



Equivalent Reactor Networks as Reduced-Order Models in a CAPE-OPEN Compliant Architecture

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LEADING THE WAY TO CLEAN COMBUSTION DESIGN

Outline

- **Reaction Design overview**
- **ENERGICO Introduction and Demonstration**
- **APECS Gasifier ROM project overview**
- **Roadmapping thoughts**
- **Summary**

Reaction Design Overview: CHEMKIN



- **CHEMKIN® is the de-facto standard for chemical kinetics calculations**
 - Most widely cited and validated kinetics software available
 - Accurate combustion and chemistry simulation for
 - Gas Turbines
 - Automotive
 - Industrial/Utility Burners
 - Chemical Processing and Refinery
 - Materials and Microelectronics
- **CHEMKIN-CFD for FLUENT**
 - Power of CHEMKIN stiff chemistry solver in FLUENT CFD
 - CHEMKIN-CFD/API to link to in-house CFD

Model Fuel Consortium: Project Synergy



MFC-I Members

● MFC-I accomplishments

- Developed momentum for accurate kinetics use
- Over 50 master mechanisms developed
- Surrogate blend optimizer
- Mechanism reduction tools

● MFC-II focus on soot

- Soot modeling tools
- Accurate soot mechanisms
- Further integration of CFD and Detailed Chemistry



reaction
DESIGN

Other Projects at Reaction Design



- **US DoD: Soot Formation in Rocket and Jet Engines (SBIR)**
 - Particle size distribution tracking module
 - Soot particle growth / oxidation chemistry model
 - Linking chemistry & particle tracking into CFD



- **NASA: Alternative Jet Fuels (Grant)**
 - Fischer-Tropsch fuels
 - Biofuels for jet applications
 - Mechanism development and reduction
 - Collaboration with USC



- **US DoE FreedomCAR: Biofuels (CRADA)**
 - Biodiesel fuels
 - Soot formation modeling
 - Collaboration with USC, Chevron



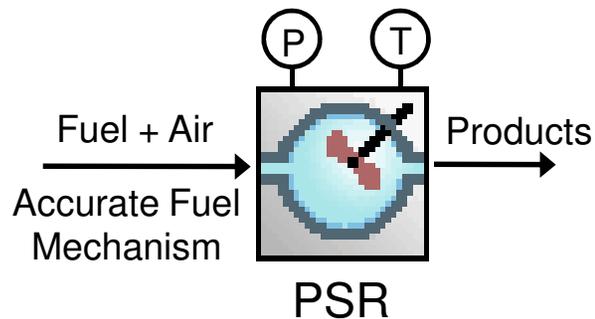
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What We're Hearing from the Market

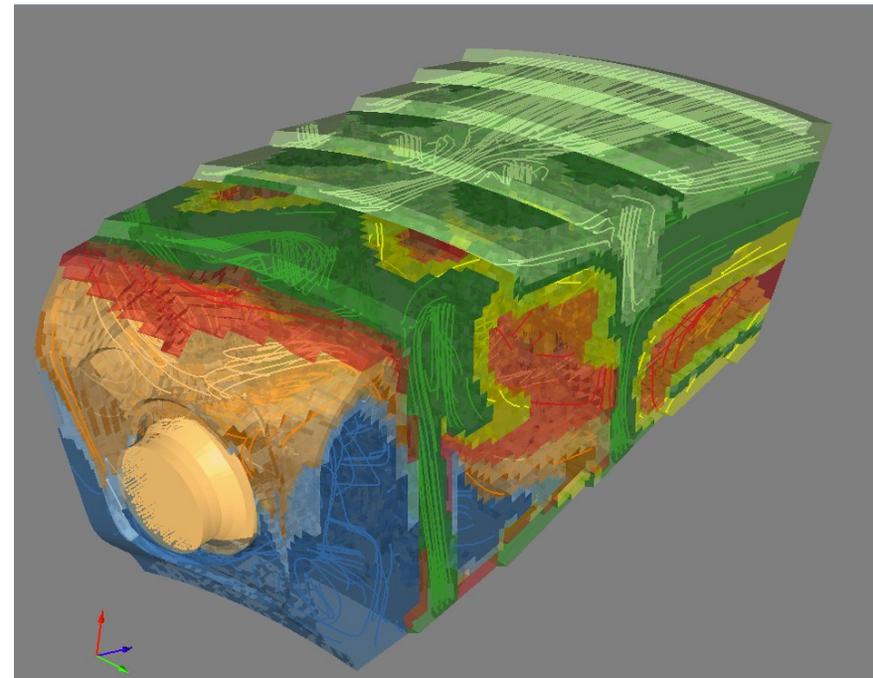
- **Most manufacturers are using CFD**
 - Healthy skepticism in CFD results inside of gasifier
- **Complexity of particle tracking and combustion limits use of accurate kinetics in CFD**
 - CFD times can exceed one month
 - Modest grid size and turbulence models employed
- **Particle surface and gas phase kinetics are considered key to simulate performance**
- **Simulation challenges for key performance guarantees**
 - Exit gas composition and emissions
 - Carbon conversion
 - Fuel composition variation
 - Maintenance schedule

Applying Reactor Modeling to Commercial Designs

- **Reduced-order models allow simulation with full kinetic details**

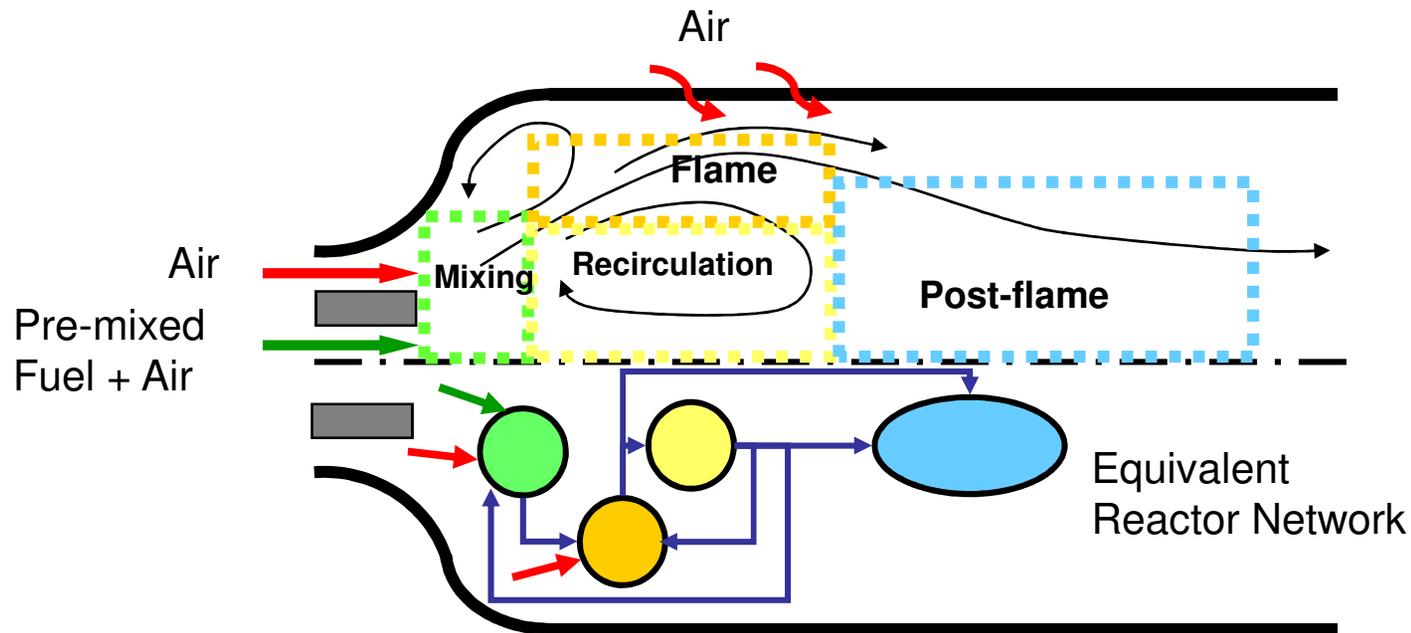


But, how do I make this ...



... look like this?

Equivalent Reactor Networks (ERNs) Provide Accuracy and Speed



Benefits of ERNs

- Quickly predict exit emissions
- Understand where and how emissions are formed

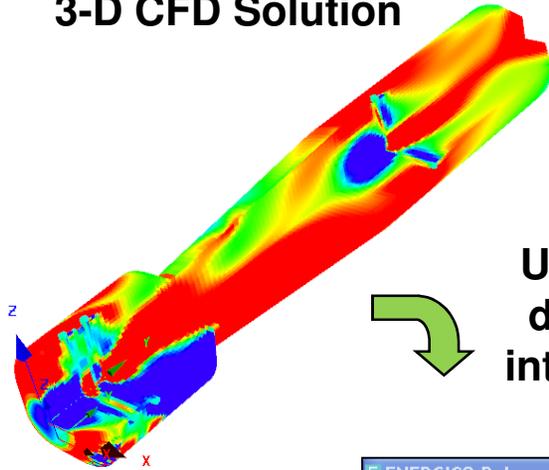
Drawbacks of ERNs

- Take too long to construct
- Hard to map results back onto combustor geometry
- Doesn't fit commercial timelines

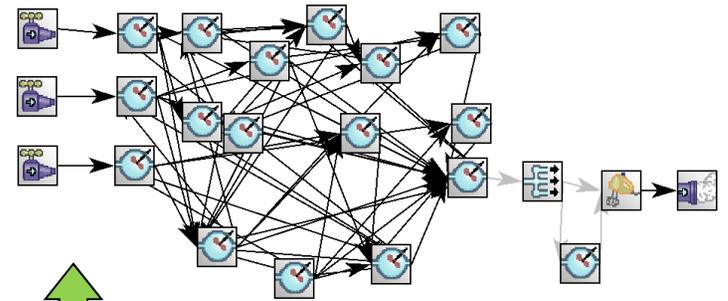


Automated ERN Generation Adds Chemistry to the Design Flow

3-D CFD Solution

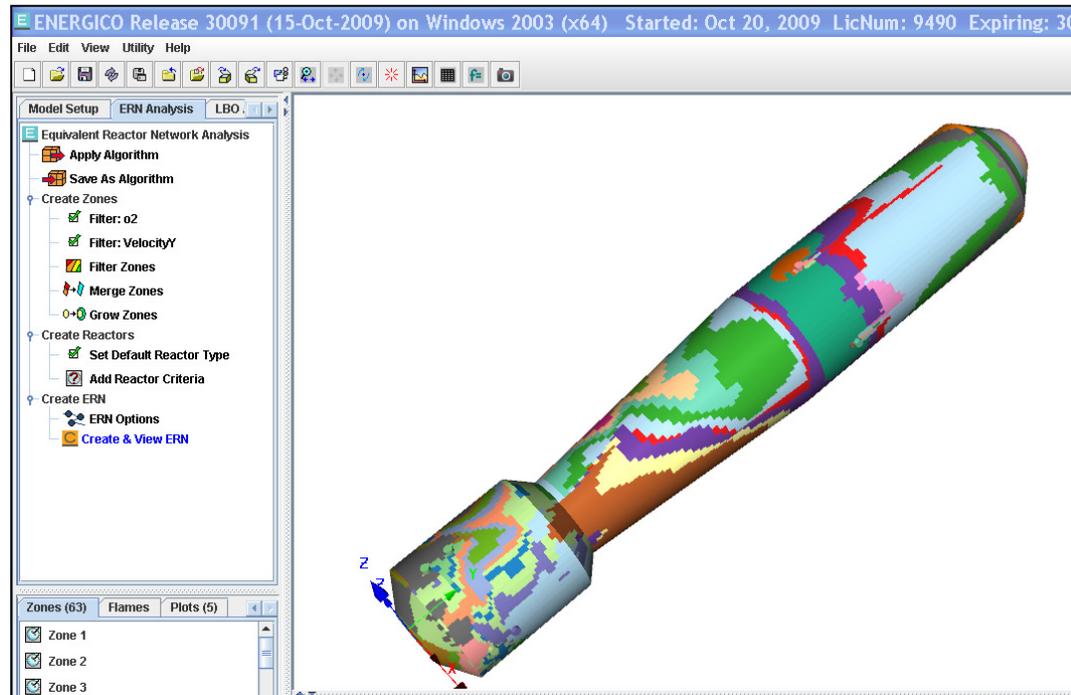


Use algorithm to divide flow field into reactor zones



Automatically create ERN

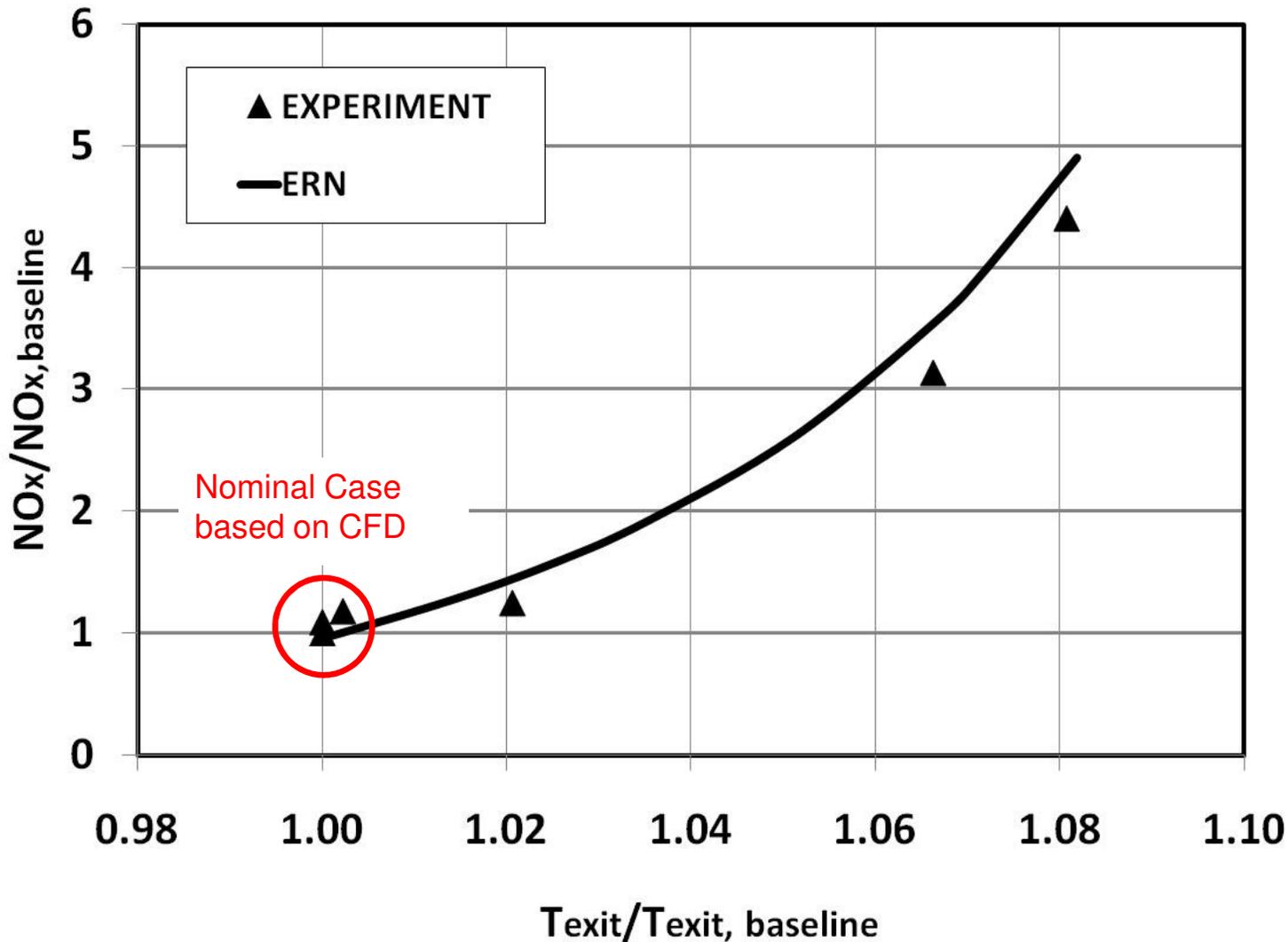
Improve your CFD model with greater kinetic understanding



Map chemistry results onto geometry view

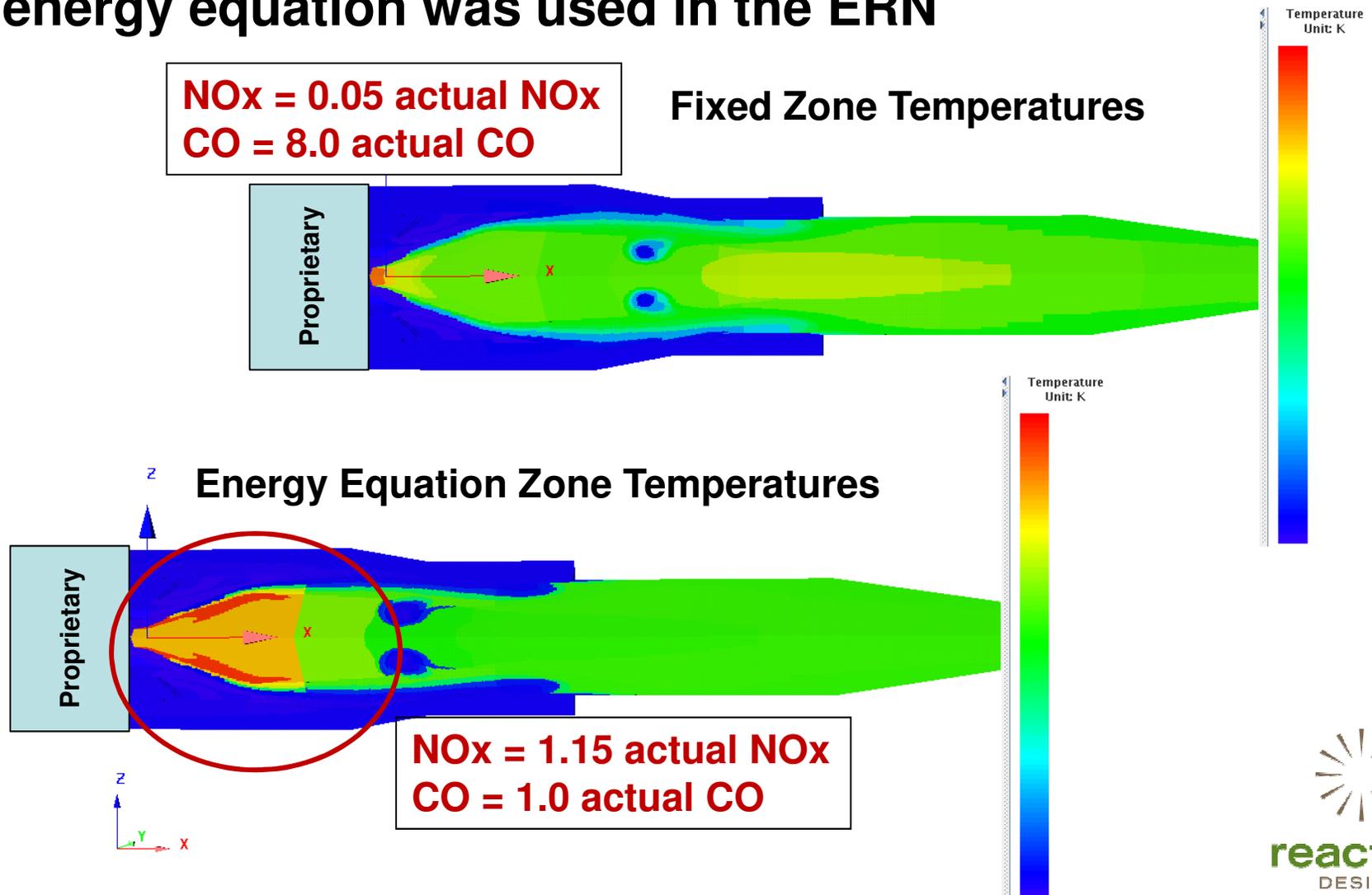
ENERGICO ERN Accurately Predicts NOx

- Increased fuel/air ratio from single data point



Comparison of CFD and ENERGICO Results

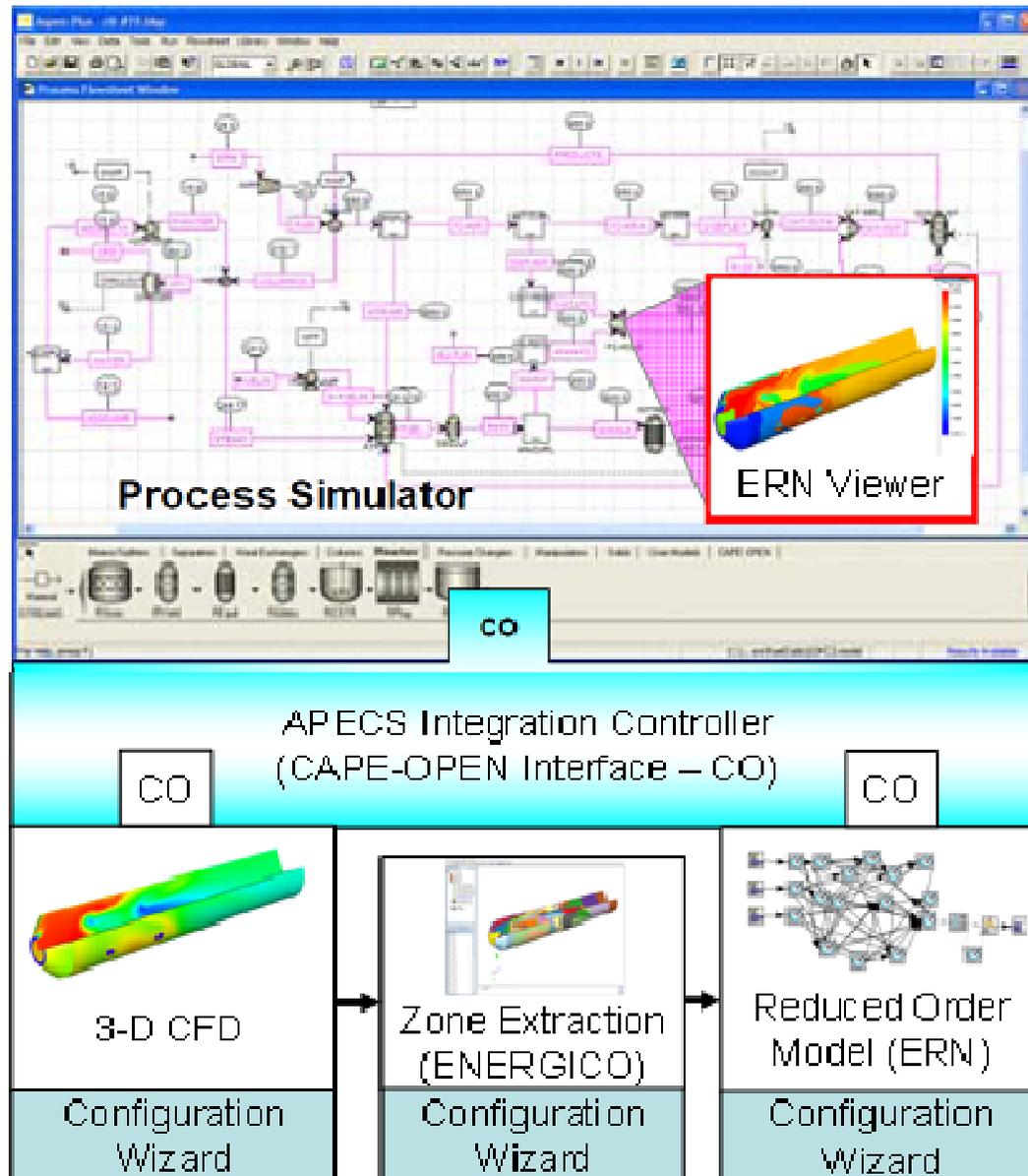
- Significant shift in flame location and NOx when the energy equation was used in the ERN



Ramping Up on This New NETL Project

- **Project duration: 3 years**
- **Start date: 10-1-2009**
- **Project Objectives:**
 - Enable advanced CHEMKIN reduced-order modeling for key unit operations in flow-sheet simulations, using CAPE-OPEN architecture
 - Use Equivalent Reactor Networks (ERNs) as basis for reduced-order models
 - Extend ENERGICO™ ERN-extraction for application to gasifiers

Big Picture Goal: Integrate into APECS



Key Contributors to the project

- **Dr. Ellen Meeks, Principal Investigator**
 - Head of Product Development at Reaction Design
- **Dr. Tony Garratt, Technical lead**
 - Senior Numerical Analyst and Team Lead at RD
 - Worked for 15+ years at Aspentech
- **Dr. Cheng Wang, Staff Development Engineer**
 - Key software architect for Reaction Design
- **Dr. C.-P. Chou, Staff Development Engineer**
 - Combustion and surface-chemistry expert
- **Scott Drennan, Director of Apps Engineering**
 - Lead in IGCC applications
 - Previously with EPRI and COEN Burner Company

Roadmapping Thoughts

- **Understand key performance trade-offs and objectives**
 - What design and performance features are important?
 - What accuracy level is *good enough*?
- **Secure validation test cases**
 - Proprietary and non-proprietary
- **Improved surface and gas phase kinetic mechanisms**
 - Various gasifier design conditions
 - Various coal types
- **Improvements in dense phase CFD**
 - Particle transport and interactions
 - Improved reduced CFD kinetics
 - Accurate turbulent models

Summary

- **ENERGICO analysis with accurate chemistry ...**
 - Proven accuracy in gas and liquid fired equipment
 - Provides great platform for extension to gasifiers
- **Goals of APECS project are to bring accurate chemistry to bear on gasifier simulation**
 - Achieve similar success that we've seen in automotive and gas turbine use of accurate chemistry to gasifiers
 - Deliver a commercial grade software tool for gasifier design and control system development
- **Project builds on previous success**
 - Improved CFD models and computer speed
 - Improved kinetics mechanisms and models
 - But, there's still much work to do



Thank You



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