Characterization of Oxy-combustion Impacts in Existing Coal-fired Boilers

Project Kick-off Meeting
November 20-21, 2008
Salt Lake City, UT
US DOE CO₂ Emissions Control R&D Activities

• Post-Combustion CO₂ Control
  – Solvents
  – Sorbents
  – Membranes

• Oxy-Combustion CO₂ Control
  – PC Oxy-combustion
  – Chemical looping

• CO₂ Compression
NETL’s Oxy-combustion CO$_2$ Capture R&D Projects for **Existing Boilers**

<table>
<thead>
<tr>
<th>Performing Organization</th>
<th>Project Title</th>
<th>Research Pathway</th>
<th>Scale</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air Products and Chemicals</td>
<td>Flue Gas Purification Utilizing SOx/NOx Reactions During Compression of CO$_2$</td>
<td>Oxycombustion - Flue Gas Cleanup</td>
<td>Laboratory</td>
</tr>
<tr>
<td></td>
<td>Derived from Oxyfuel Combustion</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Praxair</td>
<td>Near-Zero Emissions Oxy-Combustion Flue Gas Purification</td>
<td>Oxycombustion - Flue Gas Cleanup</td>
<td>Laboratory</td>
</tr>
<tr>
<td>Alstom Power</td>
<td>Oxy-Combustion Boiler Development for Tangential Firing</td>
<td>Oxycombustion Boiler Development</td>
<td>Pilot</td>
</tr>
<tr>
<td>Foster Wheeler</td>
<td>Oxy-Combustion Boiler Material Development</td>
<td>Oxycombustion Boiler Development</td>
<td>Laboratory</td>
</tr>
<tr>
<td>Reaction Engineering International</td>
<td>Characterization and Prediction of Oxy-combustion Impacts in Existing Coal-fired Boilers</td>
<td>Oxycombustion Boiler Development</td>
<td>Multi</td>
</tr>
</tbody>
</table>

* 5 of 15 new project selections announced July 31, 2008.*
Oxy-combustion Retrofit Design Issues

- Flue gas recycle composition
- FGR ratio
- Coal, O$_2$, and FGR injection location
- Boiler impacts
Retrofit Impacts

FGR and oxy-firing design affect:

• Flame characteristics
  – Ignition, char burnout
  – Heat transfer (temperature, emissivity, sooting)
  – NOx, SOx, fine particulates

• Surface characteristics
  – Slagging
  – Fouling
  – Waterwall corrosion
Data/Tools Needed for Characterization

- Fundamental Data from experiments
- Validated Mechanisms to describe oxy-combustion processes
- Simulation Tools to evaluate full-scale retrofit designs
REI’s DOE Program Overview

- **Objective:** Characterize and predict performance and operational impacts of oxy-combustion retrofit designs on existing coal-fired boilers

- Utilize multi-scale testing and theoretical investigations to develop:
  - **Fundamental data** that describe flame characteristics, waterwall corrosion, and ash properties (slagging, fouling) in oxy-firing
  - **Validated mechanisms** that describe oxy-combustion processes
  - **Firing system principles** (oxy-burner design, flue-gas recycle)

- Incorporate validated mechanisms into **CFD models**; evaluate full-scale oxy-retrofit designs
# REI Team

<table>
<thead>
<tr>
<th>Team Member</th>
<th>Project Role</th>
</tr>
</thead>
<tbody>
<tr>
<td>REI</td>
<td><em>program management, testing oversight, mechanism development, simulations</em></td>
</tr>
<tr>
<td>University of Utah</td>
<td><em>laboratory and pilot-scale testing, mechanism development</em></td>
</tr>
<tr>
<td>Siemens/ABT</td>
<td><em>burner technology</em></td>
</tr>
<tr>
<td>Praxair</td>
<td><em>oxygen and CO\textsubscript{2} supply</em></td>
</tr>
<tr>
<td>Brigham Young Univ.</td>
<td><em>soot measurements</em></td>
</tr>
<tr>
<td>Corrosion Management</td>
<td><em>corrosion tests, mechanism development</em></td>
</tr>
<tr>
<td>Sandia National Labs</td>
<td><em>bench-scale testing, mechanism development</em></td>
</tr>
<tr>
<td>Vattenfall AB</td>
<td><em>mechanism development, validation data</em></td>
</tr>
<tr>
<td>PacifiCorp, Praxair, Southern Company, Vattenfall</td>
<td><em>Advisory Panel provides industrial perspective on R&amp;D needs, retrofit requirements and constraints, suggested assessment studies</em></td>
</tr>
</tbody>
</table>
Development of Fundamental Data
Multi-scale Experiments

- **100 kW Oxy-Fuel Combustor (OFC) Tests**
  - Ash Characterization and Deposition
  - Soot Evolution
- **1.2 MW Pilot-Scale Furnace (L1500) Tests**
  - Impacts of Burner Configuration
  - Heat Flux, Corrosion and Deposition
  - Flue Gas Chemistry
- **Bench-Scale Optical Entrained Flow Reactor**
  - Char Oxidation Kinetics
100 kW Oxy-Fuel Combustor (OFC)

Unique OFC Capabilities:
- CO$_2$ from tank or FGR
- Optional particulate control
- Optional SO$_2$ control
- Optional condensation
- Variable FGR temperature
100 kW Oxy-Fuel Combustor (OFC) Experiments

Experiments

Ash Characterization and Deposition

Soot Evolution

Measurements

Low-Pressure Impactor Collection

Computer Controlled Scanning Electron Microscope (CCSEM) particle composition analysis

Scanning Mobility Particle Sizer (SMPS)

Two-Color Extinction Method

Data will be tailored for mechanism development and validation
1.2 MW Pilot-Scale Furnace (L1500)

Unique L1500 Capabilities:
- Realistic Burner Turbulent Mixing Scale
- Realistic Radiative Conditions
- Realistic Time – Temperature Profiles

Air / FGR Train

Convective and Radiant Sections

Burner

Sampling Ports

Radiant Section

Convective Section

Reaction Engineering International
1.2 MW Pilot-Scale Furnace (L1500) Experiments

Experiments

- Fuel, Oxygen and FGR Mixing in Burner
- Corrosion, Radiation and Particle Deposition

Measurements

- Flame Stabilization Location
- Flue Gas Composition and Concentrations
- Unburned Carbon in Ash
- Temperature Profile
- Real-Time Corrosion Rate, Electrochemical Noise (ECN) Technology
- Heat Flux
- Deposition Rate
Bench-Scale Optical Entrained Flow Reactor Experiments

Unique Entrained Flow Reactor Capabilities:

- Temperature measurements of individual particles
- Rapid devolutilization under boiler relevant conditions
- Relevant gas temperatures and compositions

(Shaddix, 2007)
Bench-Scale Optical Entrained Flow Reactor

Experiments

Char Oxidation

Measurements

Particle Burnout (through collection and analysis)
Optical Sizing Pyrometry (particle size and temperature profile)
Formation and Validation of Mechanisms
Mechanism Development Overview

- Mechanism Exchange
- Slagging Mechanism Development
- Fouling Mechanism Development
- Corrosion Mechanism Development
- Char Oxidation Mechanism Development
- Soot Mechanism Development
- Mechanism Validation
Mechanism Exchange

- Mechanisms and sub-models for oxy-combustion (for CFD model integration) have been developed by several researchers, including Vattenfall AB, Chalmers University and University of Newcastle.

- These mechanisms will be reviewed in order to facilitate and guide mechanism development for this program.
Slagging Mechanism Development

Slagging (Deposition in Radiant Section)

Dependent on:
- Particle size and composition
- Surface and particle temperatures
- Radiation conditions
- Local oxygen concentration

Impacted by oxy-combustion conditions

New mechanism extended from REI’s current deposition mechanism, which tracks ash particle composition and size distribution.
Fouling Mechanism Development

Fouling (Deposition in Convective Section)

Dependent on:

- Gas-phase alkali sulfates concentration
- Particle and tube temperatures
- Particle size distribution
- Tube geometry and velocity field

Impacted by oxy-combustion conditions

New mechanism extended from REI’s current deposition mechanism, which tracks ash particle composition and size distribution

\[ \text{Dew Point} < T_{\text{gas}} < \text{Melting Point (1157 K)} \]

Becomes sticky and condenses

\[ \text{Na}_2\text{SO}_4 \]
Factors Important For Corrosion

- Temperature
  - Metal and gas temperature
  - Heat flux
  - Temperature gradient
  - Temperature fluctuations
- Fuel/Deposit Characteristics
  - Sulfur, chlorine, alkali metal
- Local Gas-Phase Stoichiometry
- Tube Metallurgy
  - Cr, Ni, Al, etc.
- Boiler Design & Operation
  - Tube spacing, tube location, etc.
  - Flue gas velocity

Modify and extend current REI corrosion mechanisms for:
- Chlorine attack
- H₂S gaseous attack
- FeS corrosion

Impacted by oxy-combustion conditions

Char Oxidation Mechanism Development

Current char oxidation model assumes reactions occur only at the surface (reaction limited). Data indicate that O₂ film diffusion may be limiting for oxy-combustion conditions (O₂ thru CO₂ slower than O₂ thru N₂), necessitating an improved model.

Surface Kinetics in Porous Particles (SKIPPY) modeling will be combined with measured data to suggest the form of the new mechanism.
Soot Mechanism Development

A mechanism for soot formation and radiation under oxy-combustion conditions will be developed based on REI’s existing soot model.

Soot formation (through cracking of tars in the coal volatiles) has been shown to be dependent on oxygen concentration in oxy-flames. The relative contribution of soot to flame emissivity, compared with CO$_2$ and H$_2$O, must be evaluated. The narrow band model Radcal will be used for this evaluation.
Mechanism Validation

• All mechanisms will be validated against data taken in the experimental program and against other available data
• Mechanisms will be implemented into CFD code Glacier
• Overall model will be validated against available pilot-scale and full-scale furnace data
Firing System Principles
Firing System Principles

• Determine firing system dependencies based on:
  – Theoretical calculations extending air-firing experience and oxy-firing properties
  – Pilot-scale testing
  – CFD modeling

• Sensitivities to be investigated include:
  – Composition and amount of flue gas recycle
  – Oxy-burner design

• Develop firing system principles and use them to guide full-scale firing system design
Assessment of Oxy-Combustion Retrofit
Assessment Groundwork

- Multi-scale Test Data
- Mechanism Development
- Firing System Principles
- Validated Mechanisms
- Assess Oxy-combustion Retrofit Using
  - Design Info
  - CFD
Assessment Approach

1) Select candidate boiler
   - Suggested/reviewed by Advisory Panel
   - Access to design and operational information
   - Feasible for oxy-retrofit

2) Simulate boiler under air-fired conditions

3) Determine oxy-firing retrofit design
   - Pilot-scale data and modeling
   - Firing system principles
   - Scale-up design

4) Simulate boiler under oxy-fired conditions
   - Use established code, Glacier, with validated sub-routines (mechanisms) for simulations
5) Optimize oxy-firing design

- Key performance metrics (compared to air-fired baseline):
  - Match heat duties in air-fired boiler
  - Minimize surface impacts (corrosion, slagging, fouling)
  - Maximize combustion efficiency
  - Minimize trace pollutant emissions

- Iterate on design to optimize firing system performance
  - Burner and/or firing system
  - Quantity and composition of flue gas recycle
  - Overfire air (OFA)
Program Status

- DOE prime contract awarded
- Sub-contracts being put in place
- Program scheduled for 3 years (10/08 – 9/11), subject to continued DOE funding
- November 2008 meeting with Vattenfall AB to review available data and state of mechanisms
- Program kick-off meeting Nov 20-21, 2008 at REI
- Intermediate and final results presented at DOE and other conferences
Acknowledgment

- **Acknowledgment:** *This material is based upon work supported by the Department of Energy under Award Number DE-NT0005288*

- **Disclaimer:** “This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.”