Evaluation of Global Reaction Mechanisms for CFD Modelling of Oxy-Fuel Combustion

Fredrik Normann

Chalmers University of Technology
Background

**Purpose**
To obtain information for development of commercial oxy-fuel boilers

**Progress of work**
- Chalmers 100 kW oxy-fuel unit
- Oxy-CFB combustion
- Series of experimental and modelling studies

**Content of work**
- Combustion issues
- Emissions ($\text{NO}_x$ and $\text{SO}_x$)
- Heat transfer

**Present presentation**
Evaluation of reduced reaction mechanisms for CH oxidation in CFD simulations

Fredrik Normann
Computational Fluid Dynamics

Complex Geometries
Complex Turbulent Flames
Simplified reaction mechanisms
Limited generalizability
Applicability to oxy-fuel combustion with high CO₂ concentration?

Source: www.hightech.fi

Fredrik Normann
Global Reaction Mechanisms

<table>
<thead>
<tr>
<th>Fuel Oxidation</th>
<th>Intermediates Oxidation</th>
<th>Radical Formation</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_3H_8 + 1.5 O_2 \rightarrow 3 CO + 4 H_2$</td>
<td>$H_2 + 0.5 O_2 \leftrightarrow H_2O$</td>
<td>$O_2 \leftrightarrow 2O$</td>
</tr>
<tr>
<td>$C_3H_8 + 3 H_2O \rightarrow 3 CO + 7 H_2$</td>
<td>$CO + H_2O \leftrightarrow CO_2 + H_2$</td>
<td>$H_2O \leftrightarrow H + OH$</td>
</tr>
</tbody>
</table>

### JL

<table>
<thead>
<tr>
<th>Air</th>
<th>Oxy-fuel</th>
</tr>
</thead>
<tbody>
<tr>
<td>3-step</td>
<td>4-step</td>
</tr>
<tr>
<td>x</td>
<td>x</td>
</tr>
<tr>
<td>x</td>
<td>x</td>
</tr>
<tr>
<td>x</td>
<td>x</td>
</tr>
<tr>
<td>x</td>
<td>x</td>
</tr>
</tbody>
</table>

References:
- Jones & Lindstedt, 1988
- Leiser et al, 2007
- Glarborg et al, 2009
- Frassoldati et al, 2009

Fredrik Normann
Mapping of 100 kW Oxy-Propane Flame

Fredrik Normann
Temperature Measurements

- Contour map created entirely from measurement data
- Six measurement positions
- Temperature and Concentration Profiles

Fredrik Normann
3D CFD Model

- Sub-models:
  - k-ε Realizable turbulence model
  - Eddy Dissipation Concept
  - Discrete Ordinates model with a WSGG model for oxy-fuel conditions (grey)

- Flame shape
  - JL predicts a wider and shorter flame than the oxy-fuel derived mechanisms

- Concentration of CO
  - JL and 3-step yield the predictions which are most in line with measured data
Generation of 1D-Model

- Traced a “particle” from the fuel inlet throughout the furnace
- Recorded O$_2$ concentration and temperature

Fredrik Normann
Comparison – CO concentration

- The propane-fired Chalmers 100 kW OF27 flame
- Includes comparison with a detailed scheme
- Path-line data from CFD calculations is used in the PFR model
  - Temperature
  - O₂ concentration
- Large discrepancies between the global models.
Comparison - Reaction Dynamics

Fuel Oxidation

\[ C_3H_8 + 1.5 O_2 \rightarrow 3 CO + 4 H_2 \]

CO Oxidation

\[ CO + 0.5 O_2 \leftrightarrow CO_2 \]
\[ CO + H_2O \leftrightarrow CO_2 + H_2 \]

Fredrik Normann
Conclusion

• There is a significant improvement potential for global oxy-fuel reaction mechanisms and, thus, a need to develop a refined global reaction mechanism.

• Simply adjusting the reaction parameters to compensate for quantitative errors (such as over-predicted CO concentration or combustion temperature) may lead to errors in the reaction dynamics.

• A qualitatively incorrect behavior reduces the generic nature and applicability of the mechanism.

Fredrik Normann
Evaluation of Global Reaction Mechanisms for CFD Modelling of Oxy-Fuel Combustion

Fredrik Normann

Chalmers University of Technology