Modeling Furnaces in the Chemical Process Industry

Committed Individuals Solving Challenging Problems

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REI Profile

- Energy And Environmental Consulting Firm Specializing In:
  - Combustion System Design and Performance Analysis
  - Complex CFD Simulations
    - Performance
    - Emissions
    - Operational Impacts
  - Customized Software
  - Specialized Equipment
  - Proof-of-Concept Testing
- Strong Network of Experts

Objective: Solve Challenging Combustion Problems Using Specialist Talent & Technology
REI Modeling Strengths

- **Modeling and Analysis Expertise**
  - Combustion, Fuel Conversion & Pollutant Emissions
  - Unique, Proprietary Modeling Capabilities & Tools
    - Ability to develop and apply advanced chemistry to CFD and process modeling tools
  - “Qualified” Combustion Modelers
    - Understand physics, chemistry, mathematics, software
    - Industrial perspective
  - Experience
    - Over 200 Combustion Systems Modeled

- **Network of Consultants**
- **Objective Analyses**
## Selected Industrial Applications & Clients

### Applications
- Melting Furnaces
- Reheat Furnaces
- Blast Furnace Injection
- Flash Smelters
- Cement Kilns
- Phosphate Kilns
- CO Boilers
- Sulfur Recovery Units
- Process Heaters
- Cracking Furnaces
- Incinerators
- Thermal Oxidizers
- Burners
- Enclosed Flares

### Selected Clients
- Bayer
- BHP
- BP
- Cadence
- Callidus
- Chemtrade
- Chevron
- China Steel
- Cominco
- ConocoPhillips
- CPC
- CPChem
- Dow
- Hexcel
- Holnam
- Huntsman Chemicals
- INCO
- Inland Steel
- John Zink
- LaFarge
- Lone Star
- Monsanto
- NOVA Chemicals
- PCA
- Persee Chemical
- Philip Morris
- Praxair
- Searles Valley Minerals
- Technip
- Solena
- Solutia
- SunCoke
- SunCoke
- Thai Olefins
Chemical Process Applications

**Systems**
- Process Heaters
- Cracking Furnaces
- Thermal Oxidizers
- Incinerators
- Burners
- Flares

**Applications**
- Pollutant Emissions (NOx, CO)
- Waste Stream Disposal
- Tube Overheating
- Heat Flux & COT Uniformity
- Process Yield & Conversion
- Radiant Efficiency
Why Use CFD Modeling?

Modeling is a cost effective approach for evaluating system performance, pollutant emissions, and operational impacts

- Improve understanding
- Estimate performance
- Provide conceptual designs
- Identify operational problems
- Cheaper than testing
- More information than testing
- Does NOT make decisions for engineers, but does help them be more informed
REI’s Proprietary CFD Software

- **BANFF & GLACIER**
  - 20+ years development and application
  - Targeted to gas, oil and coal-fired utility boilers

- **ADAPT**
  - ~10 years development and application
  - Improved geometry resolution (adaptive mesh refinement)
  - Advanced chemistry
  - Improved turbulence-chemistry interaction
  - Targeted to gas-fired ultra low-NOx systems and premixed combustion
Chemical Furnace Modeling Challenges

- **Scales!**
  - Geometric resolution
  - Jet velocities
  - Chemistry vs turbulent mixing

- **Input accuracy**
  - Garbage-in garbage out

- **Trade-off between accuracy and turn-around time**
  - What are most critical factors for problem of interest

![Diagram of time scales: Slow time scale, Intermediate time scale, Fast time scales, "equilibrium chemistry"]

- **Chemical Time Scale**
  - $10^{-6}$ s
  - $10^{-4}$ s
  - $10^{-2}$ s
  - $10^{0}$ s

- **Physical Time Scale**
  - Time scales of flow, transport, turbulence
  - millimeter
  - meter
  - tens of meters
Furnace Model Requirements

- Accurately represent furnace geometry and operation

- Sub-models for:
  - Turbulent fluid mechanics
  - Combustion chemistry
  - Turbulence-chemistry interactions
  - Finite-rate kinetics for ppm-level NOx, CO
  - Surface properties
  - Gas-wall-tube heat transfer (conduction, convection, radiation)
  - Process chemistry

- Computationally efficiency (parallel execution)
Modeling Approach

- REI currently uses advanced *ADAPT* CFD software for process heaters/cracking furnaces
- Accurate modeling provides accurate flame shape, flow patterns, temperature profiles, major species profiles, heat transfer/heat flux profiles, tube temperatures, process fluid heat absorption
- Provides capability to analyze:
  - New generation ultra-low NOx burners for new furnaces and revamps
  - Burner spacing, distribution and burner-burner interactions
  - Lower emissions (CO and NOx)
  - Impacts of fuel changes
  - Non-uniform heat flux profiles and surface temperatures
  - Sources and fixes for process or convective tube overheating
  - Test furnace to full-scale furnace scale-up
Sample Uses of Modeling

- Improved Performance
  - Enhance furnace efficiency
  - Lower emissions
  - Study particulate behavior during de-coking process

- Reduce risk of new technology
  - Evaluate burner designs and spacing for new furnaces
  - Compare different burner designs for furnace revamps
  - Assess impacts of fuel changes
  - Evaluate coating impacts
  - Scale burner performance from test furnace to full-scale furnaces

- Troubleshooting
  - Identify causes and fixes for process or convective tube overheating
  - Identify source of heat flux non-uniformities
Pyrolysis Furnaces
Example - Retrofit Burner Evaluation

Full-Scale Pyrolysis Furnace

- Objectives
  - Improve flame quality
  - Maintain low NO\textsubscript{x} emissions
- Compare retrofit burners
  - Flame quality (no rollover)
  - Low NO\textsubscript{x} and CO emissions
  - Heat flux profile
- Use \(\frac{1}{4}\)-furnace model
  - Capture burner-burner interaction
  - Capture tube heat flux profiles
  - Maximize burner resolution
Retrofit Burner Evaluation

Isosurfaces of 5000 ppm CO

- Original burner: Excess fuel between burners
- Option 1: Propensity for flame rollover
- Option 2: Limited heat flux distribution
- Option 3: Good combination of flame quality and heat distribution
Retrofit Burner Evaluation

$NO_x$ Profiles

- Option 3 improved flame quality and slightly lowered $NO_x$ emissions
Example – New Furnace

- Identified improved burners for new ethylene cracking furnace, helped adjust heat flux design basis
Example – New Burner

- Evaluated new ultra low-NOx burner performance, helped guide burner spacing and port placement
Example – Burner Retrofit

- Evaluated different burner designs to determine best flux profile and NO emissions for furnace retrofit
Example – Fuel Change

- Evaluated performance of back-up fuel with new burners
Industrial Furnaces
CO Boiler

- Simulation of a CO boiler with process tubes for heating crude oil. CO plenum was simulated to predict the mixing of injection air into the CO plenum to account for impacts of non-uniform air and CO mixing.
CO Boiler

- Simulation of CO oxidation and NOx formation in a CO boiler to assess flue gas properties in the boiler that would impact SNCR design.
CO Boiler

- Simulation of flue gas flow, gas temperature, CO, and NOx distributions in approximately 10 different waste-heat recovery CO boilers augmented by natural gas combustion for assessment of SNCR for NOx control.
Refinery Process Heater

- Simulation of a refinery process furnace for evaluation of impacts of modifications of process tube arrangement to mitigate tube overheating.
Spent Acid Furnace

- Simulation of a spent acid furnace fired by fuel oil. Modeling used to verify adequate fuel burnout and aqueous spent acid vaporization achieved with limited droplet impaction on walls.
Simulation of an absorber off-gas oxidizer. Simulations were conducted in order to optimize burnout of the waste gas while minimizing NOx formation.
Detailed Example – Xylene Reboiler

- Xylene Splitter Reboiler (XSR)
- 52.5 MMBtu/hr Firing Rate
- 95/5% Oil/Gas
- 20% Excess Air
- 4 Process Tubes

- Radiant Tubes Hottest At 1/3 Height (why?)
- Bridgewall Temperatures Too Hot (measurement system reliable?)
- Convective Tube Localized Overheating (how to fix?)
Flow and Temperature Patterns

- Recirculating Flow Field
- Long Flames Mix Slowly
- CO & O₂ Have Similar Profiles
- Flames Highly Emissive
Temperature Profiles

Radial Gas Temperature Profiles

Profile Impacts:

- Flame Emission
- Tube Heat Flux & Temperatures
- Bridgewall Temperatures
- Convective Tube Temperatures
Flame Emission

- Emission Dependent on Temperature & Emissivity
- Peak Flame Emission ~1/3 Up Furnace
- Peak Incident & Net Flux at Same Height (~1/3 up)
- Peak Temp at Same Height; Location Agrees With Hot Tube Observation
Radiant Section Tube Heat Flux Profiles

- Flux peak 2/3 down tube
- Flux peak 1/3 up tube
- Top crossover
- Bottom crossover

High Flux Locations Correlate with Hot Tube Temperatures
Bridgewall Temperatures

Temperature Contours

- Probe Measures “Max” Temperature Entering Convective Section
- Hot Gas → Hot Tubes
- Gradient Impacts Measurement & Control of Temperature
Convective Section

- Tube Has 2 Passes in Each of 9 Rows
- Upper 6 Rows Have Fins, Lowest 3 Rows Are Bare
- Radiant Load Highest at Lowest Tubes
- Tube 12 Overheating

Finned Tubes

- Hotter high velocity flue gas due to more open flow area

Bare Tubes

 Tube D

2  1
3  4
6  5
7  8
10 9
11 12
14 13
15 16
18 17
Observation - Net Flux Changes w/ Finned Tubes
Convective Section Tube Temperature Profile

High Tube Temperatures Correlate w/ High Net Fluxes
Recommended Modification

- Reduce Row 4 Fins
- Add Row 3 Fins
- Evens Out Net Flux & Tube Skin Temperatures
XSR Modeling Conclusions

- Modeling Useful For Furnace Evaluation
  - Recirculating Flow with Long, Highly Emissive Flames
  - Radiant Furnace Tube Temperatures Reflect Flame Emission & Match Observation
  - Long Flames Create Gradients at Bridgewall

- Modeling Useful For Furnace Troubleshooting
  - Temperature Gradient at Bridgewall Impacts Measurements & Control
  - Convective Tube Temperatures Reflect Net Flux Change with Finned Tubes
  - Design Modification Identified to Minimize Convective Tube Hot Spots
Reaction Engineering International

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