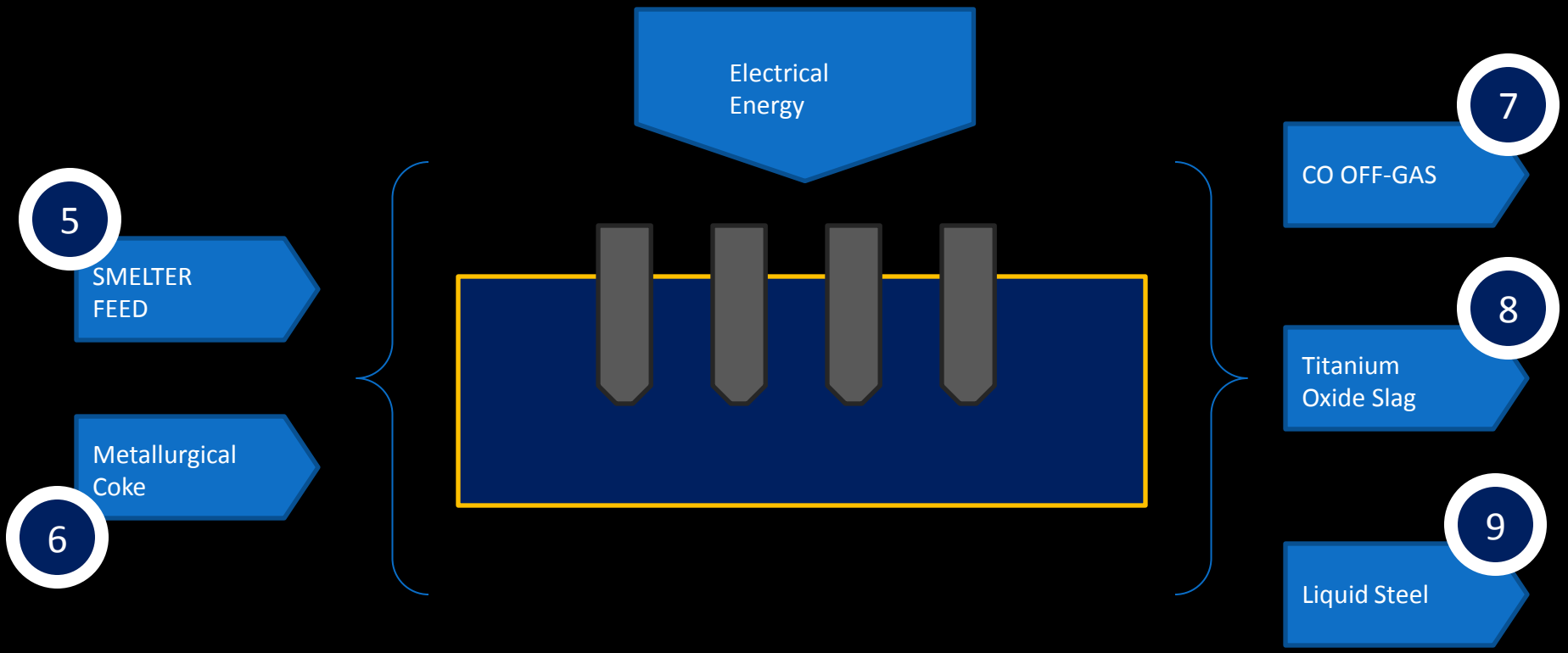


Process Flow Diagram



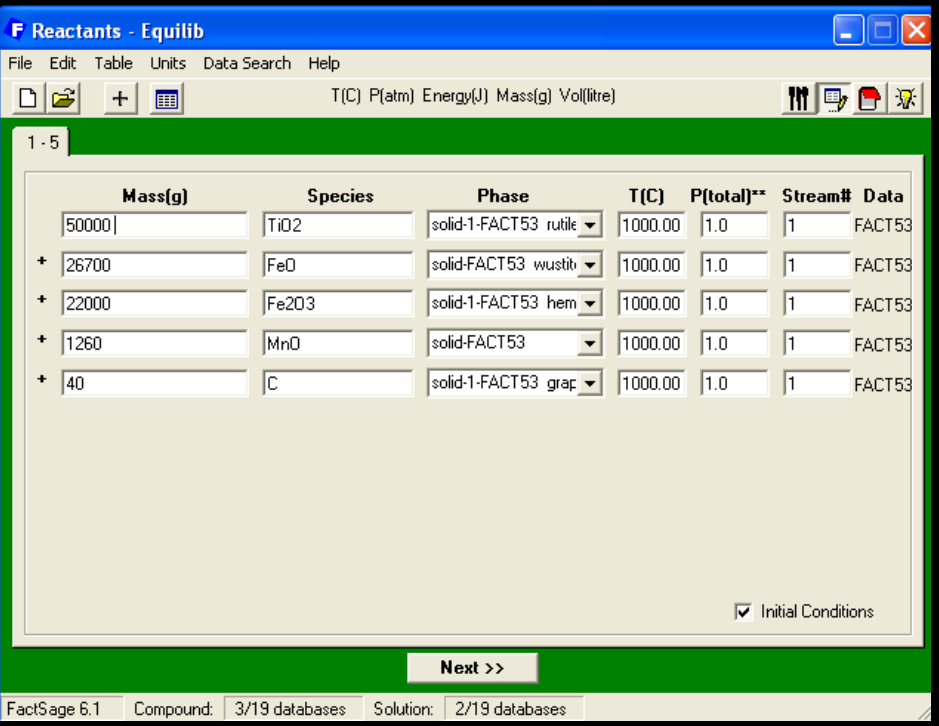
SMELTER SIMULATION

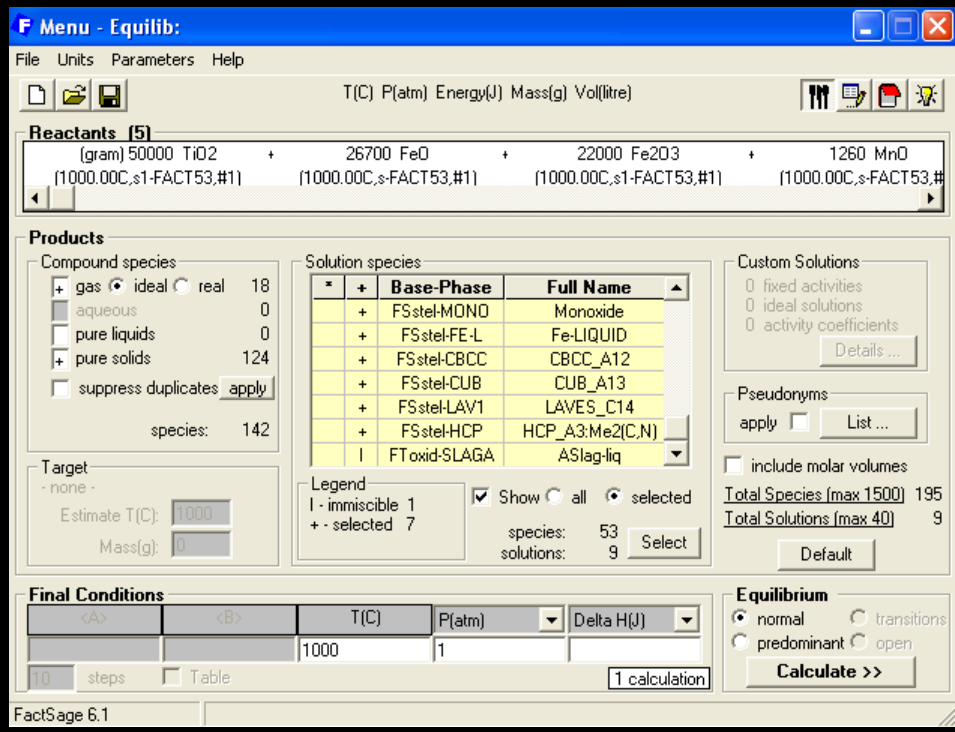
SMELTER SIMULATION



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

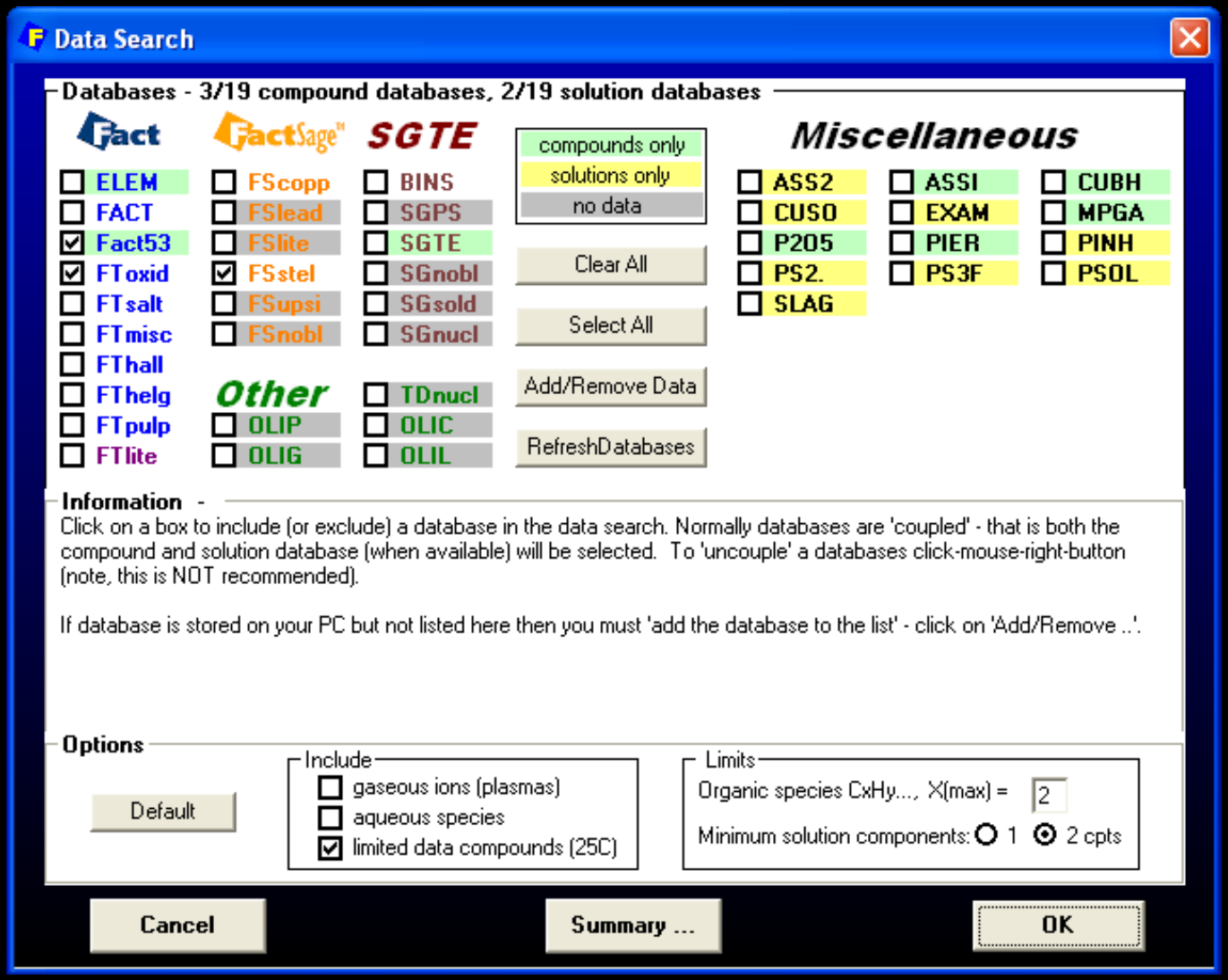
SMELTER SIMULATION
Ore Feed





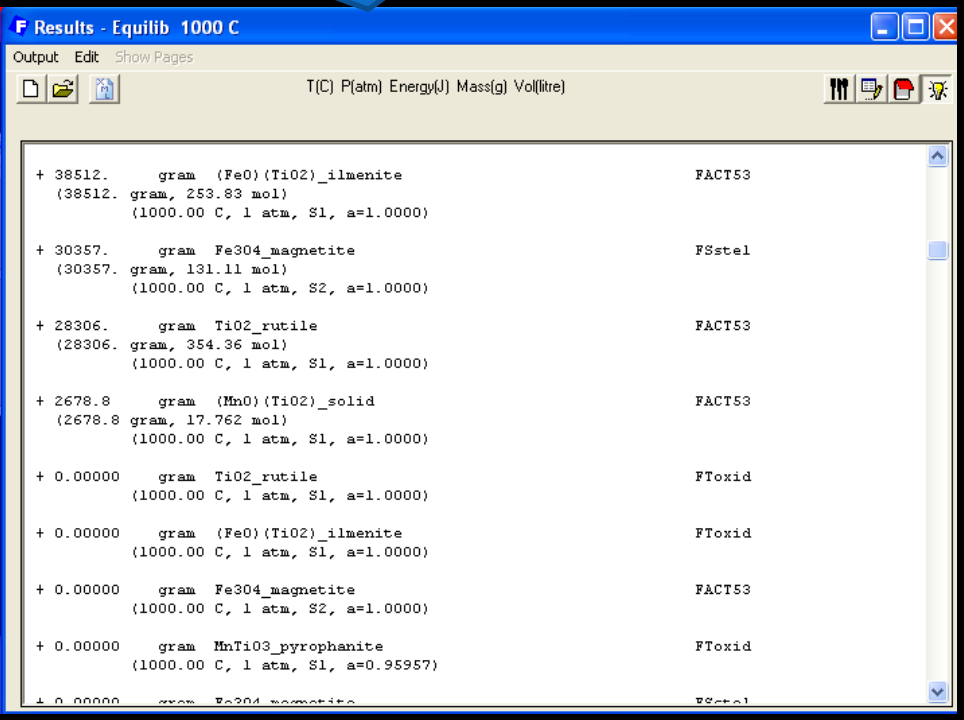
Ore feed was assumed to come from the Rotary Kiln at 1000 °C. The composition was reacted at the same temperature in order to identify the stable phases.

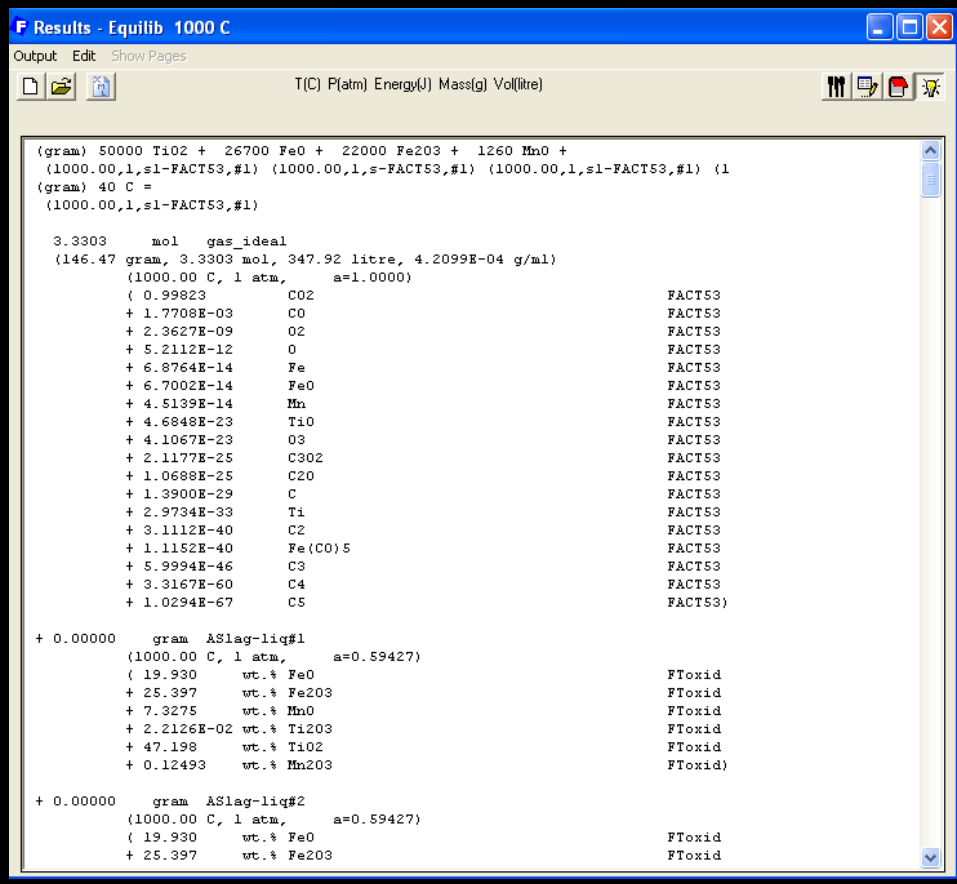
SMELTER SIMULATION
Ore Feed



SMELTER SIMULATION
Ore Feed

5 SMELTER FEED





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%
C	85
Ash	11
S	1
H2O	3
total	100

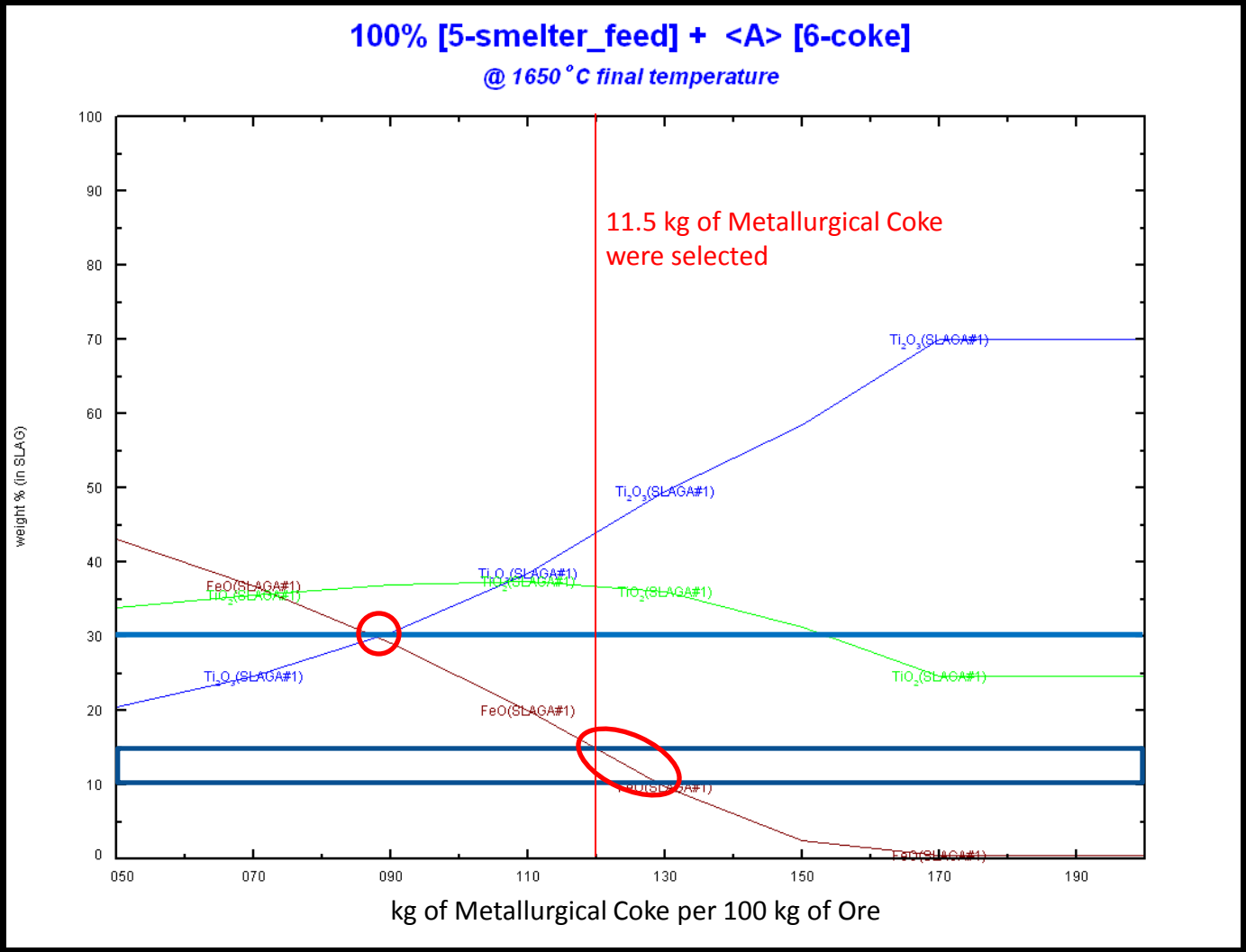
Ash	wt%
Al2O3	36
SiO2	59
Fe2O3	5
total	100

STREAM 6	**wt%**
C	**85**
Al2O3	**3.96**
SiO2	**6.49**
Fe2O3	**0.55**
S	**1**
H2O	**3**
total	**100**

SMELTER SIMULATION: ORE to COKE ratio

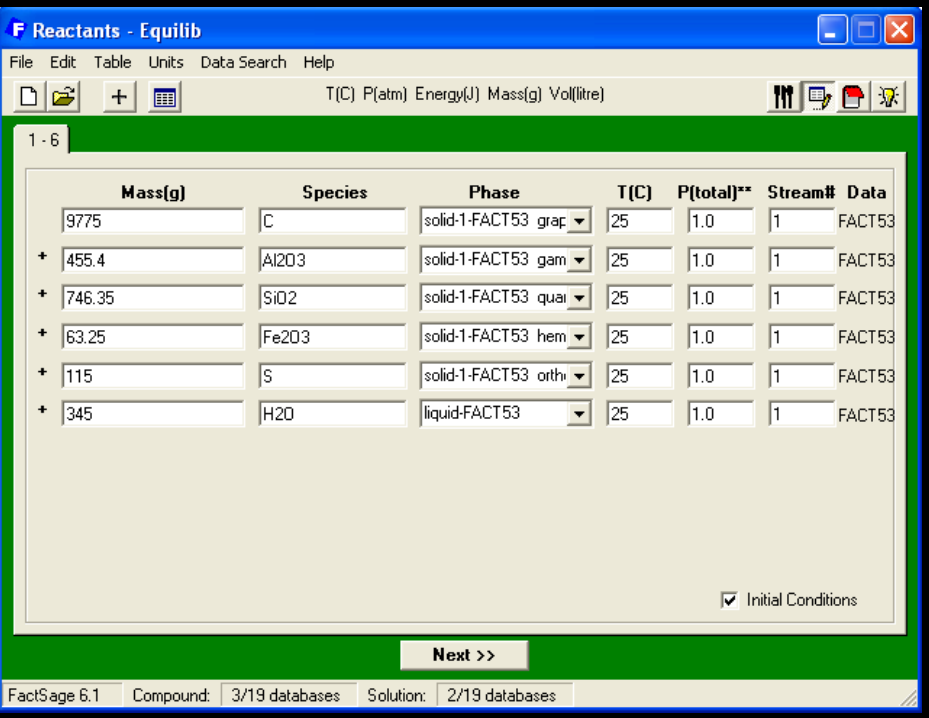
ASSUMPTION: In Titanium Slag => FeO≈ 10-15%, Ti_2O_3≈30%, Final Temp. is 1650 °C

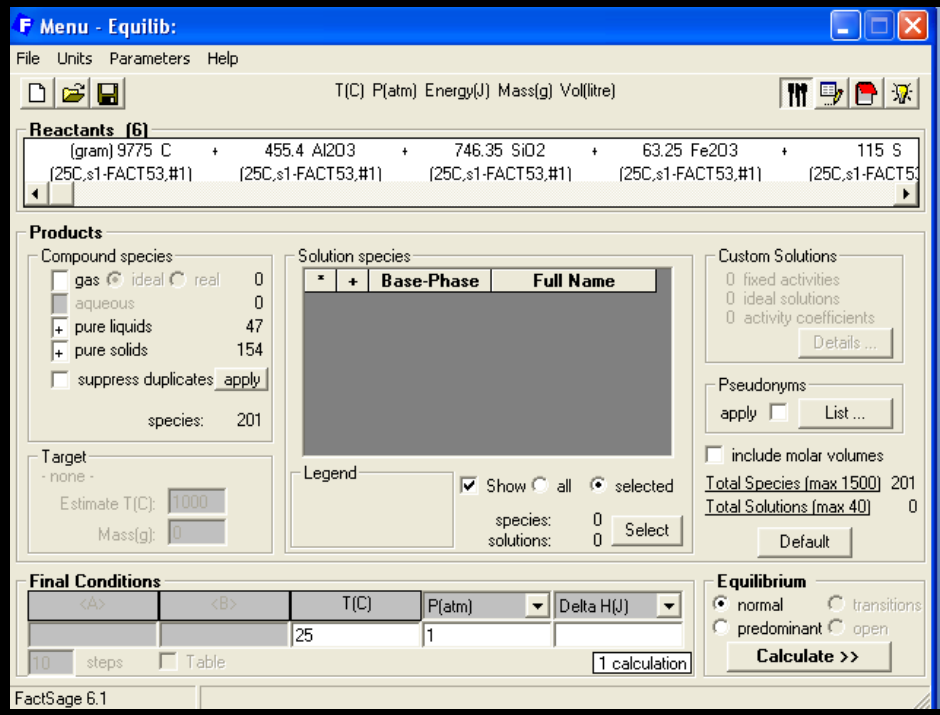
For 100 kg of Ore, what is the quantity of Metallurgical Coke that will fulfill these conditions?



SMELTER SIMULATION
Metallurgical Coke Feed

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





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

SMELTER SIMULATION
Metallurgical Coke Feed

Metallurgical Coke

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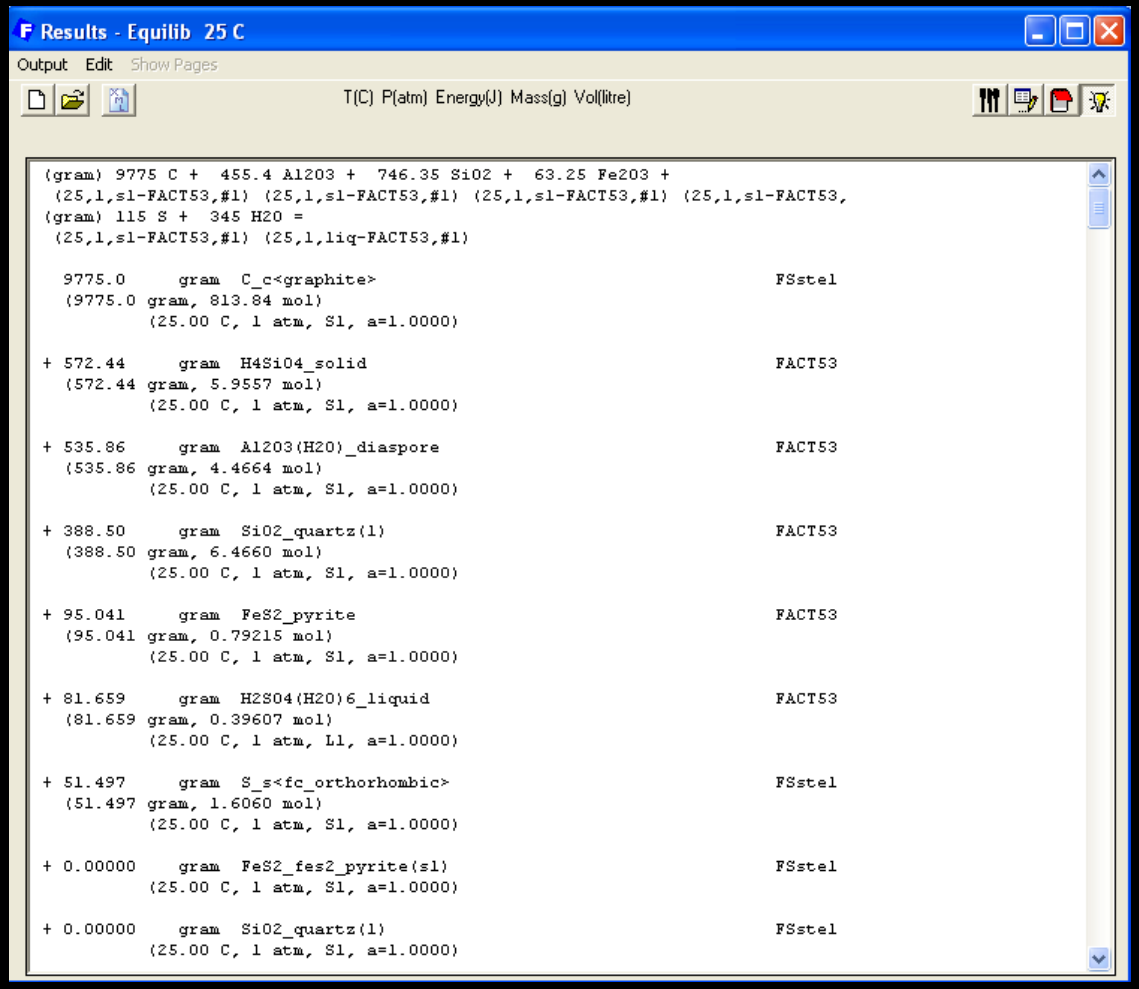
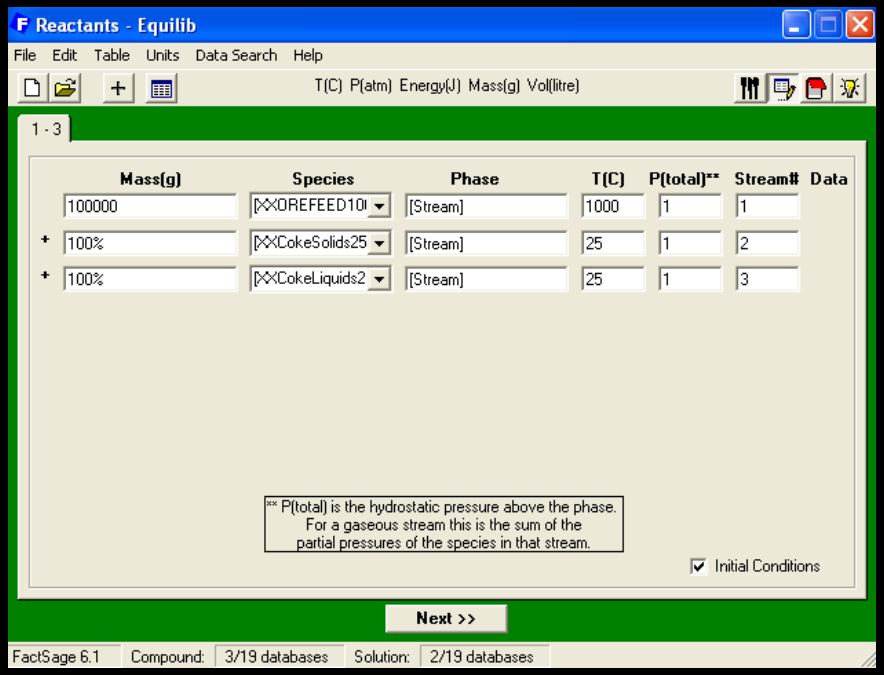
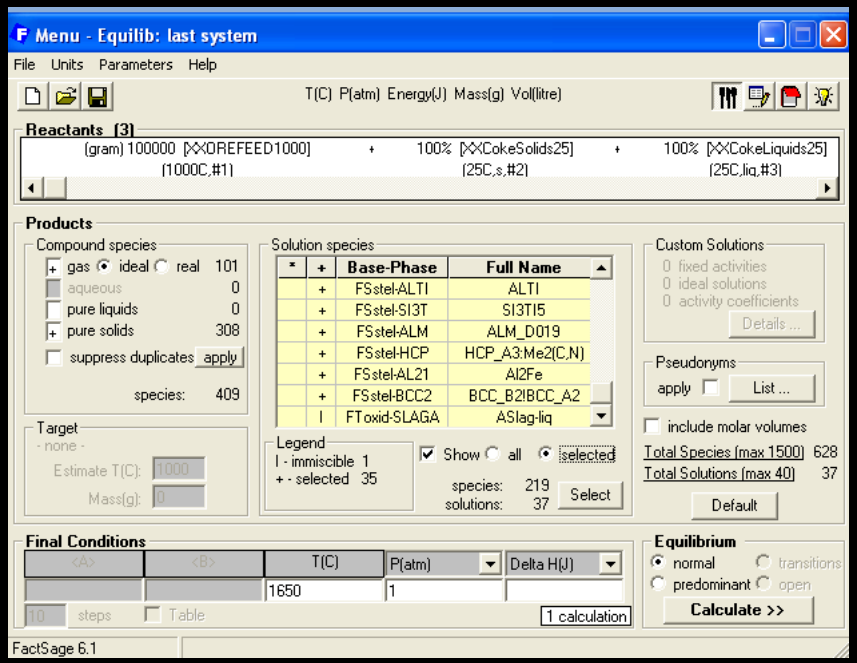


Metallurgical Coke stream was saved as 2 streams, solids + liquids

SMELTER SIMULATION
EQUILIBRIUM CALCULATIONS





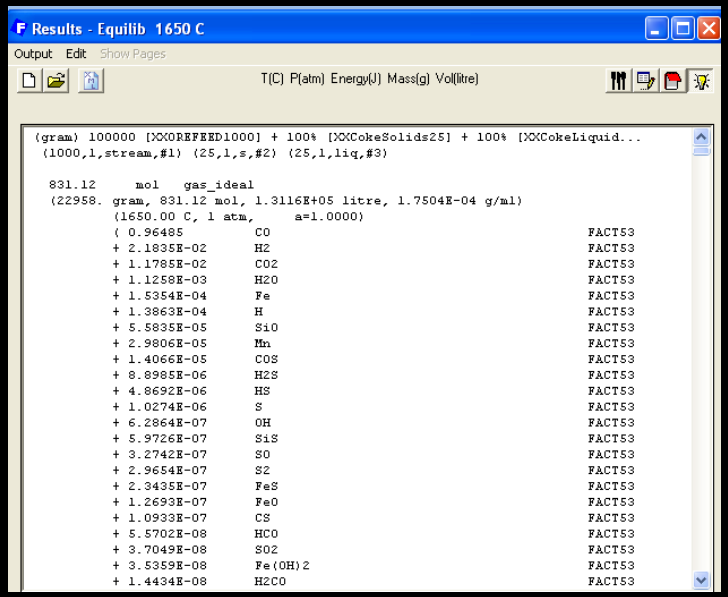
1700 °C is a typical temperature for slag while 1600 °C is a typical temperature for liquid steel. 1650 °C was fixed as the final temperature. All solution phases from the Fsstel database

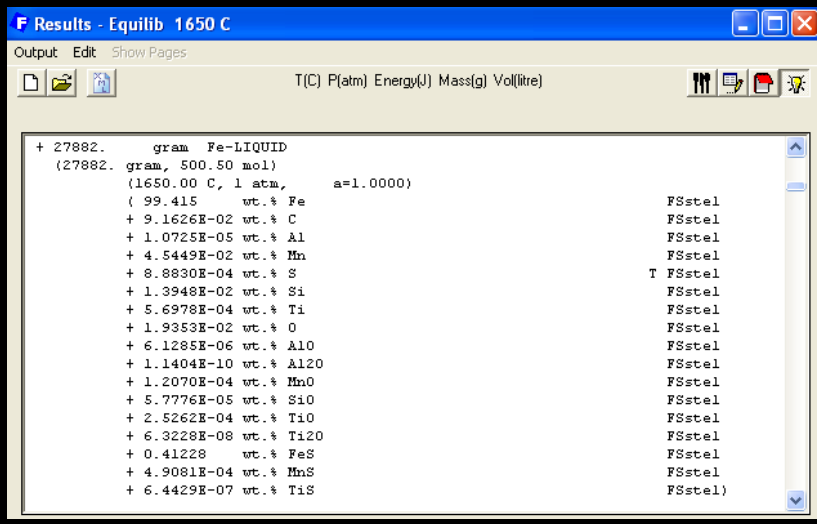
SMELTER SIMULATION
EQUILIBRIUM CALCULATIONS

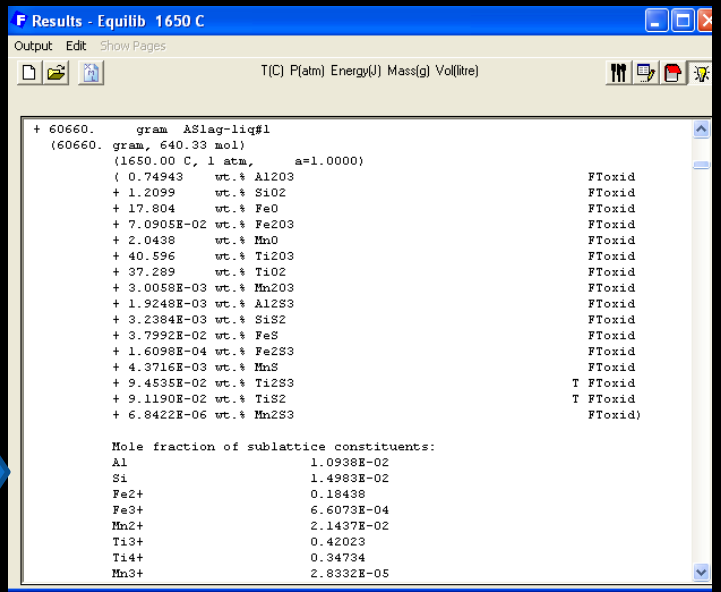
RESULTS

8

Titanium Oxide Slag







All 3 streams were saved.

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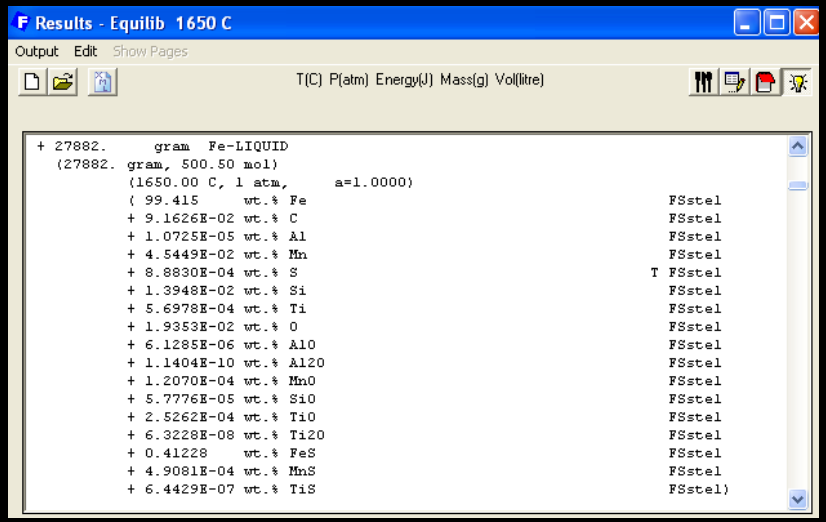
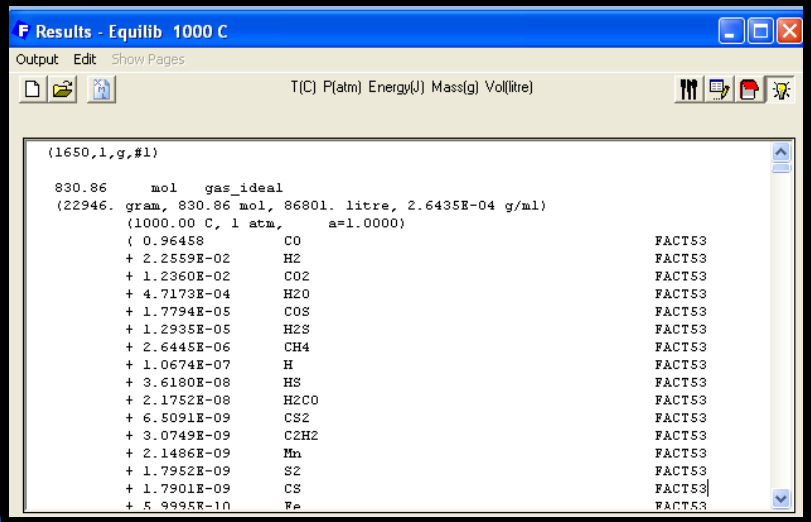
Liquid Steel

SMELTER SIMULATION
EQUILIBRIUM CALCULATIONS

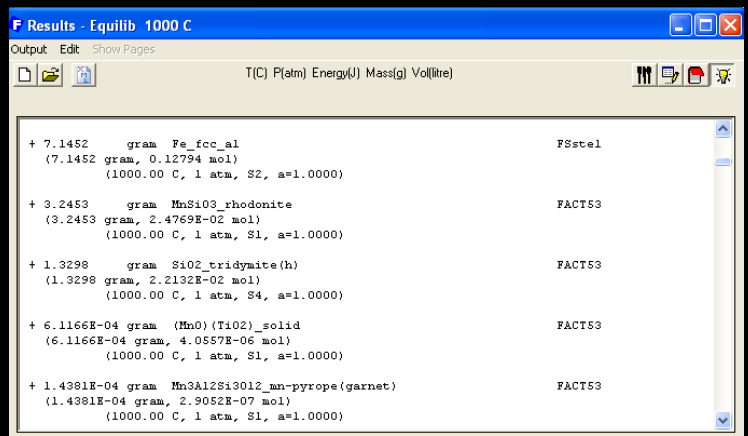
RESULTS

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





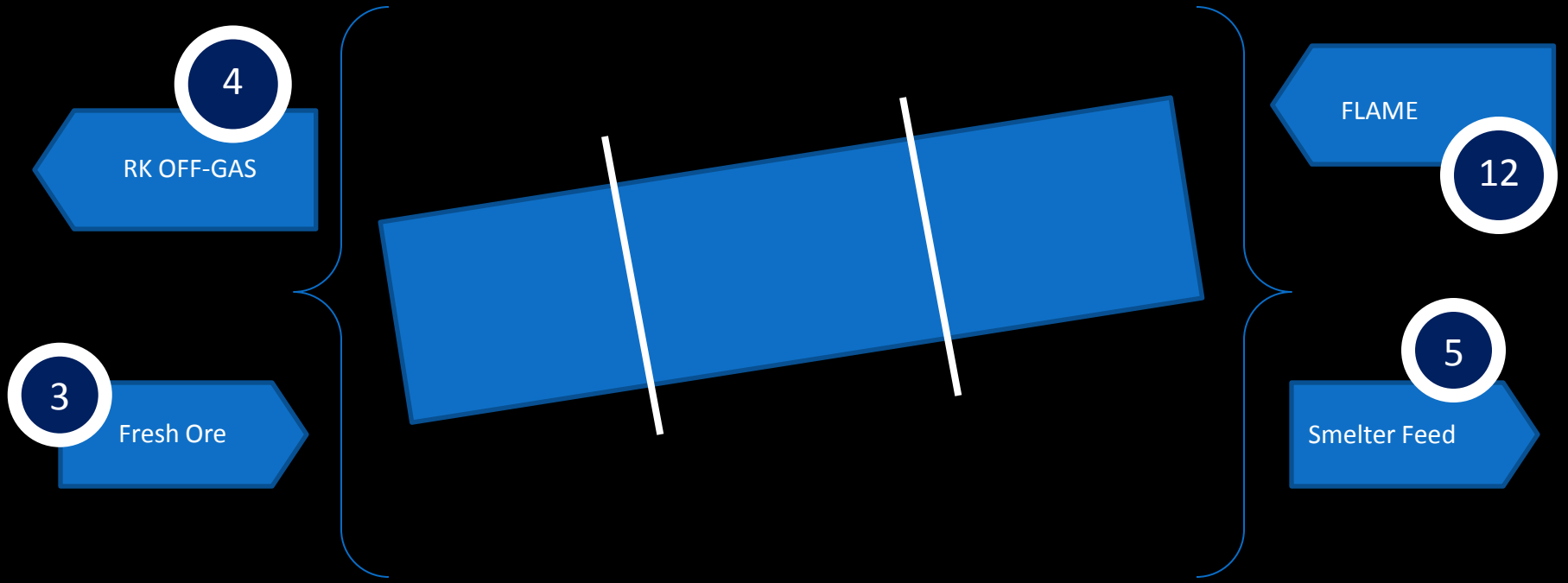
7 CO OFF-GAS



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

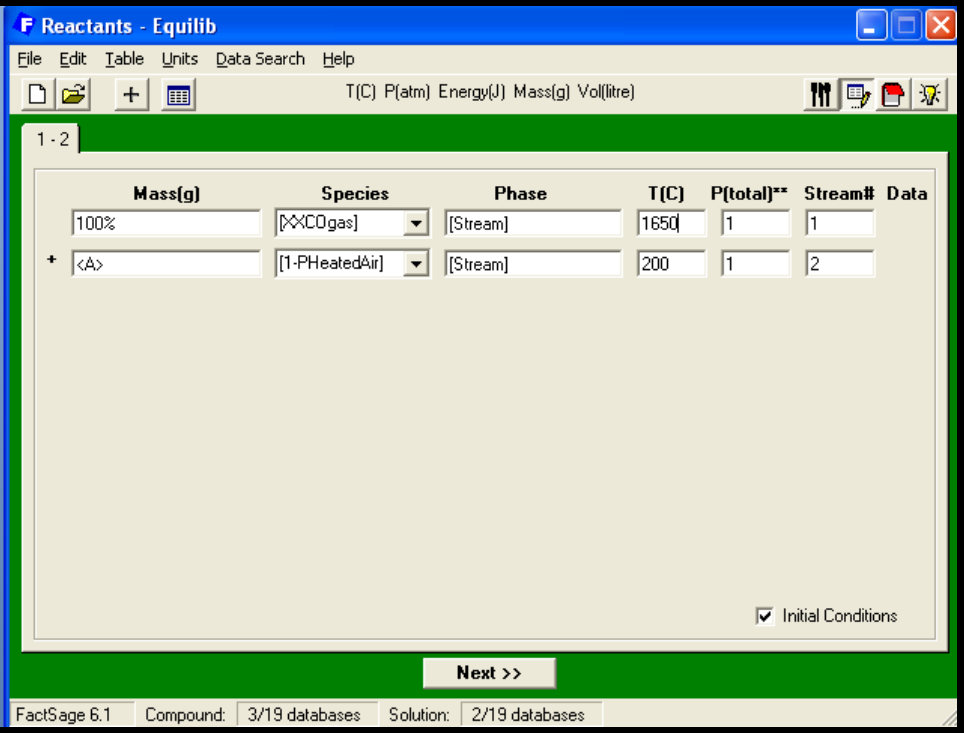
ROTARY KILN MODELLING

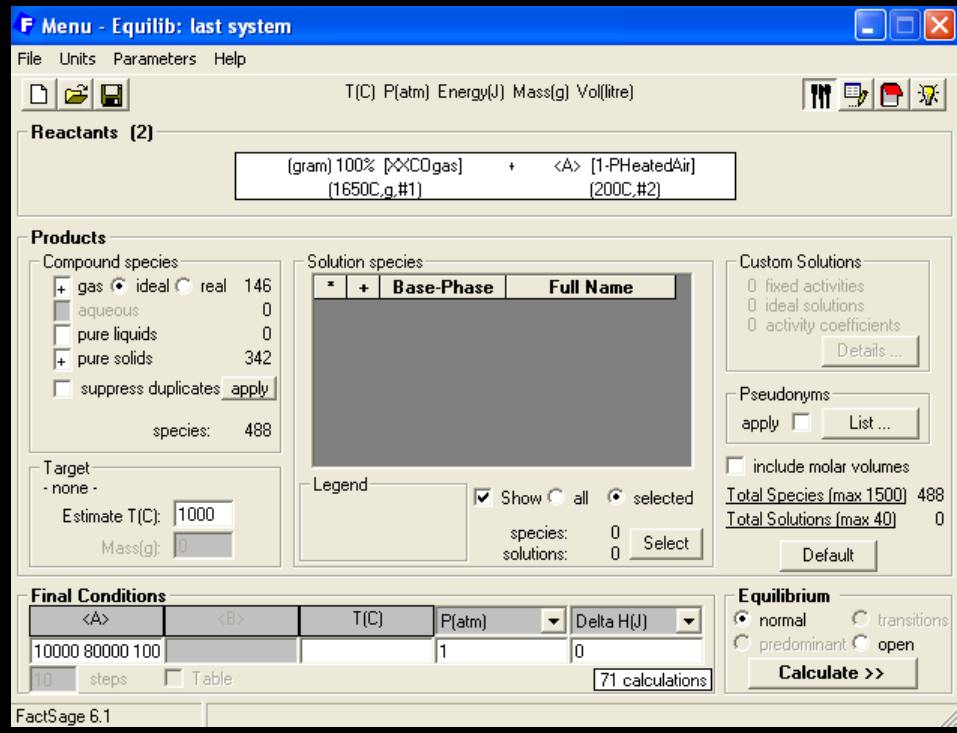
ROTARY KILN



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.

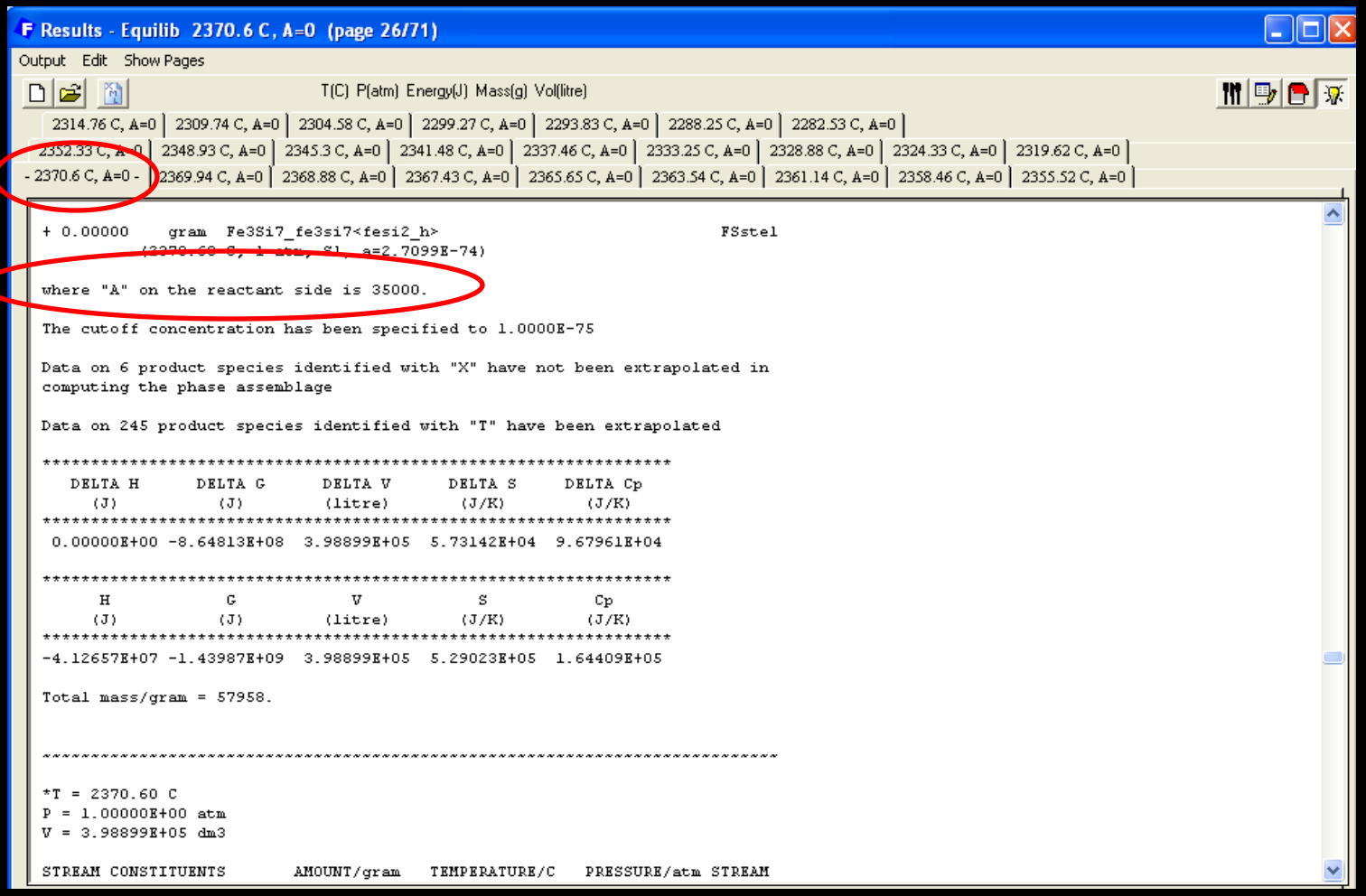




CO FLAME CALIBRATION

RESULTS

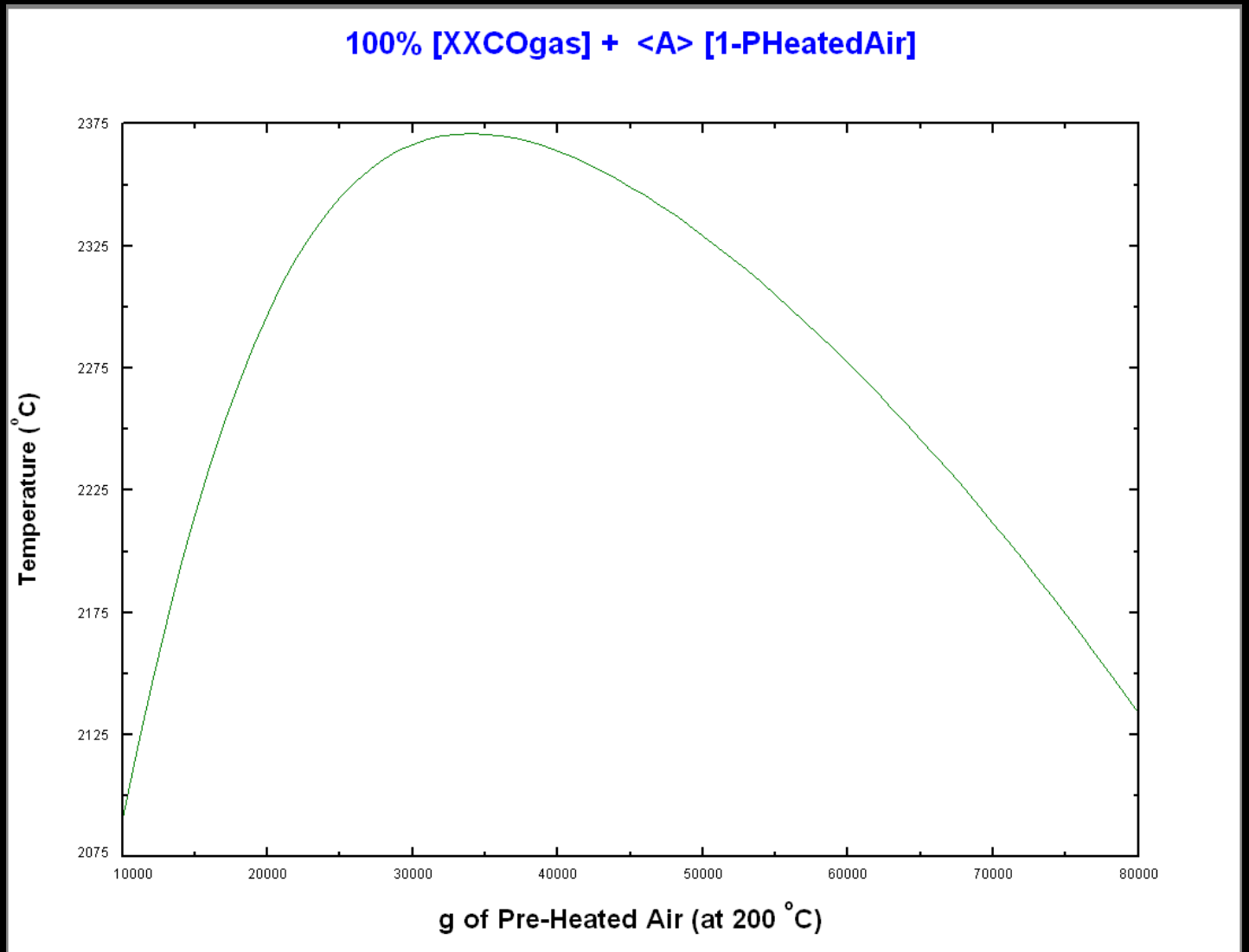
The highest temperature (≈2371 °C) is reached at around <A> = 35,000 g of Air



CO FLAME CALIBRATION

RESULTS

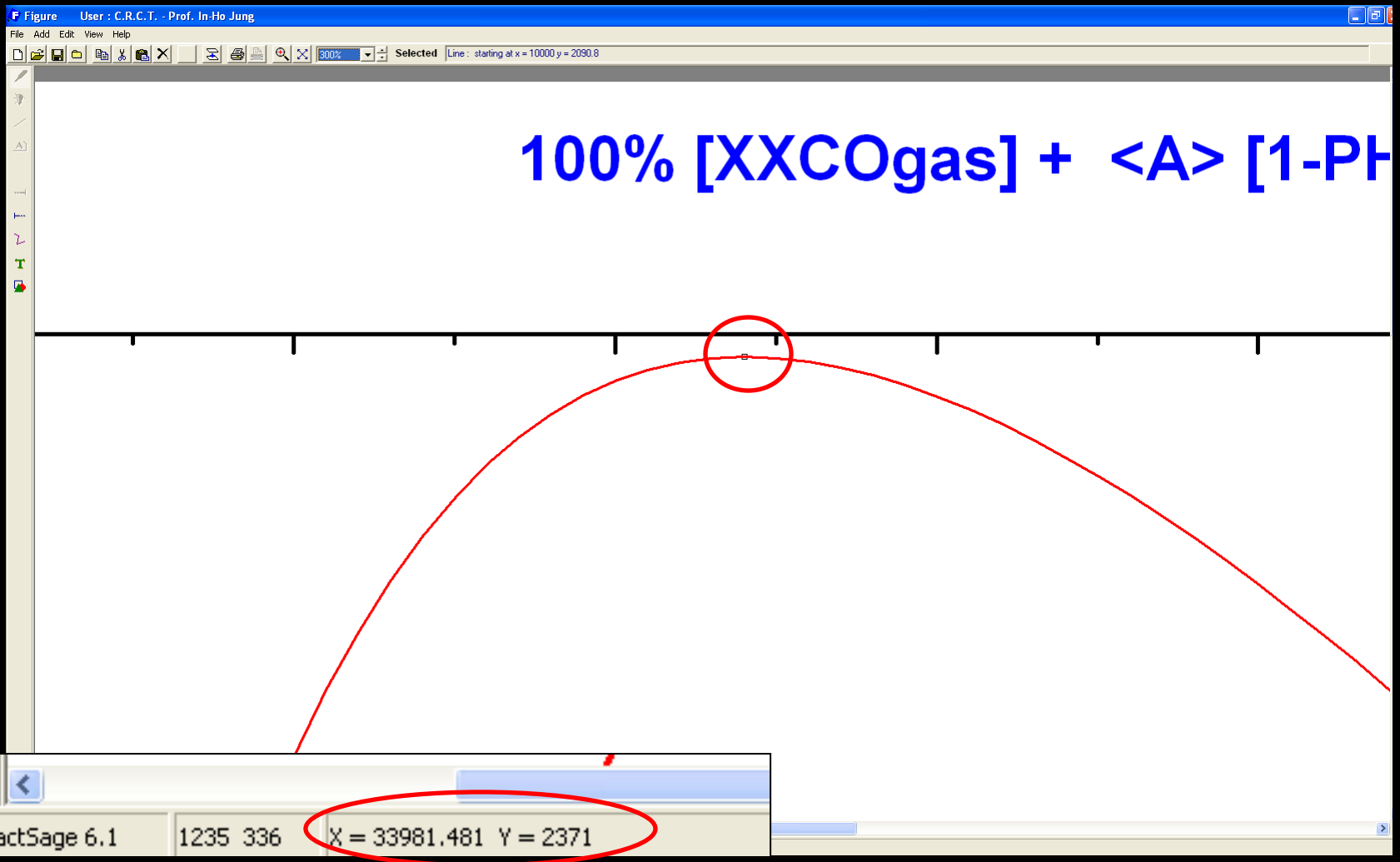
A plot of equilibrium temperature vs. g of air was generated.



CO FLAME CALIBRATION

RESULTS

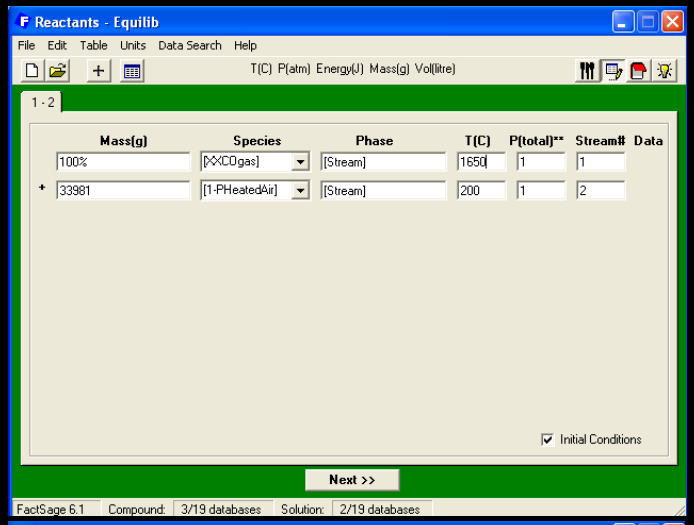
A plot of equilibrium temperature vs. g of air was generated. A peak was found at: 33,981 g of air, generating an adiabatic flame temperature of 2371 °C.

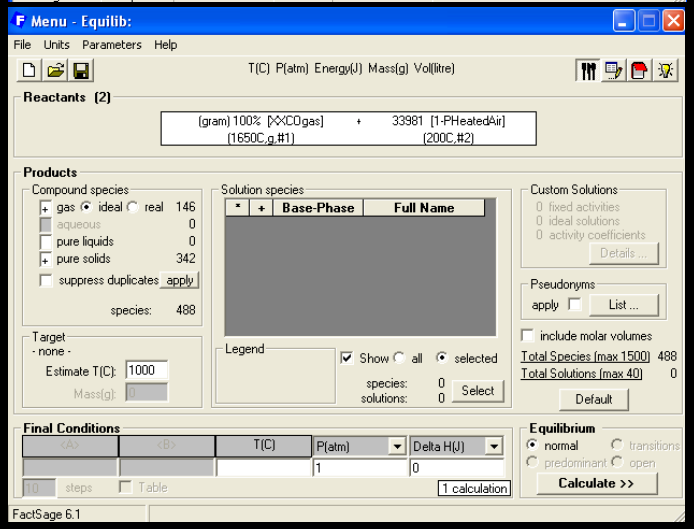


CO FLAME CALIBRATION

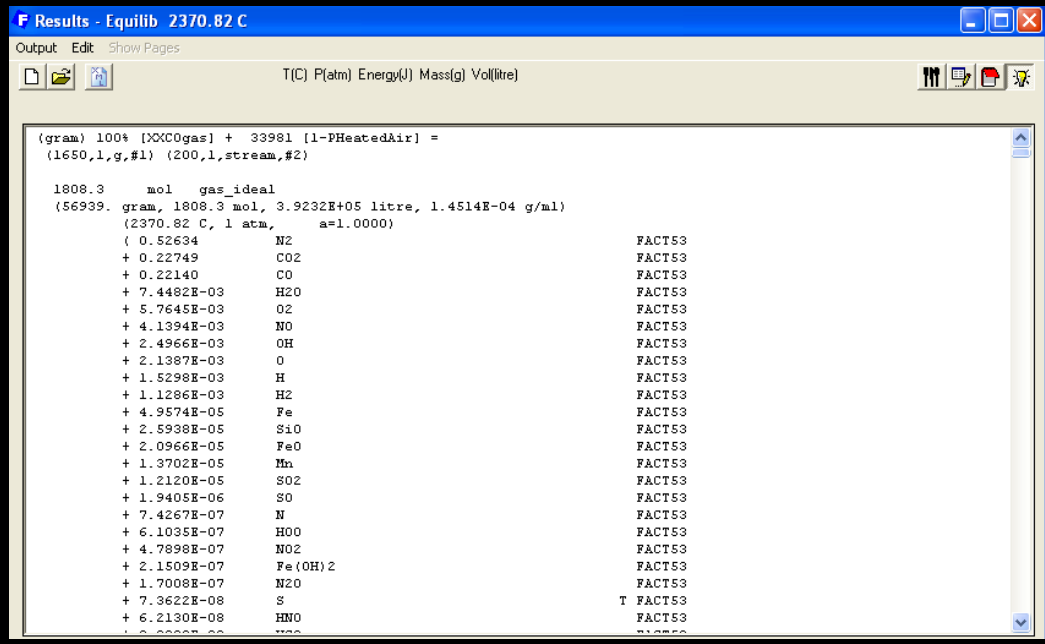
“CO FLAME”

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





“CO FLAME” stream

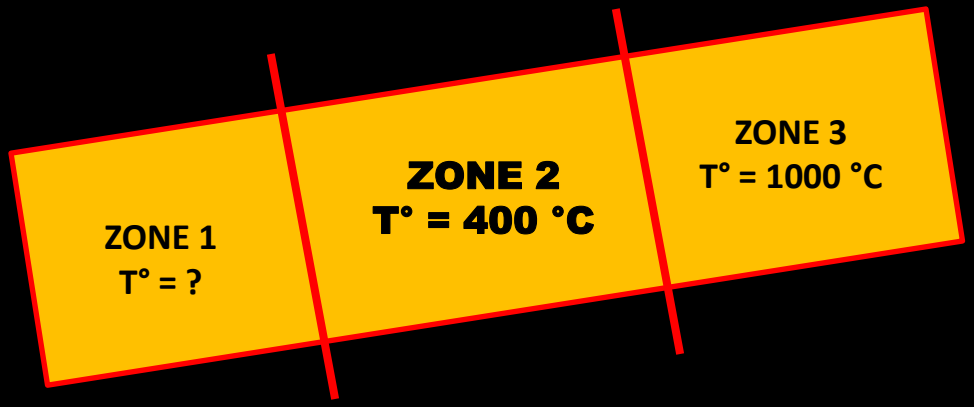


ROTARY KILN ENERGY INPUT

ASSUMPTIONS & SIMPLIFICATIONS

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

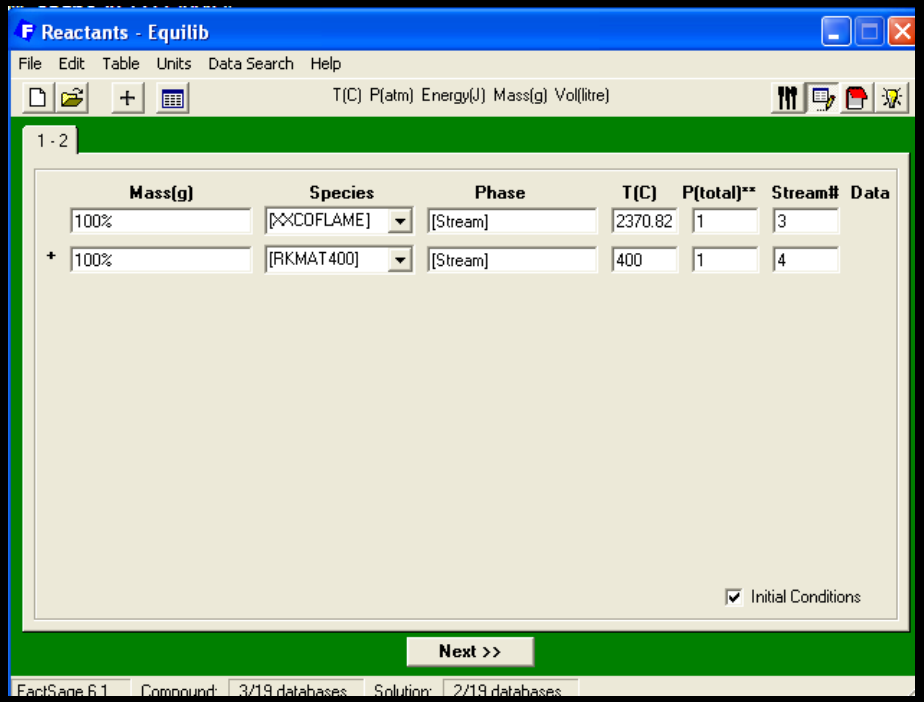
- The RK is divided in 3 zones;
- Each zone is assumed to reach equilibrium (i.e. have uniform composition and temperature);
- At steady state, the temperature in zone 2 (at the center) is 400 °C;
- At steady state, the temperature in zone 3 (at the flame and RK discharge) should be 1000 °C;

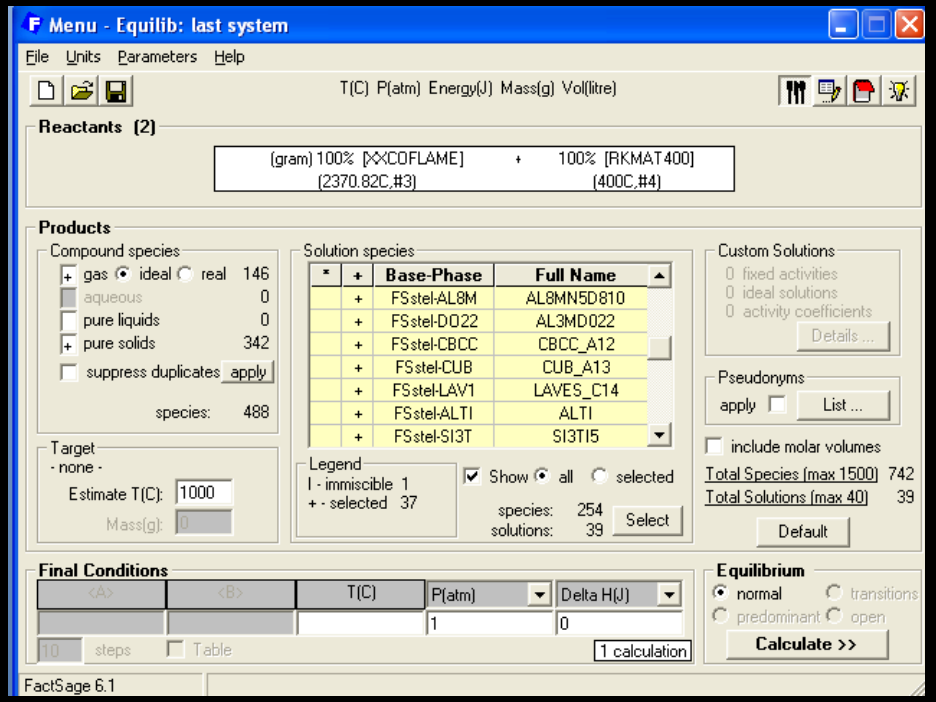


ROTARY KILN ENERGY INPUT

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.

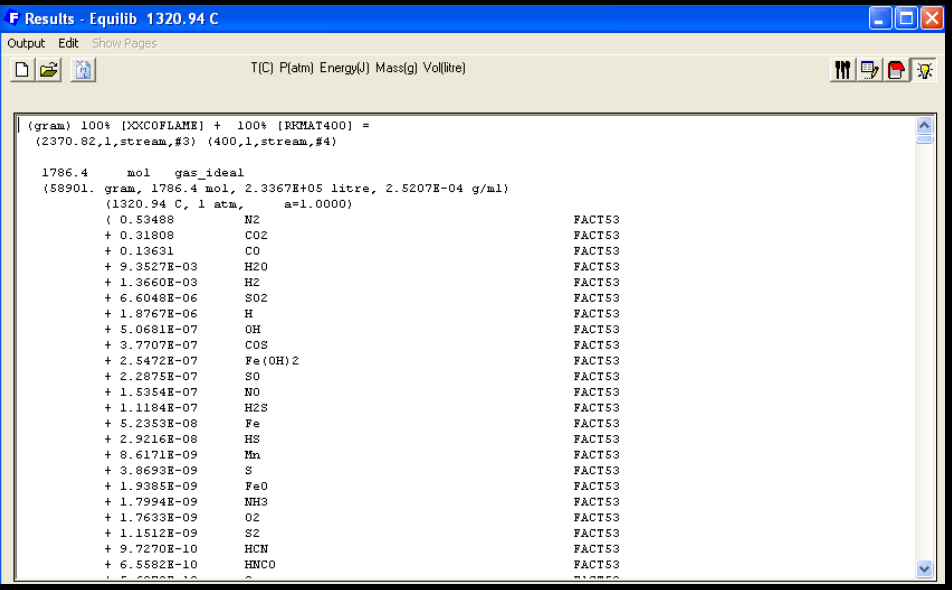


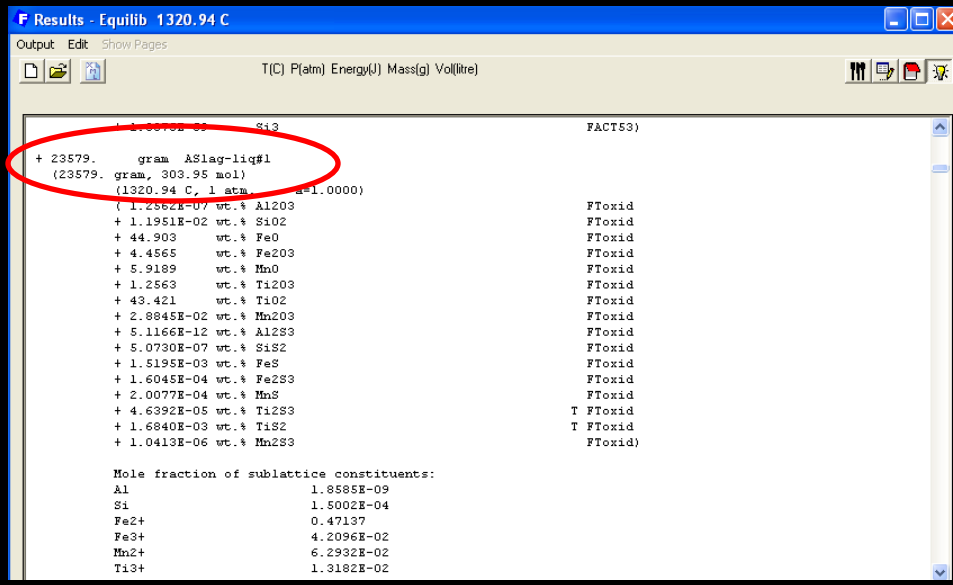


ROTARY KILN ENERGY INPUT

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.

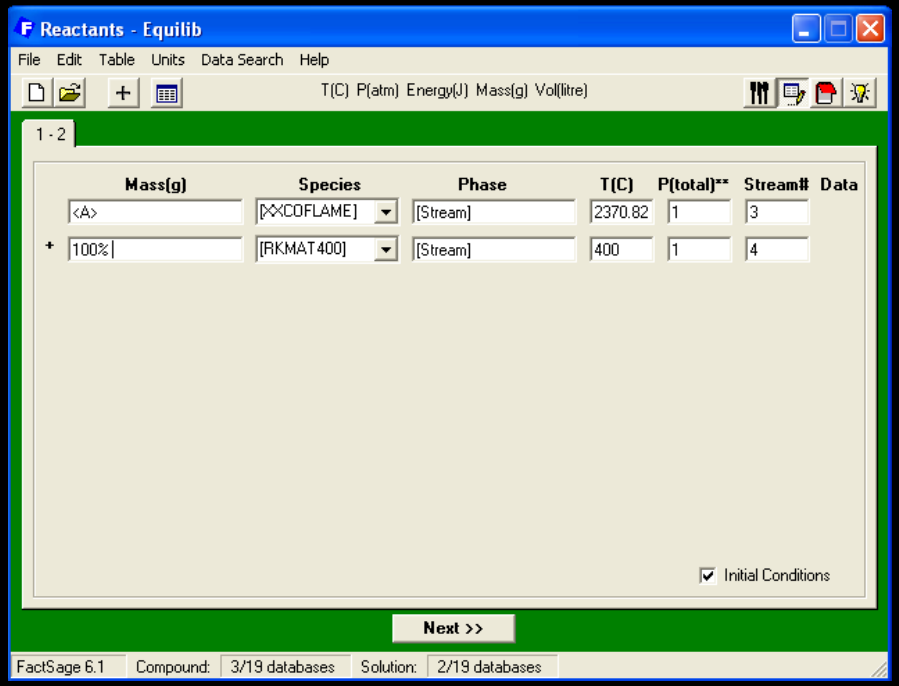


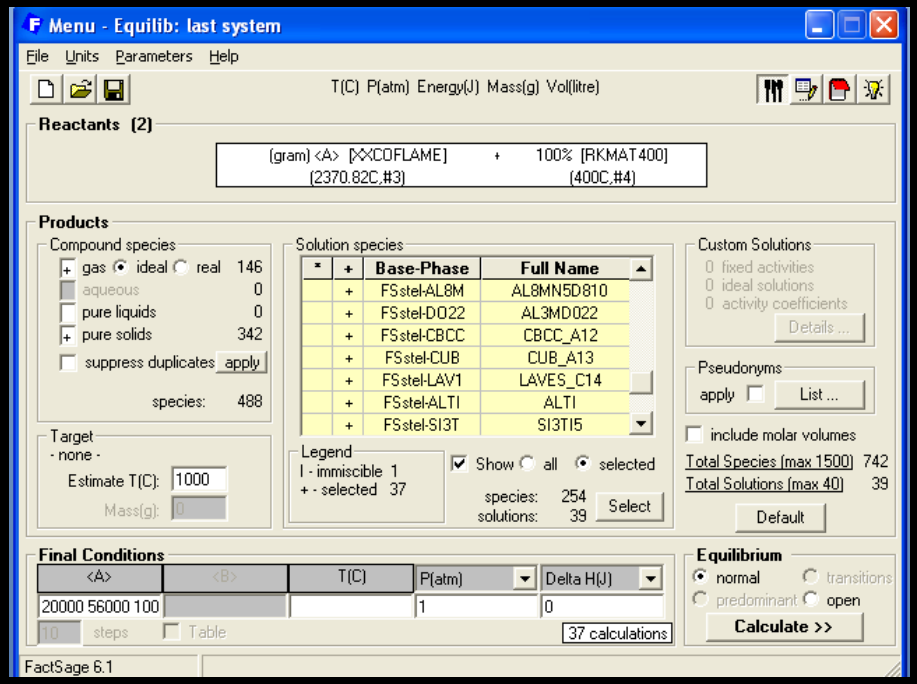


ROTARY KILN ENERGY INPUT

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.

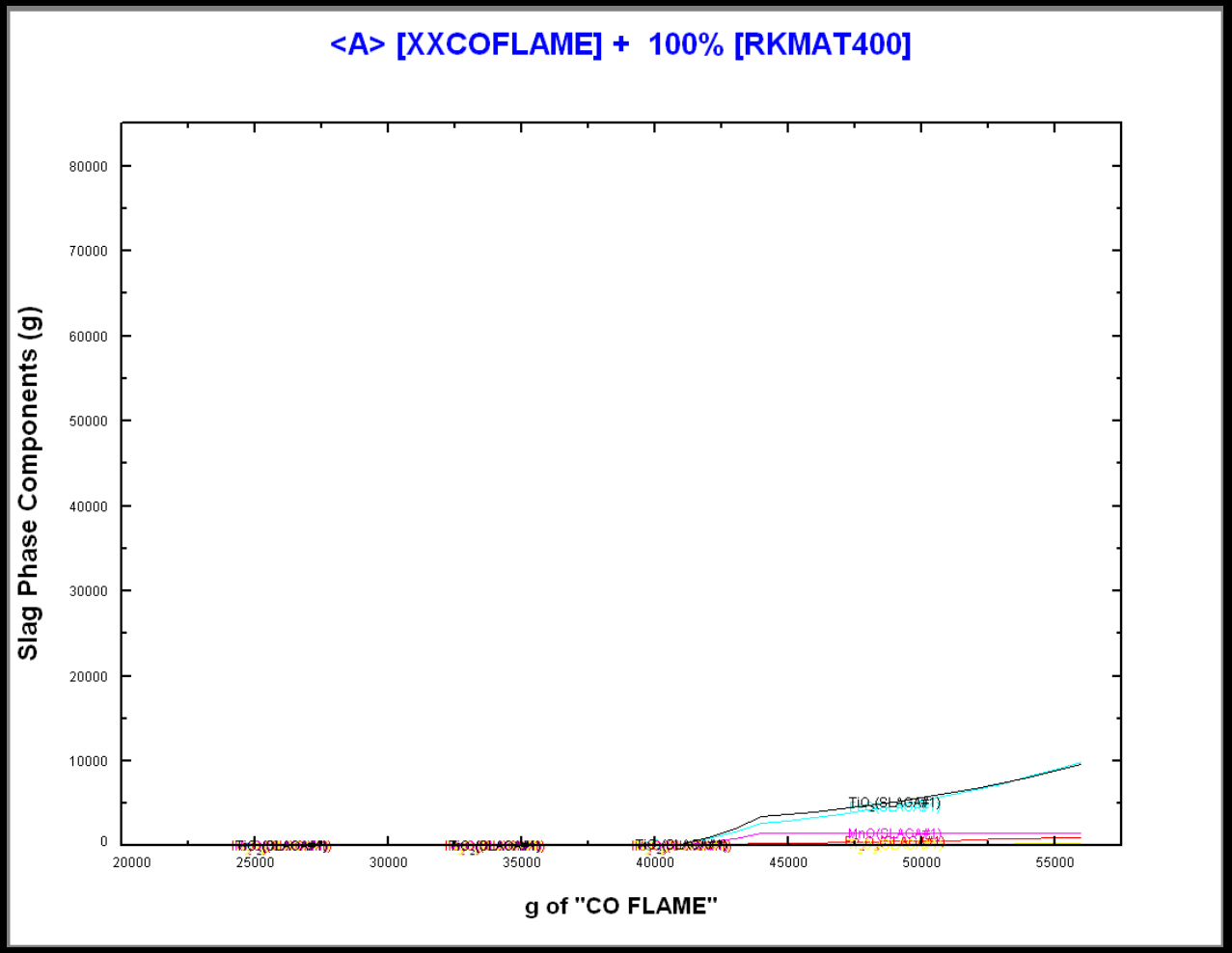




ROTARY KILN ENERGY INPUT

HOW MUCH CO FLAME SHOULD BE ADDED? RESULTS

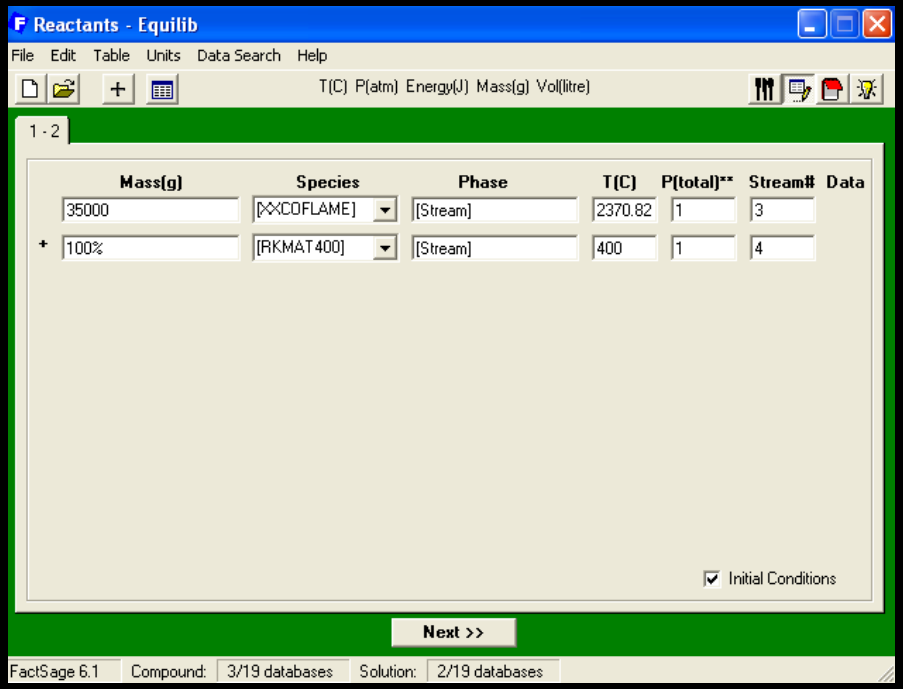
A graph was generated representing the quantity of slag present at equilibrium as a function of grams of “CO FLAME”. This graph shows slag products being created slightly after 40,000 grams of “CO FLAME” have been added.

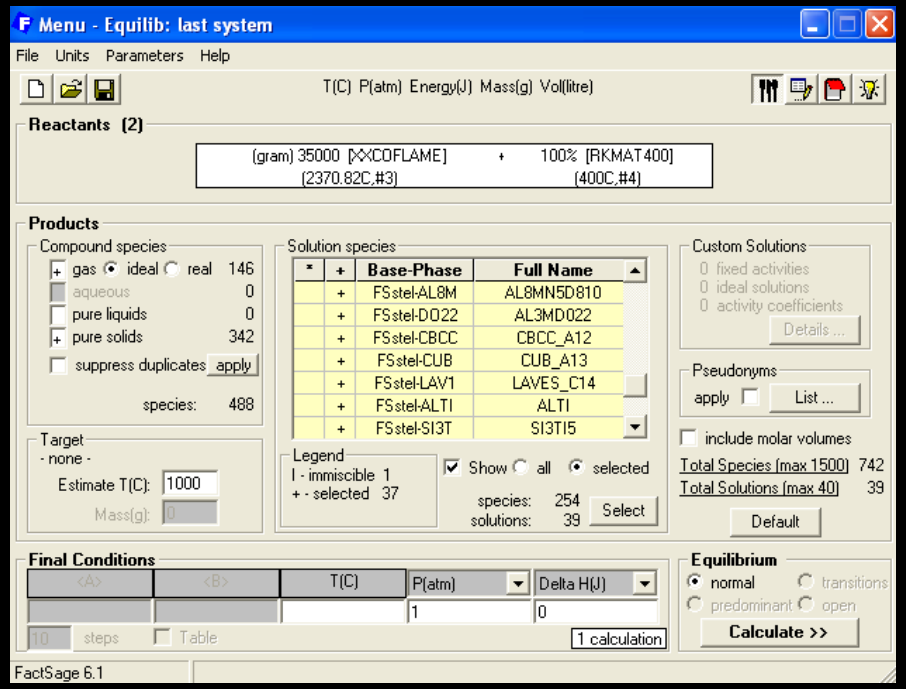


ROTARY KILN ENERGY INPUT

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.

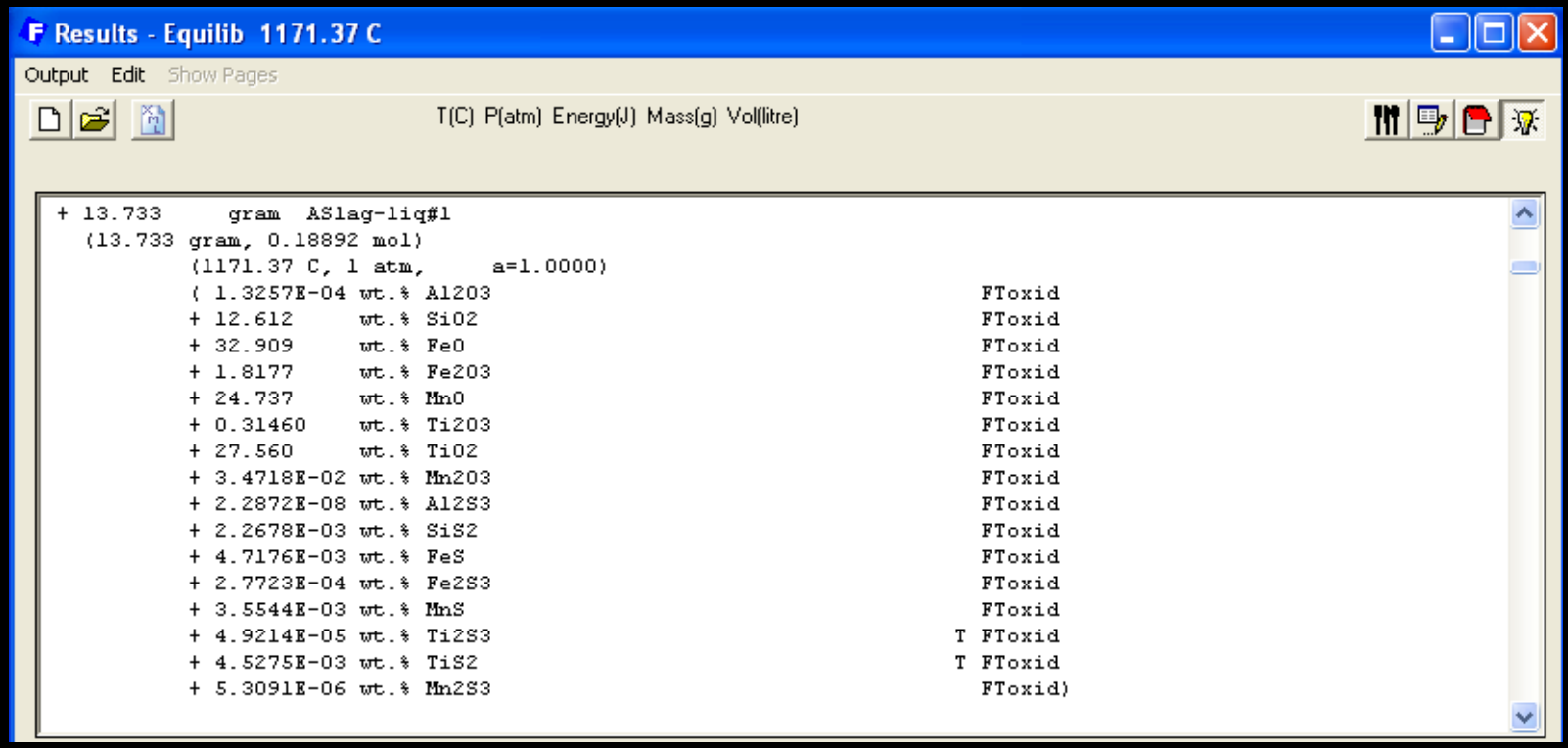




ROTARY KILN ENERGY INPUT

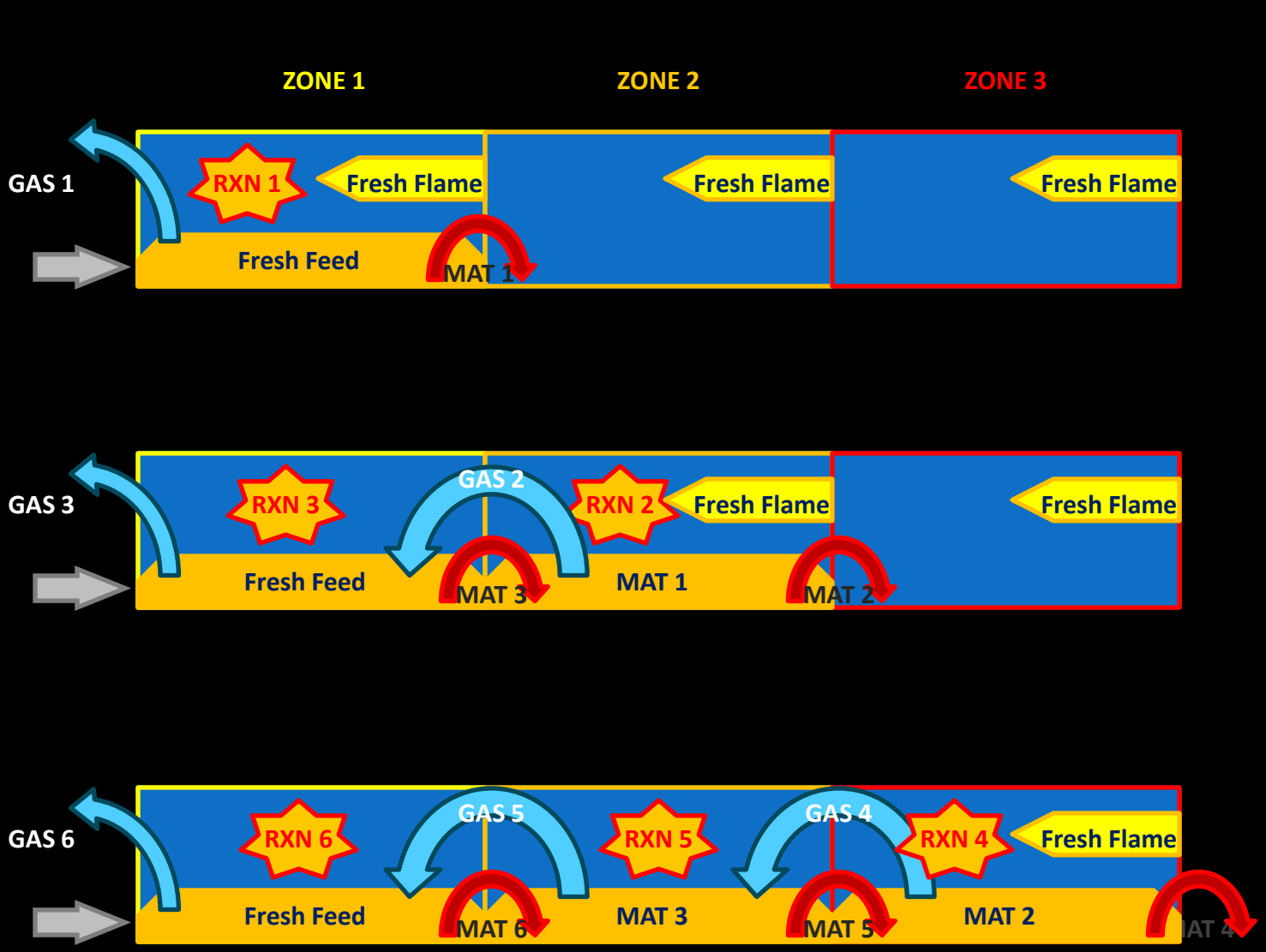
SECOND TEST: RESULTS

The resulting equilibrium produced a temperature of 1171 °C and close to 14 g of slag. This quantity was considered to be very minute and 35,000 g of “CO FLAME” were adopted as the value for the heat supply of the rotary kiln.



ROTARY KILN DYNAMIC SIMULATION

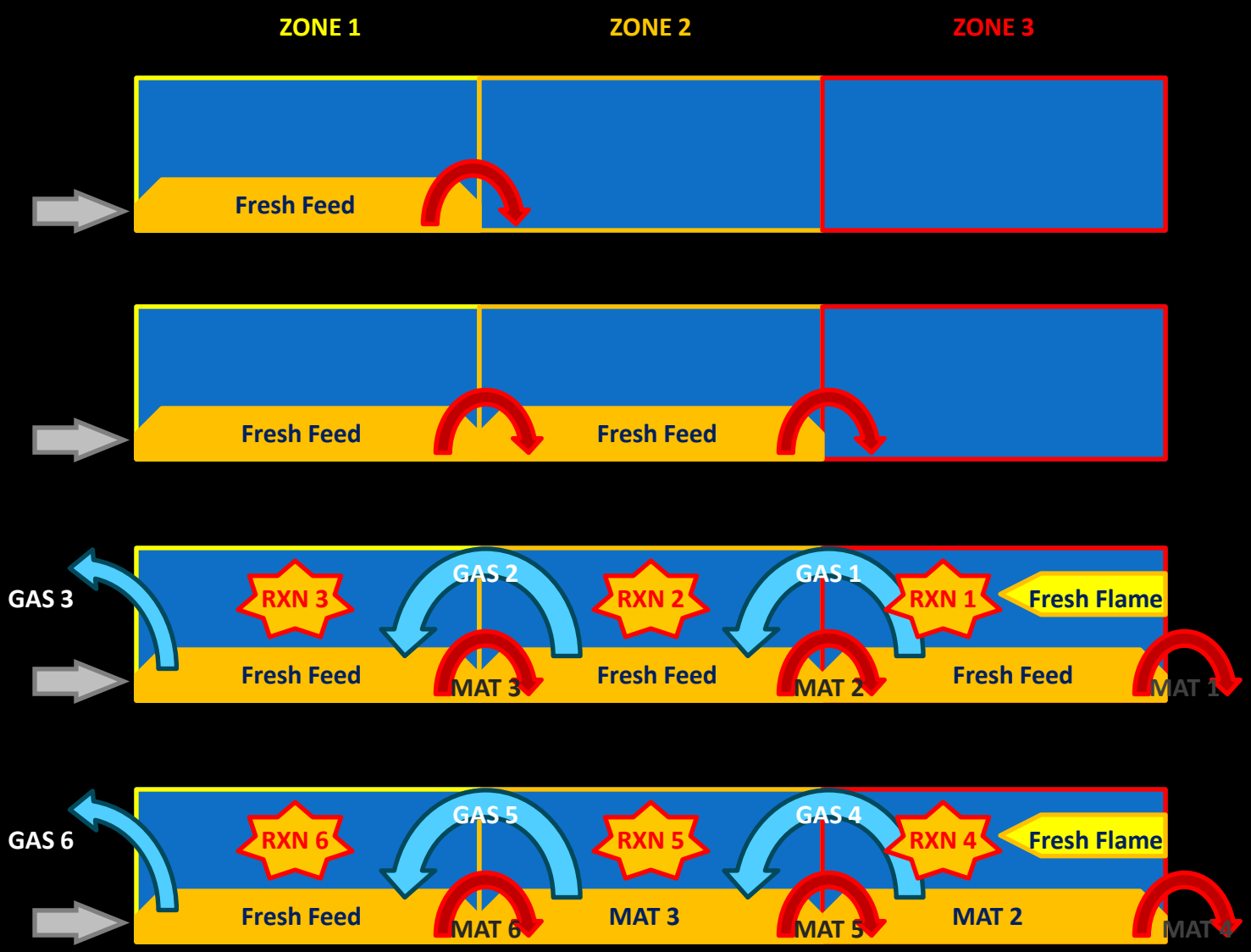
ROTARY KILN DYNAMIC SIMULATION: Principle



Rotary Kiln Calculations

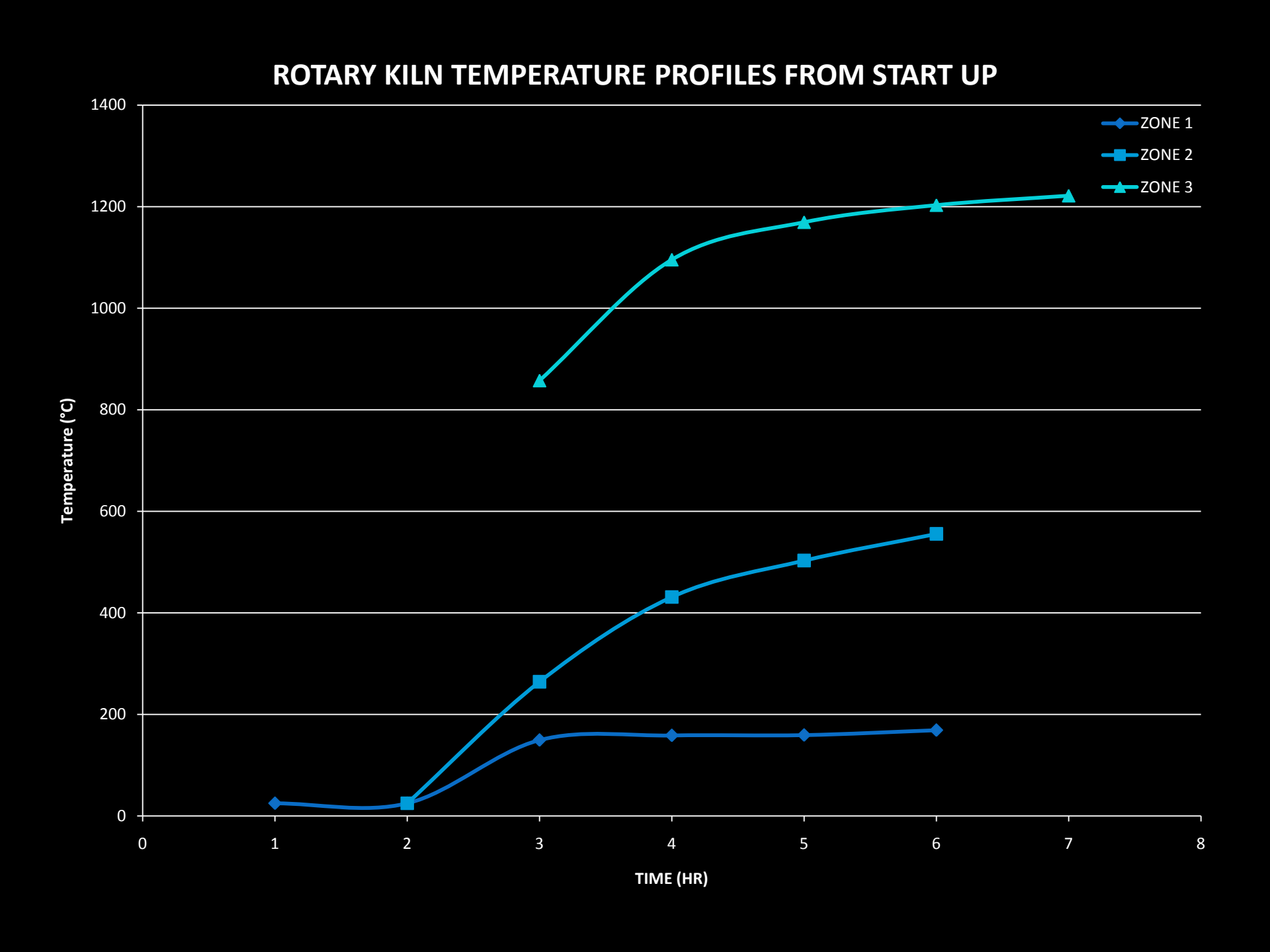
THE ROTARY KILN START-UP: 1 to 4 hrs

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

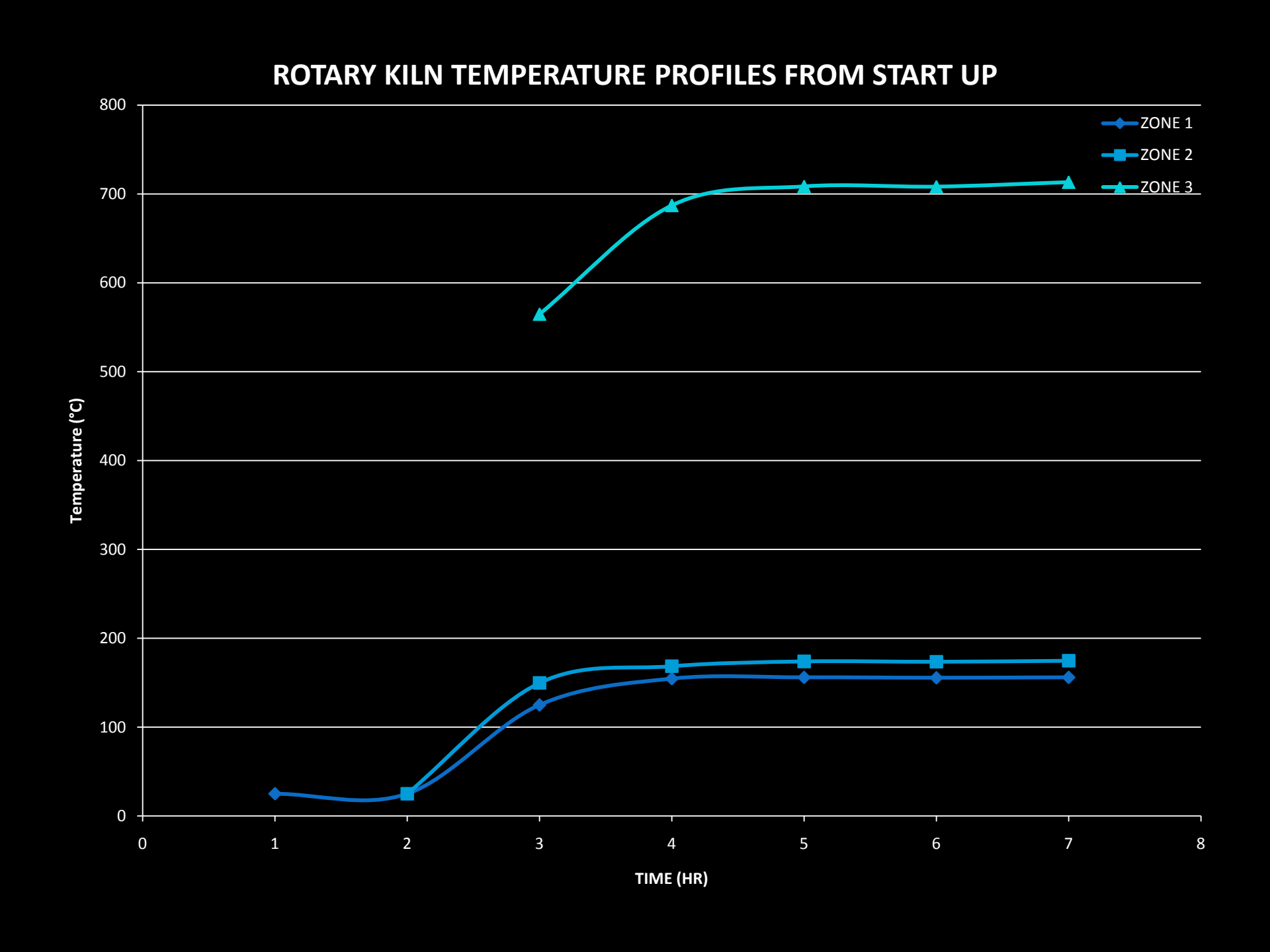


THE ROTARY KILN START-UP: 5 to 8 hrs
RK is filled and approaches Steady State

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
1400
1200
1000
800
600
400
200
0
Temperature (°C)
0
1
2
3
4
5
6
7
8
TIME (HR)
ZONE 1
ZONE 2
ZONE 3

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


ROTARY KILN TEMPERATURE PROFILES FROM START UP
800
700
600
500
400
300
200
100
0
Temperature (°C)
0
1
2
3
4
5
6
7
8
TIME (HR)
ZONE 1
ZONE 2
ZONE 3

ASSUMPTIONS vs. RESULTS

Smelter Feed (ASSUMPTION)

	wt%
$FeTiO_3$	38.57
Fe_3O_4	30.40
TiO_2	28.35
$MnTiO_3$	2.68
	100.00

Smelter Feed/RK discharge (RESULT)

	wt%
$FeTiO_3$	62.01
Fe_3O_4	2.25
TiO_2	33.72
$MnTiO_3$	2.02
	100.00

Rotary Kiln (ASSUMPTION)

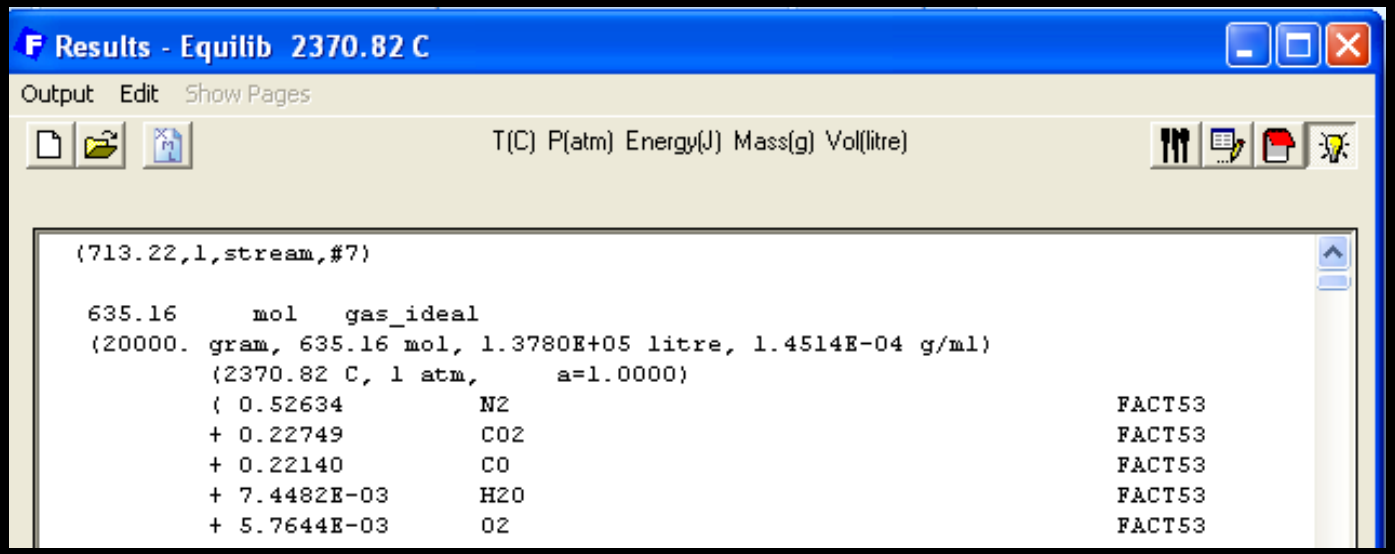
	ZONE 1	ZONE 2	ZONE 3
T (°C)	?	400	1000

Rotary Kiln (RESULT)

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

DISCUSSION

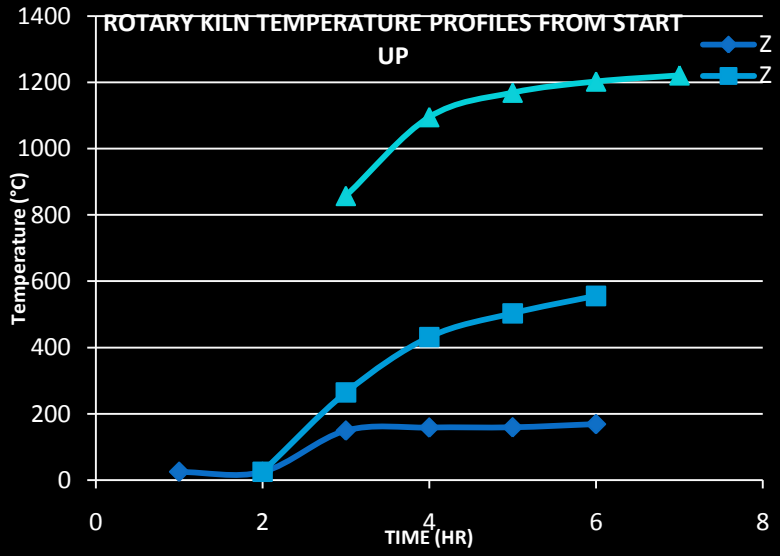
Significant difference exist between the assumptions and the RK discharge. Discrepancies in chemistries are explained by the atmosphere created by the burning of the CO gas. At peak temperature, the composition of the "CO FLAME" retains a significant amount of CO gas, almost equivalent to that of CO_2. The reducing conditions explain a higher content of $FeTiO_3$.

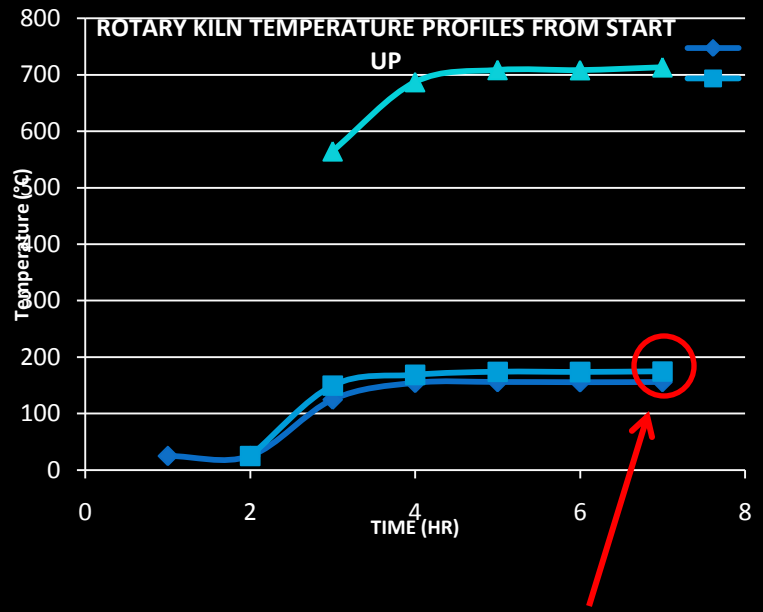


The original strategy used to determine the CO gas/air ratio was to choose a composition at which peak temperature would be achieved. This strategy should be revised as it does not consider the differences in heat capacity between CO and CO_2. Heat content should be used to determine a proper CO gas/air ratio.

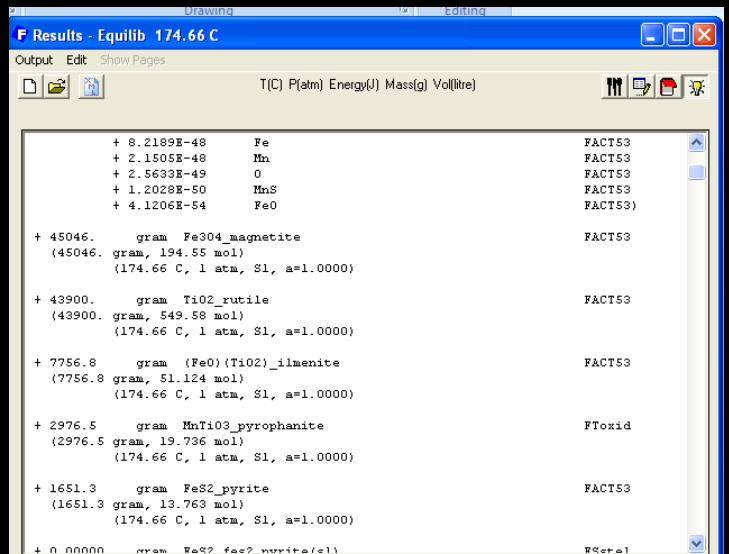
DISCUSSION

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 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 occuring 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)