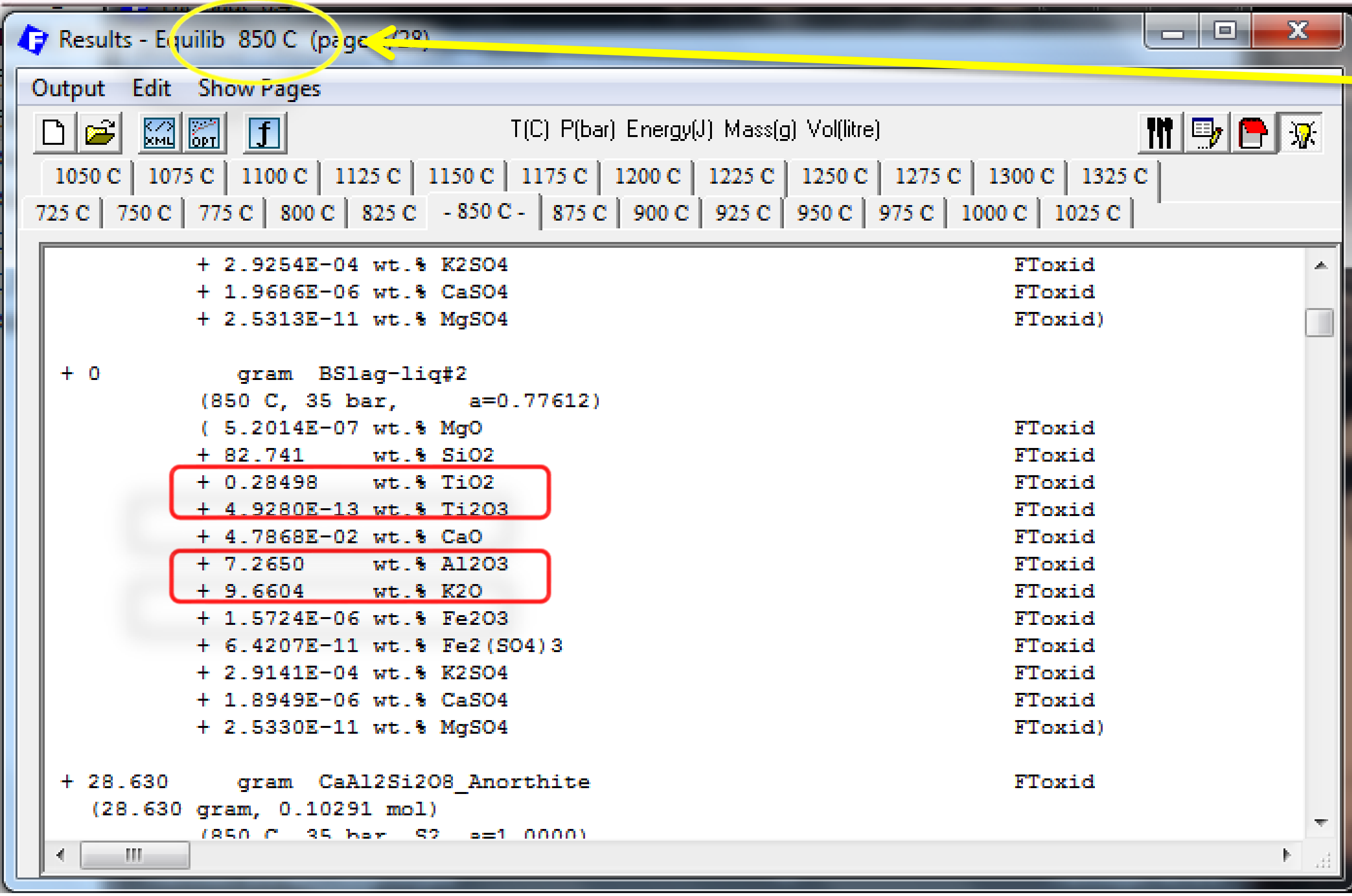
EFFECT OF GASIFICATION OPERATING TEMPERATURE ON EITHER LEACHABILITY OF ASH AND MIGRATION OF ELEMENTS DURING AN UCG PROCESS OR RECOVERY OF SPECIFIC ELEMENTS SUCH AS K, AL AND TI FROM A FIXED BED GASIFICATION PROCESS

GTT WORKSHOP, AACHEN, 1-3 JULY 2015

Prof JC van Dyk
AC Collins* (author)
Prof CA Strydom
JF Brand

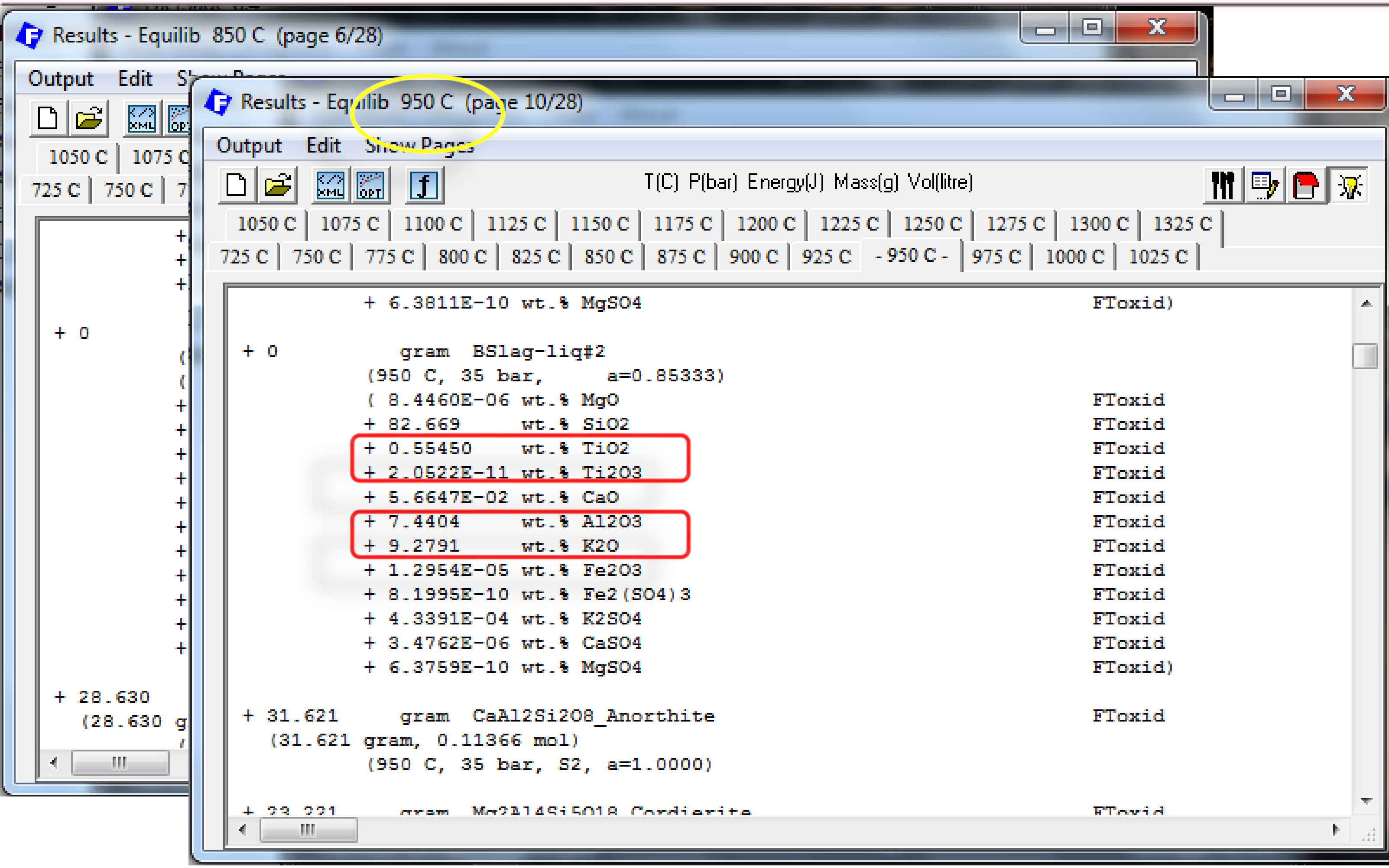
AFRICARY
CHEMICAL RESOURCE BENEFICIATION
CHEMIESE HULPBRONVEREDELING
NORTH-WEST UNIVERSITY
YUNIBESITI YA BOKONE-BOPHIRIMA
NOORDWES-UNIVERSITEIT
POTCHEFSTROOM CAMPUS

Motivation

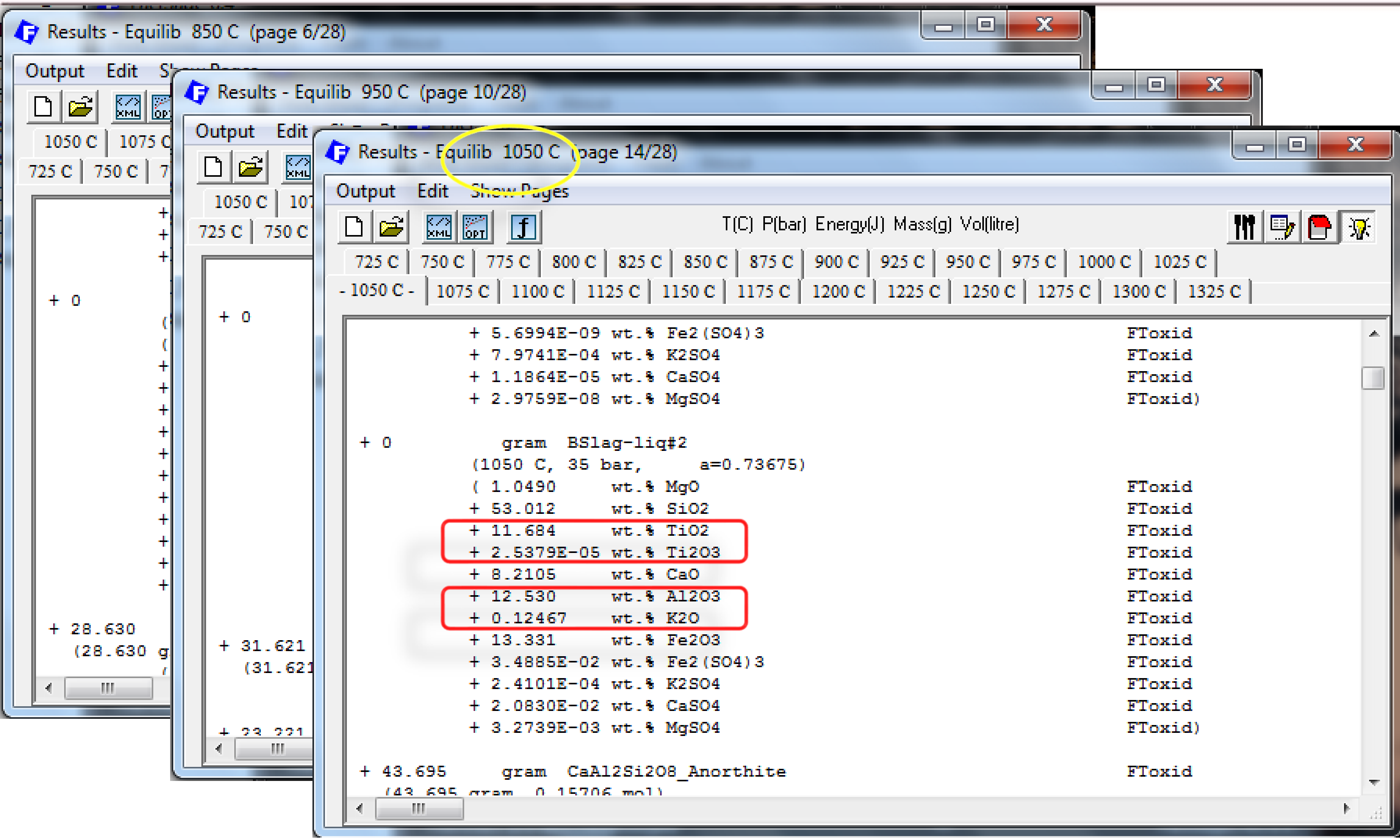


Ideal operating conditions for the recovery of minerals from the coal ash

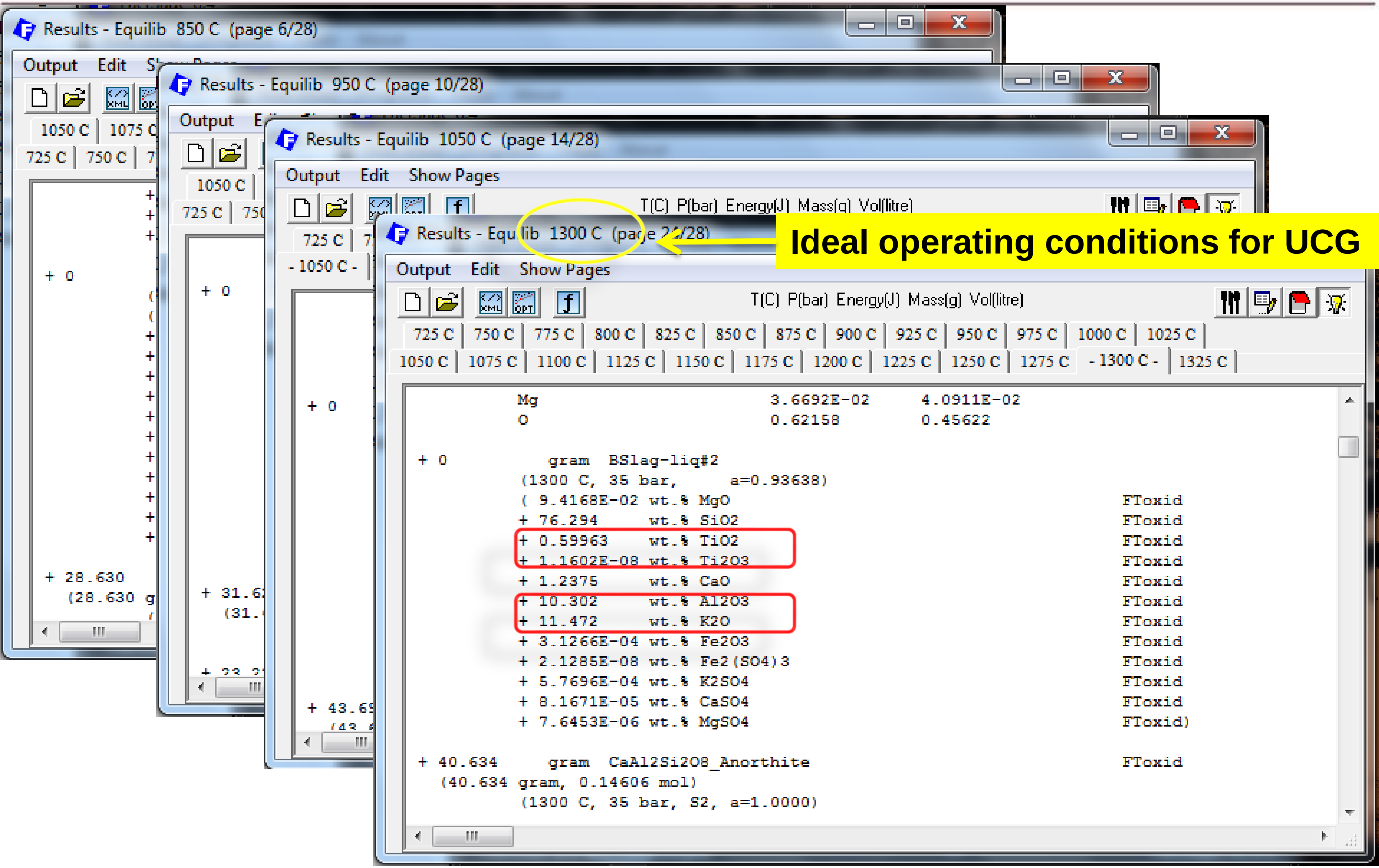
Motivation


Results - Equilib 850 C (page 6/28)
Results - Equilib 950 C (page 10/28)
Output Edit Show Pages
T(C) P(bar) Energy(J) Mass(g) Vol(litre)
1050 C 1075 C 1100 C 1125 C 1150 C 1175 C 1200 C 1225 C 1250 C 1275 C 1300 C 1325 C
725 C 750 C 775 C 800 C 825 C 850 C 875 C 900 C 925 C - 950 C - 975 C 1000 C 1025 C
+ 6.3811E-10 wt.% MgSO4 FToxid)
+ 0 gram BSlag-liq#2
(950 C, 35 bar, a=0.85333)
(8.4460E-06 wt.% MgO FToxid
+ 82.669 wt.% SiO2 FToxid
+ 0.55450 wt.% TiO2 FToxid
+ 2.0522E-11 wt.% Ti2O3 FToxid
+ 5.6647E-02 wt.% CaO FToxid
+ 7.4404 wt.% Al2O3 FToxid
+ 9.2791 wt.% K2O FToxid
+ 1.2954E-05 wt.% Fe2O3 FToxid
+ 8.1995E-10 wt.% Fe2(SO4)3 FToxid
+ 4.3391E-04 wt.% K2SO4 FToxid
+ 3.4762E-06 wt.% CaSO4 FToxid
+ 6.3759E-10 wt.% MgSO4 FToxid)
+ 31.621 gram CaAl2Si2O8_Anorthite FToxid
(31.621 gram, 0.11366 mol)
(950 C, 35 bar, S2, a=1.0000)
+ 28.630
(28.630 g

Motivation


Results - Equilib 850 C (page 6/28)
Results - Equilib 950 C (page 10/28)
Results - Equilib 1050 C (page 14/28)
Output Edit Show Pages
T(C) P(bar) Energy(J) Mass(g) Vol(litre)
725 C 750 C 775 C 800 C 825 C 850 C 875 C 900 C 925 C 950 C 975 C 1000 C 1025 C
- 1050 C - 1075 C 1100 C 1125 C 1150 C 1175 C 1200 C 1225 C 1250 C 1275 C 1300 C 1325 C
+ 5.6994E-09 wt.% Fe2(SO4)3 FToxid
+ 7.9741E-04 wt.% K2SO4 FToxid
+ 1.1864E-05 wt.% CaSO4 FToxid
+ 2.9759E-08 wt.% MgSO4 FToxid)
+ 0 gram BSlag-liq#2
(1050 C, 35 bar, a=0.73675)
(1.0490 wt.% MgO FToxid
+ 53.012 wt.% SiO2 FToxid
+ 11.684 wt.% TiO2 FToxid
+ 2.5379E-05 wt.% Ti2O3 FToxid
+ 8.2105 wt.% CaO FToxid
+ 12.530 wt.% Al2O3 FToxid
+ 0.12467 wt.% K2O FToxid
+ 13.331 wt.% Fe2O3 FToxid
+ 3.4885E-02 wt.% Fe2(SO4)3 FToxid
+ 2.4101E-04 wt.% K2SO4 FToxid
+ 2.0830E-02 wt.% CaSO4 FToxid
+ 3.2739E-03 wt.% MgSO4 FToxid)
+ 43.695 gram CaAl2Si2O8_Anorthite FToxid
+ 28.630
(28.630 g
+ 31.621
(31.621

Motivation

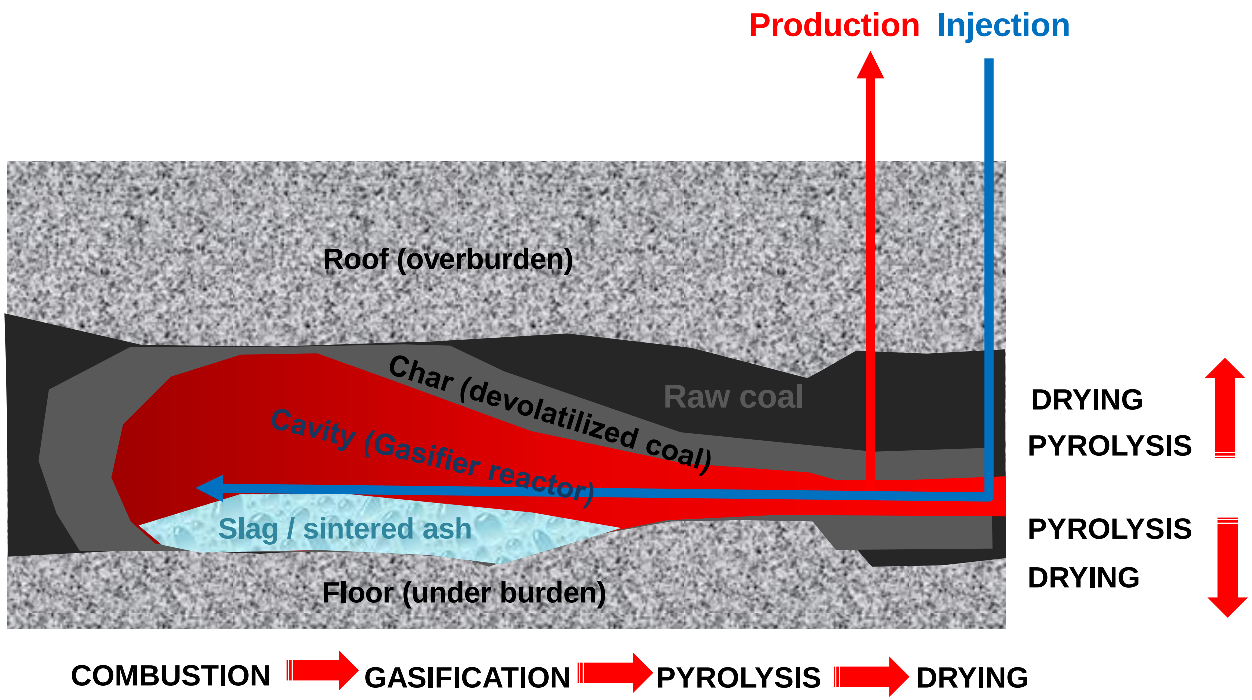

Results - Equilib 850 C (page 6/28)
Results - Equilib 950 C (page 10/28)
Results - Equilib 1050 C (page 14/28)
Results - Equilib 1300 C (page 24/28)
Ideal operating conditions for UCG
Output Edit Show Pages
T(C) P(bar) Energy(J) Mass(g) Vol(litre)
725 C | 750 C | 775 C | 800 C | 825 C | 850 C | 875 C | 900 C | 925 C | 950 C | 975 C | 1000 C | 1025 C
1050 C | 1075 C | 1100 C | 1125 C | 1150 C | 1175 C | 1200 C | 1225 C | 1250 C | 1275 C | - 1300 C - | 1325 C
Mg 3.6692E-02 4.0911E-02
O 0.62158 0.45622
+ 0 gram BSlag-liq#2
(1300 C, 35 bar, a=0.93638)
(9.4168E-02 wt.% MgO FToxid
+ 76.294 wt.% SiO2 FToxid
+ 0.59963 wt.% TiO2 FToxid
+ 1.1602E-08 wt.% Ti2O3 FToxid
+ 1.2375 wt.% CaO FToxid
+ 10.302 wt.% Al2O3 FToxid
+ 11.472 wt.% K2O FToxid
+ 3.1266E-04 wt.% Fe2O3 FToxid
+ 2.1285E-08 wt.% Fe2(SO4)3 FToxid
+ 5.7696E-04 wt.% K2SO4 FToxid
+ 8.1671E-05 wt.% CaSO4 FToxid
+ 7.6453E-06 wt.% MgSO4 FToxid)
+ 40.634 gram CaAl2Si2O8_Anorthite FToxid
(40.634 gram, 0.14606 mol)
(1300 C, 35 bar, S2, a=1.0000)

Motivation

NORTH-WEST UNIVERSITY
YUNIBESITI YA BOKONE-BOPHIRIMA
NOORDWES-UNIVERSITEIT
POTCHEFSTROOM CAMPUS

- **The influence of operating temperature on mineral species;**
- **Determination of whether these species are recoverable/leachable from the ash or lost/captured in the slag;**
- **The influence of gasification temperature on the slagging behaviour of coal samples with different characteristics;**
- **The influence of potassium on slagging behaviour when present in high concentrations within the coal;**
- **The influence of a specific potassium compound on the slagging behaviour when added to the coal in different percentages.**

FactSage Model of UCG Gasifier



$C + ½ O_2 \rightarrow CO$ $\quad$ $C + CO_2 \rightarrow 2 CO$

$C + O_2 \rightarrow CO_2$ $\quad$ $C + H_2O \rightarrow CO + H_2$

$H_2 + O_2 \rightarrow H_2O$

Water-gas shift:

$CO + H_2O \rightarrow CO_2 + H_2$

Methane formation:

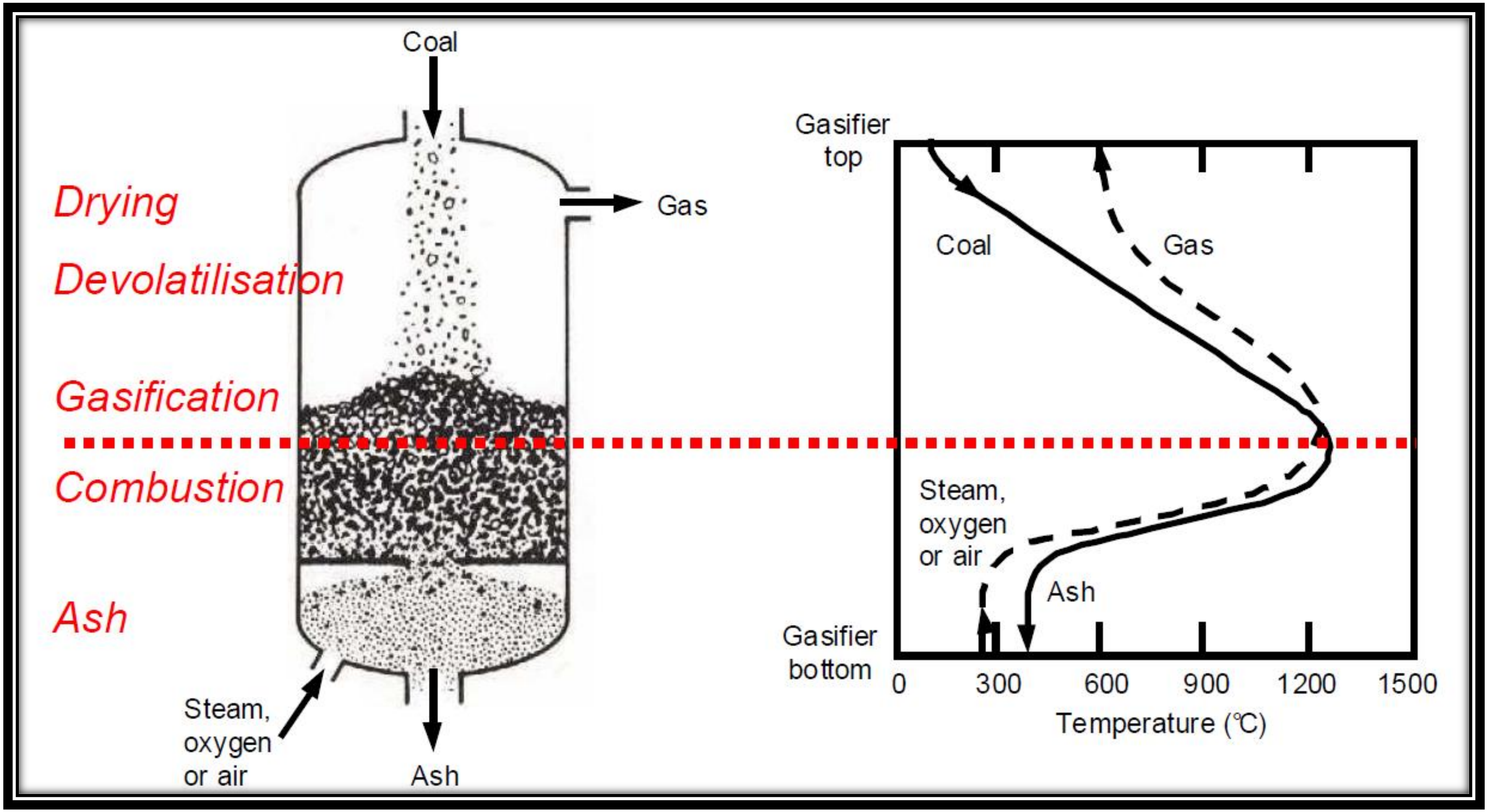
$C + 2 H_2 \rightarrow CH_4$

$CO + 3H_2 \rightarrow CH_4 + H_2O$

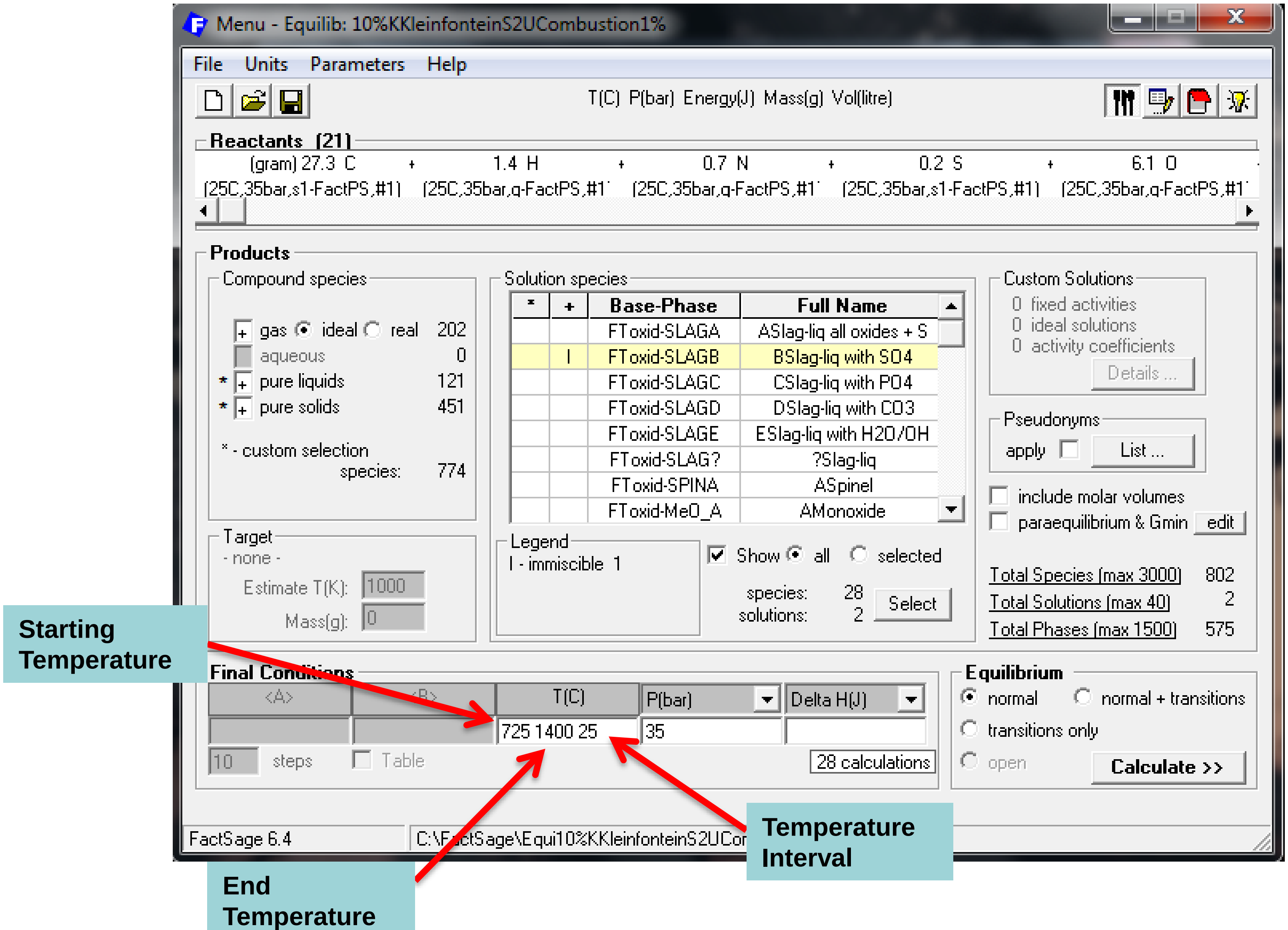
$3C + 2H_2O \rightarrow CH_4 + 2 CO$

FactSage Model of FBDB Gasifier

NORTH-WEST UNIVERSITY
YUNIBESITI YA BOKONE-BOPHIRIMA
NOORDWES-UNIVERSITEIT
POTCHEFSTROOM CAMPUS



FactSage Model



Reactants - Equilib

File Edit Table Units Data Search Help

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

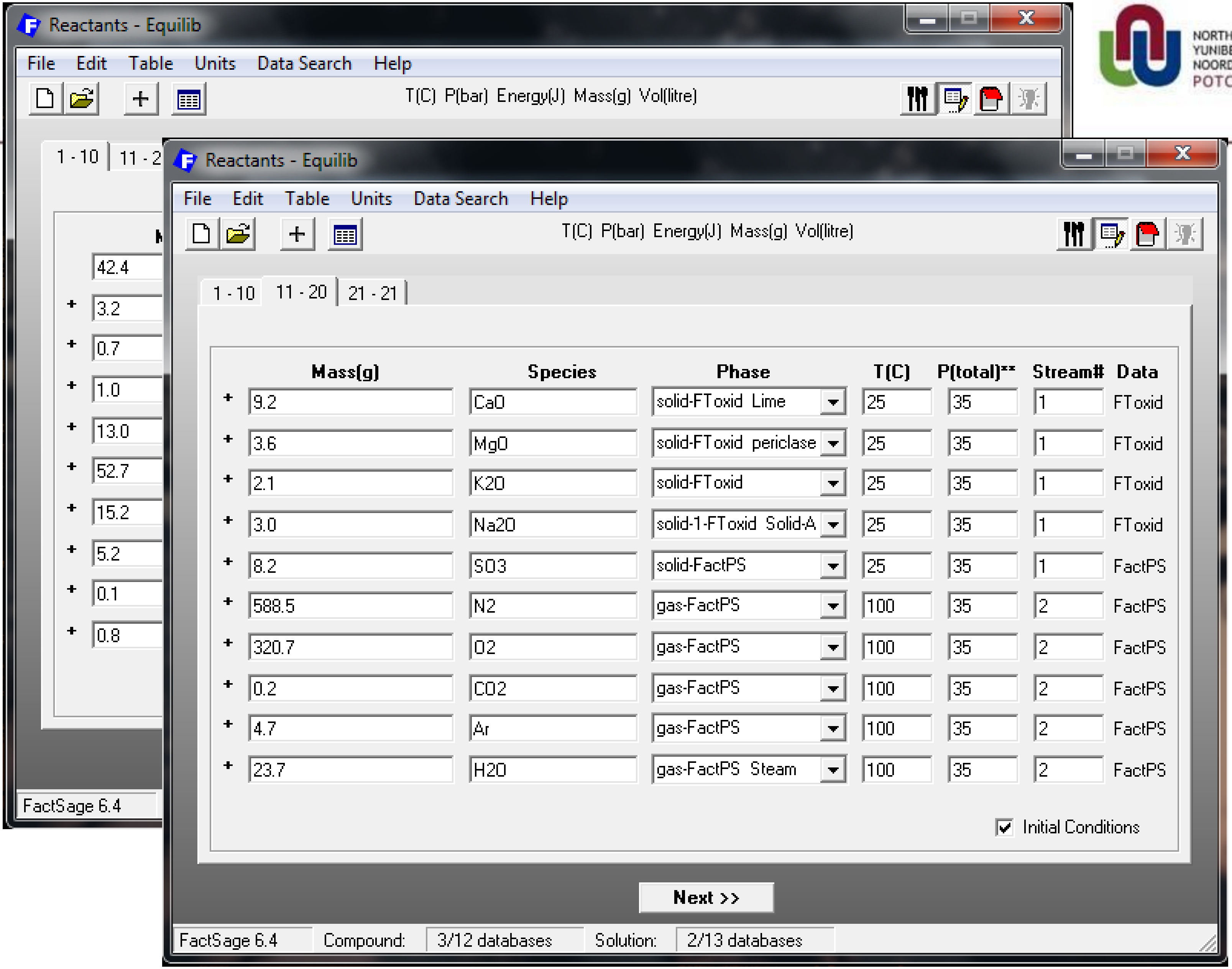
1 - 10 | 11 - 20 | 21 - 21

	Mass(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
	42.4	C	solid-1-FactPS Graphi	25	35	1	FactPS
+	3.2	H	gas-FactPS	25	35	1	FactPS
+	0.7	N	gas-FactPS	25	35	1	FactPS
+	1.0	S	solid-1-FactPS Orthorh	25	35	1	FactPS
+	13.0	O	gas-FactPS	25	35	1	FactPS
+	52.7	SiO2	solid-1-FToxid Quartz(	25	35	1	FToxid
+	15.2	Al2O3	solid-1-FToxid gamma	25	35	1	FToxid
+	5.2	Fe2O3	solid-1-FToxid hematit	25	35	1	FToxid
+	0.1	(P2O5)2	solid-FactPS	25	35	1	FactPS
+	0.8	TiO2	solid-1-FToxid Rutile	25	35	1	FToxid

☑ Initial Conditions

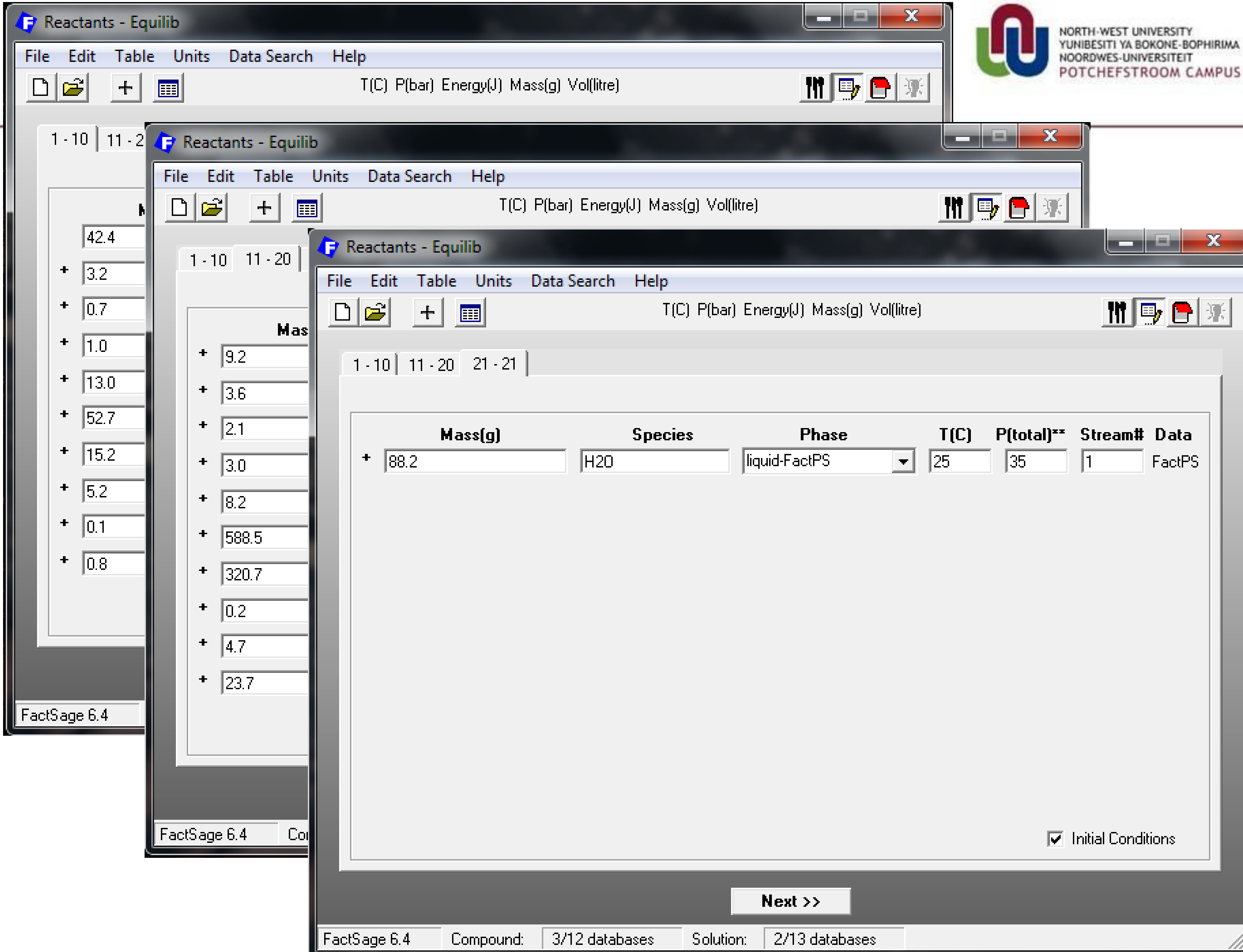
Next >>

FactSage 6.4 | Compound: 3/12 databases | Solution: 2/13 databases



	Mass(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
+	9.2	CaO	solid-FToxid Lime	25	35	1	FToxid
+	3.6	MgO	solid-FToxid periclase	25	35	1	FToxid
+	2.1	K2O	solid-FToxid	25	35	1	FToxid
+	3.0	Na2O	solid-1-FToxid Solid-A	25	35	1	FToxid
+	8.2	SO3	solid-FactPS	25	35	1	FactPS
+	588.5	N2	gas-FactPS	100	35	2	FactPS
+	320.7	O2	gas-FactPS	100	35	2	FactPS
+	0.2	CO2	gas-FactPS	100	35	2	FactPS
+	4.7	Ar	gas-FactPS	100	35	2	FactPS
+	23.7	H2O	gas-FactPS Steam	100	35	2	FactPS

NORTH-WEST UNIVERSITY
YUNIBESITI YA BOKONE-BOPHIRIMA
NOORDWES-UNIVERSITEIT
POTCHEFSTROOM CAMPUS



Coal samples

Coal sample	Coal Rank	Base/Acid Ratio	Acidity
KFS2U	Medium Volatile Bituminous Coal	0.05	18.4
L#2	Lignite Coal	0.34	2.95
MD	High Volatile Bituminous Coal	0.33	2.91
WFS1	Medium Volatile Bituminous Coal	0.16	6.31

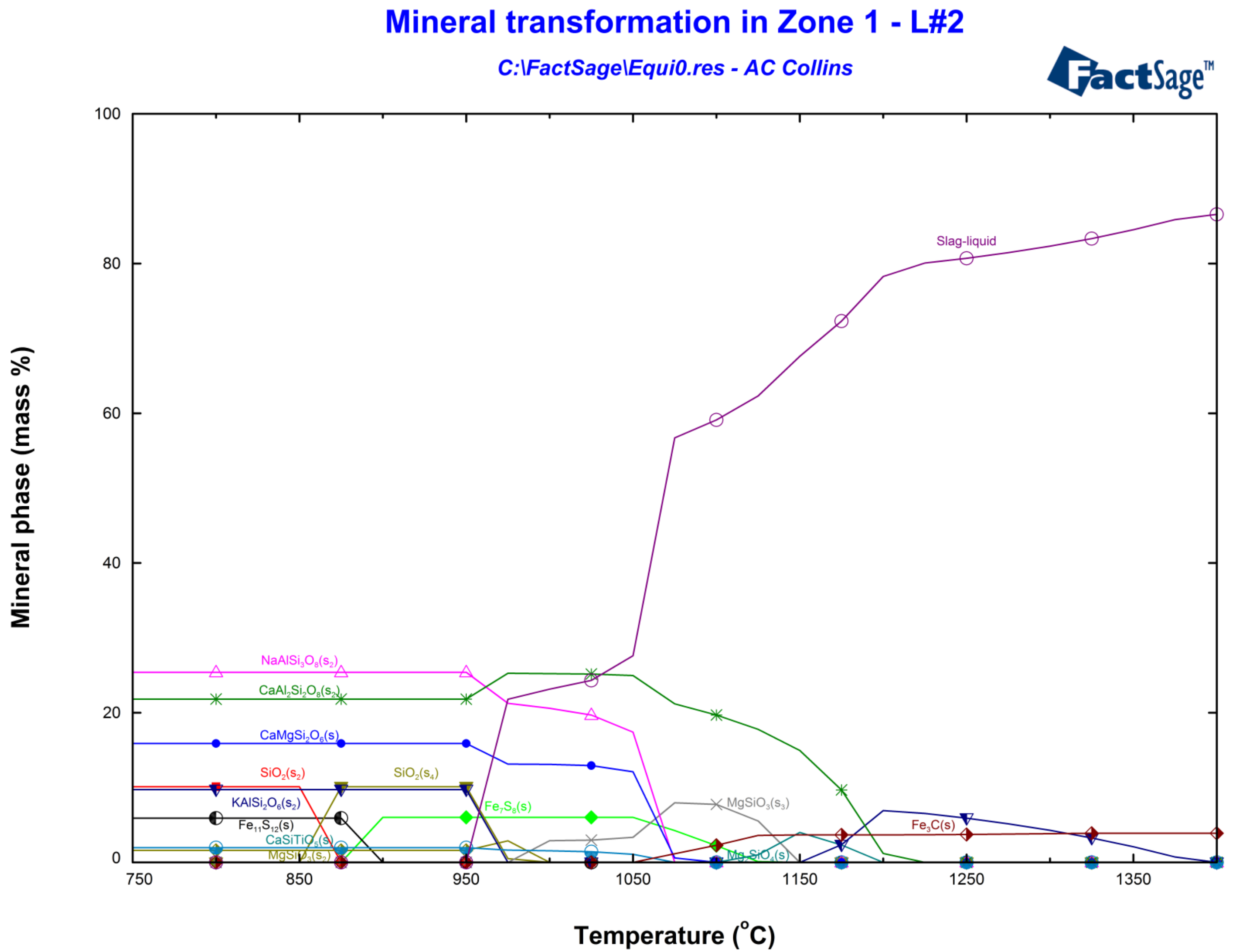
Characterization Results

	KFS2U	KFS2U + 10%K	L#2	L#2 + 10%K	MD	MD + 10%K	WFS1	WFS1 + 10%K
Proximate analysis								
Moisture content	3.3	2.7	18.0	26.2	3.7	2.9	4.0	3.8
Ash content	28.3	35.0	20.5	26.1	28.5	36.0	22.4	30.7
Volatile content	18.2	20.5	30.5	24.3	21.2	23.9	21.9	23.0
Fixed carbon	50.2	41.8	31.0	23.4	46.5	37.2	51.7	42.5
Ultimate analysis								
% C	56.4	47.8	43.3	32.8	53.7	45.6	59.1	50.6
% H	2.9	2.4	3.2	2.5	2.6	2.3	3.1	2.7
% N	1.2	1.2	0.7	0.6	1.3	1.2	1.4	1.2
% O	7.4	10.6	13.3	11.2	8.9	11.3	8.9	10.4
% S	0.5	0.3	1.0	0.5	1.3	0.8	1.1	0.8

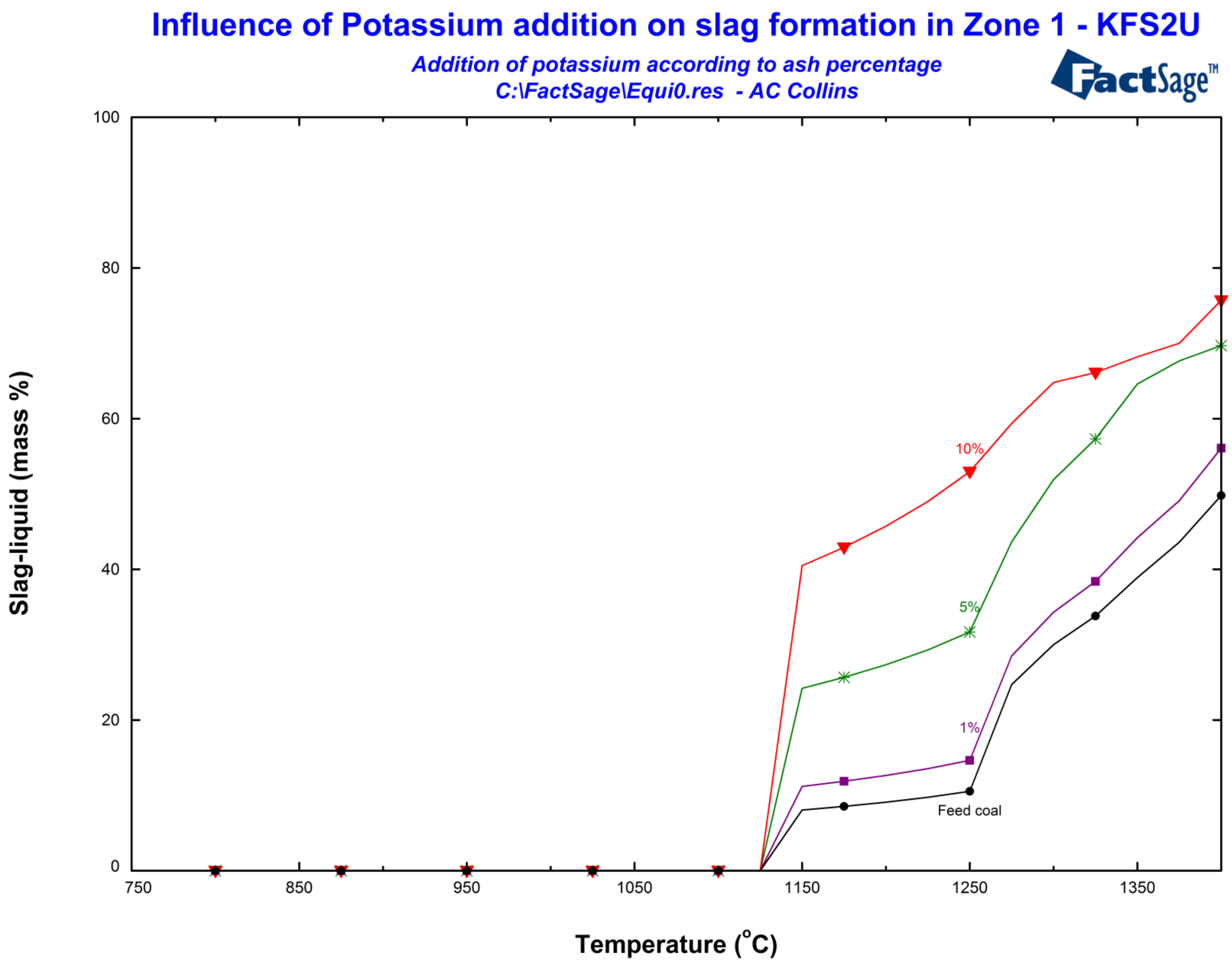
	KFS2U	KFS2U + 10%K	L#2	L#2 + 10%K	MD	MD + 10%K	WFS1	WFS1 + 10%K
<u>XRF</u>								
Al_2O_3	28.46	19.42	15.07	9.22	25.18	17.82	25.89	16.50
CaO	1.51	1.00	9.13	5.05	13.02	8.94	5.07	3.37
Cr_2O_3	0.12	0.02	0.03	nd	0.03	nd	0.03	0.02
Fe_2O_3	2.00	1.18	5.16	3.06	5.64	3.73	5.54	3.53
K_2O	0.69	29.79	2.06	38.78	1.11	27.61	0.43	31.82
MgO	0.78	0.52	3.52	2.02	3.15	2.18	1.81	1.20
MnO	0.03	0.03	0.05	0.03	0.07	0.05	0.05	0.04
Na_2O	Nd	0.17	2.94	1.88	nd	0.15	nd	0.27
P_2O_5	0.07	0.04	0.10	0.07	0.26	0.19	0.10	0.14
SiO_2	63.17	43.17	52.16	31.66	41.60	29.70	55.15	34.17
TiO_2	1.52	1.05	0.80	0.47	1.79	1.27	1.34	0.84
V_2O_5	0.02	0.02	0.02	0.02	0.02	0.02	0.03	0.03
ZrO_2	0.09	0.06	0.03	0.02	0.08	0.05	0.06	0.04
BaO	0.02	nd	0.56	0.33	0.15	0.11	0.08	0.07
SrO	0.02	0.01	0.25	0.14	0.27	0.19	0.07	0.08
SO_3	1.48	3.53	8.10	7.24	7.62	7.99	4.33	7.89

Drying, Devolatilization and Gasification Zone 1

Results

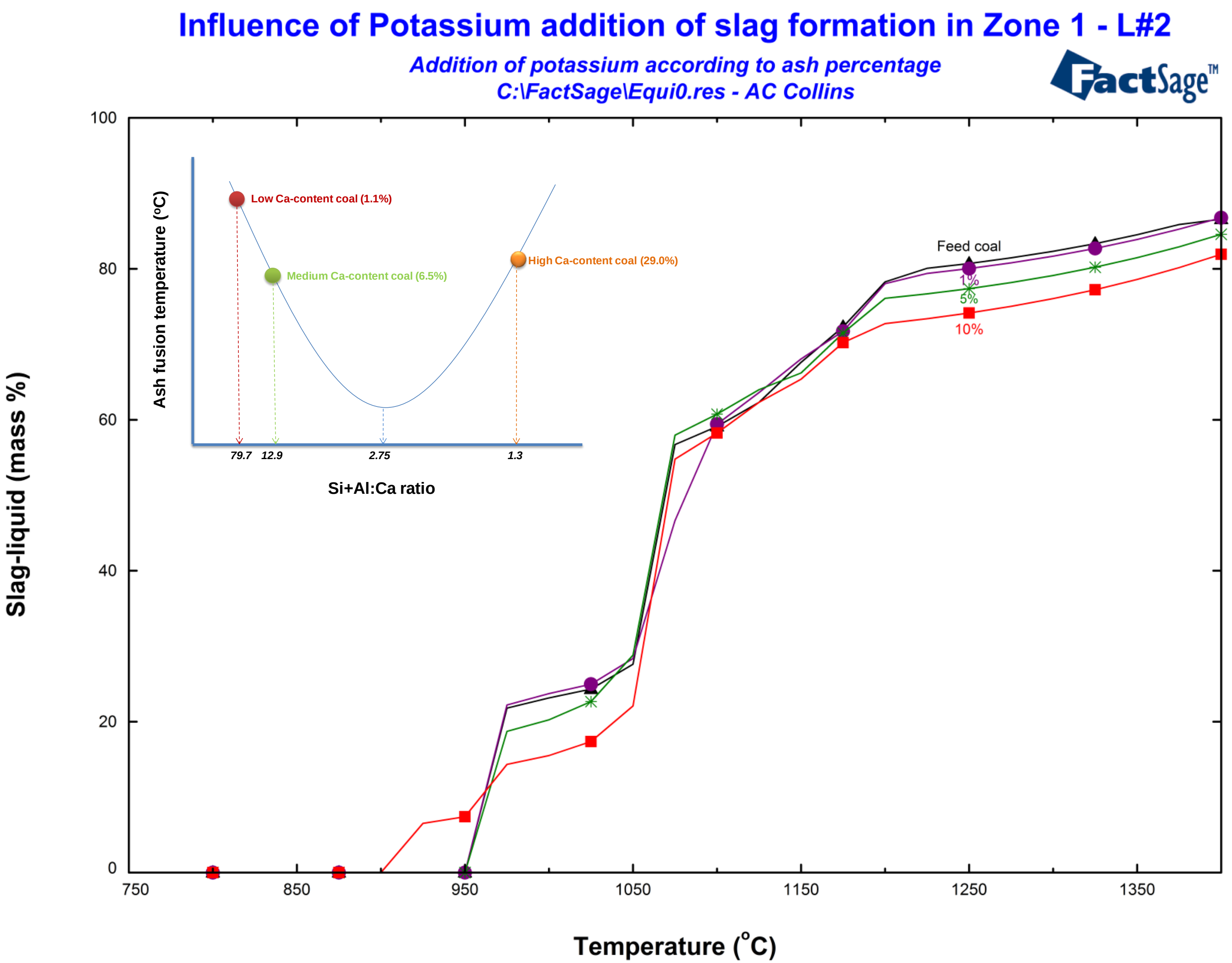

Mineral transformation in Zone 1 - L#2
C:\FactSage\Equi0.res - AC Collins
FactSage™
Mineral phase (mass %)
Temperature (°C)
0
20
40
60
80
100
750
850
950
1050
1150
1250
1350
Slag-liquid
NaAlSi3O8(s2)
CaAl2Si2O8(s2)
CaMgSi2O6(s)
SiO2(s2)
SiO2(s4)
KAlSi2O6(s2)
Fe11S12(s)
CaSiTiO5(s)
MgSiO3(s3)
Fe7S8(s)
MgSiO3(s2)
Mg2SiO4(s)
Fe3C(s)

Results


Influence of Potassium addition on slag formation in Zone 1 - KFS2U
Addition of potassium according to ash percentage
C:\FactSage\Equi0.res - AC Collins
FactSage™
Slag-liquid (mass %)
0
20
40
60
80
100
750
850
950
1050
1150
1250
1350
Temperature (°C)
10%
5%
1%
Feed coal

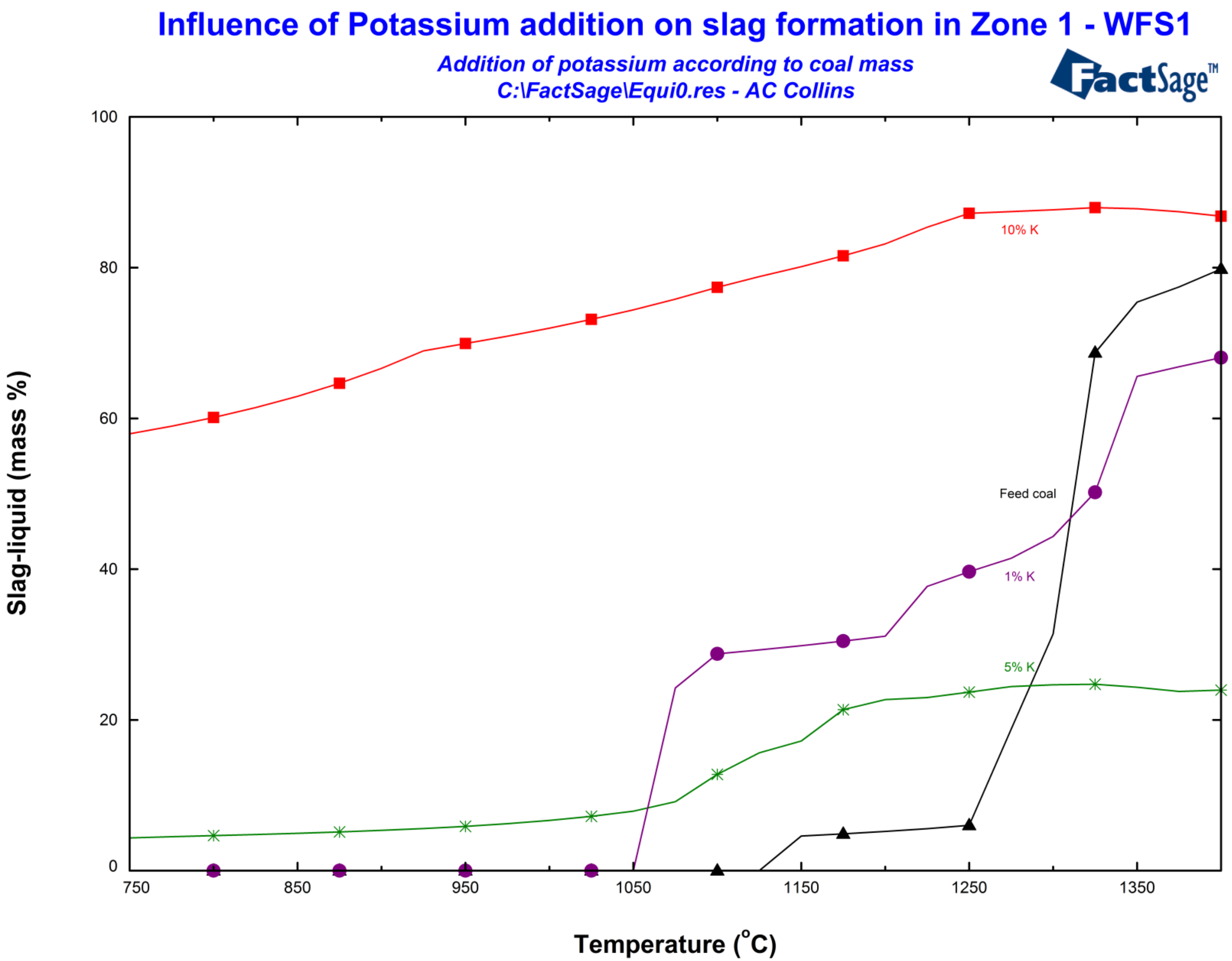
Results

NORTH-WEST UNIVERSITY
YUNIBESITI YA BOKONE-BOPHIRIMA
NOORDWES-UNIVERSITEIT
POTCHEFSTROOM CAMPUS

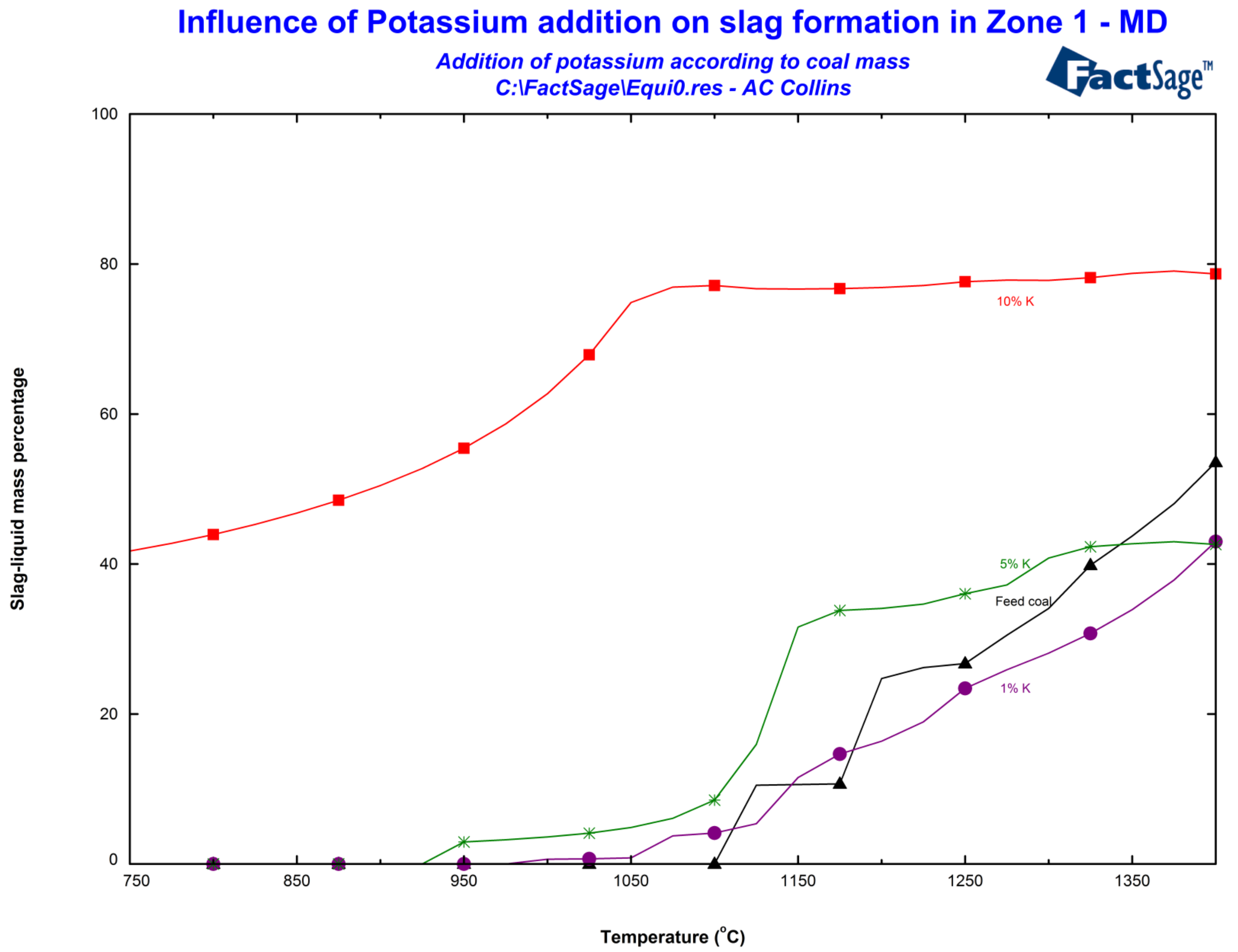


Results

NORTH-WEST UNIVERSITY
YUNIBESITI YA BOKONE-BOPHIRIMA
NOORDWES-UNIVERSITEIT
POTCHEFSTROOM CAMPUS



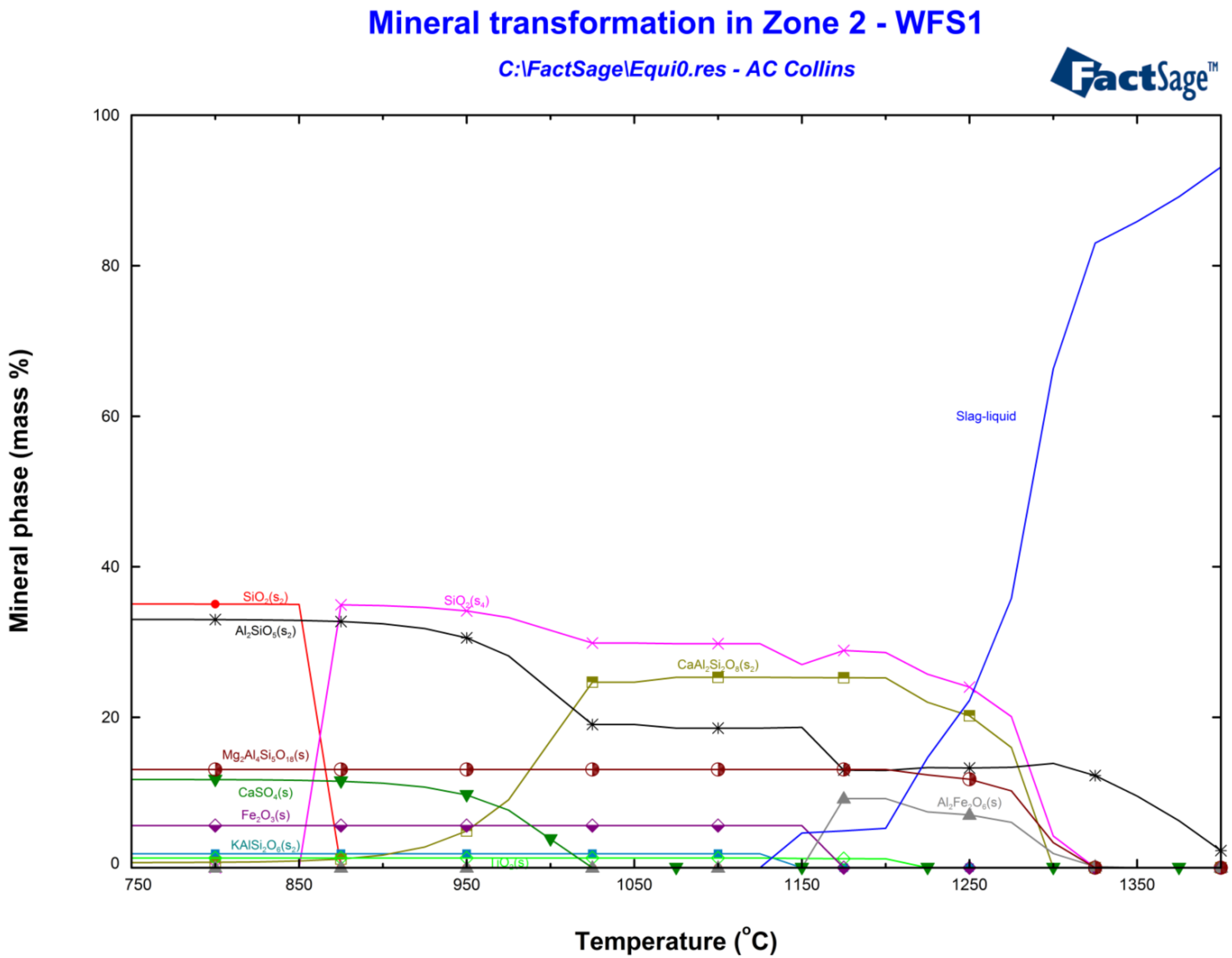
Results


Influence of Potassium addition on slag formation in Zone 1 - MD
Addition of potassium according to coal mass
C:\FactSage\Equi0.res - AC Collins
FactSage™
Slag-liquid mass percentage
Temperature (°C)
10% K
5% K
Feed coal
1% K
0
20
40
60
80
100
750
850
950
1050
1150
1250
1350

Combustion and Ash
Zone 2

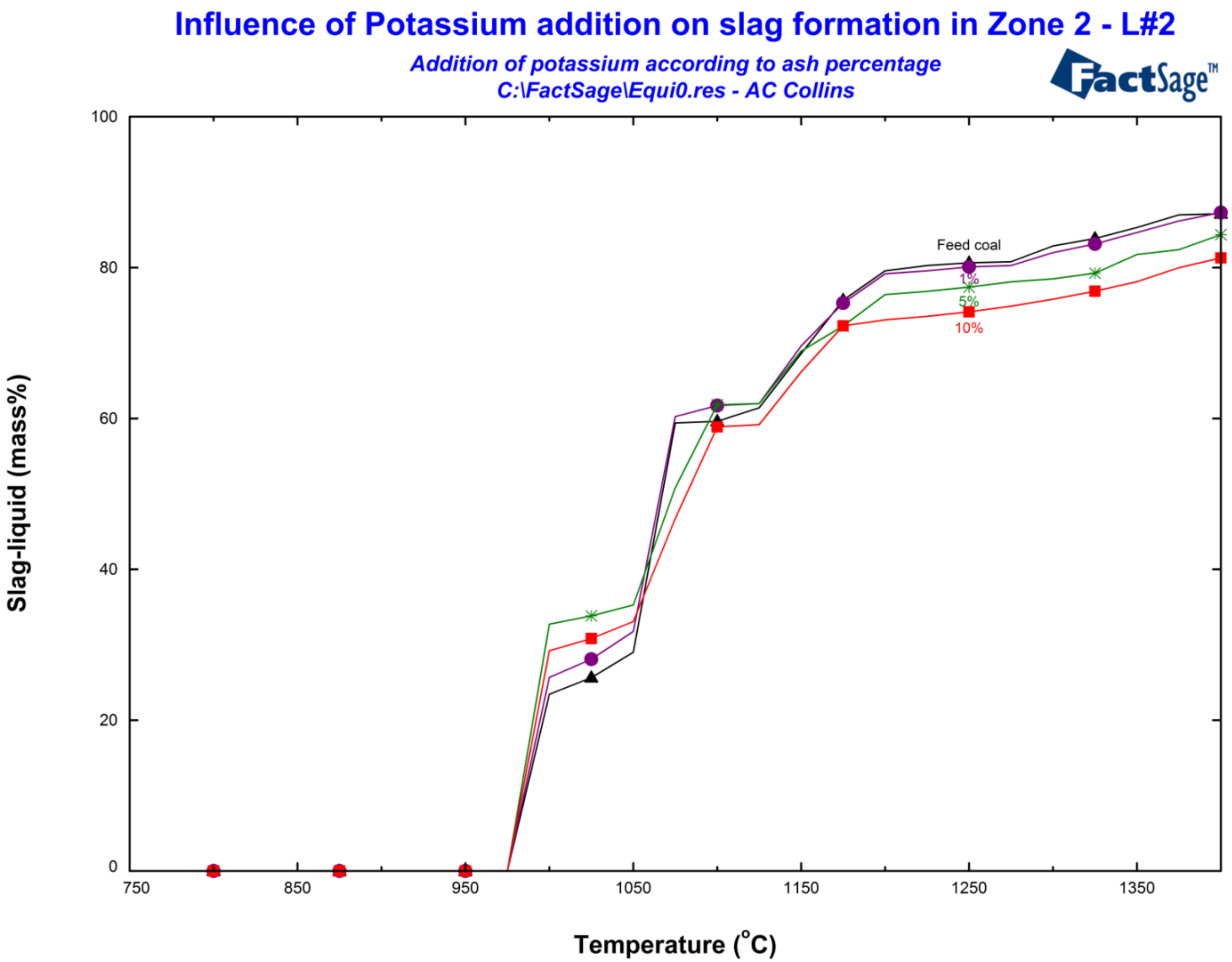
Results

NORTH-WEST UNIVERSITY
YUNIBESITI YA BOKONE-BOPHIRIMA
NOORDWES-UNIVERSITEIT
POTCHEFSTROOM CAMPUS



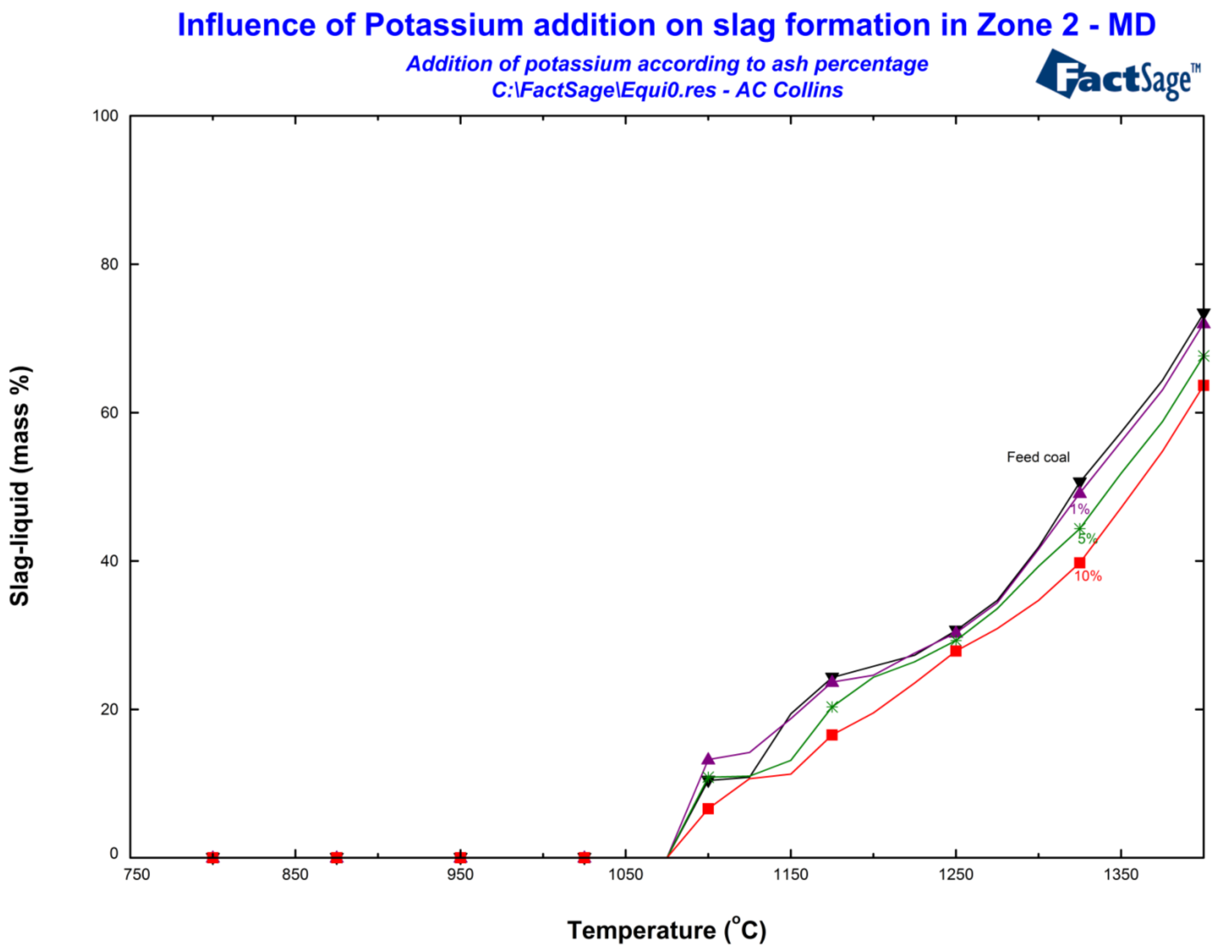
Cooling process in combustion zone

Results



Cooling process in combustion zone

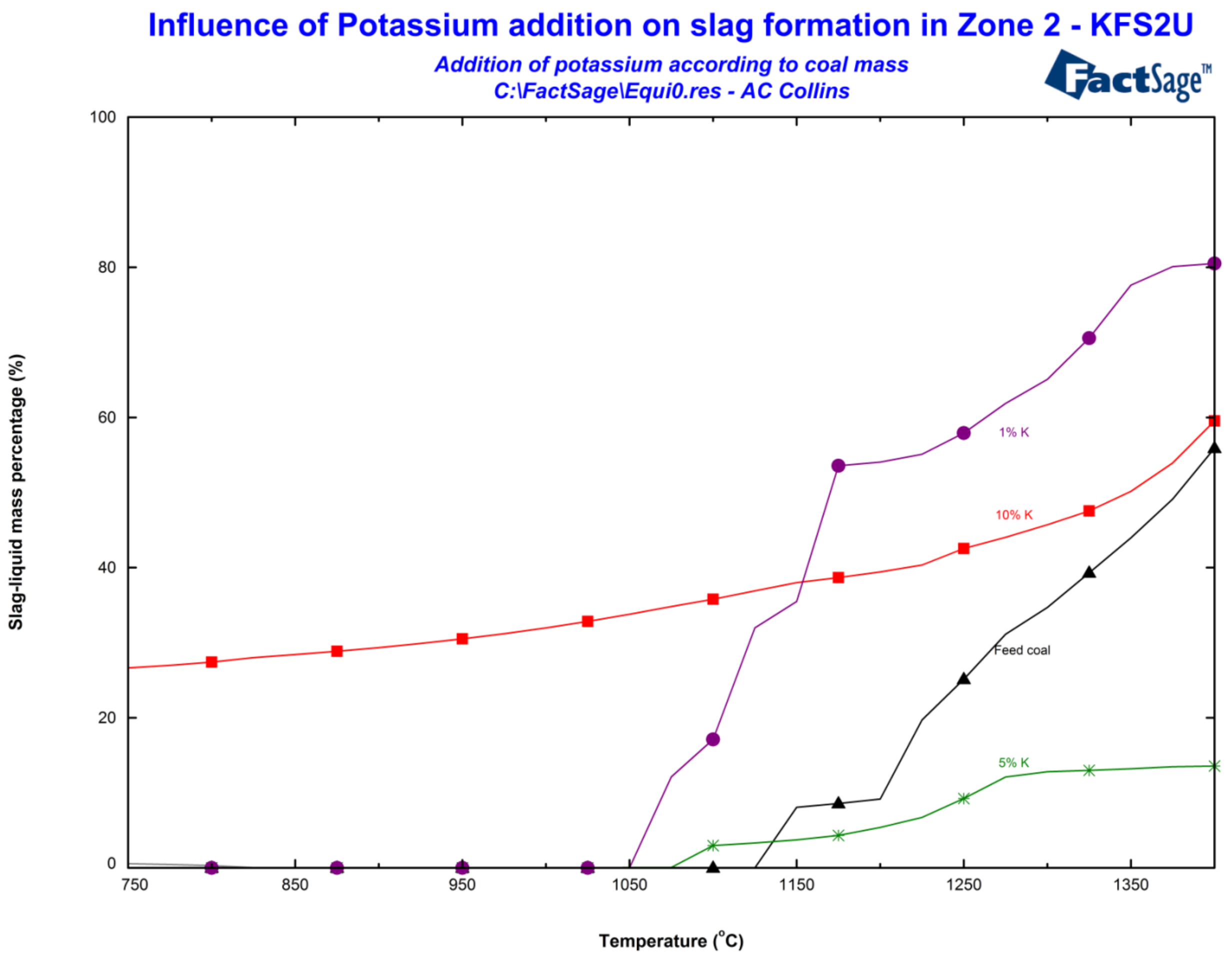
Results



Cooling process in combustion zone

Results

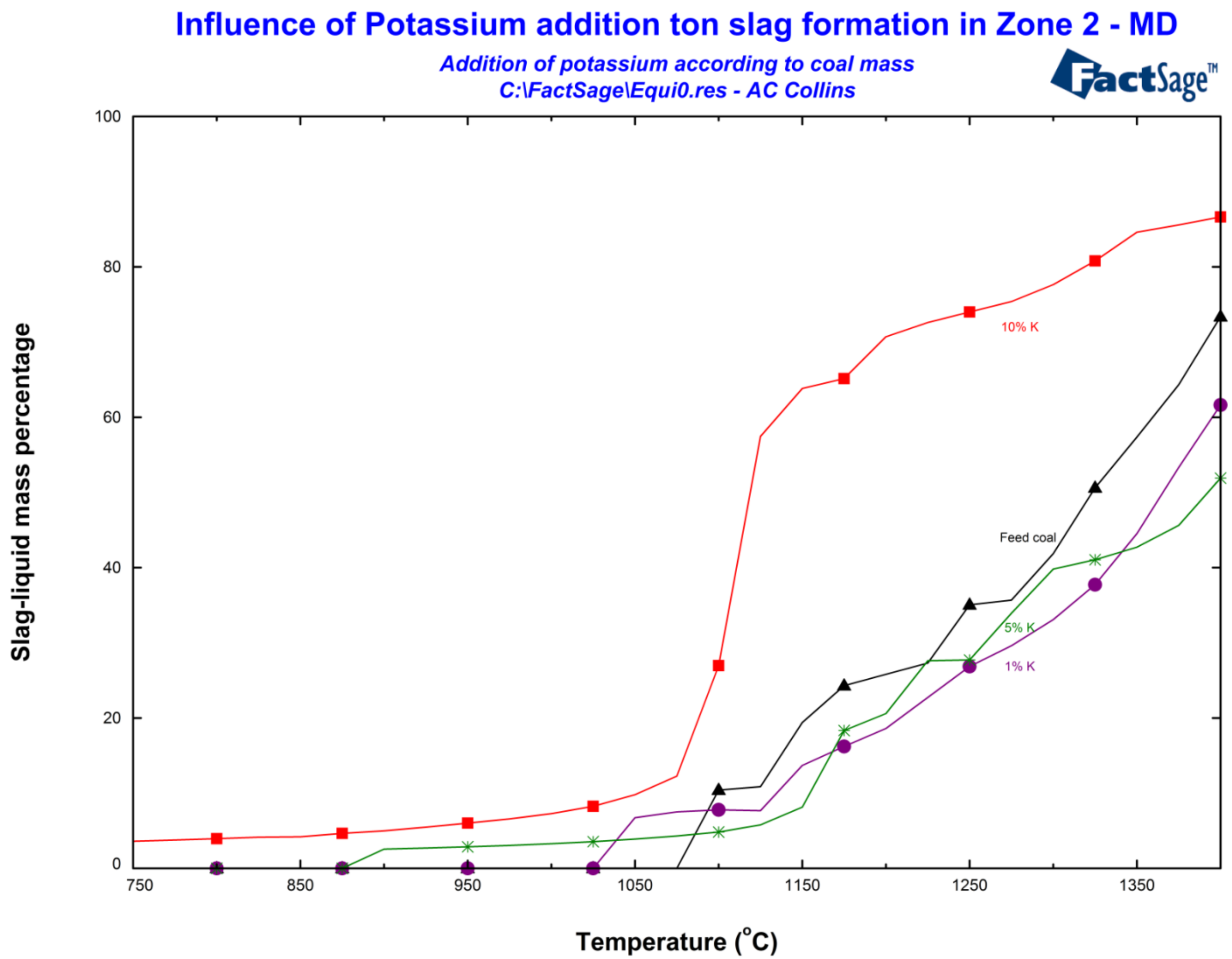
NORTH-WEST UNIVERSITY
YUNIBESITI YA BOKONE-BOPHIRIMA
NOORDWES-UNIVERSITEIT
POTCHEFSTROOM CAMPUS



Cooling process in combustion zone

Results

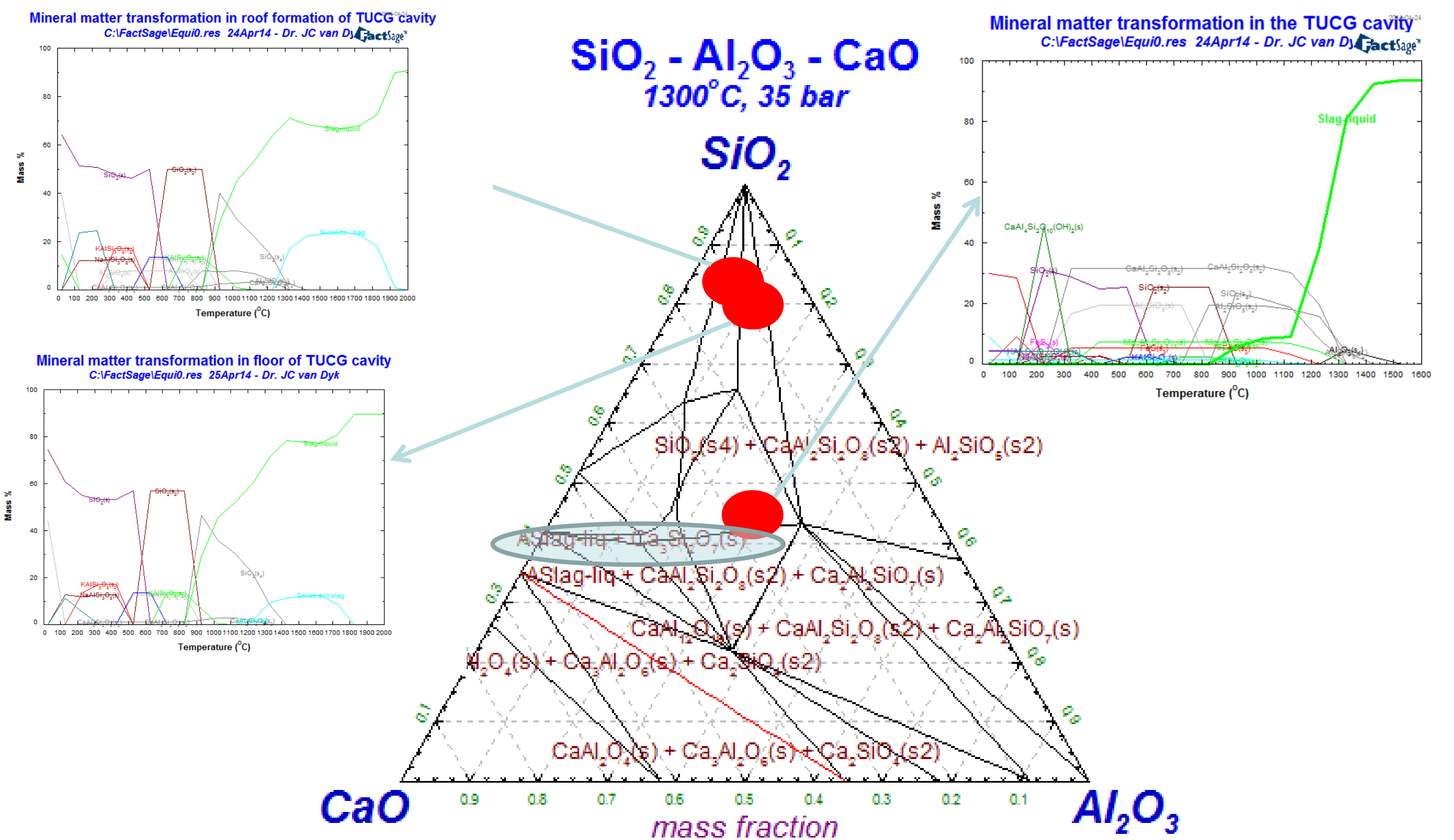
NORTH-WEST UNIVERSITY
YUNIBESITI YA BOKONE-BOPHIRIMA
NOORDWES-UNIVERSITEIT
POTCHEFSTROOM CAMPUS



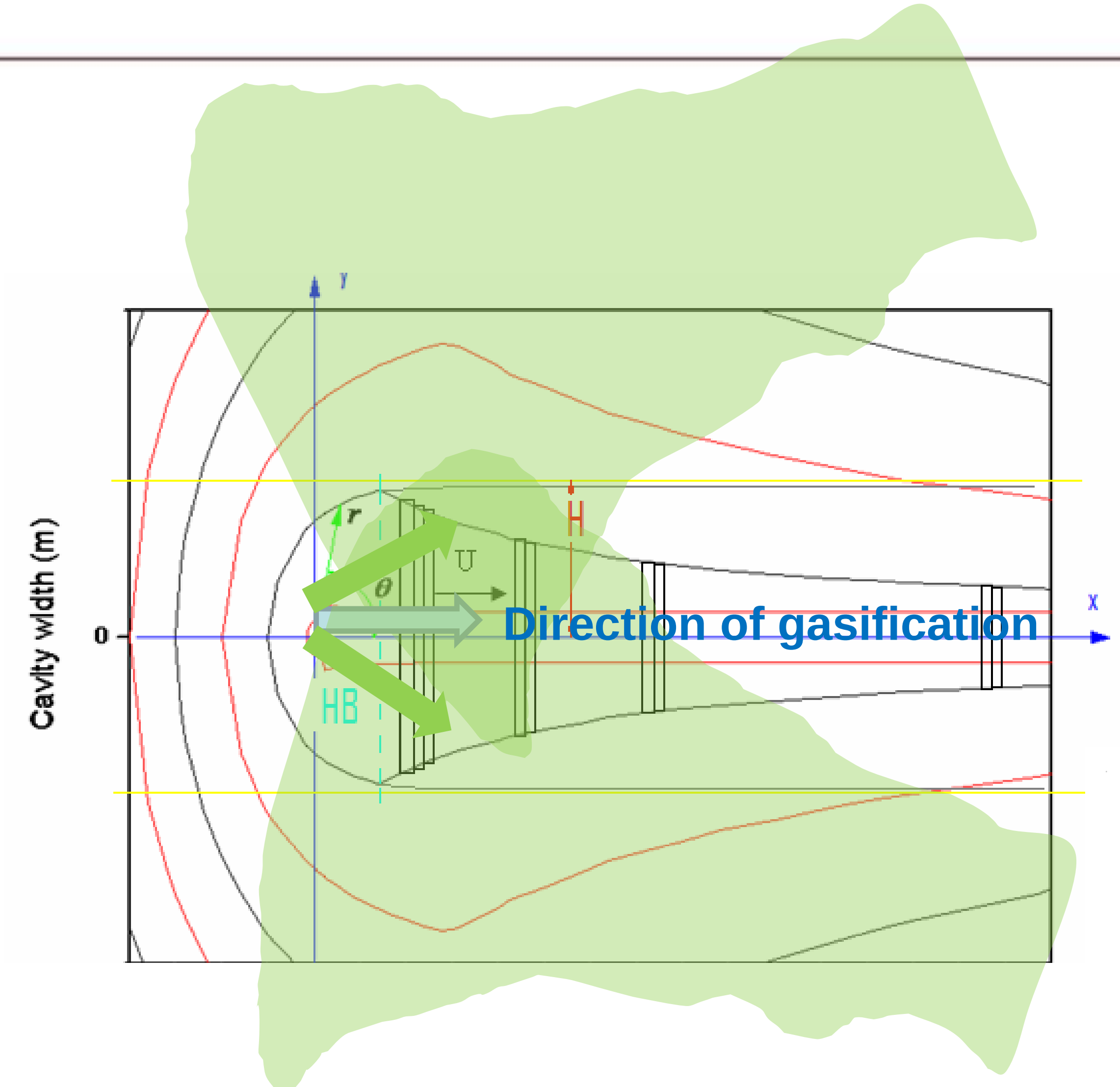
Cooling process in combustion zone

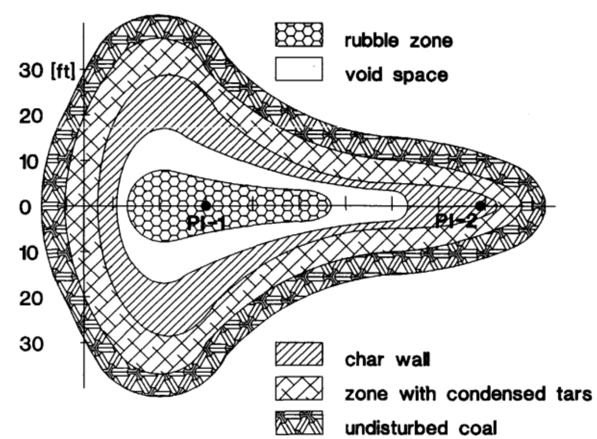
Gasification science – mineral transformation and ash behaviour

NORTH-WEST UNIVERSITY
YUNIBESITI YA BOKONE-BOPHIRIMA
NOORDWES-UNIVERSITEIT
POTCHEFSTROOM CAMPUS



What next on UCG simulations?

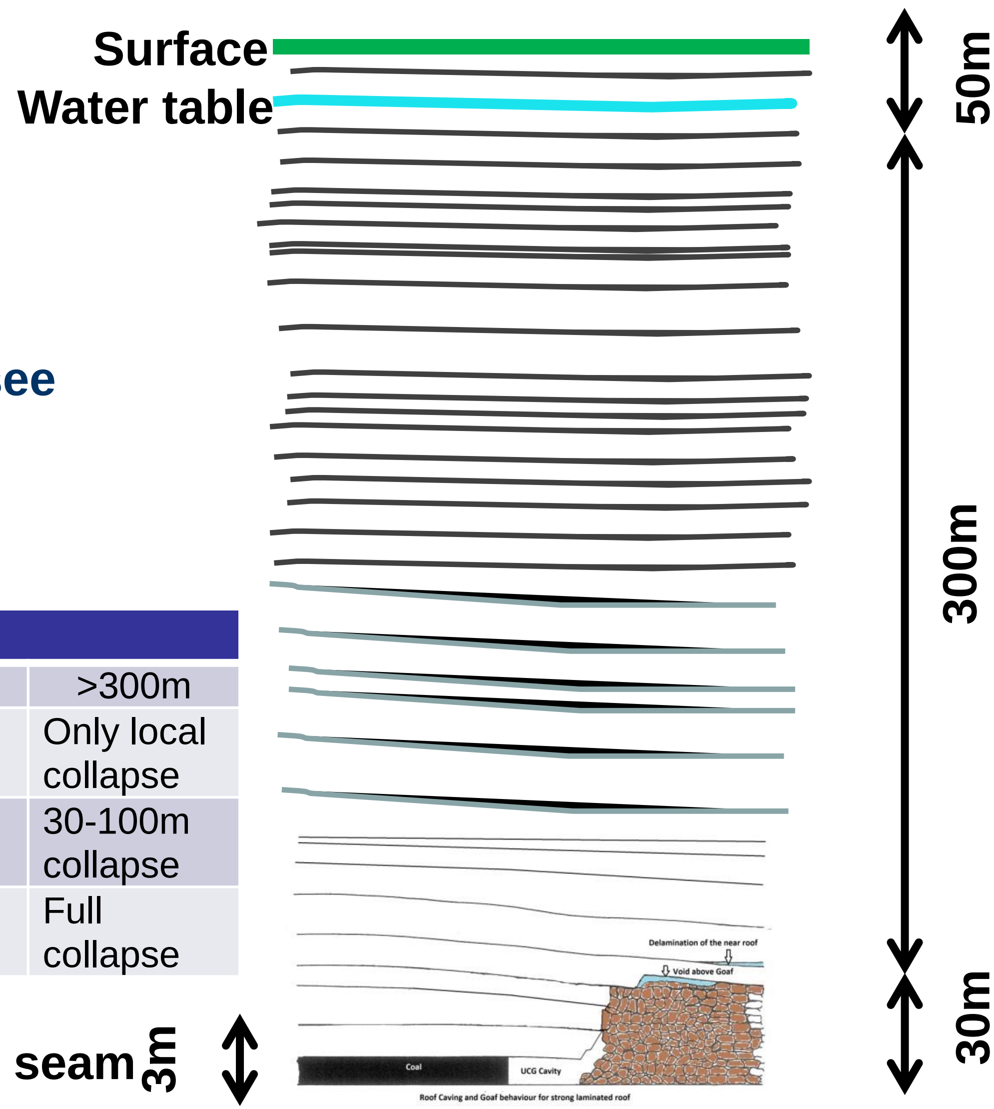




Geophysical study

NORTH-WEST UNIVERSITY
YUNIBESITI YA BOKONE-BOPHIRIMA
NOORDWES-UNIVERSITEIT
POTCHEFSTROOM CAMPUS

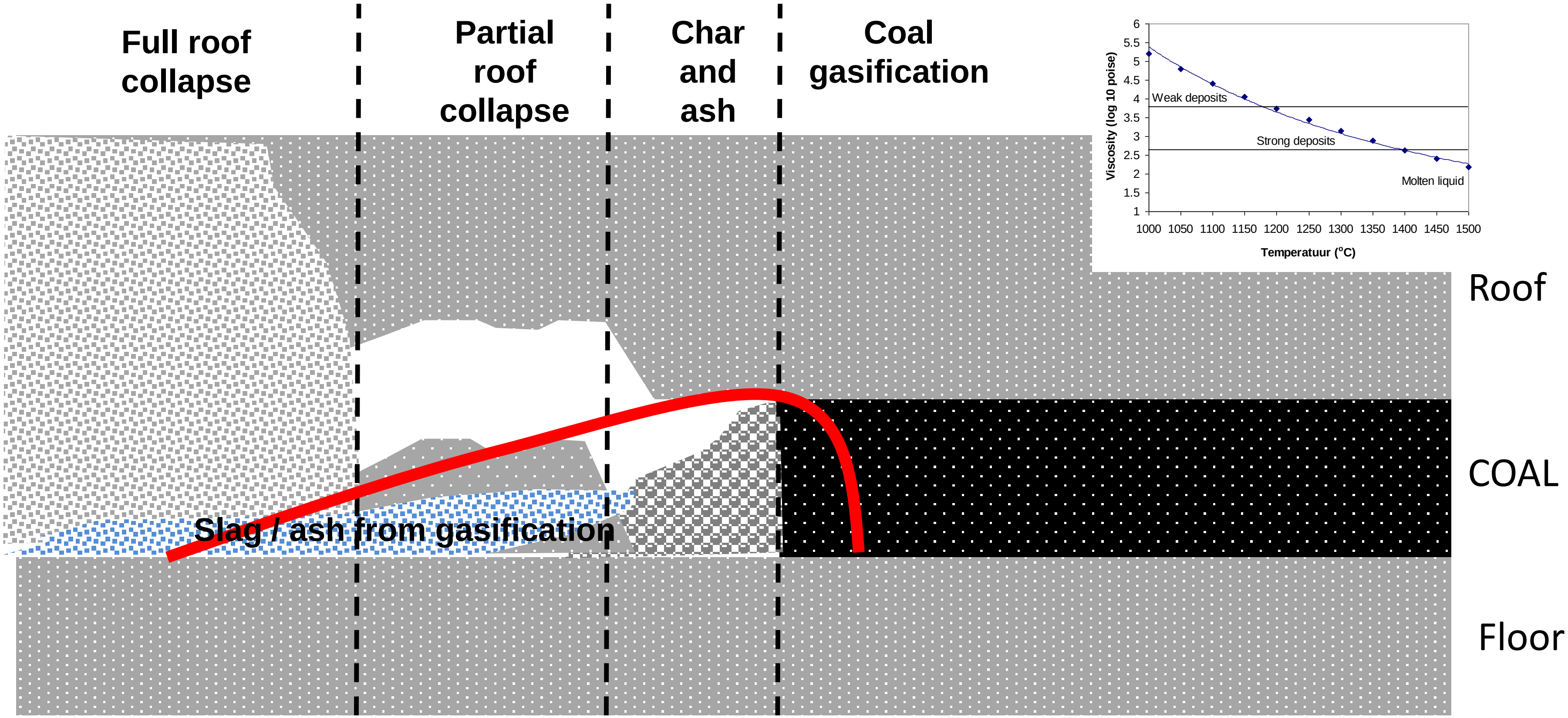
Not to Scale!
(Otherwise you will not be able to see what is happening…)



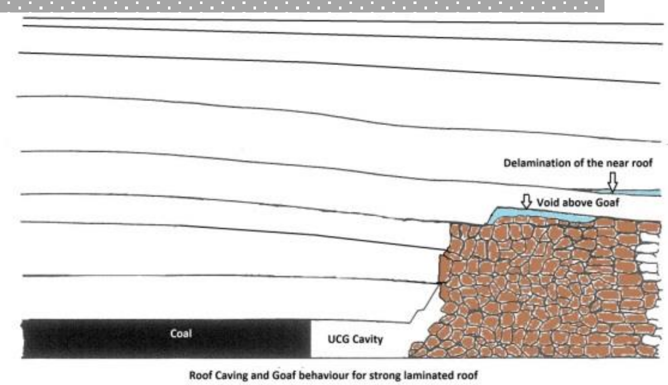
		ADVANCE		
		100m	100-300m	>300m
Cavity Width	0-100m	Only local collapse	Only local collapse	Only local collapse
	100-300m	Only local collapse	30-100m collapse	30-100m collapse
	>300m	Only local collapse	30-100m collapse	Full collapse

Stable ΣΣX Strata Consulting

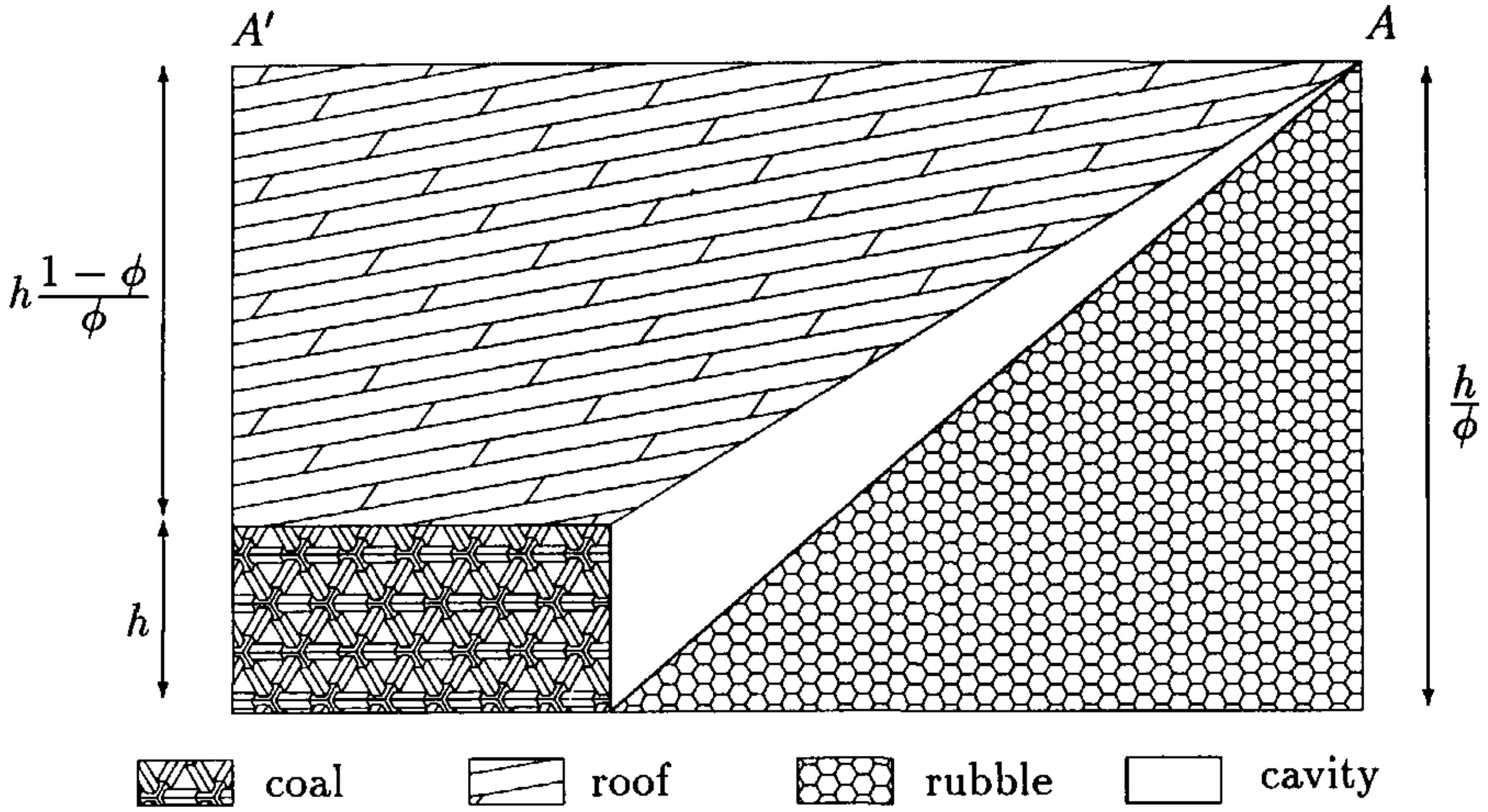
The approach!



		ADVANCE		
		100m	100-300m	>300m
Cavity Width	0-100m	Only local collapse	Only local collapse	Only local collapse
	100-300m	Only local collapse	30-100m collapse	30-100m collapse
	>300m	Only local collapse	30-100m collapse	Full collapse



Approach from Batenburg (Delft)



Conclusions

NORTH-WEST UNIVERSITY
YUNIBESITI YA BOKONE-BOPHIRIMA
NOORDWES-UNIVERSITEIT
POTCHEFSTROOM CAMPUS

- **Percentage K added according to ash percentage:**
  - Similar trend for all the percentage simulations for a coal sample;
  - Behavior dependent on the coal composition;

    i.e. KFS2U = ↑ in slag formation with ↑ % K

    L#2 = ↓ in slag formation with ↑ % K

    MD = ↓ in slag formation with ↑ % K

  Slag formation temperatures does not vary much due to small increase in % K.
- **High concentrations (10%) K added to the coal:**
  - High percentage slag formed,
  - Lower slag formation temperatures.
- **Concentrations (1 & 5%) K added to the coal:**
  - Different slag percentages, dependent on coal mineral composition,
  - Lower slag formation temperatures.

Conclusions

NORTH-WEST UNIVERSITY
YUNIBESITI YA BOKONE-BOPHIRIMA
NOORDWES-UNIVERSITEIT
POTCHEFSTROOM CAMPUS

- **Mineral transformation and slag formation is depended on the operating temperatures;**
- **Lower operating temperatures may produce mineral species, which will be leachable from the ash;**
    - Lower temperatures indicate higher percentage of solid mineral species present that at temperatures > 1000°C.
- **The mineral composition and acid/base ratio for the different coal types influences the slag formation temperatures and mineral transformation.**

Upcoming International Conference in South-Africa

NORTH-WEST UNIVERSITY
YUNIBESITI YA BOKONE-BOPHIRIMA
NOORDWES-UNIVERSITEIT
POTCHEFSTROOM CAMPUS

Thank You