Simulation of Cement Rotary Kiln at Start-up

Winter 2013

MIME 572 – Computational Thermodynamics

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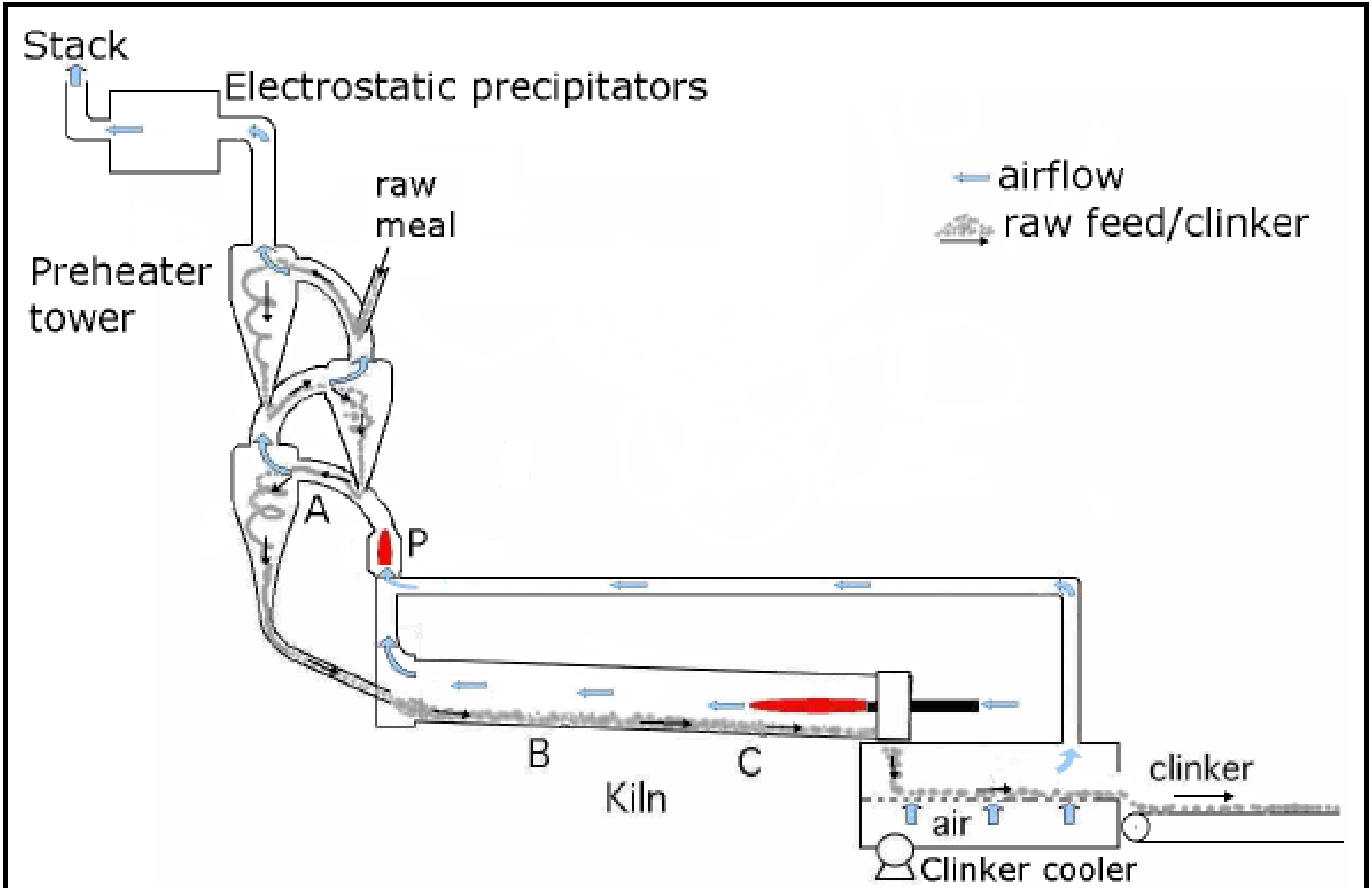
Background



http://www.understanding-cement.com/kiln.html

Objective

- Use FactSage and the macro application to develop a program to simulate the start-up of a cement rotary kiln which responds to changes in the following inputs:
  1. Input mass of solids
  2. Input mass of gas/fuel
  3. Change in kinetics
     - (i.e. the amount of solids, slag and gas reacting)
  4. Changes in input temperature of solids and/or gas-fuel

Design Concept

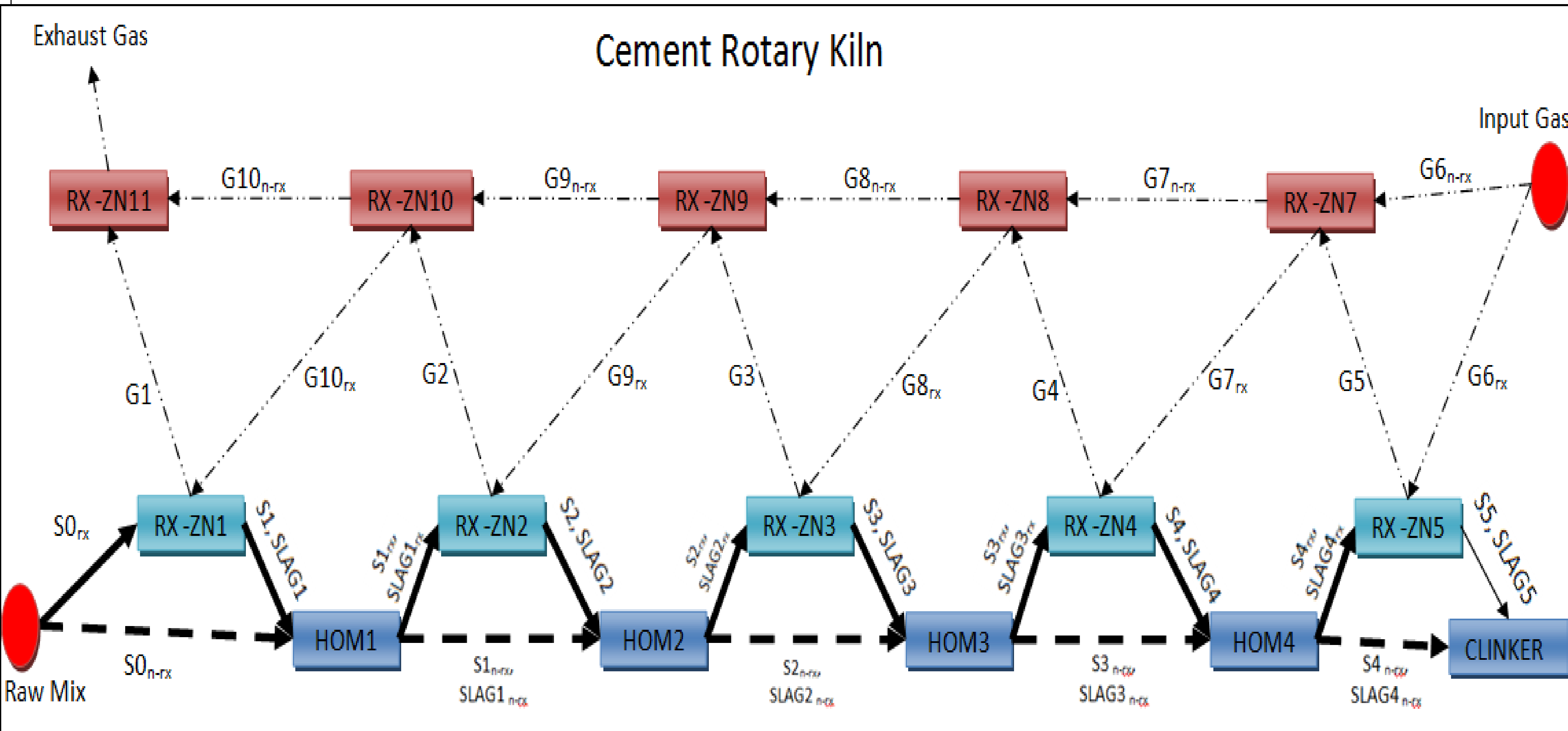
- Two primary research papers were used as the basis for the design and initial conditions:
  - *Modelling trace and alkali mobilisation in the rotary cement kiln by* Thompson, D. and B.B. Argent
    - Rxn zones
    - Composition of the input solids (raw mix)
    - Initial temperature of the solids
  - *Mathematical modelling of rotary cement kilns by the zone method by* Guruz, H.K. and N. Bac
    - Inlet fuel-gas composition
    - Ratio of fuel and gas to input solids

Design Concept

Further Assumptions:

1. Kinetic factors such as the amount of gas, solid and slag reacting during reactions.
2. Initial gas inlet temperature
3. All reactions are adiabatic
4. The kiln begins operation full of the raw mix and air at 25°C

Process Flowsheet



FactSage Setup

5 rxn's between portion of solids, slag and gas:

- 33 pure solid species were chosen from FactPS or FToxid database
- SlagA was chosen from FToxid
- All pure gas species were chosen from FactPS

5 homogenization rxn's between reacted and non-reacted solids and slags

- 33 pure solid species were chosen from FactPS or FToxid database
- SlagA was chosen from FToxid
- All pure gas species were chosen from FactPS, but no gas forms. This allows for the equilibrium calculations to consider ferrous and ferric species which would cause the model to crash if not incorporated.

5 homogenization rxn's between reacted and non-reacted gas

- All pure gas species were chosen from FactPS (160 species).

FactSage Setup

#	Species	Database	Name
1	MgO(s)	FToxid	periclase
2	Al2O3(s4)	FToxid	corundum(alpha)
3	SiO2(s)	FToxid	quartz(l)
4	SiO2(s2)	FToxid	quartz(h)
5	SiO2(s4)	FToxid	tridymite(h)
6	SiO2(s6)	FToxid	cristobalite(h)
7	MgSiO3(s3)	FToxid	proto-enstatite
8	Mg2SiO4(s)	FToxid	forsterite
9	CaO(s)	FToxid	lime
10	CaAl2O4(s)	FToxid	solid
11	CaAl4O7(s)	FToxid	solid
12	CaAl12O19(s)	FToxid	solid
13	Ca3Al2O6(s)	FToxid	solid
14	CaSiO3(s2)	FToxid	ps-wollastonite
15	Ca2SiO4(s)	FToxid	gamma(olivine)
16	Ca2SiO4(s2)	FToxid	alpha-prime
17	Ca2SiO4(s3)	FToxid	alpha
18	Ca3SiO5(s)	FToxid	hatrurite
19	Ca3Si2O7(s)	FToxid	rankinite
20	CaMgSi2O6(s)	FToxid	diopside(cl-py...
21	Ca2MgSi2O7(s)	FToxid	akermanite(meli...
22	Ca3MgSi2O8(s)	FToxid	merwinite
23	CaAl2Si2O8(s2)	FToxid	anorthite
24	Ca2Al2SiO7(s)	FToxid	gehlenite
25	Fe2O3(s)	FToxid	hematite
26	CaFe2O4(s)	FToxid	solid
27	Ca2Fe2O5(s)	FToxid	solid
28	MgAl2O4(s)	FactPS	spinel
29	Al6Si2O13(s)	FactPS	mullite
30	CaOMgOSiO2(s)	FactPS	monticellite
31	Fe3O4(s)	FactPS	magnetite
32	FeAl2O4(s)	FactPS	hercynite
33	CaFe4O7(s)	FToxid	solid

FactSage Setup – Screen Shot Examples

Writing the Macro-Code

1. **Time 0**
   a. Initialization of input solids stream (raw mix) at T= 650°C,
      i. save SOLIDS stream as **S0-S4**
      ii. save FToxid-SlagA#1 as **SLAG1-SLAG4**
      iii. output S0 composition
   b. Initialization of input gas stream (gas burner) at T= X ,
      i. save GAS stream as **G6**
      ii. Output gas stream composition
   c. Initialization of input gas stream (gas burner) at T= 25°C ,
      i. save GAS stream as **G7-G10**

Writing the Macro-Code

2. **Time 1-X (LOOP ON THIS)**
   a. RX_ZN5: react <E>S4 +<E>SLAG4+ <G>G6
      i. save the solids stream as S5
      ii. save the FToxid-SlagA#1 as SLAG5
      iii. save the gas stream as G5
   b. Homogenize <100%>S5 + <1-D> S4 <100%>SLAG5 + <1-D> SLAG4
      i. output composition of clinker
   c. RX_ZN4: react <D>S3 +<D>SLAG3+ <G>G7
      i. save the solids stream as S4
      ii. save the FToxid-SlagA#1 as SLAG4
      iii. save the gas stream as G4
   d. Homogenize <100%>S4 + <1-D> S3+ <100%>SLAG4 + <1-D> SLAG3
      i. save as S4 and SLAG4
      ii. output composition
   e. RX_ZN3: react <C>S2 +<C>SLAG2+ <G>G8
      i. save the solids stream as S3
      ii. save the FToxid-SlagA#1 as SLAG3
      iii. save the gas stream as G3

Writing the Macro-Code

1. **Time 1-X (LOOP ON THIS) Continued**
   f. Homogenize <100%>S3 + <1-C> S2+ <100%>SLAG3 + <1-C> SLAG2
      i. save as S3 and SLAG3
      ii. output composition
   g. RX_ZN2: react <B>S1 +<B>SLAG1+ <G>G9
      i. save the solids stream as S2
      ii. save the FToxid-SlagA#1 as SLAG2
      iii. save the gas stream as G2
   h. Homogenize <100%>S2 + <1-B> S1+ <100%>SLAG2 + <1-B> SLAG1
      i. save as S2 and SLAG2
      ii. output composition
   i. RX_ZN1: react <A>S0 + <G>G10
      i. save the solids stream as S1
      ii. save the FToxid-SlagA#1 as SLAG1
      iii. save the gas stream as G1

Writing the Macro-Code

1. **Time 1-X (LOOP ON THIS) Countinued**
    - j. Homogenize <100%>S1 + <1-A> S0+ <100%>SLAG1
        - i. save as S1 and SLAG1
        - ii. output composition
    - k. RX_Z11: react <100%>G1 and <1-G>G10
        - i. output EXHAUST GAS composition
    - l. RX_ZN10: react <100%>G2 + <1-G>G9
        - i. Save homogenized gas stream as G10
    - m. RX_ZN9: react <100%>G3 + <1-G>G8
        - i. Save homogenized gas stream as G9
    - n. RX_ZN8: react <100%>G4 + <1-G>G7
        - i. Save homogenized gas stream as G8
    - o. RX_ZN7: react <100%>G5 + <1-G>G6
        - i. Save homogenized gas stream as G7

Results from the Simulation

1. The slides in the following sections show attempts to simulate the temperature and correct compositional results from the original paper this simulation was based on.

2. Only three attempts are shown but several others sets of parameter were attempted and the data can be found in the files provided.

Excel Outputs for each attempt include:

- Output composition of solids after each reaction zone
- Output gas composition
- Temperature profiles of all homogenizations zones

Attempt 1 – Excel Inputs (literature values with elevated gas temperature for alite formation in clinker zone constant kinetics)

Raw Mix						
CaO	SiO2	Al2O3	Fe2O3	MgO	Total	Temp (°C)
69.0%	21.0%	5.0%	3.5%	1.5%	100%	650
111455.7	33921.3	8076.5	5653.55	2422.95	161530	Grams

Fuel			Gas		
C	H	S	N2	O2	Temp (°C)
83.50%	13.50%	3.00%	79%	21%	2500
13318.04	2153.216	478.4924503	7577.582	2014.294	grams
	Total		Total		
	100%		100%		
	15949.75		9591.876		

Gas		Temp
N2	O2	25
79%	21%	
7577.582	2014.294	grams
Total		
100%		
9591.876		

Duration of Start-up
150

Ratio of Fuel to Raw Mix	0.098742
Ratio of Air to Raw Mix	0.059381

S4 React	S4 Nonreact
50%	50%

S3 React	S3 Nonreact
50%	50%

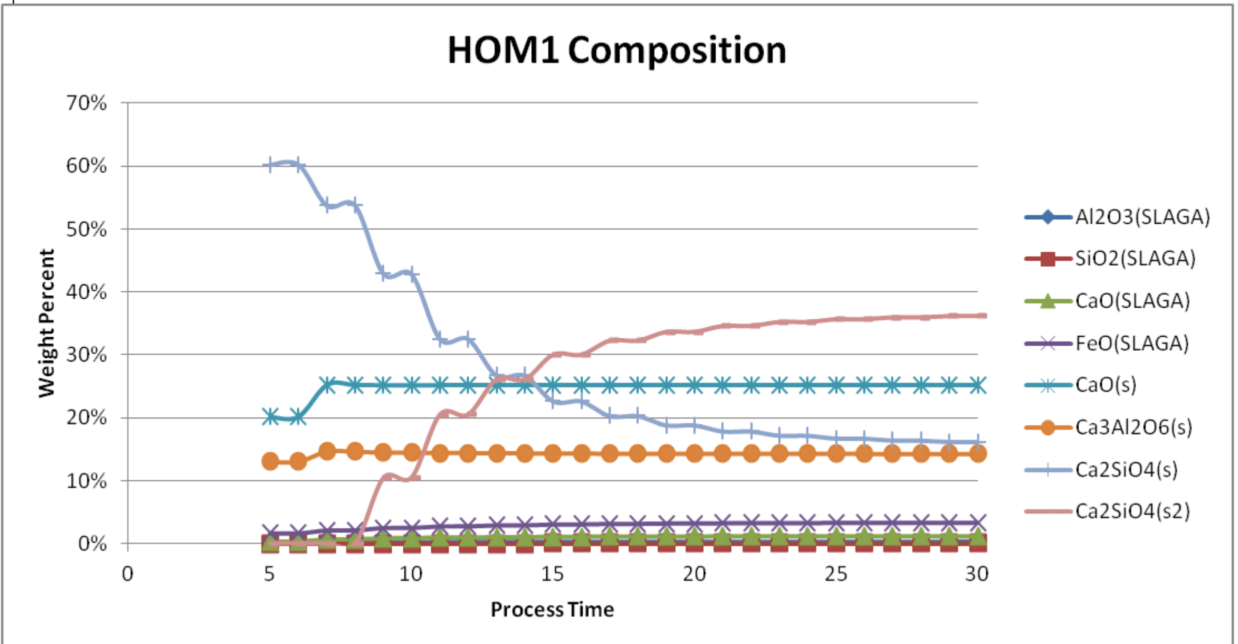
S2 React	S2 Nonreact
50%	50%

S1 React	S1 Nonreact
50%	50%

S0 React	S0 Nonreact
50%	50%

GAS React	Gas Nonreact
50%	50%

Change in Composition from ZN1 to ZN2



Start Temp: 631.53 °C

S.S. Temp: 834.86 °C

Overall Composition:

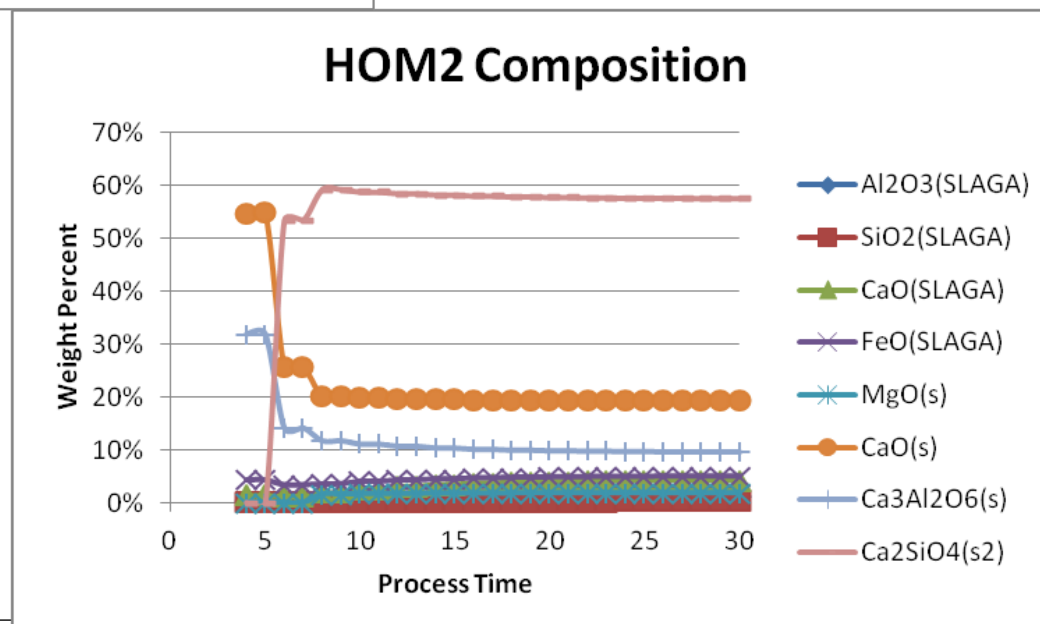
C=	69.36%
S=	18.30%
A=	5.68%

Start Temp: 631.53 °C

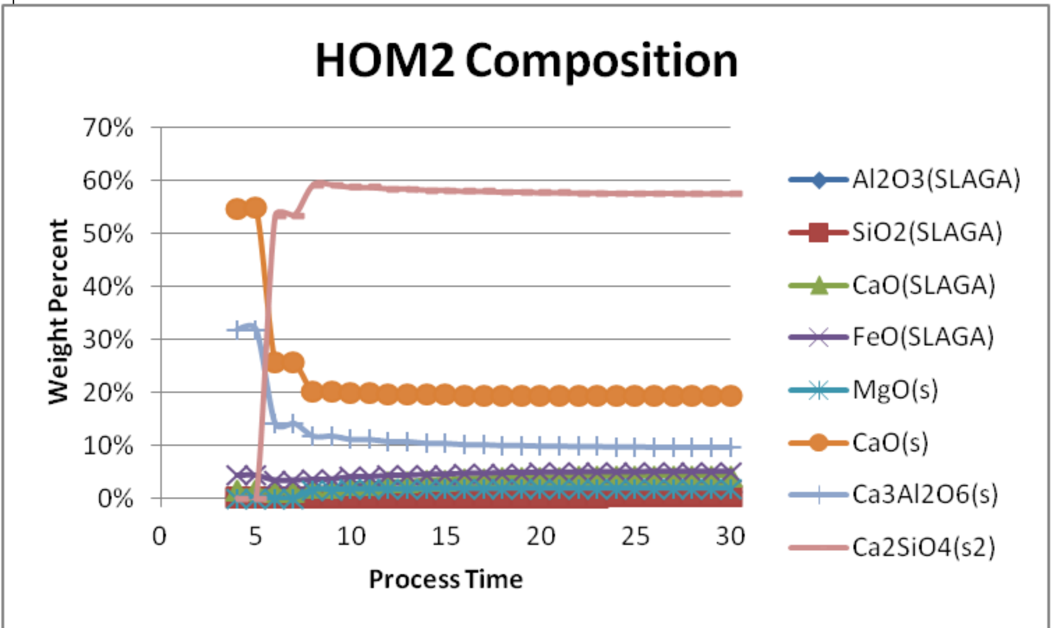
S.S. Temp: 1015.64 °C

Overall Composition:

C=	66.95%
S=	20.38%
A=	4.85%



Change in Composition from ZN2 to ZN3



Start Temp: 631.53 °C
S.S. Temp: 1015.64 °C

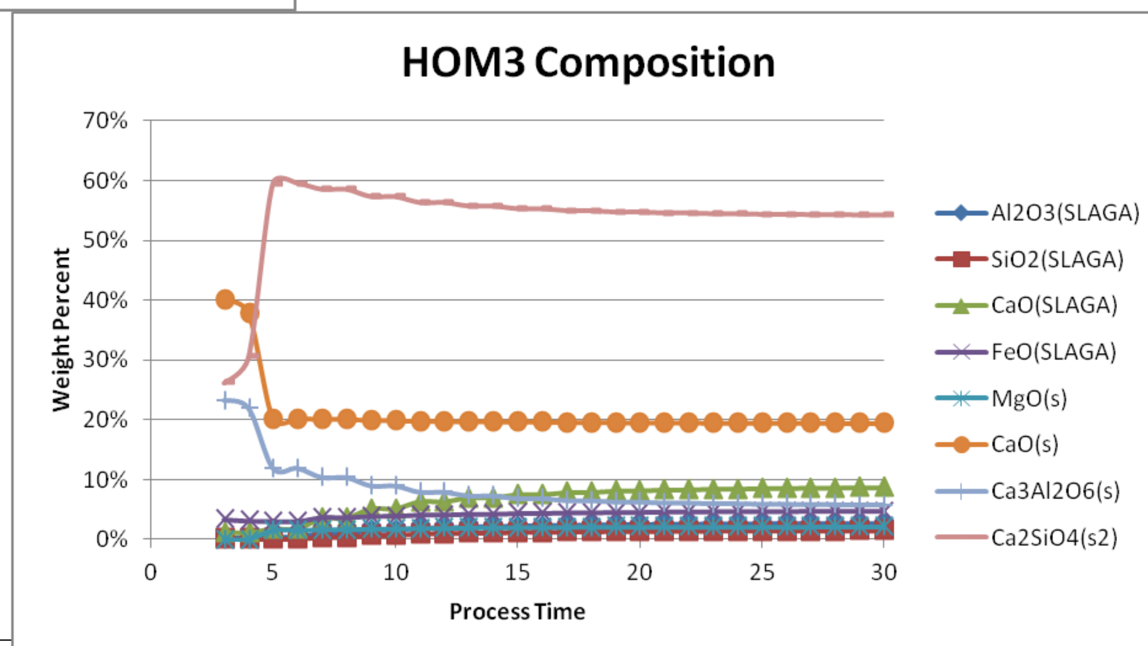
Overall Composition:

C=	66.95%
S=	20.38%
A=	4.85%

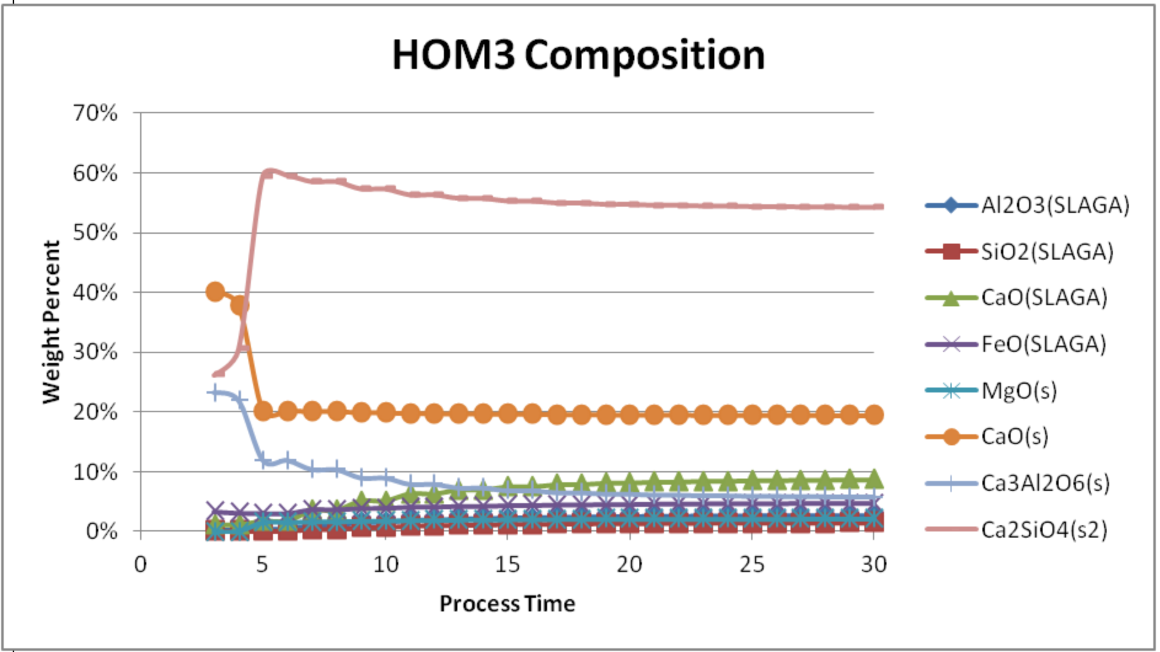
Start Temp: 631.53 °C
S.S. Temp: 1155.06 °C

Overall Composition:

C=	67.08%
S=	20.42%
A=	4.85%



Change in Composition from ZN3 to ZN4



Start Temp: 631.53 °C

S.S. Temp: 1155.06 °C

Overall Composition:

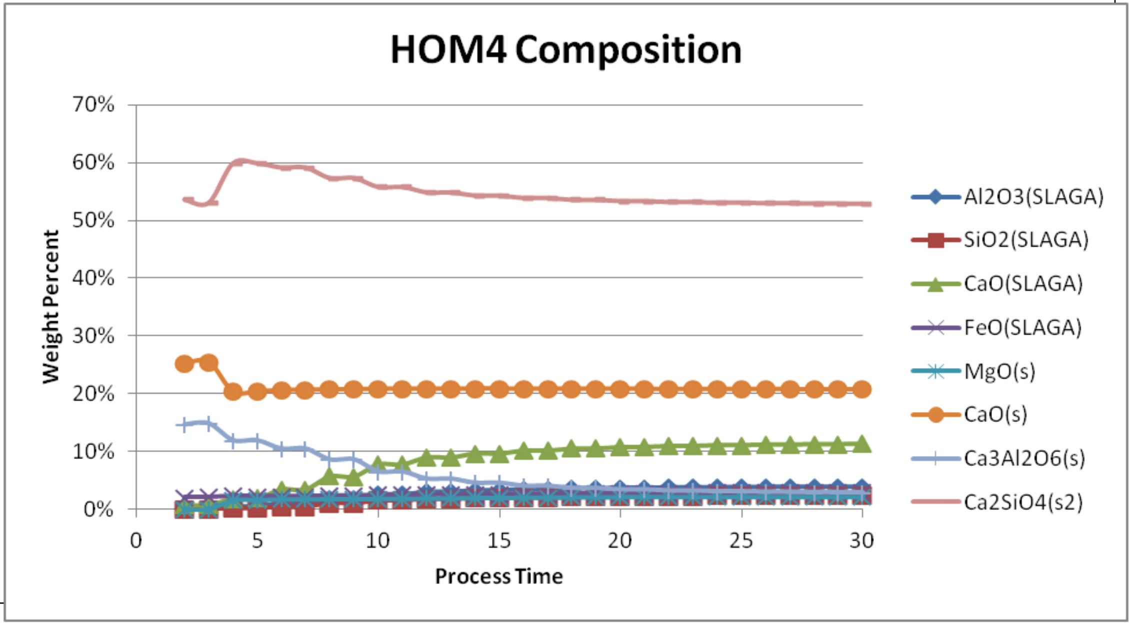
C=	67.08%
S=	20.42%
A=	4.85%

Start Temp: 631.53 °C

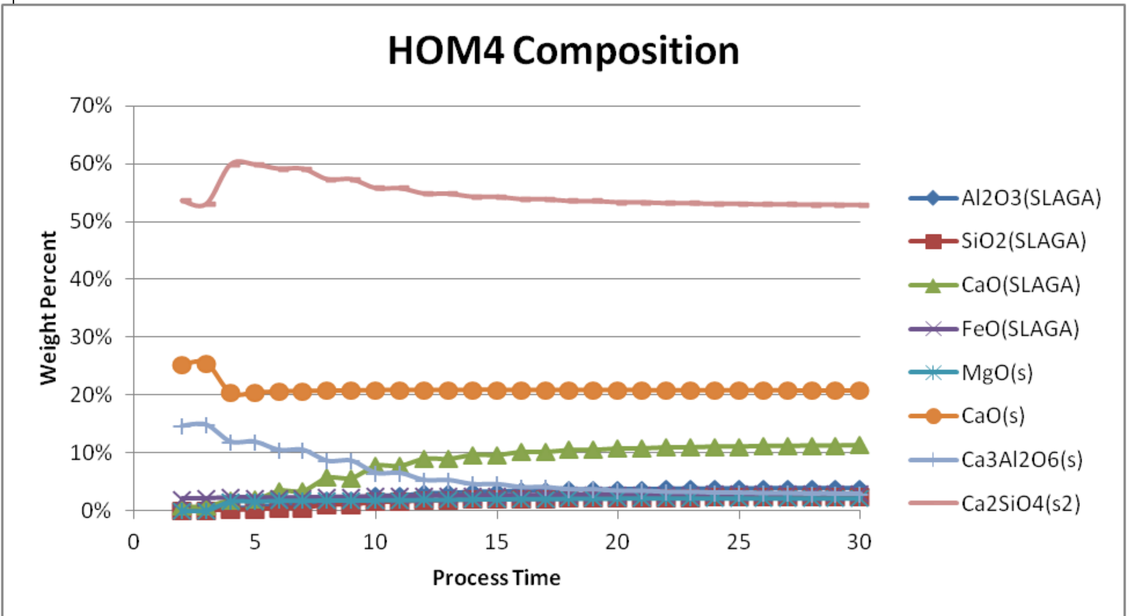
S.S. Temp: 1261.67 °C

Overall Composition:

C=	68.32%
S=	20.79%
A=	4.92%



Change in Composition from ZN4 to ZN5



Start Temp: 631.53 °C

S.S. Temp: 1261.67 °C

Overall Composition:

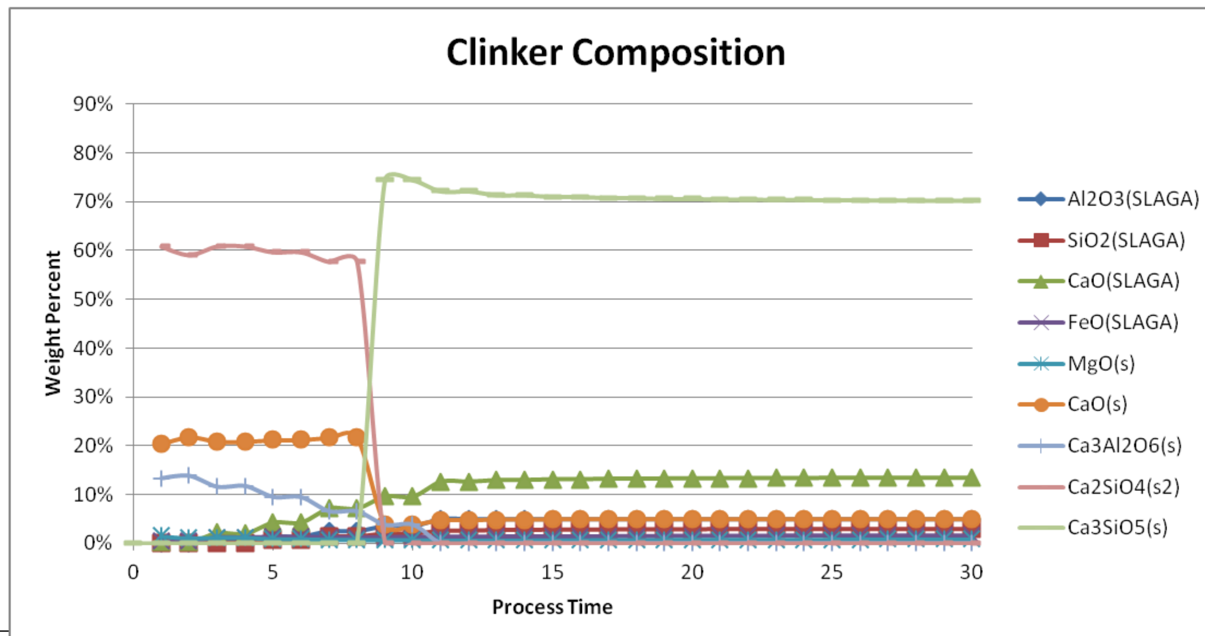
C=	68.32%
S=	20.79%
A=	4.92%

Start Temp: 900.26 °C

S.S. Temp: 1344.62 °C

Overall Composition:

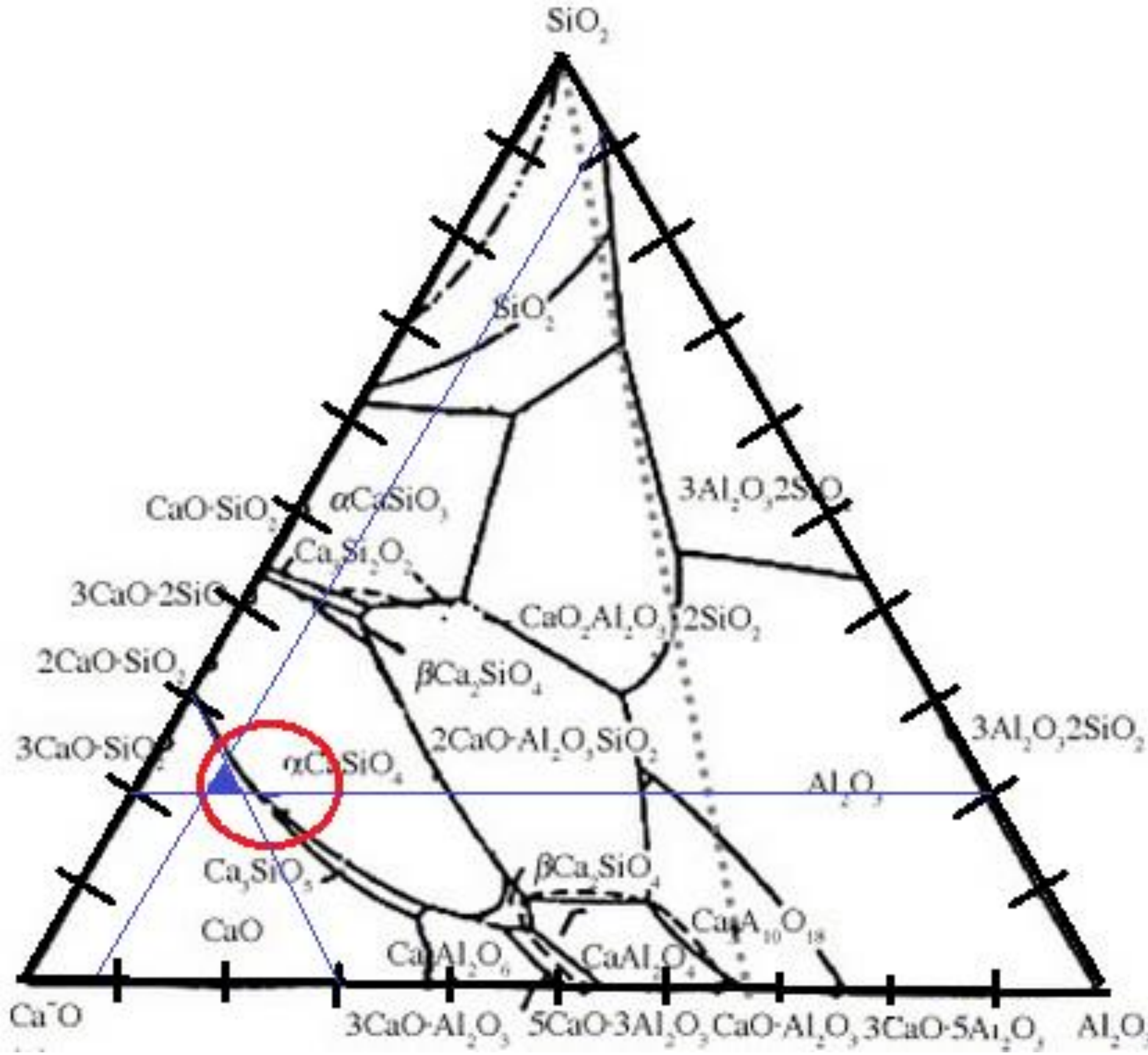
C=	70.06%
S=	21.35%
A=	5.01%



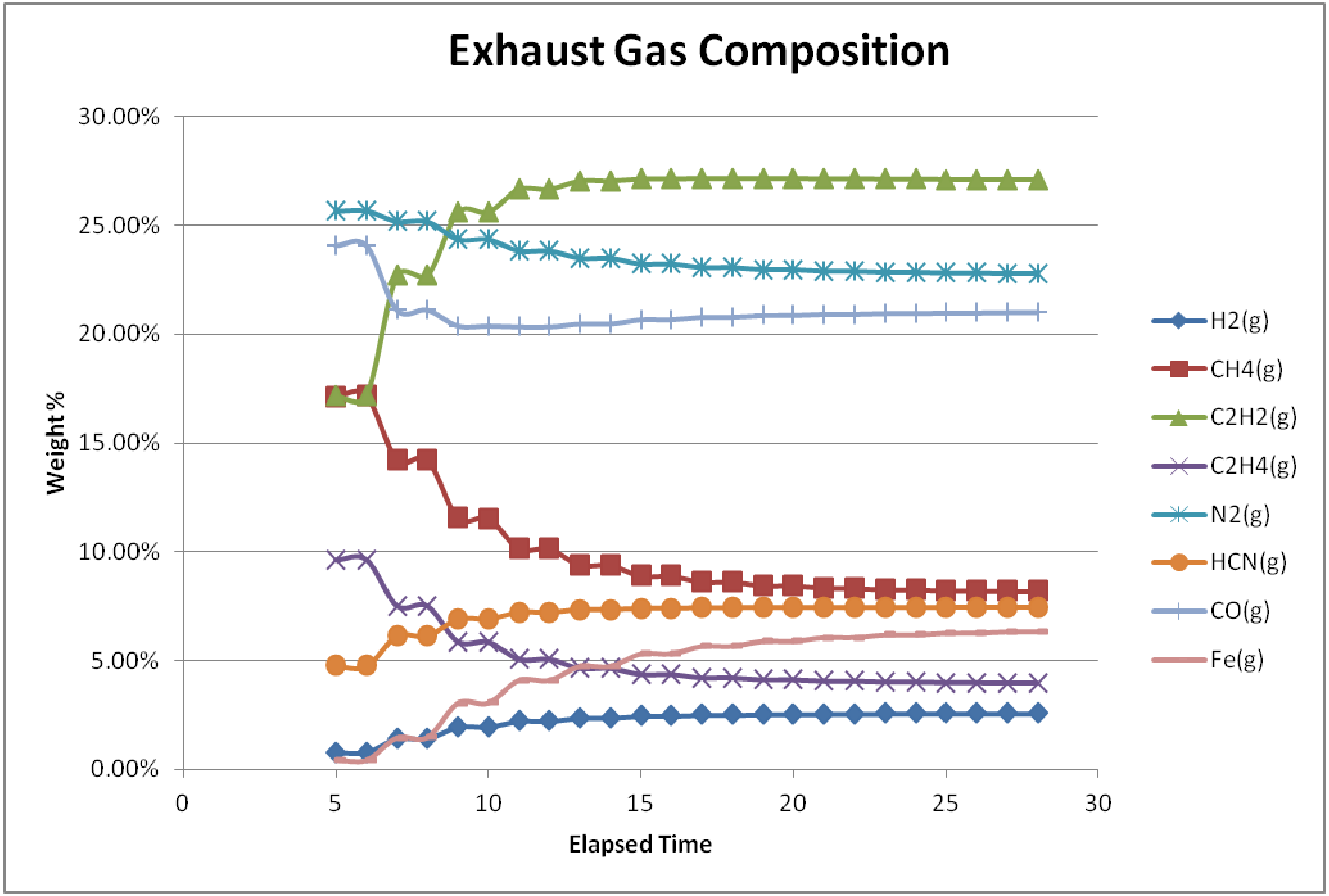
CaO-SiO2-Al2O3 Ternary Phase Diagram

Final Composition:

C=	70.06%
S=	21.35%
A=	5.01%



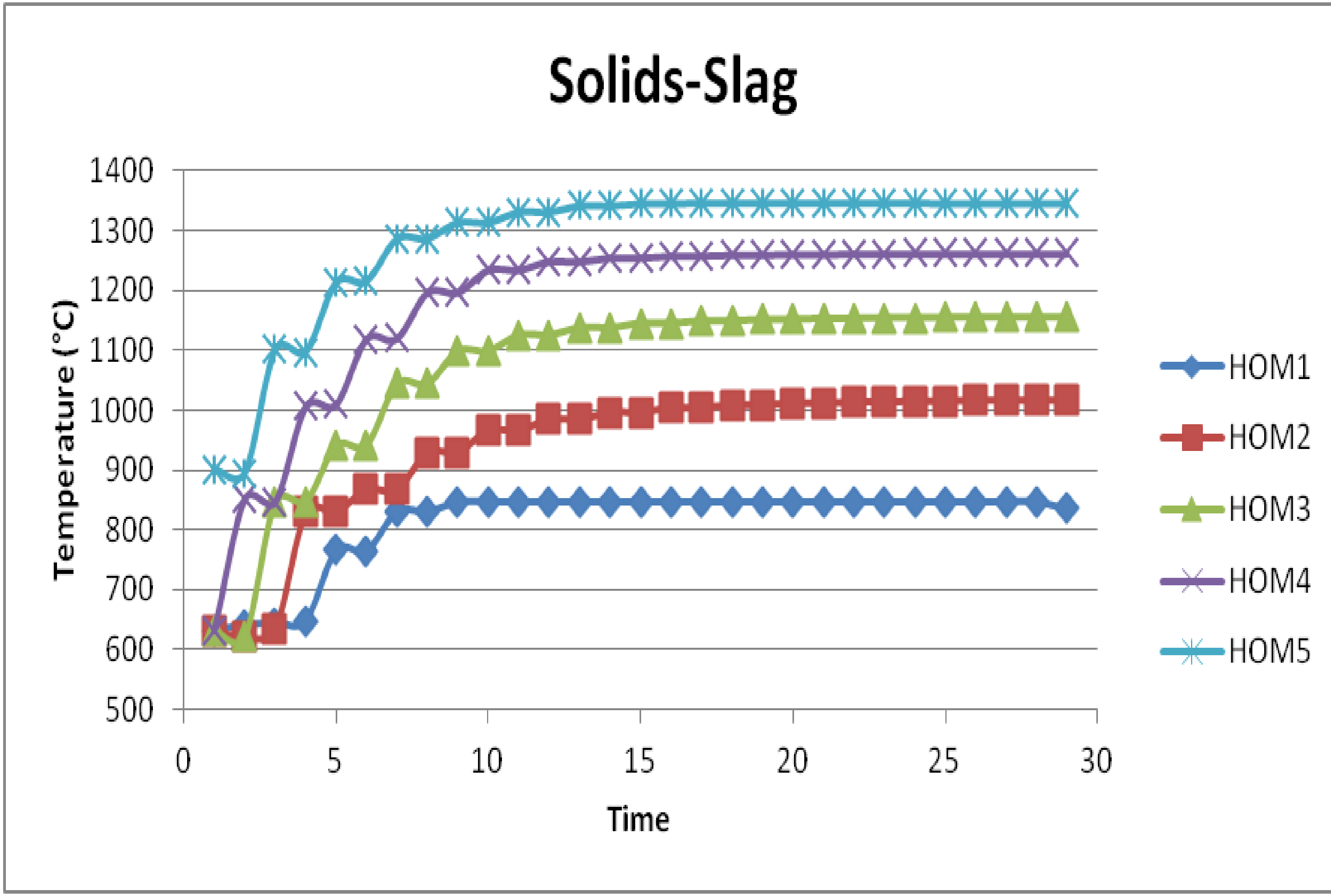
Exhaust Gas Composition



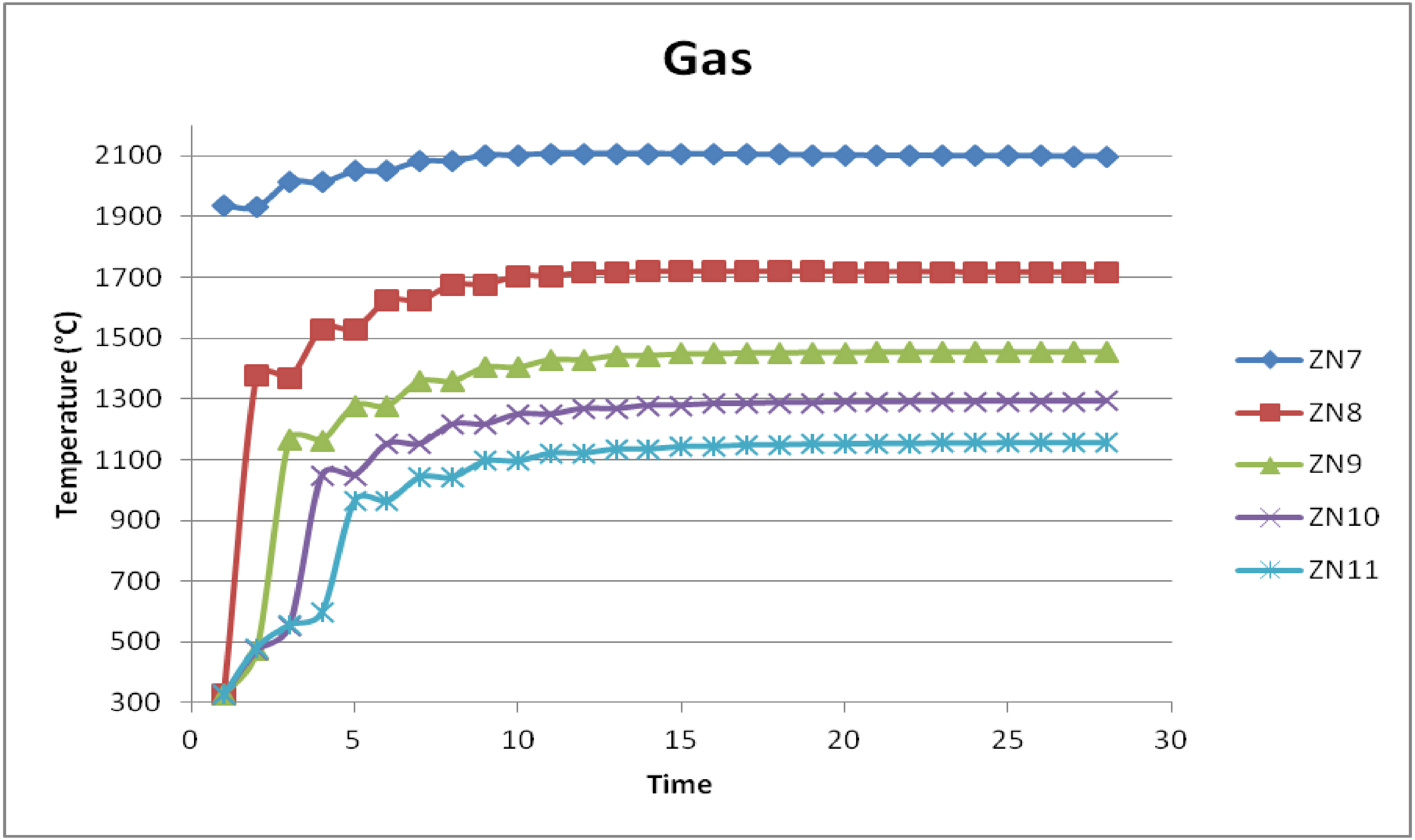
Start Temp: 327.59 °C

S.S. Temp: 1157.35 °C

Temperature Profiles



Temperature Profiles



Attempt 1 Discussion

- The presence of alite (Ca_3SiO_5) was found in the clinker as required.
- The inlet gas temperature is relatively high at 2500 °C
- The exhaust gas composition has HCN and other species forming which are not ideal and are not representative of actual exhaust gas composition in practice. This is likely due to high fuel to air ratio.
- The next attempt tries to fix the gas issue and form alite with lower fuel consumption but increased kinetics and increased ratio of air.

Attempt 2 – Excel Inputs (lower gas temperature with increasing kinetics, more hot air, but less fuel)

Raw Mix						
CaO	**SiO2**	**Al2O3**	**Fe2O3**	**MgO**	**Total**	**Temp (°C)**
69.0%	21.0%	5.0%	3.5%	1.5%	1	650
69000	21000	5000	3500	1500	100000	Grams

Fuel			Gas		
C	**H**	**S**	**N2**	**O2**	**Temp (°C)**
83.50%	13.50%	3.00%	79%	21%	2000
4175	675	150	11850	3150	grams
	Total		**Total**		
	100%		100%		
	5000		15000		

Gas		Temp
N2	**O2**	25
79%	21%	
11850	3150	
Total		
100%		
15000		

Duration of Start-up
150

Ratio of Raw Mix to Fuel	**0.05**
Ratio of Raw Mix to Air	**0.15**

S4 React	S4 Nonreact
50%	50%

S3 React	S3 Nonreact
55%	45%

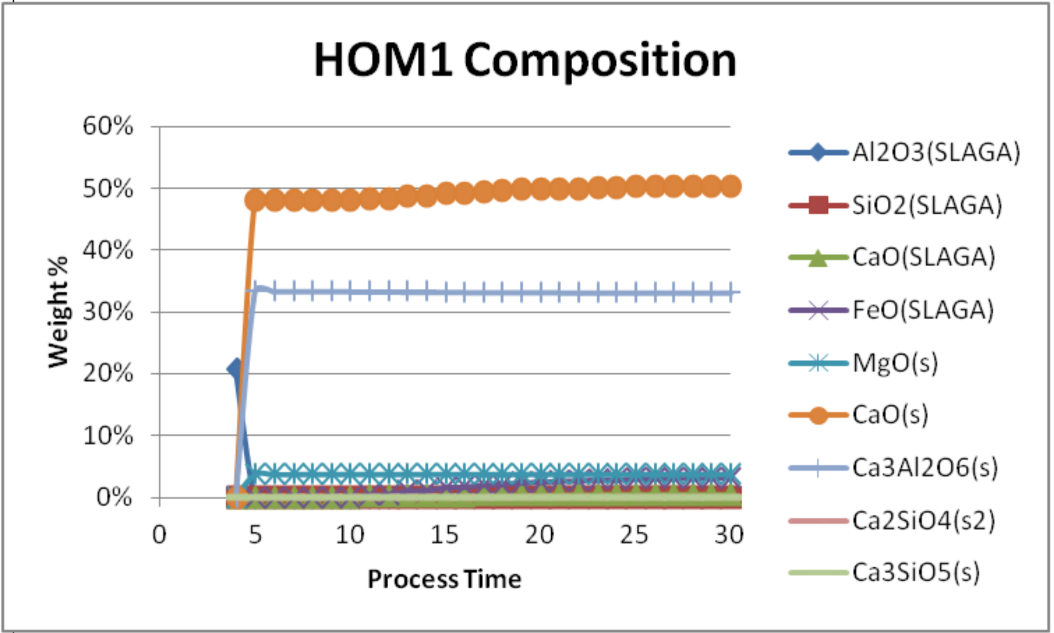
S2 React	S2 Nonreact
60%	40%

S1 React	S1 Nonreact
65%	35%

S0 React	S0 Nonreact
70%	30%

GAS React	Gas Nonreact
70%	30%

Change in Composition from ZN1 to ZN2



Start Temp: 590 °C
S.S. Temp: 692 °C

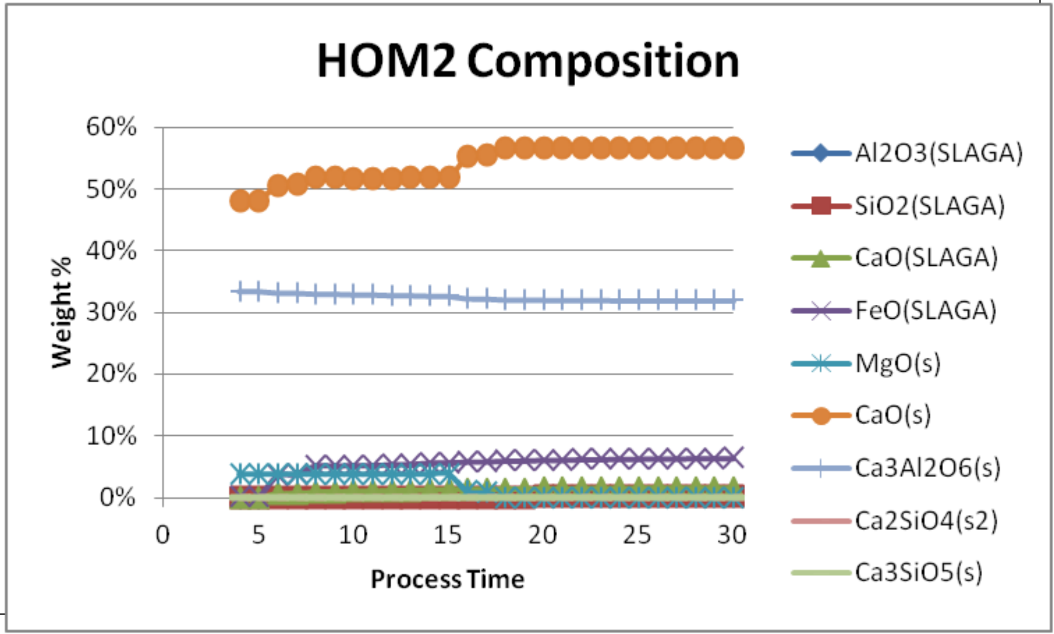
Overall Composition:

C=	71.32%
S=	0.00%
A=	12.53%

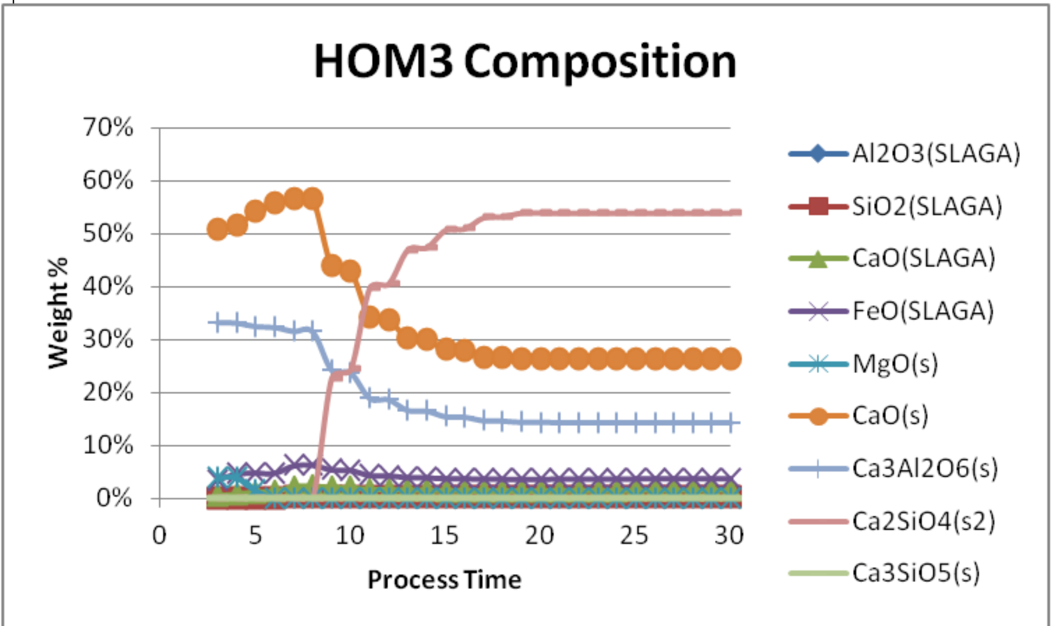
Start Temp: 590 °C
S.S. Temp: 781 °C

Overall Composition:

C=	78.07%
S=	0.04%
A=	12.41%



Change in Composition from ZN3 to ZN4



Start Temp: 592 °C

S.S. Temp: 861 °C

Overall Composition:

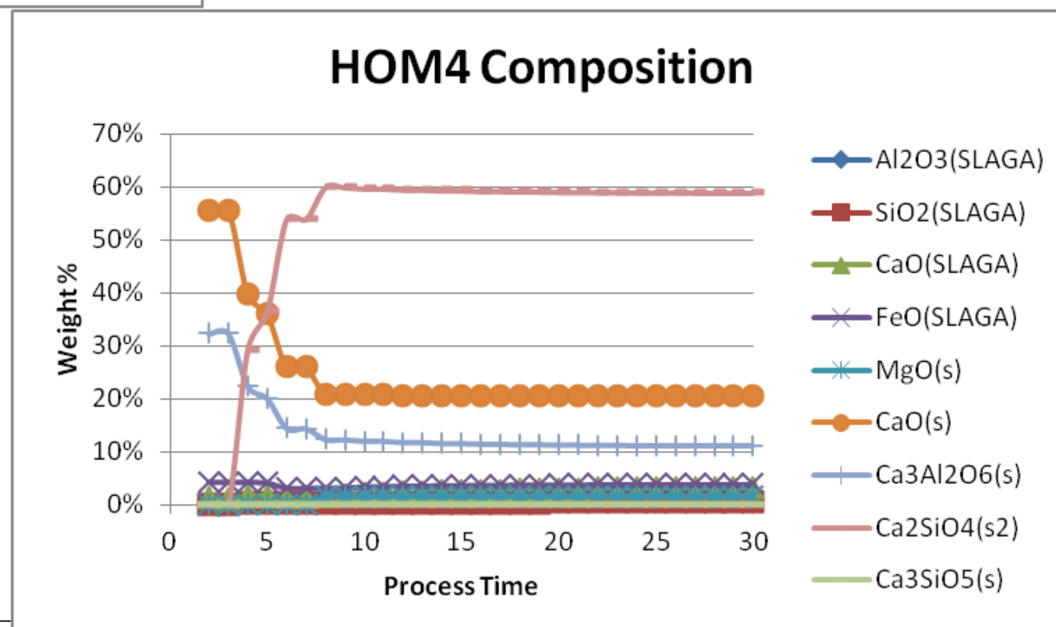
C=	71.35%
S=	18.82%
A=	5.69%

Start Temp: 592 °C

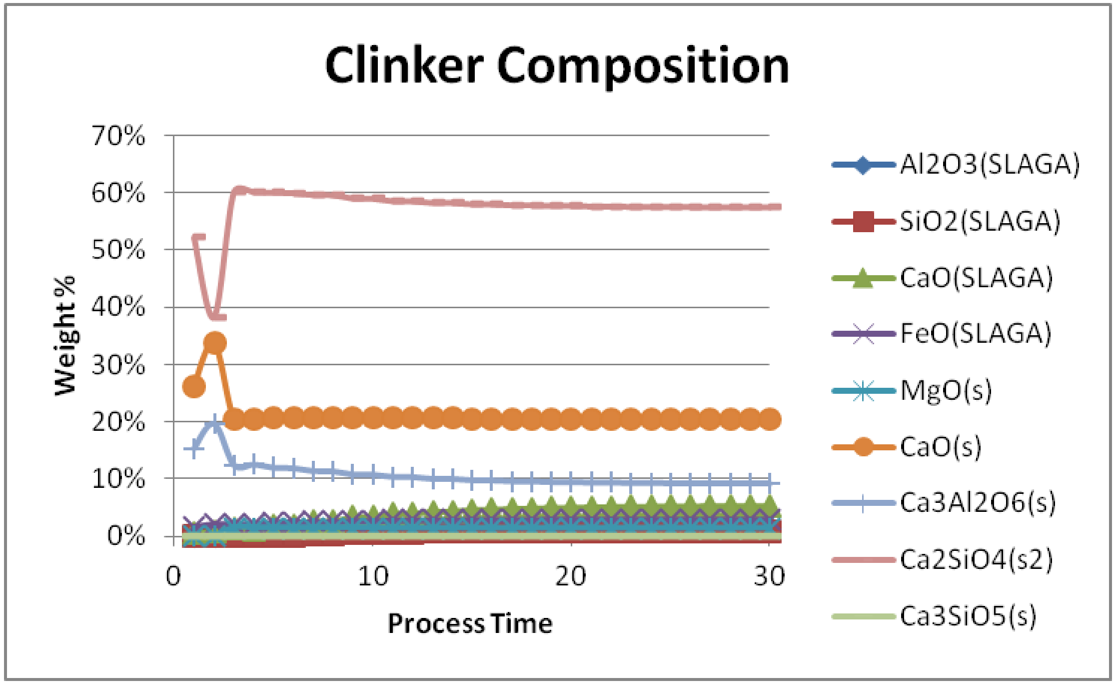
S.S. Temp: 1009 °C

Overall Composition:

C=	68.55%
S=	20.87%
A=	4.96%



Change in Composition ZN5



Start Temp: 847 °C

S.S. Temp: 1154 °C

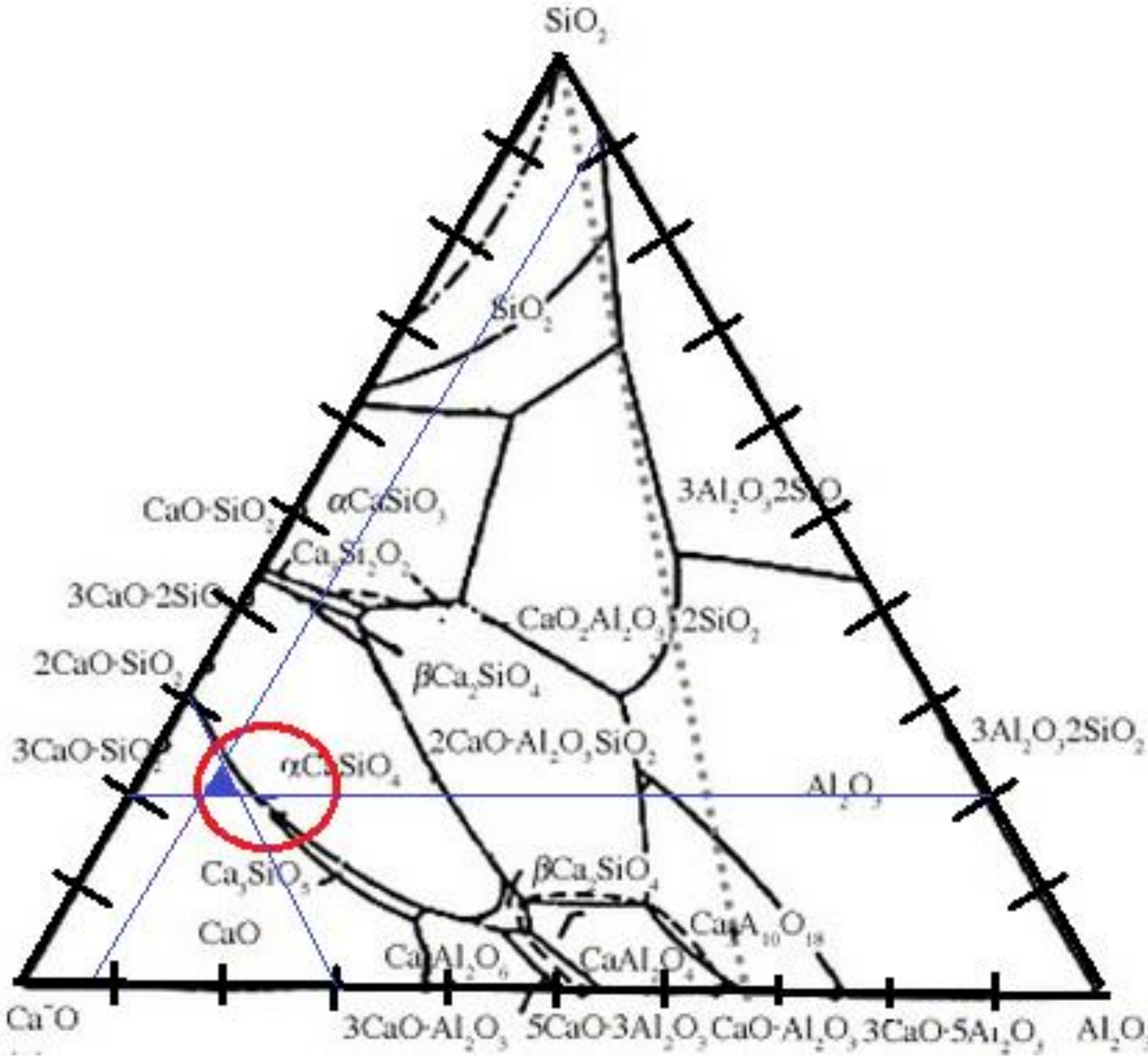
Overall Composition:

C=	69.06%
S=	21.03%
A=	4.98%

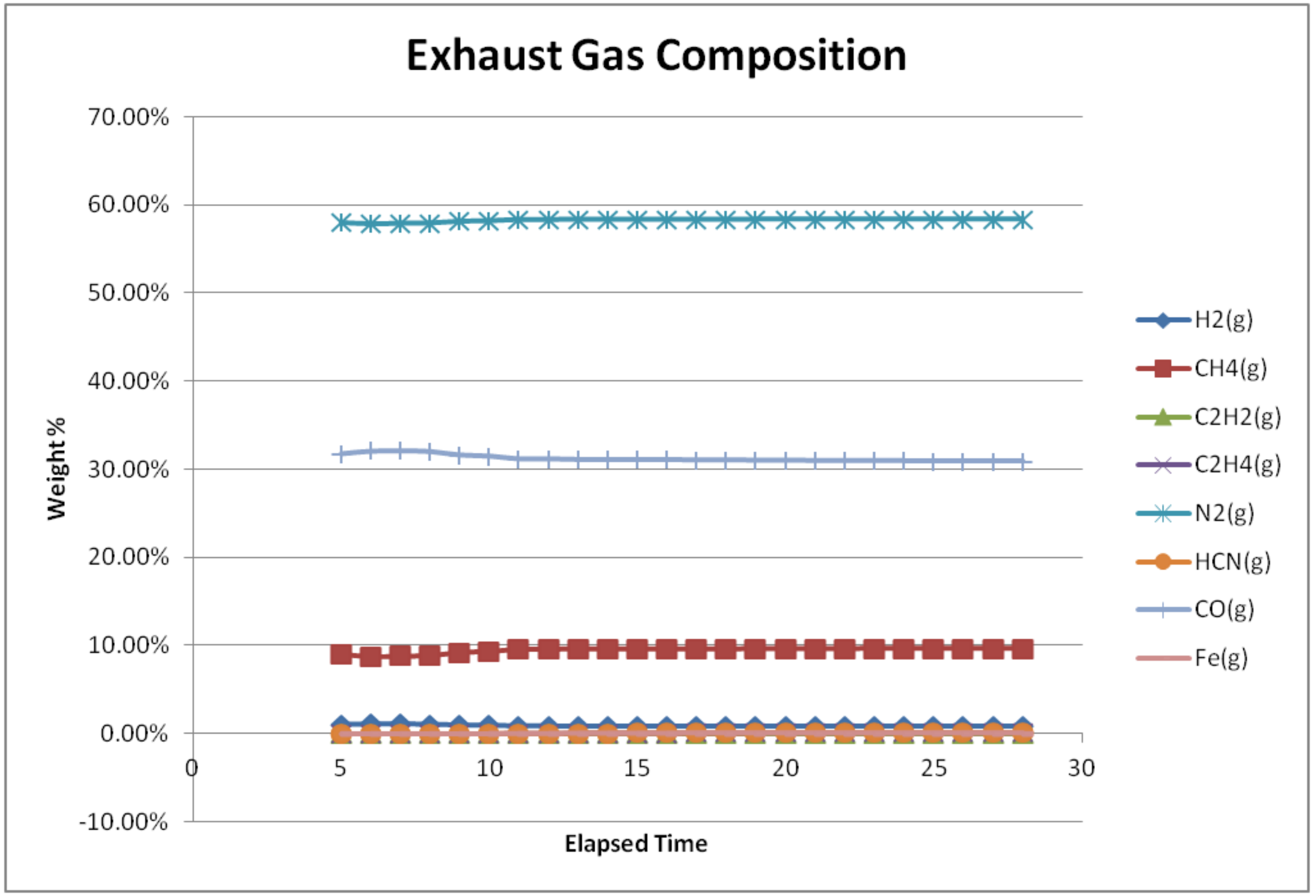
CaO-SiO2-Al2O3 Ternary Phase Diagram

Final Composition:

C=	69.06%
S=	21.03%
A=	4.98%

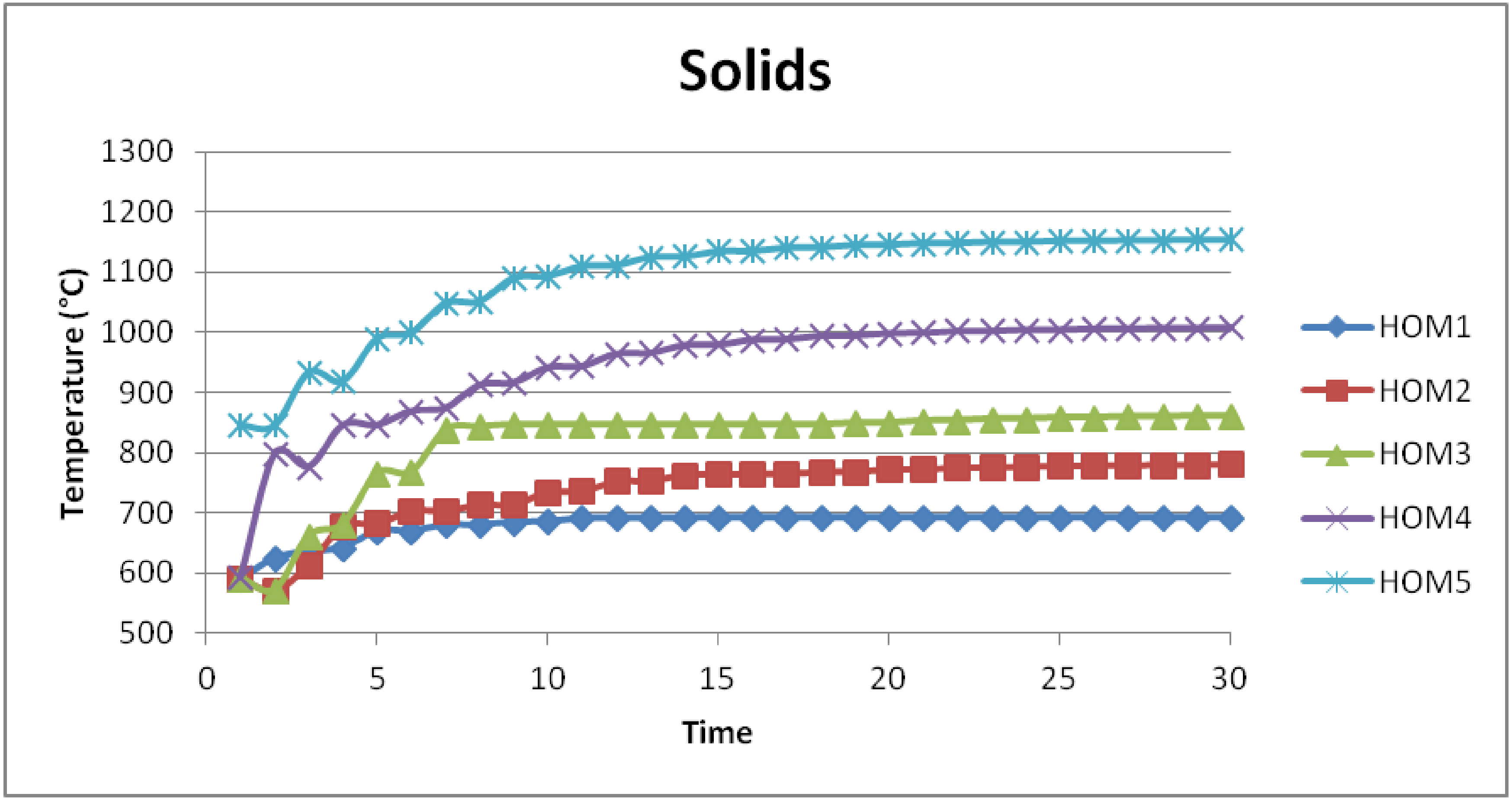


Exhaust Gas Composition

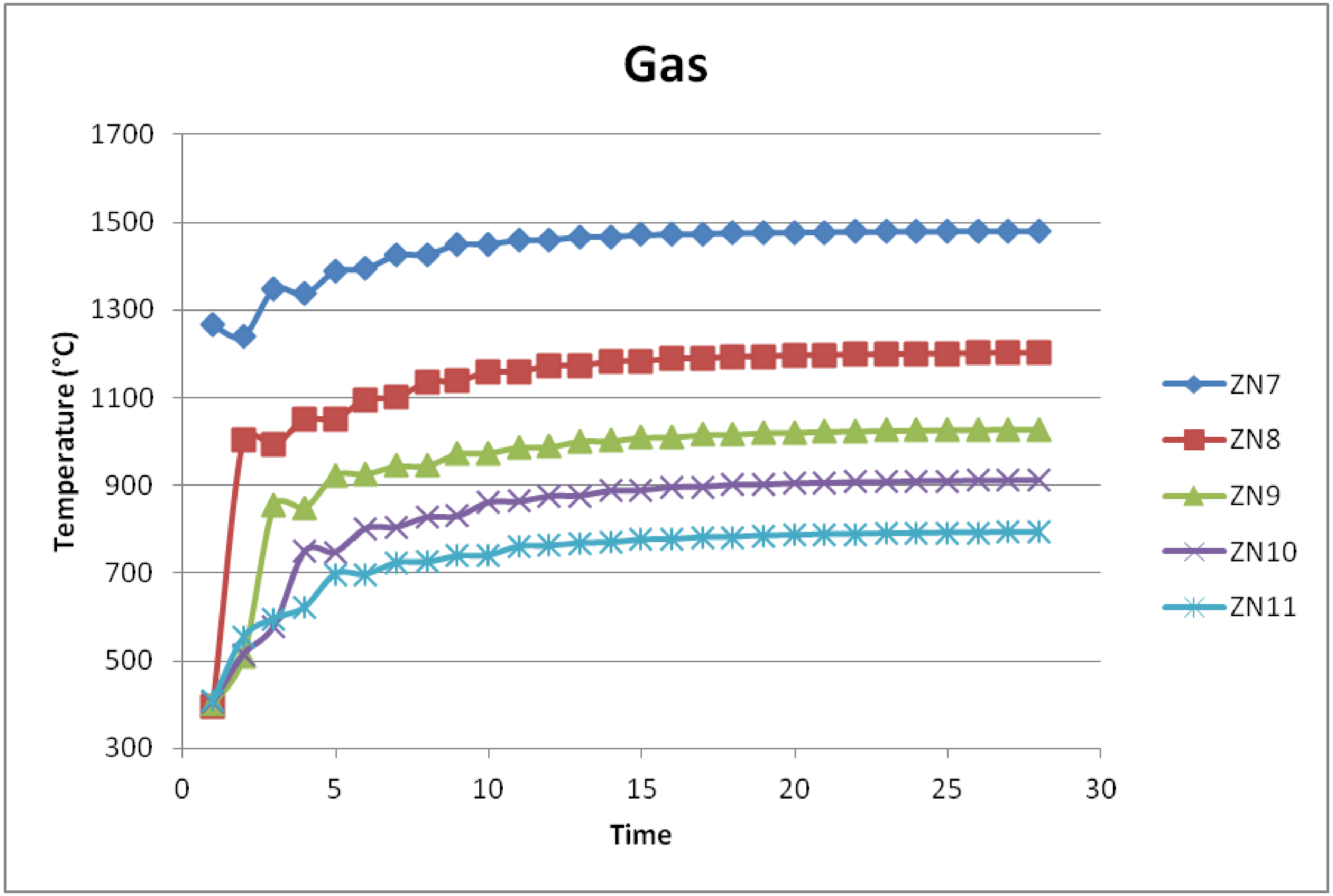


Start Temp: 408 °C
S.S. Temp: 793 °C

Temperature Profiles



Temperature Profiles



Attempt 2 Discussion

- The presence of alite (Ca_3SiO_5) was not found in the clinker as is required. Alite forms at approximately 1300 °C
- The inlet gas temperature was lower at 2000 °C
- The issue of HCN formation was corrected by decreasing the amount of fuel and increasing the amount of air. The exhaust gas composition is close to the industry composition at 58% N_2, 31% CO and 10% CH_4, 1% others.
- The next attempt tries to again form alite while keeping the corrected exhaust gas temperature.

Attempt 3 – Excel Inputs (same as attempt 2, but with higher gas temperature)

Raw Mix						
CaO	**SiO2**	**Al2O3**	**Fe2O3**	**MgO**	**Total**	**Temp (°C)**
69.0%	21.0%	5.0%	3.5%	1.5%	1	650
69000	21000	5000	3500	1500	100000	Grams

Fuel			Gas		
C	**H**	**S**	**N2**	**O2**	**Temp (°C)**
83.50%	13.50%	3.00%	79%	21%	2500
4175	675	150	11850	3150	grams
	Total		**Total**		
	100%		100%		
	5000		15000		

Gas		Temp
N2	**O2**	25
79%	21%	
11850	3150	
Total		
100%		
15000		

Duration of Start-up
150

Ratio of Raw Mix to Fuel	**0.05**
Ratio of Raw Mix to Air	**0.15**

S4 React	S4 Nonreact
50%	50%

S3 React	S3 Nonreact
55%	45%

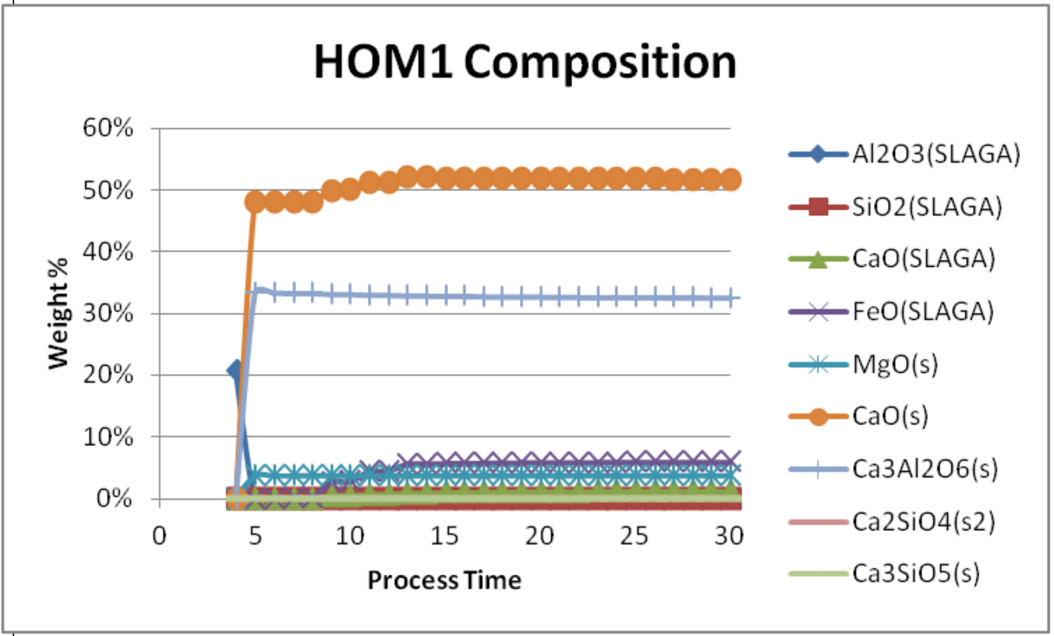
S2 React	S2 Nonreact
60%	40%

S1 React	S1 Nonreact
65%	35%

S0 React	S0 Nonreact
70%	30%

GAS React	Gas Nonreact
70%	30%

Change in Composition from ZN1 to ZN2



Start Temp: 590 °C
S.S. Temp: 746 °C

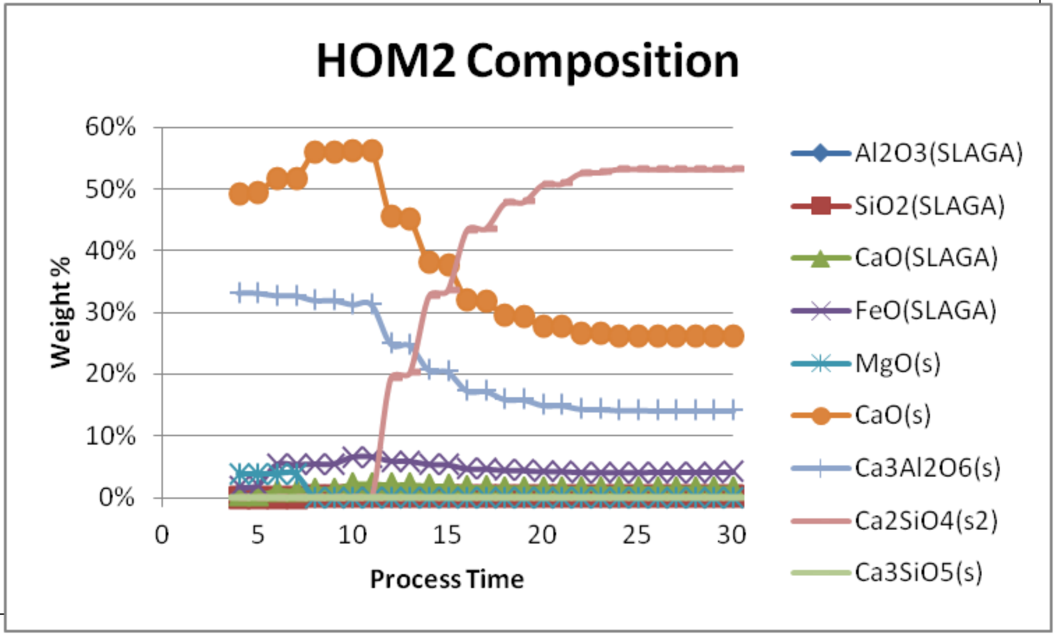
Overall Composition:

C=	73.13%
S=	0.02%
A=	12.56%

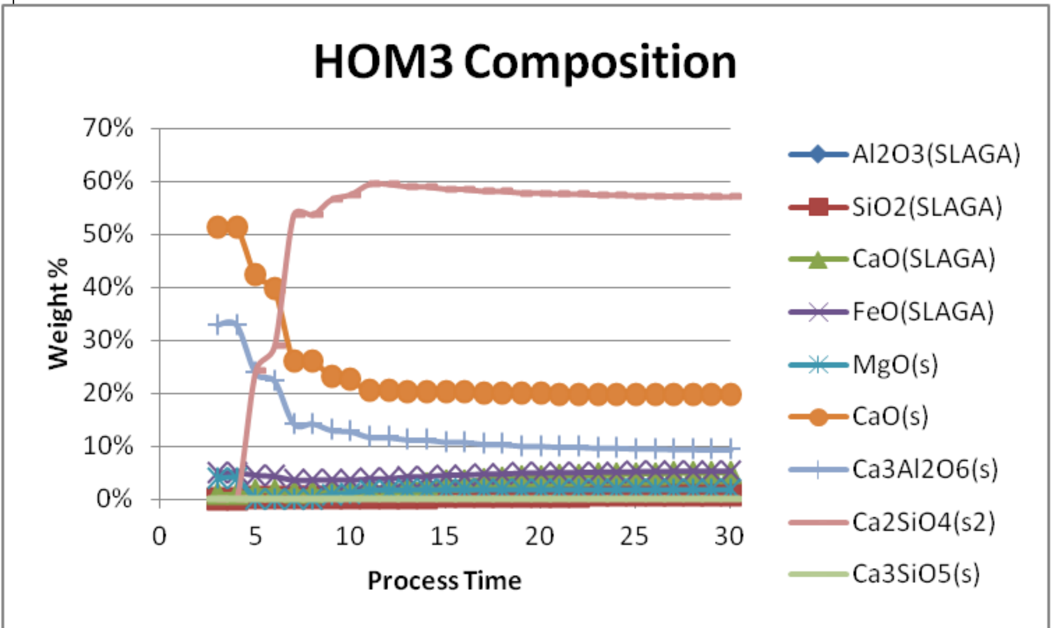
Start Temp: 590 °C
S.S. Temp: 856 °C

Overall Composition:

C=	71.02%
S=	18.59%
A=	5.70%



Change in Composition from ZN3 to ZN4



Start Temp: 592 °C

S.S. Temp: 1042 °C

Overall Composition:

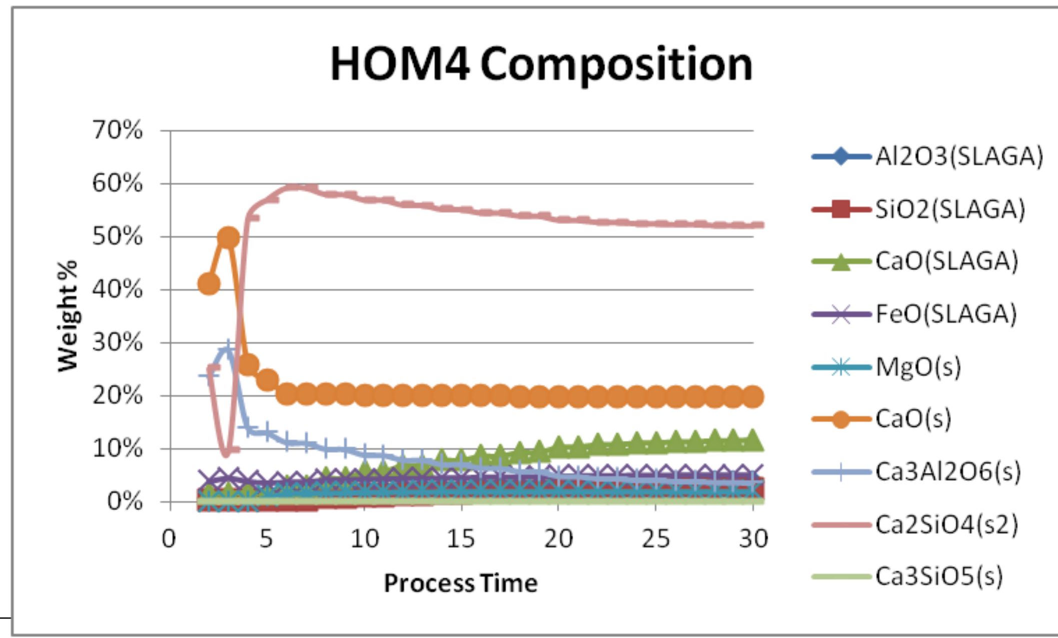
C=	67.44%
S=	20.53%
A=	4.89%

Start Temp: 592 °C

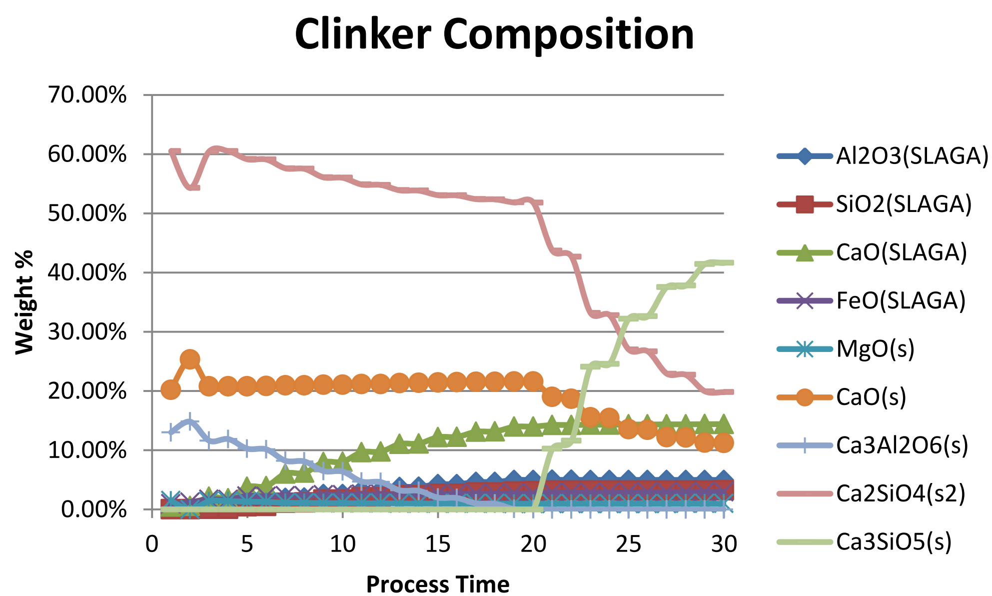
S.S. Temp: 1200 °C

Overall Composition:

C=	67.22%
S=	20.46%
A=	4.86%



Change in Composition ZN5



Start Temp: 904 °C

S.S. Temp: 1300 °C

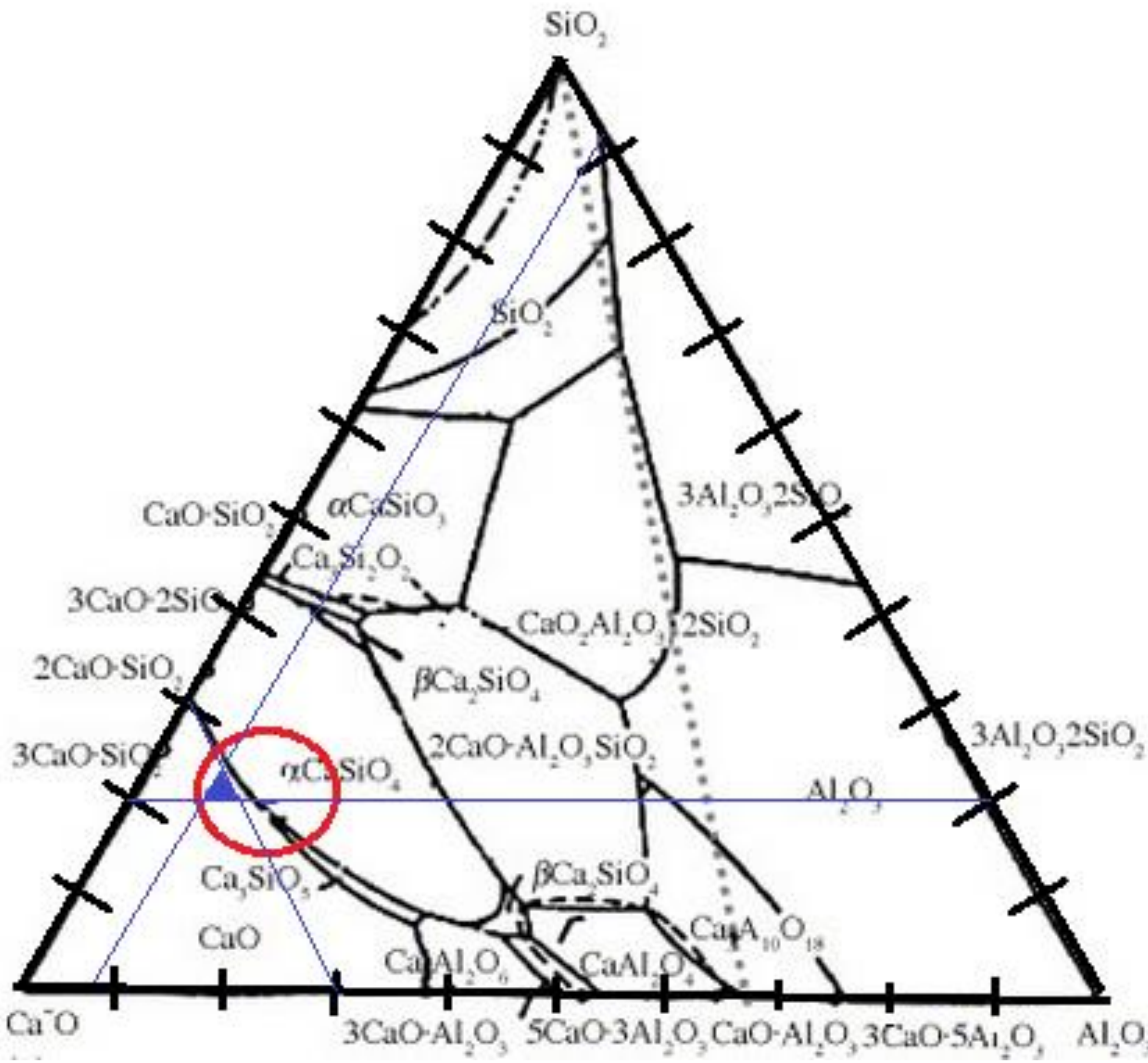
Overall Composition:

C=	69.17%
S=	21.06%
A=	4.98%

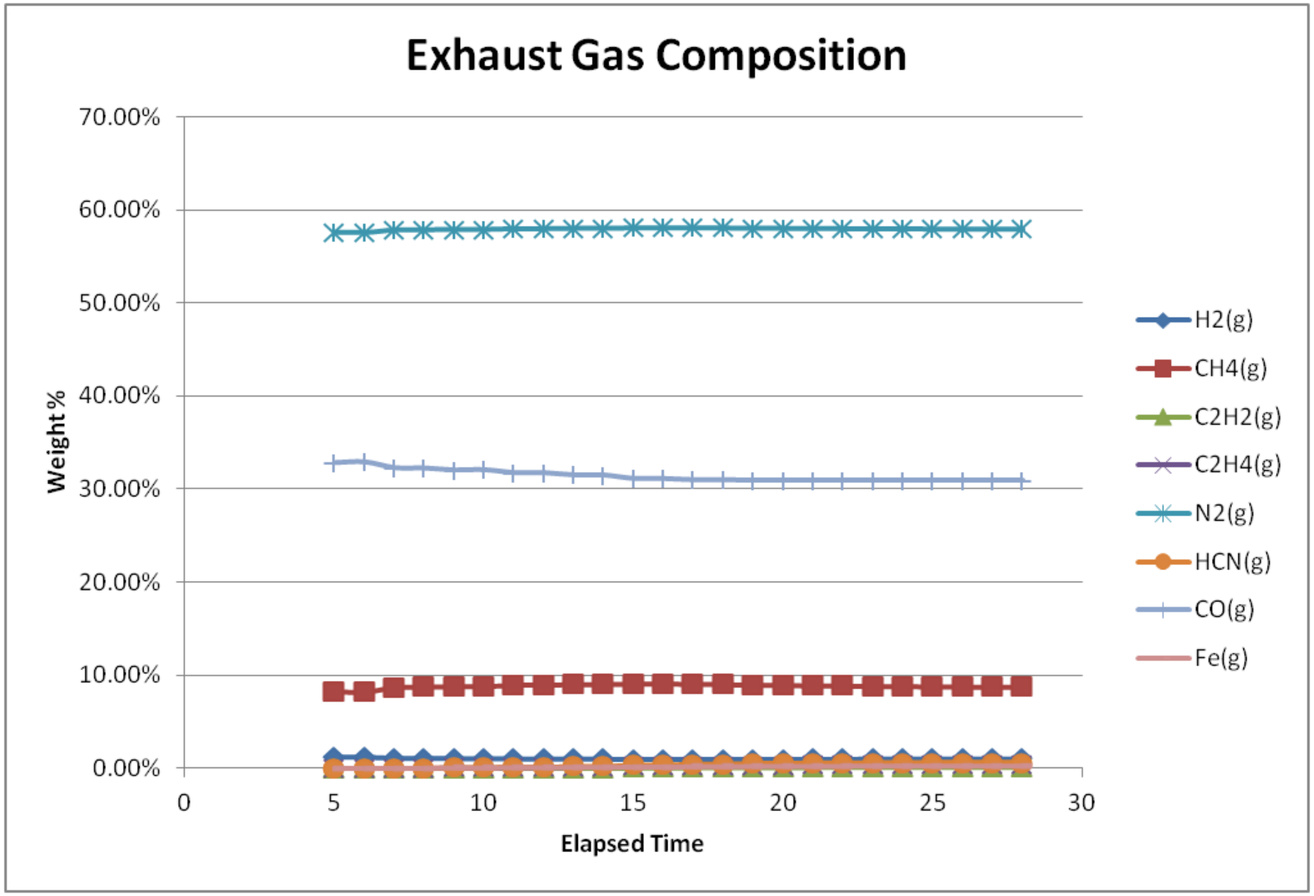
CaO-SiO2-Al2O3 Ternary Phase Diagram

Final Composition:

C=	69.17%
S=	21.06%
A=	4.98%

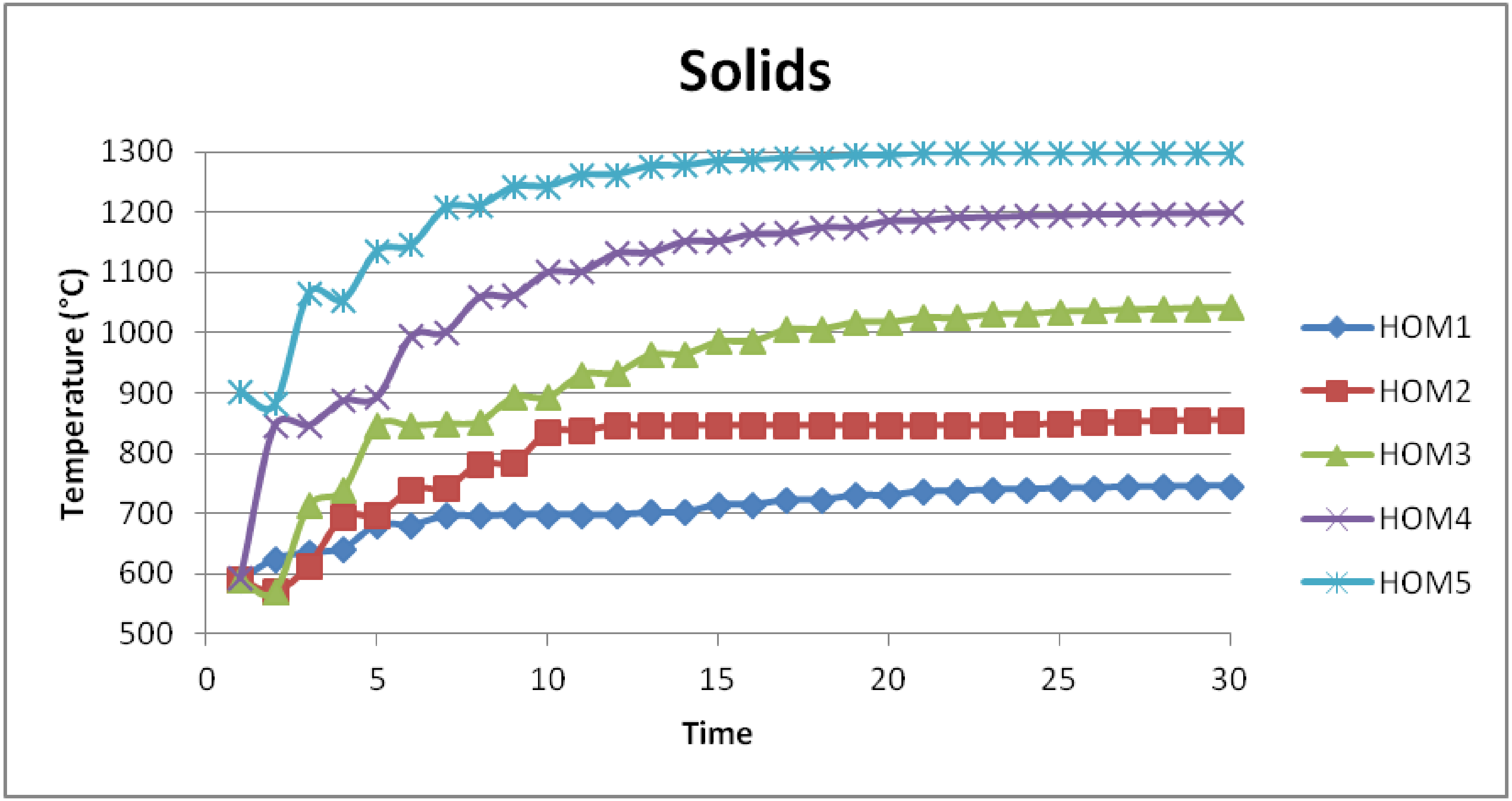


Exhaust Gas Composition

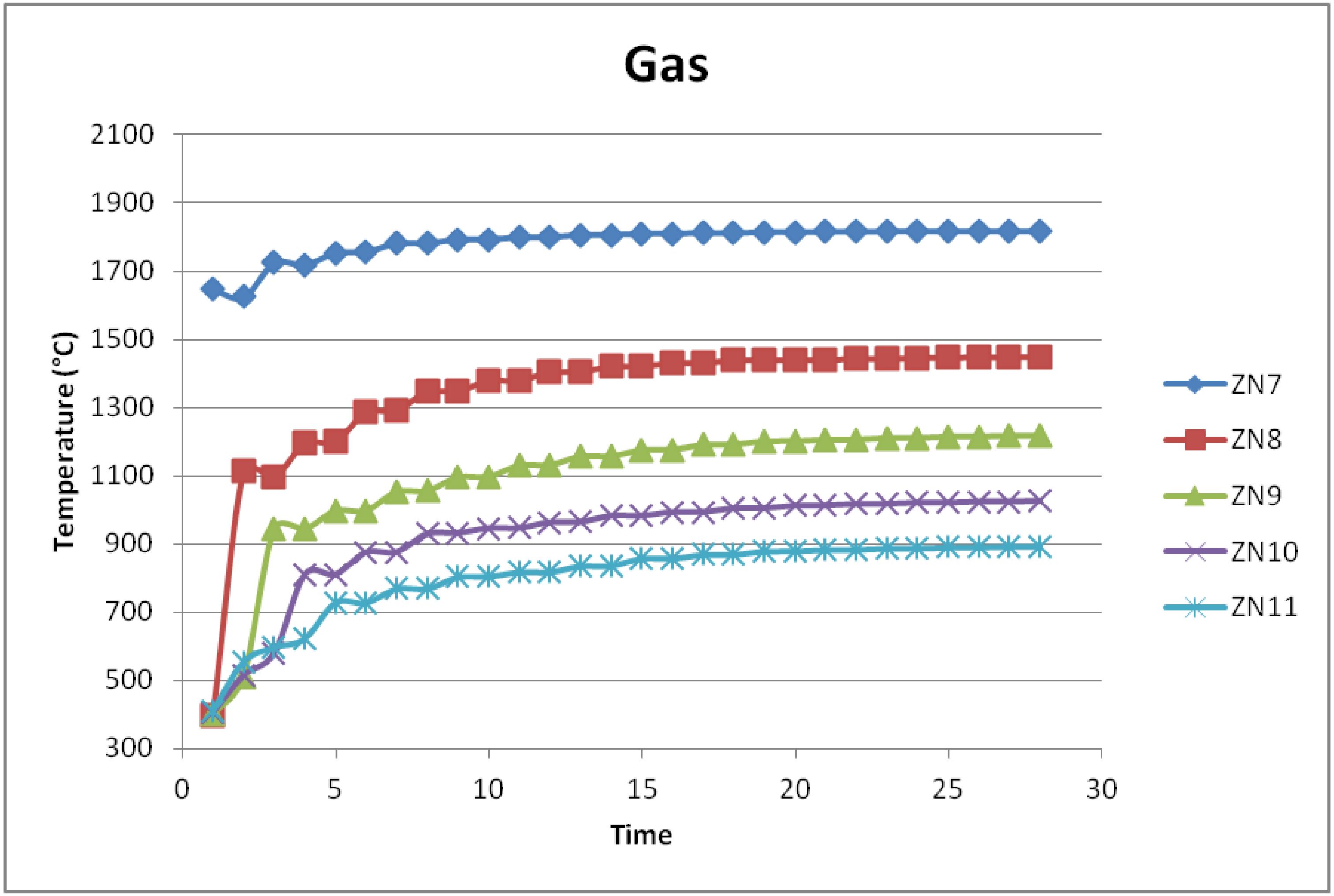


Start Temp: 408 °C
S.S. Temp: 894 °C

Temperature Profiles



Temperature Profiles



Attempt 3 Discussion

- The presence of alite (Ca_3SiO_5) was found in the clinker as is required. In addition, belite was also present which is characteristic of clinker at the ratios found in the excel output. This occurrence is likely due to the fact that the clinker homogenization zone reached steady state temperature at approximately 1300 °C.
- The inlet gas temperature was elevated at 2500 °C
- As in attempt 2, the exhaust gas composition is close to the industry composition at 58% N_2, 31% CO and 10% CH_4, 1% others.
- Many other attempts to reproduce experimental data were attempted and can be found in the provided excel files, but none were more successful than the ones presented in this document. In addition, the automatic graphs had not been incorporated into those excels, but it is incorporated into the excel sheet which the macro uses. All further simulations therefore get automatically graphed for compositions and temperature with time.

Conclusion

- Continue conducting tests to find optimal operating conditions and compare with literature results.
- Fine-tune the macro-code to only output the necessary species and cut down drastically on processing time
- Model is ideal for evaluating temperature profiles within the rotary kiln
- Currently, the exhaust gas composition of the rotary kiln simulation is not the final composition released to the environment.

References

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2. Lea FM. The Chemistry of Cement and Concrete. Third Edition ed. Great Britain: Edward Arnold Ltd; 1970. 727 p.

3. Taylor HFW. Cement Chemistry. Second Edition ed. London: Thomas Telford Publishing; 1997. 459 p.

4. Thompson D, Argent BB. Modelling trace and alkali mobilisation in the rotary cement kiln. Mineral Processing and Extractive Metallurgy. 2007;116(2):115-22.

Questions?