Simulation of Coal Particles in a Full Chemical Looping Combustion System

James Parker
CPFD Software, LLC

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Objectives

• Develop a Chemical Looping Combustion model
  – Full loop, 3D geometry
  – Fluid-particle dynamics
  – Oxidation/reduction chemistry
  – Coal devolatilization, moisture release, gasification reactions
  – Thermal characteristics
Traditional Combustion

Nitrogen
+ Excess Oxygen
+ Combustion Products

Heat

Combustion

Air
Fuel

Chemical Looping Combustion

Nitrogen
+ Excess Oxygen

Heat

Combustion Products

Solid carrier
+ Oxygen

Oxidation

Air
Fuel

Solid carrier

Reduction
Model geometry

- Design provided by NETL for **800 lb/hr** circulation of solids carrier

- Approximately 12’ tall

- Geometry contains equipment for reactions
  - Air reactor
  - Fuel reactor

- Solids circulation and separation
  - Cyclone
  - Loop seal
  - L-valve
Cold flow model

- Isothermal at 298K
- Non-reacting
Modeling CLC Reactions

• Key features
  – Multicomponent particles
  – Particle level chemistry

• Multicomponent particles provide Lagrangian tracking of particle composition

• Particle level chemistry provides a separate domain to each computational particle for reaction calculations
  – Particle composition
  – Particle temperature
  – Particle diameter, area, etc
  – Fluid properties
Ilmenite Carrier

• Primarily consists of
  – ilmenite (FeTiO$_3$)
  – rutile (TiO$_2$)
  – hematite (Fe$_2$O$_3$)

• $d_{50}$ of 156 microns

• Oxygen carrying capacity: 3.3 wt% of oxidized particle weight
Ilmenite chemistry

**Oxidation (exothermic)**

\[ 4\text{FeO} + \text{O}_2 \rightarrow 2\text{Fe}_2\text{O}_3 \]

**Reduction (endothermic)**

\[ 4\text{Fe}_2\text{O}_3 + \text{CH}_4 \rightarrow 8\text{FeO} + \text{CO}_2 + 2\text{H}_2\text{O} \]

\[ \text{Fe}_2\text{O}_3 + \text{H}_2 \rightarrow 2\text{FeO} + \text{H}_2\text{O} \]

\[ \text{Fe}_2\text{O}_3 + \text{CO} \rightarrow 2\text{FeO} + \text{CO}_2 \]

Rates from Abad et al (2001)
CLC subset models

• Apply ilmenite chemistry
  – air reactor subset model
  – fuel reactor subset models
Air reactor subset

• Ilmenite enters air reactor completely reduced

Percent Oxidation = \( \frac{W_{Fe_2O_3}}{0.307} \times 100 \)

• Max Fe_2O_3 on particle: 30.7 wt%
Oxidation level of ilmenite feed

- Ilmenite enters air reactor unoxidized
- Ilmenite enters air reactor 65% oxidized

Temperatures in Air Reactor

![Graph showing temperatures in Air Reactor for different heights and oxidized levels.](image-url)
Fuel reactor subset with methane
Temperatures in Fuel Reactor with methane
Coal chemistry

- **Coal devolatilization**
  - Temperature-dependent release of methane, carbon dioxide, carbon monoxide, water
  - Included particle swelling effects

- **Coal drying**
  - Mass transfer limited release of moisture from particle. Equilibrium between solid and gas phase.

- **Gasification of carbon**
  - Steam gasification producing carbon monoxide, hydrogen
  - CO$_2$ gasification producing carbon monoxide

- **Water-gas shift reaction**

- **Ilmenite reduction reactions**
  - Reduction reactions of Methane, Hydrogen, Carbon monoxide
Coal particle properties

- Initial particle density: 1333 kg/m³
- 50 micron – 150 micron particle diameter
- Heat of combustion: 32 MJ/kg

<table>
<thead>
<tr>
<th>Component</th>
<th>Composition (wt%)</th>
<th>Density (kg/m³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Char</td>
<td>51%</td>
<td>2150</td>
</tr>
<tr>
<td>Volatile Organics</td>
<td>34%</td>
<td>815</td>
</tr>
<tr>
<td>Ash</td>
<td>10%</td>
<td>2200</td>
</tr>
<tr>
<td>Moisture</td>
<td>5%</td>
<td>1000</td>
</tr>
</tbody>
</table>

Initial coal composition

Released Gases

<table>
<thead>
<tr>
<th>Component</th>
<th>Composition (wt%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methane</td>
<td>66.8%</td>
</tr>
<tr>
<td>Carbon monoxide</td>
<td>24.4%</td>
</tr>
<tr>
<td>Water</td>
<td>5.9%</td>
</tr>
<tr>
<td>Carbon dioxide (gas)</td>
<td>2.8223%</td>
</tr>
<tr>
<td>Carbon dioxide (trapped)</td>
<td>0.0777%</td>
</tr>
</tbody>
</table>
Coal particle subset model
Full CLC simulation with coal

• Apply ilmenite chemistry and coal chemistry to loop

• Coal feed is 2.7 lb/hr at 298K
Full CLC loop simulation

[Diagram of CLC loop simulation with various parameters such as Particle Volume Fraction, Particles by Initial Location, Percent Oxidation of tanninite, Particle Temperature (K), Pressure (Pa), Moles Fraction Oxygen, Moles Fraction Water, Moles Fraction CO2, and Time (s): 20.00]
Full CLC loop simulation

- Simulated circulation rate is close to target rate of 800 lb/hr
Conclusions

• Full reacting chemical looping combustion system was modeled in 3D

• Model highlights
  – Composition of solid ilmenite carrier was tracked on each computational particle in model
  – Oxidation/reduction of ilmenite is modeled using particle level chemistry
  – Coal particles were modeled as a fuel source, including devolatilization, moisture release, and gasification reactions

• Tool for future design and optimization work
Acknowledgements

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