Experimental Investigation and CFD Modelling of Oxy-Coal Combustion on UKCCSRC-Pilot Scale Advanced Capture Technology (PACT) Facility

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5th Oxy-fuel Combustion Research Network Meeting, Wuhan, China
27th-30th October, 2015
Overview

- PACT
- Objectives
- Experimental setup
- Experimental data
- NOx modelling
- Summary / Future Work
Objectives
• Comprehensive and detailed characterization of pf Oxy-fuel experiments
• Development and validation of CFD sub-models
Air Separation Unit

Furnace

ESP/Bag house

Condenser

Coal pulveriser

Dry recycle for primary oxidant

Coal

Air

N2

O2

Recycle gas

Vent Gases

CO2

Water

Non condensable

ESP

Bag house

C P U Compression / Purification units
Experimental Setup
Pf Combustion Test Facility

- In-flame gas temperatures - suction pyrometer
- In-flame gas composition ($O_2$, $CO_2$, $CO$, $NO$, $SO_2$)
- Heat flux - Schmidt Boelter
- 2D and 3D imaging
- Ash sampling
- Deposition studies
- Flue gas emissions
NO Injection
0.25 MW_th PACT Facility Burner

3- OxyCAP -Oxyfuel Combustion Academic Programme for the UK; EPSRC grant: EP/G062153/1

200 kW air-fired coal flame
Experimental Data
Optimum Secondary : Tertiary Partitioning Position
Experimental Data

NO injection - Primary Air

- NOx reported as NO2, mg/MJ
- NO* injected in Primary, mg/MJ

- 39 mm split (Theoretical expected NO)
- 39 mm split (Sec45: Ter 55) - Residual of injected NOx in flue
- 39 mm split (Sec45: Ter 55) - NOx Coal baseline

NO destruction ~ 98%

*reported as NO2
Experimental Data

NO injection- All Air streams

- 39 mm split (Theoretical expected NO)
- 39 mm split (Sec45: Ter 55)- NOx Coal baseline
- 39 mm split (Sec45: Ter 55)- Residual of injected NOx in flue

NO* injection- All Air streams

NO destruction ~ 80-82 %

*reported as NO₂
NOx vs Carbon burnout
Oxy 28%

Diamond: Carbon burnout
- NOx

Low ash El-Cerrejon Coal ~1.4%

NOx reported as NO₂, mg/MJ

Carbon burnout, %

Secondary - Tertiary Partitioning Position, mm
Experimental Data
NO injection- Oxy 28%

- 39 mm split (Theoretical expected NO)
- 39mm split (Sec 45: Ter 55)-NOx coal baseline
- 39 mm split (Sec45: Ter 55)- Residual of injected NOx in flue

SRF* NO destruction ~ 75- 85 %

* simulated recycle flue gas
** reported as NO₂
Experimental Data
NO injection- Oxy 28% in all streams

- 39 mm split (Theoretical expected NO)
- 39 mm split (Sec 45: Ter 55)- NOx coal baseline
- 39 mm split (Sec 45: Ter 55)- Residual of injected NOx in flue

SRF* NO destruction ~ 79-82%

* simulated recycle flue gas
** reported as NO₂
Experimental Data
Comparison Air – Oxy 28%

* reported as NO₂
## Computational modelling

### Commercial Software: ANSYS Fluent v15.0

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<td>NOx modelling</td>
<td>ANSYS model for NOx formation, including thermal, prompt, char and reburning rates</td>
</tr>
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</table>


$^2$ Porter, R. Theoretical modelling and design tools for oxy-coal combustion technology PhD thesis School of Process, Environmental and Materials Engineering, University of Leeds 2011
NOx model

NOx reburning rate significant for recycle

\[ \text{Volatile N} \rightarrow \text{HCN} \rightarrow \text{NO} \\]

\[ \text{Char N} \rightarrow \text{N}_2 \rightarrow 1 - \alpha \]

\[ \text{Volatile N} + \alpha \text{Ch}_{i} + \text{NO} \rightarrow \text{HCN} \]

\[ \text{HCN} + \text{O}_2 \rightarrow \text{NO} \]

\[ \text{Char N} + \text{NO} \rightarrow \text{N}_2 \]
Reburn mechanism

\[ R_4 = (k_a \chi_1 + k_b \chi_1^2)[CH_i][NO] \]
\[ R_5 = k_c \chi_1^2 \chi_2[CH_i][NO] \]

where \( \chi_1 = \frac{[H]}{[H_2]} \), \( \chi_2 = \frac{[OH]}{[H_2O]} \)

\[ \frac{d[HCN]}{dt} = 4 \times 10^{-4}R_4 \]
\[ \frac{d[NO]}{dt} = -4 \times 10^{-4}(R_4 + R_5) \]
In flame major species Air

- Measured CO2
- Predicted CO2
- Measured O2
- Predicted O2

Dry volume %

Radial distance (m)
Radial in flame NOx Air

- NOx measurements
- No reburning
- CH4 analogue
- CH2 analogue
Axial NOx Air

- NOx measurements
- No reburning
- CH4 analogue
- CH2 analogue

Dry ppm by volume vs. Distance from furnace ceiling (m)
Radial in flame NOx
Air + NO

- NOx measurements
- No reburning
- CH4 analogue
- CH2 analogue
Axial in flame NOx
Air + NO

- NOx measurements
- No reburning
- CH4 analogue
- CH2 analogue

Dry ppm by volume

Distance from furnace ceiling (m)
NOx contours
Air

NOx dry ppmv

0 100 200 300 400 500 600 700 800 900 1000

No reburn  CH₂ reburn  CH₄ reburn
NOx contours
Air + NO

No reburn  CH₂ reburn  CH₄ reburn
Summary / Future Work

• Measurements and CFD of NOx concentrations compared
  • Baseline measurements and with NO injection
  • Simulated recycled flue gas NO destruction of about 80-85% was achieved for Oxy 28% case.

• Different reburning analogues evaluated
  • Good agreement in developed regions for CH₂
  • Further development of advanced turbulence/combustion models required

• Work in Progress
  • NO destruction for Oxy 25, 31% ; 2D flame imaging; In-flame and axial measurements
Acknowledgements

• The project investigators would like to acknowledge the financial support of the UK CCSRC to the project.

• The in-kind supports of the industrial partners are also greatly appreciated by the project investigators.
Thank you
Extra Slides
Experimental Data
Flue gas measurement

** reported as NO₂

![Graph showing NOx measured (Air) vs. NO* injected in all streams, mg/MJ](image)

NOx measured (Air) — NOx measured (Oxy 28%)

** reported as NO₂
Fuel composition - Coal (sub-bituminous coal)

**Fuel:**

<table>
<thead>
<tr>
<th>Component</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>NCV</td>
<td>29.57 MJ/kg</td>
</tr>
<tr>
<td>Q</td>
<td>200 kW</td>
</tr>
<tr>
<td>Coal</td>
<td>24.3 kg/hr</td>
</tr>
</tbody>
</table>

**Stoichiometric O2 requirement**

<table>
<thead>
<tr>
<th>Element</th>
<th>wt% (ar)</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>73.67</td>
</tr>
<tr>
<td>H</td>
<td>5.04</td>
</tr>
<tr>
<td>O</td>
<td>11.31</td>
</tr>
<tr>
<td>N</td>
<td>2.48</td>
</tr>
<tr>
<td>S</td>
<td>0.38</td>
</tr>
<tr>
<td>Ash</td>
<td>1.31</td>
</tr>
<tr>
<td>Moisture</td>
<td>5.81</td>
</tr>
</tbody>
</table>

**Exit conc.**

- CO₂ = 95%, 45 mg/MJ
- CO = <15 ppmv
- O₂ = 3.8-4.0%

**Inflame measurement**

- Outer recirculation zone
  - CO = 50-1000 ppmv
- Inner core flame zone
  - CO = 4000-60,000 ppmv

**Tert. O₂**

<table>
<thead>
<tr>
<th>Component</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>O₂</td>
<td>30.0 vol%</td>
</tr>
<tr>
<td>CO₂</td>
<td>9.5 kg/hr</td>
</tr>
<tr>
<td>O₂+CO₂</td>
<td>52.0 kg/hr</td>
</tr>
<tr>
<td>O₂</td>
<td>61.4 wt%</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Component</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tert. O₂</td>
<td>56.7 kg/hr</td>
</tr>
<tr>
<td>Tert. CO₂</td>
<td>182.0 kg/hr</td>
</tr>
<tr>
<td>Tert. O₂+CO₂</td>
<td>238.7 kg/hr</td>
</tr>
<tr>
<td>Tert. O₂</td>
<td>23.76 wt%</td>
</tr>
</tbody>
</table>
Coal nitrogen Routes

(1) Fuel mechanism
(2) Reburning mechanism
(3) Char surface NO reduction
(4) Prompt mechanism
(5) Thermal mechanism
(6) NO – HCN reduction
(7) HCN oxidation
• 500 ppmv = 350 mg/MJ injected in all air streams for radial profile measurements
• 0-1000 ppmv was injected for Oxy 28% simulated recycle cases
• Typical ppmv: mg/MJ ratio is 1:1.5
• Typical mg/MJ to mg/Nm3 ratio is 0.75:1
Char-Nitrogen: NO conversion
Temperature, oxygen, char mass

Fig. 11. Net NO formation selectivity from char combustion in a fixed bed as a function of initial char mass for a pulverized (10–20 μm) bituminous coal char [217].

- Glarborg et al., Fuel nitrogen conversion in solid fuel fired systems, Progress in Energy and Combustion Science 2003

- The NO conversion decrease as the char mass (and so the char surface available for heterogeneous reaction) increase, due to the NO-surface reduction

Fig. 2. Net NO formation selectivity from char combustion as a function of burned char mass. Experimental data are shown as points and the lines are two model fits (reactor set-point temperatures: 850, 1050 and 1150 °C; steady-state O2 concentrations: 10%, gas flow: 1 L/min (at 20 °C and 1 atm)).

Fig. 3. Effect of nominal (steady-state) O2 concentration on net char-N to NO conversion from bituminous char combustion at low char masses. A steady-state O2 concentration of 10% corresponds to an average O2 concentration during combustion of 4%, and a steady-state concentration of 1% to 0.2%.
Reburning

\[ NO + CH_i = HCN + \text{products} \]

- **Instantaneous Approach**

\[
\frac{d[NO]}{dt} = -k_1[NO][CH] - k_2[NO][CH_2] - k_3[NO][CH_3]
\]

\( k_1, k_2, k_3 \) from Arrhenius

\[
S_{NO,reb} = M_{W,NO} \frac{d[NO]}{dt}
\]

Possible just with detailed kinetic scheme, with global scheme the real values of radical concentrations are unknown.

- **Partial-equilibrium approach**

\[
\frac{d[NO]}{dt} = 4 \times 10^{-4} (R_1 + R_2)
\]

\[ R_1 = (k_a \epsilon_1 + k_b \epsilon_1^2) [CH_4][NO] \]

\[ R_2 = (k_c \epsilon_1^3 \epsilon_2) [CH_4][NO] \]

Where \( k_a, k_b, k_c \) are Arrhenius type kinetic constants:

\[ k_i = A_i T^b \exp \left( -\frac{E_a}{RT} \right) \]

with different values of \( A, b, E_a \) for different species of \( CH_i \)

and the values of \( \epsilon_i \):

\[ \epsilon_1 = \frac{[H_1]}{[H_2]} = 1 \quad \text{and} \quad \epsilon_2 = \frac{[OH]}{[H_2O]} = \frac{k_{dr}}{k_{df}} \text{ from the reaction:} \]

\[ OH \cdot +H_2 = H_2O + H \cdot \]