OXYFUEL COMBUSTION FOR COAL-FIRED POWER GENERATION WITH CO₂ CAPTURE-
OPPORTUNITIES AND CHALLENGES

CCS Research Group, The University of Leeds

Penny Edge (PhD)  Kris Larsen (PhD)  Maryam Gharebaghi (PhD)
Richard Porter (RF)  Rachael Porter (PhD)  Mohamed Degereji (PhD)
Sreenivasa Gubba (RF)

K. Hughes, M. Pourkashanian, L. Ma, B. Nimo, and A. Williams,

CFD Support: A. Burns and D. Ingham
How carbon capture and storage (CCS) could make coal the fuel of the future

Explainer: The three main techniques for preventing carbon dioxide from coal-fired power stations contributing to global warming.

Engineers set to convert carbon dioxide into solid rock.

i read all 8 coments, you all had good ideas the O2 idea was good, less babies is good to, clean coal is good now lets do something about it. now that we got rid of the planet killing repubs maybe the tech. for clean coal can go ahead. i hope obamawill do what he said and make renuable energy first.

david loomis, black river falls 54615, usa
Growing Global Energy Demand by Sector (1971-2030)

- **1971**
- **2002**
- **2030**

**Energy Demand (bnboe)**

- **Transport**
- **Industry**
- **Other Sectors**
- **Power**
Why the Interest in CCS?

- The UNFCCC goal of stabilizing atmospheric GHG concentrations will require significant reductions in future CO$_2$ emissions
- Possible to achieve material reductions in CO2 emissions & provide a bridge to a lower carbon future
- CCS could be part of a *portfolio of options* to mitigate global climate change
- Can provide a win ~ win for both energy security and environment
- CCS has potential to reduce overall costs of mitigation
LEC = \left[ \frac{\sum_{t=1}^{n} \frac{I_t + M_t + F_t}{(1+r)^t}}{\sum_{t=1}^{n} \frac{E_t}{(1+r)^t}} \right]

IEA WEO 2006 (BAH Analysis)
LEC = \frac{\sum_{t=1}^{n} \frac{L_t + M_t + F_t}{(1+r)^t}}{\sum_{t=1}^{n} \frac{E_t}{(1+r)^t}}
- O₂/CO₂ recycle combustion is interesting an option for power generation with CCS:

- use advanced steam technology
- reduce the boiler size and cost and
- to design a zero-emission power plant
CFD Modeling: Current Challenges

- CFD Modeling can provide reasonable predictions.
- Current challenges include:
  - Radiation predictions – especially in oxy-fuel combustion due to the high participation of spectrally absorbing-emitting CO₂ and H₂O
  - Turbulence-radiation interaction – widely-used RANS averaged models do not take into account local fluid property fluctuations which have impact on radiation and chemistry
  - Lack of validation data

![Calculated flame temperatures](image)

![Combustion Test Facility](image)
Temperature Profile

Char Burnout Kinetics
Char Oxidation

Oxidizer Flow

Free Stream

Zone of the reaction

$2CO + O_2 = 2CO_2$

Porous Char Particle

Inter-Particle Diffusion

Heterogeneous Reactions

\[
\begin{align*}
C_{(s)} + O_2 &= CO_2 \\
2C_{(s)} + O_2 &= 2CO \\
C_{(s)} + CO_2 &= 2CO \\
C_{(s)} + H_2O &= 2CO + H_2
\end{align*}
\]
Fate of Mercury in Coal Combustion

- **Coal** (Containing 10-100 PPM of Hg)
  - **Char**
  - **Unburned Carbon**

- **Heat**
  - **Cl₂** + **H₂O** → **HCl**
  - **Hg(0)**

- **Homogeneous reactions**, Happen in the convection duct or Flue gas treatment line when temperature is around 200 – 500 °C.
  - **HgCl, HgCl₂, HgO - Hg (II)** and **Hg(P)**

- **Heterogeneous reactions**, Happen in the Flue gas treatment line when temperature is around 100 – 350 °C.
Interaction of Pollutants in Air-Coal Combustion

**Chlorine (Cl₂ / HCl)**
Source: Cl – Fuel

Cl – fuel (HCl/Cl₂ in flue gas) is the most important oxidizer for the Mercury. The chlorinated activated carbon is an effective sorbent for Hg removal. However, if Sulfur removes Cl from the carbon surface, Hg removal is decreased. Cl effect is not important in heterogeneous reactions.

**Unburnt Carbon (in fly ash)**
Source: Inefficient char combustion process, mainly in fuel rich zones
Removal: Using filters or bag houses (Physical separation)

**Mercury**
Source: Hg – Fuel
Removal: Activated Carbon sorbent

Interaction due to Hg Removal

**SO₂**
Source: S – Fuel. Also Sulfur may enter the system in the flue gas treatment line. Formation: During devolatilisation (as H₂S) and during char oxidation (as SO₂ which will oxidize to SO₃ in the gas phase)
Removal: FGD unit using solvents

In fuel rich zones, S – Fuel which forms SO₂ may inhibit NOₓ reduction reaction.

**NOₓ**
Source: Thermal NOₓ and Fuel NOₓ (N – Fuel)
Removal: Low NOₓ burners

Inhibition effect on Hg oxidation in presence of Cl

**Steam**
Source: Combustion product, Recycled flue gas.

There is a competition between Sulfur and Mercury for Carbon surface reaction. SO₃ generation inhibits Hg removal by activated carbon, since there is a higher concentration of Sulfur compounds in the flue gas than Hg.

**CO**
Source: Incomplete combustion of coal

SO₂ inhibits CO oxidation by affecting [OH]
Interaction of Pollutants in Oxy-CO₂-Coal Combustion

**Chlorine (Cl₂ / HCl)**
- Source: Cl – Fuel
  - Cl – fuel (HCl / Cl₂ in flue gas) is the most important oxidizer for the Mercury. The chlorinated-activated carbon is an effective sorbent for Hg removal. However, if Sulfur removes Cl from the carbon surface, Hg removal is decreased. Cl effect is not important in heterogeneous reactions.

**Unburnt Carbon (in fly ash)**
- In Oxy combustion, due to Oxygen deficiency in some zones, Unburnt Carbon in ash is higher. So there is a direct effect on the heterogeneous reactions of Carbon – Mercury.

**Mercury**
- Source: Hg – Fuel
  - Removal: Activated Carbon sorbent

**SO₂**
- In Oxy combustion, there is an increase of SO₂ in the combustion zone. So far, there is a direct effect on the heterogeneous reactions of Carbon – Mercury – Sulfur.
- SO₂ inhibits CO oxidation by affecting [OH]

**NOx**
- In Oxy combustion, there is a decrease in NOx generated in the furnace, however, there is a distinction between NO and NO₂ effect on Hg oxidation.
- In fuel rich zones, S – Fuel which forms SOₓ may inhibit NOx reduction reaction.

**Steam**
- There is more steam in the combustion Zone in Oxy combustion.
- Inhibition effect on Hg oxidation in presence of Cl

**CO**
- Source: Incomplete combustion of coal
Formulation from database of narrow band k-distributions (based on LBL data)

- **Gases**
  - Species accounted for in NB database are CO2, CO, H2O and CH4.

- **Larger particles**
  - Mie Theory for larger particles in the geometric limit – Two main properties to be predicted for non-uniform particle cloud

- **Soot**
  - Mie Theory reduces to the Rayleigh scattering limit due to the size parameter of the soot particles

- **Size distribution**
  - Char
    - Particle size distribution from Rosin-Rammler input to Fluent is possible
  - Ash
    - Fragmentation means ash not same psd as char. Size distribution must be modelled

- **Absorption extinction factor**
  - Char
    - Geometric limit: \( Q_{abs} = 1/2(f1+f2) \)
      - Dependent upon \( n \) and \( k \) for the particles and hence wavenumber
  - Ash
    - More complex expression still requires \( n \) and \( k \) dependence
Radiative properties of gases

Line by line methods

Band models

Total emissivity / absorption methods

Narrow band models

Wide band models

Statistical NBM (Malkmus, Goody etc)

K-distribution NBM – no approx based on LBL data

Edwards EWBM

Narrow band k-dist models e.g. $\Delta \nu = 25 \text{cm}^{-1}$ ($I_b$ assumed constant in band)

Full Spectrum k-distribution FSK model (Weighted by $I_b$)

Direct formulation from LBL database

Formulation from database of narrow band k-distributions (based on LBL data)
Slagging, Fouling and Corrosion Mechanism Development
Mechanism Development Overview

• Char Oxidation Mechanism Development
• Heat Transfer (Radiation Model) Development
• Soot Mechanism Development
• Pollutants Emission Mechanism Development
• Slagging & Fouling Mechanism Development
• Corrosion Mechanism Development

Mechanism Validation
Evaluation of CFD Simulation Options for Oxy-Coal Combustion

Consultation with Industry

High

Low

Low

High

Impact On Oxy-Fuel CFD Simulation Accuracy

- LES
- RANS
- Char Oxidation
- Volatile Combustion
- Devolyization
- Hg/Cl
- Metal release
- Fouling
- Slagging
- TR I
- HT
- Soot Formation
- NOx-SOX
- TCI
In-depth Studies of OxyCoal Combustion Processes through Numerical Modelling and 3D Flame Imaging

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School of Process, Environmental and Materials Engineering
FACULTY OF ENGINEERING

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Project Partner:

UNIVERSITY OF LEEDS

UNIVERSITY OF CAMBRIDGE  Cranfield University  Imperial College London  University of Kent  The University of Nottingham

ANSYS  Doosan  Doosan Babcock Energy  THE LINDE GROUP