# 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
- Thai Olefins

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### **Chemical Process Applications**

#### <u>Systems</u>

- 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 turbulencechemistry 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



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## **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**



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## **Example - Retrofit Burner Evaluation**

Full-Scale Pyrolysis Furnace

#### Objectives

- » Improve flame quality
- » Maintain low NO<sub>x</sub> emissions
- Compare retrofit burners
  - » Flame quality (no rollover)
  - » Low NO<sub>x</sub> and CO emissions
  - » Heat flux profile
- Use 1/4-furnace model
  - » Capture burner-burner interaction
  - » Capture tube heat flux profiles
  - » Maximize burner resolution





## **Retrofit Burner Evaluation**

#### Isosurfaces of 5000 ppm CO



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## **Retrofit Burner Evaluation**

*NO<sub>x</sub> Profiles* 



Option 3 improved flame quality and slightly lowered NO<sub>x</sub> emissions



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#### **Example – New Furnace**

 Identified improved burners for new ethylene cracking furnace, helped adjust heat flux design basis





**Incident Flux** 



#### **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



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## **Example – Fuel Change**

• Evaluated performance of back-up fuel with new burners



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#### **Industrial Furnaces**



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#### **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





#### **Thermal Oxidizer**

• 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 & O<sub>2</sub> 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





## **Radiant Section Tube Heat Flux Profiles**

#### Flux peak 2/3 down tube 16000-16000 Flux peak 1/3 up tube 14000-14000 Incident Flux (BTU/hr/ft<sup>2</sup> 12000-12000<sub>4</sub> 10000 10000 8000 8000 Flux 6000 6000-**Top crossover** Net 4000 4000-**Bottom crossover** 2000 2000-Qinc D Qnet D 0 0 50 0 100 150 200 250 300 350 400 450 Distance Along Tube (ft)

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

**Probe Location** 



## **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



### **Convective Section Tube Heat Flux Profiles**



**Observation - Net Flux Changes w/ Finned Tubes** 

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#### **Convective Section Tube Temperature Profile**



**High Tube Temperatures Correlate w/ High Net Fluxes** 



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#### **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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