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

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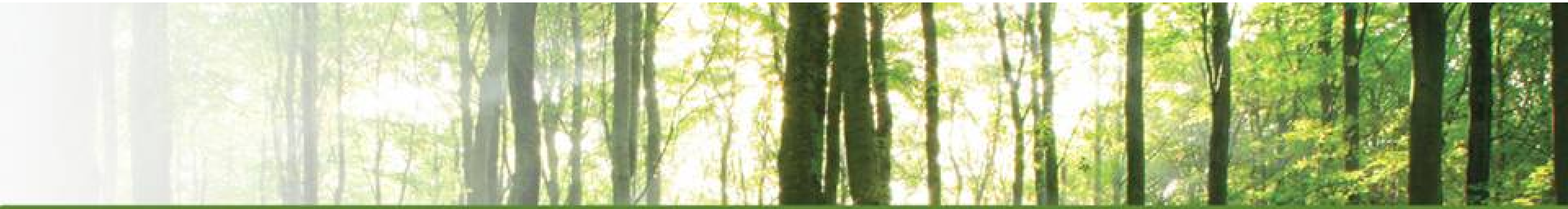
NETL
Pittsburgh, PA

DE-FE0001074



LEADING THE WAY TO CLEAN COMBUSTION DESIGN

Outline

- **Overview of project goals & scope**
- **Technical contributors**
- **Background on Reaction Design**
  - Our technology base
- **Project plan**
  - Tasks and Milestones
  - Deliverables
  - Timeline
- **Current Status**

Our main goal is to create a new reduced-order model capability for APECS

- **Project duration: 3 years**
- **Start date: 10-1-2009**
- **Project Objectives:**
  - Enable advanced 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

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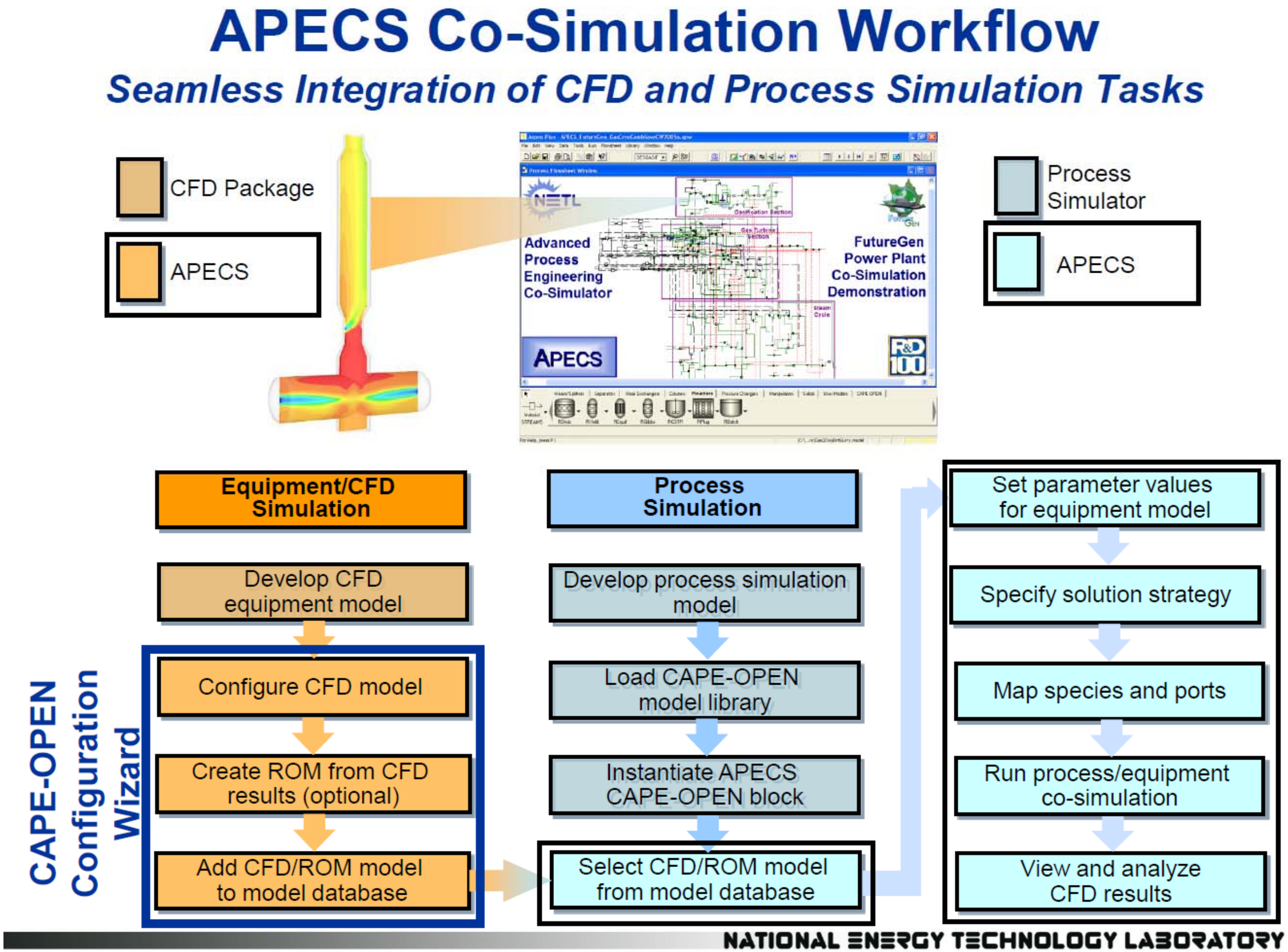
APECS is a co-simulation program at NETL*



*From S. Zitney, APECS Workshop, Oct 2009.

The application focus is on coal-gasification plants, especially involving IGCC

- **APECS integrates CFD and reduced-order-models (ROMs) into flow-sheet simulations for plant design**
  - Built on CAPE-OPEN interface to, e.g., AspenPlus
- **Our "bridge" technology between CFD and detailed-kinetics simulations provides an automated way to create ROMs**
  - Uses "equivalent reactor network" approach, or ERN
  - Gas-turbine combustors are already modeled
  - Extensions to multi-phase flow for gasifier simulations

Key Contributors to the project

- **Ellen Meeks, PI**
  - Head of product development at Reaction Design
- **Tony Garratt, Technical lead**
  - Senior Numerical Analyst and Team Lead at RD
  - Worked for 15+ years at Aspentech
- **Cheng Wang, Staff Development Engineer**
  - Key software architect for Reaction Design
- **C.-P. Chou, Staff Development Engineer**
  - Combustion and surface-chemistry expert
- **Scott Drennan, Director of Apps Engineering**
  - Lead in IGCC applications

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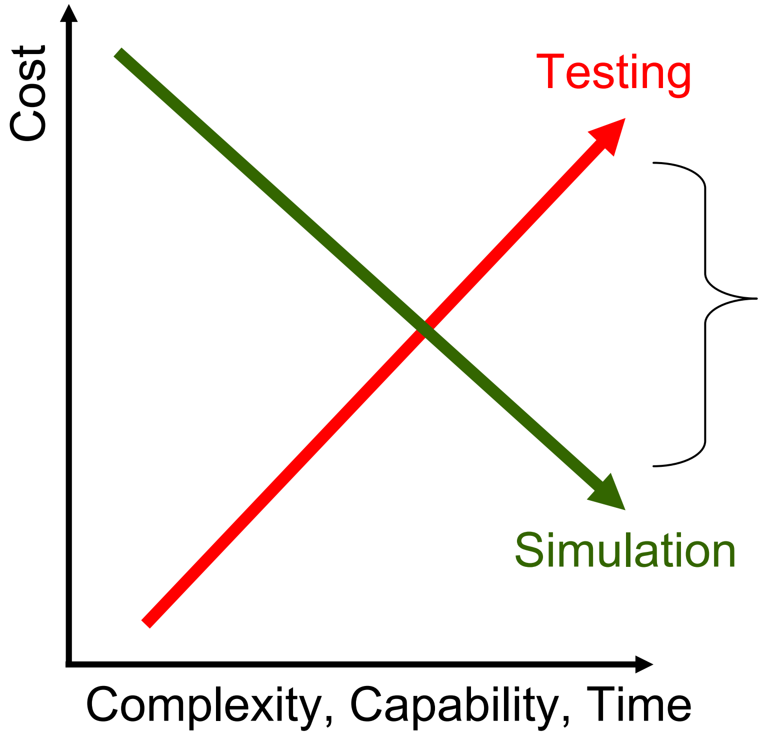
Reaction Design's mission

- Empowering transportation and energy companies to design and develop the cleanest possible combustion systems

Simulation reduces cost of development



- **There is a growing opportunity to:**
  - Reduce risk
  - Improve use of testing
  - Speed development
  - Facilitate innovation

Reaction Design's core business

We are in the business of:

- **Chemical Kinetics Software**
  - CHEMKIN® Software
    - Exclusive worldwide distributor & developer since 1997
  - CHEMKIN-CFD/API™ Module
    - Kinetics solver plug-in for CFD Simulation
  - ENERGICO™ Simulation Package
    - Emissions modeling for Gas-turbine Combustors
- **Professional Services**
  - Chemical kinetics applications
  - Mechanism development, validation, reduction
  - Custom software
- **Industry-led Consortia**

toward the development of clean technology

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CHEMKIN-PRO is our flagship product

- **CHEMKIN is the standard for chemical kinetics calculations**
  - Most widely cited and validated kinetics software available
- **Focused on accurate simulations of chemistry for:**
  - Gas Turbines
  - Automotive engines
  - Industrial/Utility Burners
  - Chemical Processing and Refinery
  - Materials and Microelectronics

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CHEMKIN-CFD™ Module -- built on CHEMKIN

CFD Simulator (e.g. FLUENT)

- Solves Navier-Stokes Eqs.
- Energy and Fluid Transport
- Turbulence Models

+

CHEMKIN-CFD™

- Solves Stiff Species Eqs.
- Surface and Gas Kinetics
- Multi-component Transport

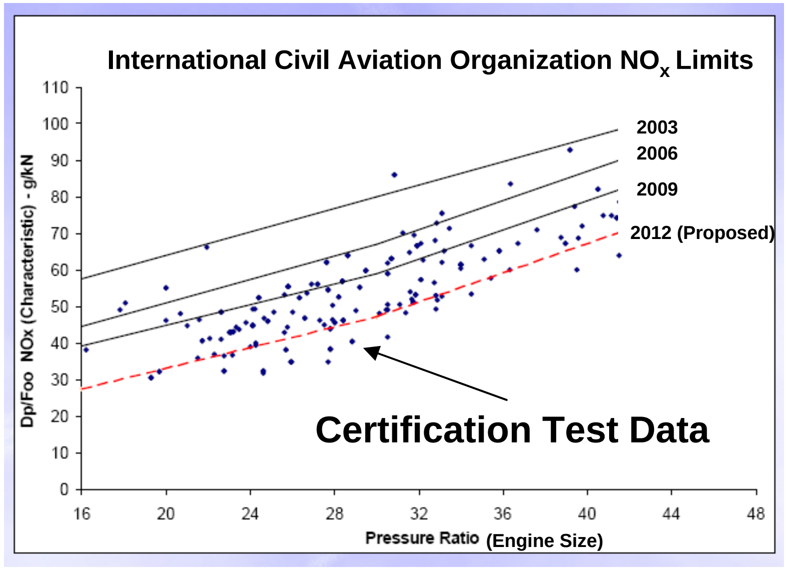
Accurate 3-Dimensional Modeling with Chemistry

Reaction Design has a track record of successful contract research and services

- **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
  - Hypersonic flow simulation
- **NASA: Alternative Jet Fuels (Grant)**
  - Fischer-Tropsch fuels
  - Biofuels for jet applications
  - Mechanism development and reduction
  - Collaboration with USC
- **US DoE FreedomCAR: Biofuels (CRA)**
  - Biodiesel fuels
  - Soot formation modeling
  - Collaboration with USC, Chevron

ENERGICO™ is Reaction Design's latest product

- **Created to address key issues facing gas-turbine combustor designers**
  - Low Emissions Regulations
    - ICAO limits on nitrogen oxides (NO_x), carbon monoxide (CO) and Unburned Hydrocarbons (UH)
    - New particulate emissions regulations
  - Fuel Flexibility
    - Alternative Fuels
    - Opportunity Fuels
    - Biofuels for carbon dioxide (CO_2) reduction
  - Combustion stability
    - Lean Blow Off assessment
    - Flash-back
    - Ignition



Source: ICAO Colloquium on Aviation Emissions, May, 2007

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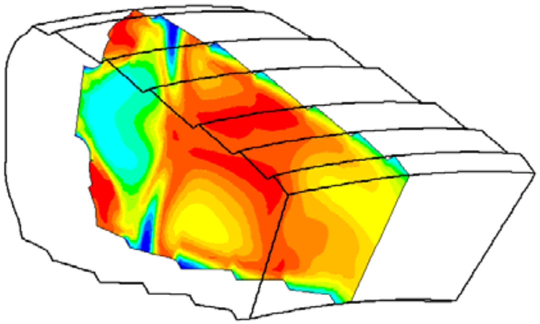
ENERGICO™ creates a bridge between CFD and required chemistry information

Goal:
Minimize emissions while maximizing efficiency

CFD Simulation:
Determine effects of fuel/air inlet locations and combustor geometry on flowfield



ENERGICO addresses the gap in design workflow

Test:
Determine emissions, stability, fuel effects

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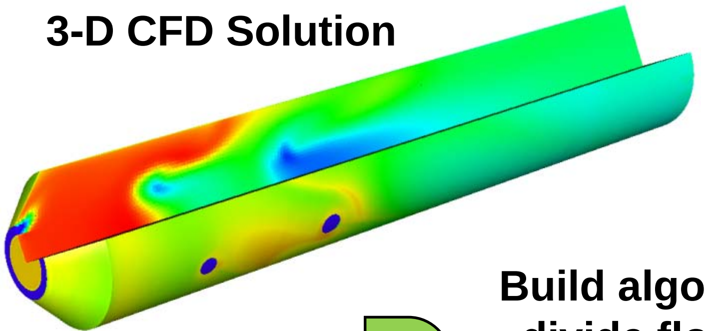
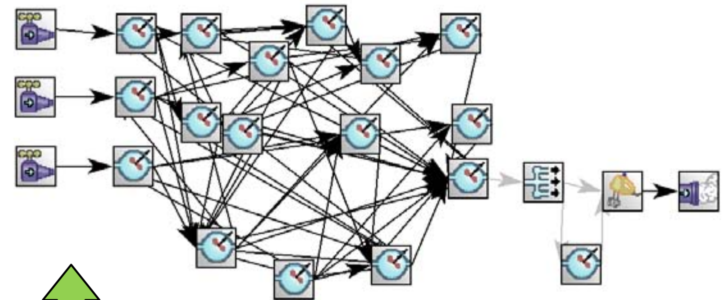
Automatic creation of Equivalent Reactor Networks adds chemistry to design flow

3-D CFD Solution

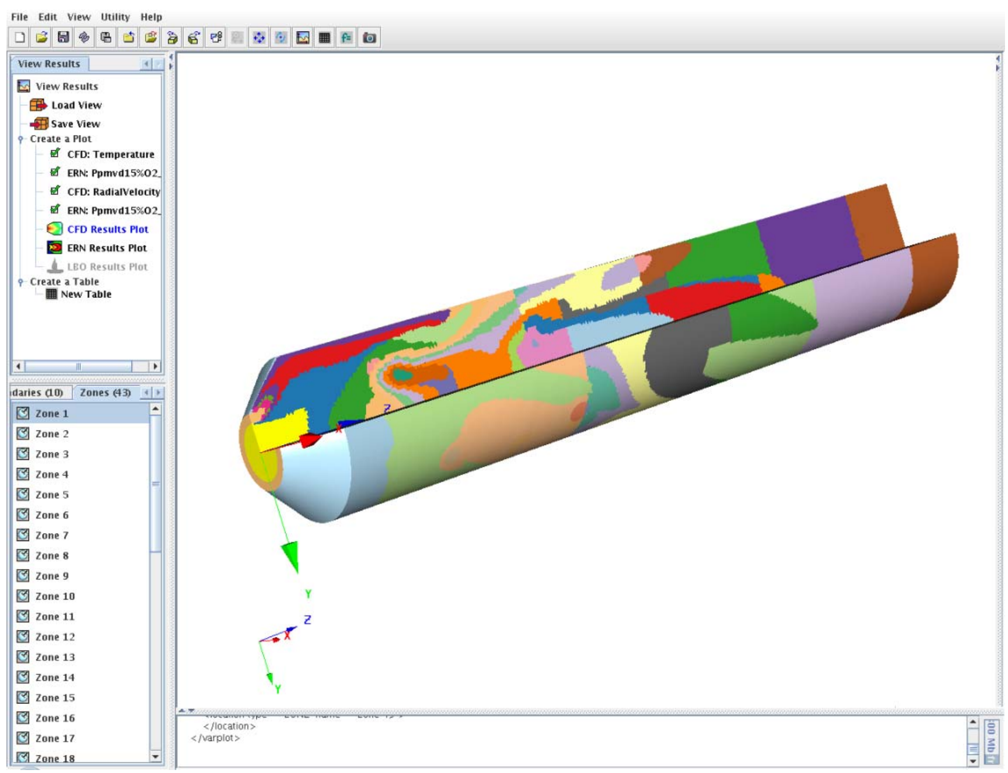


Build algorithm to divide flow field into reactor zones



Automatically create ERN

Map chemistry results onto geometry view



Improve your CFD model with greater kinetic understanding

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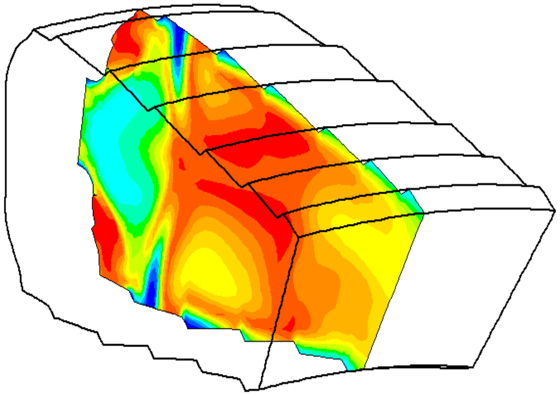
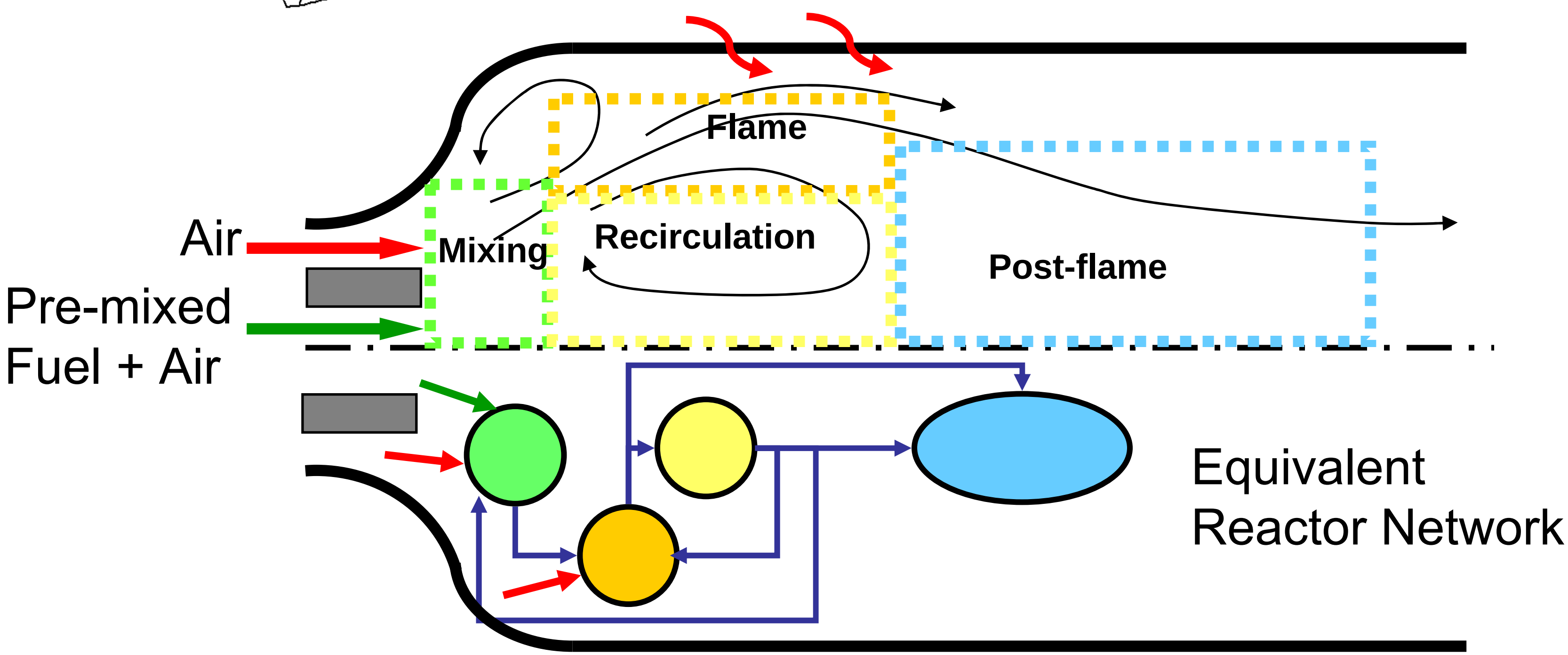
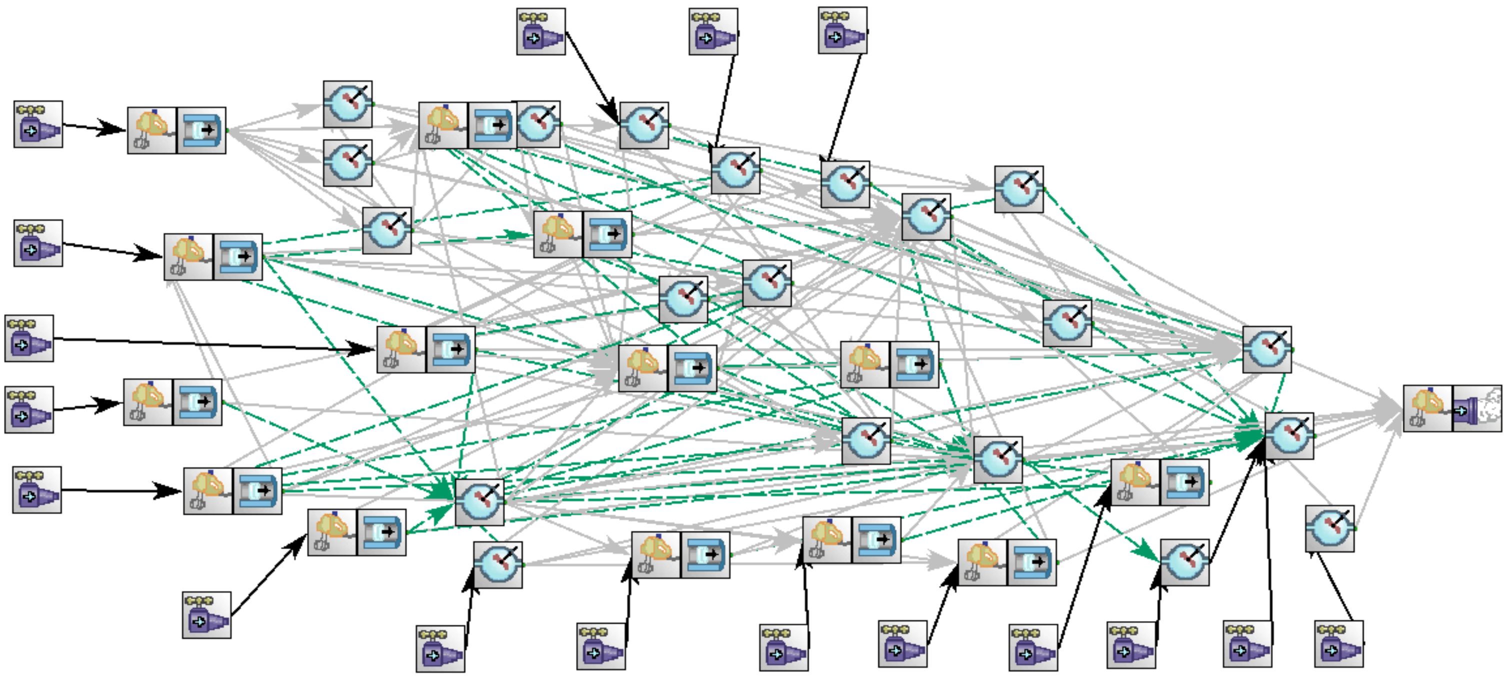
Reactor networks represent complex systems while allowing detailed kinetics



Essence of flowfield in complex geometry can be represented by reactors with mass-flow connections



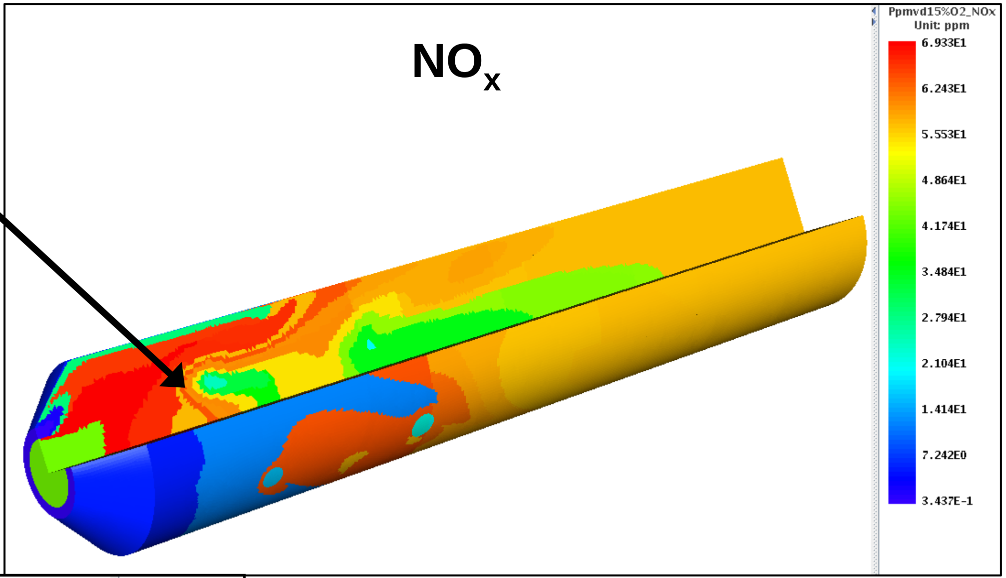
ENERGICO creates complex reactor networks quickly and automatically

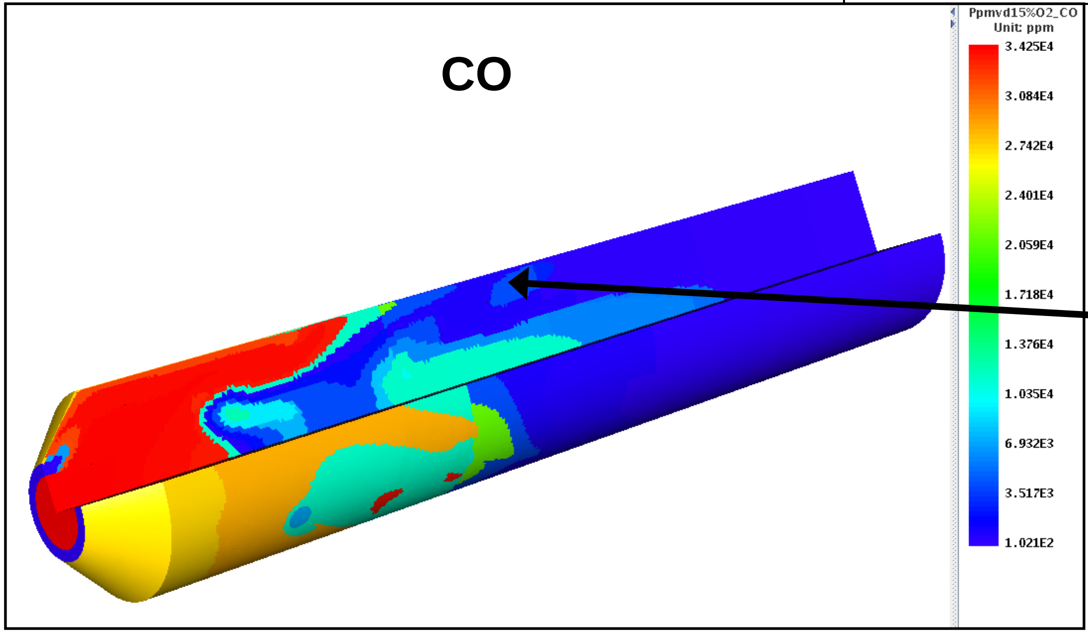


- **Automation supports commercial design timelines**
  - Creates ERNs in minutes rather than months
  - Enables widespread use by combustor designers
- **Accurately follows specific sets of rules**
  - Correct-by-Construction

Results mapped back to the CFD mesh show ERN predictions in geometric context

Identify where NO_x emissions are formed





Identify where CO emissions are quenched

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Sample ENERGICO results compared to data for gas-fired gas-turbine combustors

Class of Combustor (all CO less than 10ppm)	Fuel Type	NO Variance	CO Variance
10MW Less than 10ppm NO_x	Natural Gas	1ppm	2ppm
25MW 25ppm NO_x	Natural Gas	2ppm	2ppm
250MW Less than 10ppm NO_x	Natural Gas	1ppm	2ppm
250MW 25ppm NO_x	Natural Gas	2ppm	2ppm
250MW 25ppm NO_x	Syngas	2ppm	2ppm

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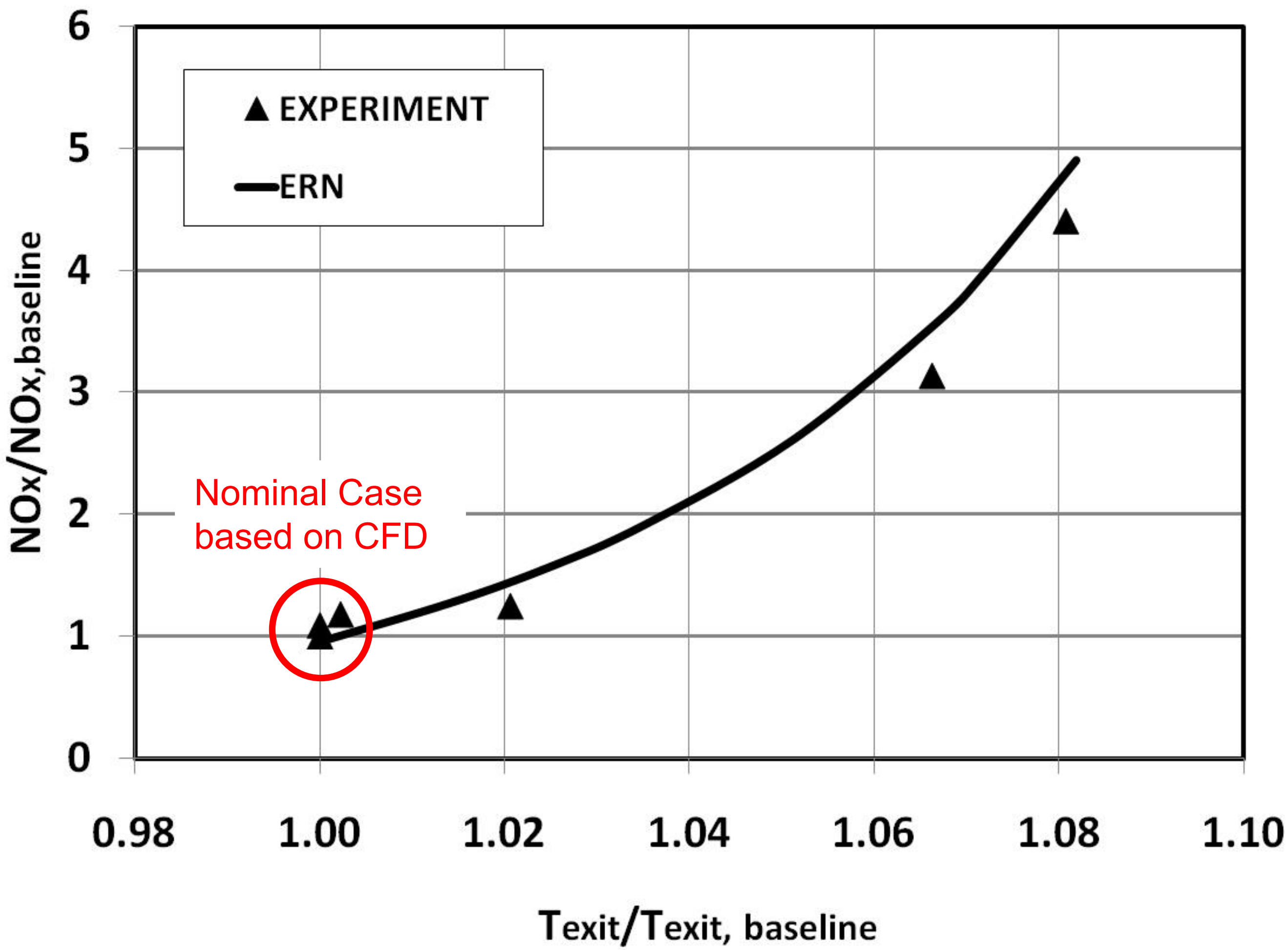
Joint work with GE demonstrated the ERN can *predict* impact of load variation on NO_x

- Increased Fuel/Air Ratio from single data point



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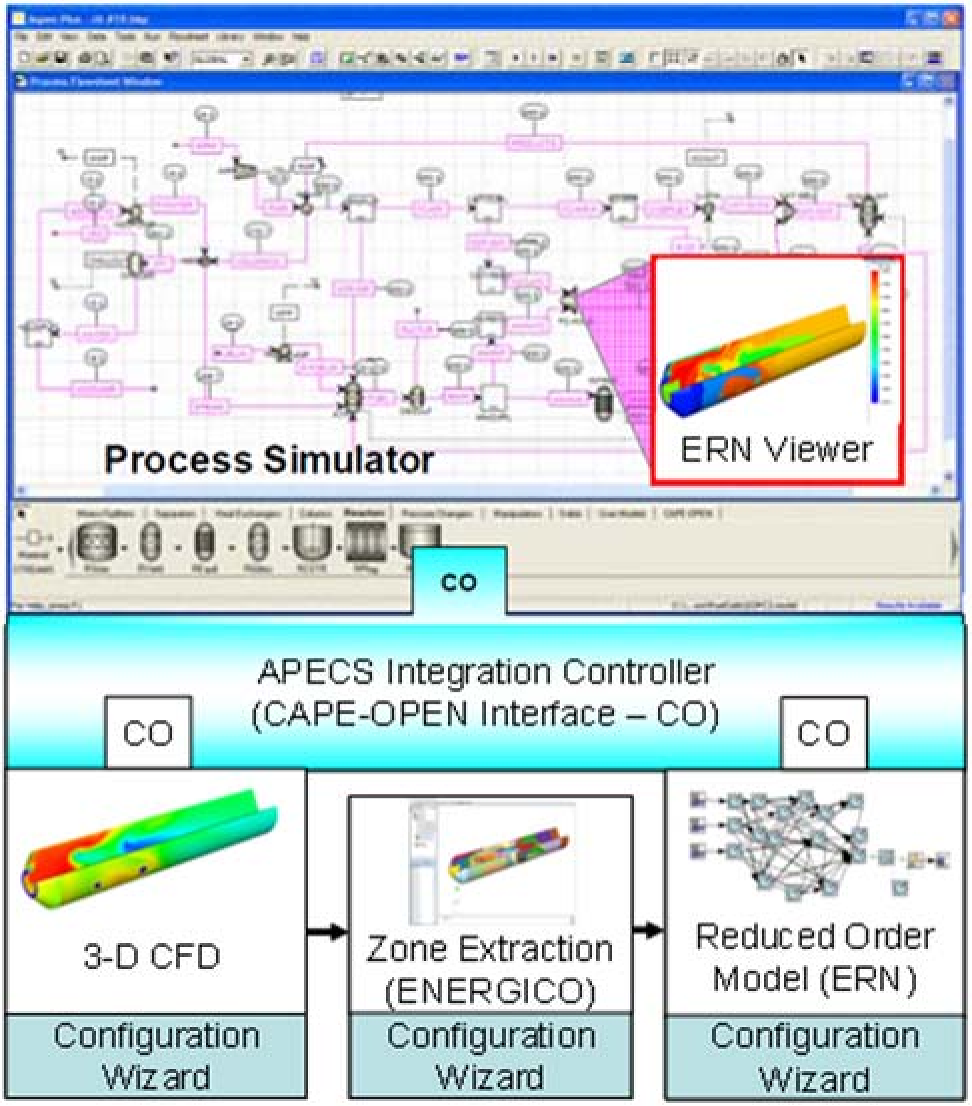
ENERGICO: Key Benefits

- **Effective integration of detailed chemistry into engineering workflow**
  - Fewer, better-directed experiments
  - Simulate conditions that cannot be experimentally tested
- **Rapid evaluation of fuel and design effects**
  - Accurate emissions predictions using overlay with CFD
    - NO_x, CO, UHC
  - Ability to determine contributions to NO_x
    - Thermal NO_x
    - Prompt NO_x
- **Platform for combustion stability analysis**
  - Lean Blow Off assessment

For this project, we will extend these concepts to gasifier simulations

- **Use ERN concept to generate “reduced order model” or ROM within a plant simulation**
- **Build the ERN automatically from CFD results**
  - Account for multi-phase flow effects
  - Identify dominant flow characteristics
- **Apply more advanced kinetics models than current practice allows**
  - More than a ROM, as it adds chemistry detail
- **Package into CAPE-OPEN architecture**
  - Allow use within APECS program

Big picture goal: integrate into APECS

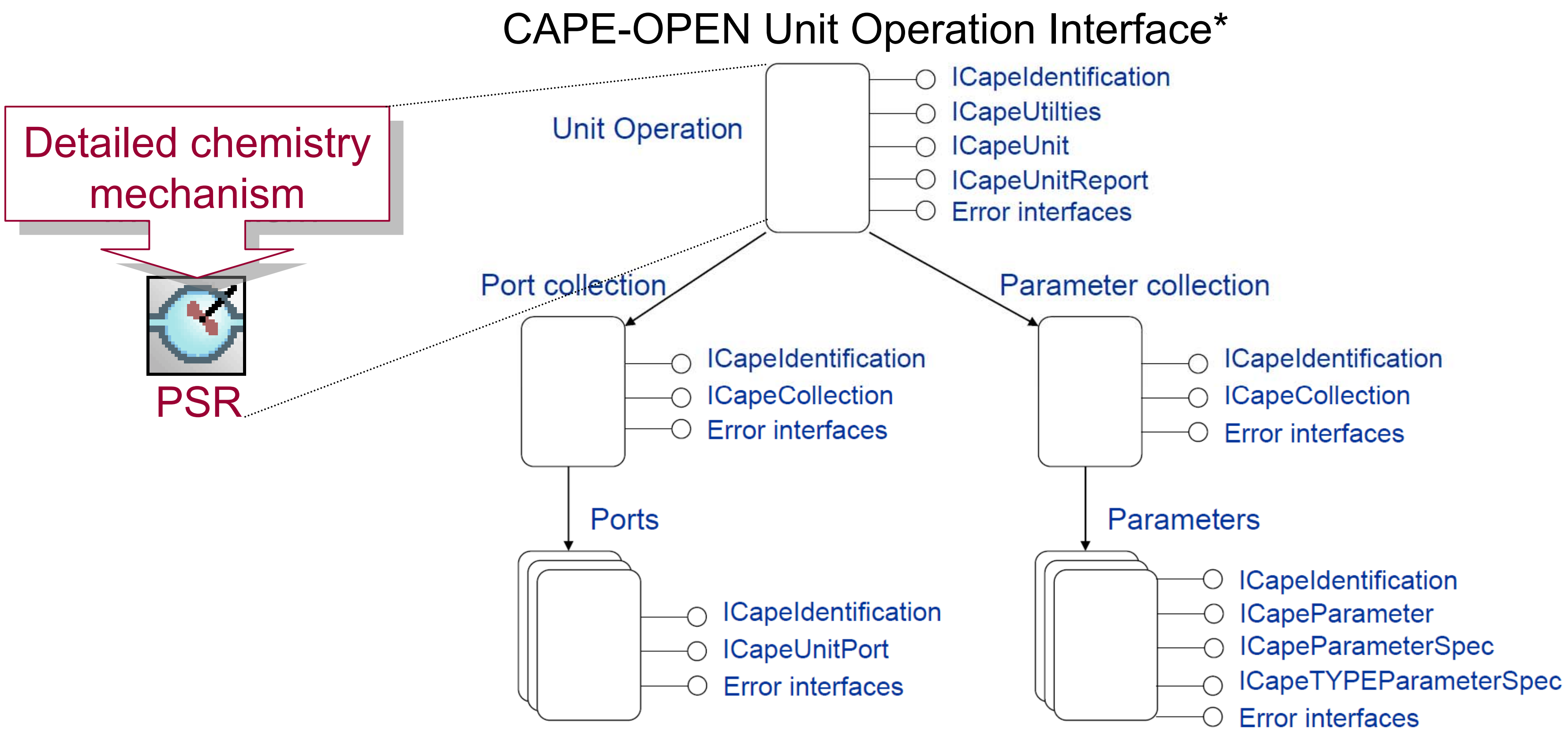


Major Tasks are identified in the SOPO

1. Project Management and Planning
2. Package CHEMKIN Models as a CAPE-OPEN Unit Reactor Model
3. Extending ENERGICO Software and Workflow for Gasifier Models
4. Evaluate Gasification Kinetics Models
5. Code and Model Integration, Testing and Validation

We begin by wrapping a single Perfectly Stirred Reactor (PSR) with CAPE-OPEN

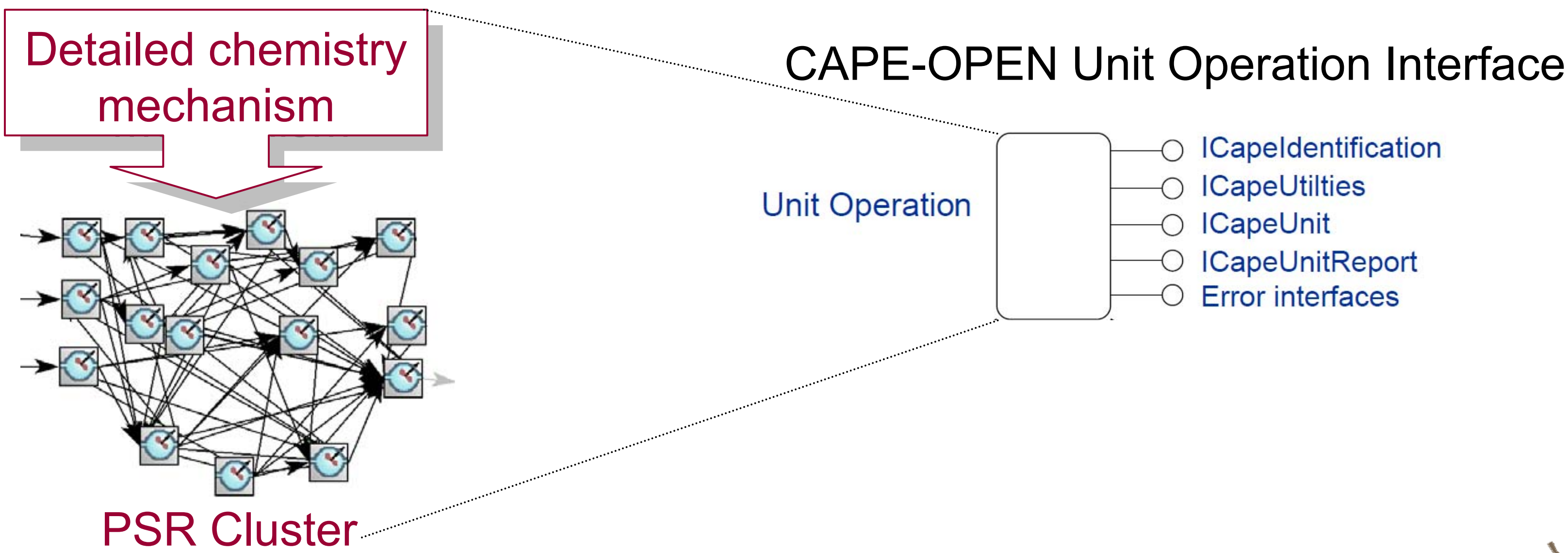
- **The CHEMKIN PSR is the core reactor model for our equivalent reactor networks**



*From S. Zitney, APECS Workshop, Oct 2009.

The next step will be to wrap a "Cluster" of PSRs to allow a network with recycle flows

- **In CHEMKIN, the PSR Cluster is solved as a single computational job**
  - Numerically, all PSRs in the Cluster are fully coupled
  - Multiple inlets, single outlet



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Concurrently, we are looking at extending ENERGICO capabilities for gasification

- **Identify key flow parameters**
  - Focus on Entrained Flow Gasifiers
  - Use as filters to generate ERN
- **Handle multi-phase flow properties**
  - Particle density, size distribution, composition
- **Test kinetics models for gasification processes**
  - Literature search
  - Incorporation into CHEMKIN's gas and surface-chemistry formalisms

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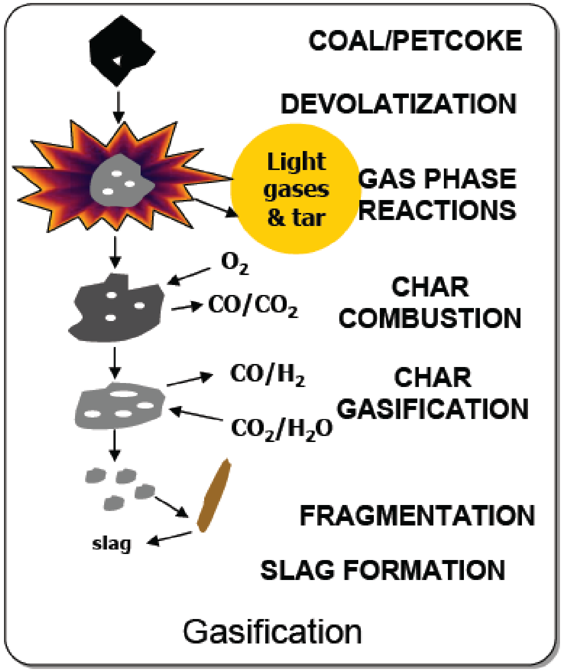
Gasification model will start by testing what's available in the literature

- **Processes that need to be considered:**
  - Early particle devolatilization, pyrolysis, and reaction
  - Char particle burn out
  - Gas phase reaction mechanisms for pyrolysis and reforming
  - Interactions with the slag (molten ash) within the gasifier



From L. Oshinowo, NETL 2009 Workshop on Multiphase Flow Science, 2009

Expected major milestones in first 18 months

A	Title: Planned Date: Verification Method:	CAPE-OPEN Interface for Single CHEMKIN PSR 6/1/2010 Test in Aspen Plus Process Simulator, compare with CHEMKIN stand-alone results, and report on success.
B	Title: Planned Date: Verification Method:	CAPE-OPEN Interface for CHEMKIN PSR Cluster 9/15/2010 Test in Aspen Plus Process Simulator, compare with CHEMKIN stand-alone results, and include in topical report.
C	Title: Planned Date: Verification Method:	ENERGICO Extended to Handle Particles in Flow 2/15/2011 Test with simplified CFD case and verify mapping of CFD to ERN zones; include in topical report

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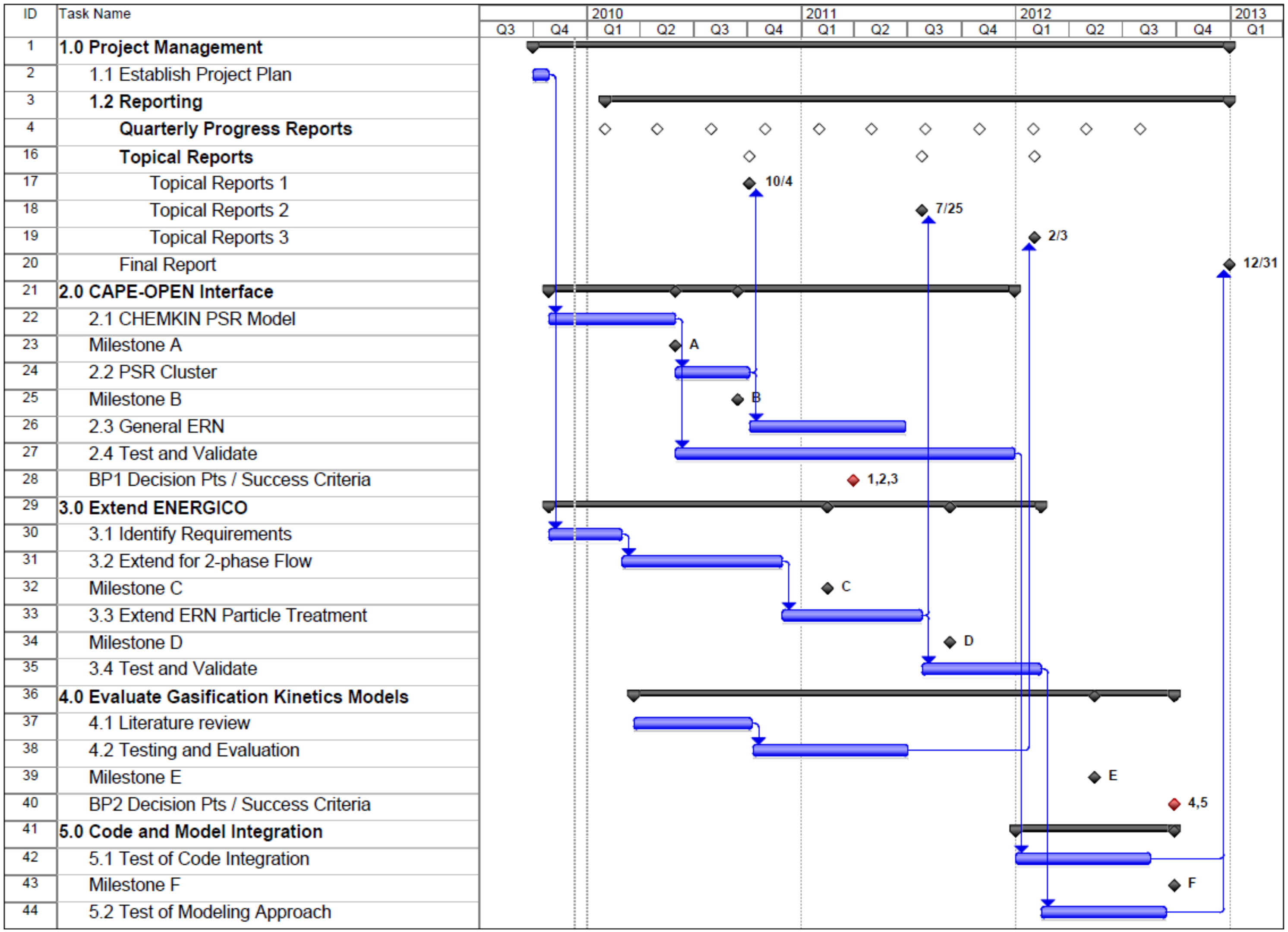
Deliverables will include reports and models

- **Topical reports**
  - CAPE-OPEN integration with CHEMKIN PSR models
  - ENERGICO extensions for gasification applications
  - Assessment of coal-gasification kinetics models
- **Models**
  - NETL access to the ENERGICO™ Simulation Package, for duration of project
  - NETL access to software modifications and enhancements made during this project
  - All model input parameters for reported results

Project Timeline



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Progress to date

- **We have a draft project plan in place for the first 12 months**
- **We are in the process of getting familiar with the details of CAPE-OPEN architecture requirements**
  - Identifying any changes needed in our CHEMKIN architecture to accommodate a wrapper approach
- **We have placed a PO for an AspenPlus License**
- **Conversations have begun with potential gasifier manufacturer partners**

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We might need some help from NETL

- **Technical contact, who could provide guidance on CAPE-OPEN implementation, in case we get stuck**
- **Sample multi-phase flow CFD case(s) we could use to test ERN extraction**
  - Test dependencies on different filters
- **Any verification data for kinetics model development for gasification process**

Summary

- **We are ramping up quickly on the new project**
- **The project is focused on the use of equivalent reactor networks to allow overlay kinetics on detailed flow (CFD) simulations**
- **The scope of the project is for coal gasifiers**
  - We are particularly interested in IGCC operations
- **Reaction Design has some unique capabilities that provide a good starting point for this work**
- **As a software company, our goal is to provide commercial product as a result of this project**

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