The Partitioning of Particles Between Slag and Flyash During Coal Gasification

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Lawrence J. Shadle
National Energy Technology Laboratory

Peter L. Rozelle
Office of Clean Energy Systems

Victor K. Der
Deputy Assistant Secretary, Office of Clean Coal
U. S. Department of Energy
An R&D Approach to Improving the Efficiency and Reliability of Gasification Systems

• The Goal- A Tool for Improved Gasification Plant Operation:
  – Minimize Unconverted Combustibles
  – Minimize Solids Fouling of Syngas Cooling and Handling Equipment

• Method- Develop a Model that can Tie Key Parameters to the Fuel Preparation System
  – Particle Population Model
  – Compatible with Grinding and Gasifier Models
An R&D Approach to Improving the Efficiency and Reliability of Gasification Systems - Uses for the Result

- Reduced need to Recycle Unconverted Combustibles
  - Reductions in Oxygen Requirement
  - Less Ash Flux through the Gasifier (Refractory Consideration)
  - More Uniform Syngas Output

- More Control over Solids Entrained in Syngas
  - Less Downtime from Fouling or Erosion of Syngas Handling Systems
  - Improved Reliability of Black Water Equipment

- Bottom Line:
  - Improved Heat Rate, Net Output and Capacity Factor
  - Reduced Production Cost per kWh
Application of a Particle Population Model to an Industrial System

- Quantifying how Different Classes of Particles Respond to a Stimulus, and Summing the Behavior
- The Classes of Particles are Grouped by Size and Specific Gravity
- 30 to 60 Years Ago, the U. S. Bureau of Mines Pioneered this for Modeling of Mineral Processing Systems
- This has been Successfully Extended to Use for Predicting Key Parameters for Power Generation Equipment
The Particle Population Model: Development and Use

- Solid Gasifier Fuels are Heterogeneous
  - Quantify the Heterogeneity (A Particle Population Model)
  - Quantify Gasification Behavior Across the Particle Population
    - Kinetics
    - Trajectories
    - Slag Entrapment and Compatibility

- Collaborators:

<table>
<thead>
<tr>
<th>U.S. Department of Energy (Model Development and Validation)</th>
<th>Leonardo Technologies, Inc. (Modeling Work)</th>
</tr>
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<tbody>
<tr>
<td>Carnegie Mellon University (Modeling and Laboratory Work)</td>
<td>Stanford Research Institute (Laboratory Work)</td>
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<td>West Virginia University (Modeling and Laboratory Work)</td>
<td>Niksa Energy Associates (Modeling Work)</td>
</tr>
<tr>
<td>Penn State University (Modeling and Laboratory Work)</td>
<td>REM Engineering Services (Laboratory Work)</td>
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</table>

Industry
The Particle Population Model: Development and Use

- Initially use for Two Effluent Streams from the System, Add more as Required.

```
F ➔ Transformations ➔ Flyash
  Reactions
  Attrition
  Agglomeration
  Adherence and Coalescence with Slag
  ➔ Slag or Bottom Ash
```
The Particle Population Model: Development and Use

- Sum the Quantifications and Tie them back to a Grinding Model.

Flowchart:
- Mill
- Fuel
- Transformations
  - Reactions
  - Attrition
  - Agglomeration
  - Adherence and Coalescence with Slag
- Slag or Bottom Ash
- Flyash
The Particle Population Model: Development and Use

- Result: A Model that Predicts Flow Rates and Characteristics of Effluent Streams Based on Grinding Parameters

- Mill
- Fuel
- Transforms to:
  - Flyash
  - Transformations:
    - Reactions
    - Attrition
    - Agglomeration
    - Adherence and Coalescence with Slag
  - Slag or Bottom Ash

NETL
Particle Trajectory Categories in an Entrained Flow Gasifier

Category 1: Particles Contact and Coalesce with Slag

Category 2: Particles do not Contact with Slag

Category 3: Particles Contact but do not Coalesce with Slag

Fine Print Disclaimer:
This diagram has been rotated to maintain a generic appearance
Particle Trajectory Categories in an Entrained Flow Gasifier

Category 1: Particles Contact and Coalesce with Slag

Category 2: Particles do not Contact with Slag

Category 3: Particles Contact but do not Coalesce with Slag

Flyash Flow = Category 2 + Category 3

Slag Flow = Category 1

Fine Print Disclaimer:

This diagram has been rotated to maintain a generic appearance
Components of Particle Population Model

- Particle Population Development
  - Particle Size and Specific Gravity
  - Linked to Grinding Model
- CFD Trajectory Model-Two Categories
  - Contacts Slag (1+3)
  - Doesn’t Contact Slag (2)
- High Pressure Kinetics Model
- Slag Entrapment Model
  - Subdivides Categories 1 and 3
Particle Population Development - Distribution of Ash Content in Rod Mill Product

*Washed Pittsburgh Seam Coal, ~8% Composite Ash*

<table>
<thead>
<tr>
<th>Microns</th>
<th>1.30 Float</th>
<th>1.30 x 1.60</th>
<th>1.60 x 2.60</th>
<th>2.60 Sink</th>
</tr>
</thead>
<tbody>
<tr>
<td>Passing</td>
<td>Retained</td>
<td>Wt%</td>
<td>% Ash</td>
<td>Wt%</td>
</tr>
<tr>
<td>600</td>
<td>600</td>
<td>2.54%</td>
<td>3.40%</td>
<td>1.86%</td>
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<tr>
<td>600</td>
<td>425</td>
<td>5.19%</td>
<td>2.90%</td>
<td>4.53%</td>
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<tr>
<td>425</td>
<td>212</td>
<td>14.90%</td>
<td>2.42%</td>
<td>10.31%</td>
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<tr>
<td>212</td>
<td>150</td>
<td>6.39%</td>
<td>2.12%</td>
<td>4.35%</td>
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<tr>
<td>150</td>
<td>106</td>
<td>5.54%</td>
<td>1.90%</td>
<td>3.51%</td>
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<tr>
<td>106</td>
<td>75</td>
<td>5.16%</td>
<td>1.68%</td>
<td>3.32%</td>
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<tr>
<td>75</td>
<td>0</td>
<td>8.12%</td>
<td>1.65%</td>
<td>19.69%</td>
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</table>
Ground Pittsburgh Seam Coal
1.3 Float Fraction

<table>
<thead>
<tr>
<th>Percentage</th>
<th>Ash Analysis</th>
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<tbody>
<tr>
<td>47.8 % of the Fuel</td>
<td>48.94% SiO₂</td>
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<tr>
<td>2.6 wt% Ash</td>
<td>26.76% Al₂O₃</td>
</tr>
<tr>
<td>14.1 wt% of Ash in Composite Fuel</td>
<td>10.71% Fe₂O₃</td>
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<tr>
<td>51.2% of Combustibles in Fuel</td>
<td>3.56% CaO</td>
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<tr>
<td></td>
<td>0.95% MgO</td>
</tr>
<tr>
<td></td>
<td>0.44% Na₂O</td>
</tr>
<tr>
<td></td>
<td>1.49% K₂O</td>
</tr>
</tbody>
</table>
Ground Pittsburgh Seam Coal
1.6 by 2.6 Fraction

3.5 % of the Fuel
52.6 wt% Ash
20.1 wt% of Ash in Composite Fuel
1.8% of Combustibles in Fuel

<table>
<thead>
<tr>
<th>Ash Component</th>
<th>% of Fuel</th>
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<tbody>
<tr>
<td>SiO₂</td>
<td>54.65%</td>
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<tr>
<td>Al₂O₃</td>
<td>21.10%</td>
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<tr>
<td>Fe₂O₃</td>
<td>15.36%</td>
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<tr>
<td>CaO</td>
<td>2.82%</td>
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<tr>
<td>MgO</td>
<td>0.72%</td>
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<tr>
<td>Na₂O</td>
<td>0.34%</td>
</tr>
<tr>
<td>K₂O</td>
<td>1.71%</td>
</tr>
</tbody>
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CFD Trajectory Model

Category 1

Category 2+3
CFD Trajectory Model

Distance from entrance (m)

Average normal velocity (m/s)
Specific Gravity Selectivity of the Grinding System

Each Specific Gravity Interval has a Different Response to the Grinding Stimulus
Particle Size and Specific Gravity Increments Before and After High Pressure Entrained Flow Reactor

Pyrolysis at 440 PSI, \( \Phi=0 \) (i.e. no \( O_2 \))

1.30 Float Particles, 2.11 wt% Ash
High Pressure Kinetics Model- Laboratory Results

Particle Size and Specific Gravity Increments Before and After High Pressure Entrained Flow Reactor

Before

440 PSI, $\Phi=0.7$

After

1.30 Float Particles, 2.11 wt% Ash
Particle Size and Specific Gravity Increments Before and After High Pressure Entrained Flow Reactor

440 PSI, $\Phi = 0.7$

1.30 Sink, 1.60 Float Particles, 12.05 wt% Ash
Compatibility of Char with the Slag Layer: A Particle Impacting at Velocity U, Experiences These Forces:

\[ F_{\text{drag}} = 6\pi AU \cdot f(\eta_S, \eta_G) \]

\[ F_{\text{added mass force}} = \frac{1}{2} \frac{4}{3} \pi A^3 \cdot h(\rho_M - \rho_I) \]

\[ F_{\text{capillary, } \sigma(Z)} = \frac{\partial E}{\partial Z} = 2\pi A \gamma_s \left[ \frac{\gamma_s - \gamma_p}{\gamma_s} - 1 + \frac{Z}{A} \right] \]

\[ = 2\pi A \gamma_s \left[ \cos \theta_{PSG} - 1 + \frac{Z}{A} \right] \]
Slag Entrapment Model
(Example)

2 m/s impact speed
$\theta_{PSG}=120^\circ$

- Entrapment via inertia
- Settling with oscillation
- Settling without oscillation

2 m/s impact speed
$\theta_{PSG}=90^\circ$

- Entrapment via inertia
- Settling with oscillation
- Settling without oscillation

Actual Distribution of Impact Velocities will come from Trajectory Model
Slag Entrapment Model
High Ash Content Fuel Particle Contacting Slag Layer under Reducing Conditions
Slag Entrapment Model
High Ash Content Fuel Particle Contacting Slag Layer under Reducing Conditions
Where this is Going

- Result: A Model that Predicts Flow Rates and Characteristics of Effluent Streams Based on Grinding Parameters

![Diagram]

- Mill
- Fuel
- Transformations
  - Reactions
  - Attrition
  - Agglomeration
  - Adherence and Coalescence with Slag
- Flyash
- Slag or Bottom Ash
Where this is Going?

The Model:

The removal rate of solids with the flyash stream, $R_\phi$, is:

$$R_\phi = F_f \left( \sum_{x=1}^{n_x} \sum_{y=1}^{n_y} \left[ 1 - K(x, y) \right] W(x, y) \right)$$
Where this is Going?

A Range of Grind Sizes from a Mill

Example for a Slurry Fed Gasifier
Using the Model and Mill Controls to Set High and Low Limits for Output

Cumulative Wt% Passing

Passing Size, Microns
Where this is Going?

• Interfacing with Grinding Models and Possibly Controls

• Model will be Available for Incorporation into Plant Simulations or Controls- i.e. a Plant Optimization Package

• Model for Fluid Bed Gasification

• Industry Input is Welcome