Lecture 3: Oxyfuel Combustion Science: Mass and energy balances, heat transfer, coal combustion and emissions

Professor Terry Wall and Dr Jianglong Yu

University of Newcastle, Australia

APP OFWG capacity building course
Oxy-fuel flowsheet for first generation technology, showing additional units for a retrofit in red.
Issues with Oxy-combustion CCS

- ASU
- CO₂ handling
  - Purification; compression; transportation; storage
- Replacement of nitrogen with recycled CO₂
  - Combustion environment of fuel
    - Fuel reactivity
    - Retrofit
    - Impurity formation and emission
  - Impurity impact on CO₂ handling
Lecture context and content

Oxyfuel science used here to compare air and oxy-fuel furnace performance, for retrofit of an existing air-fired boiler while maintaining heat transfer, considering

- Conditions for matched heat transfer
- Changed burner flows, with flame and heat transfer impacts
- Coal reactivity and burnout impacts

Developments and gaps in knowledge will be suggested
Mass and energy balances and heat transfer
AFT of air and oxy cases

Adiabatic flame temperature (K) vs O2 fraction at burner inlet

- Blue line: oxy-wet
- Red line: oxy-dry
- Green data point: air
Oxy-fuel: differences of combustion in $\text{O}_2$/CO$_2$ compared to air firing

- To attain a similar AFT the $\text{O}_2$ proportion of the gases through the burner is $\sim 30\%$.
- The high proportions of CO$_2$ and H$_2$O in the furnace gases result in higher gas emissivities.
- The volume of gases flowing through the furnace is reduced.
- The volume of flue gas (after recycling) is reduced by about 80%.
- Recycle gases have higher concentrations in the furnace.
Gas property differences 1: Emissivity
Triatomic gas (H$_2$O+CO$_2$) emissivity ~ beam length comparisons

Oxy-fuel fired furnace
Air fired furnace

\[ \varepsilon = \sum_{i=0}^{\infty} a_{\varepsilon,i} (T) \left[ 1 - e^{-k_i (p_{CO2} + p_{H2O})L} \right] \]
Gas property differences 2: Heat capacity etc

Impact for air to oxyfuel retrofit

- Higher O2 thru burner
- Lower burner velocity, higher coal residence time in furnace
- Slower flame propagation velocity

Gas property ratios for CO₂ and N₂ at 1200 K

Properties from Shaddix, 2006
Therefore secondary RFG reduced

Recirculated Flue Gas, RFG

27% \( O_2 \) % v/v fixed for same HT

Secondary air/ RFG

\( \sim 3\% \) v/v \( O_2 \)

Fixed velocity

Primary air/ RFC

Furnace

Burner

Flue gas Stack

Coal
# 1 MWt test conditions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Full load</th>
<th></th>
<th>Partial load</th>
<th></th>
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</thead>
<tbody>
<tr>
<td></td>
<td>Air case</td>
<td>Oxy case</td>
<td>Air case</td>
<td>Oxy case</td>
</tr>
<tr>
<td>Coal flow rate</td>
<td>kg/hr</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Primary velocity</td>
<td>m/s</td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>Secondary velocity</td>
<td>m/s</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>Secondary swirl number</td>
<td>-</td>
<td>0.2</td>
<td></td>
<td>0.2</td>
</tr>
<tr>
<td>Primary momentum flux</td>
<td>kg/s.m²/s²</td>
<td>35.7</td>
<td>54.1</td>
<td>20.9</td>
</tr>
<tr>
<td>Secondary momentum flux</td>
<td>kg/s.m²/s²</td>
<td>270.2</td>
<td>74.1</td>
<td>38.2</td>
</tr>
<tr>
<td>Momentum flux ratio (Pri/Sec)</td>
<td>-</td>
<td>0.13</td>
<td>0.73</td>
<td>0.55</td>
</tr>
</tbody>
</table>

Preheated air/RFG: primary 350 - 400K and secondary 450 - 550 K, Wall 1200 K
IFRF Flame types from swirl burners

Type-0
Lo S

Type-1
Hi S (S>0.6), Lo v₂

Type-2
Hi S, Hi v₂
1 MWt – Temperature contours at full load

Air-case

X 1.5m

Type-0 flame

Oxy-case
Coal combustion in Sandia’s entrained flow reactor under the intermediate gas temperature conditions.

(Murphy and Shaddix 2006)
Sensitivity analysis – full & partial load

The graph shows the temperature (K) as a function of the axial distance from the burner (m) under different load conditions:
- **Air-full load**
- **Air-partial load**
- **Oxy-full load**
- **Oxy-partial load**

The temperature increases as the axial distance from the burner increases, with the oxy-full load showing the highest temperature and the air-partial load showing the lowest.
Effect of momentum flux

- Confirms the significance of momentum flux and Gas properties on flame ignition
1 MWt Temperature comparisons for matching furnace heat transfer

Diagram showing temperature comparisons for Flame and FEGT.
Coal combustion in Sandia’s entrained flow reactor under the intermediate gas temperature conditions.

(Murphy and Shaddix 2006)
Particle imaging of ignition and devolatilization of pulverized coal during oxy-fuel combustion.

Devolatilization of coals under fluidized bed conditions in oxygen-enriched air

(Borah, Ghosh et al. 2008)
30 MWe Burner plane – Temperature contours

Air case

Oxy case
30 MWe – heat transfer results

![Graph showing total surface heat flux (kw/m²) for different furnace wall areas (m²) for air and oxy-fuel.]
425 MWe – burner zone temperatures
Summary plot relating gas emissivity changes to burner oxygen

- Wet recycle
- Dry recycle

Gas Emissivity (oxy to air)

Fraction at burner inlet (-)

Beam Length (L) (m)

Gas Emissivity (%)
Through early modelling although CO$_2$ has a different thermodynamic properties, under the same oxygen content, oxy-combustion heat transfer does not differ much from air combustion because oxy-combustion has a lower flame temperature;

CFD based modelling indicated that when oxygen content in the oxy-combustion increases from 21% to 29%, combustion efficiency and boiler efficiency increase. But further increase in oxygen content does not significantly improve the efficiency and 30% above oxygen causes other problems and safety concerns. The oxygen content in oxy-combustion therefore vary from 21% to 29%. 

**Heat transfer: Other relevant study (CFB (Zhejiang 2003))**
And O₂ fraction at the burner can be determined by flue gas recycle ratio (here, for wet recycle)
Coal combustibility
1 MWt Combustibility comparison

Parity, equal C-in-ash air/oxy
Unburnt carbon in ash: oxy vs air combustion

Electric Power Development & IHI, Kimura 1995

Coal swirl burner
Illustrative differences in air and oxyfuel which influence burnout

For matched furnace heat transfer:

Oxyfuel has longer furnace residence time, ~20% Good
Oxyfuel has lower temperatures, ~ 50 °C Bad
In oxyfuel, coal experiences an environment with higher $O_2$ Good
Pyrolysis and oxidation reactivities of Coal A & Coal B in TGA

![Graph showing reactivities of Coal A and Coal B in TGA](image-url)
Heat flow during pyrolysis & oxidation of Coal A & Coal B in TGA

- Coal A Pyrolysis & gasification Endothermic
- Coal B Oxidation Exothermic
- Coal A Oxidation Exothermic
- Coal B Pyrolysis
- Oxidation

Temperature (°C) vs Heat flow (mW)
### Volatile yields in DTF at 1400 °C

<table>
<thead>
<tr>
<th></th>
<th>Coal B</th>
<th>Coal C</th>
<th>Coal D</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V^\ast$ ($N_2$)</td>
<td>36.7</td>
<td>30.9</td>
<td>53.5</td>
</tr>
<tr>
<td>Q factor ($N_2$)</td>
<td>1.52</td>
<td>1.43</td>
<td>1.76</td>
</tr>
<tr>
<td>$V^\ast$ ($CO_2$)</td>
<td>43.3</td>
<td>32.2</td>
<td>66.2</td>
</tr>
<tr>
<td>Q factor ($CO_2$)</td>
<td>1.79</td>
<td>1.49</td>
<td>2.18</td>
</tr>
</tbody>
</table>

$V^\ast$ - Volatile yield at 1400 °C  
Q factor – Ratio of $V^\ast$ and volatile yield obtained by proximate analysis
Char burnout in DTF taking $V^*(N_2)$ to estimate char yield

![Graph showing char burnout as a function of oxygen concentration for Coal B](image)
Summary of reactivity data for 63-90 micron size cuts of four coals from DTF experiments at 1400 °C

Volatile yield

Coal Burnout
DTF-char reactivity in TGA

Coal B

Char Reactivity (s\(^{-1}\))

Temperature (°C)

- Air 2% O\(_2\)
- Oxy 2% O\(_2\)
- Air 5% O\(_2\)
- Oxy 5% O\(_2\)
- Air 10% O\(_2\)
- Oxy 10% O\(_2\)
- Air 21% O\(_2\)
- Oxy 21% O\(_2\)
- Air 50% O\(_2\)
- Oxy 50% O\(_2\)
Char reactivity comparison for air and oxyfuel conditions at the same O$_2$ level
Combustion efficiency (cfb)
Emissions and impurity impacts

PM, SOx, NOx, Hg
Concentration in the flue gas and in furnace and Impacts on CO₂ handling
Impurity impacts on the purification process in oxy-fuel combustion based CO₂ capture and storage system

Li, H., J. Yan, et al. (2009)
Size distribution (mass fraction) of the particles collected using DLPI under oxy and air combustion conditions  

Sheng, 2008
Size distribution (mass fraction) of the particles collected using DLPI under oxy and air combustion conditions

Sheng, 2008
Size distribution (mass fraction) of the particles collected using DLPI under oxy and air combustion conditions  

Sheng, 2008
Formation of Submicron Particulates (PM1) from the Oxygen-Enriched Combustion of biomass

Zhang, 2007
Impurity impacts on the purification process in oxy-fuel combustion

Impurity impacts on the purification process in oxy-fuel combustion

Fig. 5. Enthalpies of different CO$_2$-mixtures in gas phase.

Impurity impacts on the purification process in oxy-fuel combustion

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Impurity impacts on the purification process in oxy-fuel combustion


2-stage-flash
Impurity impacts on the purification process in oxy-fuel combustion

2-stage-flash


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Impurity impacts on the purification process in oxy-fuel combustion


distillation
SO₂ formation (CFB)

(CFD, Zhejiang 2003)
NOx emission (PF)

Electric Power Development & IHI, Kimura 1995

Coal swirl burner
Fuel-N conversion into NOx (PF)

IHI, T.Kiga, 1997
NOx emission (CFB)

SO2 emission

Normalized SO2 emission

(CFD, Zhejiang 2003)
Additional research required

Heat transfer and combustion

- Hot spot evaluation, and burner impacts (cfd based)
- Quantify potential $O_2$ reduction

Gas quality and furnace

- Sulfur gases and corrosion (using pilot-scale data and calculation)
- Mercury levels and form, and impact on $CO_2$ handling

Gas quality for transport, compression and storage

- Plant impacts, regulation and safety issues
Thank you for your attention!
Phase Diagram of CO2
Flame propagation speed (mm/s) vs oxygen content in different atmosphere

(T. Kiga, 1997)