2004 ACERC Conference

Use of Modeling to Solve Industrial Combustion Problems

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Reaction Engineering International

"Committed Individuals Solving Challenging Problems"

Why Use Combustion Modeling?

Modeling is a cost effective approach for evaluating combustion performance, operational impacts & emissions

- **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**

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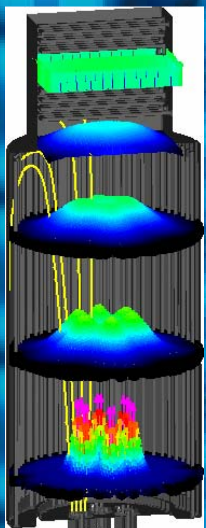
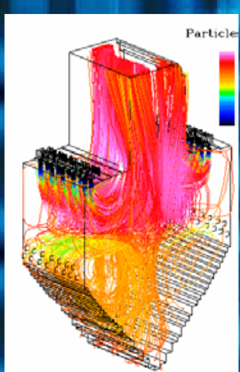
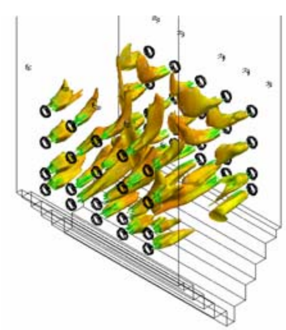
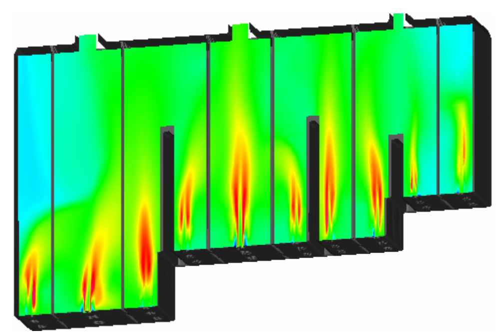
Key Elements to Successful Combustion Modeling

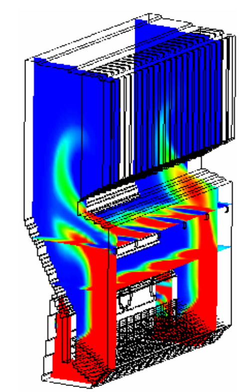
- REI has modeled ~150 combustion systems, focusing on performance and emissions
- Experience suggests successful applications involve:
  - Guiding application of modeling tools with physical insight and experience
  - Interacting with customer to ensure problem understanding and solution applicability
  - Maintaining combustion expertise in modeling tools and engineers









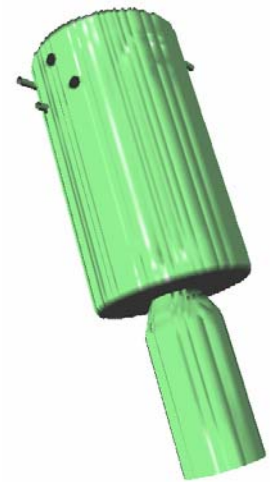


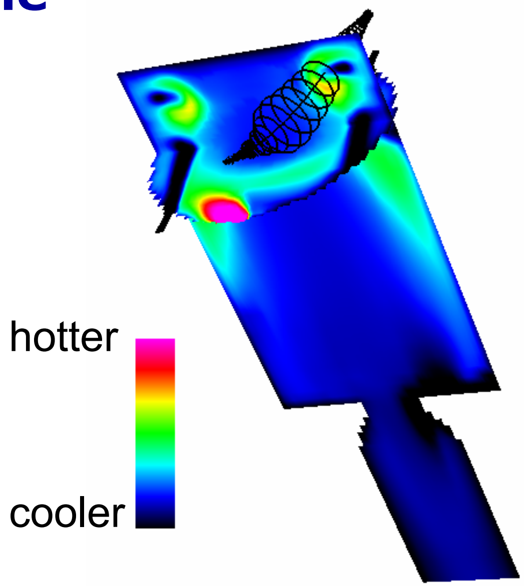
Problem Solving Examples

- **Copper Smelting Cyclone Operation**
- **NOx Reduction in Cyclone-fired Boilers**
- **Chemical Weapons Incineration**

Cyclone Smelter Example

- Grass Roots Design Cyclone Copper Smelter
  - Tangentially-fed concentrate heated by oxy-fuel burners & reactions
  - Hot, partially oxidized concentrate deposits on cyclone walls, melts, and runs out bottom of cyclone
- Operational Problems
  - Accretion buildup
  - Dust carryover
  - Surface damage
- Unacceptable Capacity and Availability

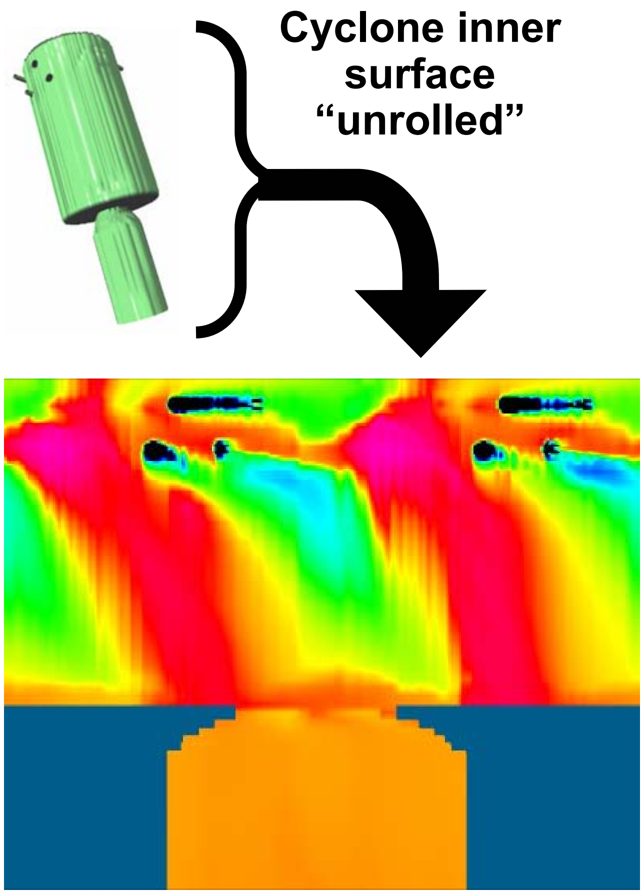




Analysis Approach

- Work with smelter personnel to understand problems and potential solutions
- Use CFD model of cyclone to analyze:
  - Cyclone flow patterns & gas properties
  - Concentrate transport, heating & reactions
  - Concentrate deposition rates & properties
  - Oxy-fuel burner performance
  - Cyclone surface properties
  - Exit gas properties & concentrate carryover
- Use analysis results to develop alternative cyclone designs & operating conditions
- Evaluate potential changes with model

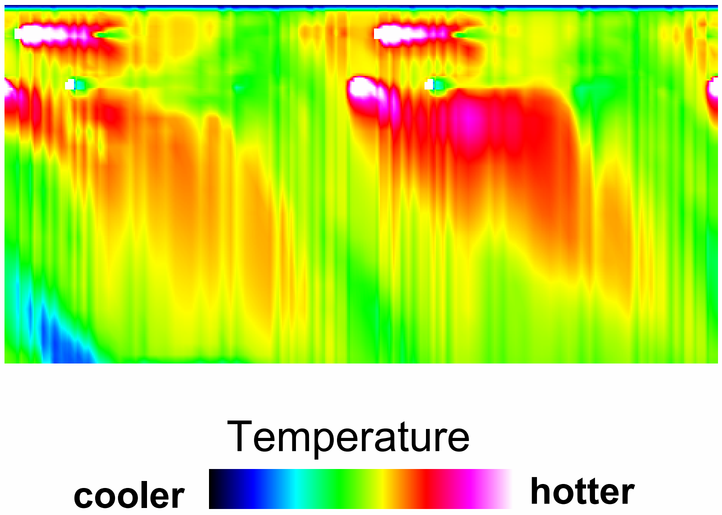
Accretion Build-up

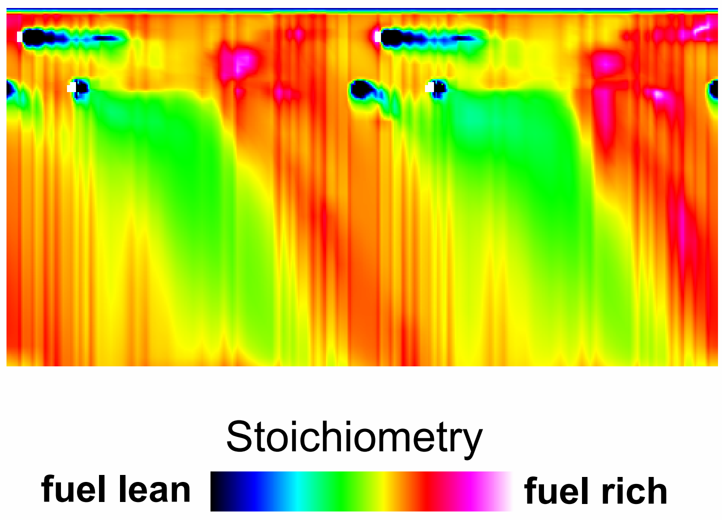


SO_2 Concentration

- Accretions controlled by
  - Deposit rheology
  - Deposition rate
- Rheology dependent on
  - Temperature
  - Composition
- Properties dependent on
  - Reaction rates
  - Heat transfer
  - Residence time
- Model with deposition rates and particle and gas properties

Surface Damage



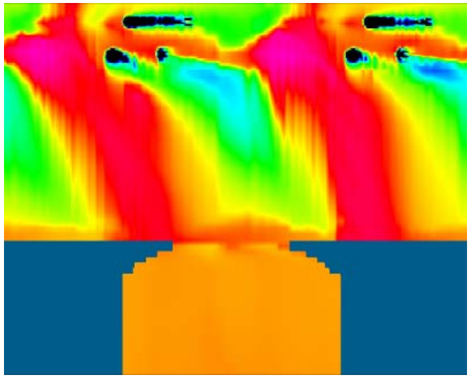


- **Surface damage from warpage and material loss**
- **Caused by**
  - **Erosion (near throat)**
  - **Acid attack (condensation)**
  - **Local hot spots**
- **Model with mass flux, stoichiometry, and gas temperature**

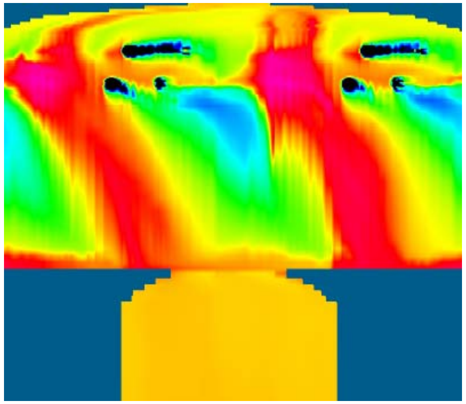
Analysis Conclusions

- **Original Design Produces**
  - **Non-uniform concentrate reactions, temperatures, and deposition patterns**
  - **Poor burner fuel-air mixing leading to long flames**
- **Recommended Changes**
  - **Change cyclone geometry**
  - **Modify concentrate carrier gas composition**
  - **Adjust burner properties**

Flat Top



Cylindrical Top



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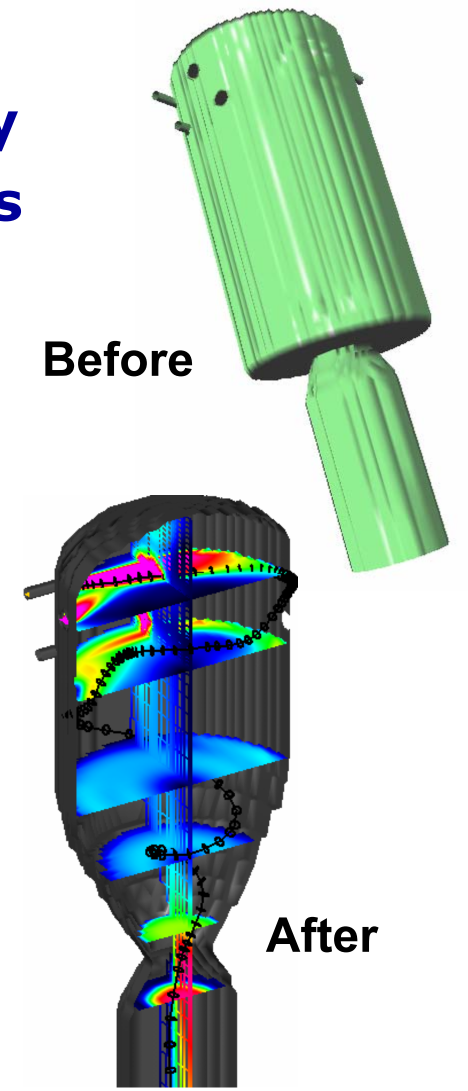
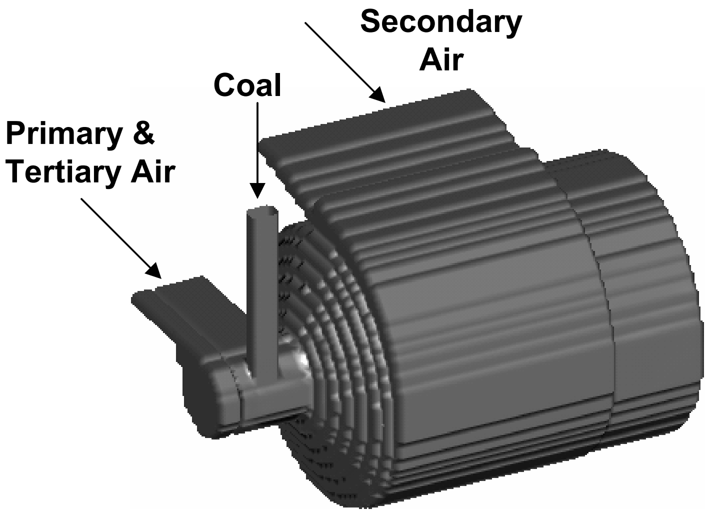
Modification Impacts

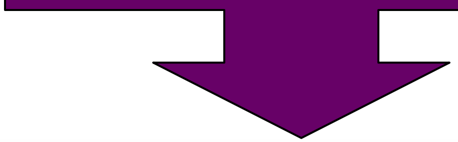
- Oxygen addition to carrier gas improved conversion uniformity
- Improved concentrate reactions minimized accretion buildup & stabilized matte quality
- Modified shaft geometry improved deposition patterns, reduced carryover ~5x
- Improved burner mixing reduced hot spots & enhanced concentrate reactions
- Capacity increased from 50% to 120%
- Availability increased from days/weeks to months



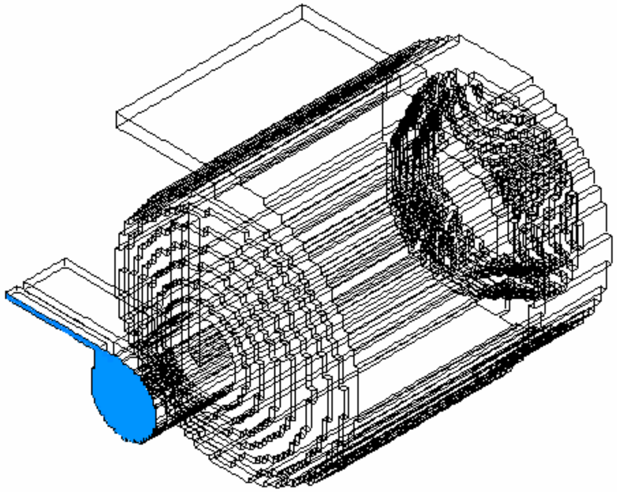
Cyclone-Fired Boiler Example



Industry Expectation: Turbulent mixing makes flow & species homogeneous

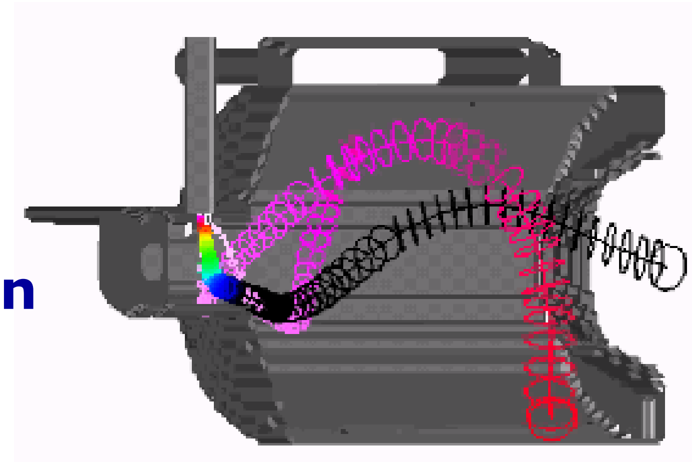


- Identify low cost NOx control strategies
- Key Processes:
  - Particle dispersion, deposition & reaction
  - Turbulent mixing & chemical reaction
  - NOx formation



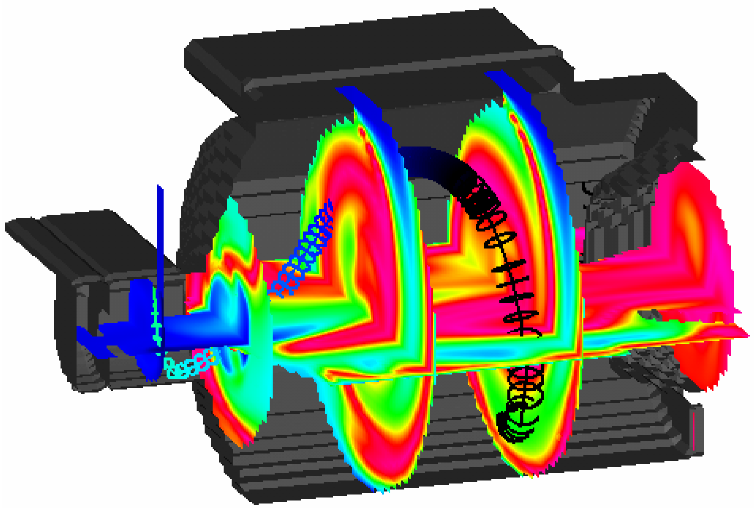
Barrel Summary

- Flow very stratified
- Only smallest particles burn in suspension
- Ignition front depends on fines, tertiary air & front tube deposition
- Very fuel rich regions near walls
- Barrel modifications have minimal impact on NOx



Particle Burnout & Deposition

Gas Temperature



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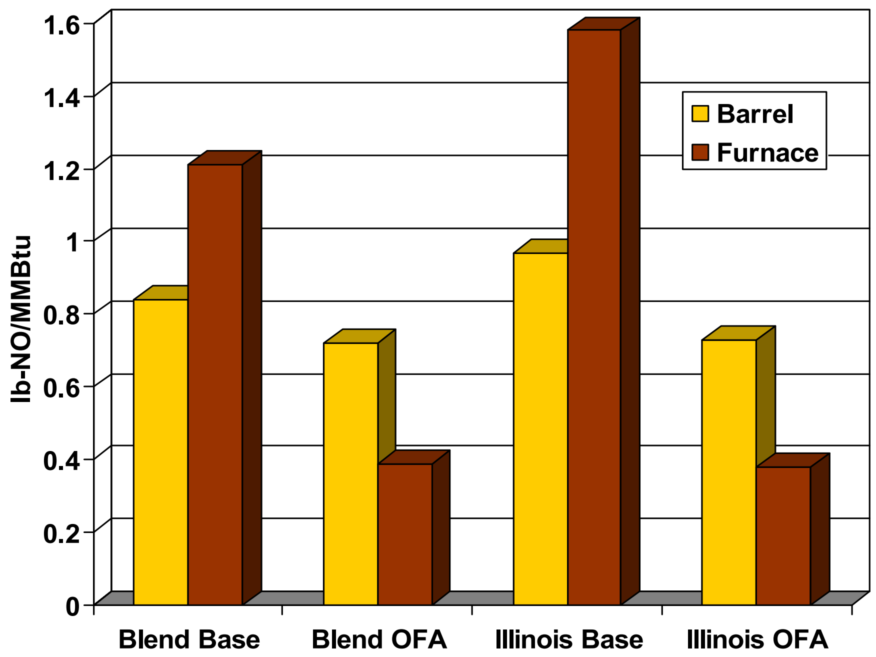
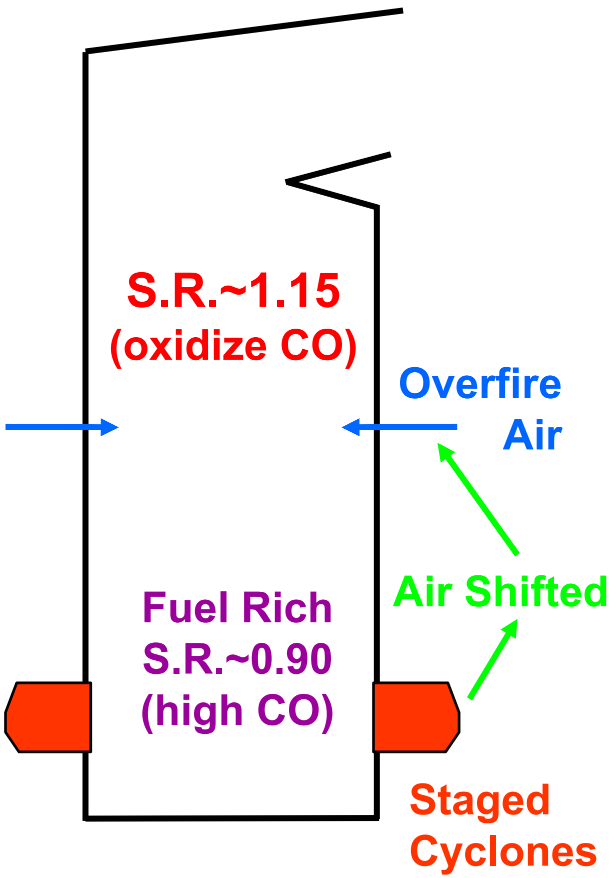
Barrel vs. Furnace NOx

- Barrel NOx alone insufficient to predict boiler NOx
- Need to extend barrel model to include furnace
- Significant NOx formation in furnace (~40%)
- Potential furnace NOx reduction via OFA

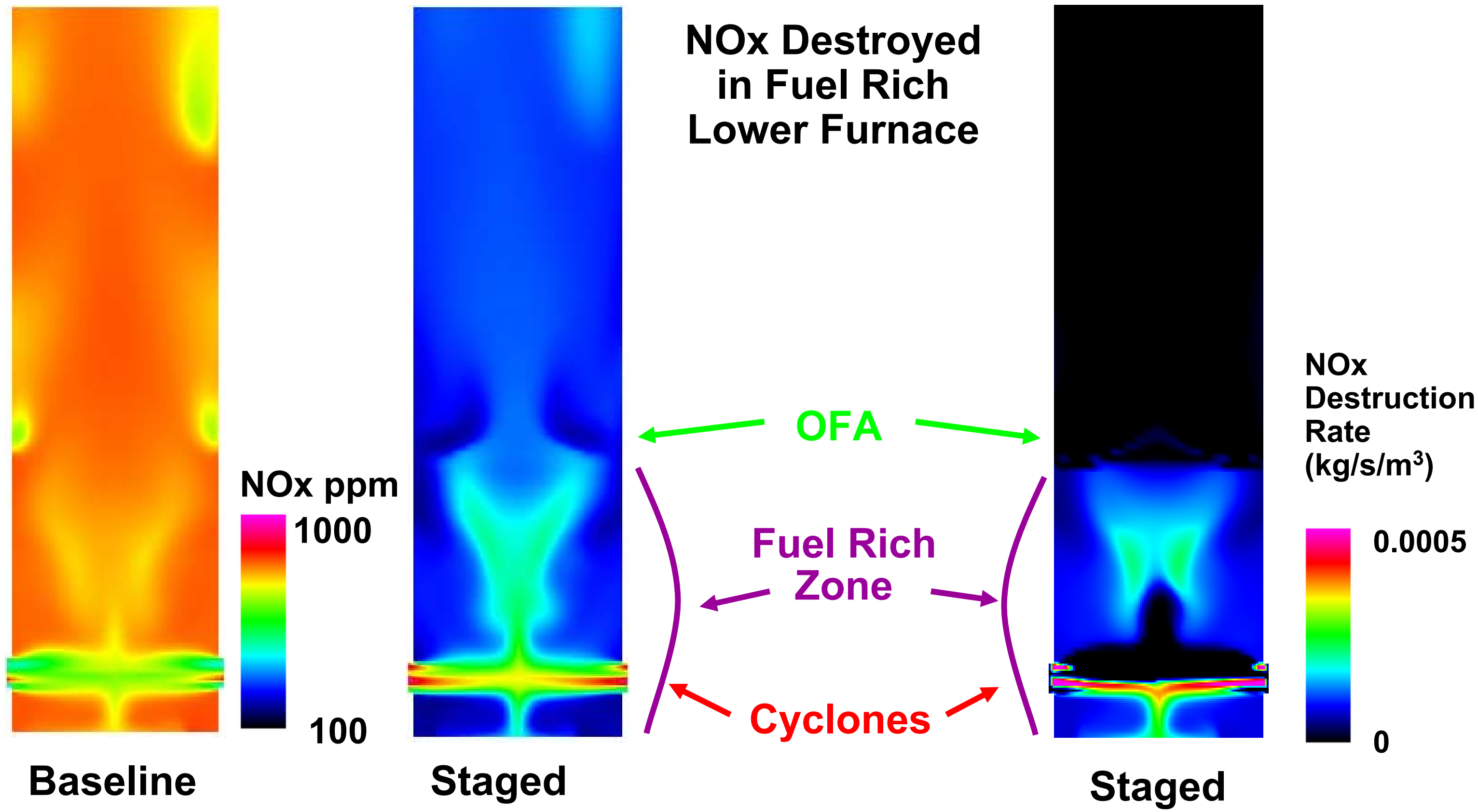


Overfire Air (OFA) Concept



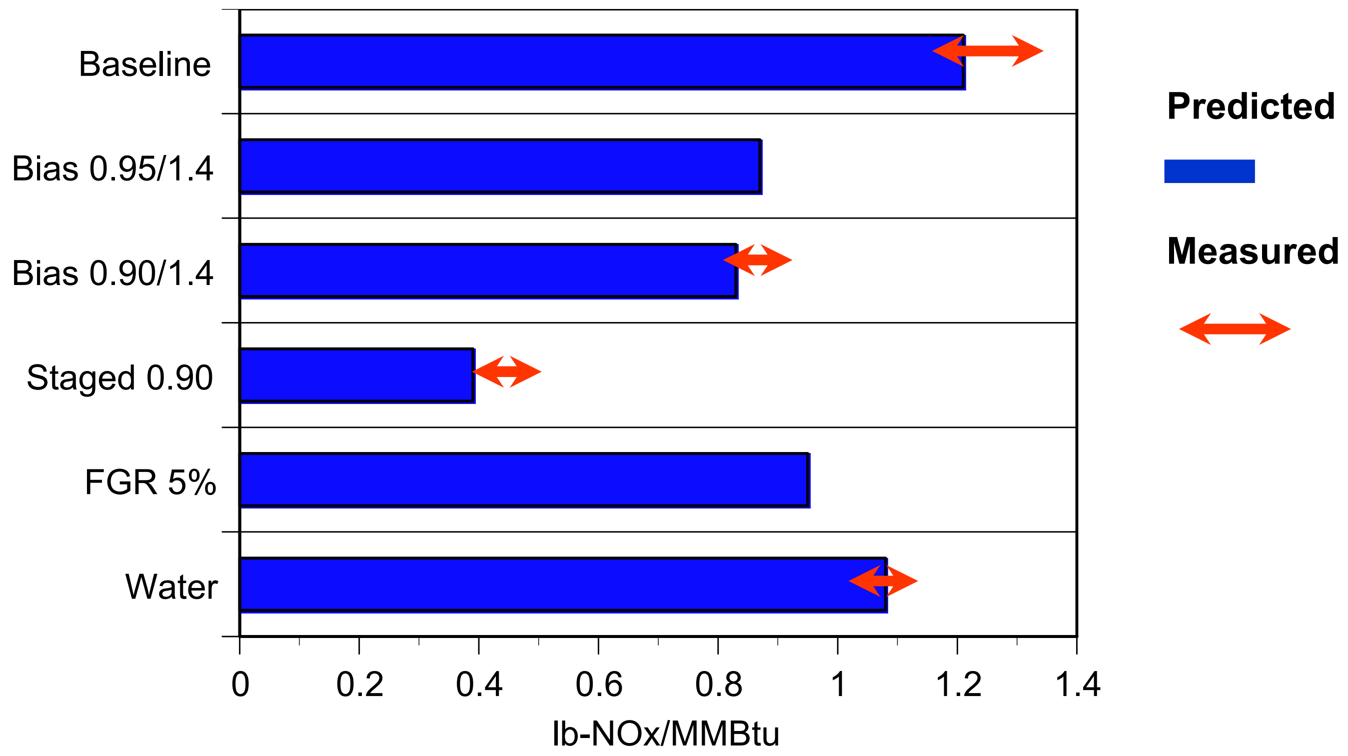
- Staged barrels create fuel rich lower furnace
- Staging results in less NOx formation
- NOx is destroyed in fuel rich zone (dependent on time, temperature, S.R.)
- OFA added to complete combustion after heat removal & NOx reduction

Furnace NOx Reduction



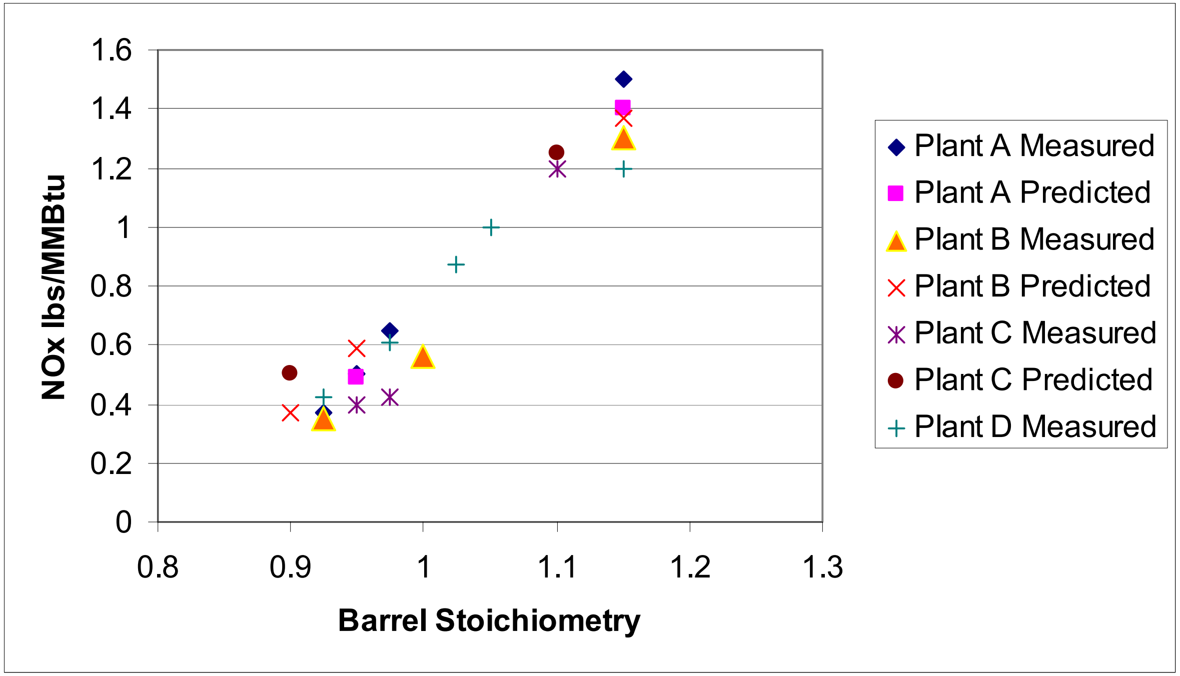
- ➢ **Reduction increases with staging & residence time**

In-Furnace NOx Control Options



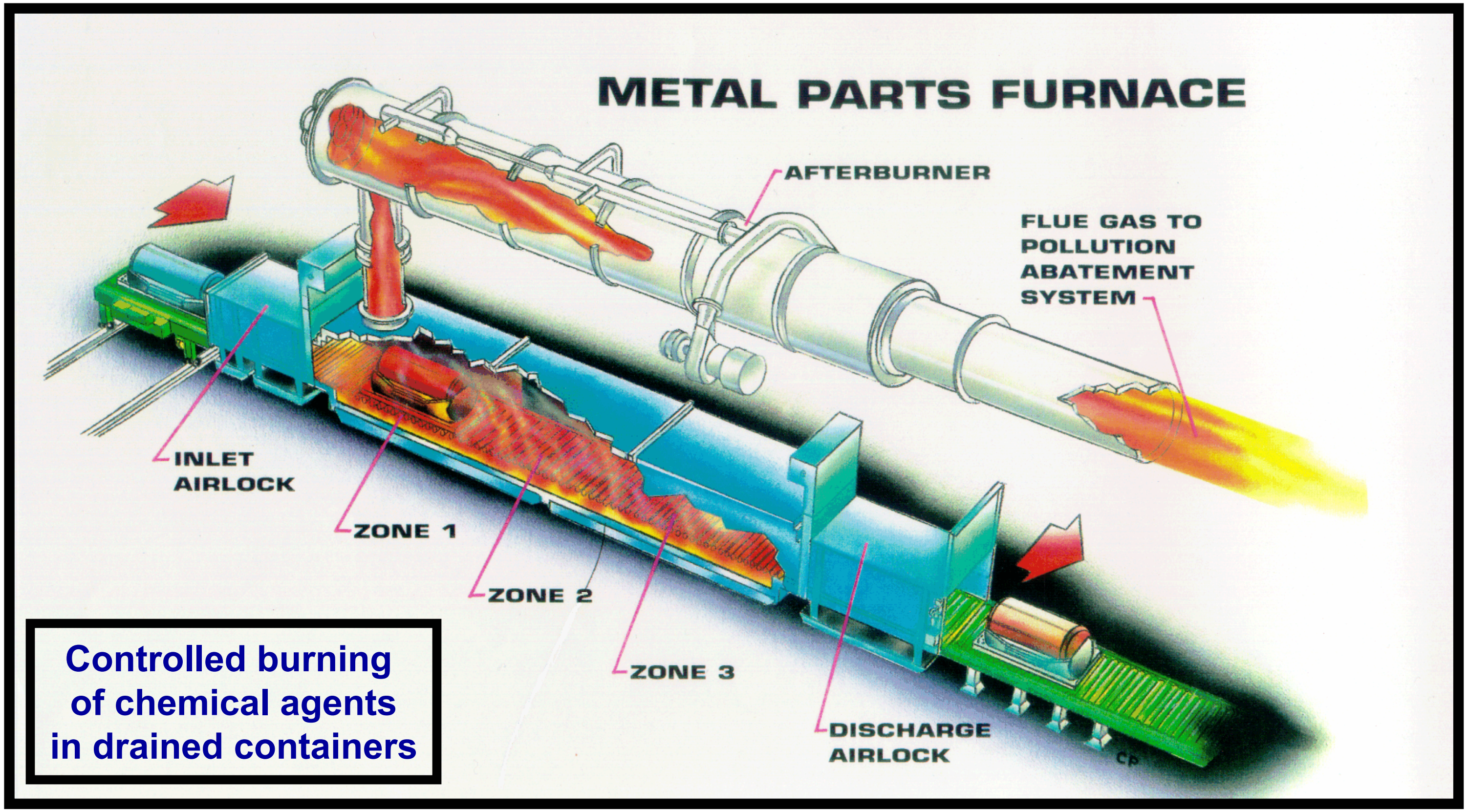
- Model is able to *predict* furnace performance

Plant NOx Reductions With OFA



- **Over 90% of U.S. cyclones have installed or plan to install OFA (50-70% NOx reduction for \$2-\$3/kW)**
- **Savings of >\$500M over other reduction technologies**

Chemical Incineration Example



Controlled burning of chemical agents in drained containers

- **Objective: develop modeling capability for chemically complex, transient combustion system**

Approach

- Assemble Team of Experts to develop chemistry models and provide oversight
- Develop a zone-based transient model to capture time dependent behavior of furnace operation
- Use CFD model to compute
  - Detailed combustion flow field
  - Agent time-temperature history

  at selected times (e.g., peak vaporization rate)
- Use detailed chemical kinetics to assess agent destruction rates

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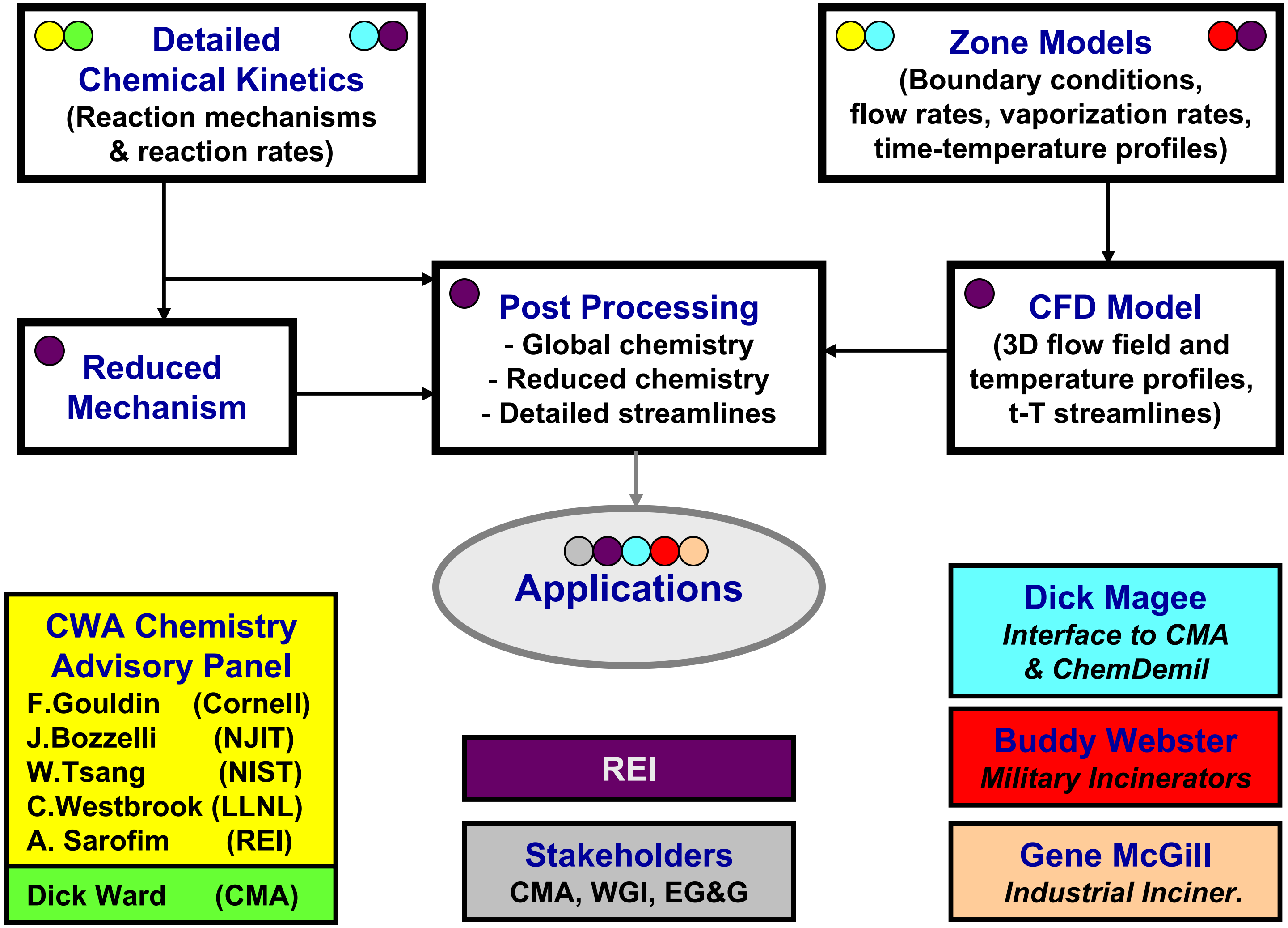
Modeling Approach
(with Team of Experts)



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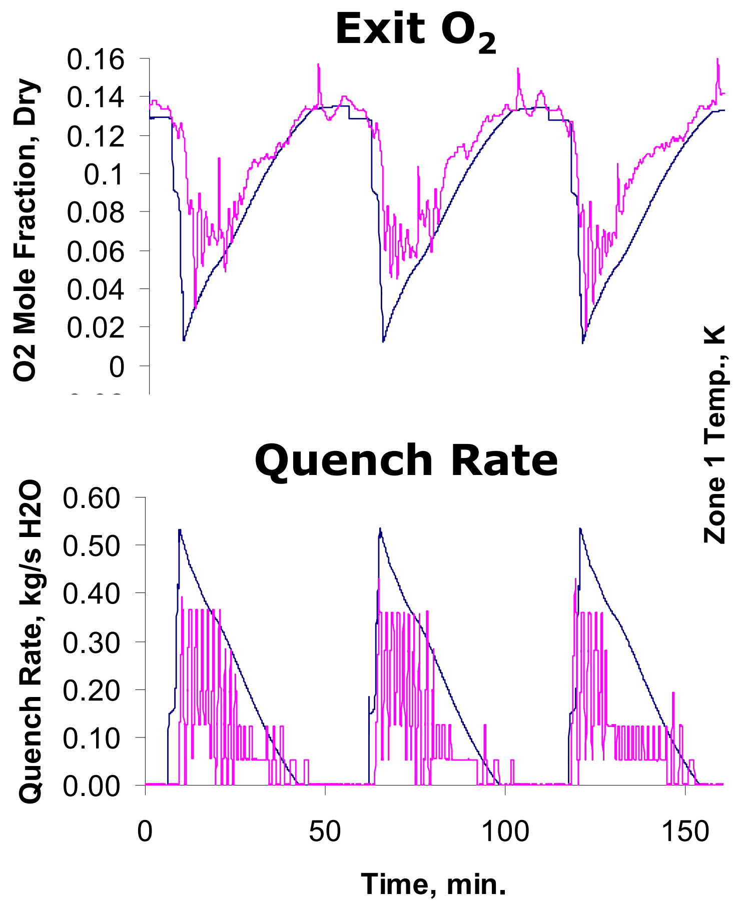
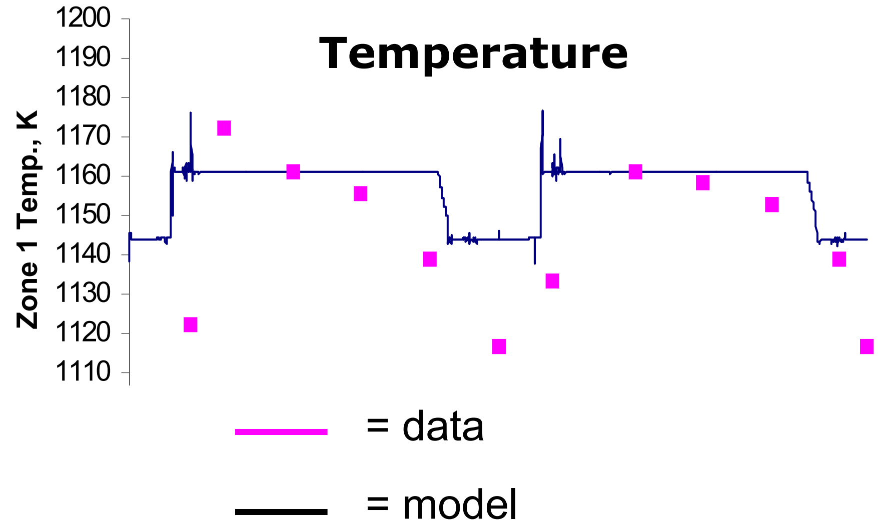
Transient Zone Model
(Primary Furnace Zone)





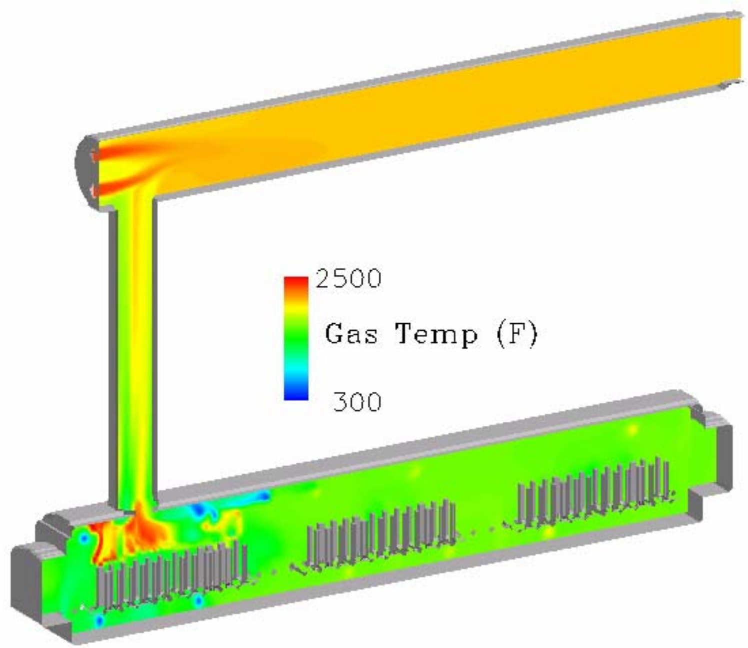
Note: model simulates smooth (rather than discrete) PID control

- **Results at specific time provide inputs for CFD model**

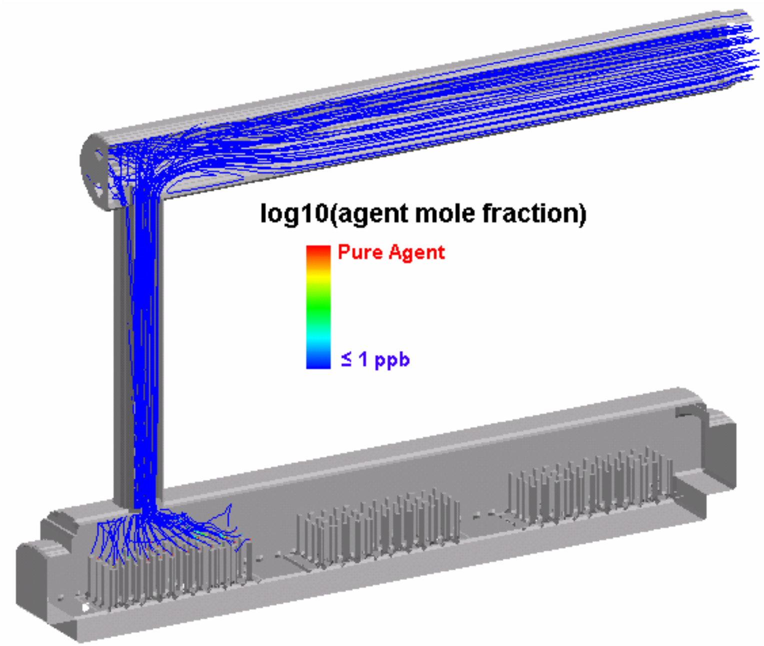
CFD Model Results

CFD results based on inputs from zone model at conditions of interest

Results provide details about agent destruction along streamlines



Gas Temperature



Agent Destruction

Incinerator Summary

- Team of Experts used to develop chemistry and zone model, extend CFD model, and provide reality check of results
- Series of models (zone, CFD, streamlines) provides capability to analyze chemically complex combustion system
- Results shown to predict system performance
- Results used by operators to
  - Better understand system behavior
  - Better manage system processes
  - Evaluate alternate processing procedures

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Conclusion

- **Combustion modeling can be successfully utilized to solve a wide variety of industrial problems, IF**
  - **Application of modeling tools is guided with physical insight and experience**
  - **Customers are consistently involved to ensure problem understanding and solution applicability**
  - **A high level of expertise is maintained in combustion modeling tools and engineers**

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End

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