VISCOSITY PREDICTION OF THE SLAG COMPOSITION OF GASIFIED COAL, UTILIZING FACTSAGE EQUILIBRIUM MODELLING

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Background

- Mineral matter transformations in coal during gasification and ash flow behaviour provide information on suitability of a coal for gasification purposes
- Detail insight of mineral matter transformations during S-L FBDB gasification obtained with Factsage modelling and HT-XRD[1]
- Equilibrium phases as calculated with Factsage confirmed with experimental work on gasifier ash[2]
- Even when operated below the flow temperature, a percentage of slag is formed[3]

1. VAN DYK, J.C., Manipulation of coal feed to gasification in order to increase the AFT of the coal, September 2006, PhD Thesis, NWU.
2. MATJIE, R.H., Van Alphen, C. and Pistorius, P.C., *Mineralogical characterization of Secunda gasifier feedstock and coarse ash*, Minerals Engineering, 19, 2006, p. 256-261.
3. VAN DYK, J.C. (b), Melzer, S. and Sobiecki, A., Mineral matter transformations during Sasol-Lurgi fixed bed dry bottom gasification – utilization of HT-XRD and FactSage modelling, Minerals Engineering, 19, 2006, p. 1126-1135.

Background (cont.)

- Applicability of AFT test results to reliably predict coal ash behaviour during gasification has been questioned[4]
- Shortcomings are its subjective nature, poor accuracy, etc.[5]
- Approaches were made to apply viscosity modelling with FACT[6]
  - *Study coal slagging characteristics during gasification in IGCC process*
  - *IGCC operating conditions allow slagging regimes when solids can be present*
  - *Describing the molten phase and crystallised slag / liquid portion are important*
  - *If the liquid phase is highly fluid (low viscosity), it will enhance flow, but the un-melted solids can make the cone behave as a pseudo-plastic solid*

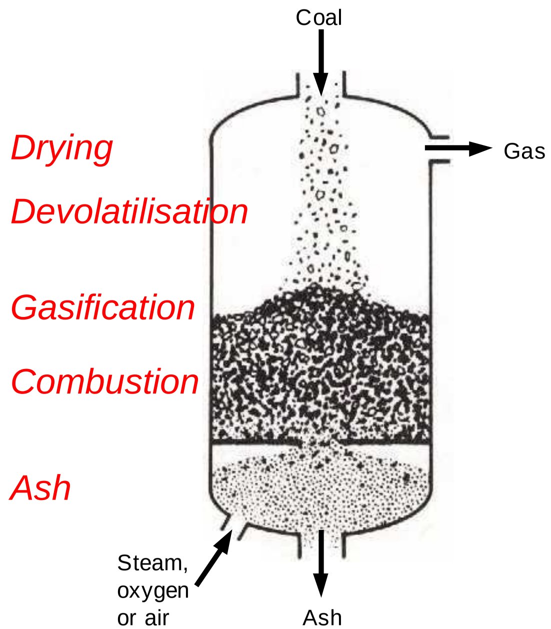
4. REIFENSTEIN, A.P., Kahraman, H., Coin, C.D.A., Calos, N.J., Miller, G. and Uwins, P., *Behaviour of selected minerals in an improved ash fusion test: quartz, potassium feldspar, sodium feldspar, kaolonite, illite, calcite, dolomite, siderite, pyrite and apatite*, **Fuel**, 1999, 78, p. 1449-1461.
5. COLLET, A.G., *Matching gasifiers to coal*, **IEA Clean Coal Centre**, 2002, p.1-64.
6. KONDRATIEV, A. AND JAK, E., Predicting coal ash slag flow characteristics (viscosity model for the Al_2O_3-CaO-FeO-SiO_2 system), Fuel, 2001, 80, p. 1989-2000.

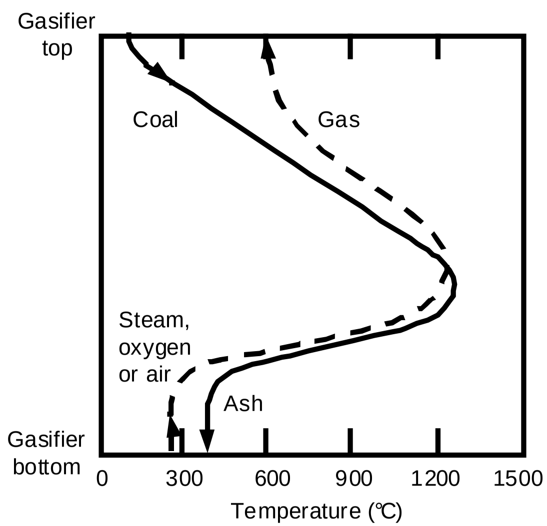
Objective of study

- Application of FactSage thermo-equilibrium modelling results for a gasification process to **determine the viscosity of the slag-liquid component within a heterogeneous mixture of crystalline phases and slag-liquid phases**.
- The combination of viscosity predictions together with FactSage will result in viscosity predictions of the **actual liquid component** rather than just an **average or pseudo viscosity prediction of the total mineral system** at a specific temperature.
- The focus will be on the application of viscosity modelling together with FactSage modelling.

Experimental

- Coal sample represents the coal blend gasified in Secunda, South Africa
- 6 different coal sources properly blended before gasified
- Factsage used to model mineral transformations and slag formation during the fixed bed gasification process[1]





- Mineral transformation can be extracted at specific T
- Slag-liquid quantity and composition at specific T available

Experimental (cont.)

- The key to the behaviour of ash deposits lies in understanding their consolidation by a viscous flow mechanism and the effect of the main fluxing agents on the viscosity of the minerals - AFT and cone deformation alone can be meaningless[7]
- In this study the focus will be on the application of viscosity modelling together with FactSage modelling
- Experimental evidence shows that the slag performance of blended coals can be either worse or better than the performance of the individual coals, which is the reason why viscosity modelling also has to be investigated[8]

7. GIBB, W.H., The UK collaborative research programme on slagging pulverised coal-fired boilers: summary and findings, PowerGen, Power Technology, Nottingham NG11 OEE, England, Applications to Advanced Technology to Ash-related problems in boilers, 1996, p.41-65.
8. GONI, C., Helle, S., Garcia, X., Gordon, A., Parra, R., Kelm, U., Jimenez, R. and Alfaro, G., *Coal blend combustion: fusibility ranking from mineral matter composition*, **Fuel**, 2003, 82, p. 2087-2095.

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Experimental (cont.)

- The model used in this study to determine viscosities is that of Kalmanovitch or the so-called "modified Urbain model"[9]

Step 1:Determine the mole fraction of all components based on the chemical oxide composition. Fe_2O_3 is converted to equivalent FeO.

Step 2: Calculate M where, M = CaO + MgO + Na_2O + K_2O + FeO + $2TiO_2$ mole fractions

Step 3: Calculate alpha where, Alpha = M / (M + Al_2O_3) mole fractions

Step 4: Calculate B where

$B = BO + (B1*SiO_2) + (B2*(SiO_2)2) + (B3*(SiO_2)3)$

$BO = 13.8 + 39.9355*alpha - 44.049*(alpha)2$

$B1 = 30.481 - 117.1505*alpha + 129.9978*(alpha)2$

$B2 = -40.9429 + 234.0486*alpha - 300.04*(alpha)2$

$B3 = 60.7619 - 153.9276*alpha + 211.1616*(alpha)2$

*Step 5: ln[A] = -(0.2812*B + 11.8279)*

Step 6: Calculate the natural log of the viscosity at a given temperature T in degrees K

$ln[viscosity] = ln[A] + ln[T] + (1000*B/T)$

9. KALMANOVITCH, D.P. and Frank, M., *An effective model of viscosity for ash deposition phenomena*, University of North Dakota, Energy and Mineral Research Center, Grand Forks, **Energy Foundation Conferences**, 1988, p.89-101.

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Experimental (cont.)

- The modified Urbain model can predict both viscosities of bulk coal ash melts as well as simple oxide glasses, with specific emphasis on $CaO-MgO-Al_2O_3-SiO_2$ systems
- Scanning Electron Microscopy Point Count (SEMPC) together with viscosity modelling is the preferred way to study ash-related materials[9, 10]
- The real advantage of SEMPC is that it does not rely on the bulk composition, but is capable of determining the chemical composition and relative amount of phases actually responsible for the ash behaviour[9]. It has also been published that the Kalmanovitch models work the best for coals high in SiO_2 and lower in Fe[10], which is appropriate for the coal sources used in this study.

10. LAUMB, M.; Benson, S.A.; Laumb, J. *Ash Behavior in Utility Boilers: A Decade of Fuel and Deposit Analyses*, *United Engineering Foundation Conference on Ash Deposition and Power Production in the 21st Century*, Snowbird, UT, Oct. 28 – Nov. 2, 2001.

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Results (ash flow temperature)

TEMPERATURE STAGE	Temperature (°C) of coal used in this study	Coal characteristic as used during previous base case tests	
		Average (°C)	Variation of base case coal sample (minimum and maximum) (°C)
IDT	1300	1290	1230-1390
ST	1320	1300	1240-1420
HT	1330	1320	1200-1440
AFT	1340	1340	1270-1470

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Results (Ash composition)

ELEMENT	Result of coal sample used in this study (mass %)	Coal characteristic as used during previous base case tests	
		Average (mass %)	Variation (minimum and maximum) (mass %)
SiO_2	50.1	48.7	40.0-51.9
Al_2O_3	23.3	24.1	20.9-30.2
Fe_2O_3	6.4	4.8	2.5-9.3
P_2O_5	0.7	0.7	0.5-2.2
TiO_2	1.0	1.4	1.0-1.6
CaO	8.1	7.9	6.1-11.6
MgO	2.7	2.5	1.9-3.2
K_2O	0.8	1.0	0.6-4.1
Na_2O	0.4	0.7	0.2-0.9
SO_3	6.1	7.3	5.3-9.5

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Results (Factsage – mineral matter composition at specific temperature)

MINERAL COMPOSITION (mass %)	TEMPERATURE (ºC)					
	1000	**1050**	**1100**	**1150**	**1200**	**1250**
Mullite	0.0	0.0	1.4	2.0	4.3	4.4
Slag-Liquid	9.1	23.1	35.5	47.5	70.5	78.9
Slag-liquid composition						
MgO	3.2	3.9	3.6	4.0	4.2	3.8
FeO	10.7	19.0	17.7	13.3	8.9	8.0
Na_2O	4.7	1.9	1.2	0.9	0.6	0.6
SiO_2	58.7	52.5	53.3	56.1	59.1	58.4
CaO	4.0	4.5	4.6	5.7	6.7	7.8
Al_2O_3	18.5	17.9	19.3	19.8	20.1	21.2
K_2O	0.0	0.0	0.0	0.0	0.1	0.2

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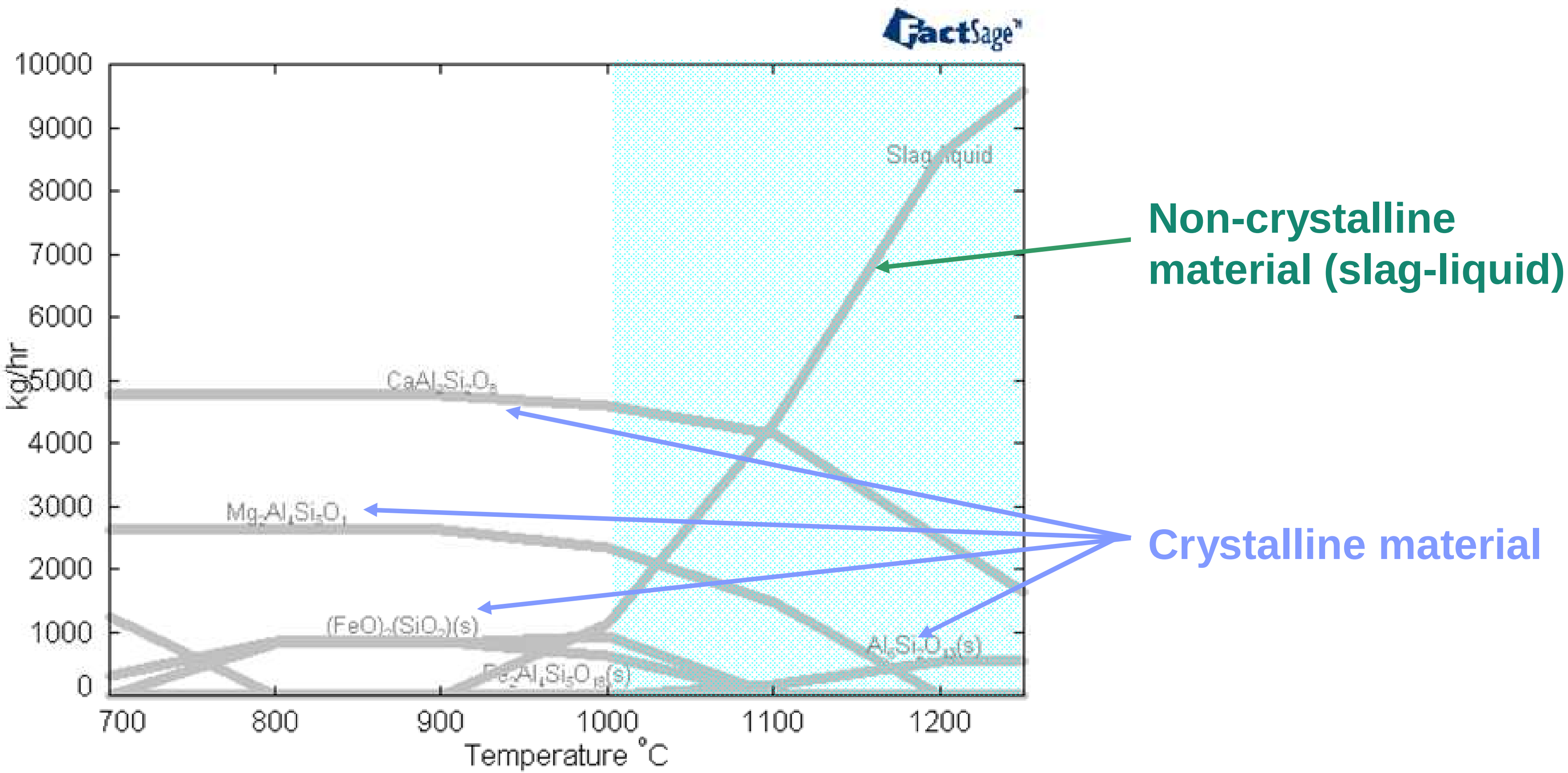
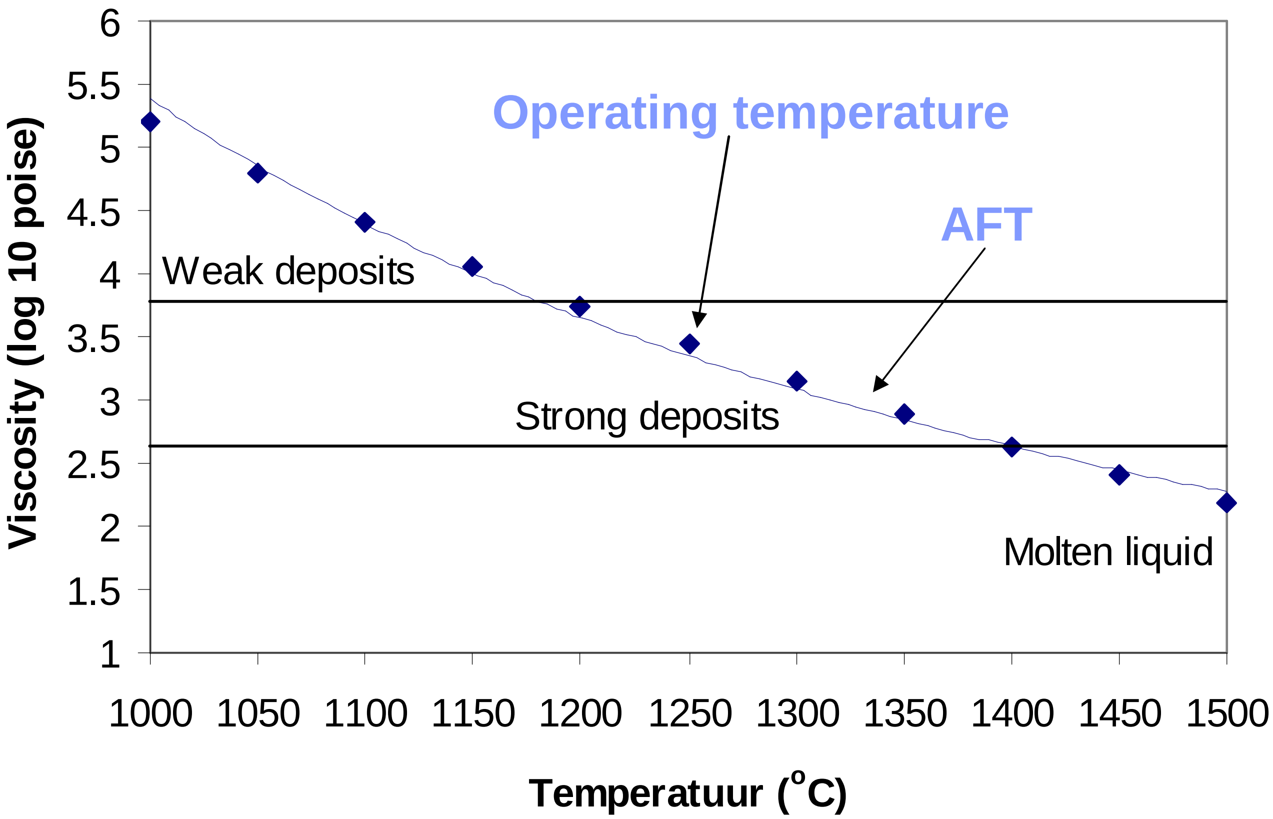
Results (Factsage – mineral matter composition at specific temperature)

MINERAL COMPOSITION (mass %)	TEMPERATURE (°C)					
	1000	1050	1100	1150	1200	1250
$CaAl_2Si_2O_8$ Feldspar	37.5	34.2	34.1	30.6	20.3	13.4
SiO_2 tridymite(h)	16.0	14.0	12.4	8.5	1.3	0.0
$KAlSi_2O_6$ leucite(rhf)-b	4.0	4.0	4.0	3.9	3.6	3.3
$Mg_2Al_4Si_5O_{18}$ cordierite	19.2	14.7	12.0	7.5	0.0	0.0
$Fe_2Al_4Si_5O_{18}$ ferrocordierite	7.5	8.5	0.0	0.0	0.0	0.0
$(FeO)_2(SiO_2)$ fayalite	5.2	0.0	0.0	0.0	0.0	0.0
$Ca_3(PO_4)_2$	1.7	1.6	0.6	0.0	0.0	0.0

Results (Factsage – graphical illustration of mineral transformations from 700-1250^{o}C)

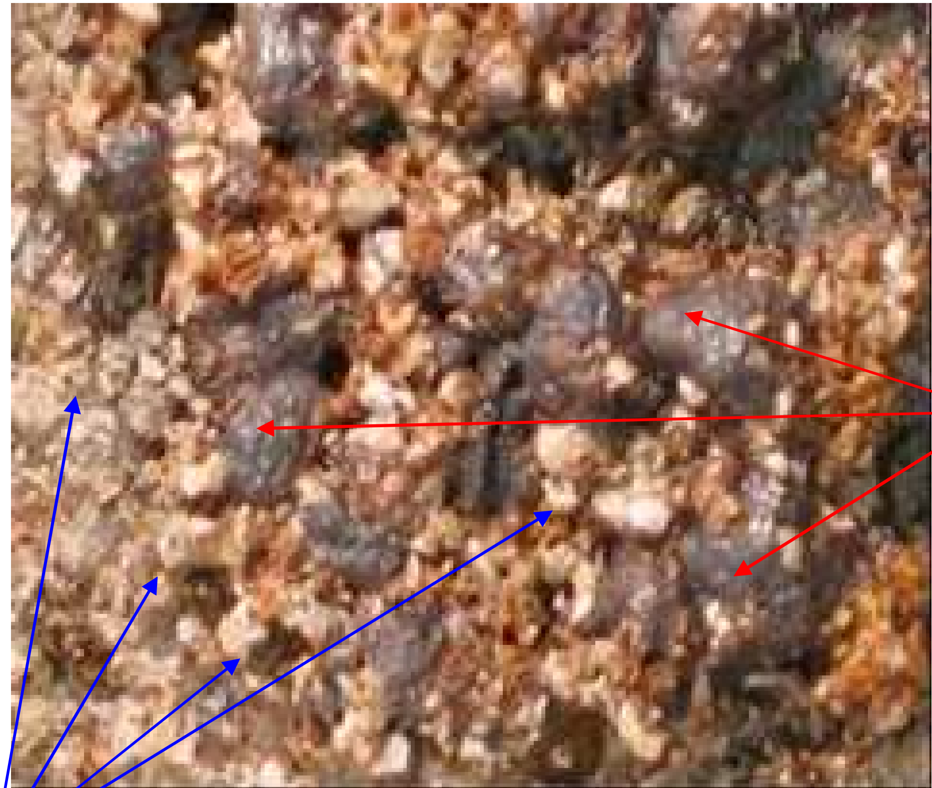


Results (Viscosity – based on overall ash composition)



- Assumes composition 100% liquid or molten
- Not true for fixed bed gasification
- More accurate results can be obtained by using Factsage results

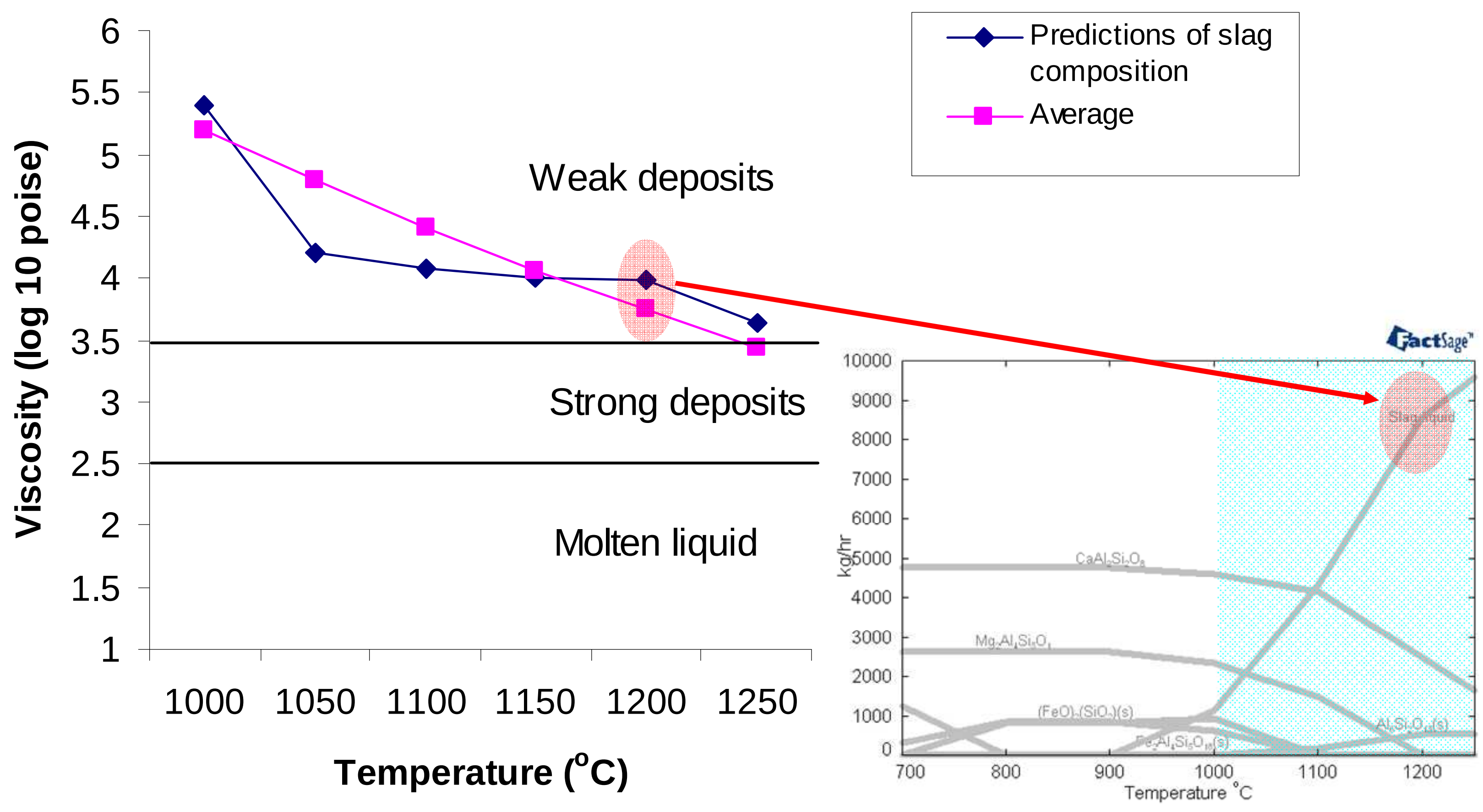
Results (sintered gasification ash)



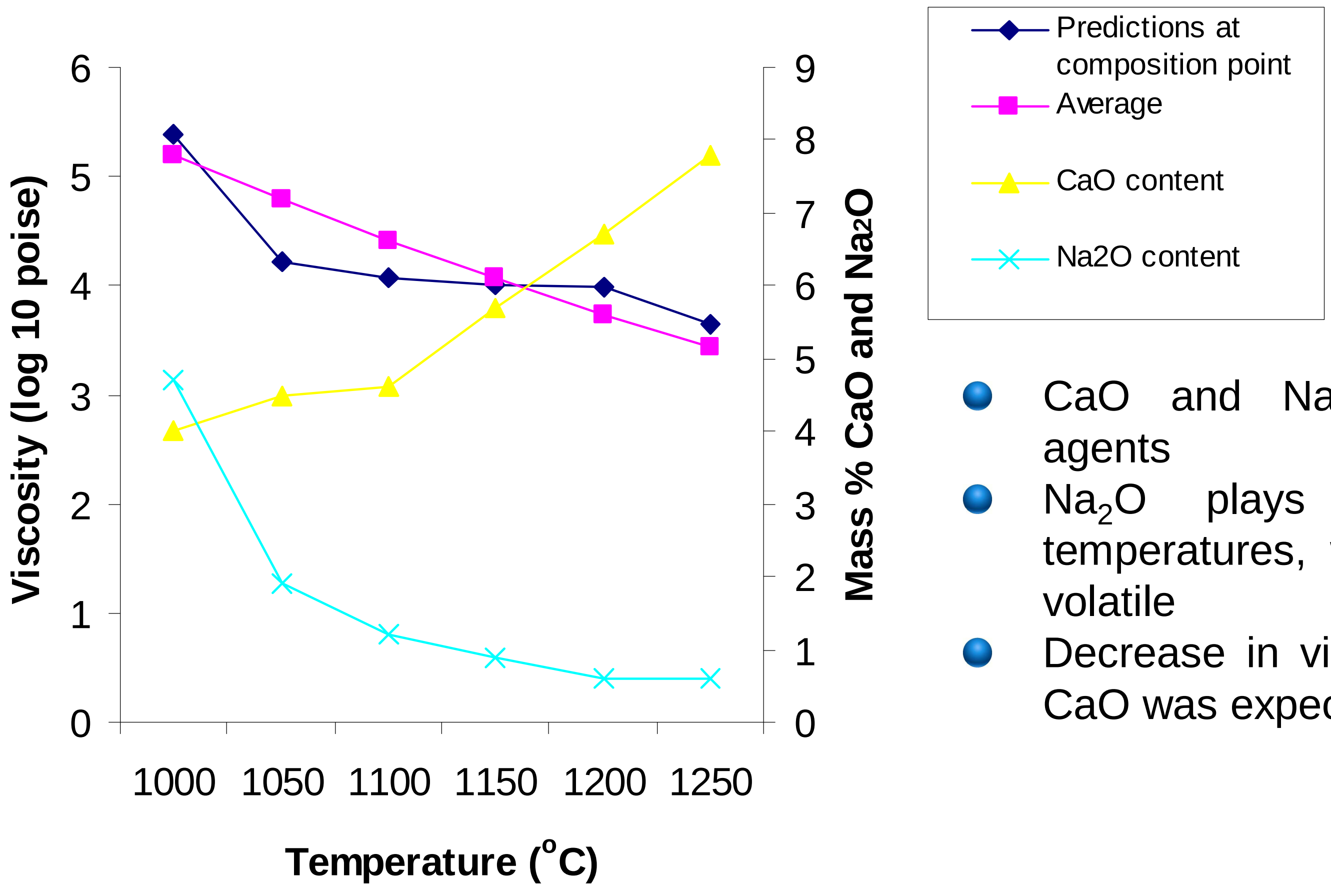
Cooled slag or glas

Crystalline material

Results (viscosity based on Factsage results versus ash composition)



Results (viscosity versus CaO and Na_2O content)



- CaO and Na_2O are both fluxing agents
- Na_2O plays a role at lower temperatures, whereafter it becomes volatile
- Decrease in viscosity with increasing CaO was expected

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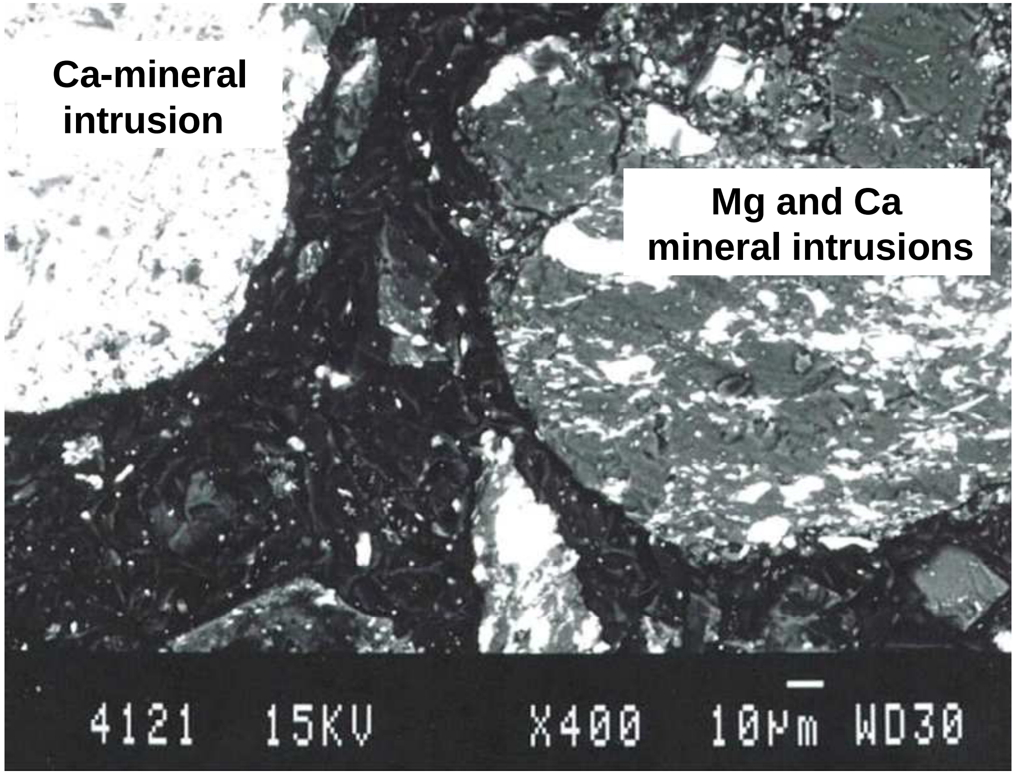
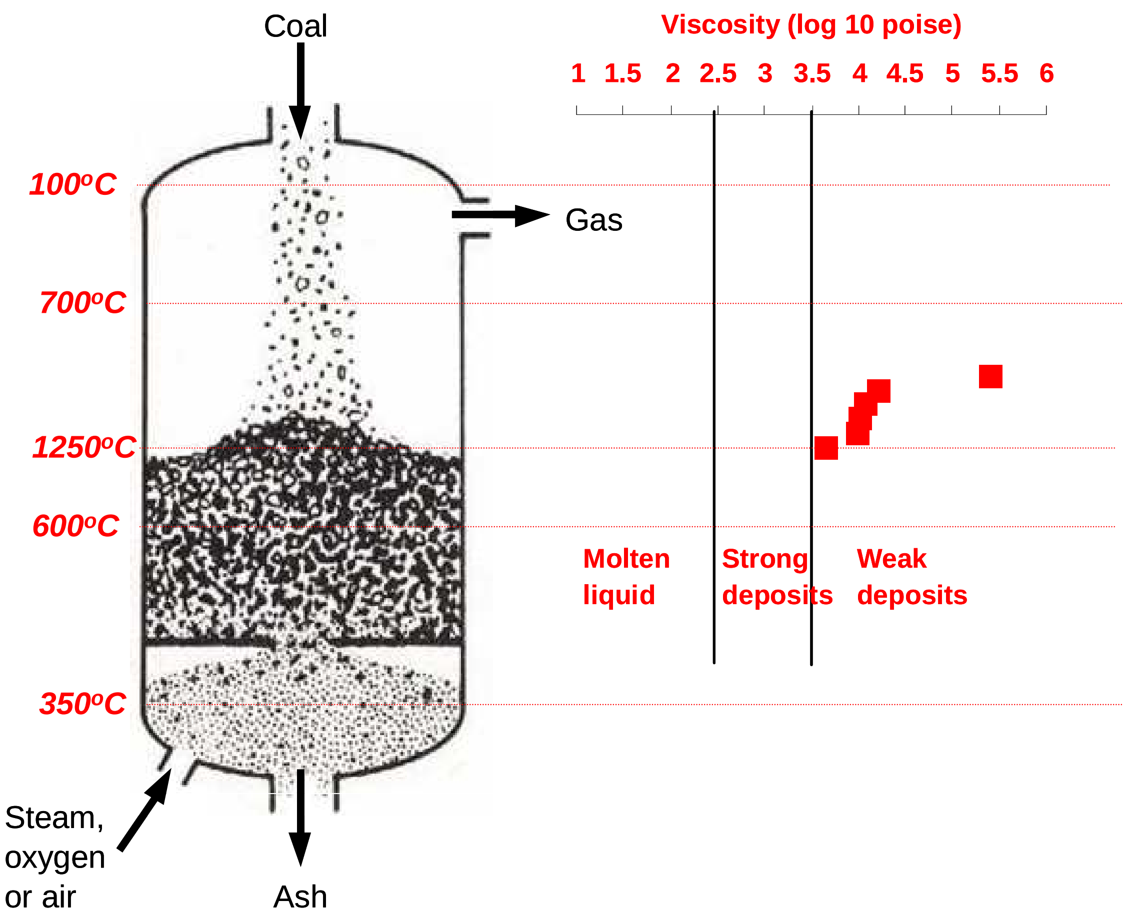
Results (Ca intrusions within coal structure)

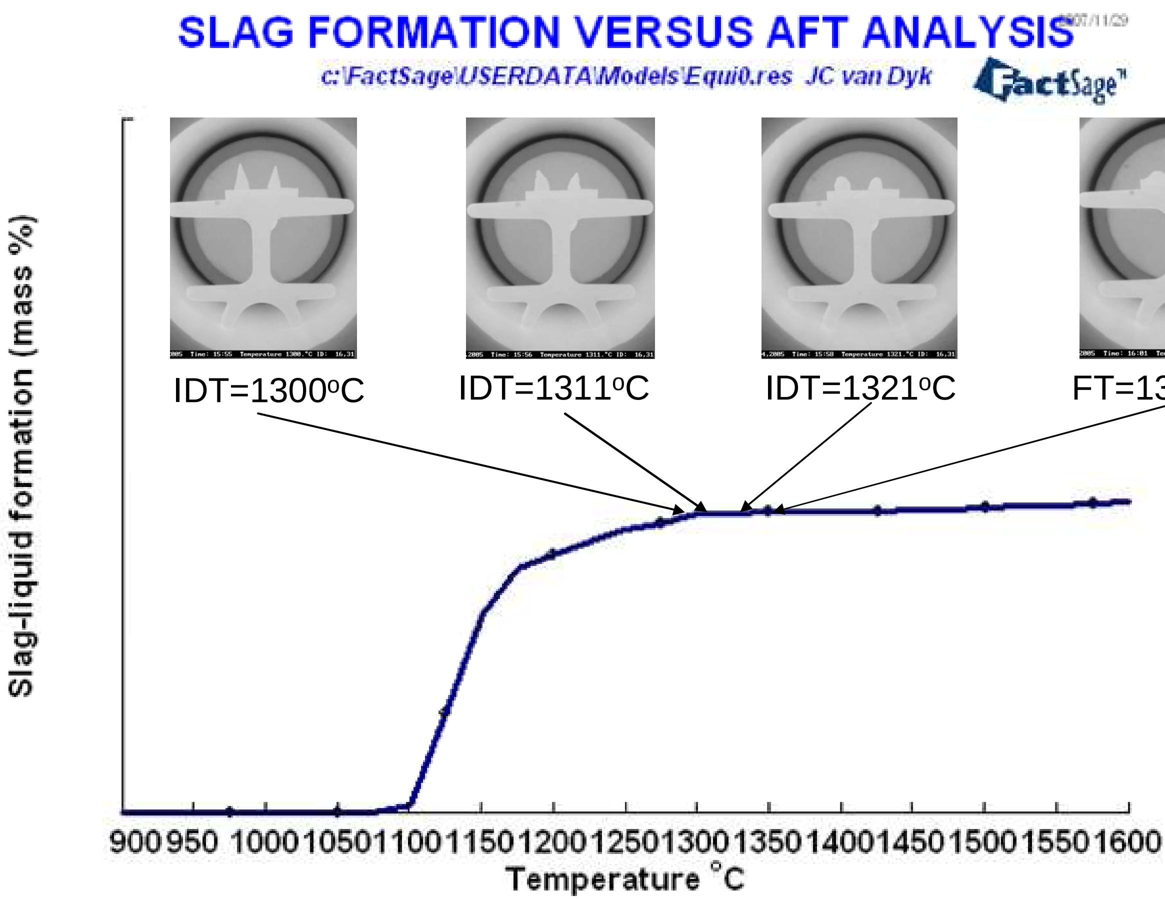


- Areas of high CaO will have lower viscosity and slag compositions forming strong glue (deposits) than areas with high SiO_2
- Anorthite major crystalline component produced from melts that contain higher Ca contents

Results (change in viscosity through gasification)



Results (slag formation versus AFT)



Conclusions

- Between 1000-1250oC the mineral composition is a mixture of both slag-liquid and crystalline material
- Urbain model with ash composition input assumed the system as 100% molten
- Viscosity predictions within fixed bed gasification conditions thus not accurate by only using the Urbain model predictions
- Viscosity predictions on the slag composition based on Factsage results supply a more accurate prediction of the actual molten material
- Correlations between trends in slag formation based on Factsage and viscosity trends on the slag composition can be explained
- Na_2O plays a role in slag formation at lower temperatures and CaO at higher temperatures

Conclusions (cont.)

- Areas of high CaO will have lower viscosity predictions, thus a general predictions is not as accurate as specific predictions on fractions
- Anorthite was formed as major crystalline component present in the slag particle and produced from melts that contain higher Ca contents
- Coal currently used for gasification in Secunda does not form strong deposits at current operating temperatures – low viscosity melts
- AFT analysis does not indicate slag formation at starting temperatures and only supply information where the material is enough to deform the structure of the cone
- **The use of viscosity predictions together with Factsage supplies a better understanding of slag and ash properties**


THANK YOU