Institut für Energieverfahrenstechnik und Chemieingenieurwesen

“Thermochemical modeling of the Combustion of Rheinland lignite coal”

Application of Simusage

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Project „SIMEX"- Overview

- **Background :** Sulfate-rich deposition (fouling and sintering) during combustion of Rheinland lignite coal

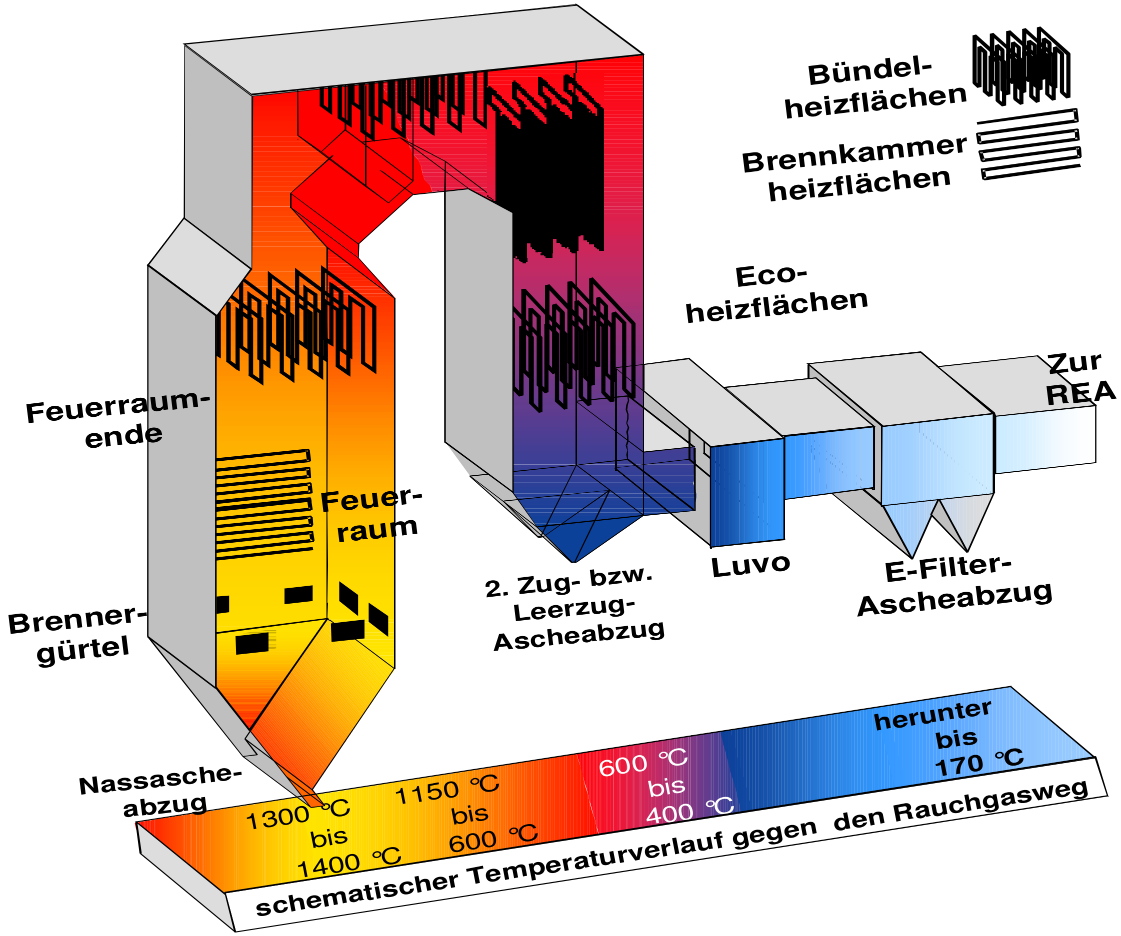
- **Objective :** Develop models, that improve understanding of ash formation and deposition mechanisms in coal fired boiler on the basis of the research in project "**SIMEX**"

- **Project Partners:** RWE Power AG, Research Center Jülich, Applied University Zittau, TU Freiberg

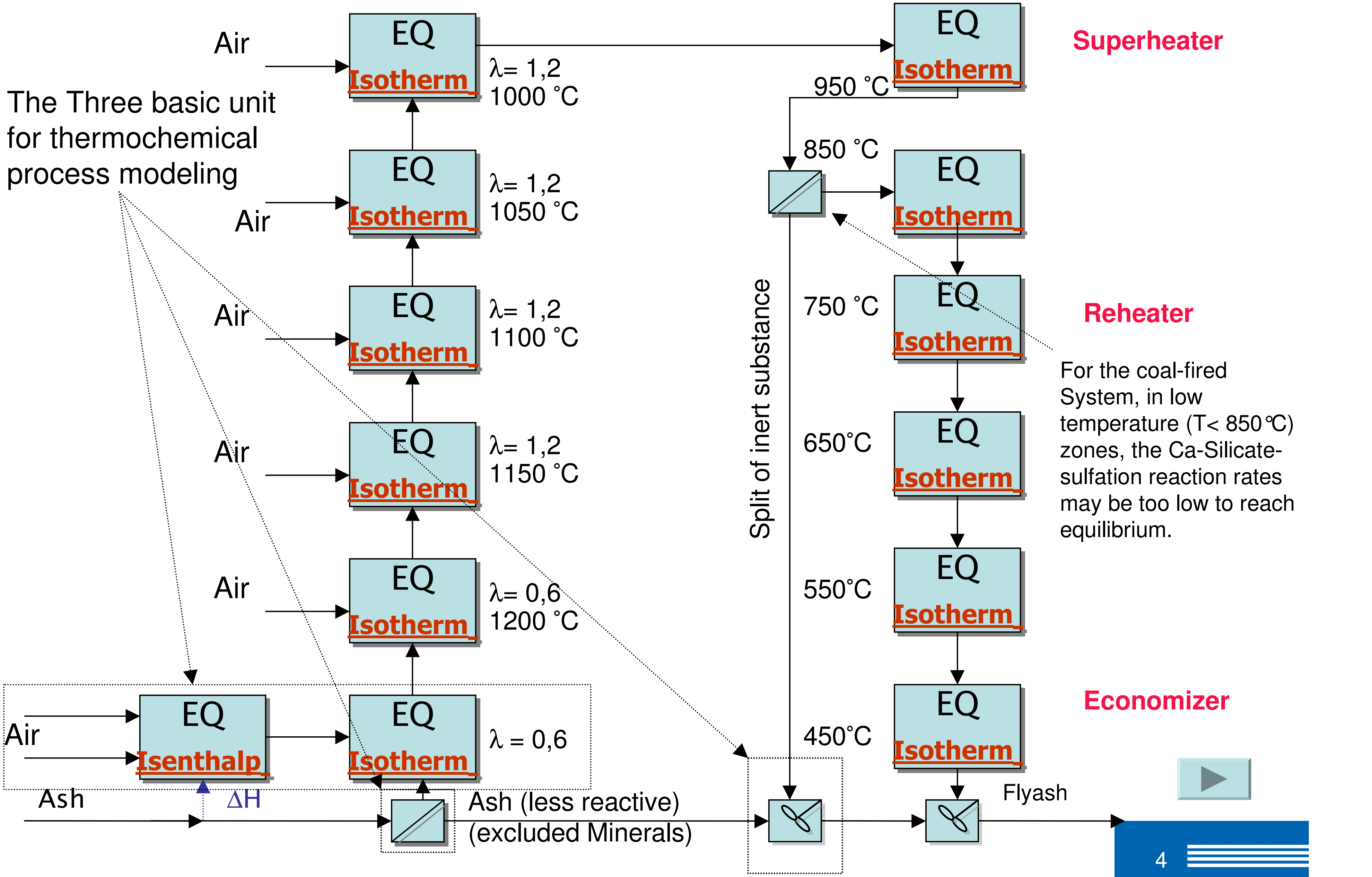
- **Subjects:**

➢ Interaction of S-, Na-, Ca-, Si- amount in the ash.
➢ Effect of O_2-level in the fuel gas on the deposition behavior.
➢ Influence of the included und excluded minerals.
➢ Reduce the deposition during mixed coal combustion.
➢ Thermodynamic investigation on the sulfate system (Na_2SO_4-K_2SO_4-$CaSO_4$-$MgSO_4$).

Schematic of a steam plant

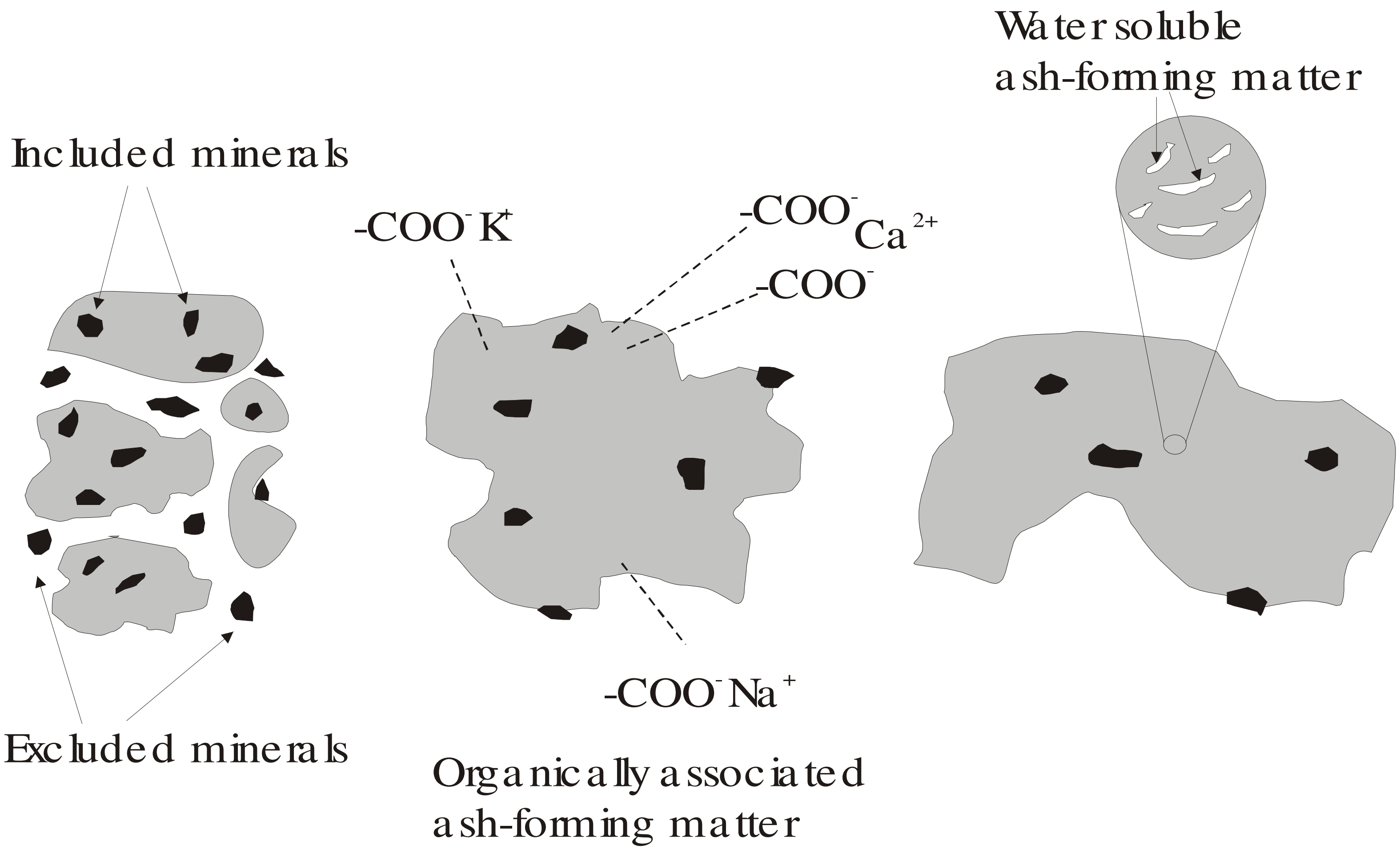


Schematic of a steam plant



Excluded and included minerales

Different forms of ash-forming matter in coals and biomass



Daniel Lindberg 2002
Thermodynamic equilibrium calculations on the combustion of five different biomass fuels

Theoretical air requirement and excess air coefficient

- Calculation table of o_{min} of solid and liquid fuels

column	1	2	3
row	Feed material	Combustion product	Oxygen demand $\frac{m^3_{O_2}}{kg_F}$
1	C	CO_2	$1.867 \cdot C$
2	H	H_2O	$5.600 \cdot H$
3	S_c	SO_2	$0.700 \cdot S$
4	O	-	$- 0.700 \cdot O$
			Sum: o_{min}

$$l_{min,dry} = \frac{100}{21} \cdot o_{min} \qquad \frac{m^3_{A,dry}}{kg_F} \text{ or } \frac{m^3_{A,dry}}{m^3_F} \qquad [1]$$

$$l_{min,wet} = l_{min,dry} + f_{W,A} \cdot 1.244 \cdot 10^{-3} \cdot l_{min,dry} \qquad \frac{m^3_{A,wet}}{kg_F} \text{ or } \frac{m^3_{A,wet}}{m^3_F} \qquad [2]$$

$$l_{dry} = \lambda \cdot l_{min,dry} \qquad \frac{m^3_{A,dry}}{kg_F} \text{ or } \frac{m^3_{A,dry}}{m^3_F} \qquad [3]$$

$$l_{wet} = \lambda \cdot l_{min,wet} \qquad \frac{m^3_{A,wet}}{kg_F} \text{ or } \frac{m^3_{A,wet}}{m^3_F} \qquad [4]$$

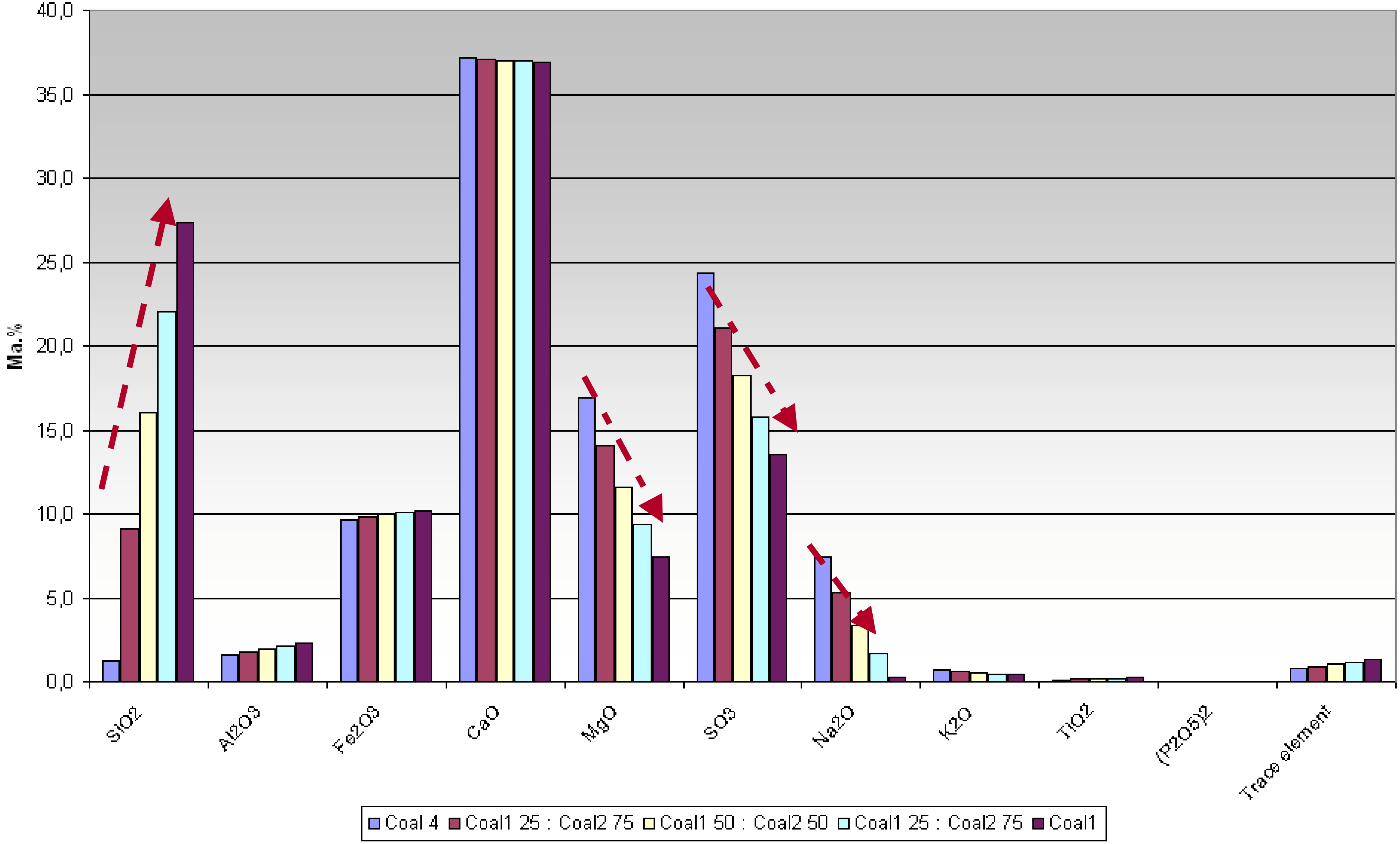
The ultimate and proximate analyses

		Coal1	Coal2	Coal3	Coal4	Coal5	Coal6	Coal7
C	Ma.-%	26,0	25,0	32,5	33,0	31,4	29,6	30,16
H	Ma.-%	1,9	1,9	2,4	2,5	2,4	2,1	2,32
N	Ma.-%	0,4	0,3	0,4	0,5	0,4	0,4	0,38
O	Ma.-%	10,6	10,8	13,0	12,4	13,1	12,4	13,19
Sc	Ma.-%	0,1	0,1	0,0	0,2	0,1	0,2	0,02
Aschegehalt	Ma.-%	2,8	1,7	1,7	2,2	3,3	7,1	5,03
W	Ma.-%	58,2	60,2	49,9	49,4	49,4	48,2	48,9
Summe	Ma.-%	100,0	100,0	100,0	100,0	100,0	100,0	100
Hu	kJ/kg	8359,0	8003,0	11081,0	11434,0	10643,0	9808,0	10109
Cfix	Ma.-%	16,9	15,6	21,9	20,0	18,8	19,8	18,36
Flüchtige	Ma.-%	22,1	22,5	26,5	28,5	28,6	24,9	27,71
Cl	mg/kg	122	246	182	283	202	140	207
SiO_2	Ma.-%	27,38	1,83	1,46	1,28	23,01	44,52	23,33
Al_2O_3	Ma.-%	2,30	7,23	1,74	1,55	4,18	19,21	7,23
Fe_2O_3	Ma.-%	10,21	31,90	9,93	9,65	10,60	2,75	25,79
CaO	Ma.-%	36,90	29,68	38,29	37,16	29,60	13,60	20,89
MgO	Ma.-%	7,47	7,37	17,73	16,93	12,88	5,89	8,58
SO_3	Ma.-%	13,52	19,52	19,52	24,36	12,88	9,01	9,93
Na_2O	Ma.-%	0,23	0,53	9,44	7,47	4,18	2,13	1,67
K_2O	Ma.-%	0,41	0,27	0,74	0,71	0,52	0,75	0,35
TiO_2	Ma.-%	0,24	0,31	0,11	0,11	0,29	1,05	0,46
$(P_2O_5)_2$	Ma.-%	0,02	0,02	0,01	0,01	0,02	0,08	0,10
Trace element	Ma.-%	1,30	1,34	1,02	0,76	1,83	1,00	1,73
	Total	100,00	100,01	100,00	100,00	100,00	99,98	100,05

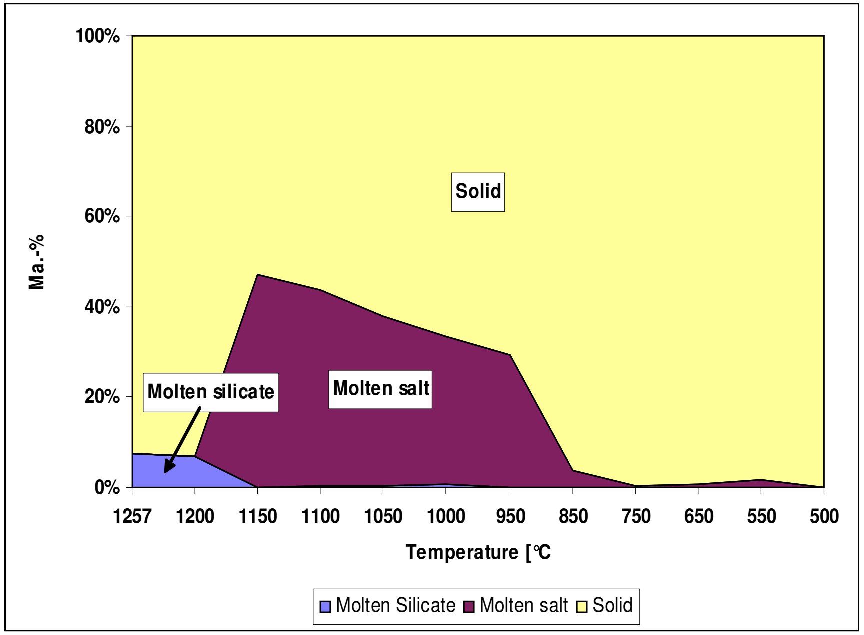
The ultimate and proximate analyses

		Coal 4	Coal1 25 : Coal2 75	Coal1 50 : Coal2 50	Coal1 25 : Coal2 75	Coal1
C	Ma.-%	33,0	31,3	29,5	27,8	26,0
H	Ma.-%	2,5	2,3	2,2	2,1	1,9
N	Ma.-%	0,5	0,4	0,4	0,4	0,4
O	Ma.-%	12,4	11,9	11,5	11,1	10,6
Sc	Ma.-%	0,2	0,2	0,1	0,1	0,1
Ash	Ma.-%	2,2	2,3	2,5	2,6	2,8
W	Ma.-%	49,4	51,6	53,8	56,0	58,2
Total	Ma.-%	100,0	100,0	100,0	100,0	100,0
Hu	kJ/kg	11434,0	10665,3	9896,5	9127,8	8359,0
Cfix	Ma.-%	20,0	19,2	18,4	17,6	16,9
Volatiles	Ma.-%	28,5	26,9	25,3	23,7	22,1
Cl	mg/kg	283,0	242,8	202,5	162,3	122,0
SiO_2	Ma.-%	1,3	9,2	16,0	22,0	27,4
Al_2O_3	Ma.-%	1,6	1,8	2,0	2,2	2,3
Fe_2O_3	Ma.-%	9,7	9,8	10,0	10,1	10,2
CaO	Ma.-%	37,2	37,1	37,0	37,0	36,9
MgO	Ma.-%	16,9	14,1	11,6	9,4	7,5
SO_3	Ma.-%	24,4	21,1	18,2	15,7	13,5
Na_2O	Ma.-%	7,5	5,3	3,4	1,7	0,2
K_2O	Ma.-%	0,7	0,6	0,5	0,5	0,4
TiO_2	Ma.-%	0,1	0,1	0,2	0,2	0,2
$(P_2O_5)_2$	Ma.-%	0,0	0,0	0,0	0,0	0,0
Trace element	Ma.-%	0,8	0,9	1,1	1,2	1,3

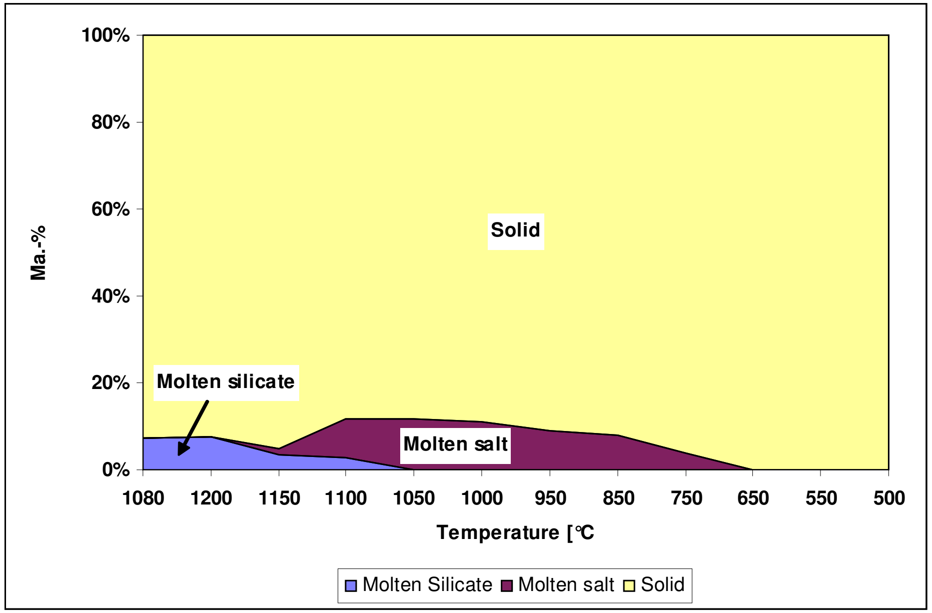
Ash analysis



Solid-Slag diagram of condensed phase

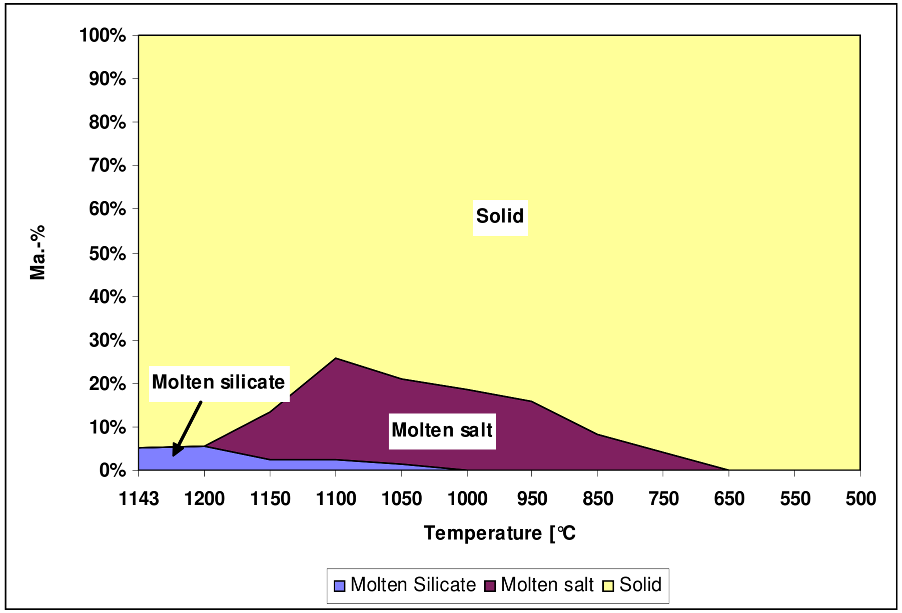


Coal4

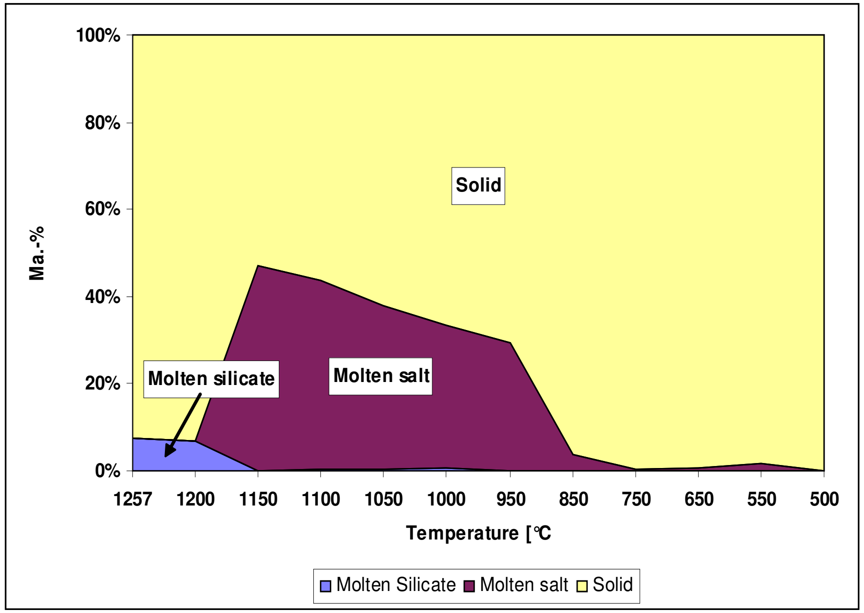


Coal1 :Coal4 (75:25)

Solid-Slag diagram of condensed phase

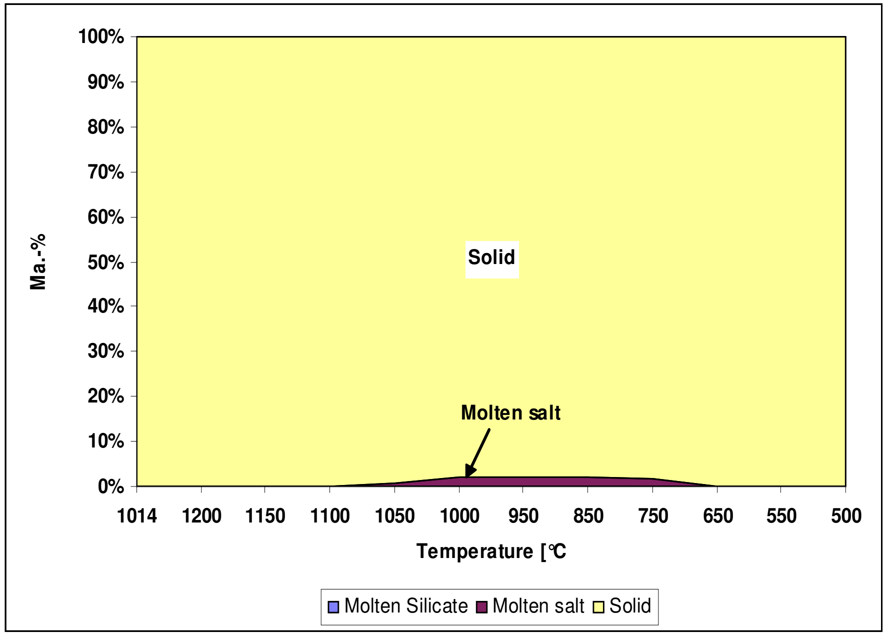


Coal1 :Coal4 (50:50)



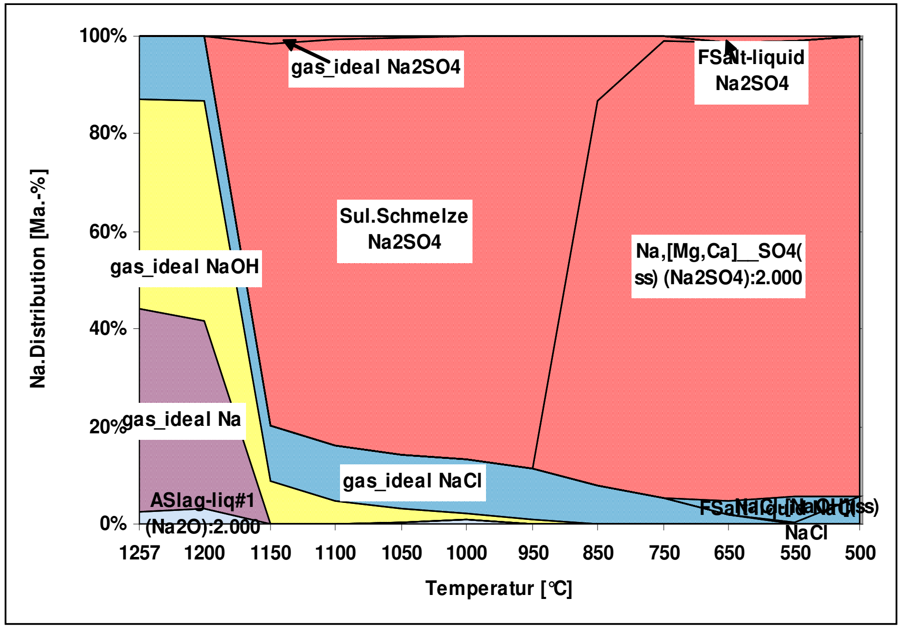
Coal1 :Coal4 (25:75)

Solid-Slag diagram of condensed phase

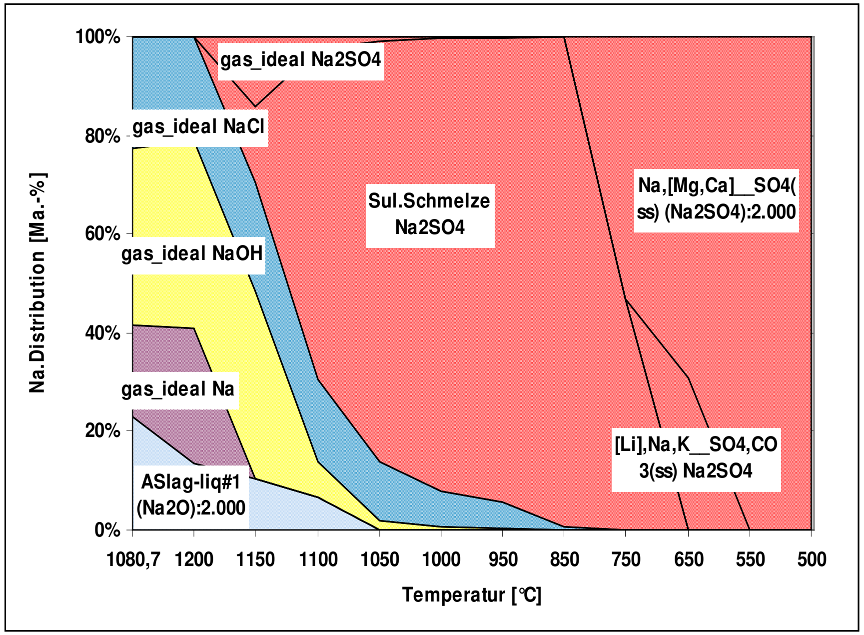


Coal1

Na-distribution: Coal1 & Coal4

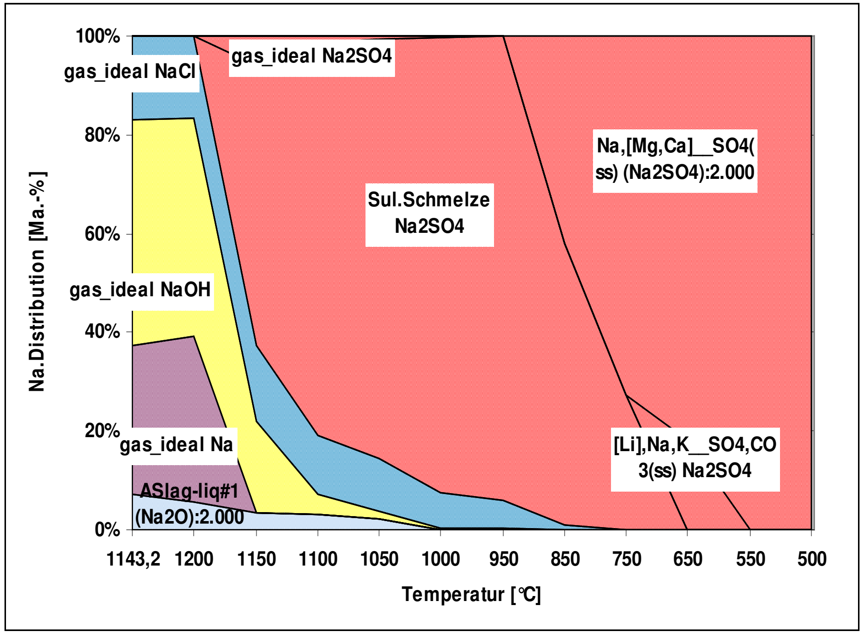


Coal4

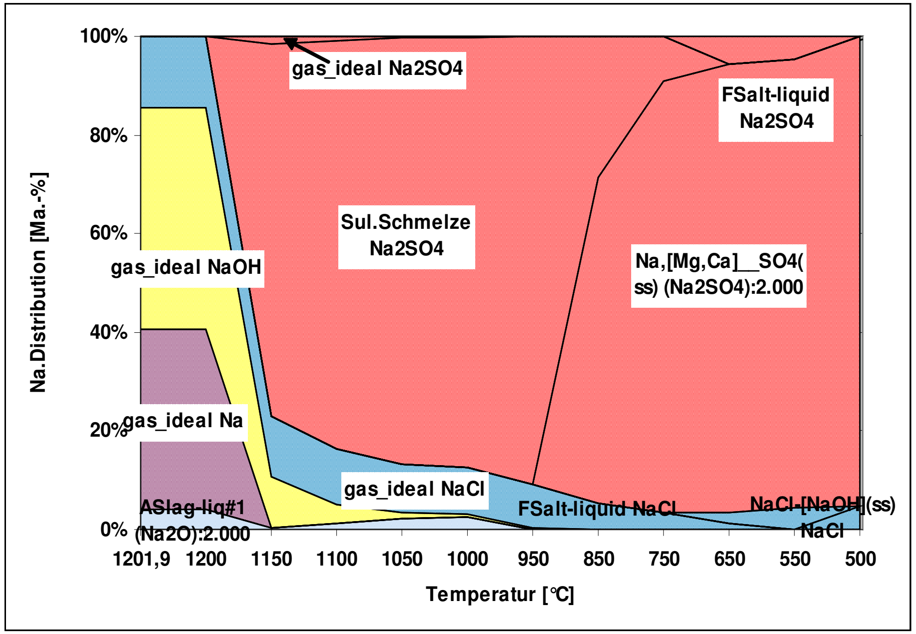


Coal1 :Coal4 (75:25)

Na-distribution: Coal1 & Coal4

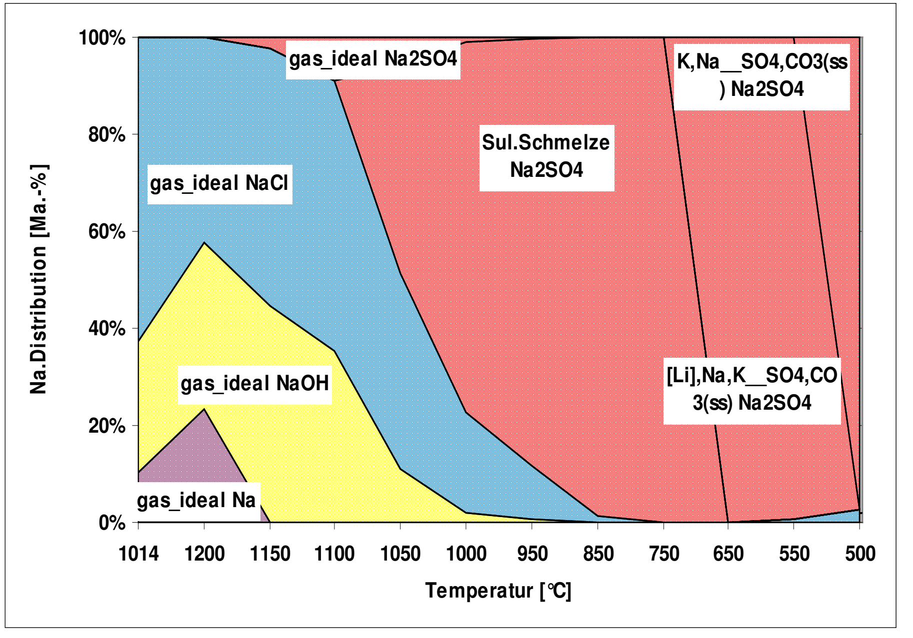


Coal1 :Coal4 (50:50)



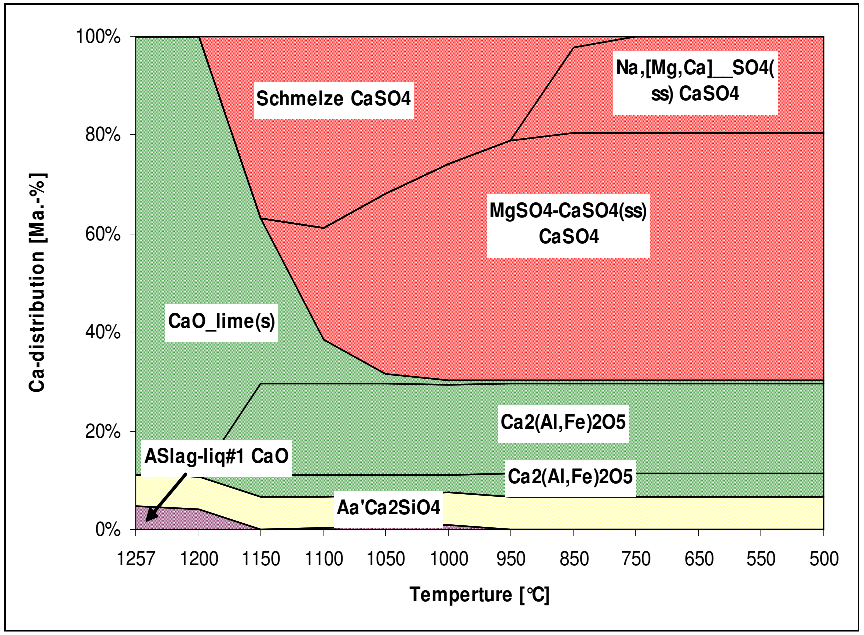
Coal1 :Coal4 (25:75)

Na-distribution: Coal1 & Coal4 +

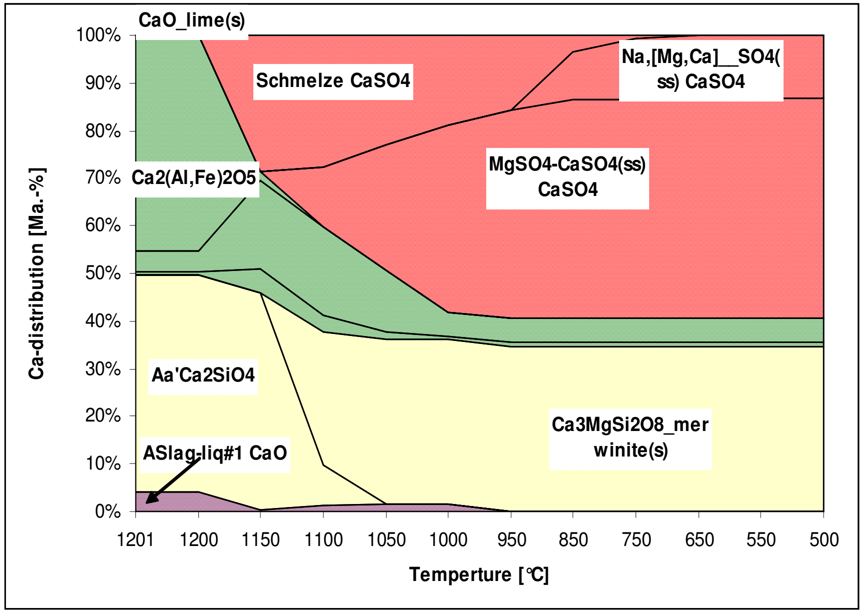


Coal1

Ca-distribution: Coal1 & Coal4

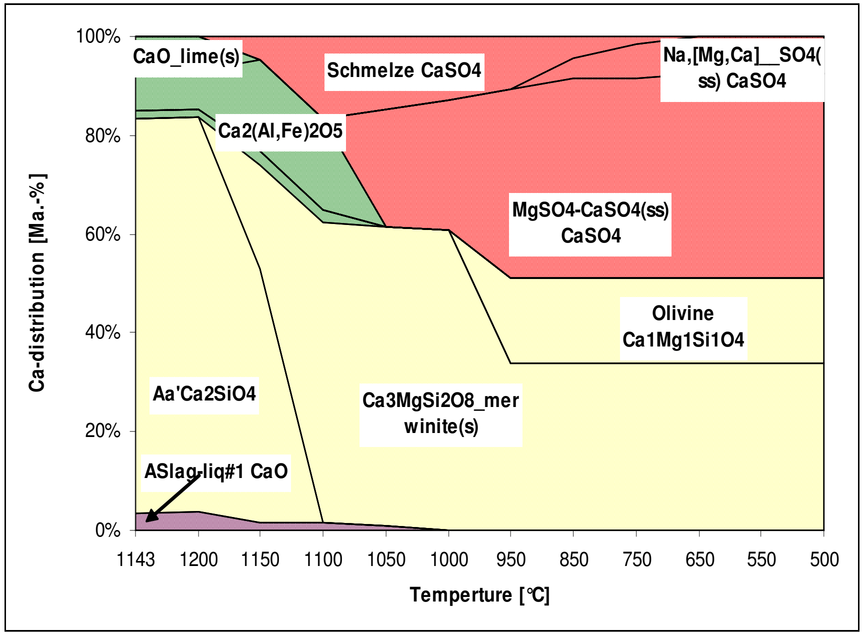


Coal4

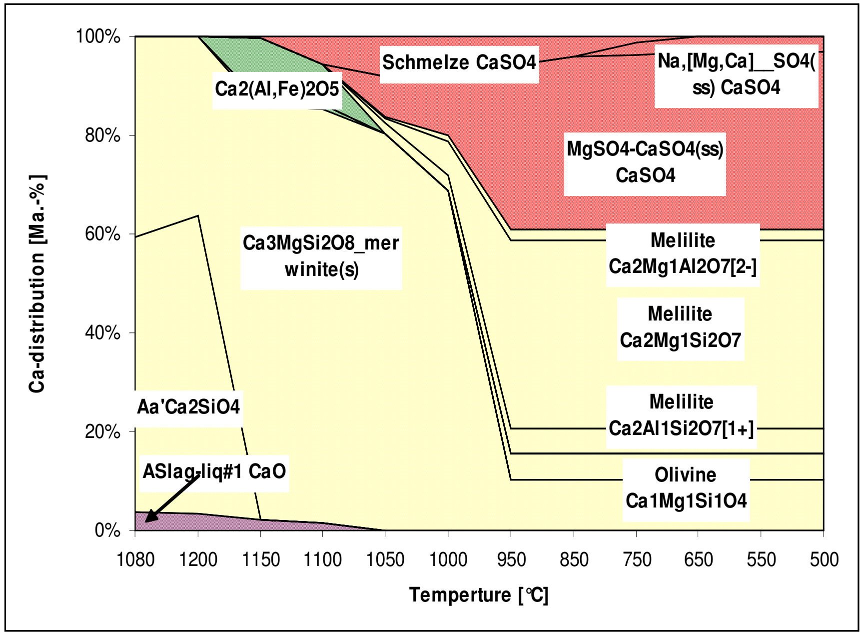


Coal1 :Coal4 (25:75)

Ca-distribution: Coal1 & Coal4 +

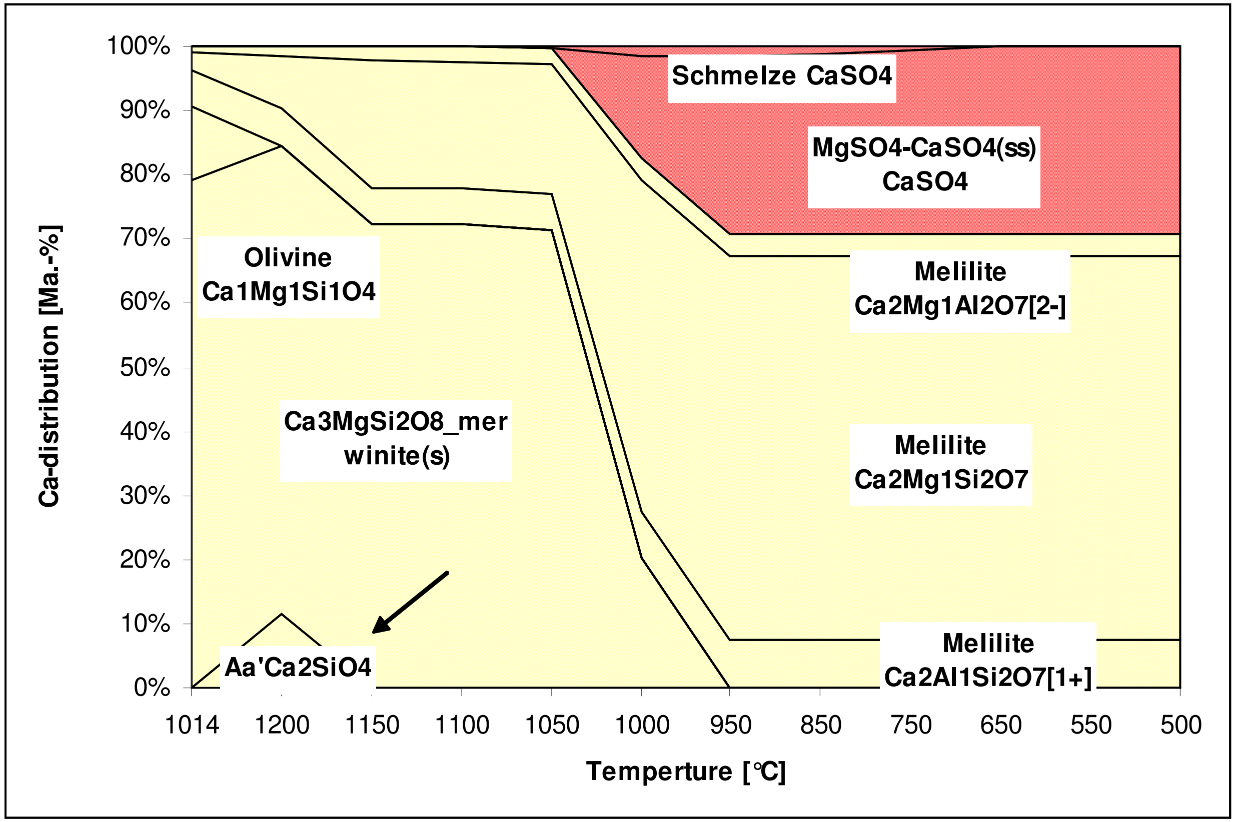


Coal1 :Coal4 (50:50)



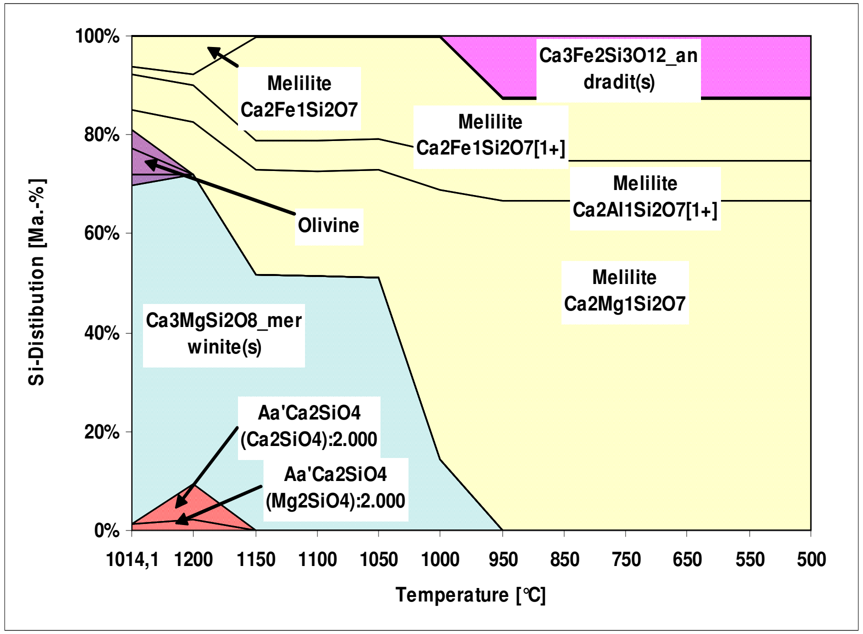
Coal1 :Coal4 (75:25)

Ca-distribution: Coal1 & Coal4

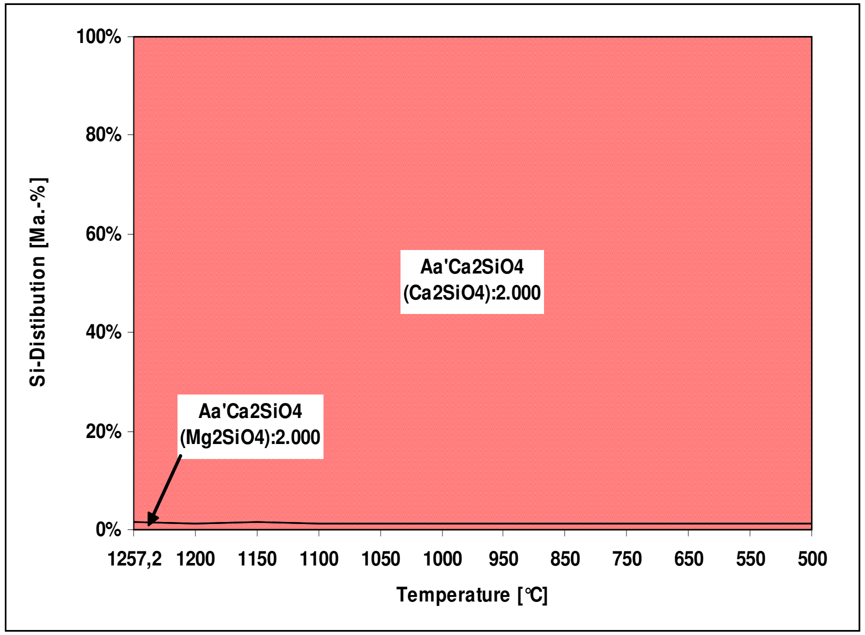


Coal1

Si-distribution: Coal1 & Coal4

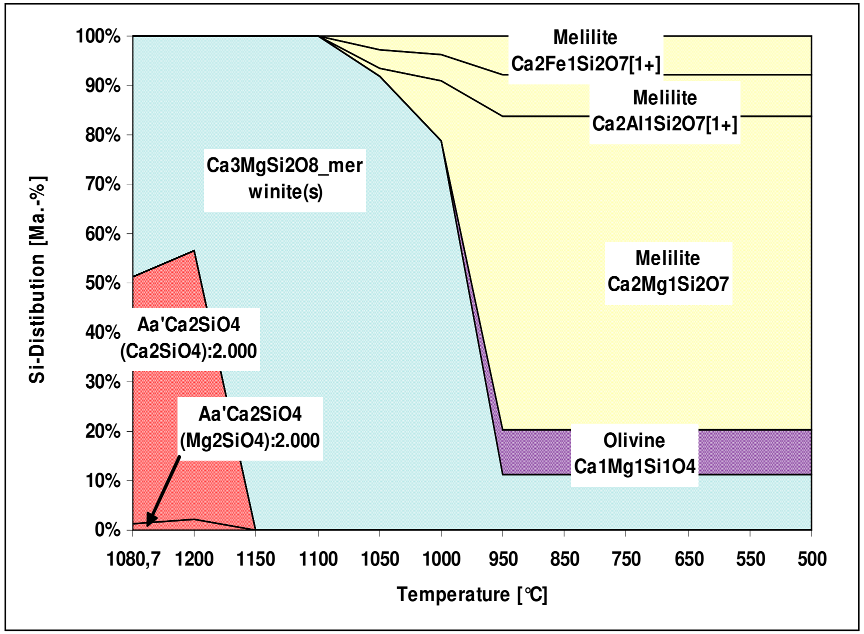


Coal1

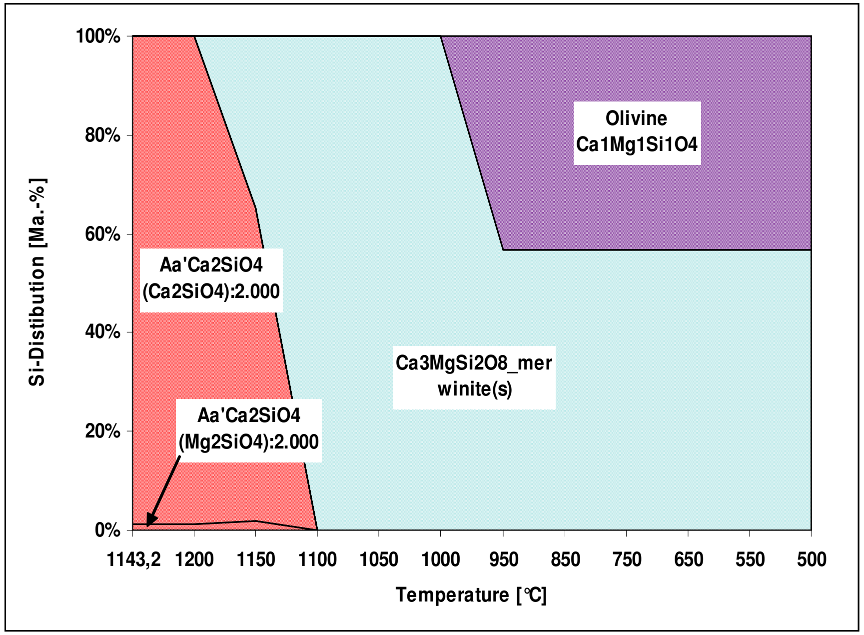


Coal4

Si-distribution: Coal1 & Coal4

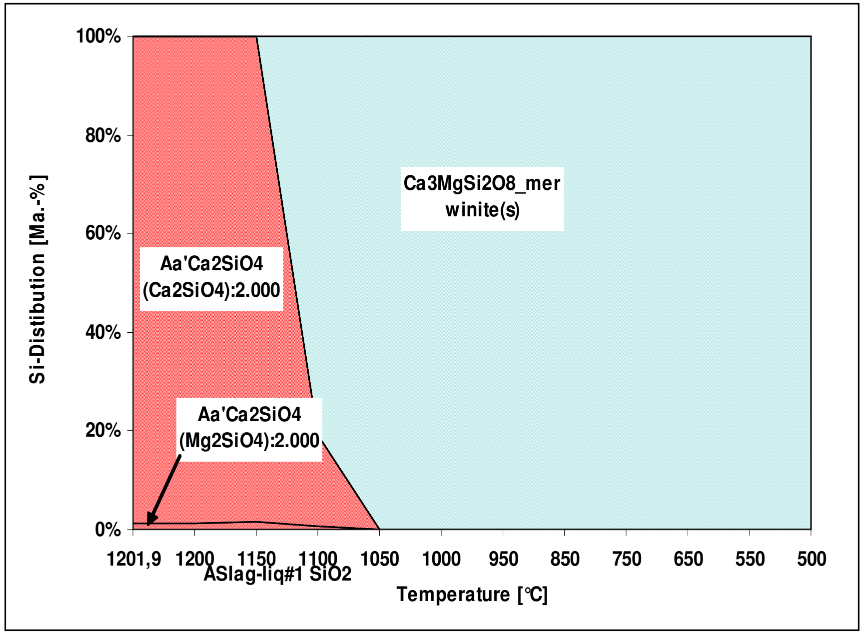


Coal1 :Coal4 (75:25)



Coal1 :Coal4 (50:50)

Si-distribution: Coal1 & Coal4



Coal1 :Coal4 (25:75)

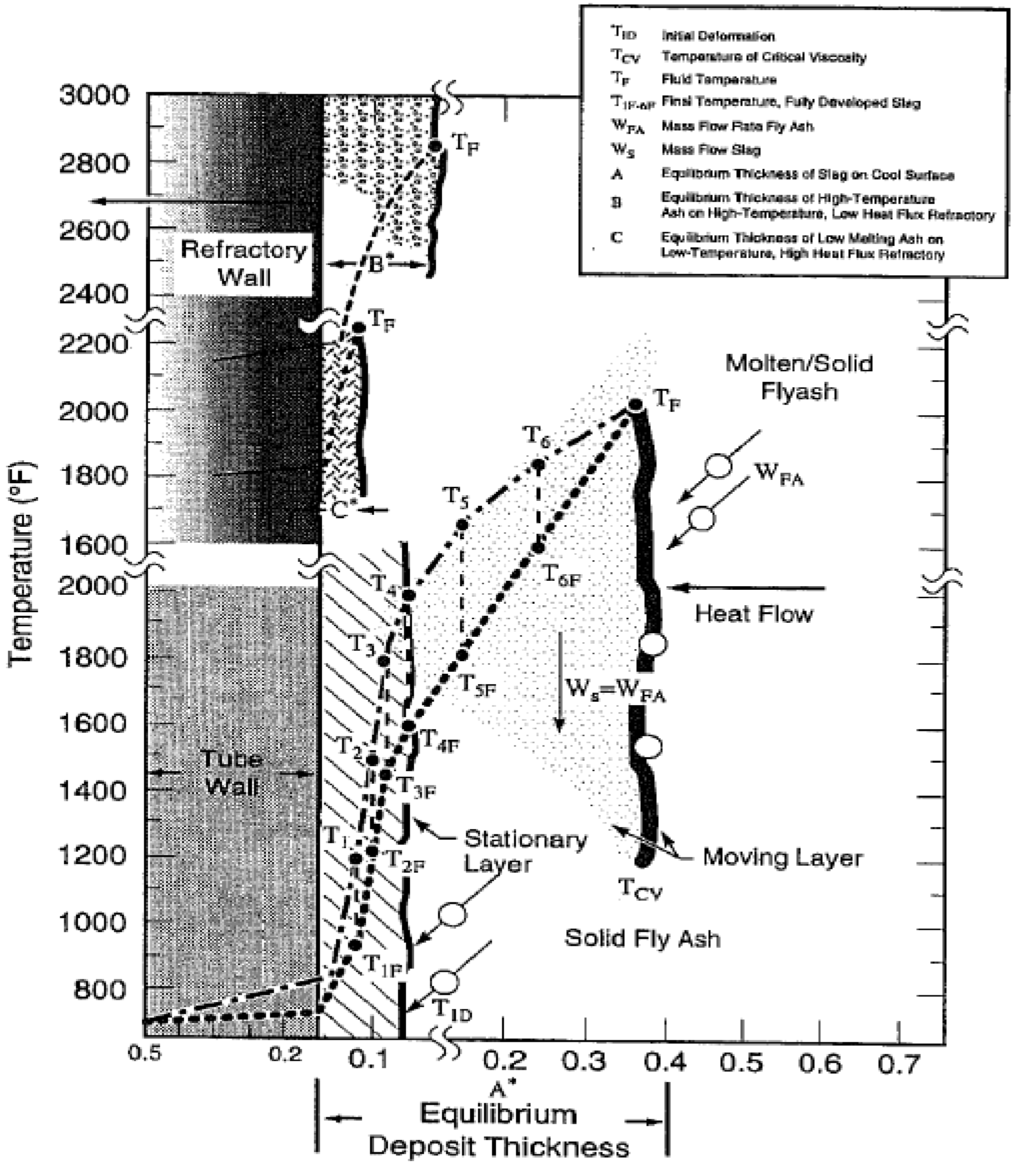
Summary and Conclusions

- Ash deposition behavior has been simulated in consideration of the mixed coal combustion and O_2-level as well as the slow reaction rats of excluded minerals in the combustion atmosphere .
- Increasing the Coal1 fraction reduces the molten salt faction (reducing the fouling risk) due to the higher content of silicon in ash.
- Increasing the Coal2 fraction results in the formation of Ca-silicate (Melilite) and reduce the Na-Ca-sulfate fraction as well as lower combustion temperature.
- Most sodium is released as $NaOH_{(g)}$.$Na_2SO_{4(g)}$ and $NaCl_{(g)}$.
- Na_2SO_4(l) is formed between 1050-750 ℃ and it may induce the Fouling of ash on the furnace wall.
- The reactions of capture of gaseous Alkali can be summarized as follows :

➢ Gaseous alkali hydroxide NaOH(g) and alkali chloride NaCl(g) combine with SO_2 to from sulfates

➢ Alkali chloride and sulfates directly condense during the gas cooling

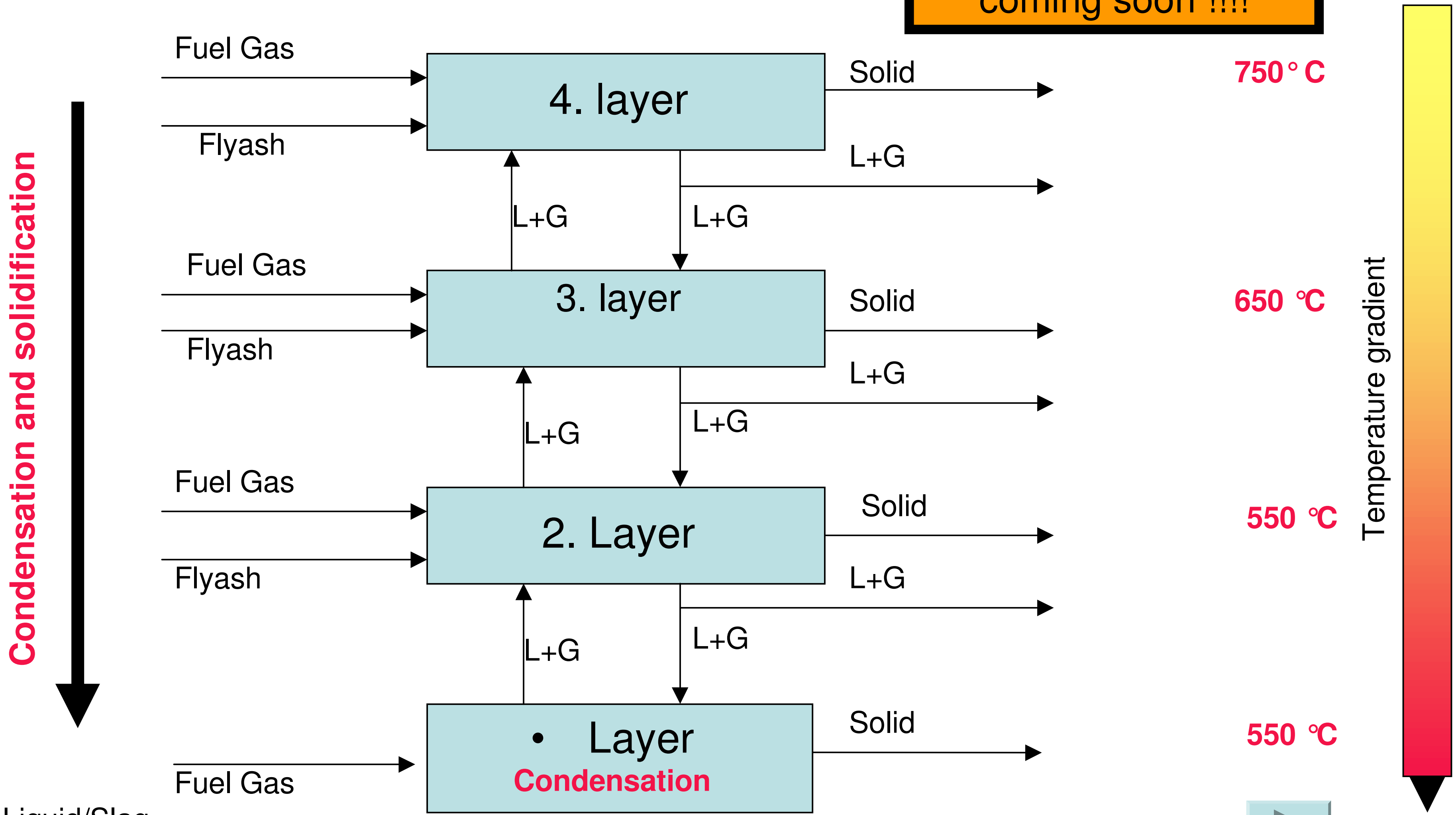
Generic Model of temperature profiles in furnace with slag



Richard Bryers
1999

Monolayer model /ash deposition

Further works on IEC coming soon !!!!



L: Liquid/Slag
G: Gas
S: Solid