

# **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**

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JF Brand



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# Motivation

F Results - Equilib 850 C (page 2)

Output Edit Show Pages

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

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

```

+ 2.9254E-04 wt.% K2SO4                                FToxicid
+ 1.9686E-06 wt.% CaSO4                                FToxicid
+ 2.5313E-11 wt.% MgSO4                                FToxicid)

+ 0      gram BSlag-liq#2
(850 C, 35 bar,          a=0.777612)
( 5.2014E-07 wt.% MgO                                FToxicid
+ 82.741      wt.% SiO2                                FToxicid
+ 0.28498      wt.% TiO2                                FToxicid
+ 4.9280E-13 wt.% Ti2O3                                FToxicid
+ 4.7868E-02 wt.% CaO                                FToxicid
+ 7.2650      wt.% Al2O3                                FToxicid
+ 9.6604      wt.% K2O                                FToxicid
+ 1.5724E-06 wt.% Fe2O3                                FToxicid
+ 6.4207E-11 wt.% Fe2(SO4)3                                FToxicid
+ 2.9141E-04 wt.% K2SO4                                FToxicid
+ 1.8949E-06 wt.% CaSO4                                FToxicid
+ 2.5330E-11 wt.% MgSO4                                FToxicid)

+ 28.630      gram CaAl2Si2O8_Anorthite
(28.630 gram, 0.10291 mol)
(850 C, 35 bar, S? =1 00000)                                FToxicid

```

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

# Motivation

The screenshot shows the Equilib software interface with two windows open. The main window is titled 'Results - Equilib 850 C (page 6/28)' and contains a list of mineral compositions. A secondary window, titled 'Results - Equilib 950 C (page 10/28)', is overlaid and has a yellow circle drawn around its title bar. This secondary window also lists mineral compositions. Several specific entries in the 950 C window are highlighted with red boxes: TiO2, Ti2O3, Al2O3, and K2O.

```

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 |

+ 0
+ 0      gram BSlag-liq#2
(950 C, 35 bar, a=0.85333)
+ 8.4460E-06 wt.% MgO
+ 82.669   wt.% SiO2
+ 0.55450   wt.% TiO2
+ 2.0522E-11 wt.% Ti2O3
+ 5.6647E-02 wt.% CaO
+ 7.4404    wt.% Al2O3
+ 9.2791    wt.% K2O
+ 1.2954E-05 wt.% Fe2O3
+ 8.1995E-10 wt.% Fe2(SO4)3
+ 4.3391E-04 wt.% K2SO4
+ 3.4762E-06 wt.% CaSO4
+ 6.3759E-10 wt.% MgSO4

+ 28.630
(28.630 g)
+ 31.621    gram CaAl2Si2O8_Anorthite
(31.621 gram, 0.11366 mol)
(950 C, 35 bar, S2, a=1.0000)

+ 23.221    gram Mn2Al4Si5O18_Cordierite

```

# Motivation

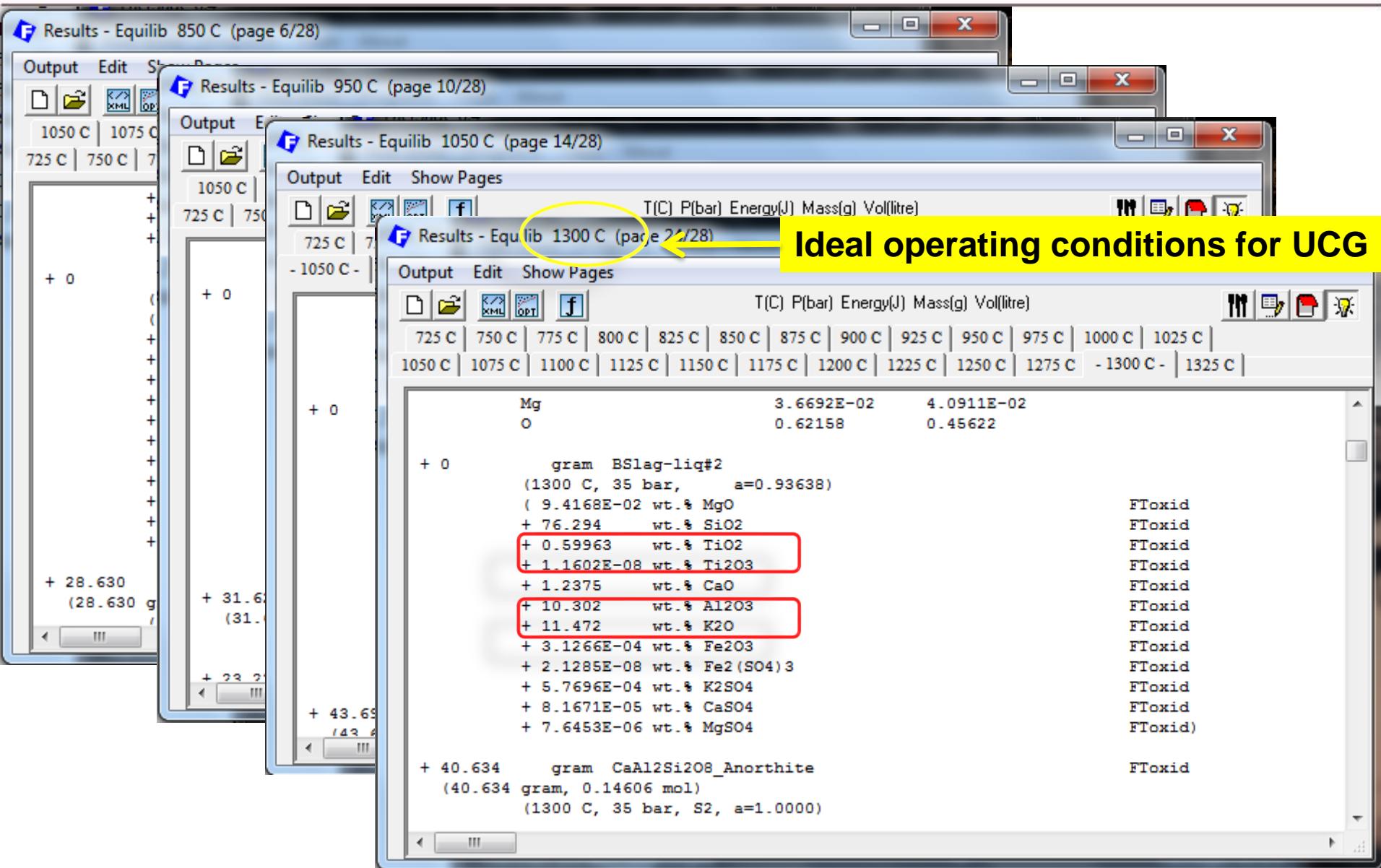
The screenshot displays three windows of the Equilib software, each representing a different temperature run:

- Top Window (850 C):** Shows results for 850 C, with a list of components including Fe<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub>, K<sub>2</sub>SO<sub>4</sub>, CaSO<sub>4</sub>, and MgSO<sub>4</sub>.
- Middle Window (950 C):** Shows results for 950 C, with a list of components including Fe<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub>, K<sub>2</sub>SO<sub>4</sub>, CaSO<sub>4</sub>, and MgSO<sub>4</sub>.
- Bottom Window (1050 C):** Shows results for 1050 C. This window has a yellow circle around its title bar. It lists various components with their compositions and toxicity information (FToxid). Two specific entries for TiO<sub>2</sub> and Al<sub>2</sub>O<sub>3</sub> are highlighted with red boxes.

**1050 C Results (Bottom Window):**

Component	Composition (wt.%)	Toxicity
+ 5.6994E-09	wt.% Fe <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>	FToxid
+ 7.9741E-04	wt.% K <sub>2</sub> SO <sub>4</sub>	FToxid
+ 1.1864E-05	wt.% CaSO <sub>4</sub>	FToxid
+ 2.9759E-08	wt.% MgSO <sub>4</sub>	FToxid)
+ 0	gram BSlag-liq#2 (1050 C, 35 bar, a=0.73675)	
+ 1.0490	wt.% MgO	FToxid
+ 53.012	wt.% SiO <sub>2</sub>	FToxid
+ 11.684	wt.% TiO <sub>2</sub>	FToxid
+ 2.5379E-05	wt.% Ti <sub>2</sub> O <sub>3</sub>	FToxid
+ 8.2105	wt.% CaO	FToxid
+ 12.530	wt.% Al <sub>2</sub> O <sub>3</sub>	FToxid
+ 0.12467	wt.% K <sub>2</sub> O	FToxid
+ 13.331	wt.% Fe <sub>2</sub> O <sub>3</sub>	FToxid
+ 3.4885E-02	wt.% Fe <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>	FToxid
+ 2.4101E-04	wt.% K <sub>2</sub> SO <sub>4</sub>	FToxid
+ 2.0830E-02	wt.% CaSO <sub>4</sub>	FToxid
+ 3.2739E-03	wt.% MgSO <sub>4</sub>	FToxid)
+ 43.695	gram CaAl <sub>2</sub> Si <sub>2</sub> O <sub>8</sub> _Anorthite (43.695 gram 0 15706 mol)	FToxid

# Motivation

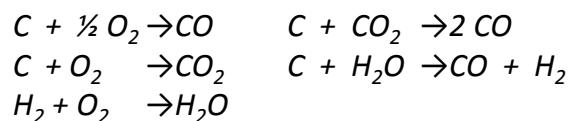
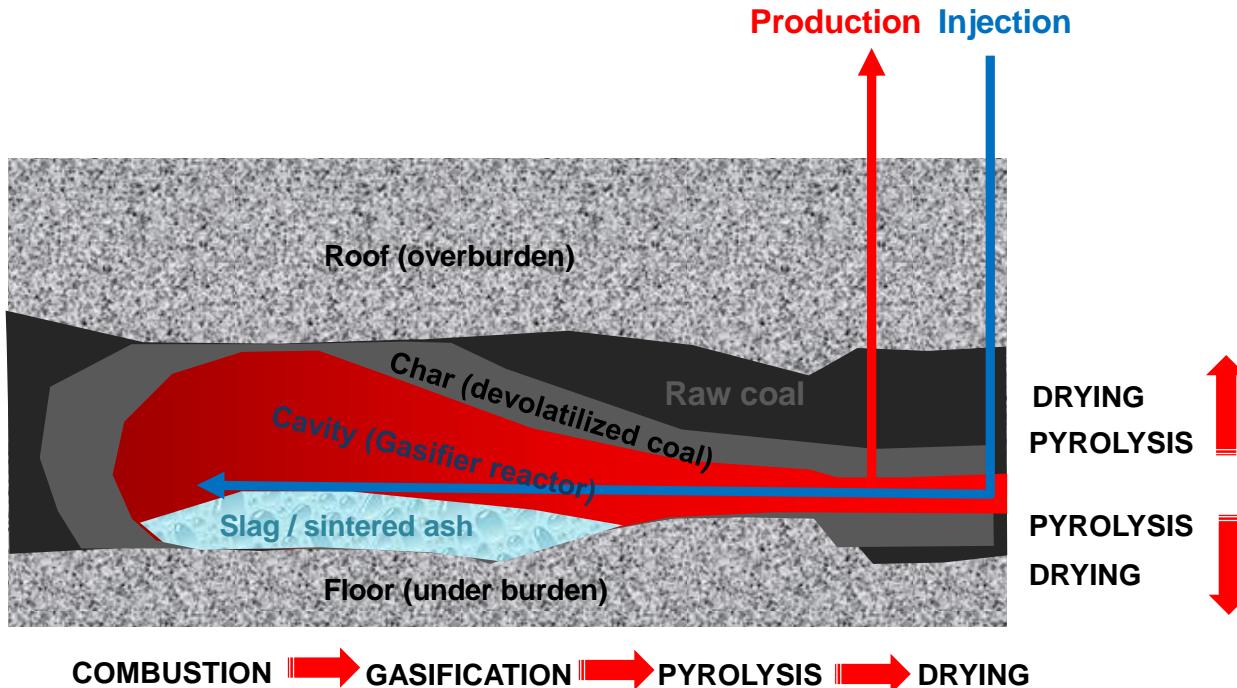


# Motivation

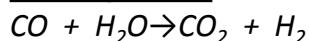
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- The influence of operating temperature on mineral species;
- Determination of whether these species are recoverable/leachable from the ash or lost/captured in the slag;
- The influence of gasification temperature on the slagging behaviour of coal 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.

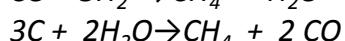
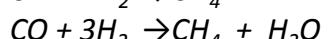
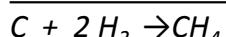
# FactSage Model of UCG Gasifier



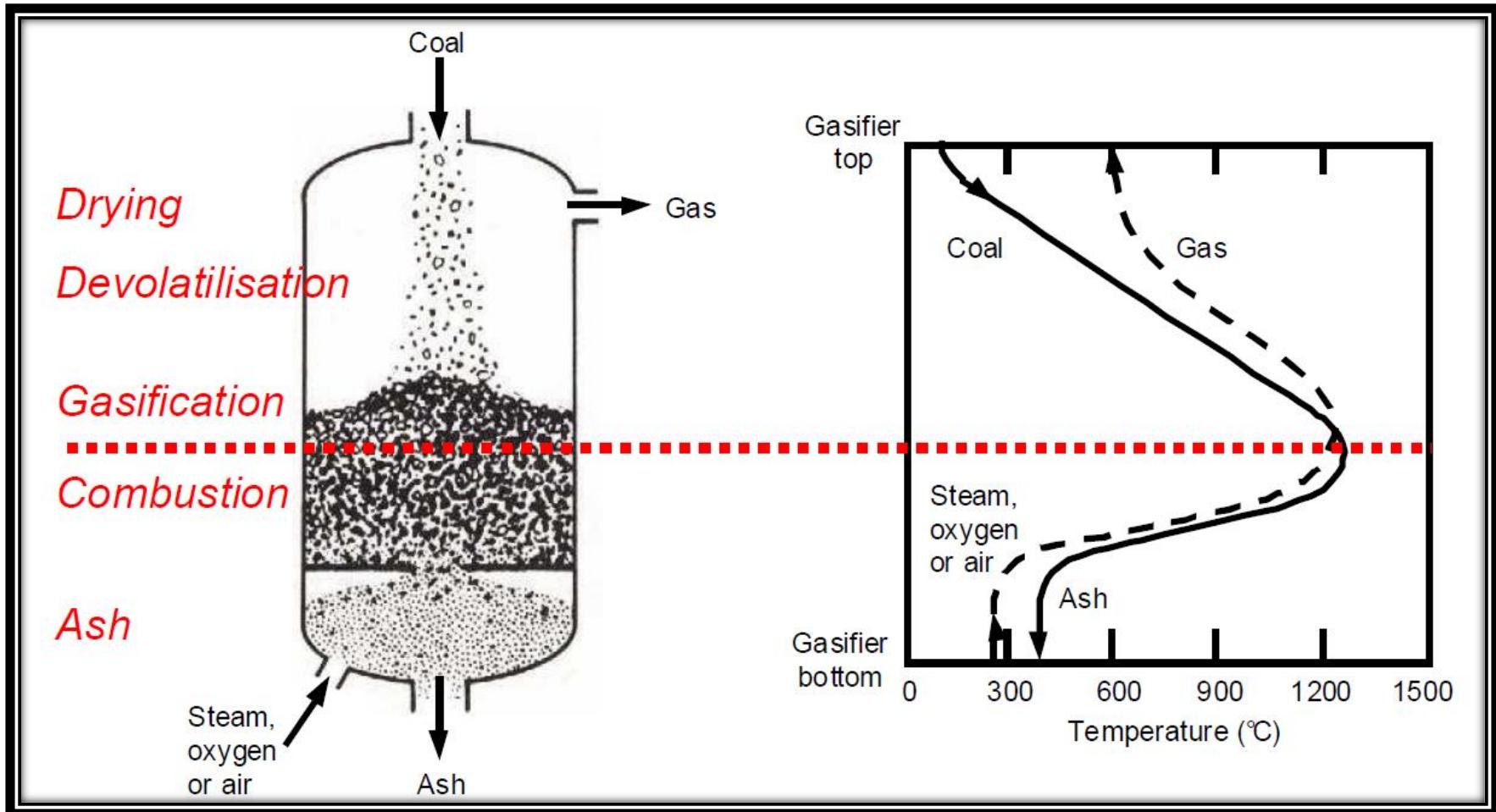
Water-gas shift:



Methane formation:



# FactSage Model of FBDB Gasifier



# FactSage Model

Starting Temperature

Final Conditions

Temperature Interval

End Temperature

Menu - Equilib: 10%KKleinfonteinS2UCombustion1%

File Units Parameters Help

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

**Reactants (21)**

(gram) 27.3 C + 1.4 H + 0.7 N + 0.2 S + 6.1 O

(25C,35bar,s1-FactPS,#1) (25C,35bar,q-FactPS,#1) (25C,35bar,q-FactPS,#1) (25C,35bar,s1-FactPS,#1) (25C,35bar,q-FactPS,#1)

**Products**

Compound species

- + gas  ideal  real 202
- aqueous 0
- \* + pure liquids 121
- \* + pure solids 451
- \* - custom selection species: 774

Target

- none -

Estimate T(K): 1000

Mass(g): 0

Solution species

*	+	Base-Phase	Full Name
*	FToxid-SLAGA	ASlag-liq all oxides + S	
I	FToxid-SLAGB	BSlag-liq with SO4	
	FToxid-SLAGC	CSlag-liq with PO4	
	FToxid-SLAGD	DSlag-liq with CO3	
	FToxid-SLAGE	ESlag-liq with H2O/OH	
	FToxid-SLAG?	?Slag-liq	
	FToxid-SPINA	ASpinel	
	FToxid-MeO_A	AMonoxide	

Legend

I - immiscible 1

Show  all  selected

species: 28

solutions: 2

Select

Custom Solutions

- 0 fixed activities
- 0 ideal solutions
- 0 activity coefficients

Details ...

Pseudonyms

apply  List ...

include molar volumes

paraequilibrium & Gmin  edit

Total Species (max 3000) 802

Total Solutions (max 40) 2

Total Phases (max 1500) 575

Equilibrium

normal  normal + transitions

transitions only

open

Calculate >

FactSage 6.4 C:\FactSage\Equi10%KKleinfonteinS2UCom

T(C) 725 1400 25

P(bar) 35

Delta H(J) 28 calculations

10 steps Table

## F 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 Graphite	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 Orthorhombic	25	35	1	FactPS
+ 13.0	O	gas-FactPS	25	35	1	FactPS
+ 52.7	SiO <sub>2</sub>	solid-1-FToxid Quartz	25	35	1	FToxid
+ 15.2	Al <sub>2</sub> O <sub>3</sub>	solid-1-FToxid gamma	25	35	1	FToxid
+ 5.2	Fe <sub>2</sub> O <sub>3</sub>	solid-1-FToxid hematite	25	35	1	FToxid
+ 0.1	(P <sub>2</sub> O <sub>5</sub> ) <sub>2</sub>	solid-FactPS	25	35	1	FactPS
+ 0.8	TiO <sub>2</sub>	solid-1-FToxid Rutile	25	35	1	FToxid

Initial Conditions

Next >>

FactSage 6.4

Compound: 3/12 databases

Solution: 2/13 databases



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## F Reactants - Equilib

File Edit Table Units Data Search Help



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



1 - 10 | 11 - 2

## F 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
+	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	S03	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	C02	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

 Initial Conditions

Next &gt;&gt;

FactSage 6.4

FactSage 6.4

Compound:

3/12 databases

Solution:

2/13 databases

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# F Reactants - Equilib

File Edit Table Units Data Search Help



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



1 - 10 | 11 - 2

# F Reactants - Equilib

File Edit Table Units Data Search Help



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



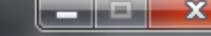
1 - 10 | 11 - 20

# F 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

42.4
+ 3.2
+ 0.7
+ 1.0
+ 13.0
+ 52.7
+ 15.2
+ 5.2
+ 0.1
+ 0.8

FactSage 6.4

FactSage 6.4 | Com

Mass(g)	Species	Phase	T(C)	P[total]**	Stream#	Data
+ 88.2	H2O	liquid-FactPS	25	35	1	FactPS

Initial Conditions

Next >>



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# 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
<b><u>Proximate analysis</u></b>								
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
<b><u>Ultimate analysis</u></b>								
% 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

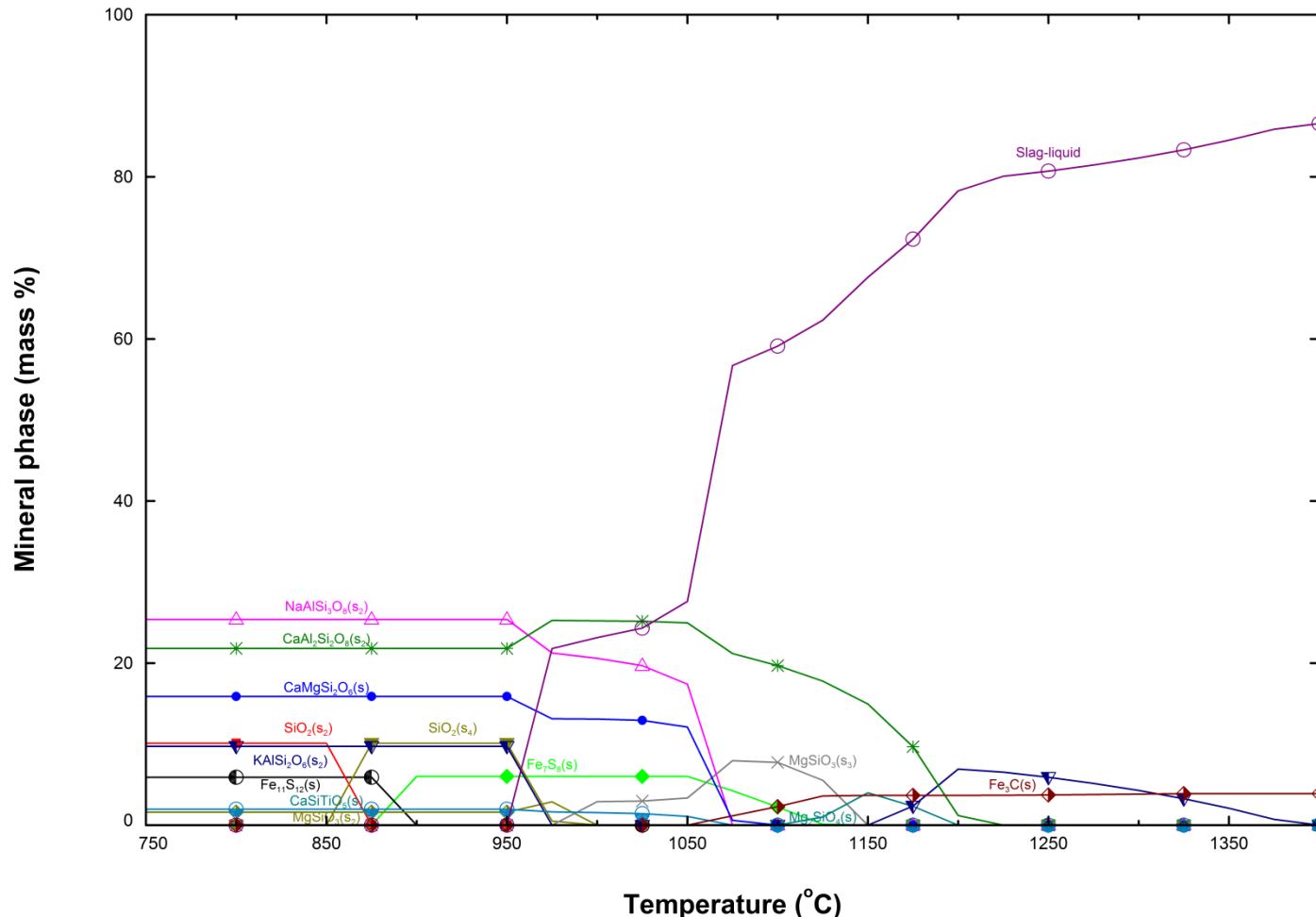
	KFS2U	KFS2U + 10%K	L#2	L#2 + 10%K	MD	MD + 10%K	WFS1	WFS1 + 10%K
<b>XRF</b>								
Al <sub>2</sub> O <sub>3</sub>	28.46	19.42	15.07	9.22	25.18	17.82	25.89	16.50
CaO	1.51	1.00	9.13	5.05	13.02	8.94	5.07	3.37
Cr <sub>2</sub> O <sub>3</sub>	0.12	0.02	0.03	nd	0.03	nd	0.03	0.02
Fe <sub>2</sub> O <sub>3</sub>	2.00	1.18	5.16	3.06	5.64	3.73	5.54	3.53
K <sub>2</sub> O	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 <sub>2</sub> O	Nd	0.17	2.94	1.88	nd	0.15	nd	0.27
P <sub>2</sub> O <sub>5</sub>	0.07	0.04	0.10	0.07	0.26	0.19	0.10	0.14
SiO <sub>2</sub>	63.17	43.17	52.16	31.66	41.60	29.70	55.15	34.17
TiO <sub>2</sub>	1.52	1.05	0.80	0.47	1.79	1.27	1.34	0.84
V <sub>2</sub> O <sub>5</sub>	0.02	0.02	0.02	0.02	0.02	0.02	0.03	0.03
ZrO <sub>2</sub>	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 <sub>3</sub>	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

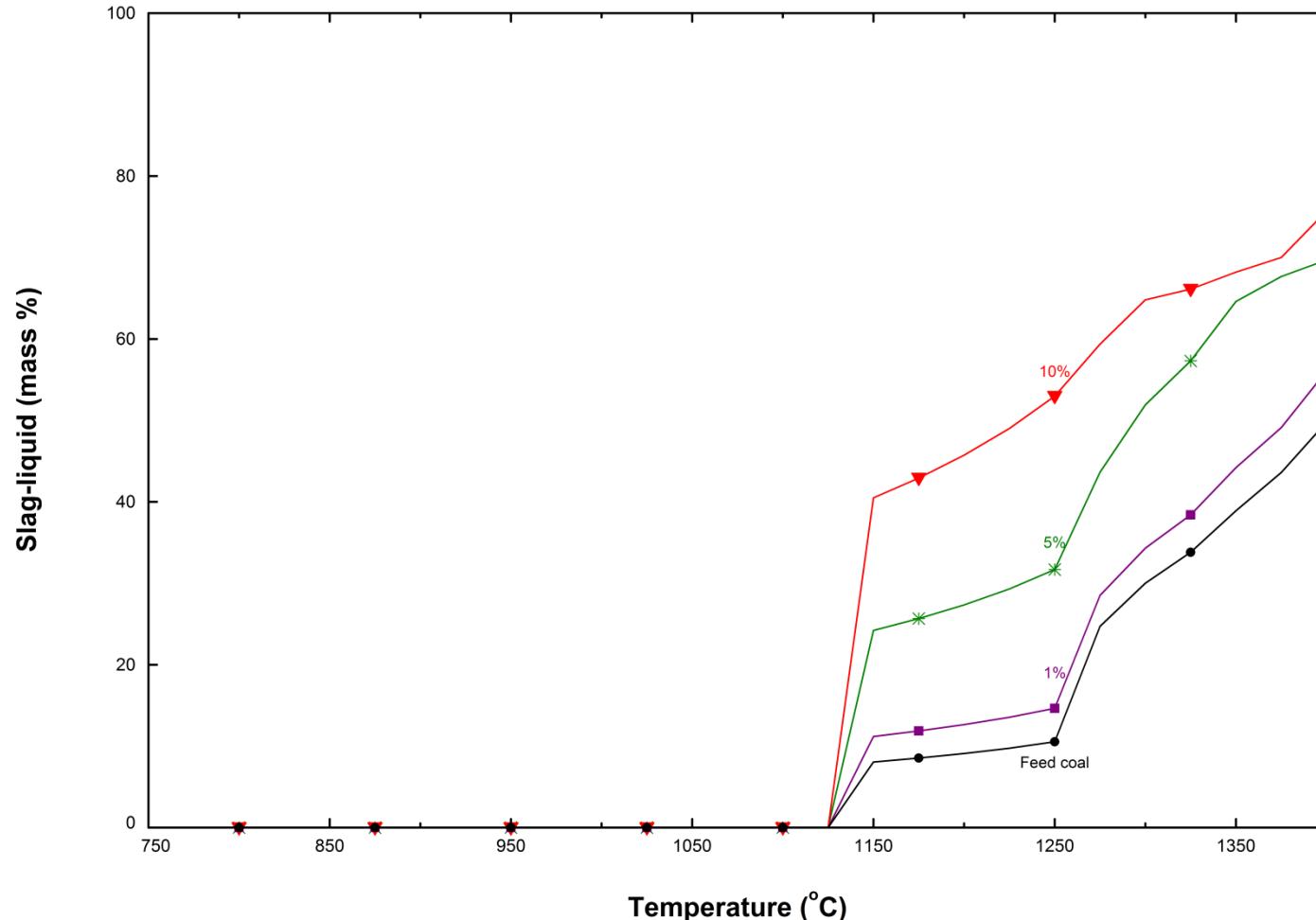


# Results

## 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™

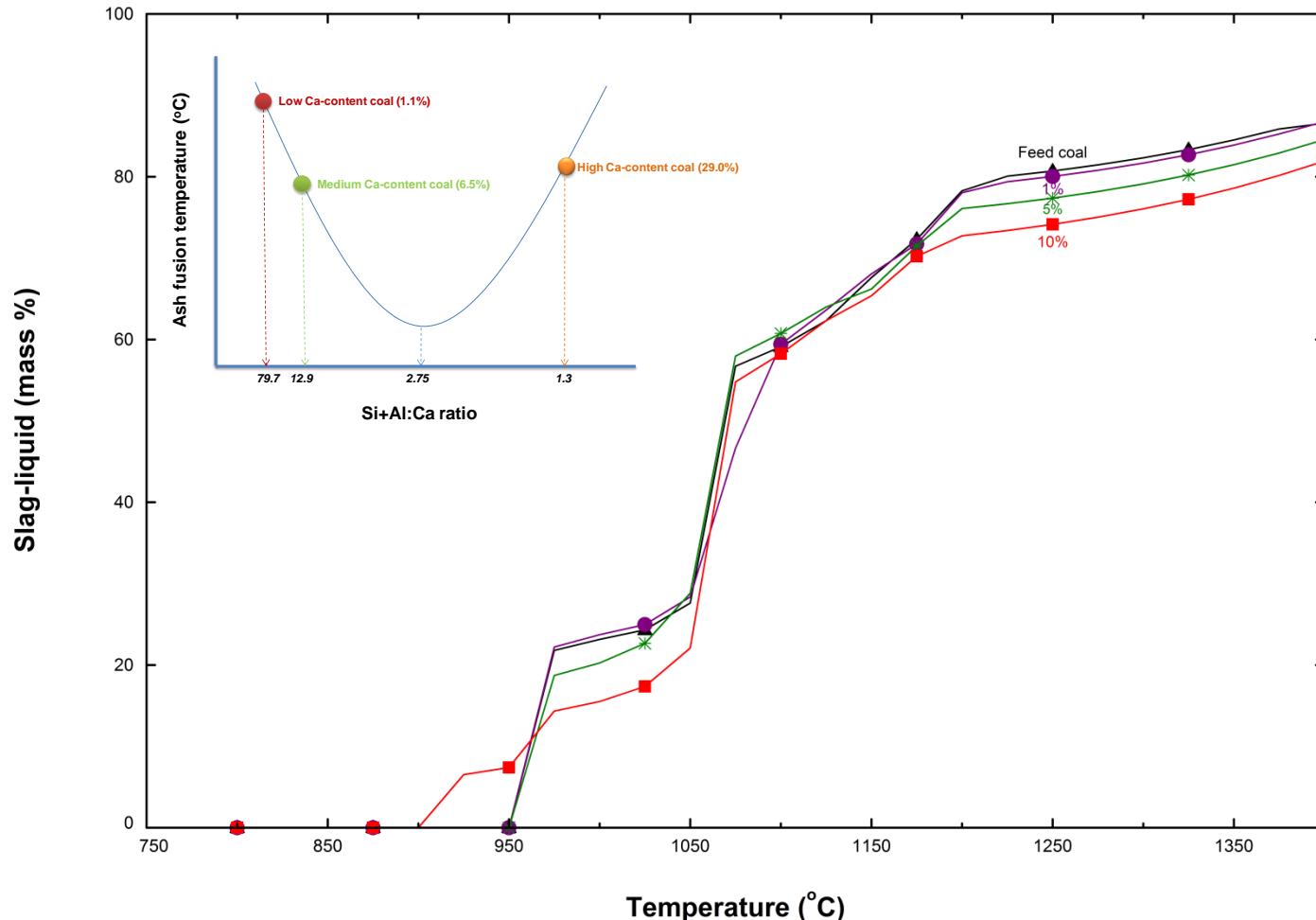


# Results

## Influence of Potassium addition of slag formation in Zone 1 - L#2

Addition of potassium according to ash percentage  
C:\FactSage\Equi0.res - AC Collins

 FactSage™

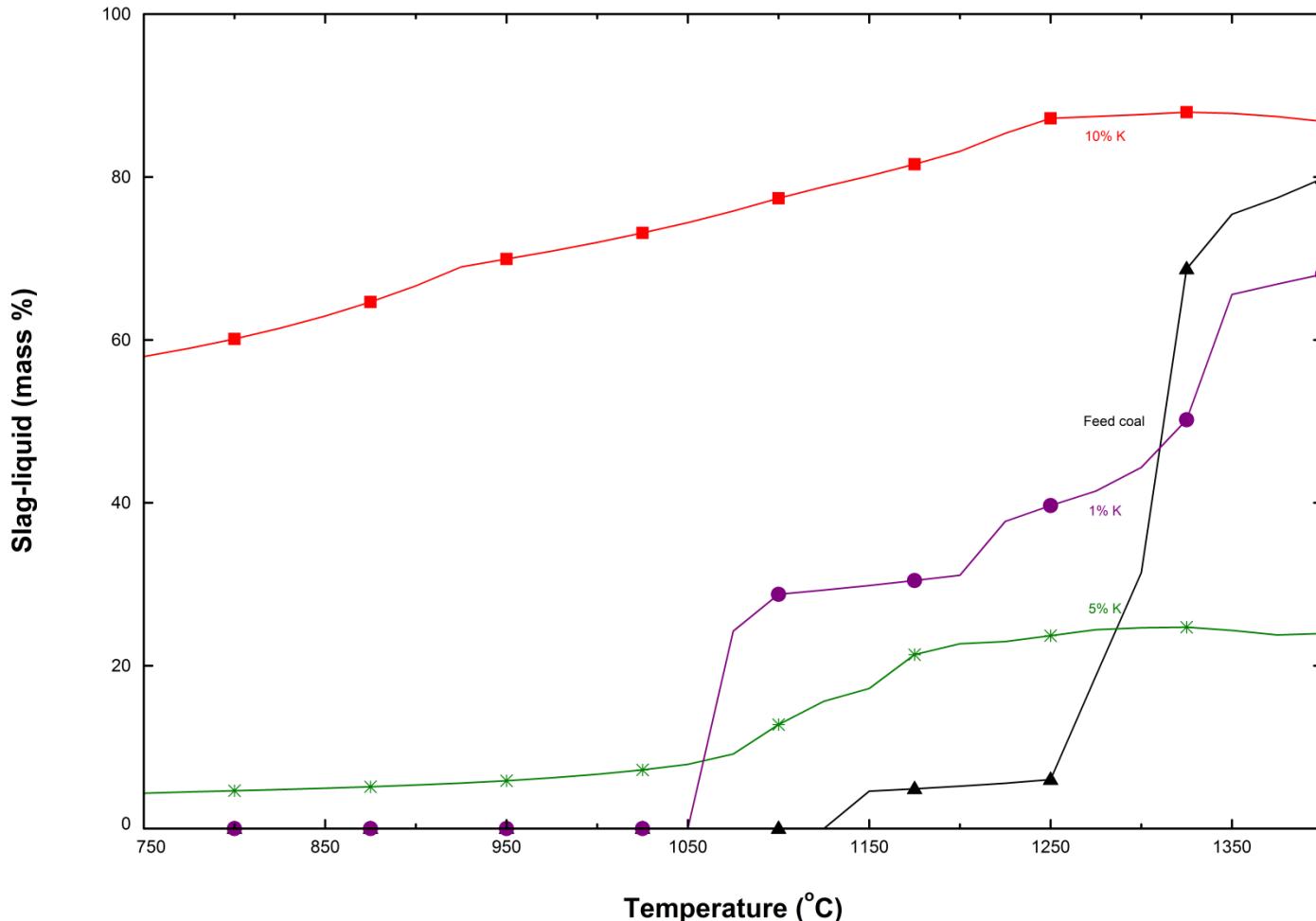


# Results

## Influence of Potassium addition on slag formation in Zone 1 - WFS1

Addition of potassium according to coal mass  
C:\FactSage\Equi0.res - AC Collins

 FactSage™

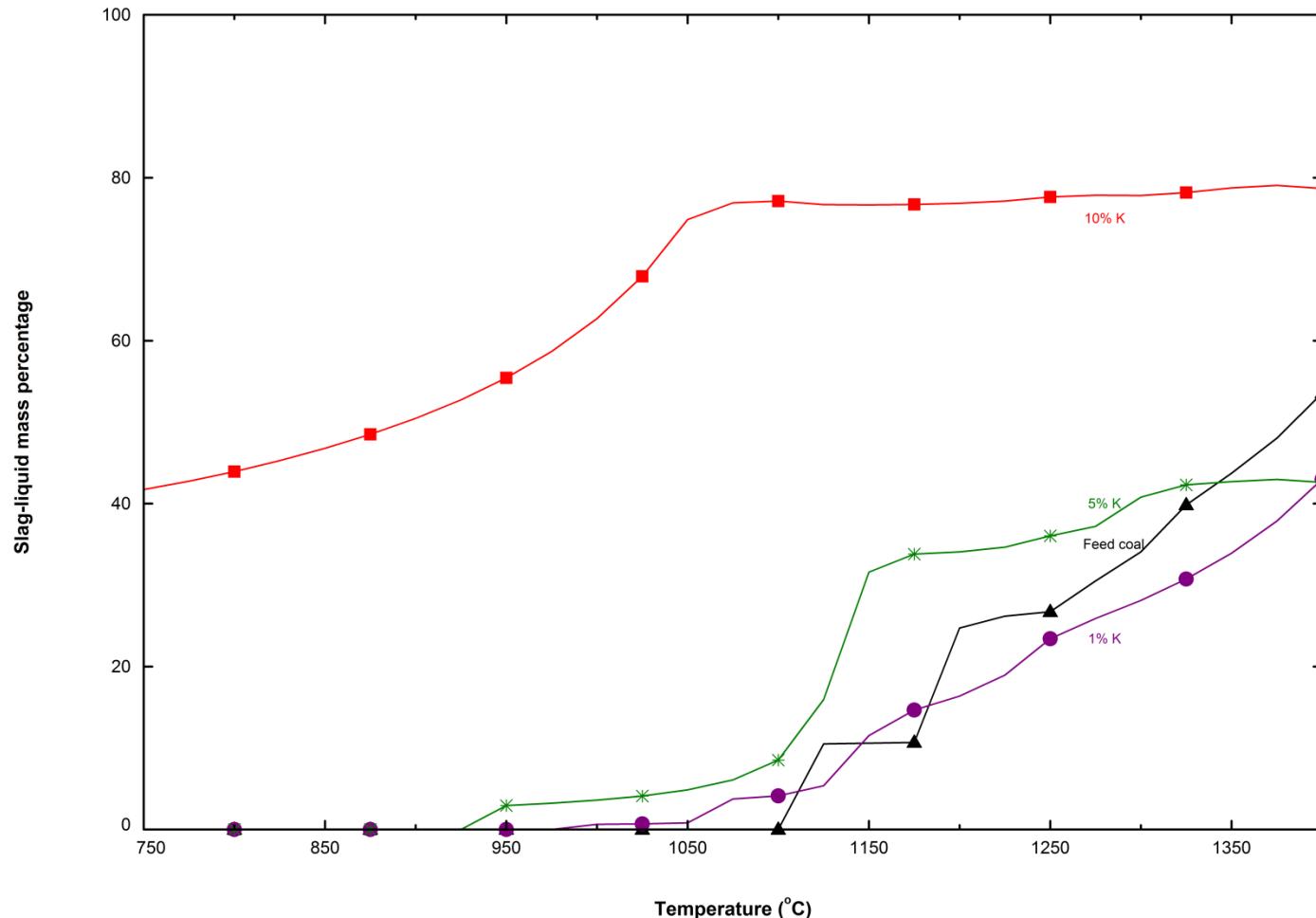


# Results

## Influence of Potassium addition on slag formation in Zone 1 - MD

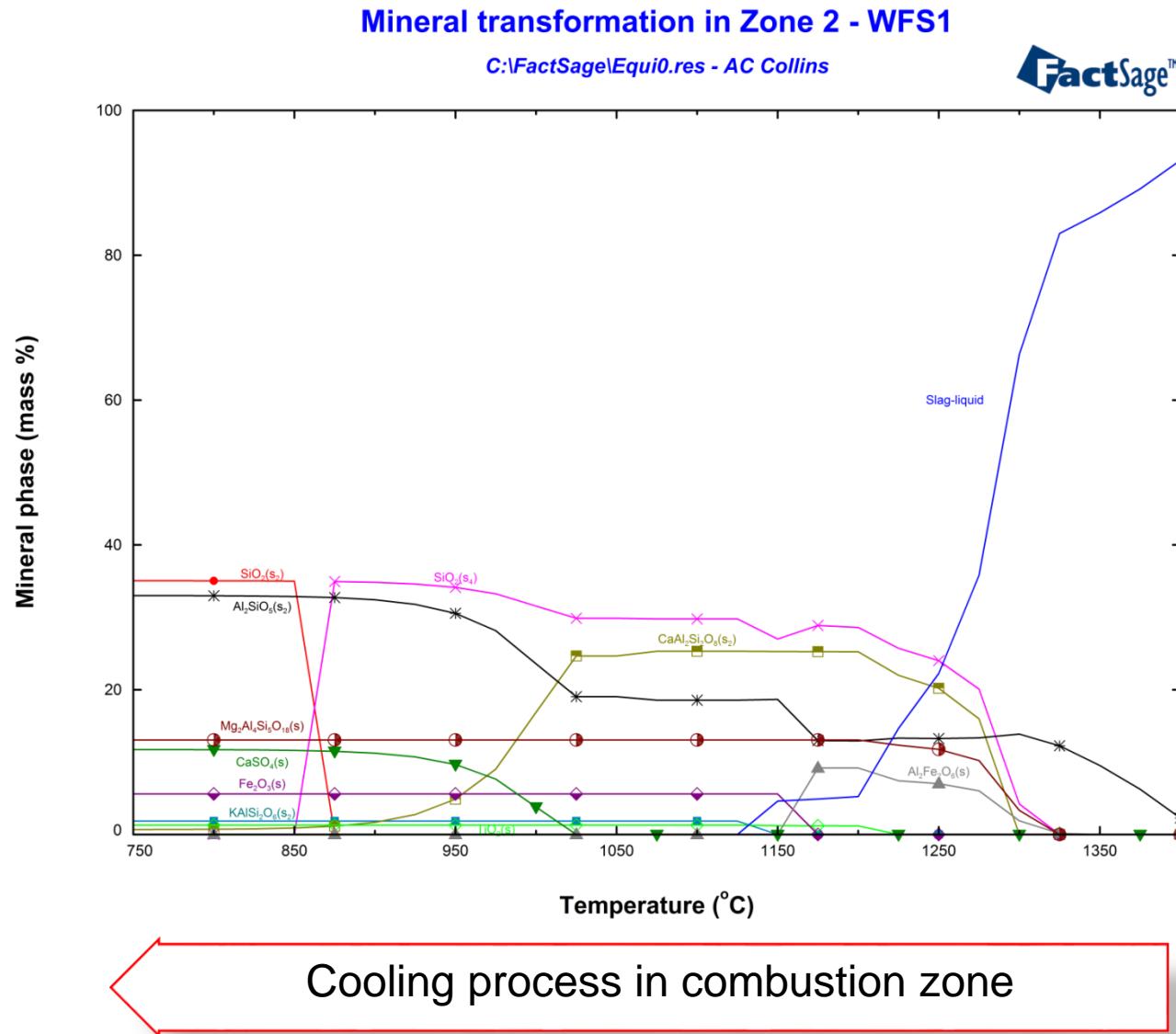
Addition of potassium according to coal mass  
C:\FactSage\Equi0.res - AC Collins

FactSage™

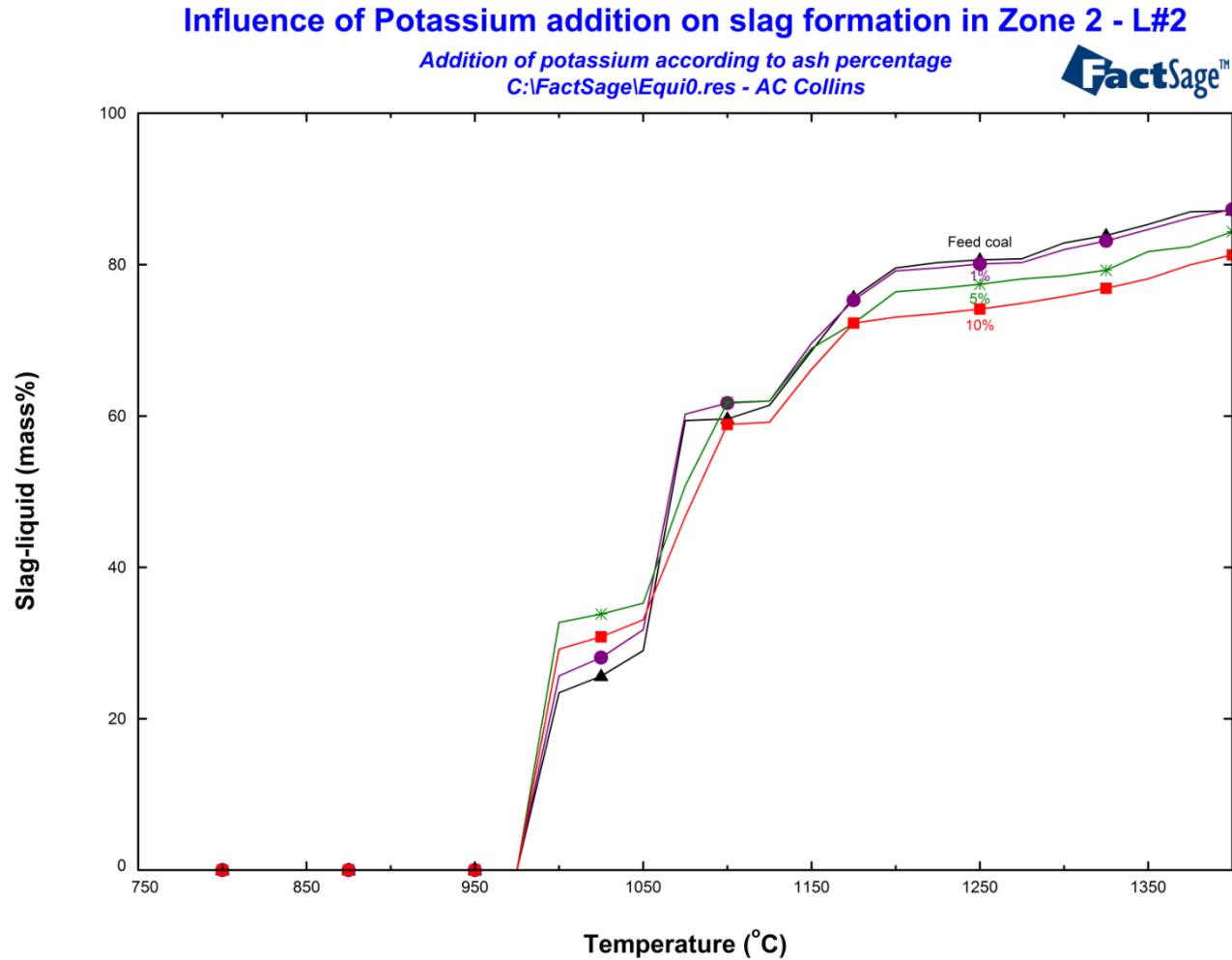


# Combustion and Ash Zone 2

# Results

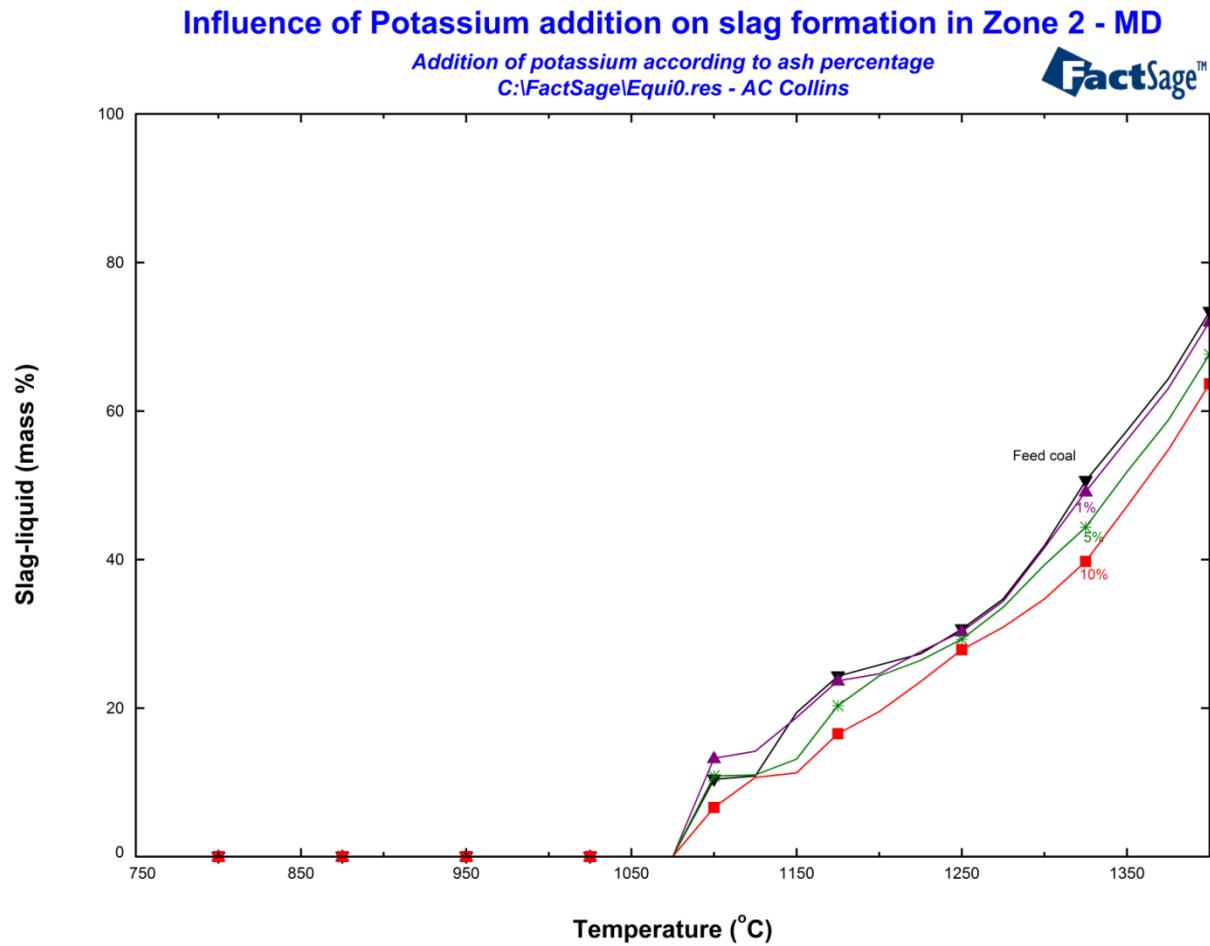


# Results



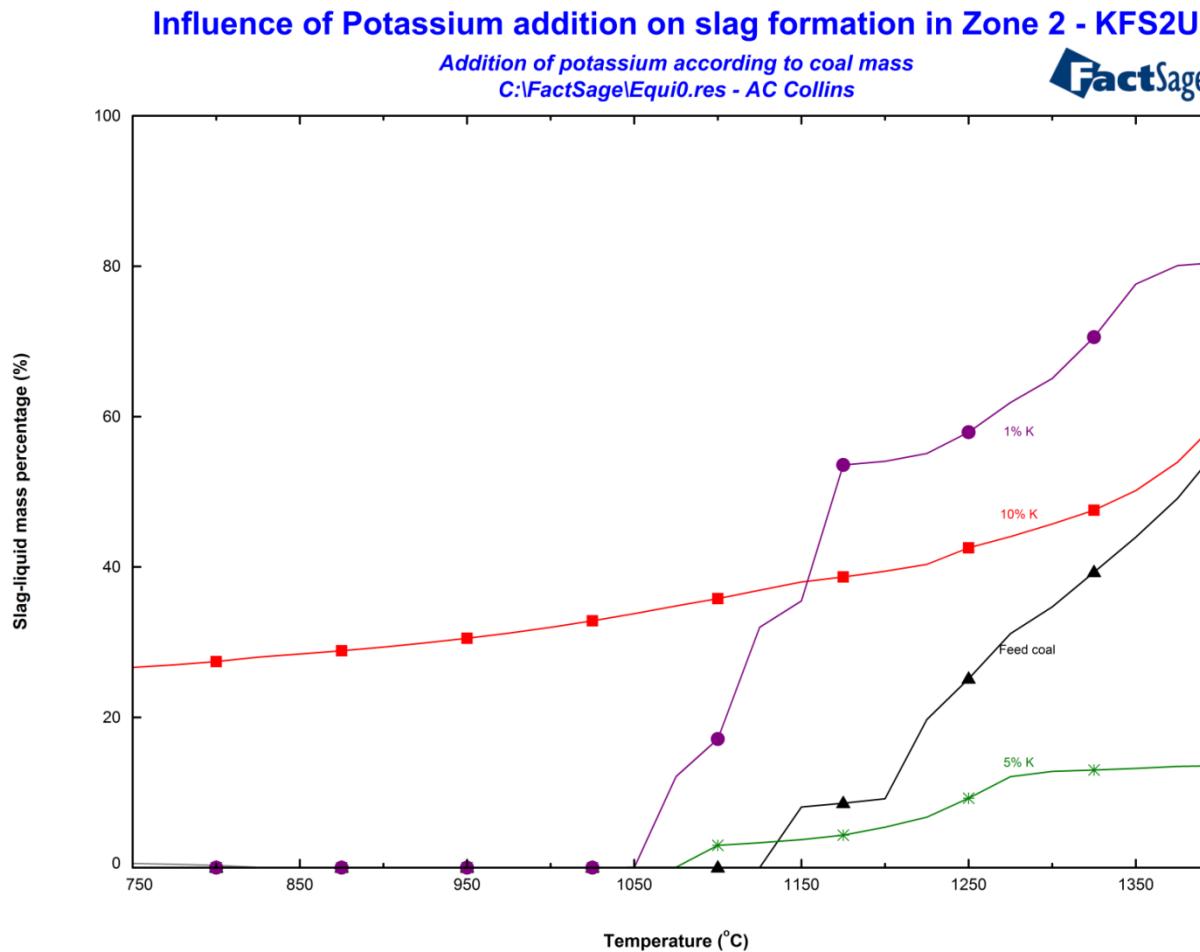
Cooling process in combustion zone

# Results



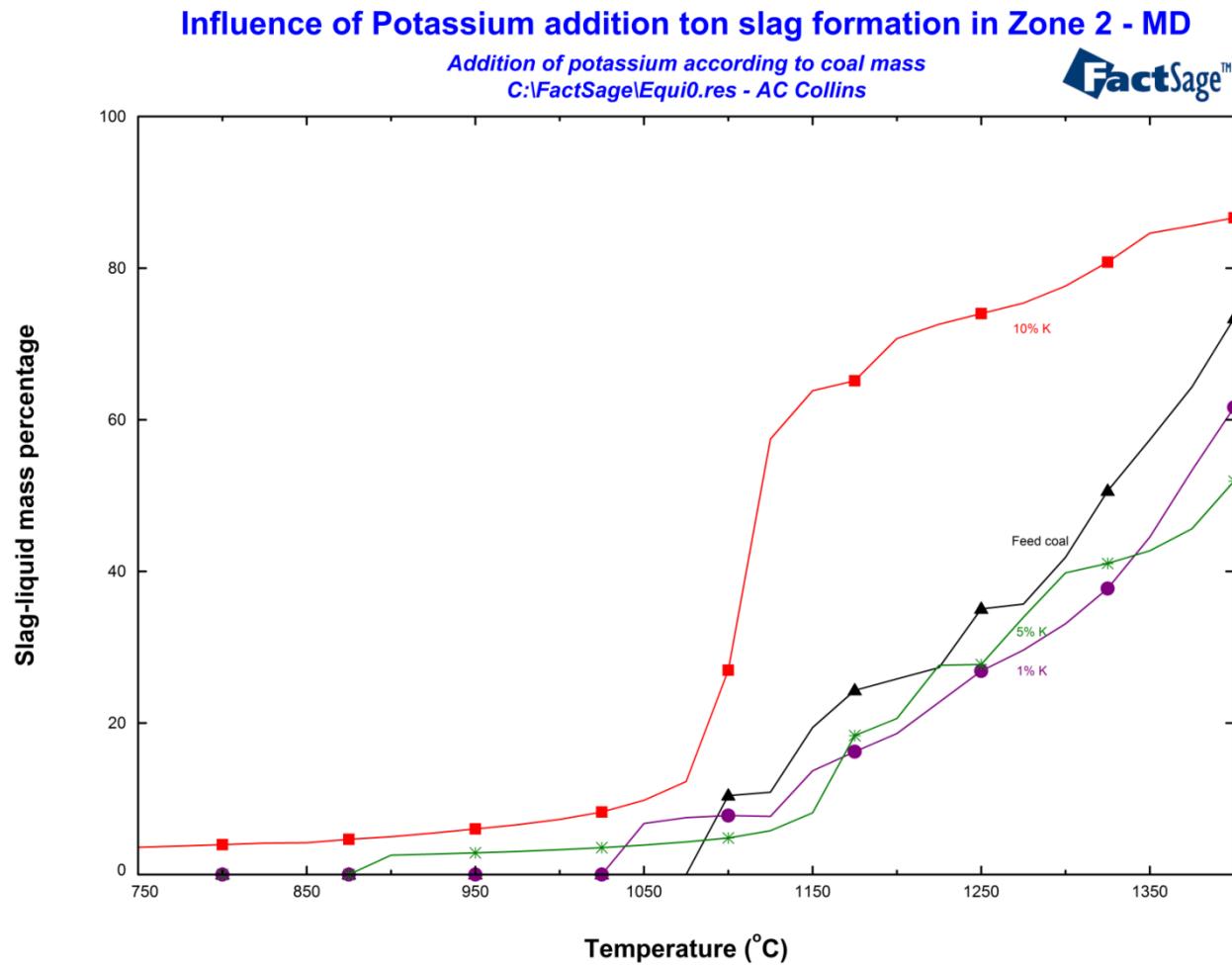
Cooling process in combustion zone

# Results



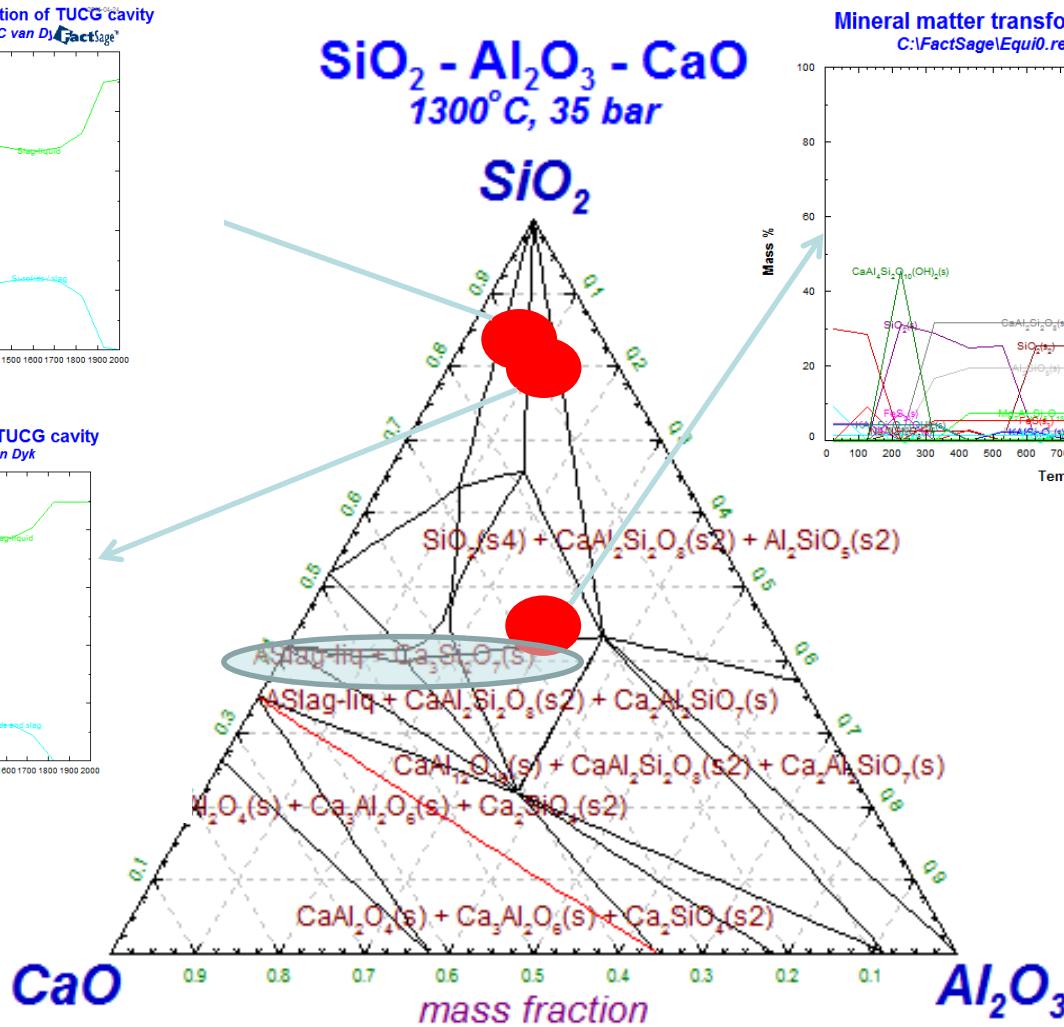
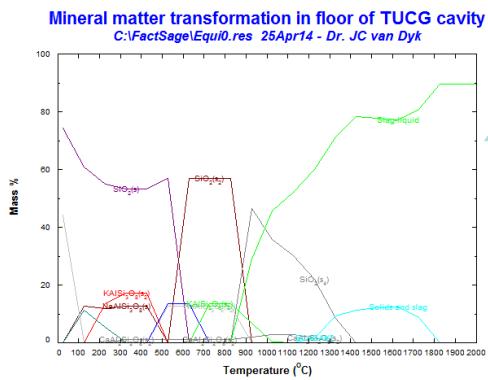
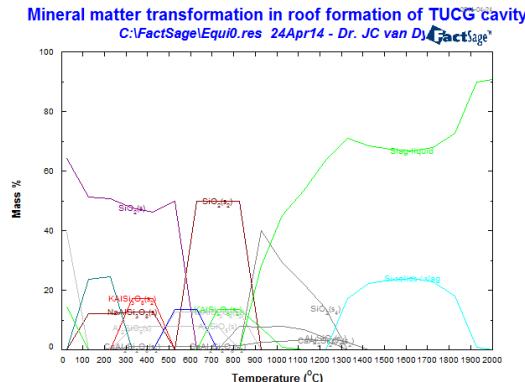
Cooling process in combustion zone

# Results

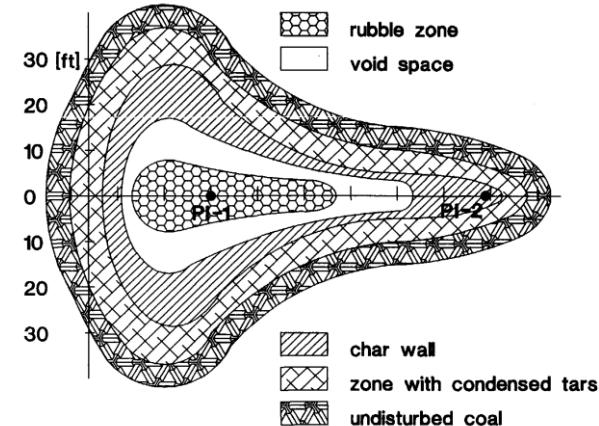
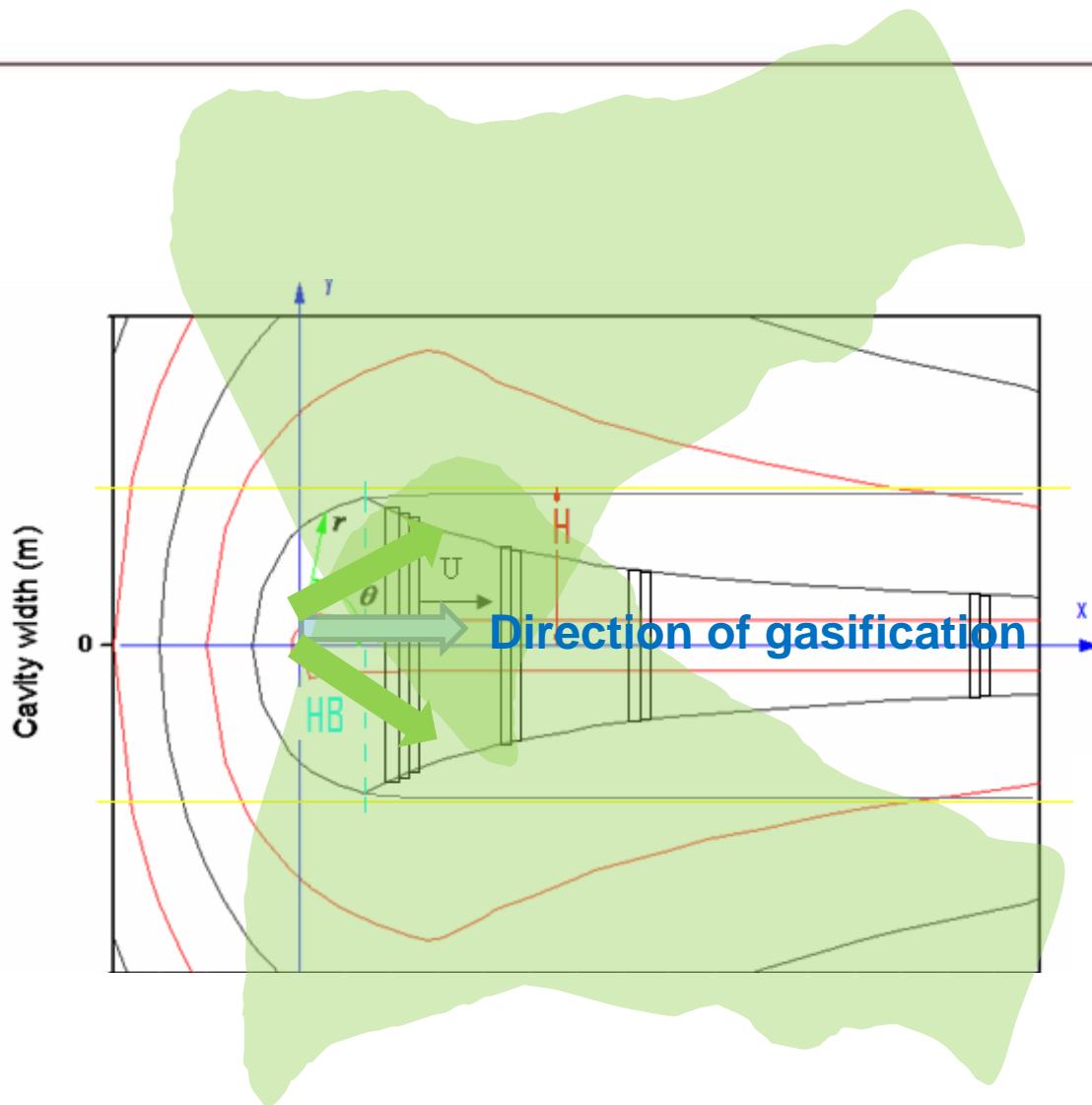


Cooling process in combustion zone

# Gasification science – mineral transformation and ash behaviour



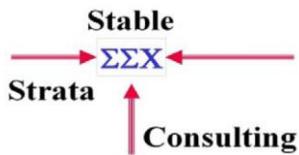
# What next on UCG simulations?



# Geophysical study

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

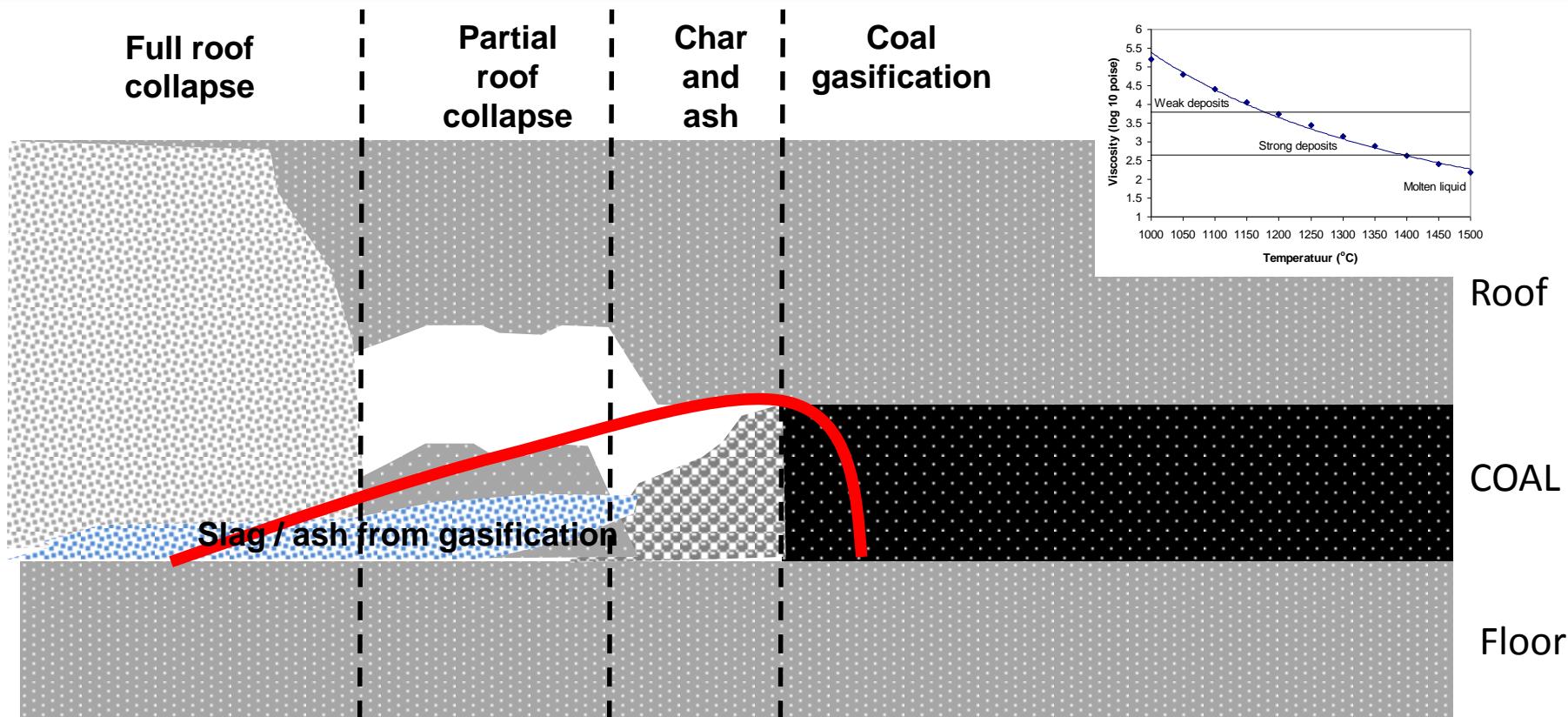
		ADVANCE		
Cavity Width	0-100m	100m	100-300m	>300m
	100-300m	Only local collapse	Only local collapse	Only local collapse
	>300m	Only local collapse	30-100m collapse	30-100m collapse
				Full collapse



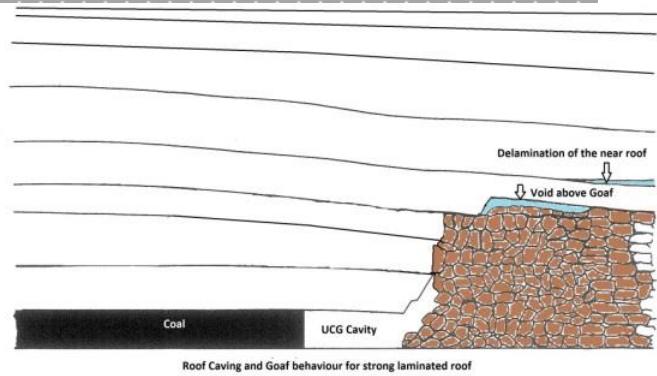
Coal seam 3m



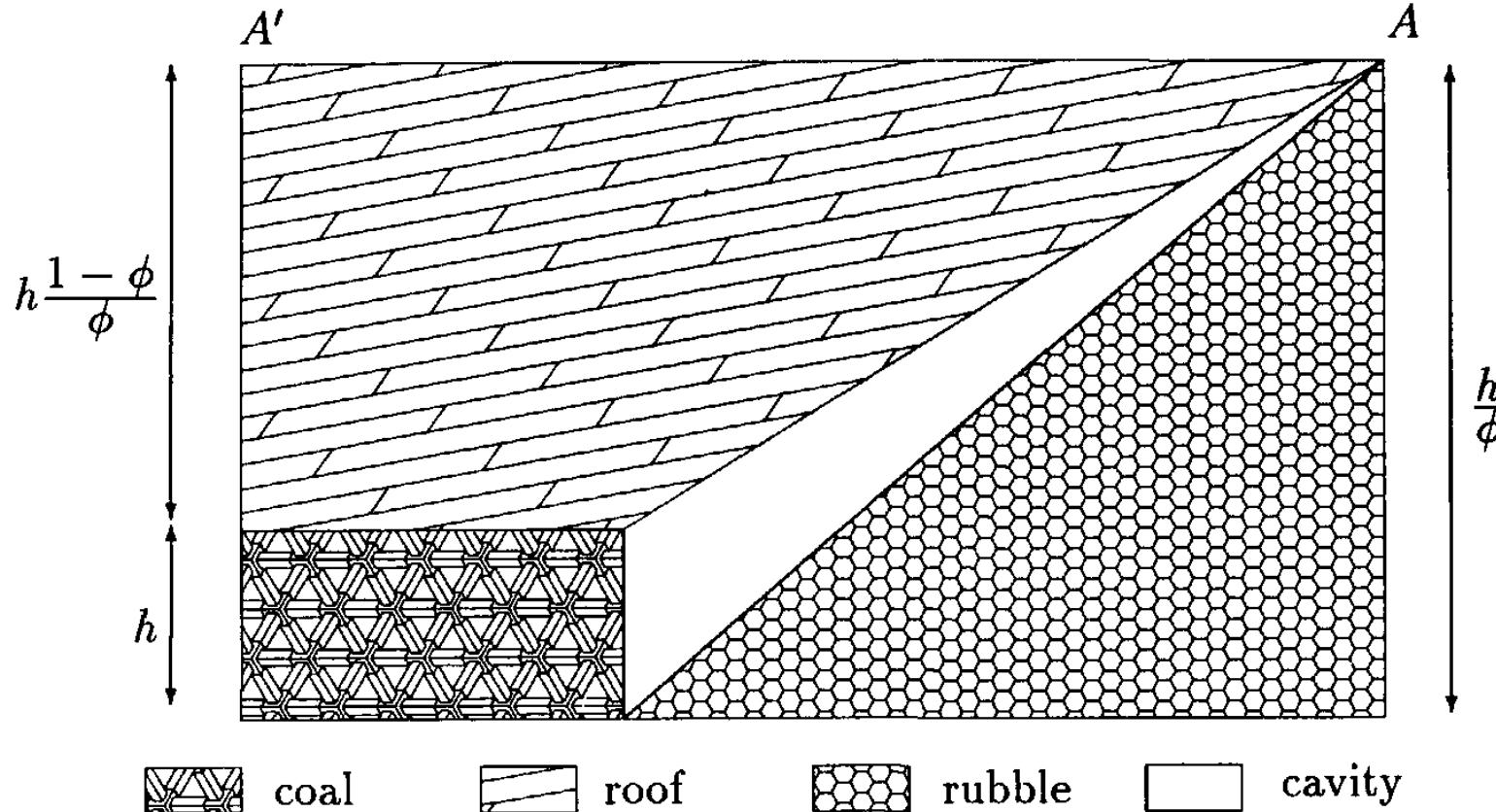
# The approach!



		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

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- **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 =  $\uparrow$  in slag formation with  $\uparrow$  % K
    - L#2 =  $\downarrow$  in slag formation with  $\uparrow$  % K
    - MD =  $\downarrow$  in slag formation with  $\uparrow$  % 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

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- 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 than at temperatures  $> 1000^{\circ}\text{C}$ .
- 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

A banner for the SAUCGA conference. It features three panels: the left panel shows a close-up of a worker's gloved hands; the middle panel shows a shovel digging into coal; and the right panel shows a pile of coal. The text on the banner reads:

SAUCGA - SOUTH AFRICAN UNDERGROUND COAL GASIFICATION ASSOCIATION  
*UNDERGROUND COAL GASIFICATION : UNLOCKING SOUTHERN AFRICA'S UNMINEABLE COAL RESERVES*

24 AUGUST 2015



## Thirty Third Annual International PITTSBURGH COAL CONFERENCE

*Conference Announcement and Call for Papers*

Abstracts Due 1 March 2016

8 – 12 August 2016

Cape Town, South Africa

International Convention Centre



# Thank You