Oxy-Fuel Combustion

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Presentation Outline

- Clean Coal Overview
- Work Done on this Project
  - Laboratory Experiments
  - Numerical Simulations
  - Pilot Scale Experiments
  - Equilibrium Calculations
- Conclusions
- Future of Oxyfuel
Oxy-fuel Motivation

“Cleaner” Coal Options:
- Oxygen combustion (Oxyfuel)
  - Concentrated CO$_2$ in products
- Amine (or others) scrubbing for new or existing plants
  - Extracts the CO$_2$ from the flue gas
  - Can be implemented Slip Stream
- Integrated Gasification Combined Cycle (IGCC)
  - Concentrated CO$_2$ in products
  - Complexity of operation
  - Can not be retrofitted to current pulverized fuel plants
  - Requires “all-in” carbon capture

Efficiency?

Jury still out for the most cost effective/efficient “cleaner” coal option

For CCS: generally thought to be between IGCC and Oxy-fuel
Oxy-fuel

- Increases CO₂ concentration
  - Easier to recover

- Could be used in retrofit existing coal plants

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Purdue’s Oxy-fuel Project Focus

- Radiative Heat Transfer
  - Dominant heat transfer mode in boiler furnace
  - Non-gray body behavior (spectral dependence)

- Temperature Measurements in Oxy-Fuel Boilers
  - Pilot scale
  - Above 3,000 K in Jupiter burner
  - Challenging to measure
Laboratory Experiments - Objectives and Apparatus

**Oxy-Coal Dust Cloud Combustion**

**Experiment Configuration**

**Objectives**

Document
- Flame Speed
- Spectral Radiation

Vary
- Coal type
- Particle size
- Oxygen content
- Diluent

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**Coal Analysis**

<table>
<thead>
<tr>
<th>Coal Type</th>
<th>Indonesian Coal</th>
<th>Illinois Basin #6</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coal Classification</td>
<td>Bituminous (low sulfur, low ash)</td>
<td>Bituminous</td>
</tr>
<tr>
<td></td>
<td><strong>Ultimate Analysis (%)</strong></td>
<td></td>
</tr>
<tr>
<td>Carbon</td>
<td>73.70%</td>
<td>68.30%</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>5.20%</td>
<td>5.00%</td>
</tr>
<tr>
<td>Oxygen</td>
<td>18.80%</td>
<td>13.80%</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>1%</td>
<td>1.30%</td>
</tr>
<tr>
<td>Sulfur</td>
<td>0.10%</td>
<td>3.50%</td>
</tr>
<tr>
<td>Ash</td>
<td>1.30%</td>
<td>8.10%</td>
</tr>
<tr>
<td></td>
<td><strong>Typical Proximate Analysis (%)</strong></td>
<td></td>
</tr>
<tr>
<td>Moisture</td>
<td>16.12%</td>
<td>10.10%</td>
</tr>
<tr>
<td>Ash</td>
<td>1.06%</td>
<td>7.30%</td>
</tr>
<tr>
<td>Volatile</td>
<td>42.59%</td>
<td>35.90%</td>
</tr>
<tr>
<td>Fixed Carbon</td>
<td>40.23%</td>
<td>46.70%</td>
</tr>
</tbody>
</table>

Further Classify Coal using Sieves:
- >106 µm
- 106 µm - 75 µm
- 75 µm - 53 µm
- 53 µm - 25 µm
- < 25 µm
How Flame Speed was Obtained

Both cases:
Cloud density - 0.539 kg/m$^3$
40% O$_2$ and 60% CO$_2$
Indonesian Coal

Automated MatLab analysis
Less Sensitive to Human Error in choosing effective diameter

Effect of Oxygen On Flame Speed

All cases:
Cloud density - 0.539 kg/m$^3$
Particle Dia. – 25-53 µm
Carbon Dioxide Diluent
Effect of Particle Diameter On Flame Speed

- Decrease in flame speed with smallest particle size can be attributed to:
  - Material Sticking to windows (leaner mixture)
  - Agglomeration (can be seen in videos)

All cases:
- Cloud density - 0.539 kg/m³
- 40% O₂ and 60% CO₂

Effect of Diluent On Flame Speed

All cases:
- Particle Dia – 25-53 microns
- Indonesian Coal
- Cloud density - 0.539 kg/m³
Laboratory Experiments – Results (Spectral)

- Fast Infrared Array Spectrometer (FIAS)
  - Portable
  - Staggered PbSe linear array sensor cooled by TEC
  - 160 wavelengths from 1.4 to 4.8 \( \mu m \)
  - Scan frequency: 6,250 Hz
  - Acquisition frequency: 1,320 Hz

Test Specs:
- 40% CO\(_2\), 60% O\(_2\)
- Particle Dia – 25-53 microns
- Cloud density - 0.539 kg/m\(^3\)
**Trends**
- Same General Shape
- Carbon Dioxide
  - Combating factors of increase in temperature vs. increased radiative potential
- Nitrogen
  - Increase in Intensity for increase $O_2$, decrease in Diameter
- Peak at 2.7 microns for Water and $CO_2$

**Test Specs:**
- 40% $O_2$, 60% Diluent
- Particle Dia – 25-53 microns
- Cloud density - 0.539 kg/m$^3$
- Indonesian Coal
Laboratory Experiments – Results (Spectral)

40% O₂

50% O₂

60% O₂

Test Specs:
- Fire Ball Diameter ~ 48mm
- CO₂ Diluent
- Particle Dia – 25-53 microns
- Cloud density - 0.539 kg/m³

Test Specs:
- 40% O₂, 60% CO₂
- Particle Dia – 25-53 microns
- Cloud density - 0.539 kg/m³
Numerical Simulations of Transient Flame Propagation in a Spherical Coal Dust Cloud

We investigated the transient combustion characteristics of a spherically symmetric cloud containing coal particles, as shown in Fig. 1. The cloud has a radius of $R_0$. Coal particles, with diameter $d_p$ and number density $n_p$, are uniformly distributed in the cloud. The cloud is numerically ignited using a hot spot.

- The Three-Level Fully Implicit (TLFI) scheme of second-order accuracy was applied to transient terms of the gas phase equations.
- The convective and diffusive terms are discretized using QUICK scheme and second order central difference, respectively.
- The time dependent equations of particle phase were solved using a standard ODE solver for stiff system, DVODE.
Governing Equations

The transient combustion is modeled by conservation equations for mass, species and energy with detailed consideration of devolatilization, homogeneous gas phase reaction, heterogeneous char surface reaction, and radiative heat transfer.

Assumptions:
(1) Gas phase and particles are uniformly mixed in space;
(2) The particles remain quiescent;
(3) Coal particles are spherical of various sizes;
(4) Each particle has uniform temperature because of its small size.

Gas-Phase Equations

\[
\frac{\partial (\varepsilon \rho)}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \varepsilon \rho u) = n \dot{m}_p
\]

\[
\frac{\partial (\varepsilon \rho Y_i)}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \varepsilon \rho u Y_i) = \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \varepsilon \rho Y_i V_i) + \omega_i W_i + \dot{w}_i W_i
\]

\[
\varepsilon \rho C_p \frac{\partial T}{\partial t} + \varepsilon \rho C_p u \frac{\partial T}{\partial r} = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 k \frac{\partial T}{\partial r} \right) - h A_p (T_g - T_p) - \sum_{i=1}^{k} \rho Y_i V_i C_{p,i} \frac{\partial T}{\partial r} - \sum_{i=1}^{k} \omega_i h_i W_i + \sum_{i=1}^{k} \dot{w}_i (h_{i,p} - h_i) W_i + Q_r
\]

where \( \varepsilon \) is the volume fraction of the gas mixture. The volume fraction of the particles, \( 1-\varepsilon \), equals to the product of particle number density and particle volume. \( \dot{m}_p \) are the mass production rate of species \( i \), due to gas phase reaction and char reaction, respectively. \( \rho \) is the molecular weight of species \( i \). \( V_i \) is diffusion velocity of species \( i \). \( h_i \) and \( h_{i,\text{p}} \) are the enthalpy of species \( i \) at gas temperature and particle temperature respectively. \( k \) is the thermal conductivity of the gas mixture. \( Q_r \) is radiative heat transfer rate from the gases to the ambient.
Particle-Phase Equations

The mass of a coal particle changes due to devolatilization and char reaction. Considering devolatilization occurs volumetrically and heterogeneous char reaction takes place on the particle surface, the governing equations of particle density and particle diameter can be approximated following:

\[
\frac{\partial \rho_p}{\partial t} = -\frac{6 \dot{m}_V}{\pi d_p^3}, \quad \frac{\partial d_p}{\partial t} = -\frac{2 \dot{m}_C}{\pi \rho d_p^2}
\]

where \( \dot{m}_V \) and \( \dot{m}_C \) are the mass loss rate due to devolatilization and char reaction respectively.

Particle temperature is obtained by solving the energy balance equation for particles:

\[
m_p C_p \frac{\partial T_p}{\partial t} = \dot{Q}_V + \dot{Q}_C + q_e + hA_p (T_g - T_p)
\]

where \( q_e \) is the radiative heat transfer between particles and the ambient gases. The last term is the convective heat transfer between particles and the surrounding gases.

Devolatilization Model

The volatiles from the coal particles are assumed to consist of \( \text{CH}_4 \) and \( \text{C}_3\text{H}_8 \) in this study. The rate of devolatilization for each volatile is expressed based on the Two Competing Rate Model:

\[
\dot{m}_{V,i} = k_{V,i}(m_{0,i} - m_{V,i})
\]

where \( m_{0,i} \) is the ultimate yield of volatile \( i \) and \( m_{V,i} \) is the amount already evolved. \( k_{V,i} \), the rate constant, is correlated with the particle temperature, \( T_p \), by

\[
k = A_i \exp \left( -\frac{E}{RT_p} \right)
\]

where \( A_i \) is the frequency factor, \( E \) the activation energy, and \( R \) the universal gas constant.
Homogeneous and Heterogeneous Reactions

The gas phase homogeneous combustion considers the following reactions with the one-step reaction rate:

\[ 2CH_4 + 3O_2 \rightarrow 2CO + 4H_2O \]
\[ 2C_3H_8 + 7O_2 \rightarrow 6CO + 8H_2O \]
\[ 2CO + O_2 \rightarrow 2CO \]
\[ 2CO_2 \rightarrow 2CO + O_2 \]

Three heterogeneous reactions are assumed to take place at the surface of particles:

\[ C + O_2 \rightarrow CO_2 \]
\[ 2C + O_2 \rightarrow 2CO \]
\[ C + CO_2 \rightarrow 2CO \]

The overall reaction rate is simulated by the diffusion-kinetic model, which is the first-order of \( O_2 \) and \( CO_2 \) concentrations.

Flame Speed

Note:
1. The velocity is defined by tracking the location of gas temperature at 1500 K.
2. The coal property and flame conditions are the same as those of the experiments.
3. As \( O_2 \) concentration increases, the discrepancy between measurements and simulations becomes large.
Note:
1. The above figure shows the transient gas-phase temperature as a function of radius.
2. The initial coal particle temperature is assumed to be room temperature.
3. This is for $O_2/CO_2=30/70$ case.

Note:
1. The above figure shows the species concentration profiles at 6 ms.
2. This is for $O_2/CO_2=30/70$ case.
3. Note, in this case, $O_2$ is not enough to consume all of the volatiles.
Experimental vs Theoretical

Flame Speed (m/s)

0 0.5 1 1.5 2 2.5 3

20 25 30 35 40 45 50 55 60 65 70

O2 (% by Volume)

Eric will do more comparisons as a class project

All cases:
Cloud density - 0.539 kg/m³
Particle Dia. – 25-53 µm
Carbon Dioxide Diluent
Indonesian Coal

Pilot Scale Experiments

From Jupiter Oxygen in Hammond Indiana
Pilot Scale Experiments - Objectives

- Measure spectral radiation intensities of a pilot-scale oxy-fuel boiler at various locations (by Jupiter engineers)
- Analyze measured radiation data
- Estimate temperate profile at one cross-section of the boiler furnace using inverse radiation interpretation

Pilot Scale Experiments - Details

- **The Pilot Scale Boiler**
  - Doosan Backcock 23.4 MW boiler
  - Four Maxson 2.93 MW
  - Total heating rate during tests: < 8.79 MW
- **Test Matrix**
  - HT oxy-natural gas without CO$_2$ recycling
  - HT oxy-natural gas with CO$_2$ recycling (blanket)*
  - LT oxy-natural gas with CO$_2$ recycling (synthetic air)
  - Air firing natural gas
  - HT oxy-coal without CO$_2$ recycling

* http://www.jupiteroxygen.com
The temperature profile was described as the following:

\[ T(r) = T_p \exp \left[ - \left( \frac{r - r_c}{c} \right)^2 \right] + T_b \]

- Assumed Temperature Profile and best fit to boundary conditions and spectral data
- First time this technique applied to coal and pilot scale experiments
Pilot Scale Experiments – Results

Jupiter Oxy-Coal Spectral Results

Coal Test 08, IR Port 2-0 ♦ Meas.
Pilot Scale Experiments – Results

Comparison of estimated temperature profiles

- Peak temperatures of HT oxy-fuel flames are MUCH higher
- Temperatures of LT oxy-fuel air-firing flames are comparable
- Gas temperature near the wall of the HT oxy-fuel without FGR configuration is the highest

Oxy-Coal Equilibrium Calculations

- Equilibrium Calculations are a valuable tool for predicting combustion
  - Product temperature
  - Pressure
  - Species concentrations

- Due to the complicated mechanisms in which coal burns, there is a lack of such a method for coal combustion

- Method developed for coal equilibrium calculations
Oxy-Coal Equilibrium Calculations

Using a molecular analysis, coal is assumed to be a sum of its parts:

\[ 1 \text{ mol Coal} \rightarrow .661 \text{C} + .013 \text{S} + .269 \text{H}_2 + .006 \text{N}_2 + .032 \text{O}_2 + .0115 \text{SiO}_2 + .003 \text{Al}_2\text{O}_3 + .002 \text{Fe}_2\text{O}_3 + .002 \text{CaO} + .00045 \]

Energy balance to define the enthalpy of formation of the coal

\[ HV = \sum_{\text{prod}} N_i [h_f + \Delta h] - \sum_{\text{react}} N_i [h_{f,\text{coal}} + \Delta h] \quad (27) \]

Assumed:
- Constant weight percentage of coal to be 25% (laboratory experiments varied from 22-27%)
- Illinois Coal molecular composition
Assumed:
• Constant weight percentage of coal to be 25% (laboratory experiments varied from 22-27%)
• Illinois Coal molecular composition

Conclusions
This work achieved the following:

• Developed and performed small scale laboratory testing to characterize coal dust cloud combustion and its radiative properties under different scenarios

• Created a Numerical Model that accurately simulates the laboratory experiments

• Examined oxy-fuel pilot scale radiative emissions under different operating scenarios and determined a temperature profile

• Developed a method to performing equilibrium calculations for coal combustion
Thesis Work yet to be Done on this Project

- Additional equilibrium calculations
- Spectral radiation estimates based on Numerical Calculations
  - Compare laboratory radiation results to predicted results
  - Perform more comparisons with model

The Future of CCS

- CCS could become cost-effective with future carbon legislation and increased efficiencies
- Need more research projects like this one to continue advancing CCS technologies

Socolow, 2005, Scientific American
Quickly approaching Oxy-Fuel projects at output levels that could replace existing large pf coal power production plants.

Acknowledgements

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We thank Jupiter Oxygen engineers for gathering the data and providing pilot scale apparatus. In particular, we thank Brian Patrick and Steve Nied.

We thank the Center for Coal Technology Research for funding under contract number 7-PSC-CTR-002. In particular, we thank Marty Irwin and Brian Bowen for their support of this work.
Estimation of temperature profile was made using the following assumptions:

1. Turbulent effects are not considered as a first approximation.
2. Negligible radiation from the wall.
3. Constant species (CO$_2$, H$_2$O, O$_2$, etc.) concentrations. The species concentrations were obtained by thermodynamics calculations using HYSYS (Jupiter's calculation).
4. The temperature profile was described as the following,

\[ T(r) = T_p \exp \left[ -\left( \frac{r - r_p}{c} \right)^2 \right] + T_b \]

where the normalized position, \( r \), is zero at the center and unity at the water wall boundary. The four parameters (\( T_b \), \( T_p \), \( c \), and \( r_p \)) are related to the gas temperature at the boundary (\( T_b \)), the normalized location of the flame front (\( r_p \)), the flame front temperature (\( T_p + T_b \)), and the gas temperature at the flame center. These parameters were first guessed and then determined when the calculated \( I_l \) based upon these parameters were optimized to yield the best fit to the measured \( I_l \) at four (at least) specifically chosen wavelengths.

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**References**

