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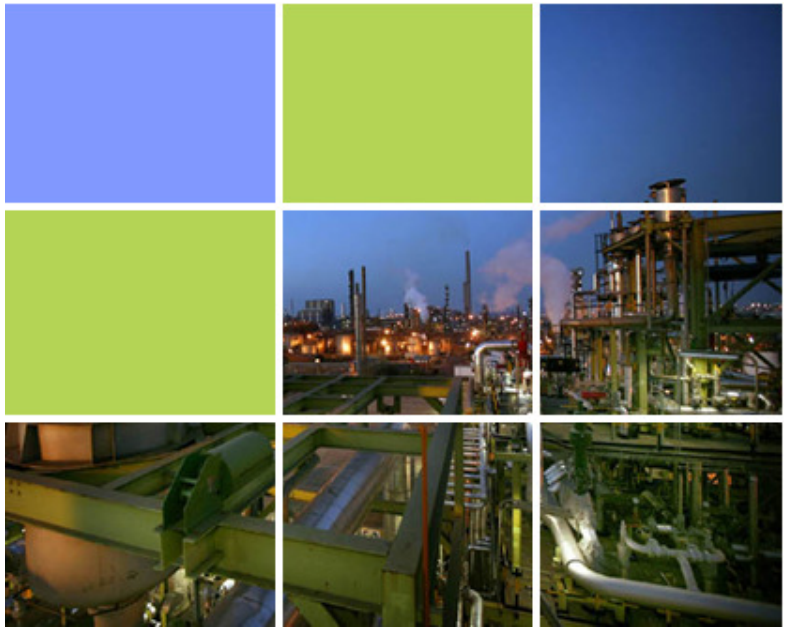
THE USE OF THERMO-EQUILIBRIUM SIMULATION (FACTSAGE) FOR INORGANIC MINERAL MATTER TRANSFORMATION IN GASIFICATION

VALUE ADDITION TO COAL AND GASIFICATION RESEARCH

JC van Dyk, Sasol Technology

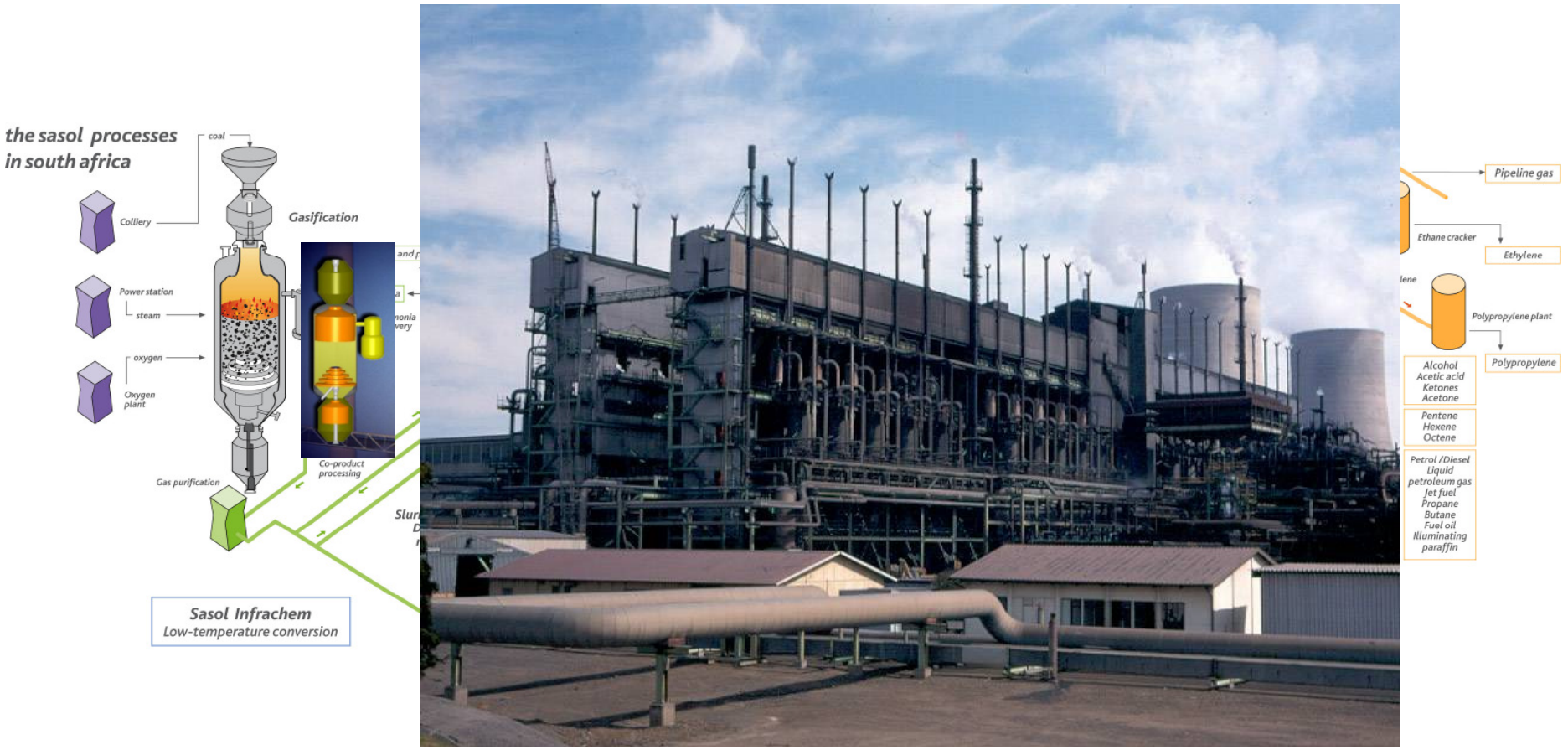
GTT Workshop, 2-4 June 2009



Roadmap of presentation

- Gasification Technologies
- Understanding mineral matter transformations - WHY?
- Applications of FactSage from 2005 in the Sasol R&D environment

Sasol fixed bed dry bottom (FBDB) gasification



Fixed bed gasifiers – where the work started

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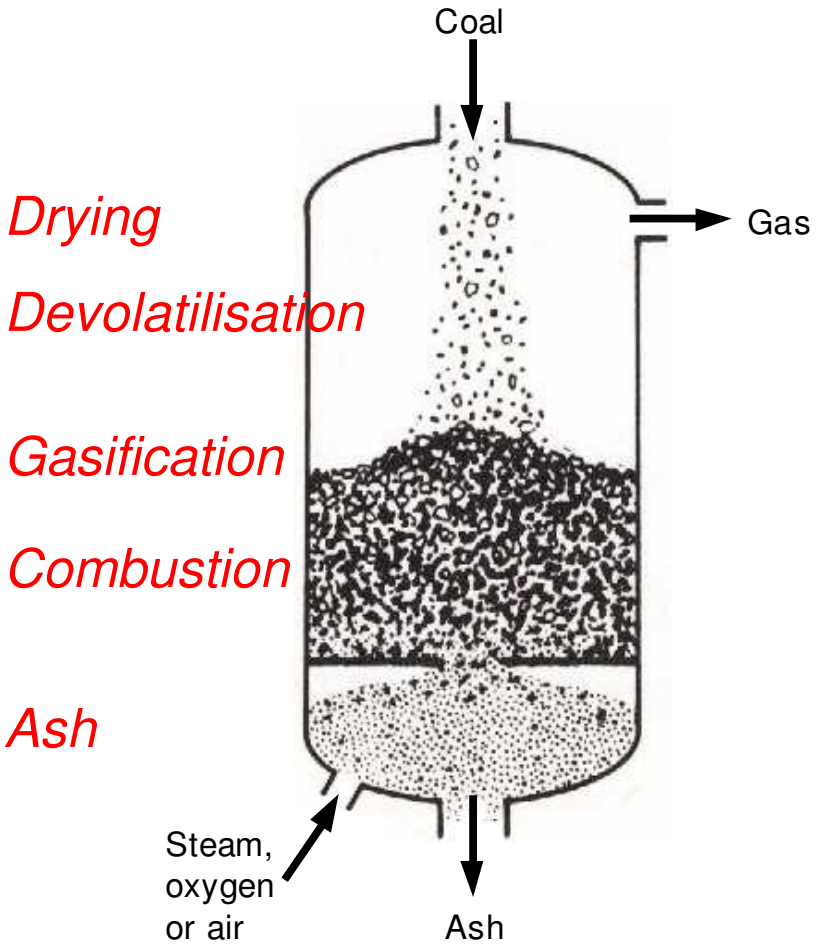
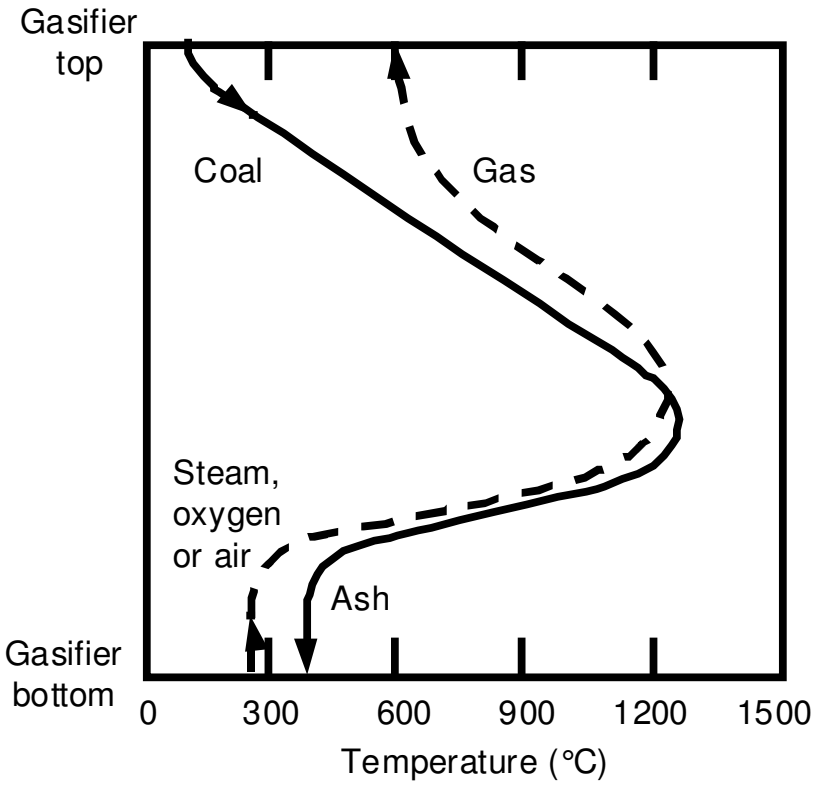
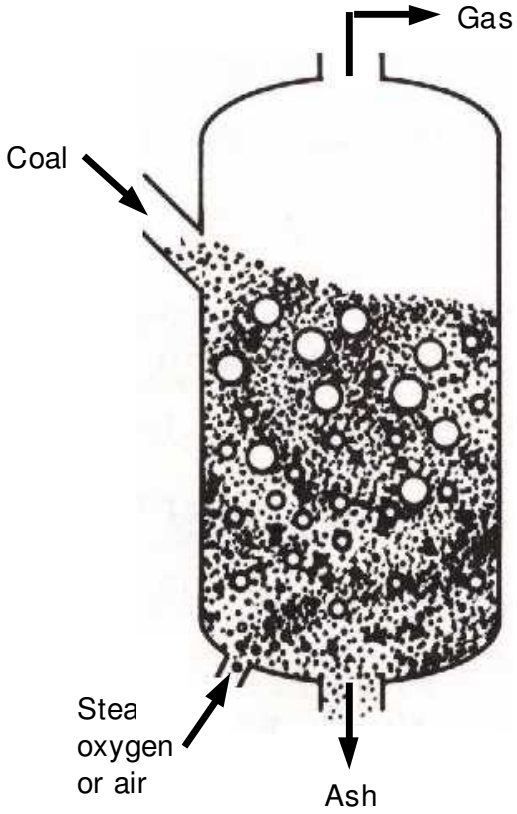
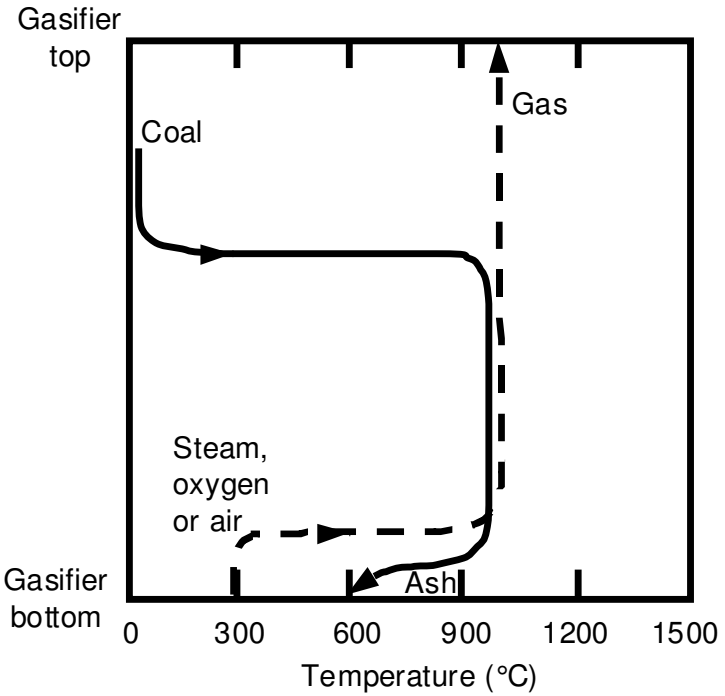


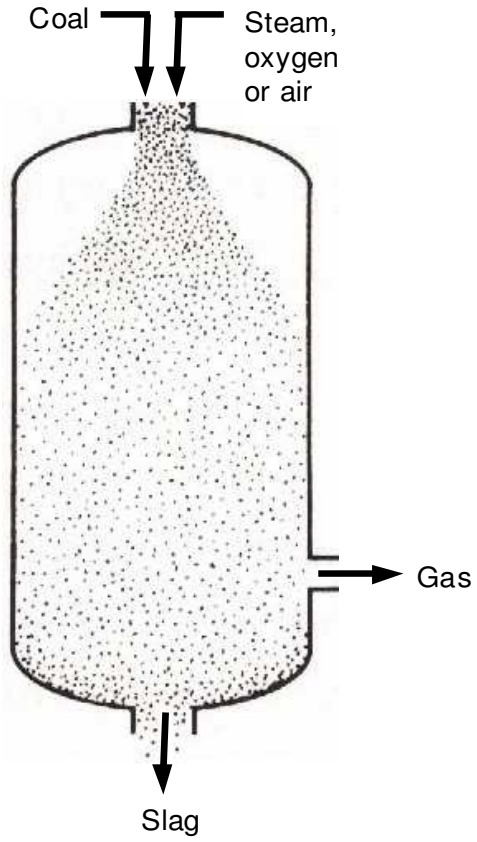


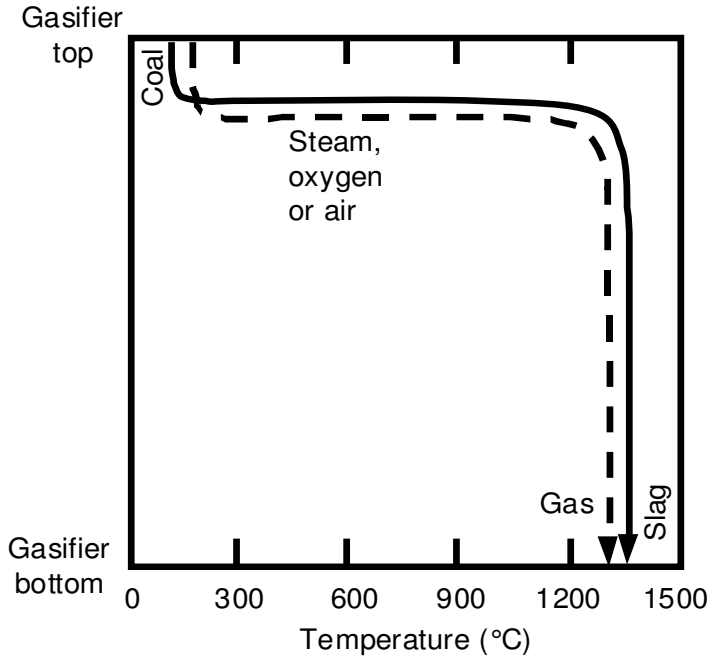
Fluidized bed gasifiers





Entrained flow gasifiers





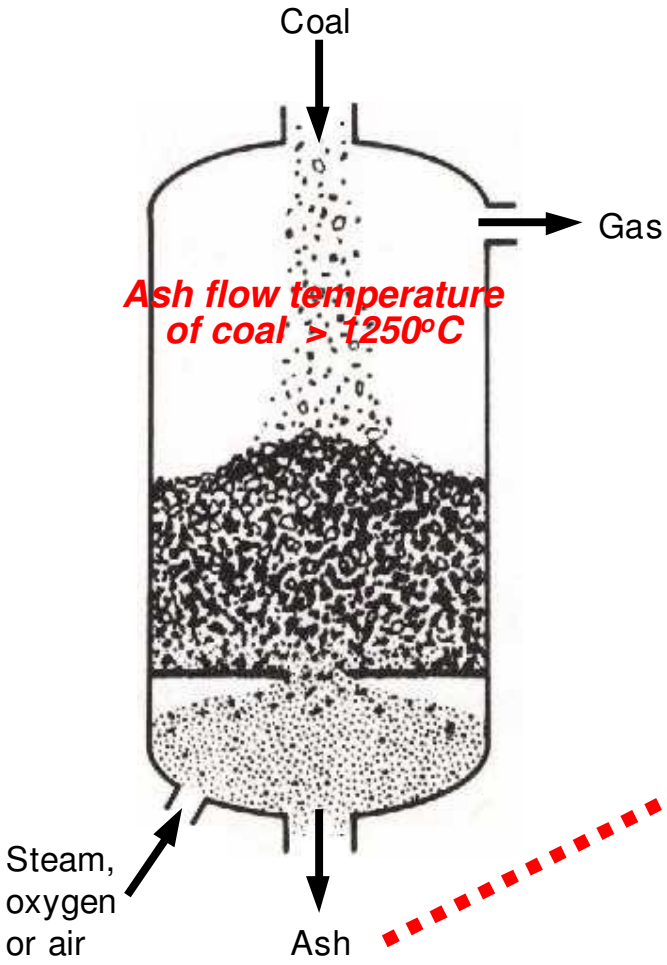
Understanding mineral matter transformations, slag formation and viscosity – WHY?

- **Ash fusion temperature (AFT)** AND **slag properties** of coal that give an indication of suitability for gasification purposes

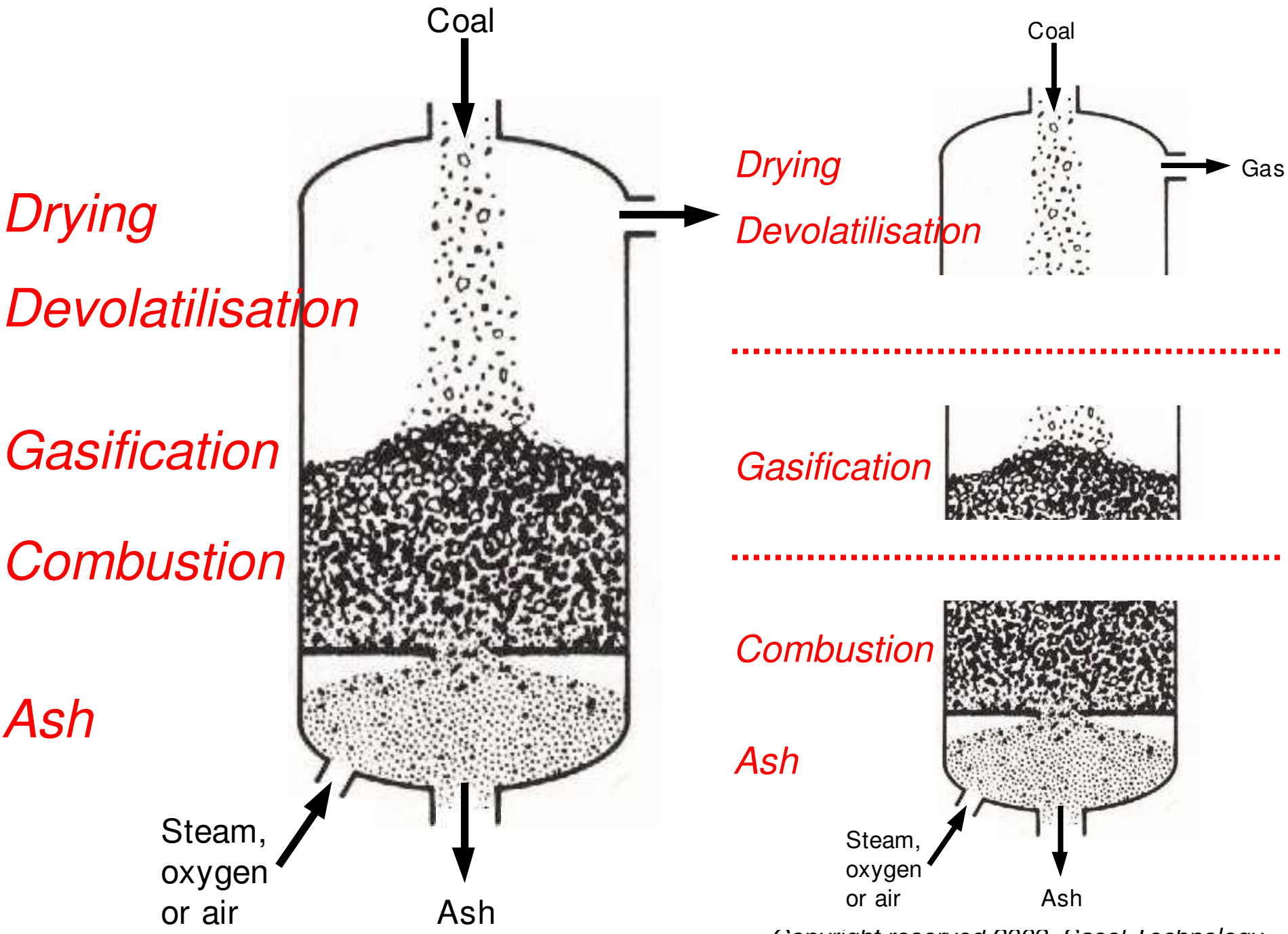
- Ash fusion temperature
  - *results in an average temperature where bulk mineral composition starts to become soft and melt*
  - *is an indication to what extent agglomeration / clinkering is likely to occur within the gasifier*
  - *is currently used to predict average slagging properties of coal sources and not at what temperature the first melt/sinter occurs*

- Ash clinkering in fixed bed gasifiers can cause channel burning, pressure drop problems, unstable gasifier operation, etc.

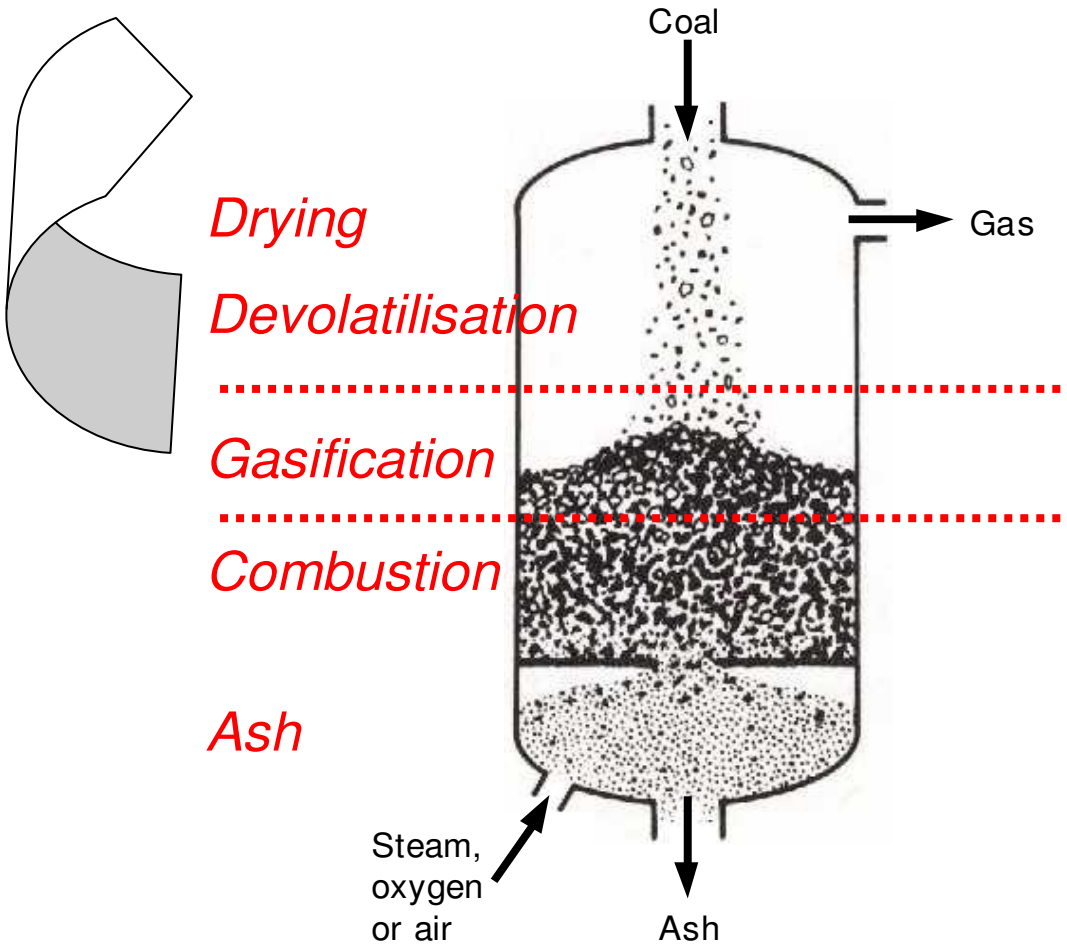
Syngas and ash producer



Courtesy of RH Matjie



FACTSAGE modelling approach



FACTSAGE input w.r.t. coal properties

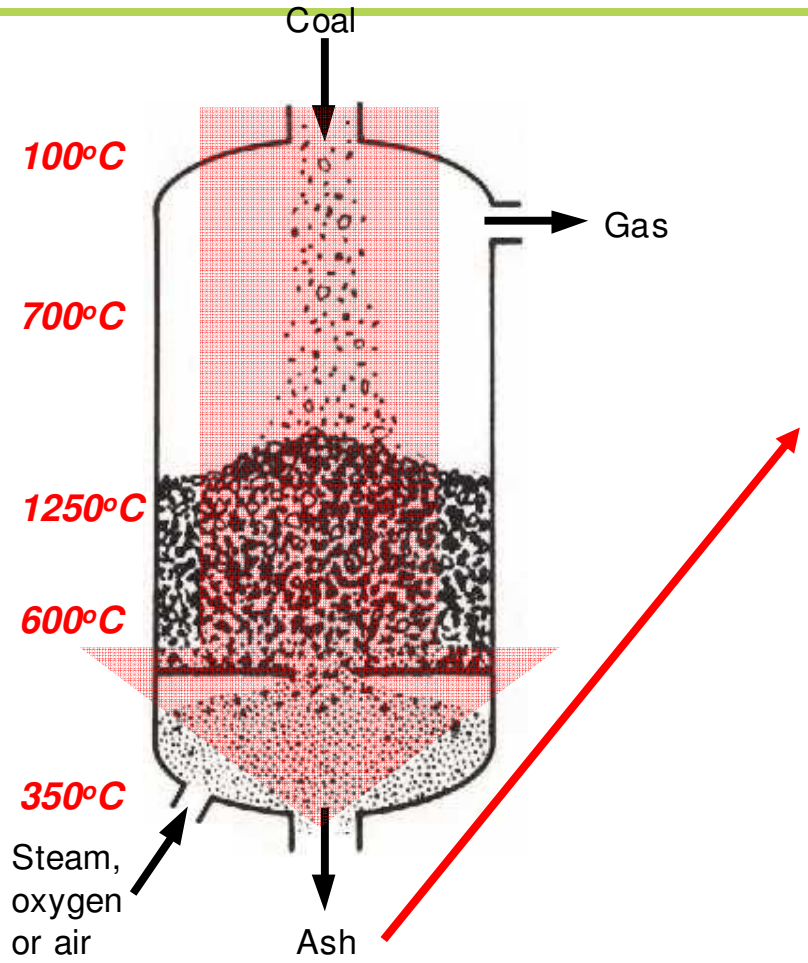
Component	Mass %	Mass flow (kg/hr)
Moisture	5.0	2550
Fixed carbon	46.3	23613
Volatile matter	22.9	11679
Ash	25.8	13158
TOTAL	100	51000

Mineral	Formula	Mass %	Mass flow (kg/hr)
Pyrite	FeS_2	4.0	526
Quartz	SiO_2	20.0	2631
Microline	$KalSi_3O_8$	1.9	250
Muscovite / Illite	$Kal_3Si_3O_{10}(OH)_2$	2.9	381
Kaolinite	$(Al_2O_3)(SiO_2)_2(H_2O)_2$	52.5	6913
Anatase	TiO_2	0.3	39
Calcite	$CaCO_3$	6.7	881
Dolomite	$CaMg(CO_3)_2$	10.1	1328
Apatite	$Ca_3(PO_4)_3(FOH)$	0.5	65
Gypsum	$CaSO_4(H_2O)_2$	1.1	144
TOTAL		100	13158

Property	Mass %	Mass flow (kg/hr)
H_2O	2.9	1479
H_2	0.15	76
CH_4	4.01	2045
CO	0.98	499
CO_2	7.2	3672
N_2	2.1	1050
Tar and oils	5.6	2858
TOTAL	22.9	11679

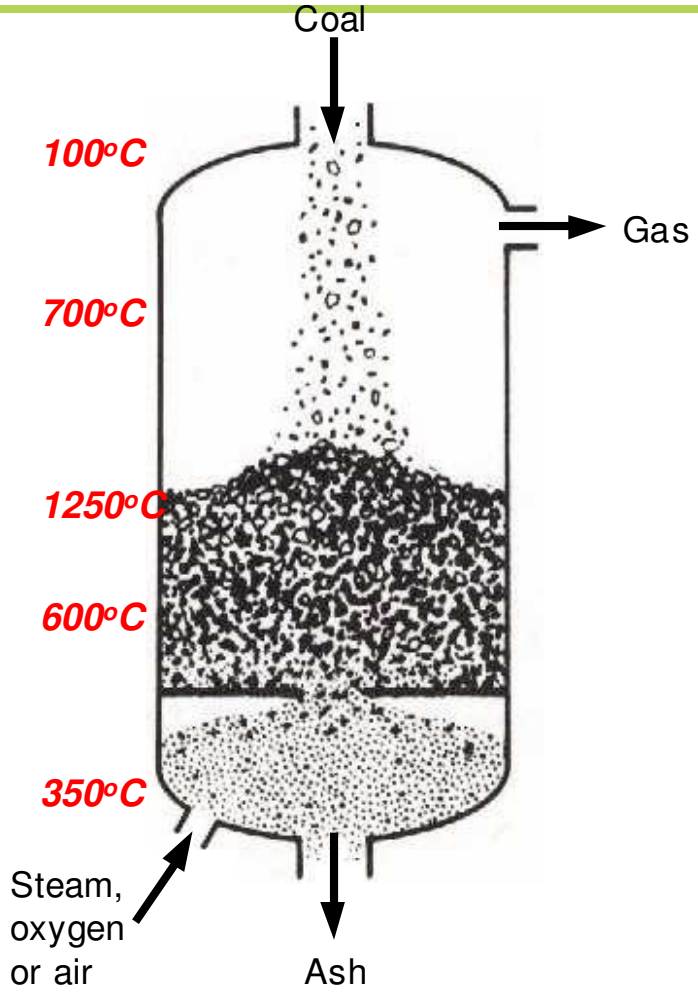
Property	Mass %	Mass flow (kg/hr)
Carbon (C)	78.8	25557
Hydrogen (H)	4.1	1329
Nitrogen (N)	2.2	713
Sulphur (S)	2.1	681
Oxygen (O) by difference	13.0	4154
TOTAL	100	32434

Combustion zone – actual ash characteristics



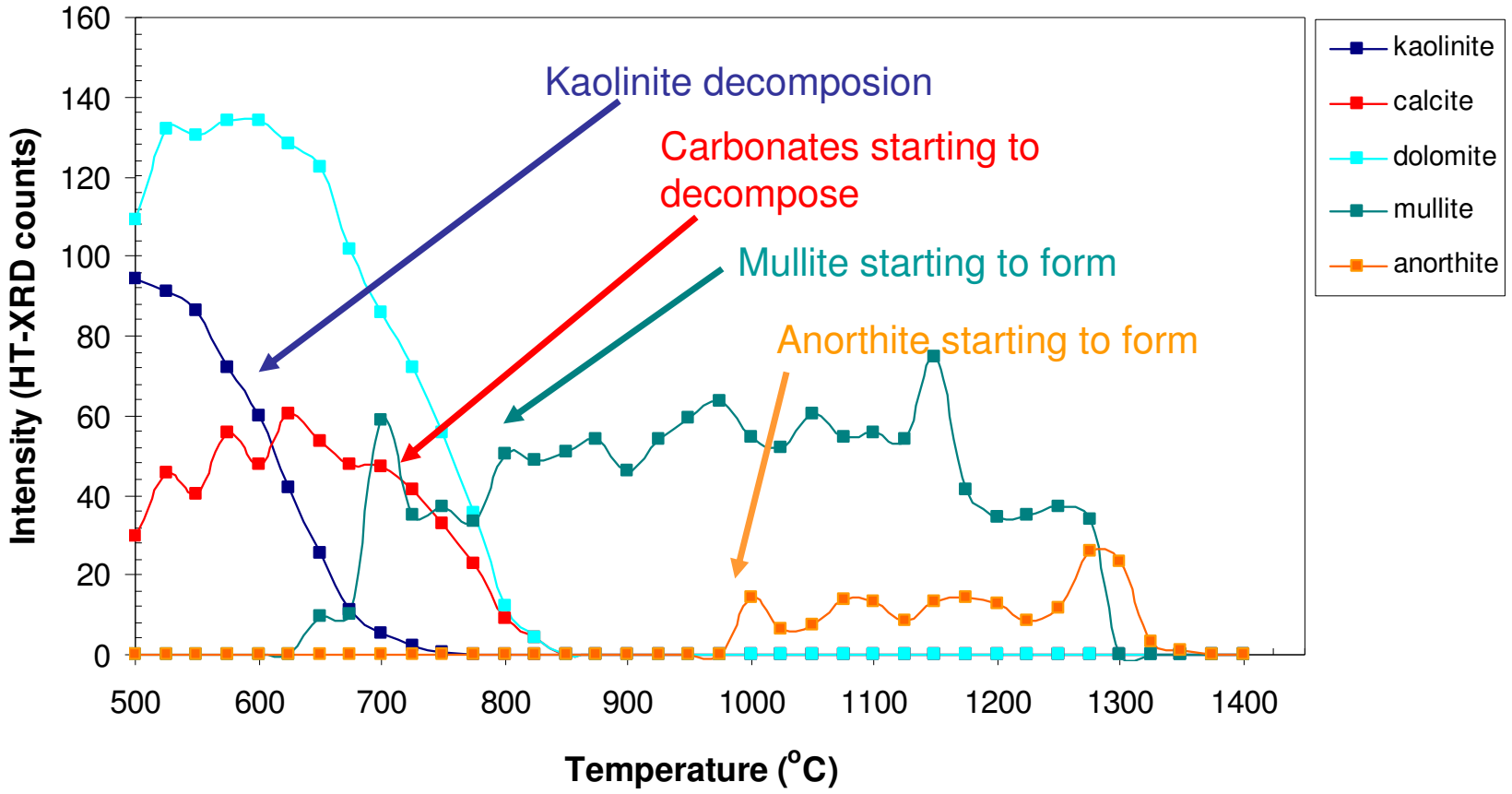
Mineral composition of ash (crystalline material)
SiO_2 quartz
$CaAl_2Si_2O_8$ anorthite
$CaAl_4Si_2O_{10}(OH)_2$ margarite
$Mg_5Al_2Si_3O_{10}(OH)_8$
$KAl_3Si_3O_{10}(OH)_2$ muscovite
$Fe_3Al_2Si_3O_{12}$ almandine
$(FeO)(TiO_2)$ ilmenite

Combustion zone – simulation results

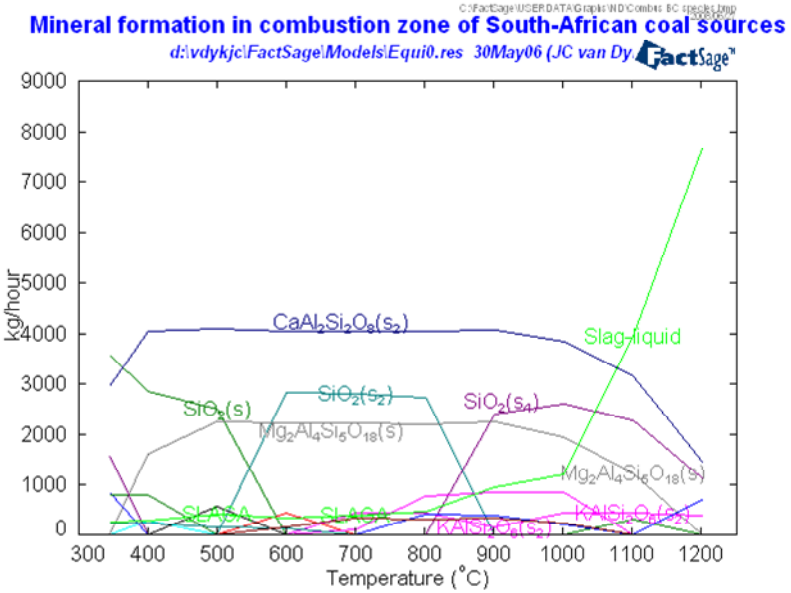


- *Kaolonite disappeared between 600°C and 650°C*
- *>650°C meta-kaolonite forms from kaolonite*
- *Carbonates, calcite and dolomite decompose*
- *Mullite starts to form*
- *Intensities of mullite and quartz reflections decrease as a result of melt formation*
- *Anorthite crystallizes between 1000°C - 1100°C*
- *Above 1200°C only quartz and anorthite remain stable in the liquidus*

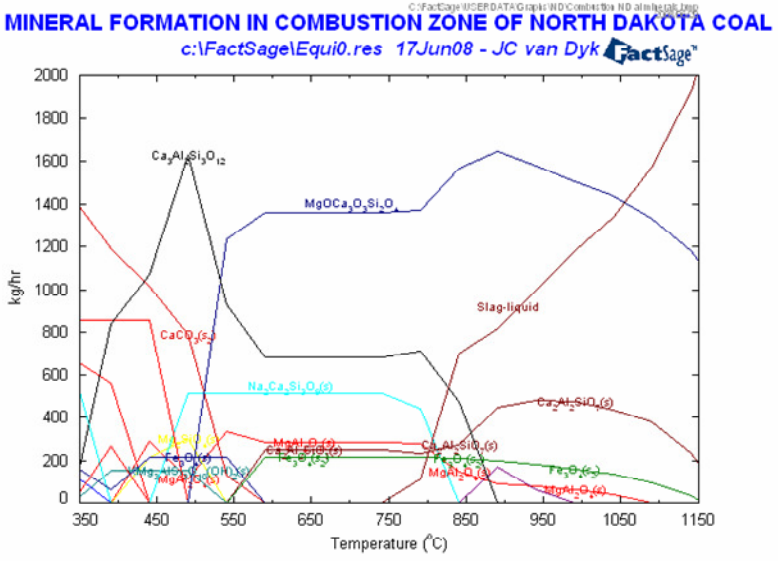
Summary of HT-XRD results



Oxygen capture in mineral structure during gasification

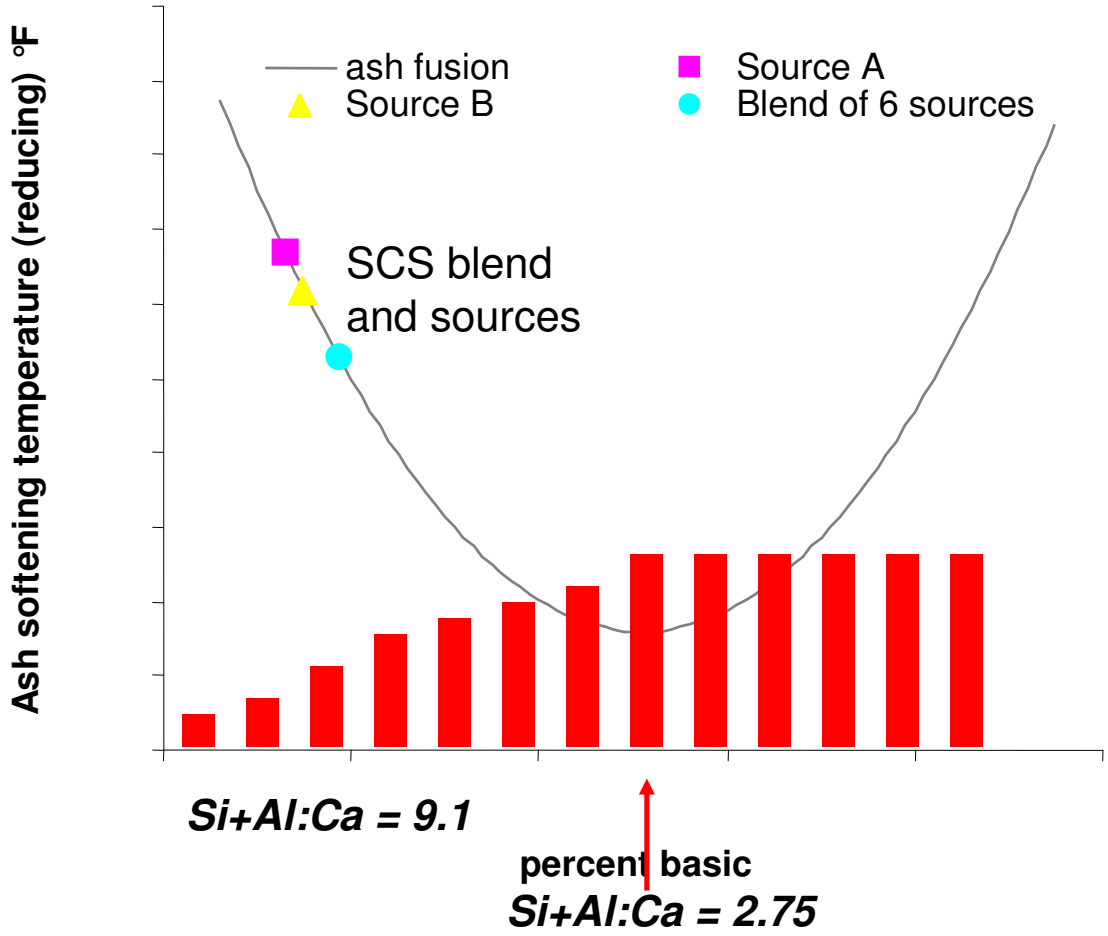


Cooling process

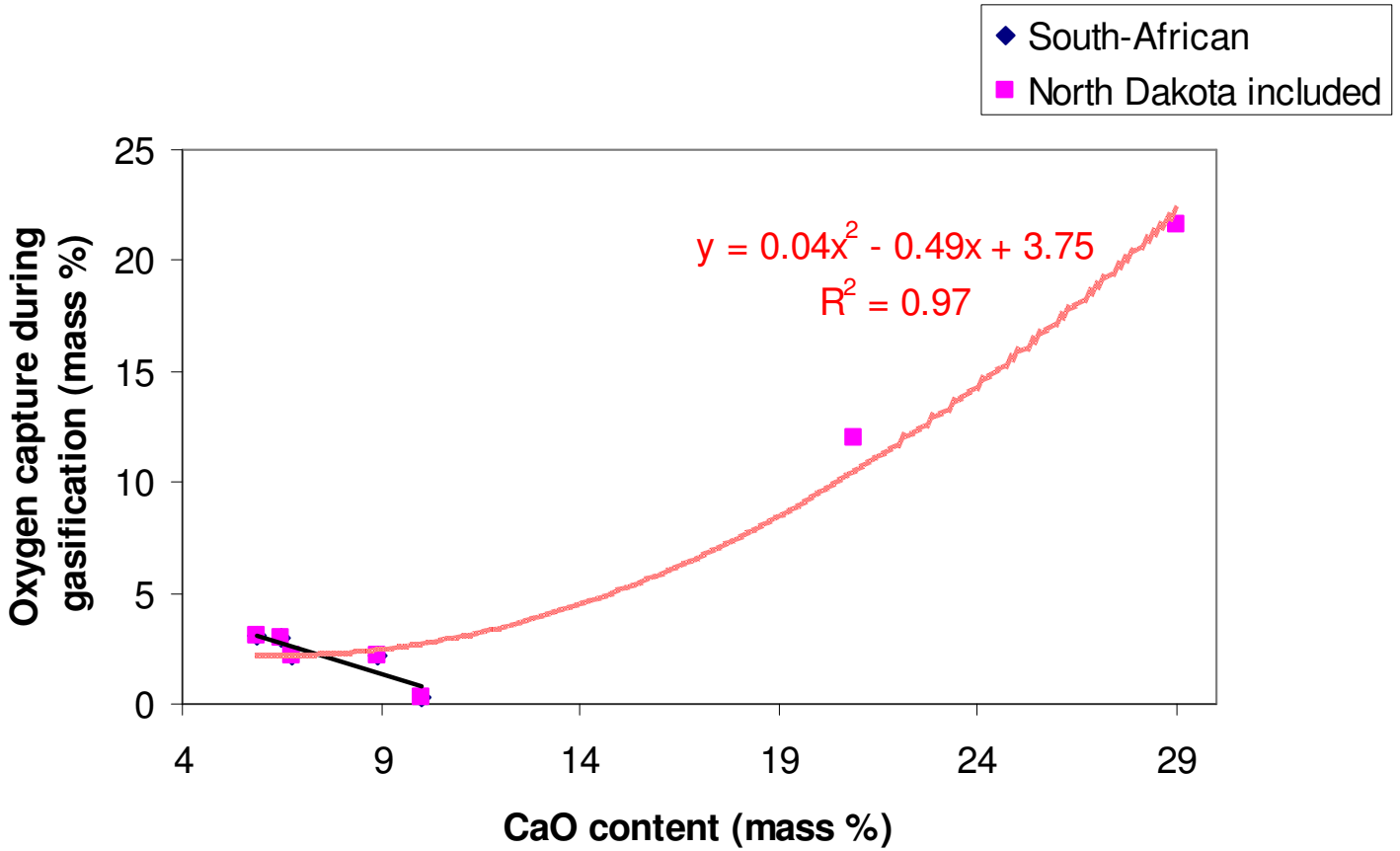


Cooling process

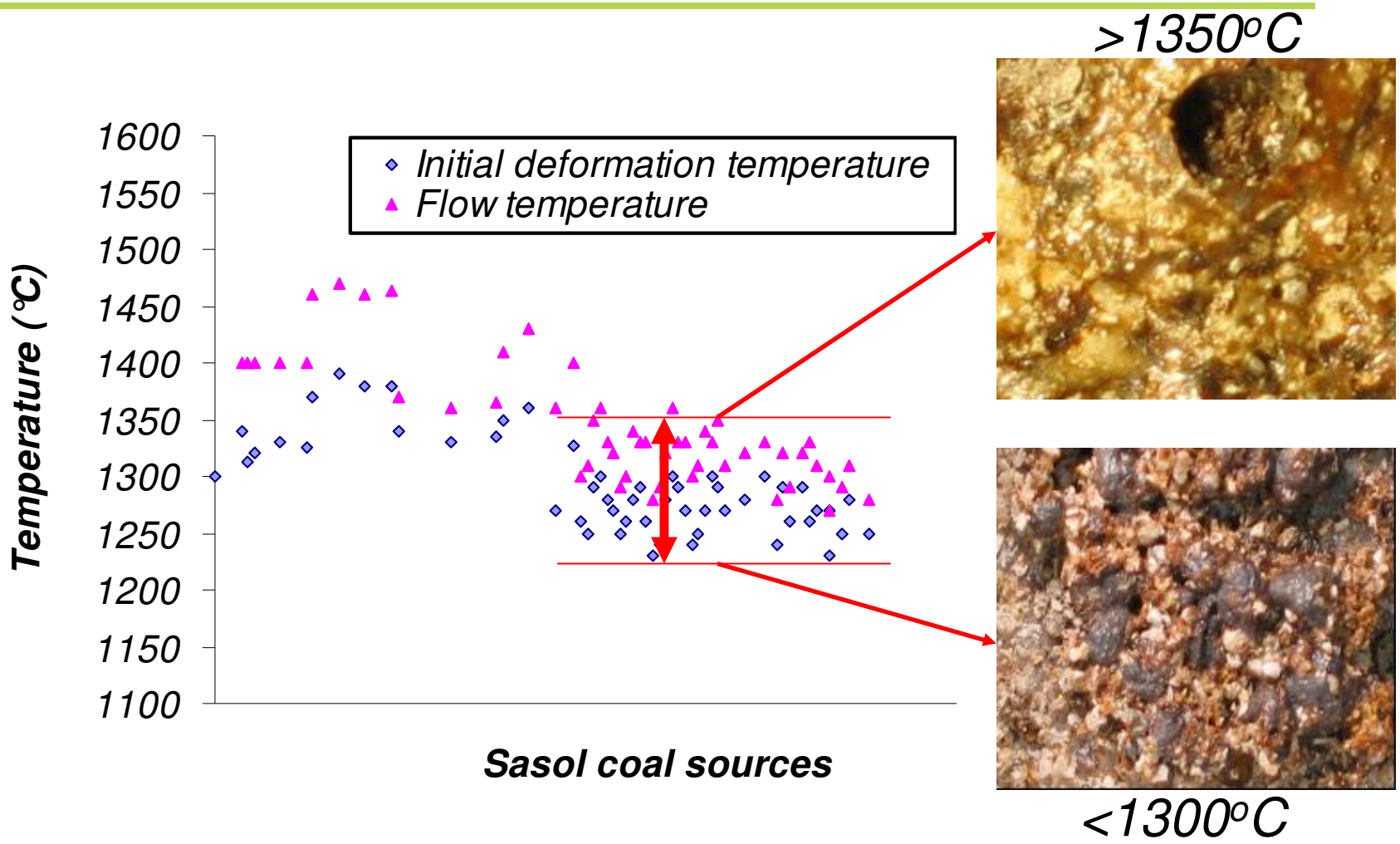
Why the difference in intensity?



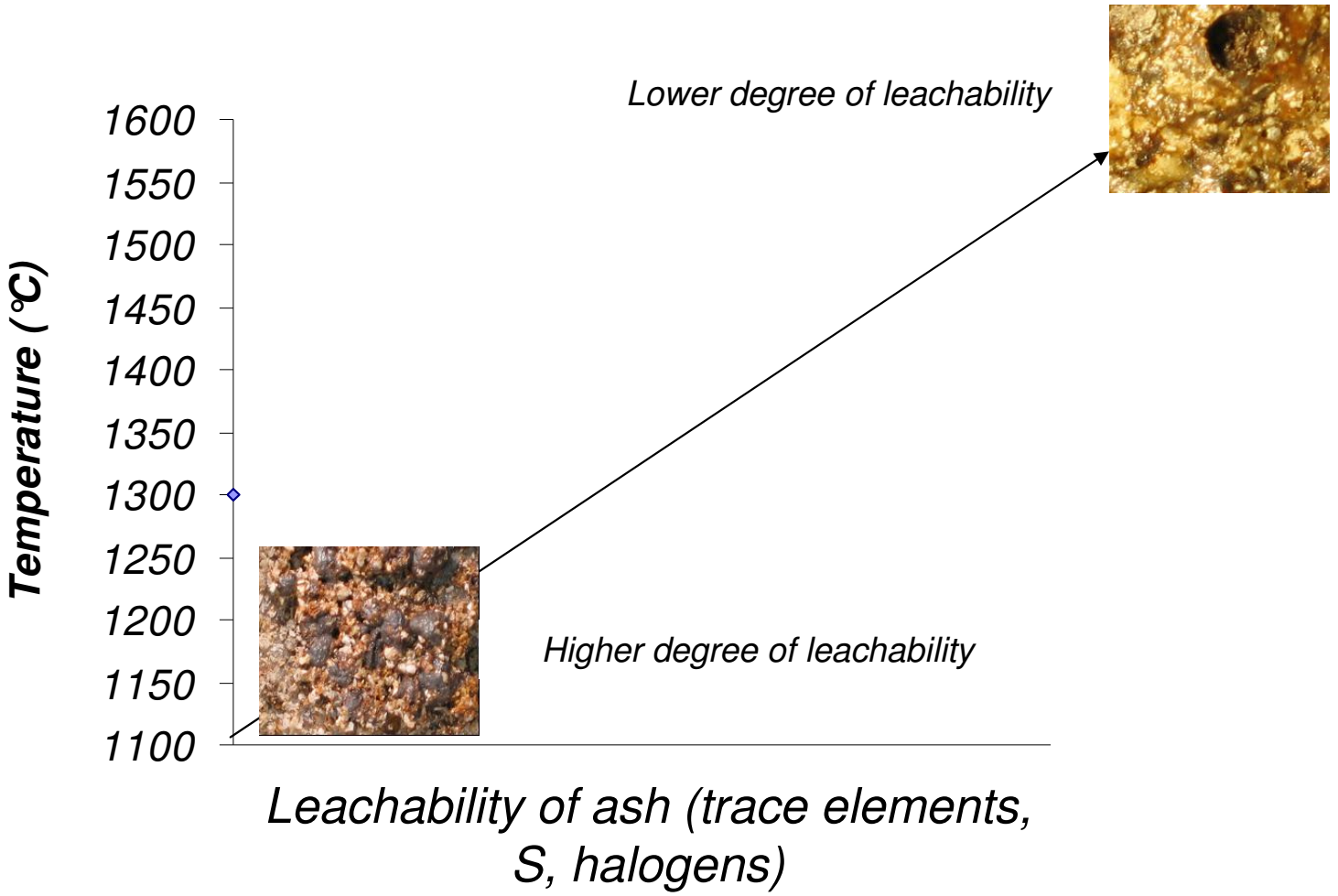
Oxygen capture versus CaO



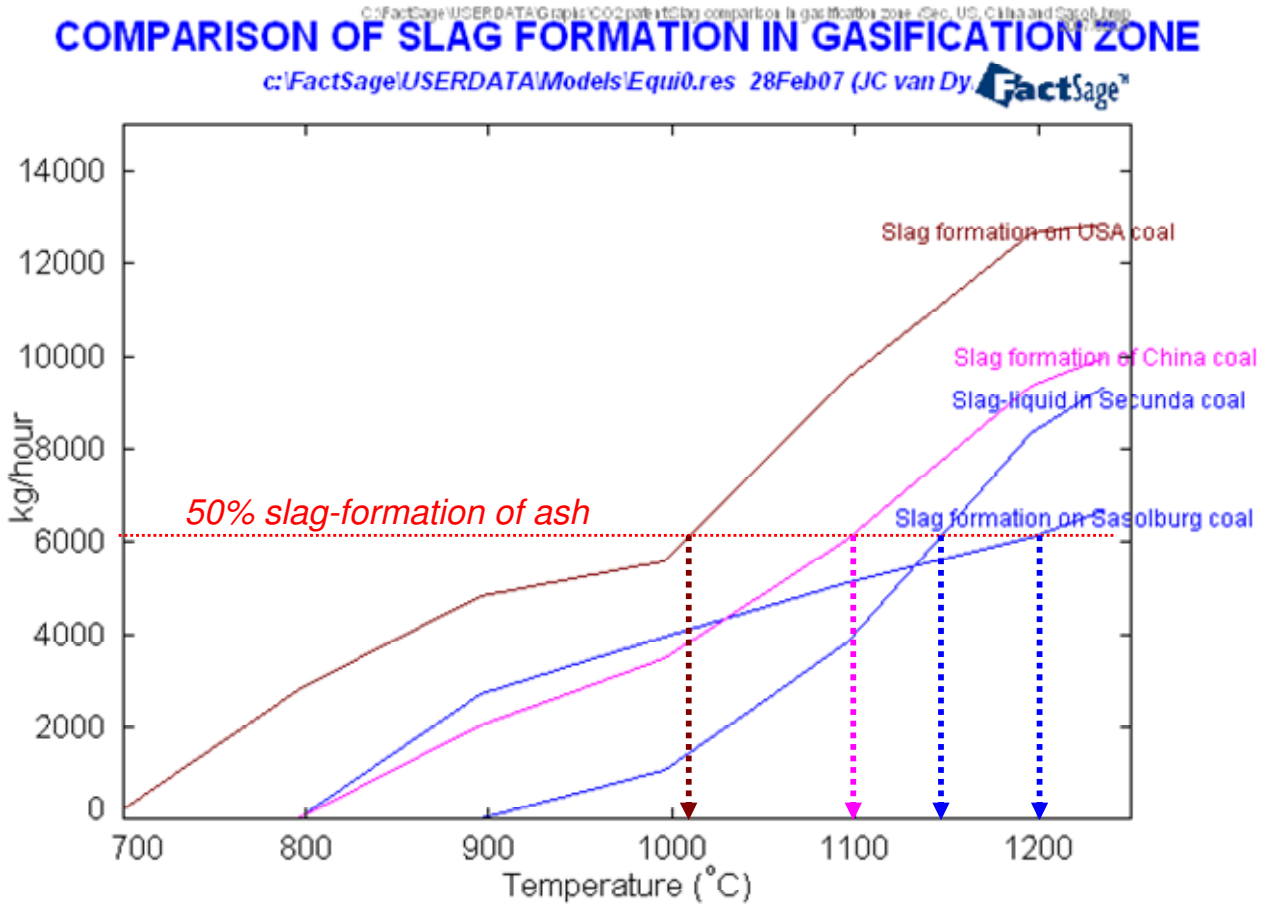
Window of operation between sintering and slagging



Leachability of ash (in progress)

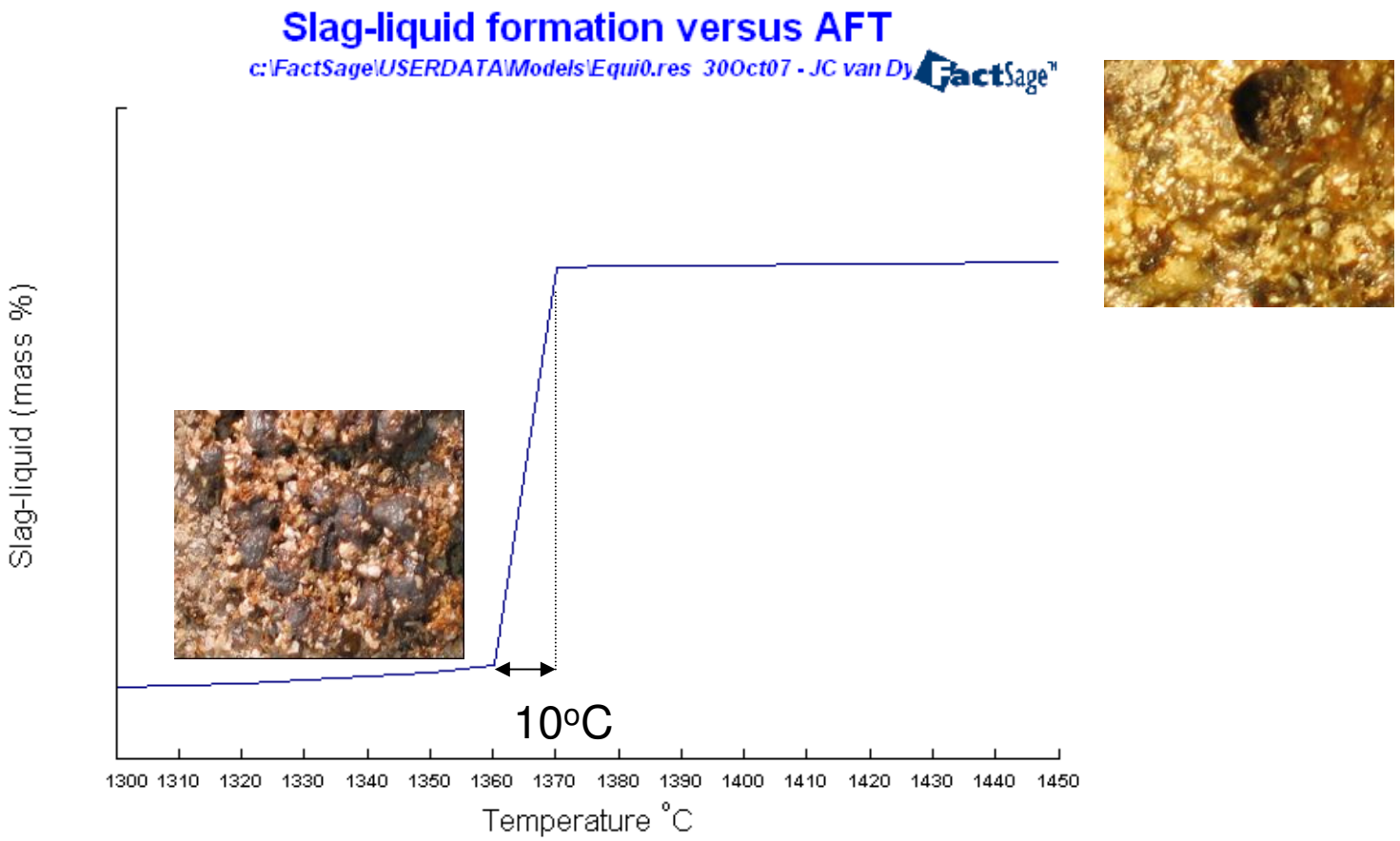


Prediction of ash flow temperatures

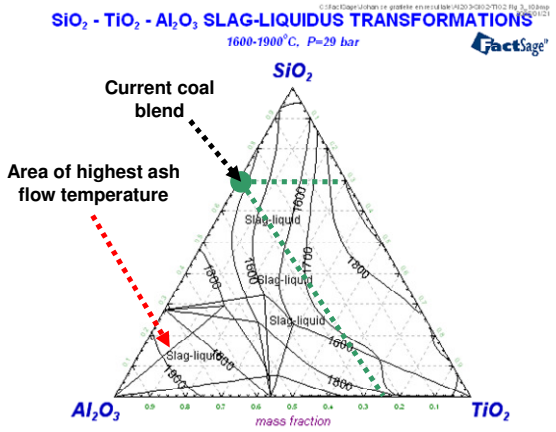


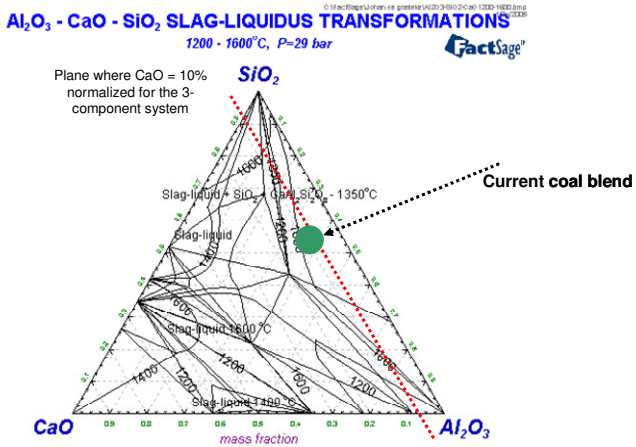
Predicted IDT

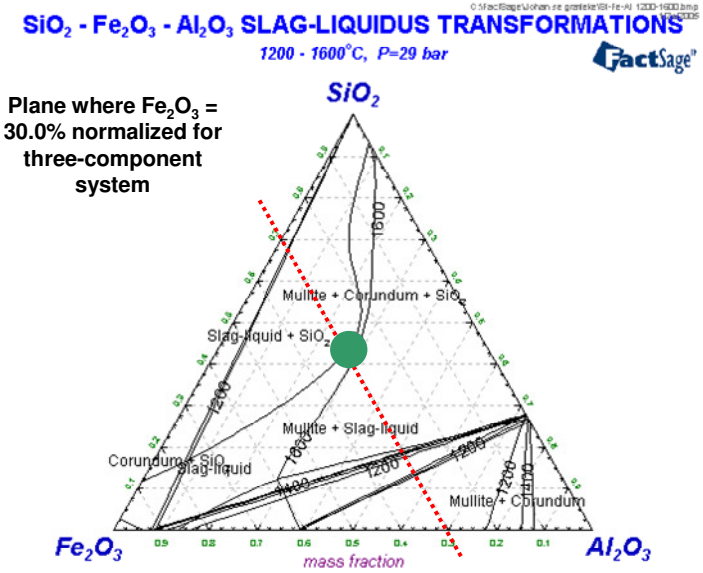
Window of operation between sintering and slagging

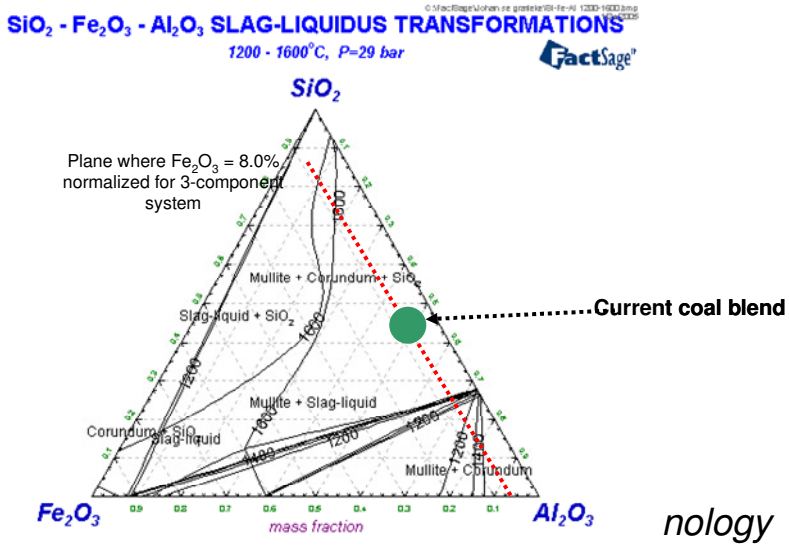


Discussion of mineral matter results by means of 3-component systems









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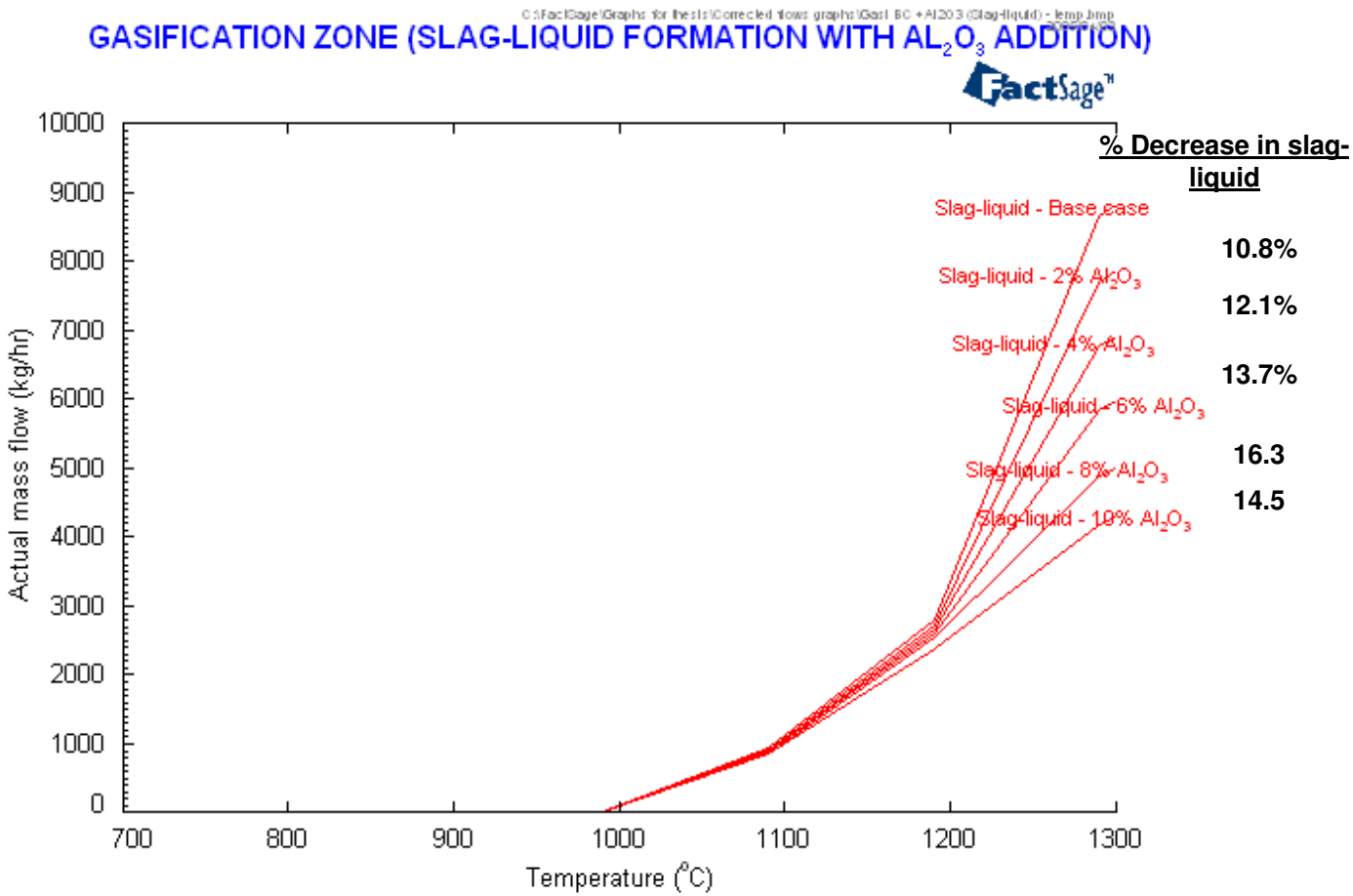
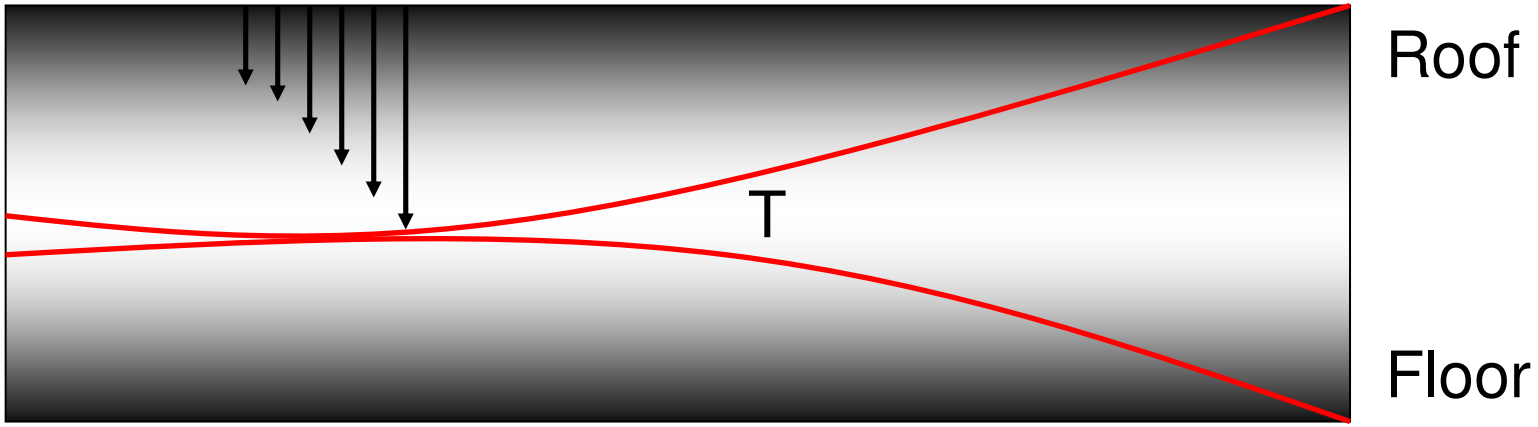
AFT Manipulation



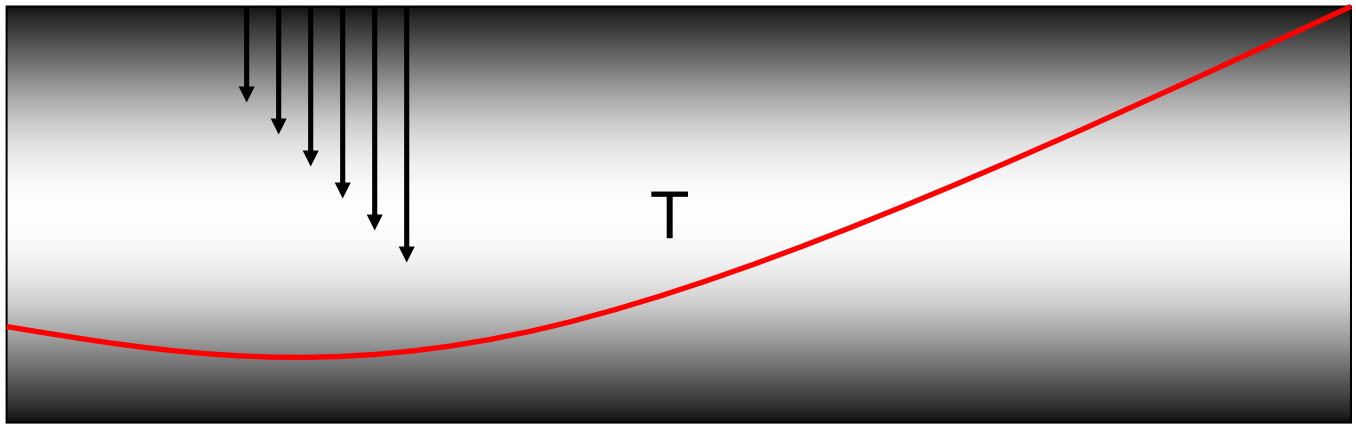
Effect of temperature on slag formation, mineral transformation and ash leaching - UCG

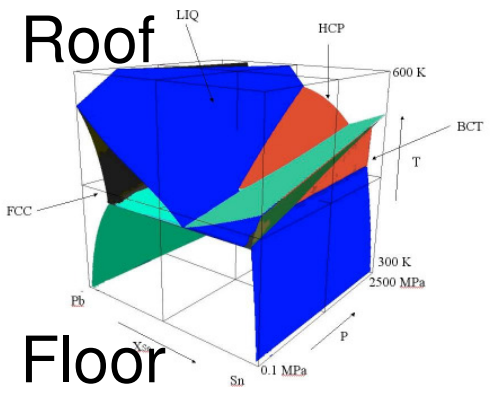
- HT-XRD – simulate mineral transformations and mineral formations with varying operating T (work not started yet)
  - *Roof*
  - *Floor*
  - *Effect of collapsing roof on ash structure and behavior*



Effect of temperature on slag formation, mineral transformation and ash leaching

- Factsage thermo-equilibrium simulation – simulate slag formation, mineral transformations and mineral formations with varying operating T (in progress)
  - *Roof*
  - *Floor*
  - *Effect of collapsing roof on ash structure and behavior*






THANK YOU