Oxy-Fuel Combustion

E. J. Miklaszewski, Y. Zheng, L. Qiao and S. F. Son
Department of Mechanical Engineering

Purdue University
West Lafayette, IN 47907

PURDUE UNIVERSITY

Presentation Outline

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

PURDUE UNIVERSITY

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

PURDUE UNIVERSITY

Efficiency?

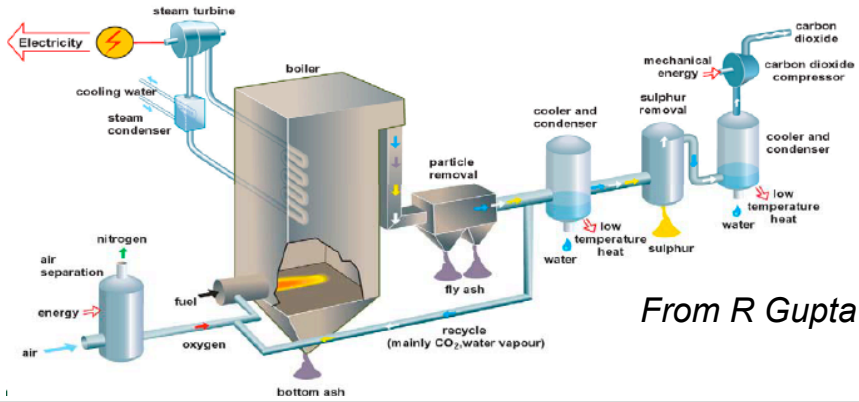
Jury still out for the most cost effective/ efficient "cleaner" coal option

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

Oxy-fuel

- Oxyfuel
  - Pure oxygen as oxidizer (often diluted with flue gas)
  - Reduces or eliminates NOx (no Nitrogen in oxidizer flow)
  - Increase in cost due to large scale oxygen production
- Increases CO_2 concentration
  - Easier to recover

Could be used in retrofit existing coal plants



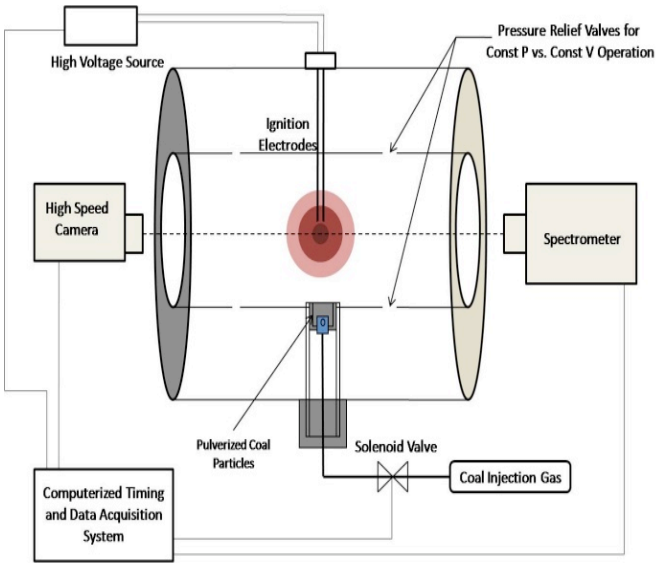
From R Gupta

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

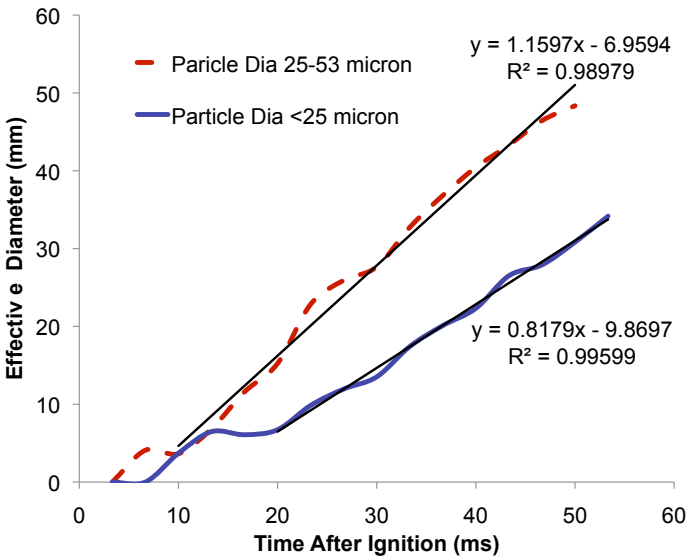
Coal Analysis

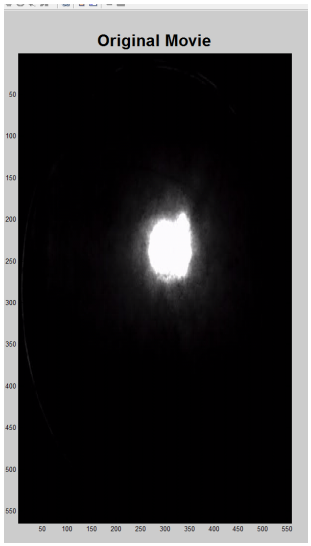
Coal Type	**Indonesian Coal**	**Illinois Basin #6**
Coal Classification	Bituminous (low sulfur, low ash)	Bituminous
	Ultimate Analysis (%)	
Carbon	73.70%	68.30%
Hydrogen	5.20%	5.00%
Oxygen	18.80%	13.80%
Nitrogen	1%	1.30%
Sulfur	0.10%	3.50%
Ash	1.30%	8.10%
	Typical Proximate Analysis (%)	
Moisture	16.12%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

Further Classify Coal using Sieves:
- >106 µm
- 106 µm - 75 µm
- 75 µm - 53 µm
- 53 µm - 25 µm
- < 25 µm

PURDUE UNIVERSITY

How Flame Speed was Obtained





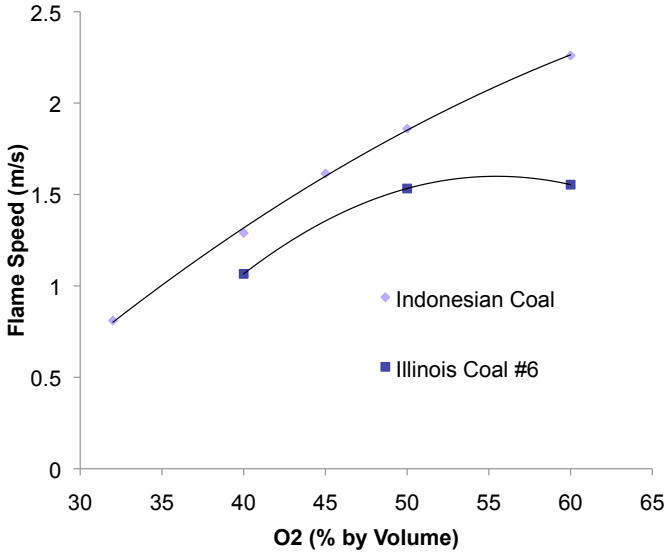
Automated MatLab analysis

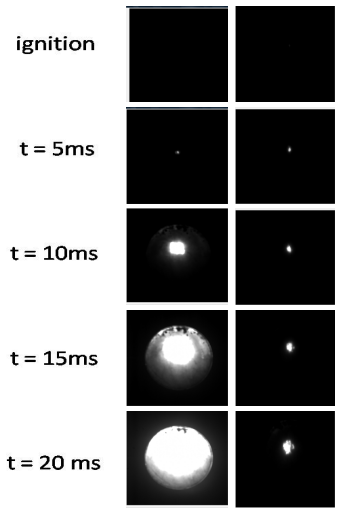
Less Sensitive to Human Error in choosing effective diameter

Both cases:
Cloud density - 0.539 kg/m^3
40% O_2 and 60% CO_2
Indonesian Coal

PURDUE UNIVERSITY

Effect of Oxygen On Flame Speed



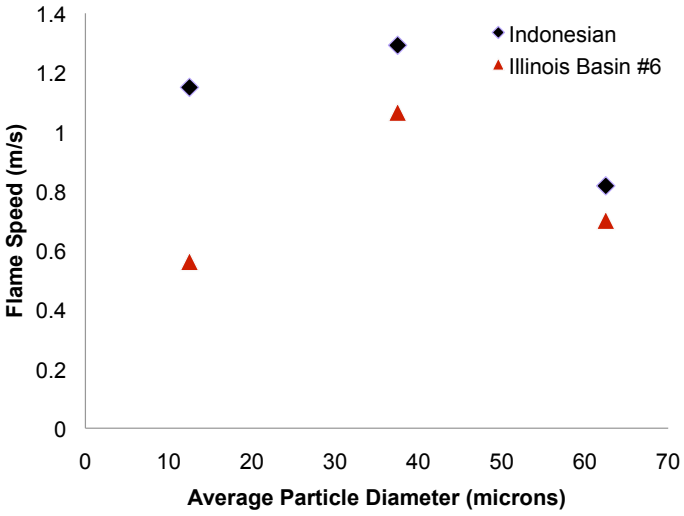


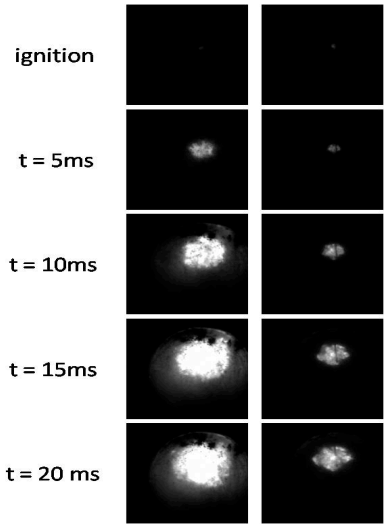
60% O_2 40% O_2

All cases:
Cloud density - 0.539 kg/m^3
Particle Dia. – 25-53 µm
Carbon Dioxide Diluent

PURDUE UNIVERSITY

Effect of Particle Diameter On Flame Speed





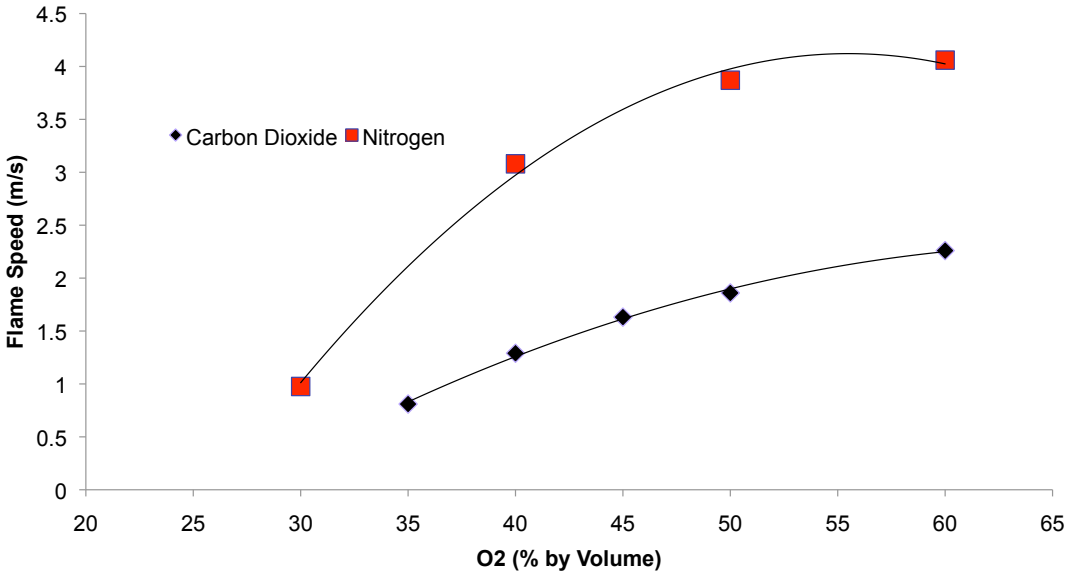
- Decrease in flame speed with smallest particle size can be attributed to:
  - Material Sticking to windows (leaner mixture)
  - Agglomeration (can be seen in videos)

Dia. <25 µm Dia. 53-75 µm

All cases:
Cloud density - 0.539 kg/m^3
40% O_2 and 60% CO_2

PURDUE UNIVERSITY

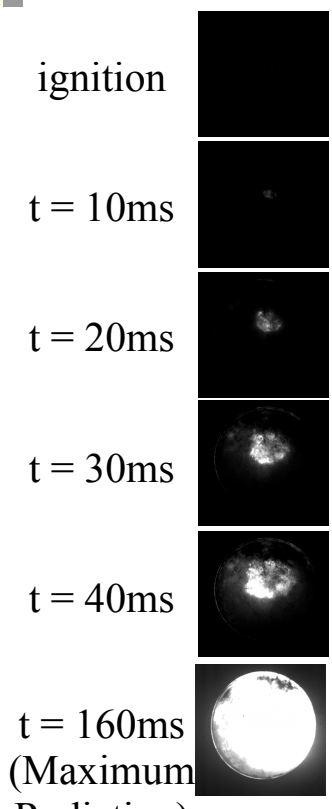
Effect of Diluent On Flame Speed

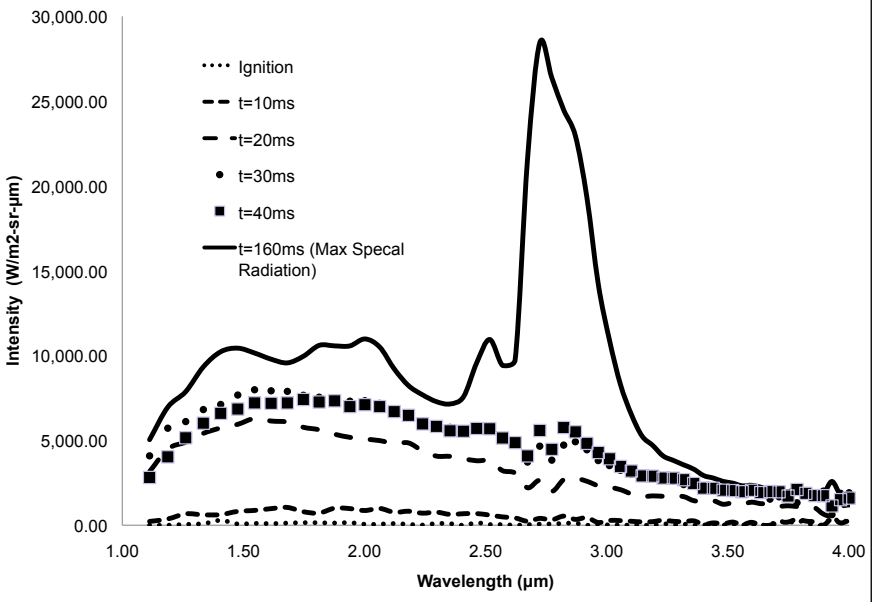


All cases:
Particle Dia – 25-53 microns
Indonesian Coal
Cloud density - 0.539 kg/m^3

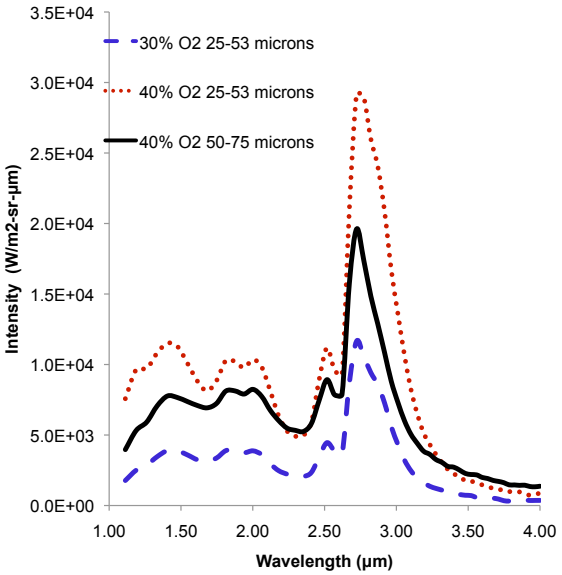
Laboratory Experiments – Results (Spectral)

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

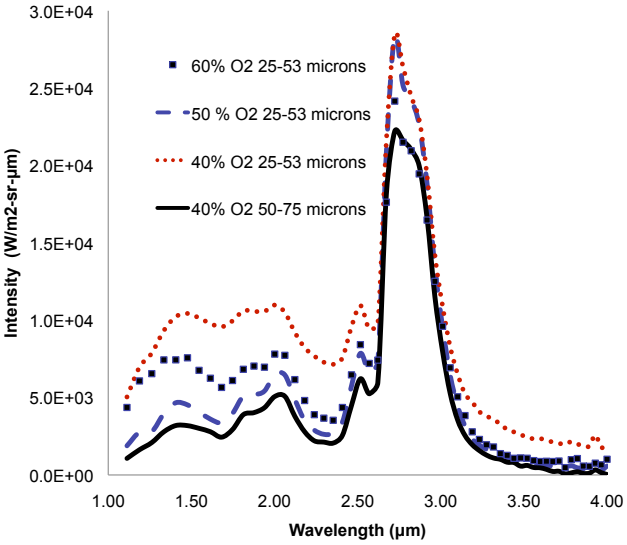




Test Specs:
40% CO_2, 60% O_2
Particle Dia – 25-53 microns
Cloud density - 0.539 kg/m^3



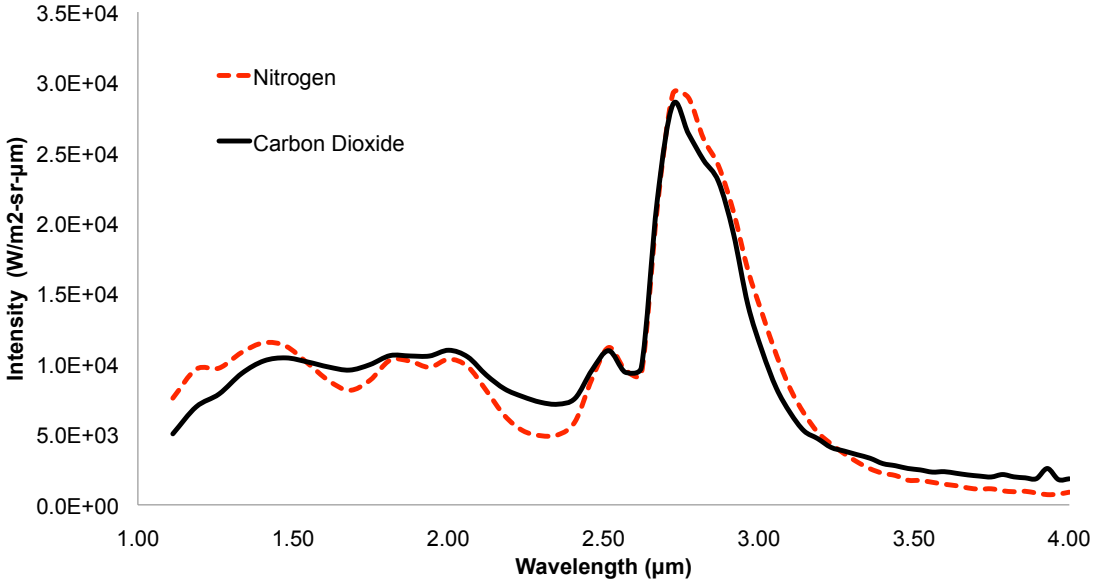
N_2 Diluent



CO_2 Diluent

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

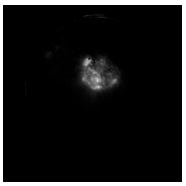


Test Specs:
40% O_2, 60% Diluent
Particle Dia – 25-53 microns
Cloud density - 0.539 kg/m^3
Indonesian Coal

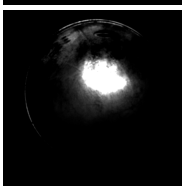
PURDUE UNIVERSITY

Laboratory Experiments – Results (Spectral)

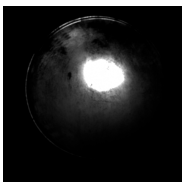
40% O_2

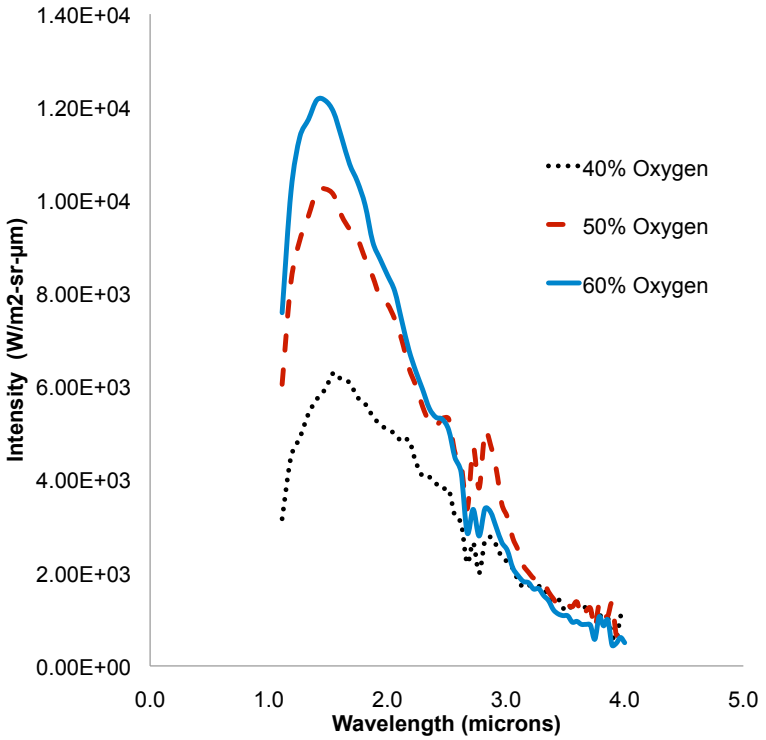


50% O_2



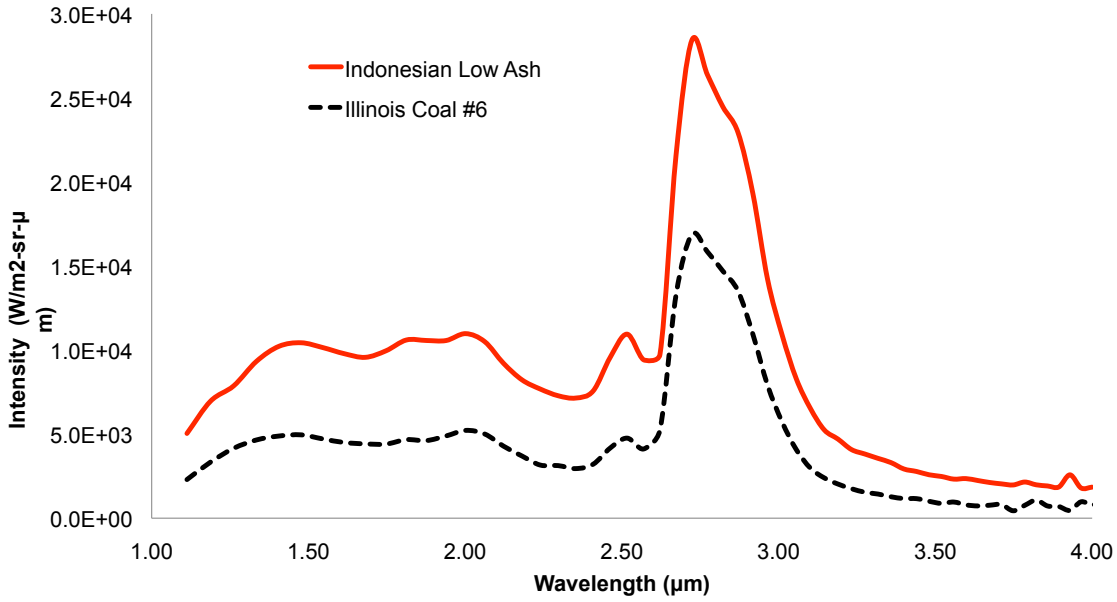
60% O_2





Test Specs:
Fire Ball Diameter ~ 48mm
CO_2 Diluent
Particle Dia – 25-53 microns
Cloud density - 0.539 kg/m^3

PURDUE UNIVERSITY



Test Specs:
40% O_2, 60% CO_2
Particle Dia – 25-53 microns
Cloud density - 0.539 kg/m^3

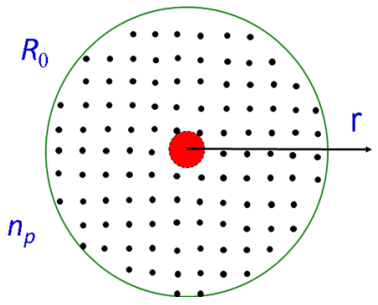
PURDUE UNIVERSITY

Numerical Simulations of Transient Flame Propagation in a Spherical Coal Dust Cloud

PURDUE UNIVERSITY

Physical Model

- 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.

PURDUE UNIVERSITY

Gas-Phase Equations

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

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

$$\varepsilon\rho C_p\frac{\partial T}{\partial t}+\varepsilon\rho C_p u\frac{\partial T}{\partial r}=\frac{1}{r^2}\frac{\partial}{\partial r}(r^2 k\frac{\partial T}{\partial r})-hA_P(T_g-T_P)-\sum_1^K\rho Y_i V_i C_{p,i}\frac{\partial T}{\partial r}-\sum_{i=1}^K\dot{\omega}_i h_i W_i+\sum_{i=1}^K\dot{w}_i(h_{i,Tp}-h_i)W_i+Q_r$$

where ε is the volume fraction of the gas mixture. The volume fraction of the particles, 1-ε, equals to the product of particle number density and particle volume. and are the mass production rate of species *i*, due to gas phase reaction and char reaction, respectively. is the molecular weight of species *i*. V_i is diffusion velocity of species *i*. h_i and $h_{i,0}$ 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 :

$$\frac{\partial \rho_P}{\partial t} = -\frac{6\dot{m}_V}{\pi d_P^3} \qquad \frac{\partial d_P}{\partial t} = -\frac{2\dot{m}_C}{\pi \rho d_P^2}$$

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:

$$m_P C_P \frac{\partial T_P}{\partial t} = \dot{Q}_V + \dot{Q}_C + q_r + hA_P(T_g - T_P)$$

where q_r 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 CH_4 and C_3H_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:

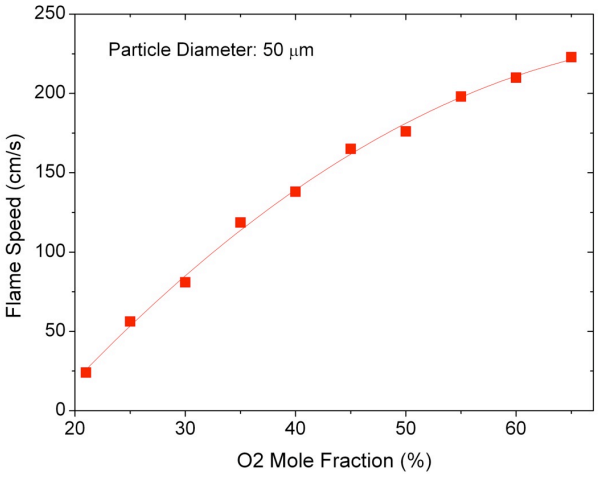
$$C + O_2 \rightarrow CO_2$$

$$2C + O_2 \rightarrow 2CO$$

$$C + CO_2 \rightarrow 2CO$$

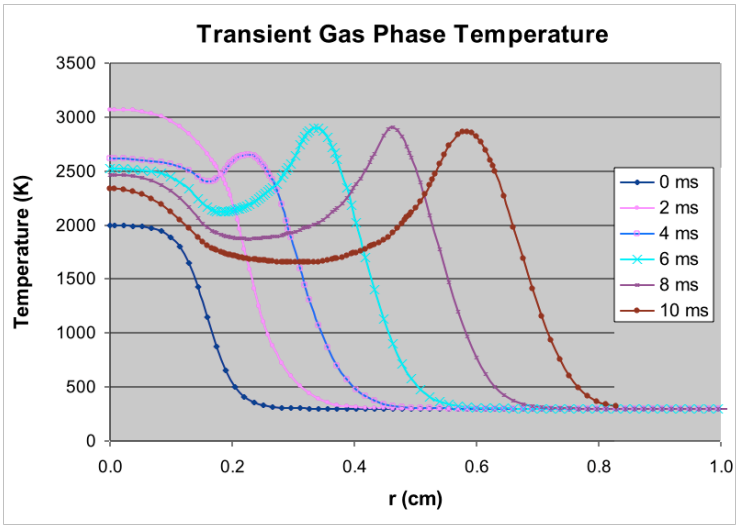
The overall reaction rate is simulated by the diffusion-kinetic model, which is the first-order of O_2 and CO_2 concentrations.

Flame Speed



O2 %	U (cm/s)
21	24.00
25	56.26
30	80.95
35	118.68
40	138.00
45	165.00
50	176.00
55	198.00
60	210.00
65	222.94

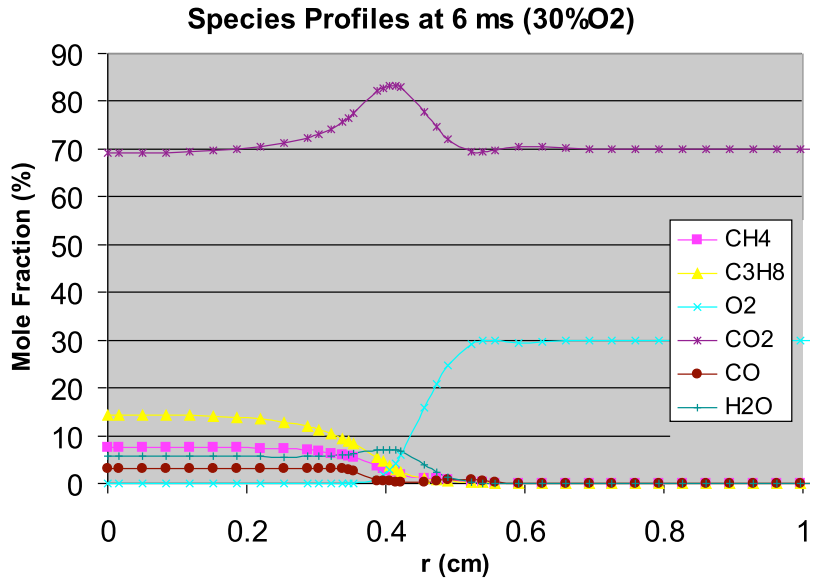
Note:
1. The velocity is defined by tracking the location of gas temperature at 1500 K.
2. The coal property and flame conditions are the same as those of the experiments.
3. As O_2 concentration increases, the discrepancy between measurements and simulations becomes large.



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.

PURDUE UNIVERSITY

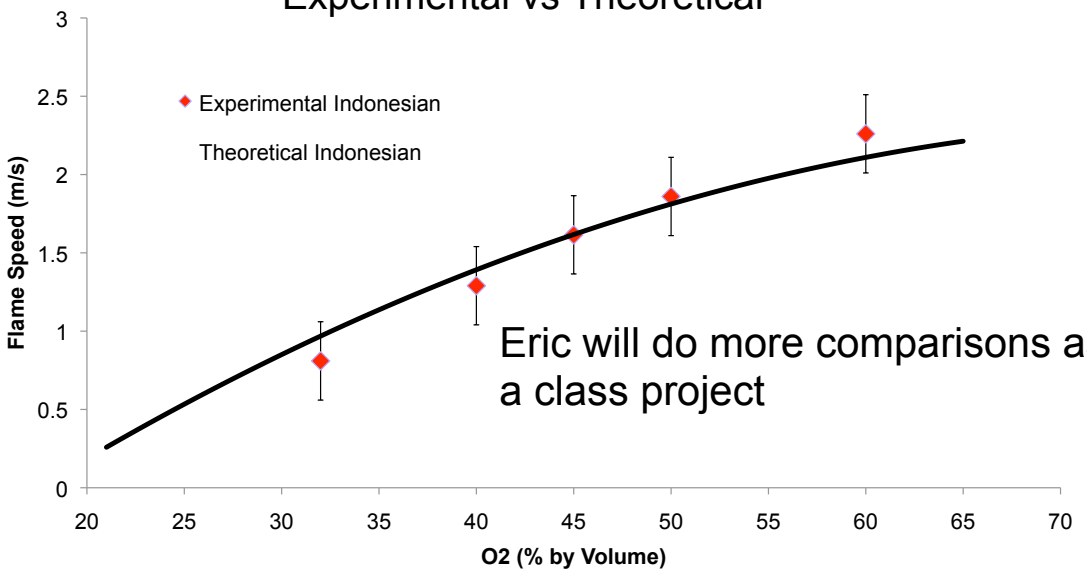


Note:

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.

PURDUE UNIVERSITY

Experimental vs Theoretical



Eric will do more comparisons as a class project

All cases:
Cloud density - 0.539 kg/m^3
Particle Dia. – 25-53 μm
Carbon Dioxide Diluent
Indonesian Coal

PURDUE UNIVERSITY

Pilot Scale Experiments

From Jupiter Oxygen in Hammond Indiana

PURDUE UNIVERSITY

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

PURDUE UNIVERSITY

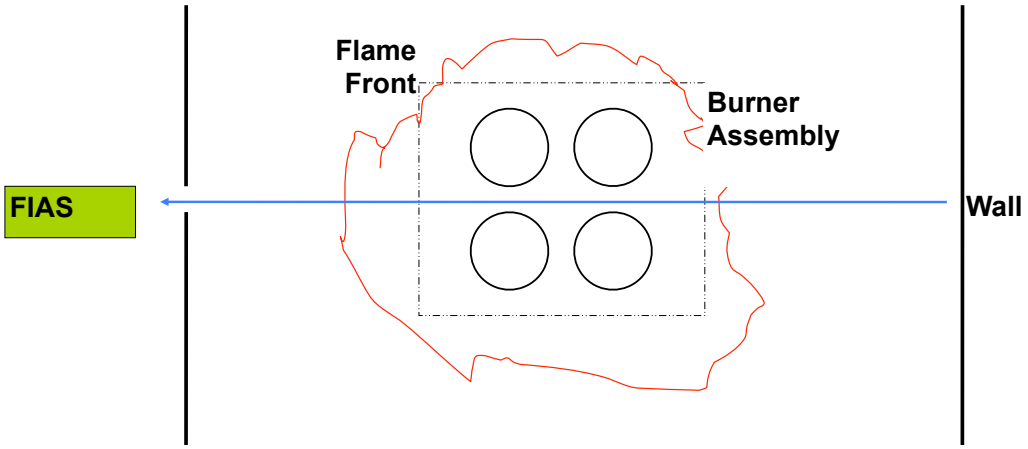
Pilot Scale Experiments - Details

- 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

Pilot Scale Experiments – Pilot Scale Apparatus

Spectral Measurement Configuration



Pilot Scale Experiments – Inverse Flame Temperature Technique

The temperature profile was described as the following:

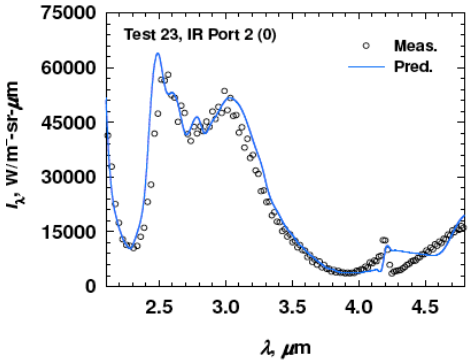
$$T(r) = T_p \exp\left[-\left(\frac{r - r_p}{c}\right)^2\right] + T_b$$

- Assumed Temperature Profile and best fit to boundary conditions and spectral data

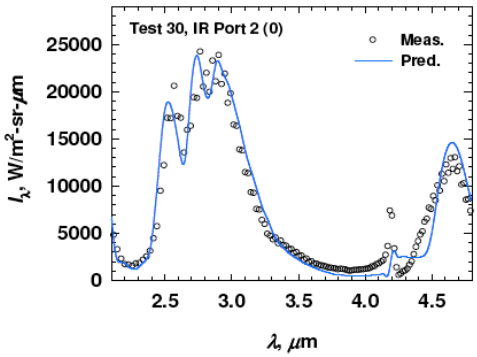
- First time this technique applied to coal and pilot scale experiments

PURDUE UNIVERSITY

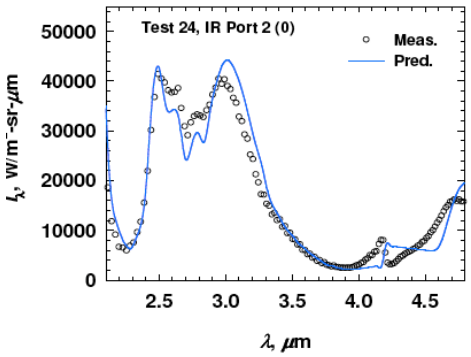
Pilot Scale Experiments – Results

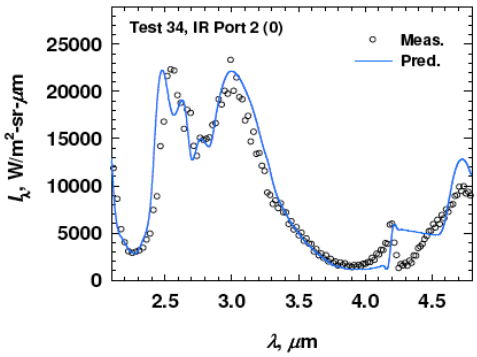


Spectral Emissions of HT oxy-fuel w/o CO_2 recirculation



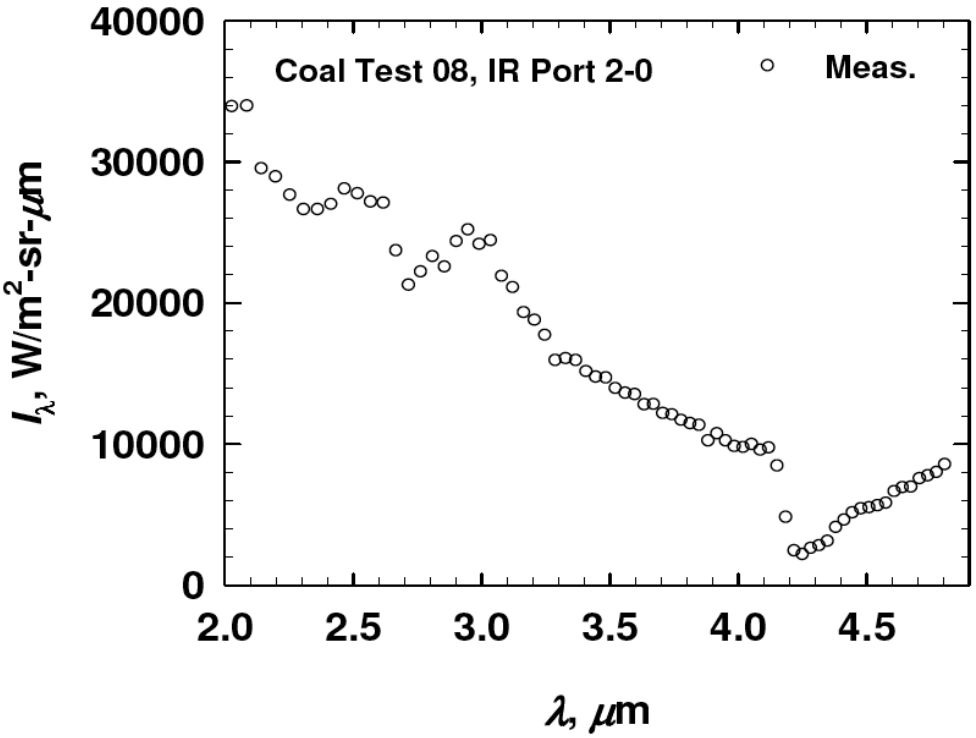
Air-Fire Spectral Emissions



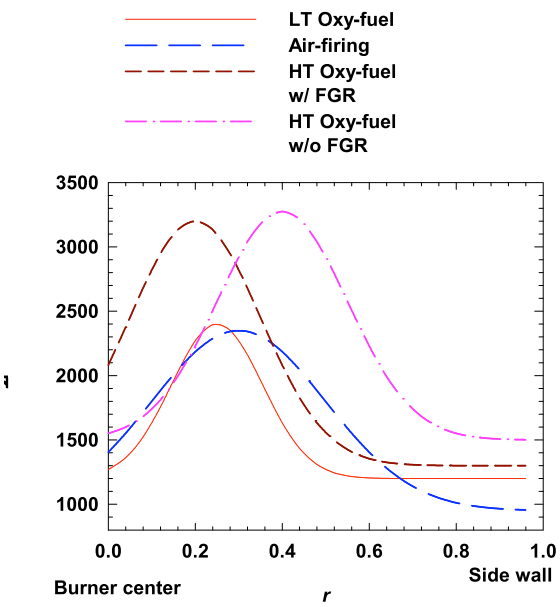


PURDUE UNIVERSITY

Jupiter Oxy-Coal Spectral Results



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

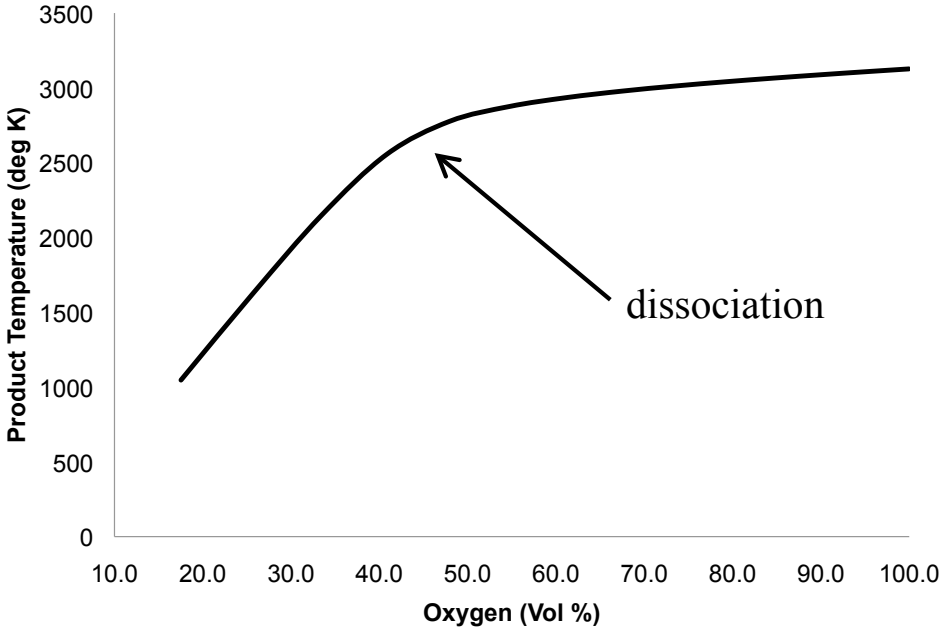
Oxy-Coal Equilibrium Calculations

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

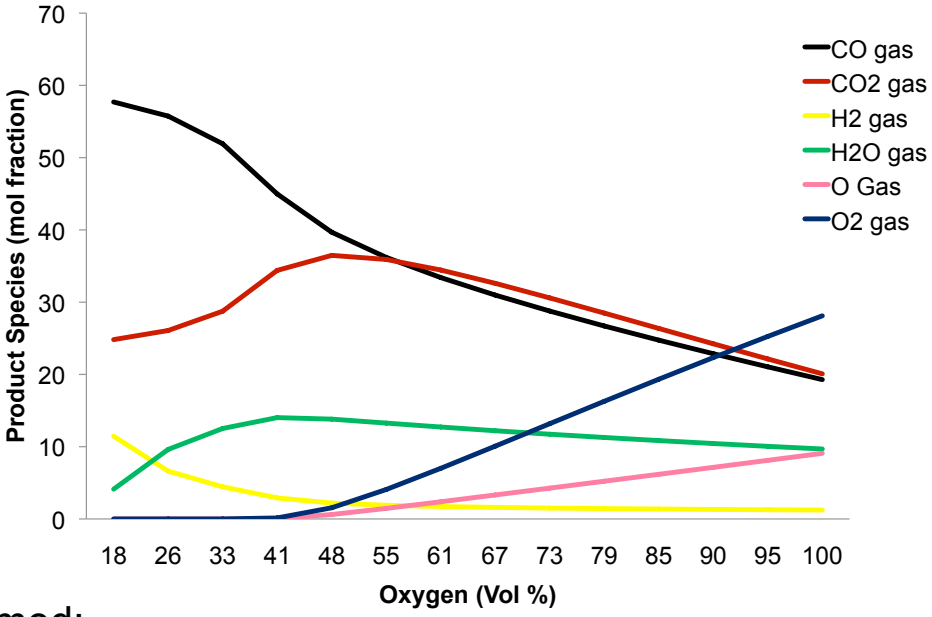
$$1\,mol\,Coal \rightarrow .661\,C + .013\,S + .269H_2 + .006N_2 + .032O_2 + .011SiO_2 + .003Al_2O_3 + .002Fe_2O_3 + .002CaO + .0004S$$

Energy balance to define the enthalpy of formation of the coal

$$HV = \sum_{prod} N_i[h_f + \Delta h] - \sum_{react} N_i[h_{f_coal} + \Delta h] \quad (27)$$



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

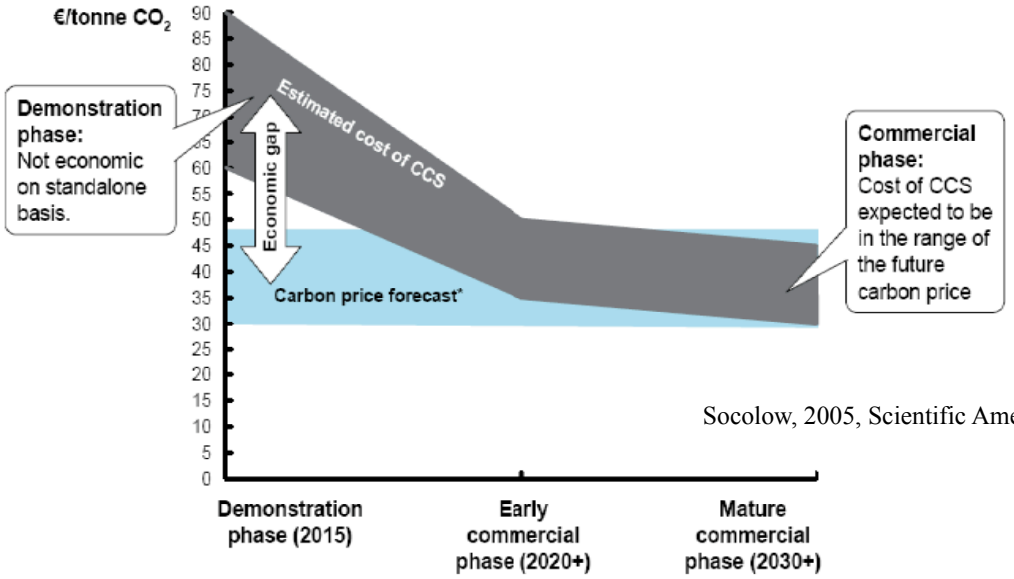
This work achieved the following:

- 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

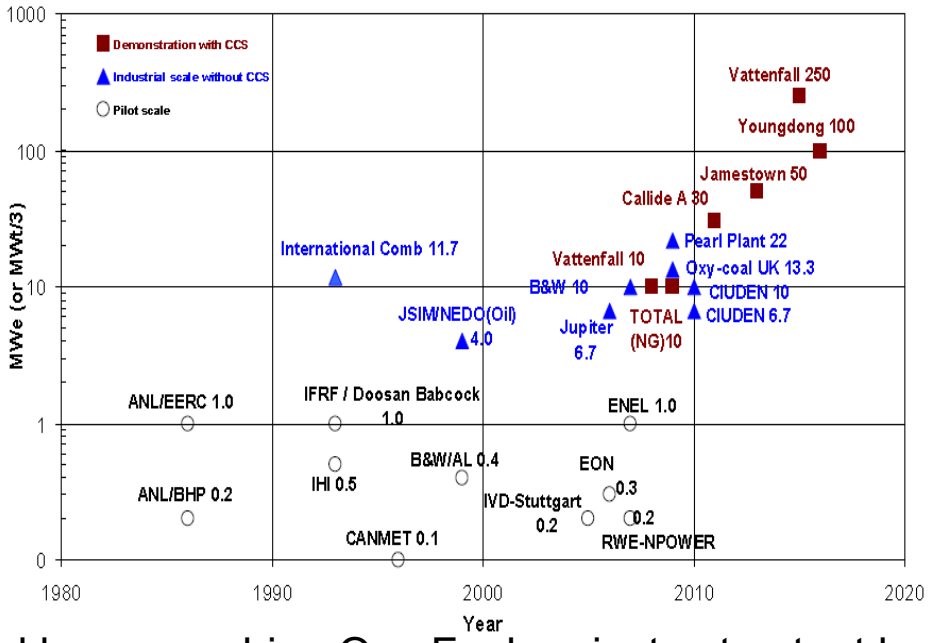
The Future of CCS



Socolow, 2005, Scientific American

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

Major Oxy-Fuel Projects



- Quickly approaching Oxy-Fuel projects at output levels that could replace existing large pf coal power production plants

Acknowledgements

We'd like to thank Prof. Timothee Pourpoint for use of his Matlab Code for analyzing the high-speed images.

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.

APPENDIX - Pilot Scale Experiments – Inverse Flame Temperature Technique

PURDUE UNIVERSITY

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_2O, 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.

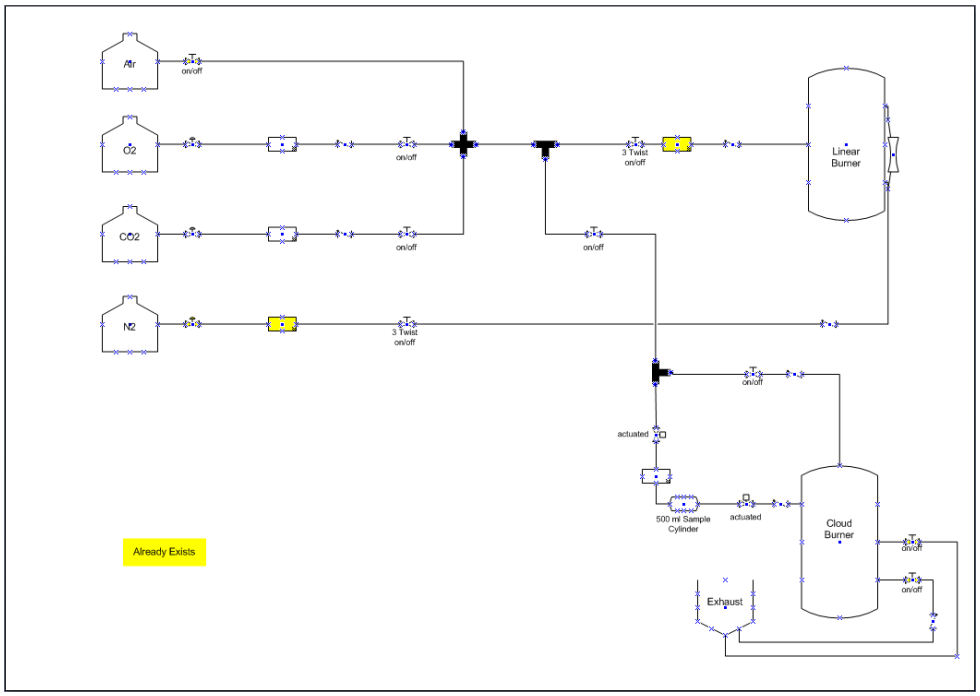
References

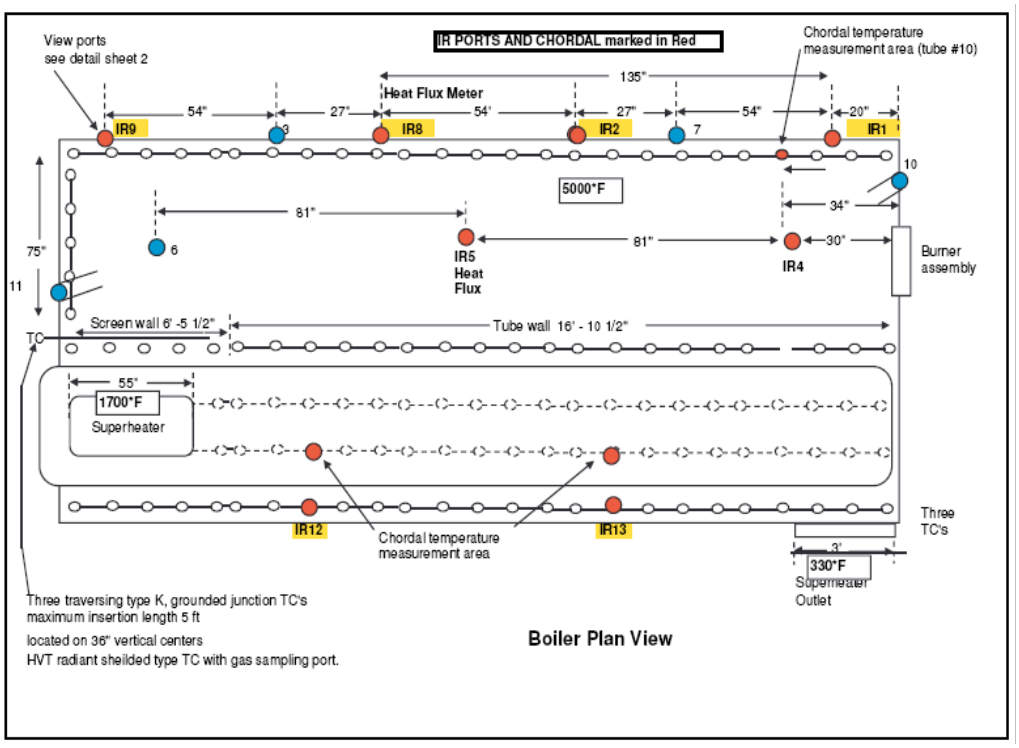
PURDUE UNIVERSITY

- 1)Suda T, Masuko K "Effect of carbon dioxide on flame propagation of pulverized coal clouds in CO2/O2 combustion", Fuel (2007), doi:10.1016/j.fuel.2006.11.038
- 2) Kiga T, Takano S, Kimura N, Omata K, Okawa M, Mori T "Characteristics of Pulverized Coal Combustion in the System of Oxygen/Recycled Flue Gas Combustion" Energy Conversion Management , 1997; 38: S129-S34

APPENDIX - Piping Diagram

PURDUE UNIVERSITY



APPENDIX - Test Arrangement

PURDUE UNIVERSITY