



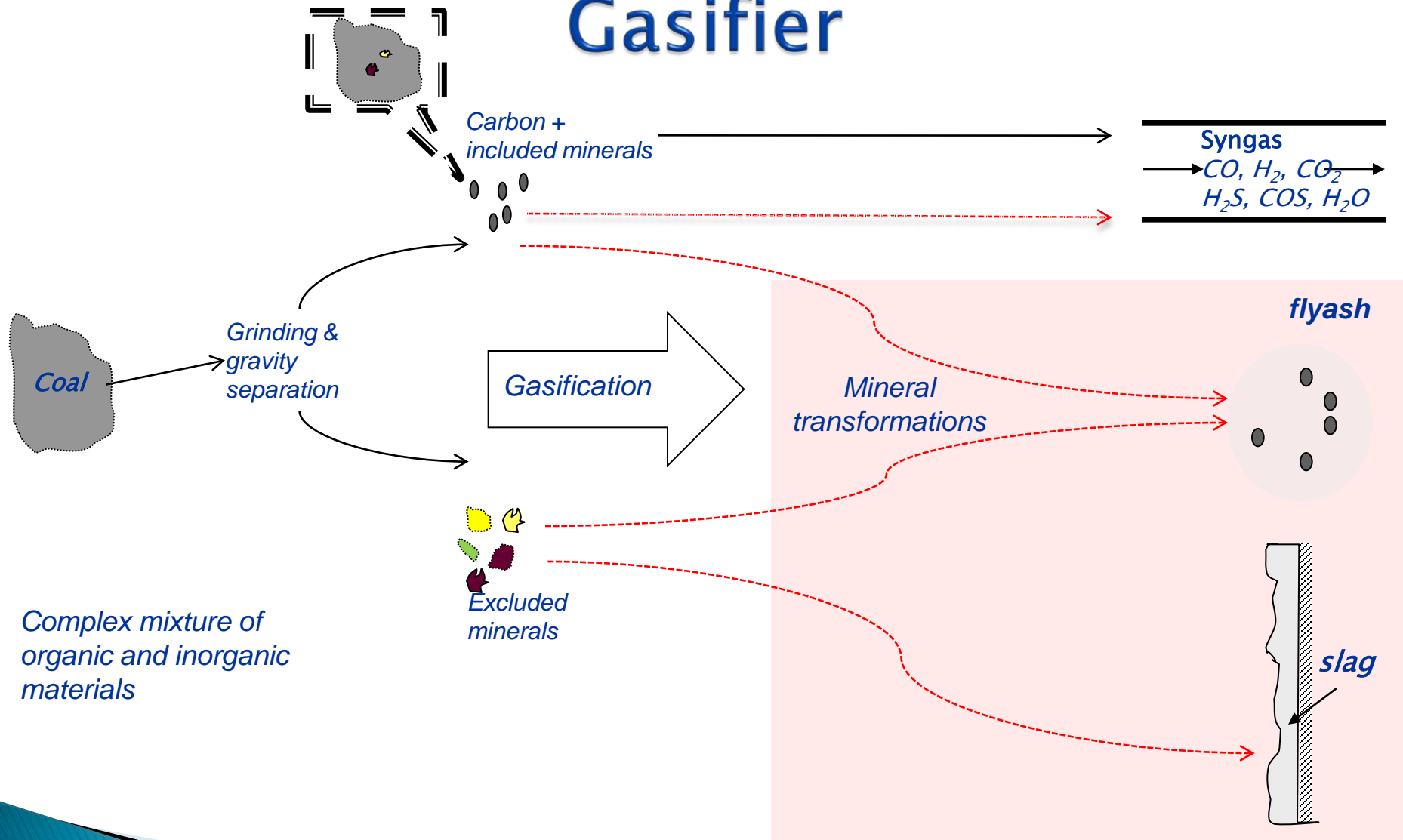
# Physical and Chemical Property Variations of Segregated Coal Fractions for Modeling Entrained Flow Slagging Gasifier

Nari Soundarrajan, Nandakumar K., Latosha Gibson, Sarma Pisupati

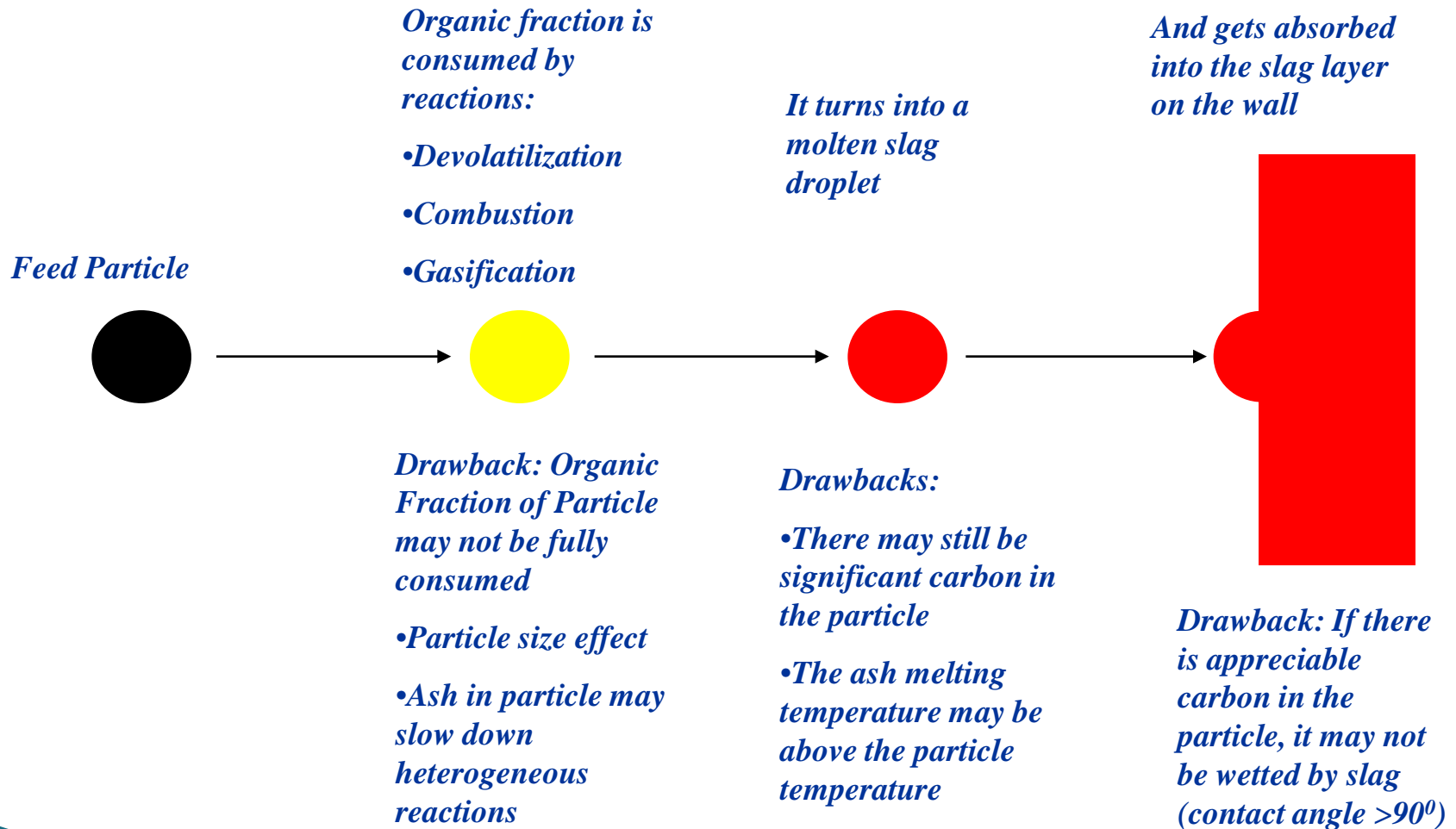
Department of Energy and Mineral Engineering and EMS Energy Institute  
Penn State University

**NETL Multiphase Flow Workshop,  
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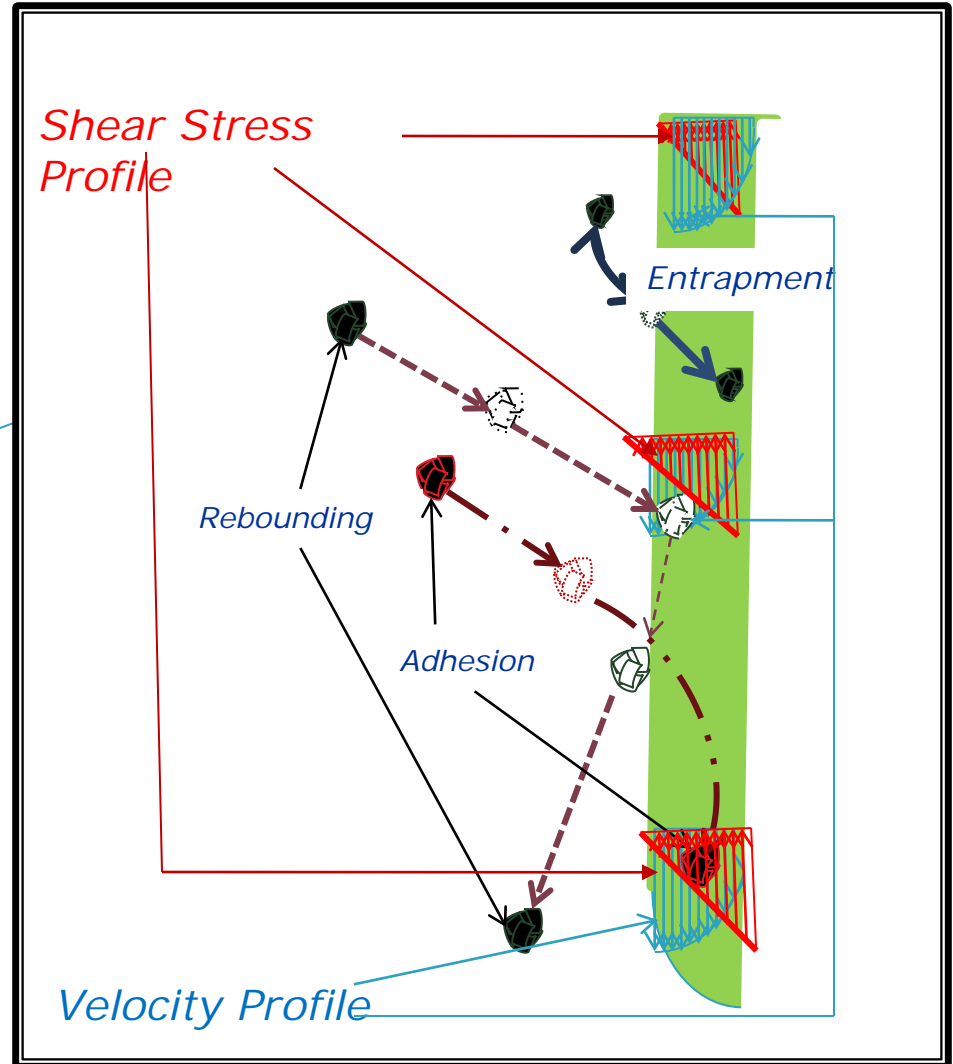
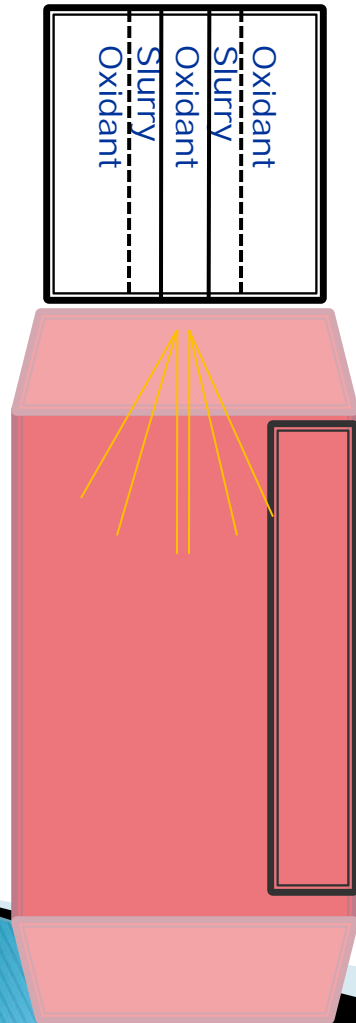
# Background – Coal Conversion in Gasifier



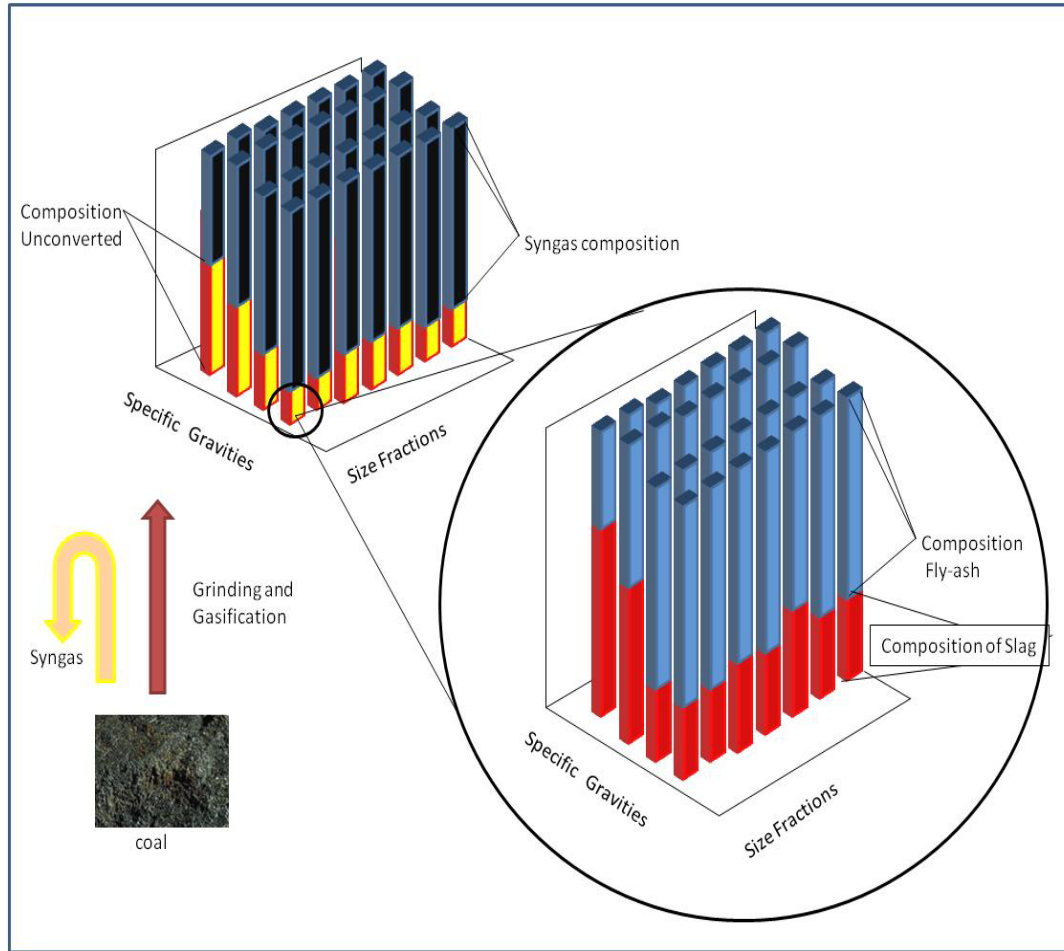
# Assumed Particle Transformation in an Entrained Flow Gasifier



# Char and Slag Interaction



# Particle Population Model for Lab Scale



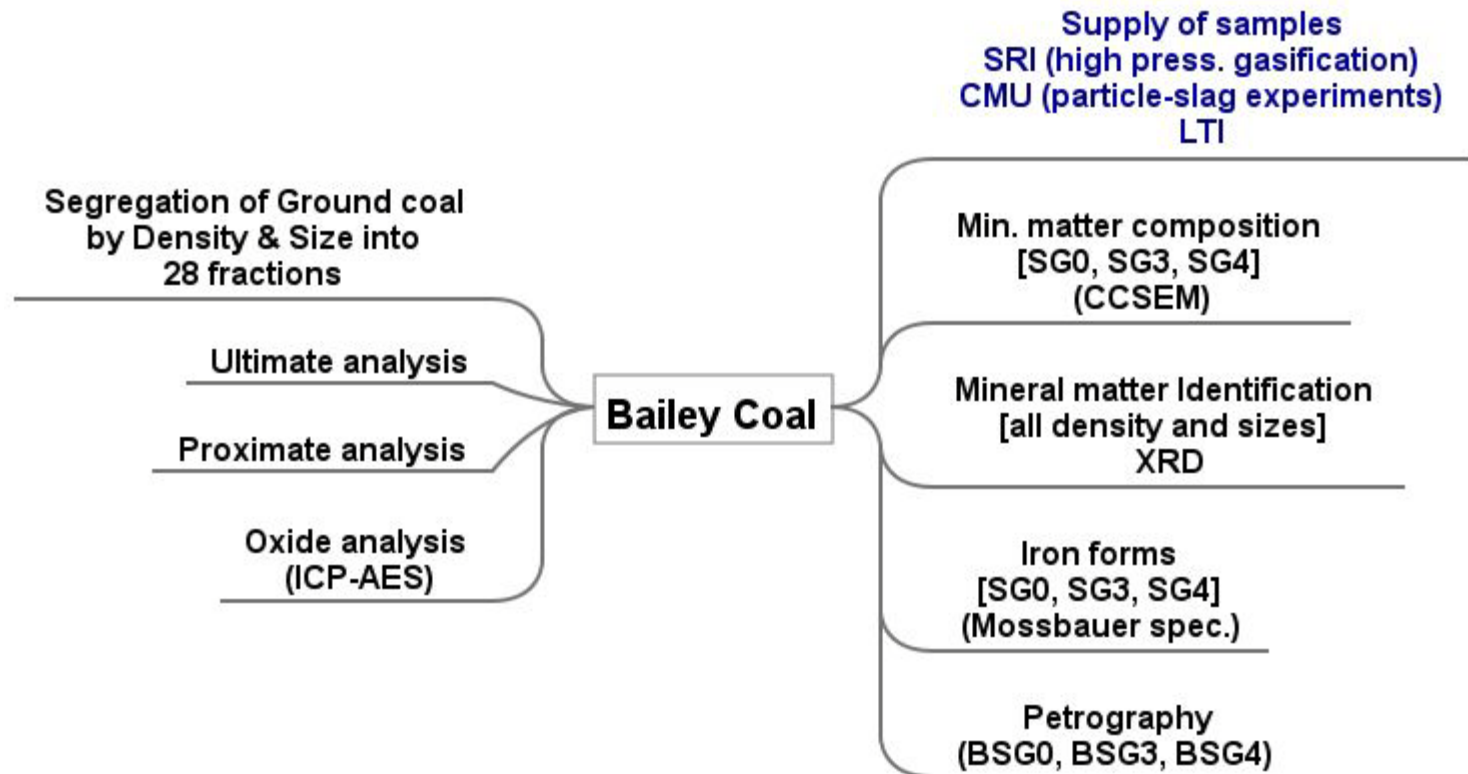
Particle Partitioning

# Overall Goal

To determine whether an analysis based on the fuel PSD, mineral compositions, carbon conversion, and capture efficiencies of the slag layer can interpret the historical backlog of entrained gasifier's syngas cooler's fouling problems for different fuels.

Based on particle size and specific gravity distributions, to quantify key fuel parameter distributions that can contribute to flyash formation

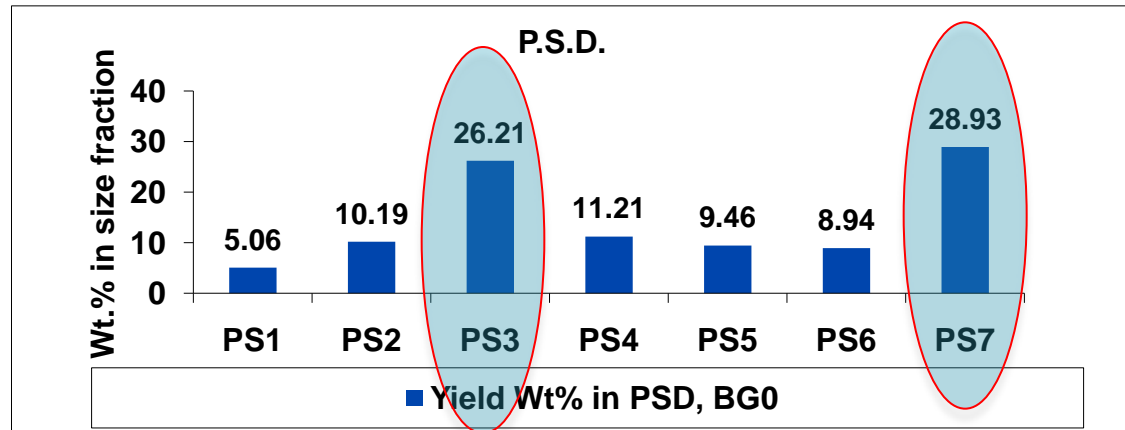
# Methodology for Evaluating Heterogeneity



**Heterogeneity in coal samples was determined with respect to organic and inorganic components**

# Yield and HHV Segregation

Property	Whole Coal	SG1	SG2	SG3	SG4
Unit		< 1.3	1.3 -1.6	1.6-2.6	> 2.6 g/cc
Yield, %	100 %	47.8	47.6	3.5	1.1
HHV MJ/kg	33.79	17.35	15.65	0.45	0.08
HHV in fractions %	100%	52.1	46.3	1.3	0.3



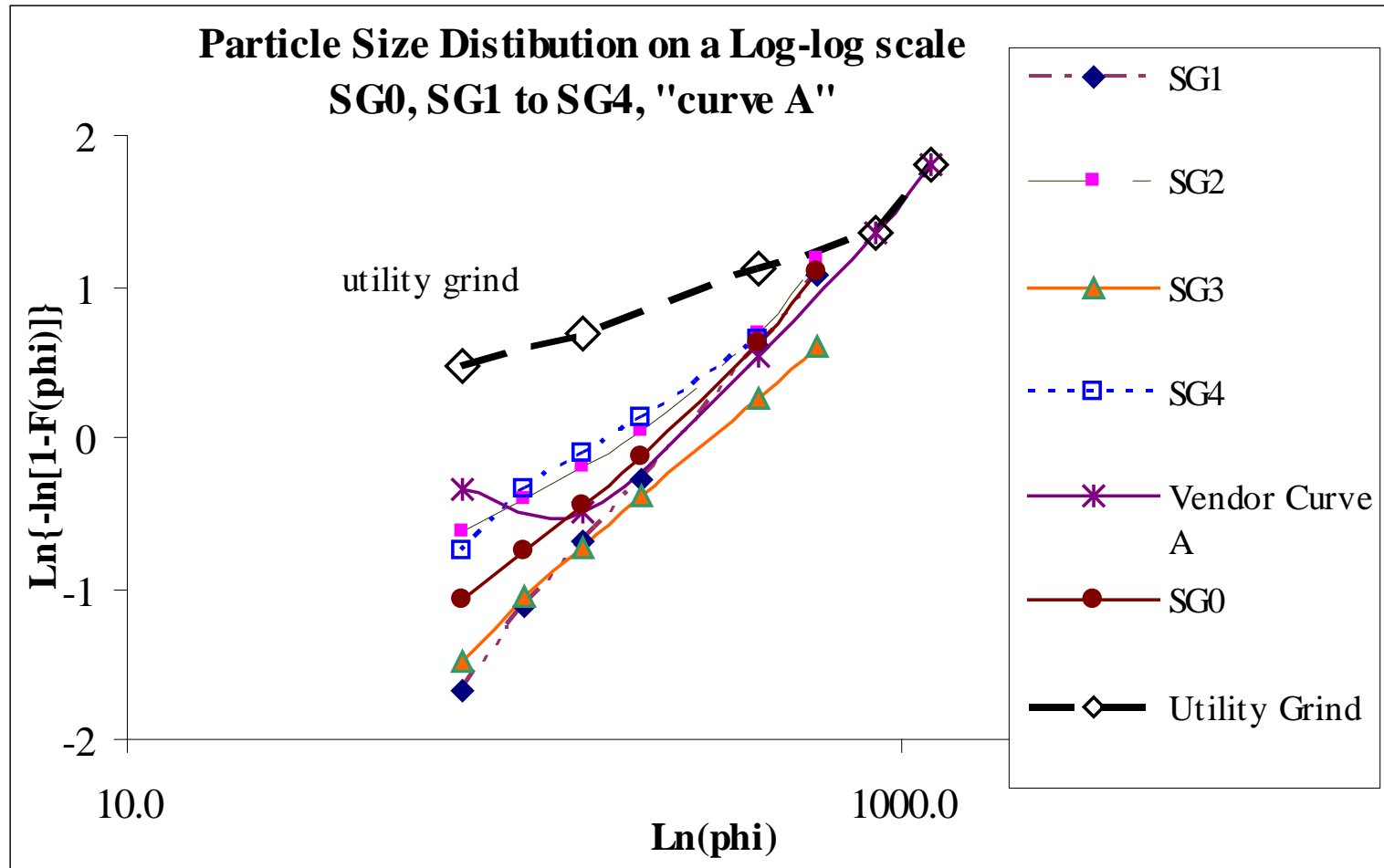


# Sample Array Showing Yield

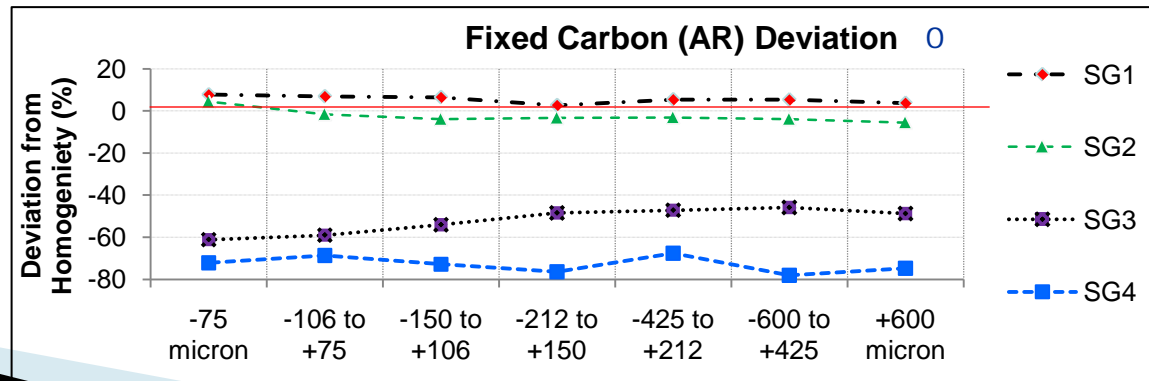
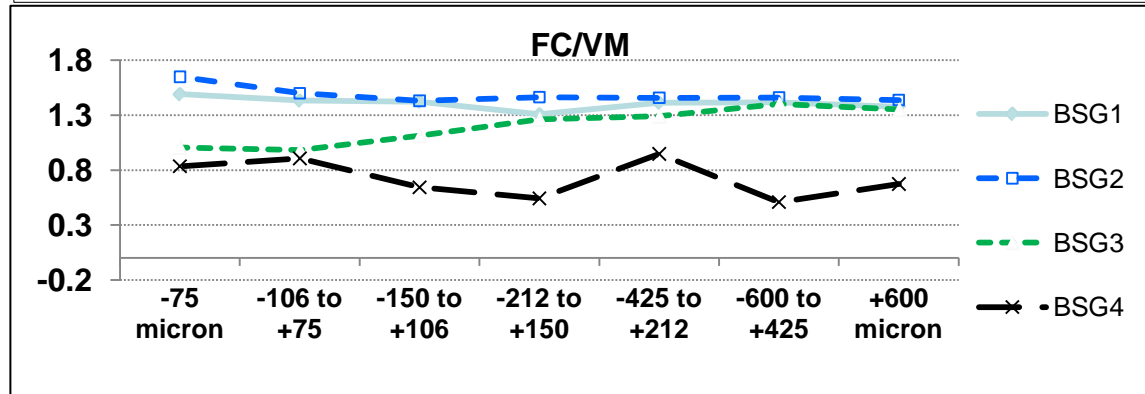
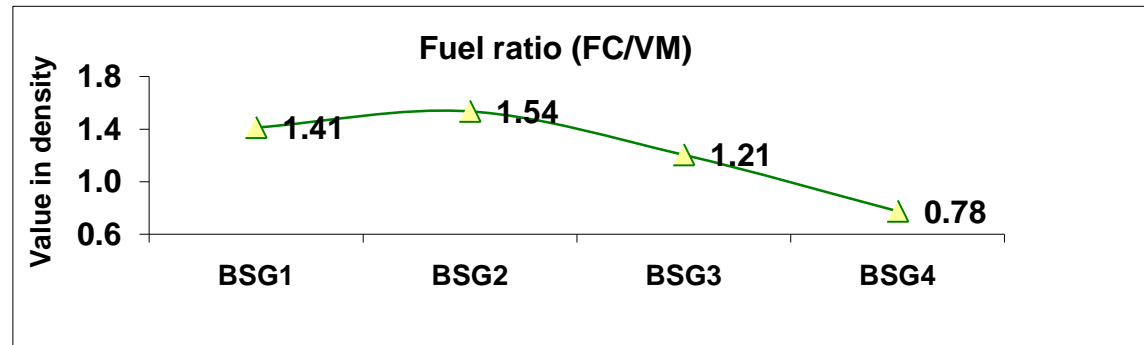
		+600 micron	-600 to +425	-425 to +212	-212 to +150	-150 to +106	-106 to +75	-75 to 0 micron
		PS1	PS2	PS3	PS4	PS5	PS6	PS7
1.3 < $\rho$	SG1	2.54	5.19	14.90	6.39	5.54	5.16	8.12
1.3 to 1.6	SG2	1.86	4.53	10.31	4.35	3.51	3.32	19.69
1.6 to 2.6	SG3	0.56	0.40	0.81	0.37	0.32	0.30	0.71
$\rho > 2.6$	SG4	0.10	0.07	0.20	0.09	0.10	0.15	0.42

*These samples  
were  
investigated by  
by SRI and  
CMU*

# PSD comparison with Utility Grind



# Heterogeneity in Fixed Carbon and Volatiles

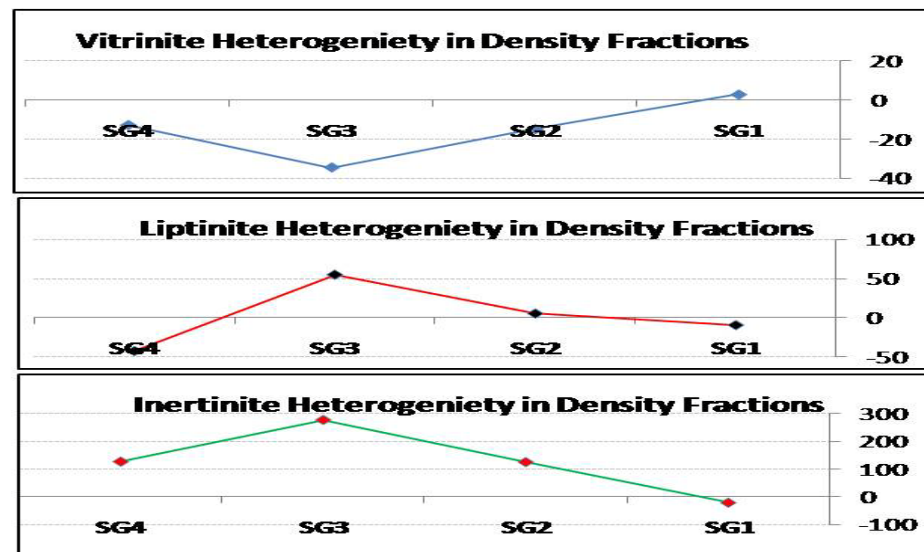
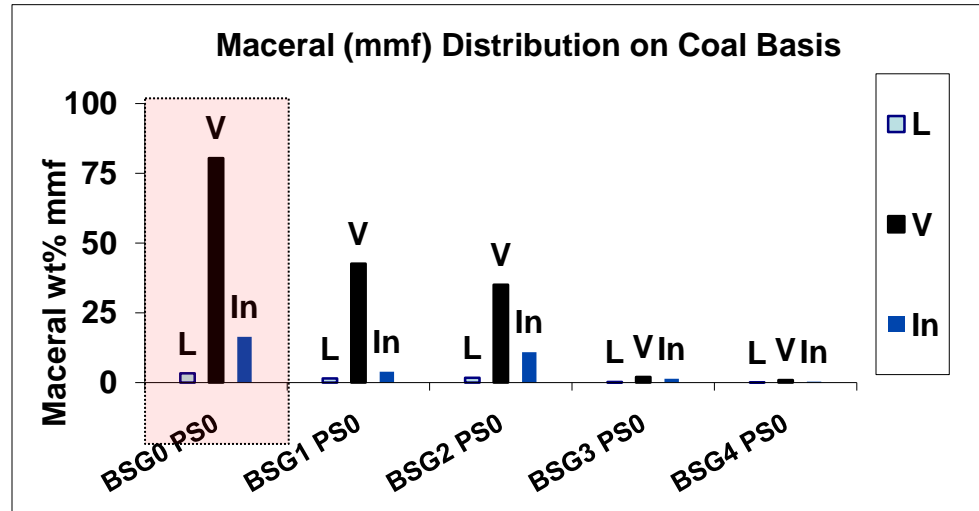


# Maceral Segregation

SG1    SG2    SG3    SG 4  
 max. V    V/I    L&I    MM

Maceral mmf	BSG0 PS0	BSG1 PS0	BSG2 PS0	BSG3 PS0	*BSG4 PS0
Vitrinite	83.7	87.2	70.5	53.1	75.2
Liptinite	3.3	3.0	3.4	5.0	1.9
Inertinite	13.0	9.9	26.0	41.8	23.4
<i>Vitrinite/ Inertinite</i>	<i>6.4</i>	<i>8.8</i>	<i>2.7</i>	<i>1.3</i>	<i>3.2</i>

- ▶ SG4 data is out of 360 counts vs. the normal 1000 count
- ▶ Based on literature\*, reactivities of chars of fractions are expected to reflect respective heterogeneity in macerals
- ▶ Vitrinites form porous char



\* Wall, T. et al. The Effect of Pressure on Char Characteristics, Burnout and Ash Formation in Entrained Flow Reactors, IFRF Combustion Journal, Art. # 200105, May 2001

# Burnout differences in Macerals: Observations

- ▶ Reactivity of Lab chars of BSG1, BSG2 (in TGA at atmospheric pressure ) are slower to start burning (confirmed from reactivity plots) but achieve higher  $R_{max}$ .
- ▶ BSG3 is very quick to burn compared to others. This could be explained by the presence of fast burning Liptinites and lower overall fixed carbon.
- ▶ Anomaly: BSG4, as it is found to start burning quite late (after BSG1) but burnout is quicker. This could be due to lower fixed carbon which in combustion reactivity settings reacts away quickly.

# Ash yield variation

Ash yield varies widely with density

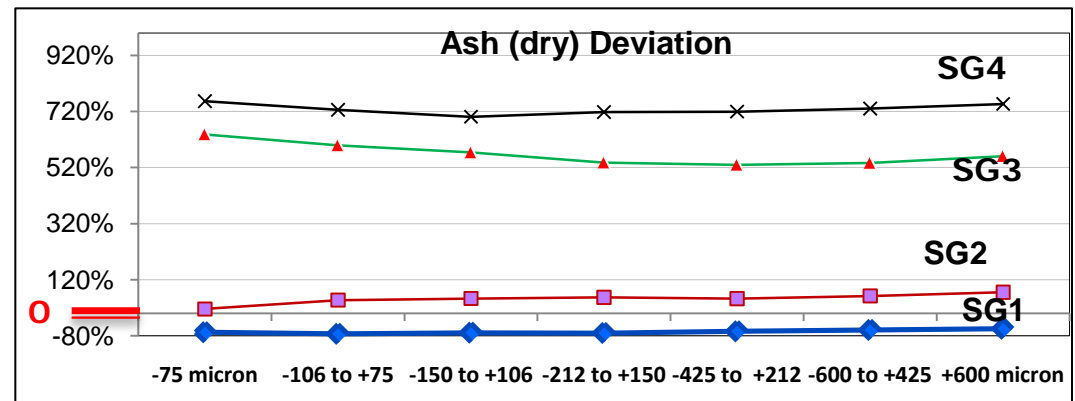
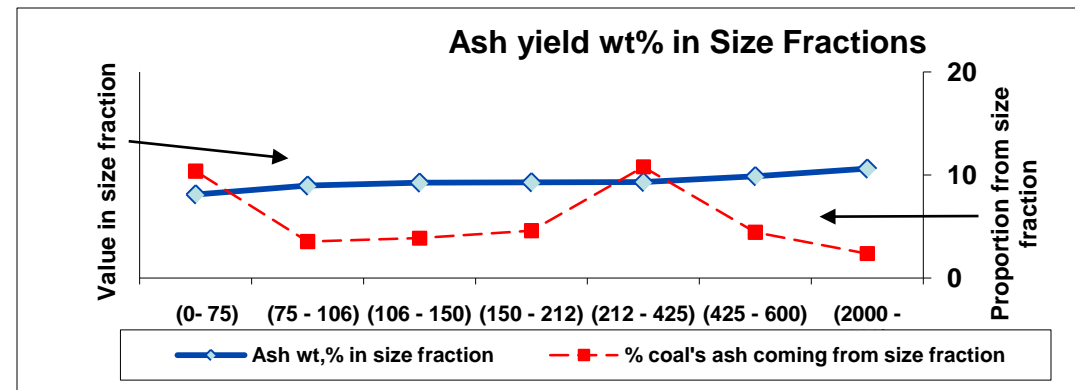
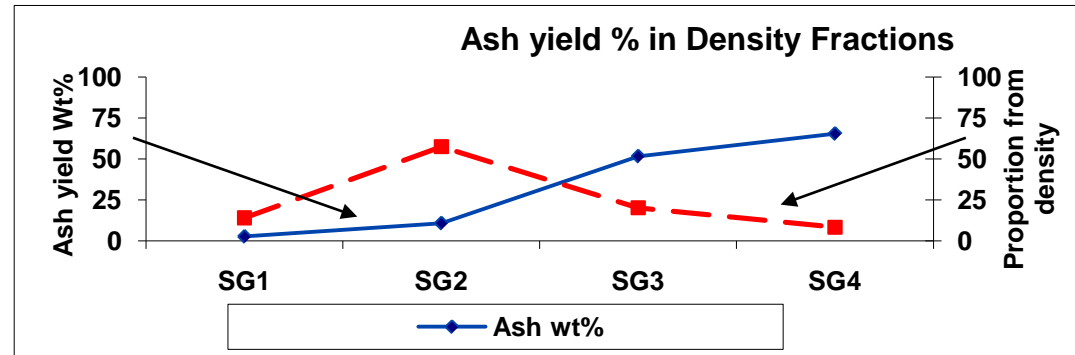
Contribution to total ash yield of coal is highest from SG2 (included nature of minerals)

Size fractions 0-75  $\mu\text{m}$  and 212-425  $\mu\text{m}$  contribute max towards the whole coal ash yield

Ash yield variation with size fraction is not significant

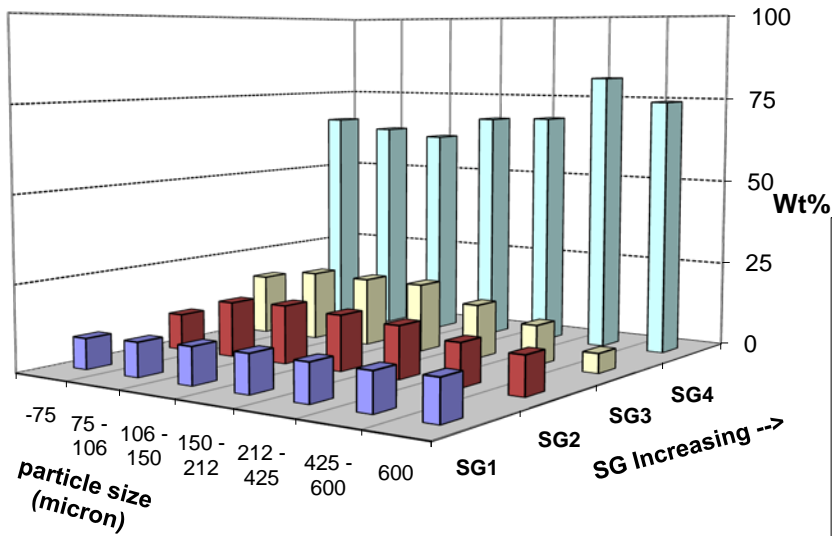
Heterogeneity in ash yield (about)

SG1 - 80 %, SG2 + 80 %  
 SG3 + 570 % SG4 + 720 %

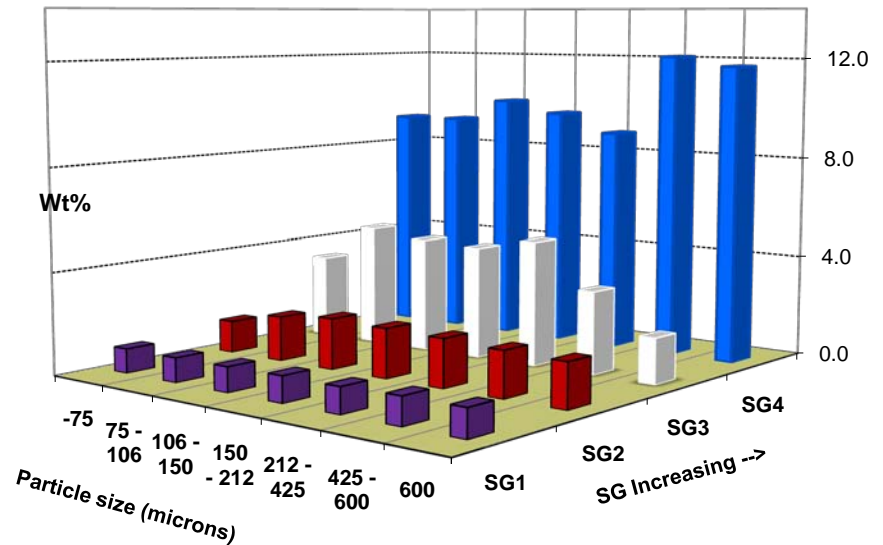


# Iron and Sulfur Distribution in Coal

**Fe<sub>2</sub>O<sub>3</sub> Distribution (on ash basis)**



**Sulfur Distribution (coal)**



# Mineral Matter Makeup SG0, SG3 & SG4

SG4 (84.23 wt.% MM)	TOTALS (%)	EXCLUDED
PYRITE (2)	90.4	88
IRON OXIDE	5.4	87.1
OXIDIZED Pyrrhotite	2.1	86.8
UNCLASSIFIED	1.9	66.8
PYRITE (1)	0.1	100
SG3 (60.04 wt.% MM)	TOTALS (%)	EXCLUDED
PYRITE (2)	33.4	80.8
UNCLASSIFIED	17.7	69
K Al Silicate	12.6	52.7
QUARTZ	8.6	59.7
KAOLINITE	4.6	29.9
MONTMORILLONITE	4	26.3
MIXED Al Silicate	3.5	37.7
CALCITE	3.1	49.2
FE Al Silicate	2.9	59
SI-RICH	2.5	42.9
GYPSUM	1.7	82.7
ALUMINOSILICATE	1.6	37
PYRITE	1.5	80

PYRITE (2) - reported as pyrrhotite by UND CCSEM software

Parent Coal (non segregated)		
SG0 (5.76 wt.% MM)	TOTALS (%)	EXCLUDED
PYRITE (2)	30.8	44.2
UNCLASSIFIED	17.9	14.2
K Al Silicate	11.7	11.1
KAOLINITE	8	14.4
QUARTZ	7.4	26.9
MONTMORILLONITE	4.5	34.6
PYRITE	3.9	25.6
SI-RICH	3.3	35.1
FE Al Silicate	3.1	11.5
MIXED Al Silicate	2.1	22.6
OXIDIZED Pyrrhotite	1.5	33.5
CALCITE	1.3	38.9
GYPSUM	1.2	70.3
IRON OXIDE	1	40.3



# CCSEM Analysis: Mineral matter Composition

## Major Minerals CCSEM\* (on coal basis)

Pyrites:  
37 %

Carbonates and  
sulphates: 3 %

Silica (with impurities): 3 %

Quartz:  
7 %

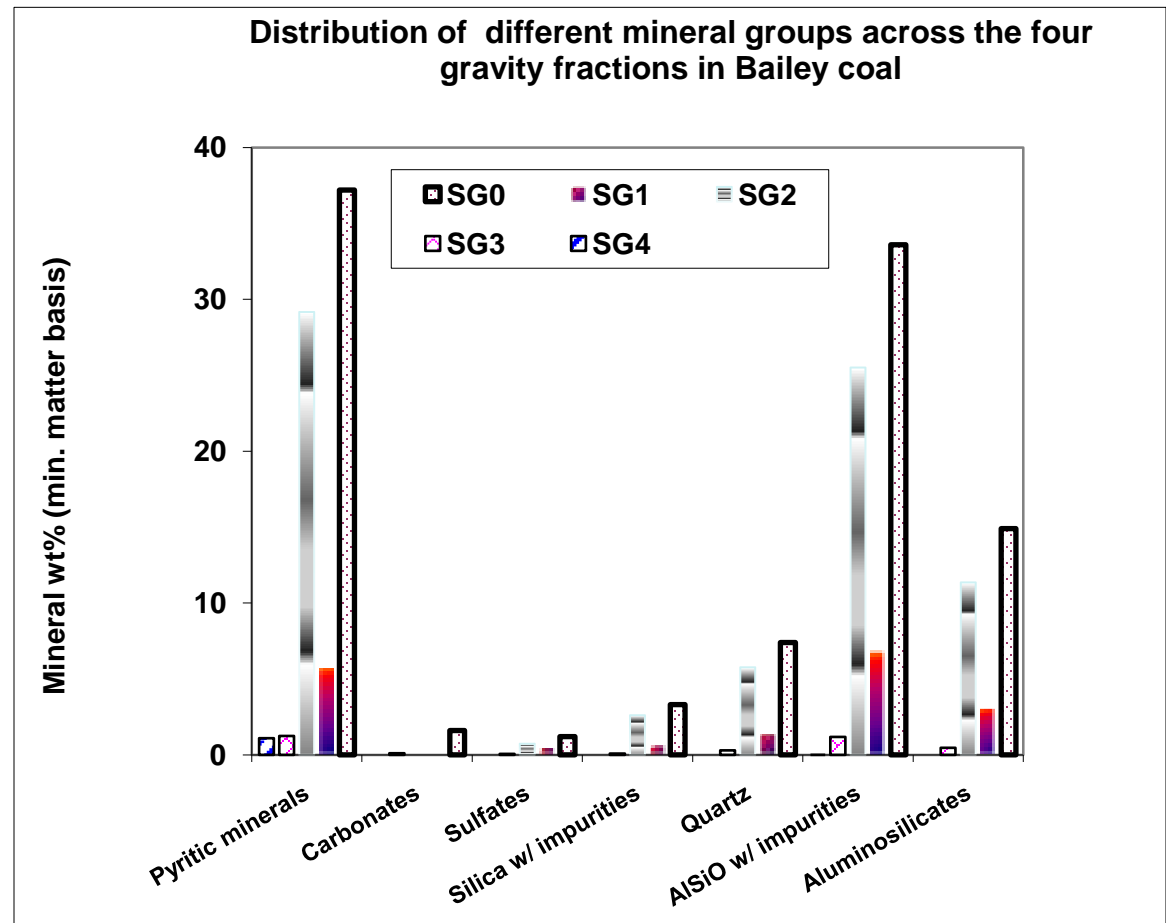
Aluminosilicates  
(with impurities): 35 %

Aluminosilicates:  
15 %

Significant presence of  
Al-silicates and silica  
with impurities

Iron, as impurity helps  
melting

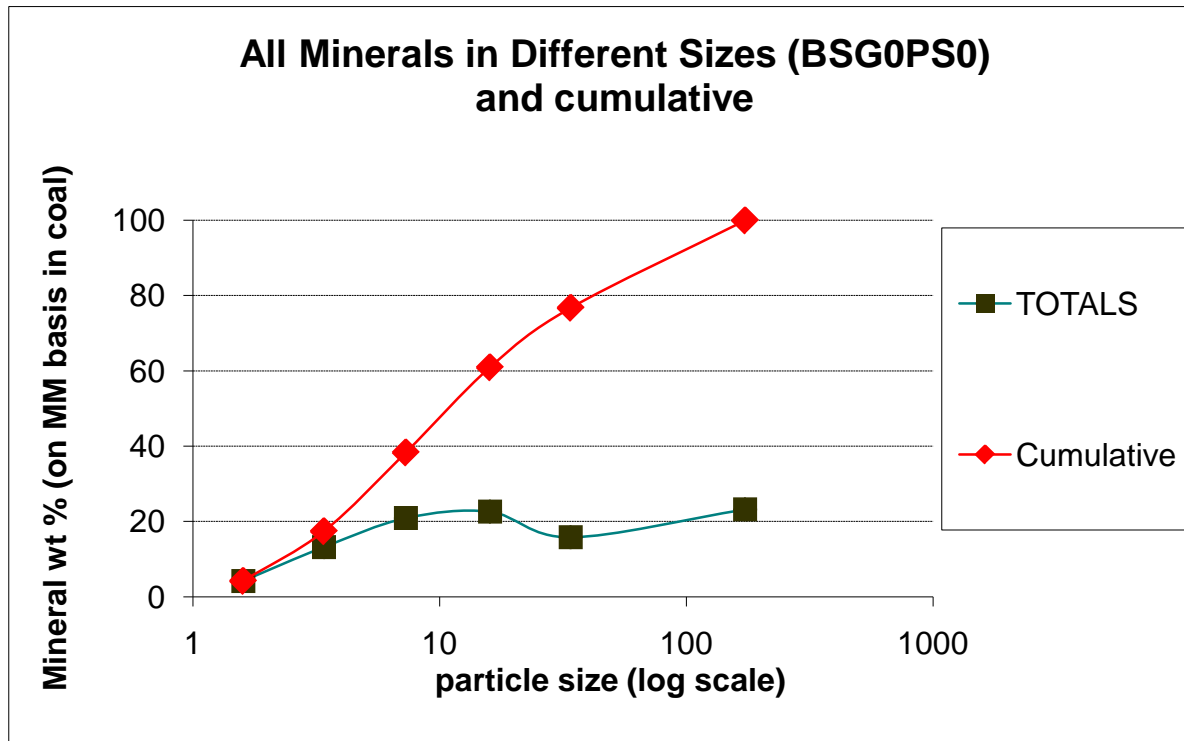
Potassium, as impurity



From left to right: SG4, SG3, SG2, SG1 and SG0 (whole coal)

**Preparation Limitation:** particles > 300  $\mu\text{m}$  were crushed and added

# Mineral matter by Size



Minerals present in extremely fine form

- ▶ 76% minerals are less than 46  $\mu\text{m}$
- ▶ 60% less than 22  $\mu\text{m}$
- ▶ 38% less than 10  $\mu\text{m}$

# CCSEM: Included vs Excluded Minerals

In whole coal, over 72% (v/v) minerals present as included;

Proportion present in the included form

- Aluminosilicates: 78 %
- Aluminosilicates (with impurities) at 87%
- Quartz: 73 %
- Silica (with impurities): 65%
- Sulfates: 30 %
- Carbonates: 62%
- Iron minerals (pyrites) 58%

## Size wise distribution of minerals

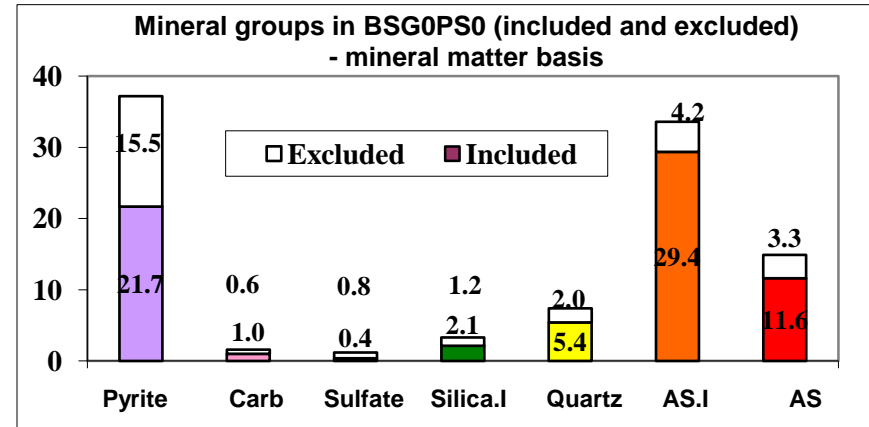
Over 42% clay particles,  $d < 10 \mu\text{m}$   
 ~ 71.6% of clay particles,  $d < 22 \mu\text{m}$

Maximum amount of aluminosilicates are present in 4.6 to  $10 \mu\text{m}$  size fraction

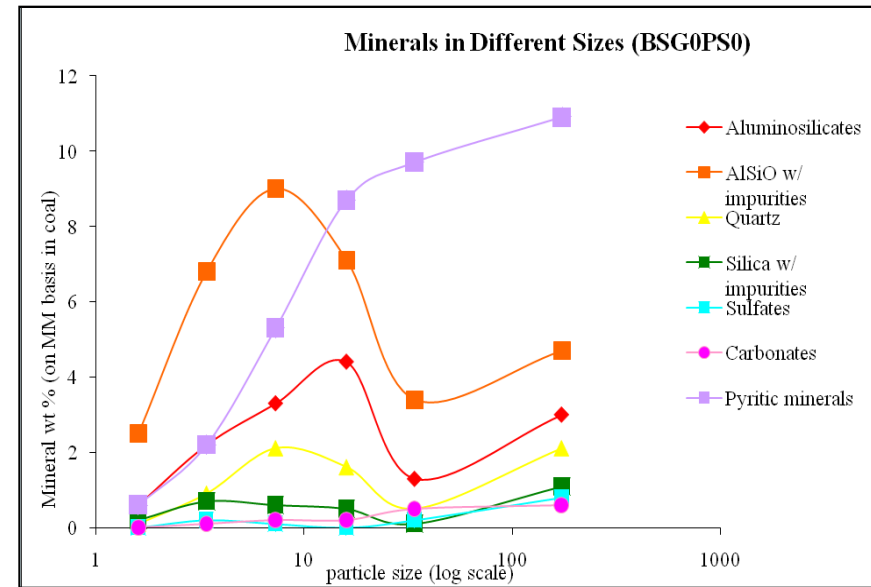
Fine sized minerals present as inclusions  
 → higher propensity to convert to fly ash particles

[Barroso et al. 2006, Study of coal ash deposition in an entrained flow reactor : Influence of coal type, blend composition and operating conditions, Fuel Proc. Technology, 87, p. 737]

NB: Preparation: particles  $> 300 \mu\text{m}$  were crushed



Carb: carbonates; AS: aluminosilicate; .I = with impurities



# Technical Approach- Future Work

- ▶ Perform gasification tests on specific sizes SG2, SG3 and SG4 fractions to obtain reactivity parameters
- ▶ Perform kinetic studies on chars obtained at different conversions to study the kinetics of char conversion as a function of starting mineral matter composition
- ▶ Modification of mineral processing circuit based on the identification of the “Bad Actors”

# Summary

Partitioning of coal by density & size distribution is a magnifying lens to select samples widely varying in constituents to identify the outliers that cause problems in entrained flow gasifiers

Three density fractions show varying macerals

- Vitrinite to inert ratios of SG1 and SG2 significantly different
- SG3 has maximum amount of liptinites (relative basis)

Minerals are predominantly aluminosilicates, pyrites and quartz

Majority of minerals present as very fine particles ( $d < 22 \mu\text{m}$ )

Bulk of fine minerals are present as included mineral matter

Feed particle size distribution into a slurry fed gasifier does not follow Rosin Rammer function.

# Acknowledgements

- ▶ This work was supported by NETL/DOE through West Virginia University.
- ▶ Discussions with NETL Scientists/Partner Institutions are greatly appreciated.