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

DE-FE0001074

reaction DESIGN

Ellen Meeks

March 13, 2012
NETL, Morgantown, WV

LEADING THE WAY TO CLEAN COMBUSTION DESIGN

Outline

- **Overview of project**
  - Project goals & scope
  - Technical contributors
  - Base technology for project
- **Summary of Current Status**
  - Tasks and Milestones
  - Deliverables
  - Timeline and Status

Our main goal is to provide innovative reduced-order models for APECS

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

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

- **Tony Garratt, Technical lead**
  - Senior Numerical Analyst and Team Lead at RD
  - Worked for 15+ years at Aspentech
- **C.-P. Chou, Staff Development Engineer**
  - Combustion and surface-chemistry expert
- **Devin Hodgson, Software Engineer**
  - Programming expert
- **Scott Drennan, Director of Apps Engineering**
  - Liaison with potential customers and applications
- **Ellen Meeks, PI**
  - Head of Product Development at Reaction Design

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ENERGICO™ and CHEMKIN-PRO® provide the baseline technology for the project

- **CHEMKIN is Reaction Design's flagship product**
  - 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
- **ENERGICO applies kinetics to complex flows**
  - Creates equivalent-reactor network model from CFD
  - Addresses key issues for gas-turbine combustor designers
    - Low Emissions Regulations
    - Fuel Flexibility
    - Combustion stability

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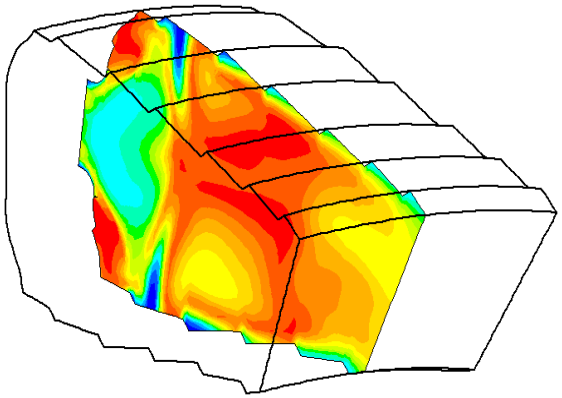
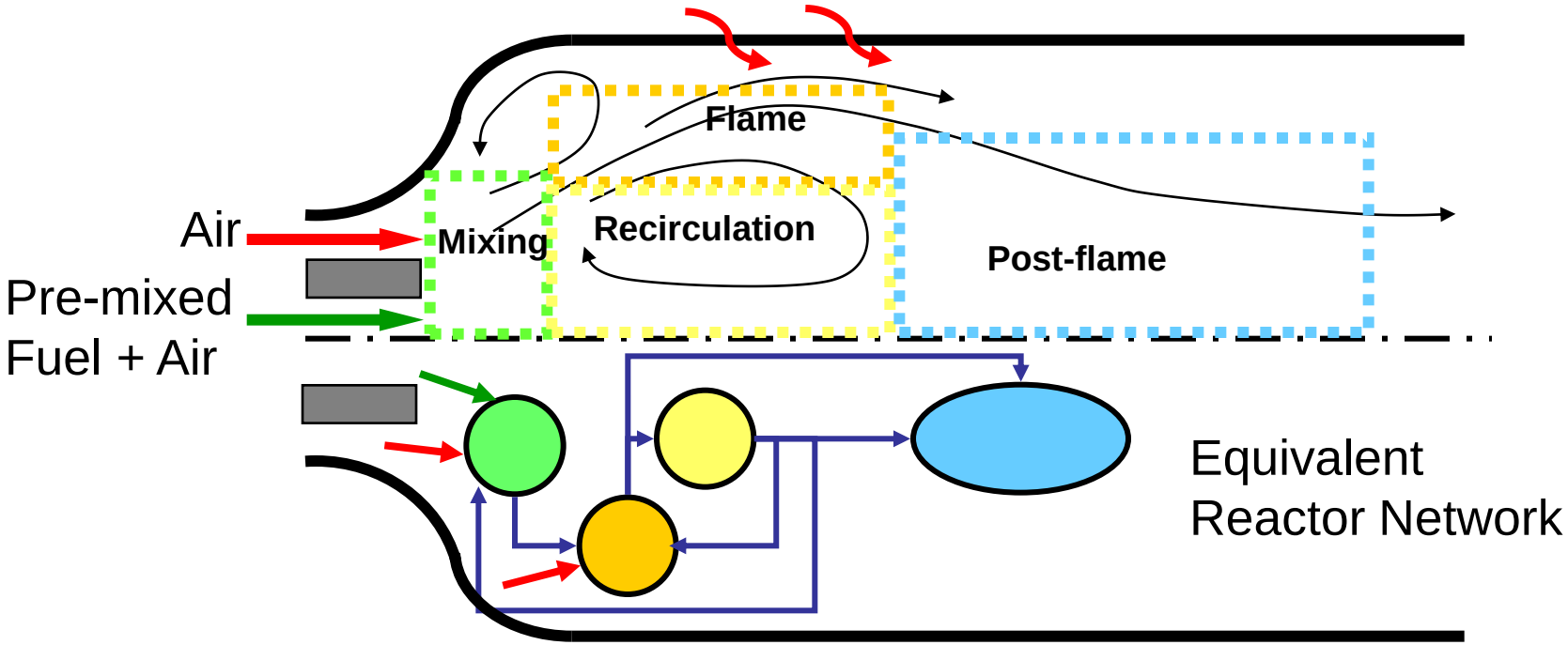
Reactor networks represent complex systems while allowing detailed kinetics



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



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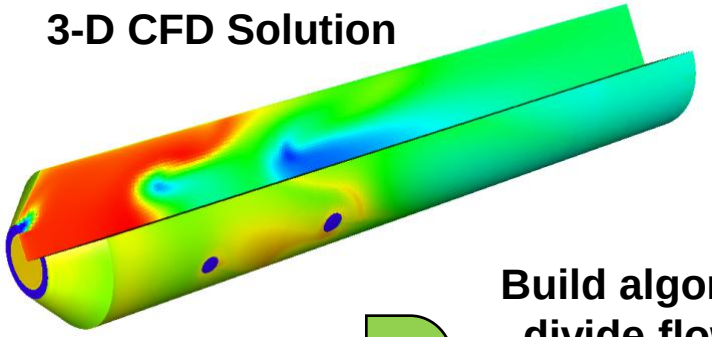
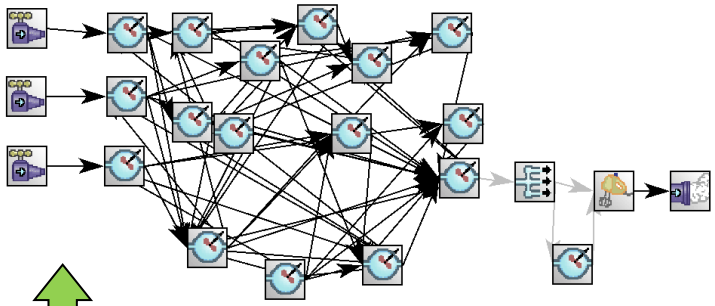
Automatic creation of Equivalent Reactor Networks adds chemistry to design flow

3-D CFD Solution

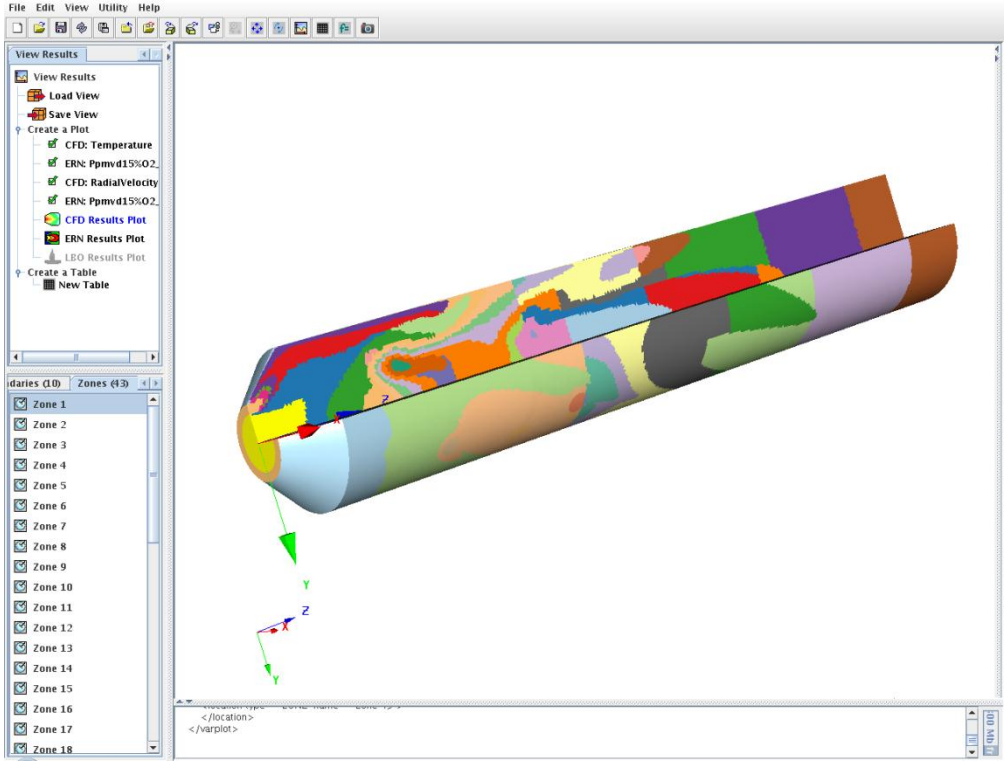


Build algorithm to divide flow field into reactor zones



Automatically create ERN

Improve your CFD model with greater kinetic understanding



Map chemistry results onto geometry view

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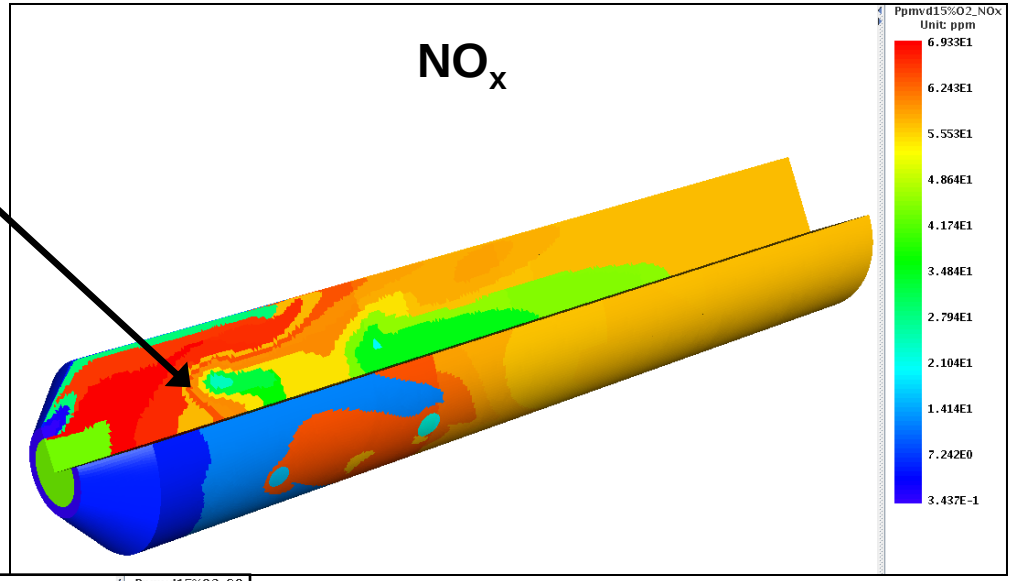
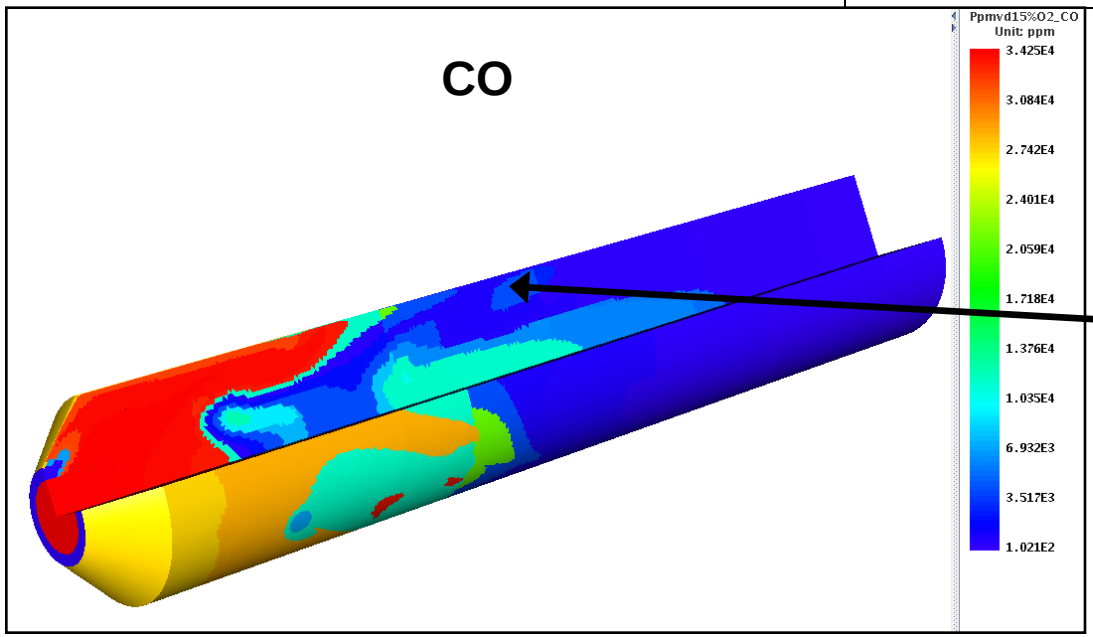
Results mapped back to the CFD mesh show ERN predictions in geometric context

Identify where NO_x emissions are formed





Identify where CO emissions are quenched

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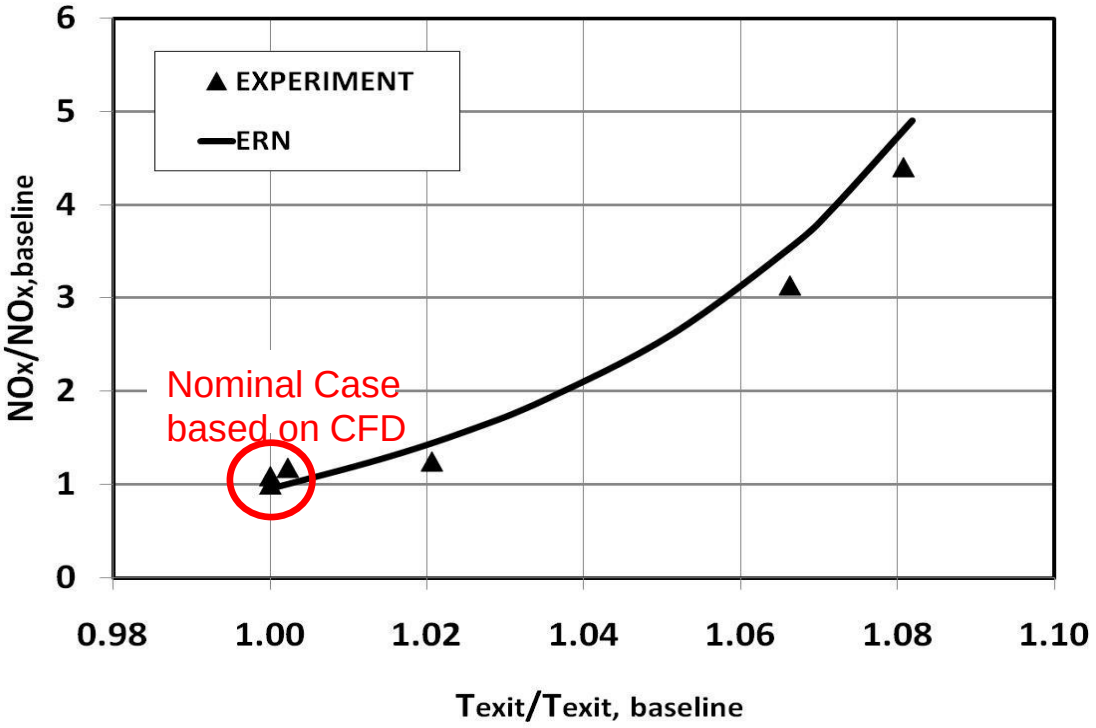
Joint work with GE demonstrated the ERN can *predict* impact of load variation on NO_x

- Affect of increased Fuel/Air Ratio predicted using ERN generated by a single CFD case
  - No change to ERN structure is needed to vary fuel load
  - No need to rerun CFD for every condition to predict kinetics effects



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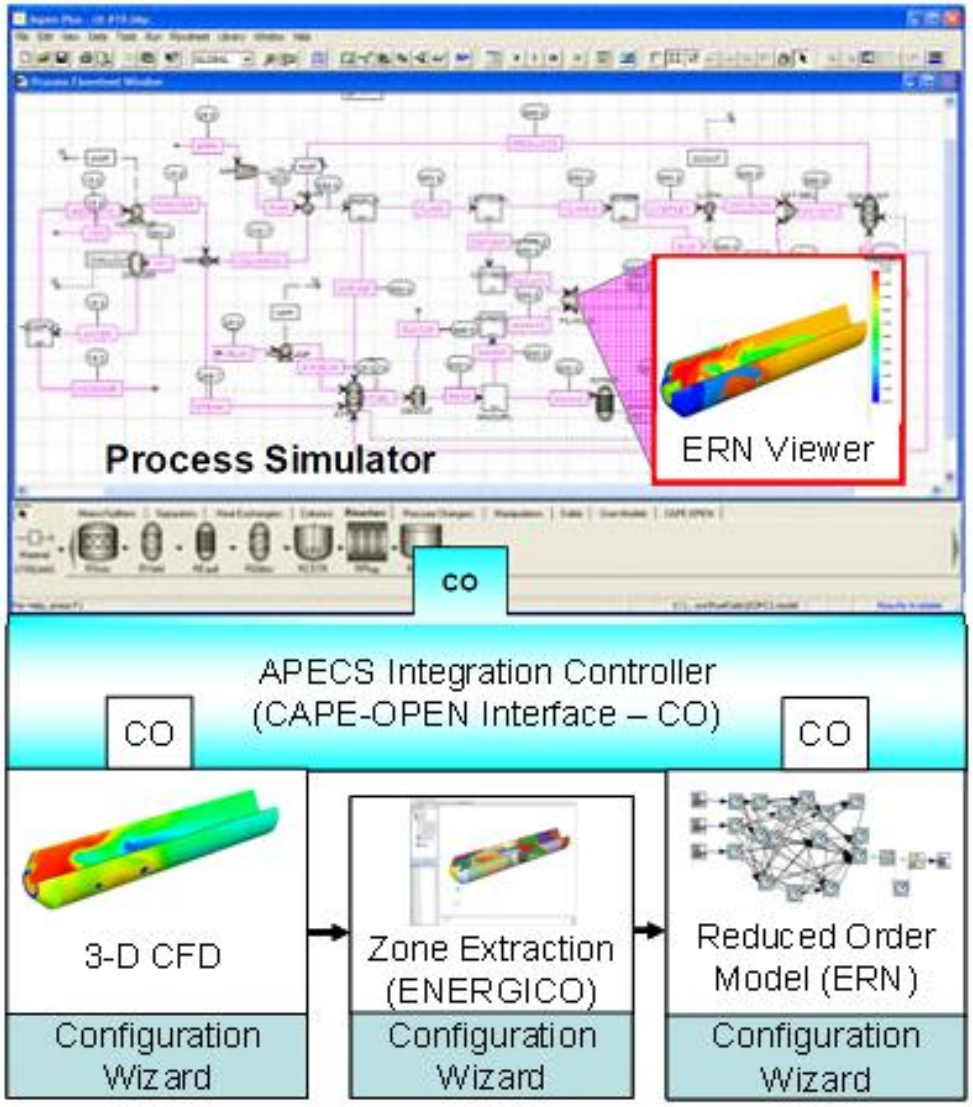
For this project, we are extending these concepts to gasifier simulations

- **Use ERN concept to generate "reduced order model" (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



Co-simulation project involving flowsheet simulation, CFD simulation, and Reduced-order Models (ROMs)

CAPE-OPEN architecture allows plug-and-play of different model hierarchies

*Adapted from S. Zitney, APECS Workshop, Oct 2009.

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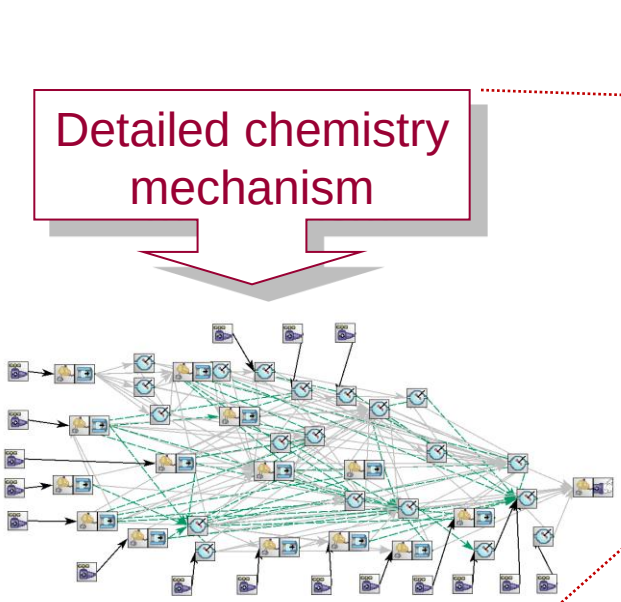
Major Tasks

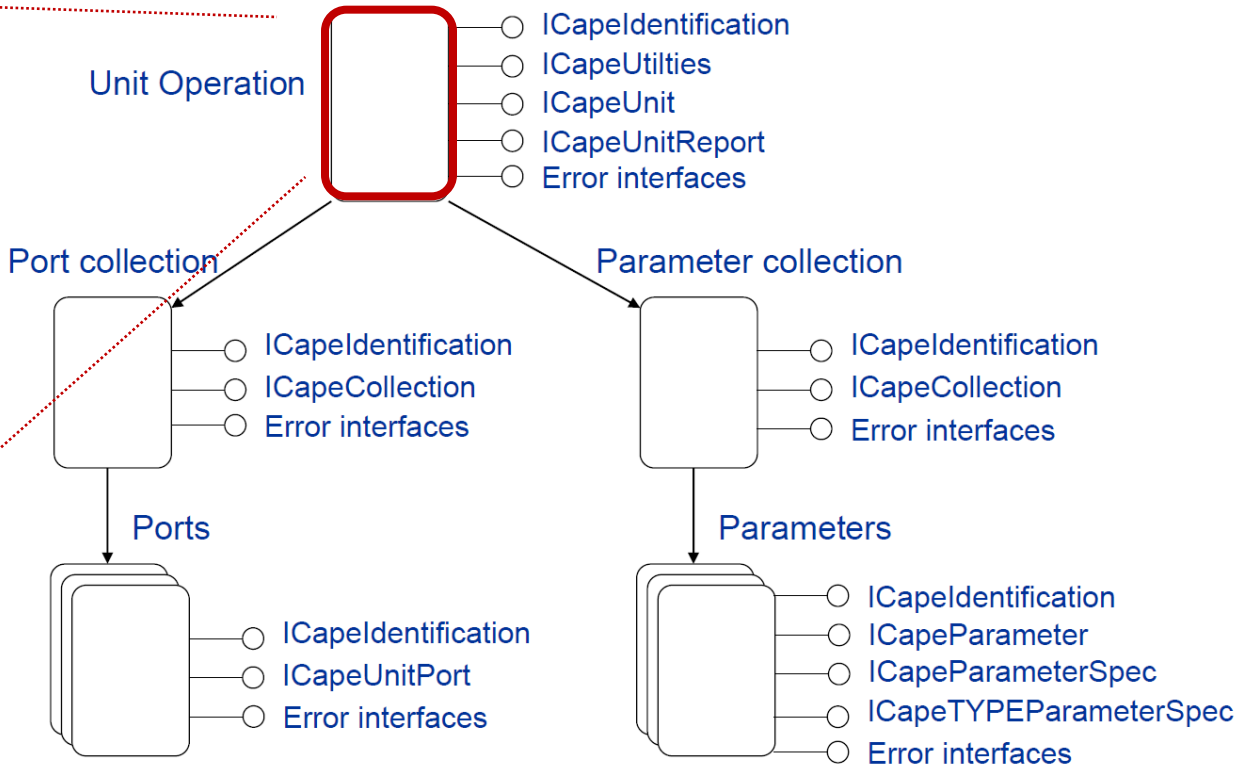
1. Project Management and Planning
2. Package CHEMKIN Models as a CAPE-OPEN Unit Reactor Model
3. Extending ENERGICO Software and Workflow for Gasifier Models
4. Evaluate Gasification Kinetics Models
5. Code and Model Integration, Testing and Validation

Task 2: The goal of this task is to wrap a complex ERN into a single Unit Operation

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



CAPE-OPEN Unit Operation Interface*



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

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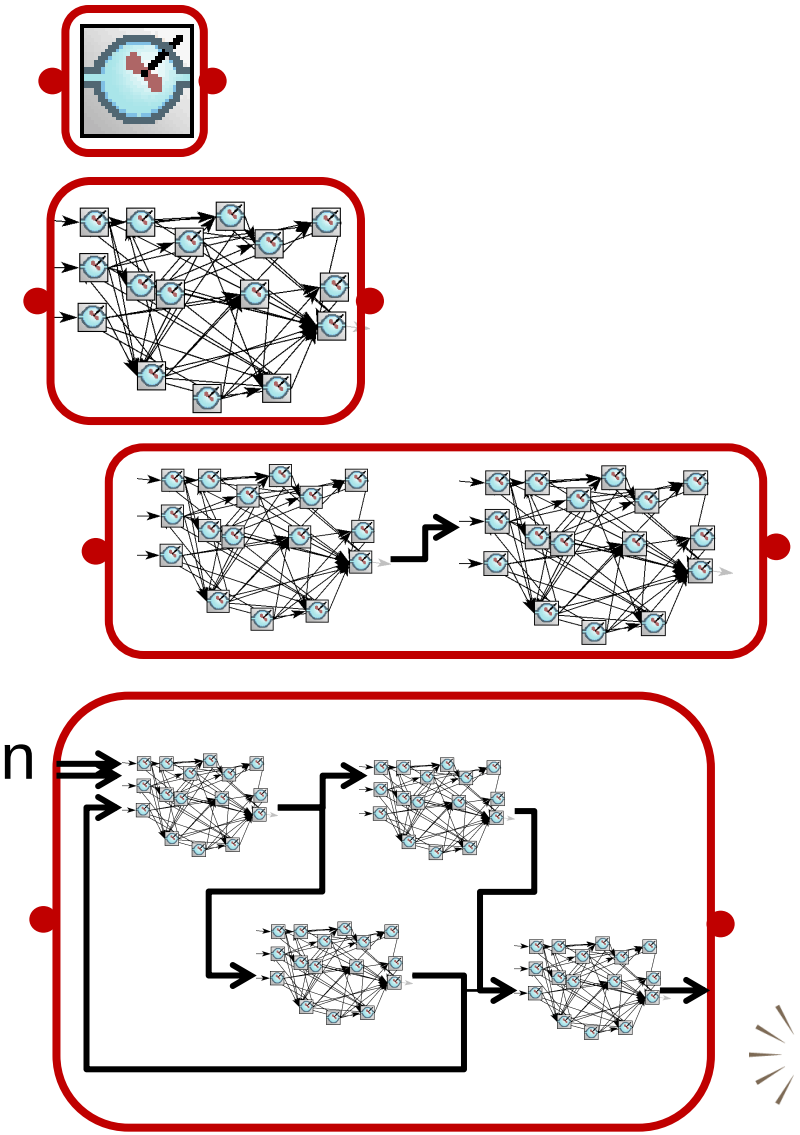
Task 2: We are near completion of this task

- ✓ **Single Perfectly Stirred Reactor (PSR)**
- ✓ **"Cluster" of PSRs**
  - PSRs within a Cluster are solved in one executable
- ✓ **Serial network of PSR Clusters or PFRs**
  - Multiple computations within one Unit Operation
- ▪ **Fully General ERN**
  - Tear-stream algorithm required inside CO object



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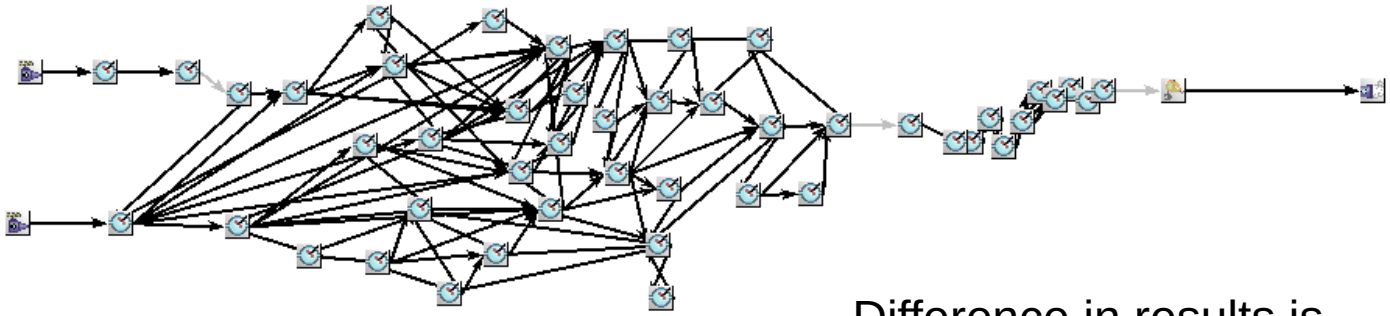
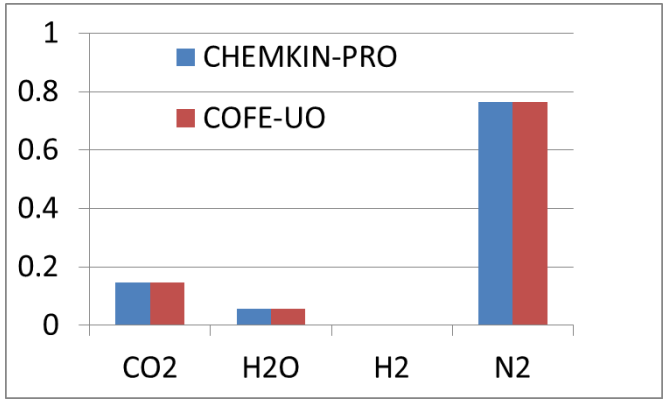
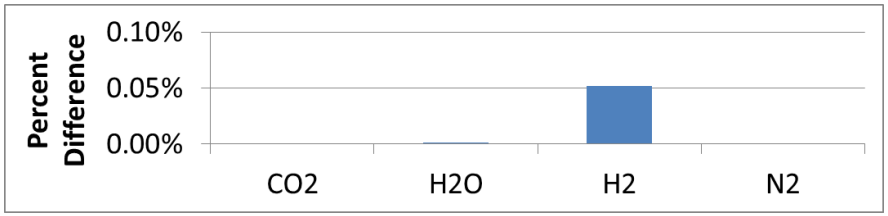
Task 2: Validation of a Serial Network of Clusters was validated in COFE Simulator

- **Results compared to stand-alone CHEMKIN-PRO simulation for ENERGICO-generated ERN representing a coal gasifier**





Difference in results is less than 0.1 % for even the trace species



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Task 2: Summary of Status

- **Major accomplishments in last year:**
  - Entire ERN packaged as one Unit Operation
  - Allows Gasifier “Unit” to be defined easily in APECS
  - Allows use of ENERGICO algorithms to generate ERN
  - New export option implemented in CHEMKIN-PRO to export CAPE-OPEN ERN definition
  - The CO Unit Operation DLL reads this ERN definition file to set up the entire ERN within one Unit in the Flowsheet Simulation
- **Work remaining**
  - Implement tear-stream algorithm within the UO object

Task 3: We have completed extensions needed to ENERGICO for gasifier workflow

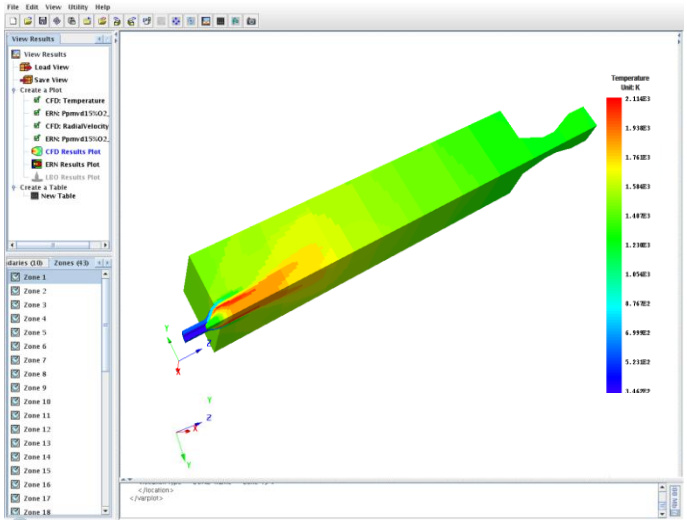
- **Identified key flow parameters**
  - Focused on Entrained Flow Gasifiers
  - Determined best filters to extract ERN from CFD
- **Handle multi-phase flow properties**
  - Particle density, size distribution, composition
  - ENERGICO was modified to handle discrete-phase sources of chemical species
    - Tested first with vaporization from FLUENT spray models
    - Verified with gasification source terms
- **Tested full workflow from CFD => ROM execution in CAPE-OPEN flowsheet**

NETL helped us acquire sample problems for application of ERN concepts

- **Acquired a 2-D and 3-D version of tutorials in FLUENT for coal gasification**
  - Includes discrete phase and reacting flow
- **Acquired real-world case from Steve Zitney (NETL)**
  - Also a FLUENT case, uses the discrete-phase model in reacting flow

CFD=>ROM workflow starts with the import of a (FLUENT) CFD model

FLUENT CFD Simulation results file for coal gasifier simulation



ENERGICO User Interface

Step 1: Read CFD file into ENERGICO

Step 2: Read in Chemistry Set

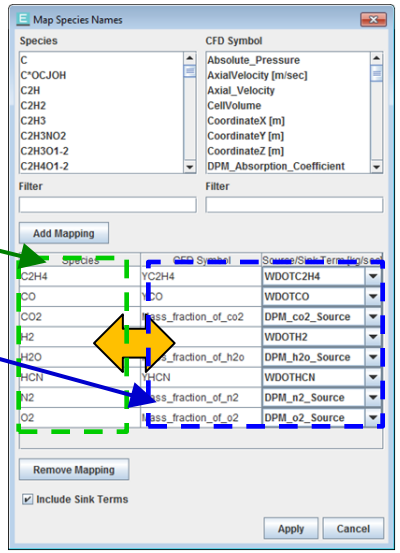
- Identify chemistry to be used in ERN

Step 3a: Map Variables

- Temperature
- Pressure
- Composition

Species Symbols in CHEMKIN mechanism

CFD variable names and source terms



Step 3b: Special Mapping

- Map the lumped pseudo-volatile in the CFD DPM source to an equivalent gas mixture of actual chemical species

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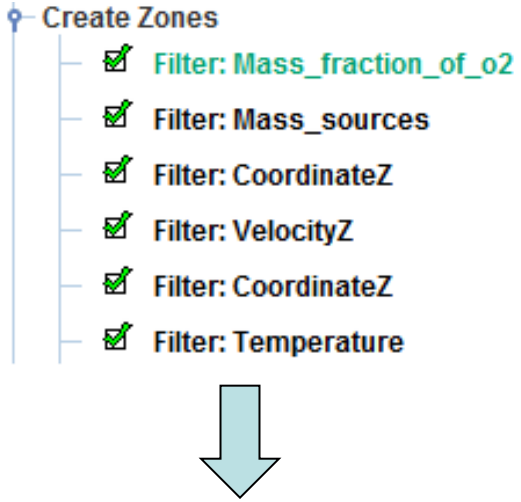
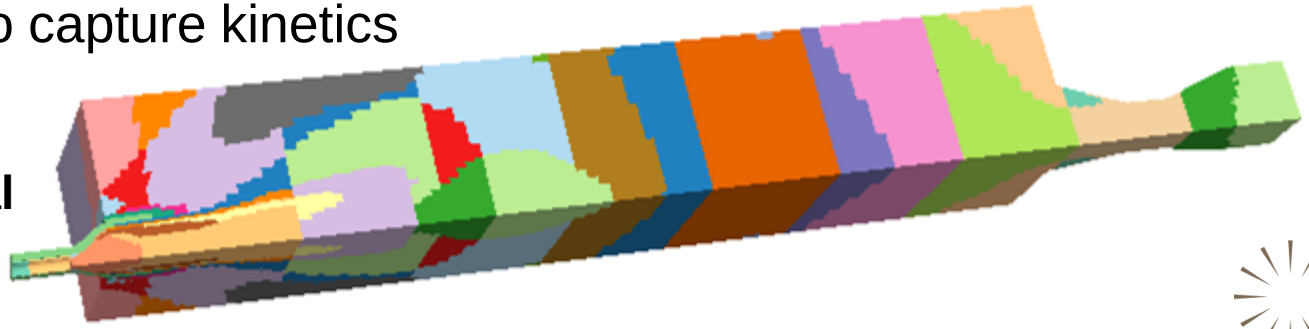
The next step is to define the zones that will separate regions by kinetics similarity

- **Step 4: Apply Filters to define ERN-generation algorithm within ENERGICO**
  - O_2 filter isolates the air inlets
  - DPM source filter isolates coal devolatilization and combustion regions
  - Z-coordinate filter separates fuel inlets
  - Axial velocity filter isolates recirculation zones
  - Z-coordinate filter divides the post-flame zone into a series of PSRs
  - Temperature filter refines all zones in the combustor to capture kinetics



Resulting 47-zone partition of the coal combustor



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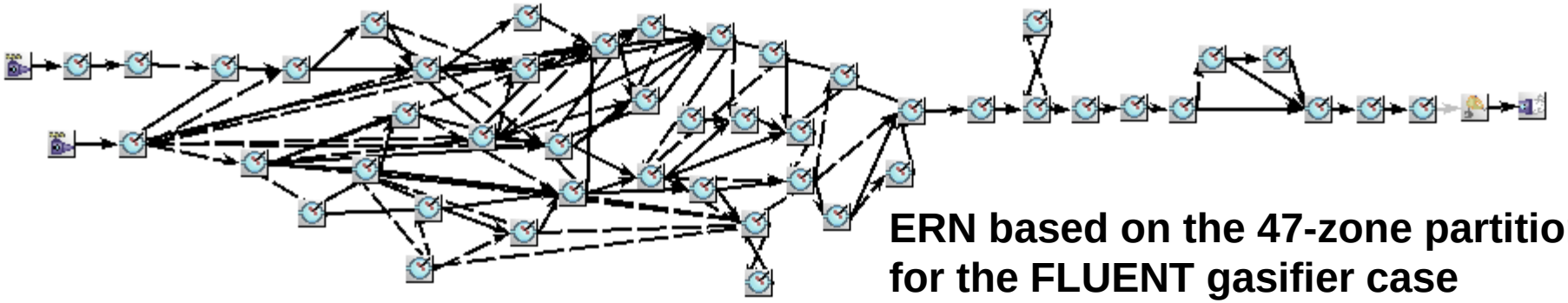
ENERGICO then automatically calculates flow connections and generates the ERN

- **Step 5: Create ERN, which opens CHEMKIN-PRO**



ERN based on the 47-zone partition for the FLUENT gasifier case

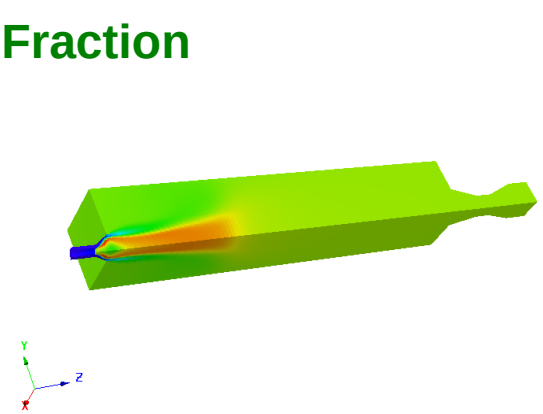
  - Set up to use the more detailed kinetics model within CHEMKIN-PRO
- **Step 6: Verification**
  - Solve the ERN within CHEMKIN-PRO (within ENERGICO)
    - Verifies connectivity, tests convergence behavior
  - Visualize results in ENERGICO, to see geometric results

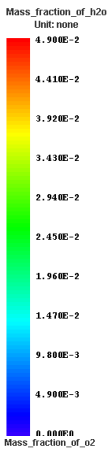
Comparison of results between original CFD and the ERN Solution (H_2O and O_2)

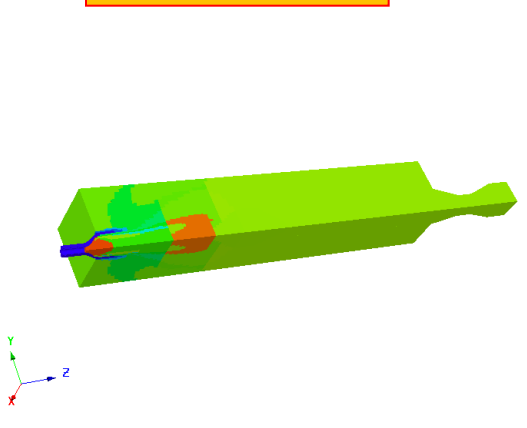
CFD Result

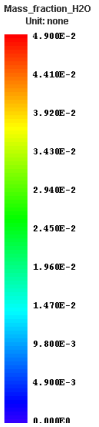
ERN Result

H_2O Mass Fraction

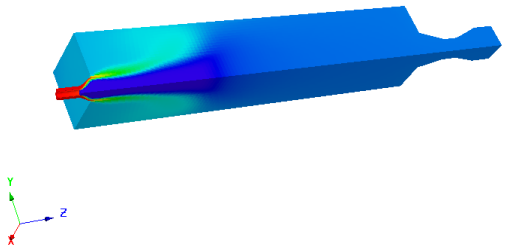


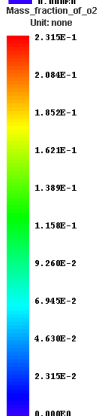


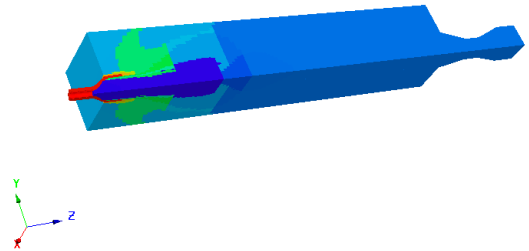


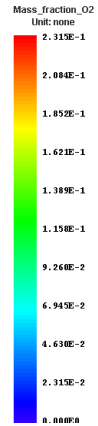


O_2 Mass Fraction









- H_2O and O_2 contours agree well between CFD and ERN

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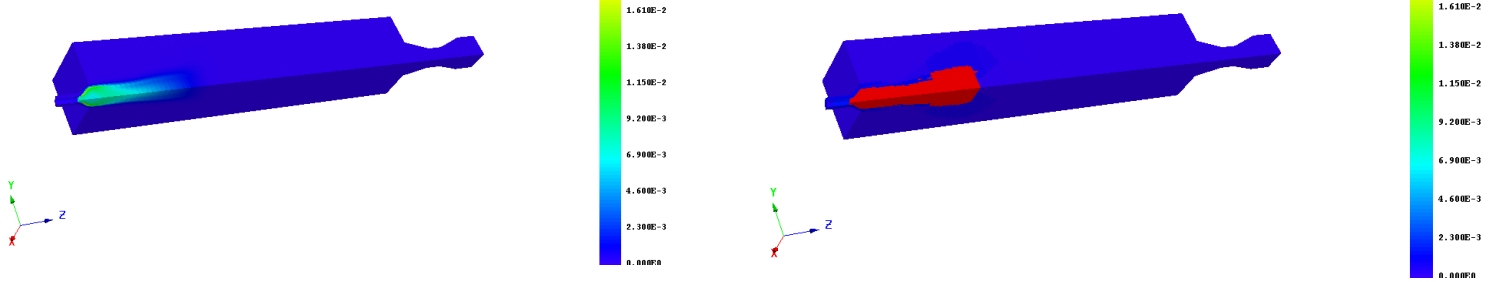
Comparison of results between original CFD and the ERN Solution (CO and CO_2)

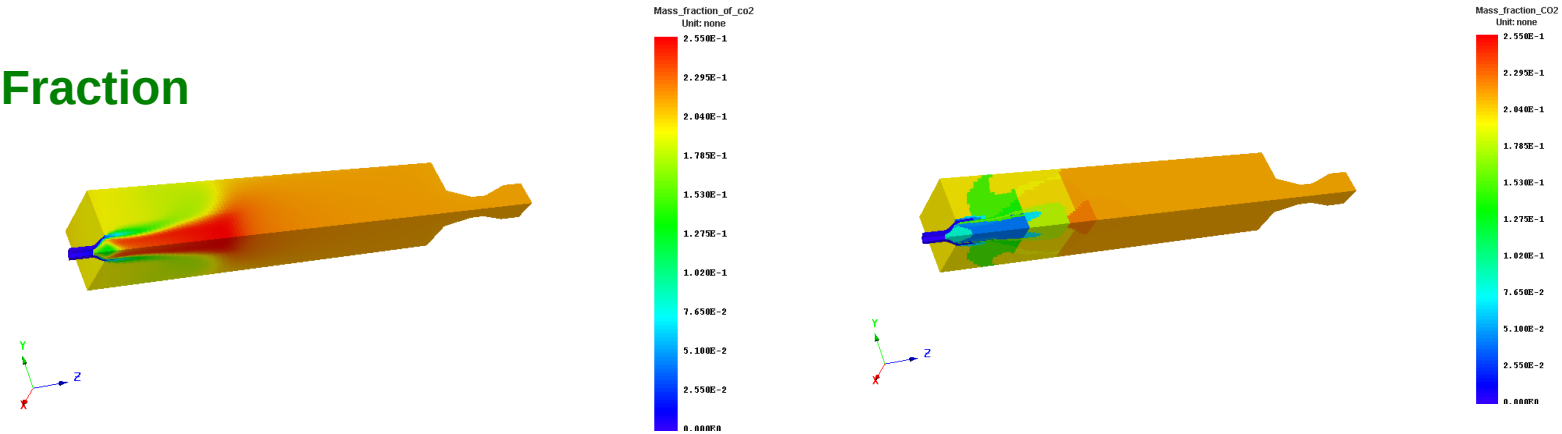
CFD Result

ERN Result

CO Mass Fraction



CO_2 Mass Fraction



- **Differences are due to the different assumptions between ERN and CFD models, regarding coal devolatilization (gaseous) products**

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The ERN can predict values for species that could not be included in the CFD model

NO (PPM on dry basis)

ERN Result

- **In this way, the ROM Is more than just a ROM**

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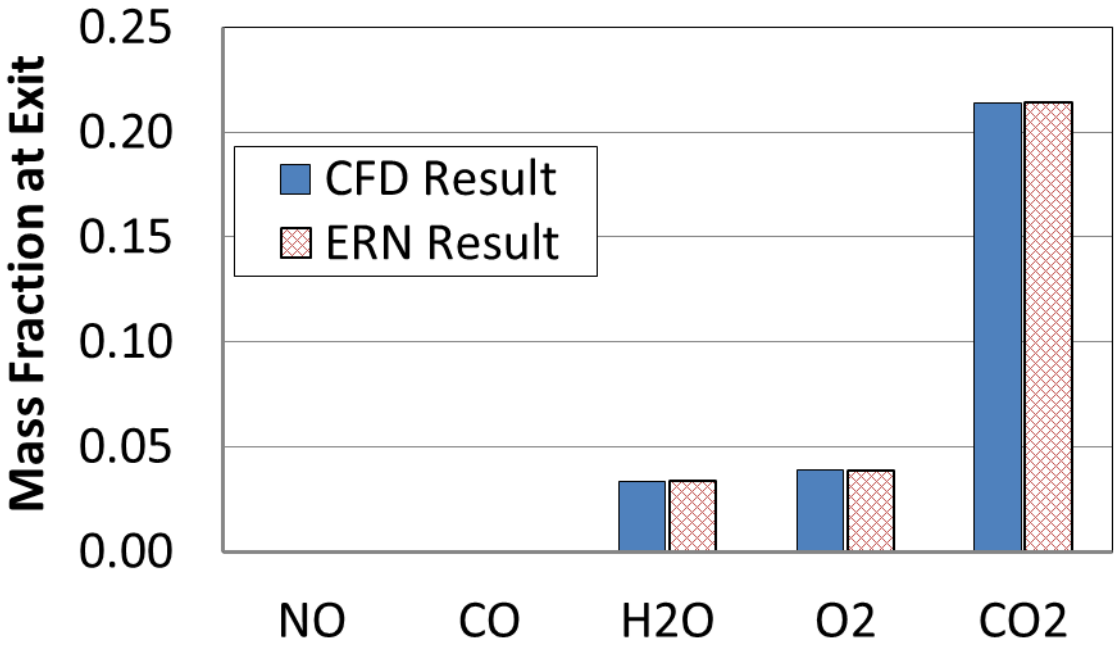
Quantitative comparison at the gasifier exit confirm that the ERN represents the CFD well

- **Predictions of average outlet species mass fractions are in good agreement**
- **With detailed chemistry, ERN can provide additional information, such as NO_x emissions**



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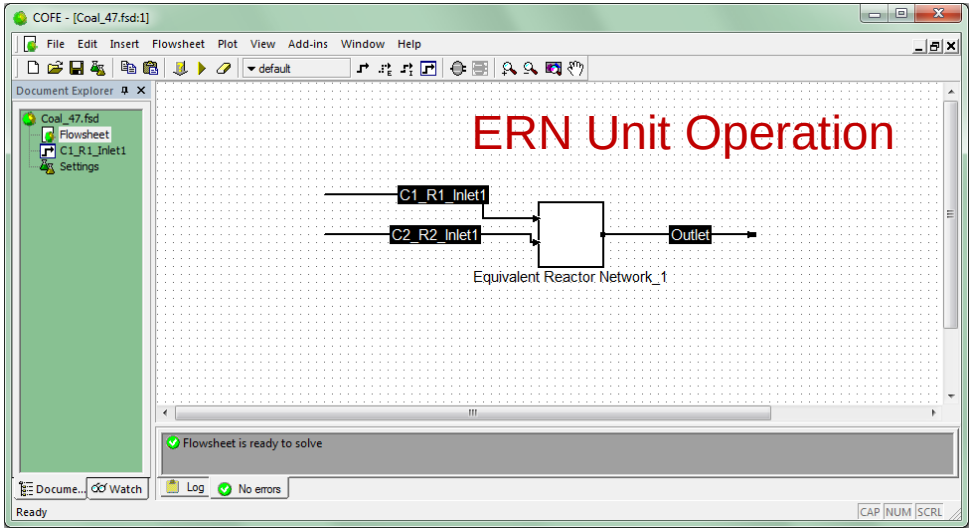
After verification, the next step is to export the ERN for input to the CAPE-OPEN object

- **Step 7: Export the ERN from CHEMIN using CKCAPE export (new button on "Run" panel)**

Custom file format defining CO ERN object

COFE Flowsheet, with Cape-Open Encapsulated Object for the ERN Unit Operation



- **Set up flowsheet with identical inlets but solve ERN via CAPE-OPEN Unit Operation**

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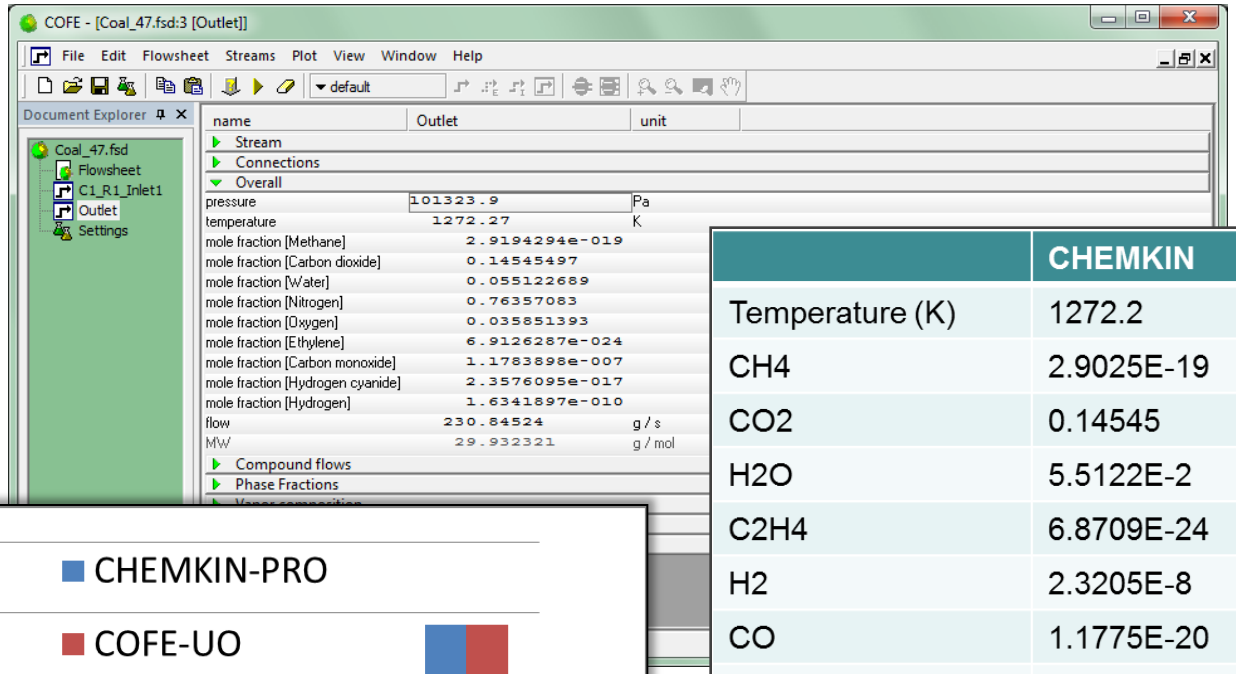
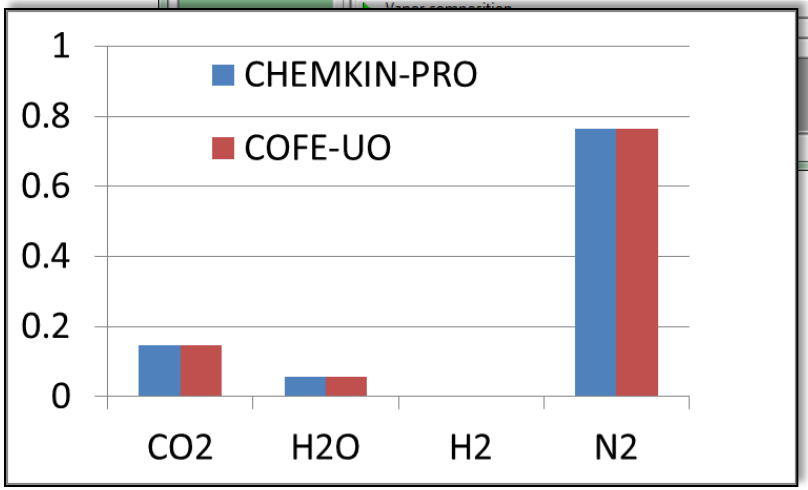
Final step in workflow: hook ERN into flowsheet model and run; verify results

- **Step 8: Verification of results within Flowsheet**

Results reported in COFE Interface





	CHEMKIN	COFE
Temperature (K)	1272.2	1272.2
CH4	2.9025E-19	2.9194E-19
CO2	0.14545	0.14545
H2O	5.5122E-2	5.5123E-2
C2H4	6.8709E-24	6.9126E-24
H2	2.3205E-8	2.3217E-8
CO	1.1775E-20	1.1783E-20
HCN	2.3443E-17	2.3576E-17
N2	0.76321	0.76321

Comparison to CHEMKIN Results for same ERN

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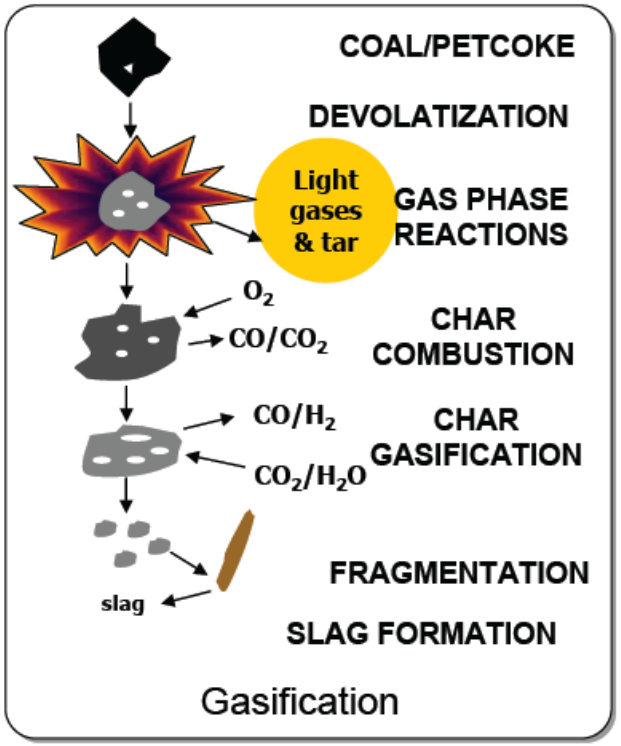
Task 3 Summary: Implementation of changes to ENERGICO is complete

- ✓ **Obtained Gasifier CFD test cases**
- ✓ **Extended ENERGICO to allow use of 2-phase flow information from CFD; particles in flow**
- ✓ **Determined appropriate filters for extracting ERN form CFD**
- ✓ **Tested and Validated expected results for generated ERNs**
  - ✓ CHEMKIN-PRO results agree with CFD
  - ✓ CO Flowsheet with encapsulated ERN agrees with CHEMKIN results
  - ✓ Tested initial detailed reaction mechanism

Task 4: Evaluation of kinetics models is complete; implementation underway

- ✓ Performed Literature search and selected modeling approach
- ✓ Tested semi-empirical model with ENERGICO-ERN-CAPE-OPEN workflow
- ● In process of implementing higher-order kinetics model



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

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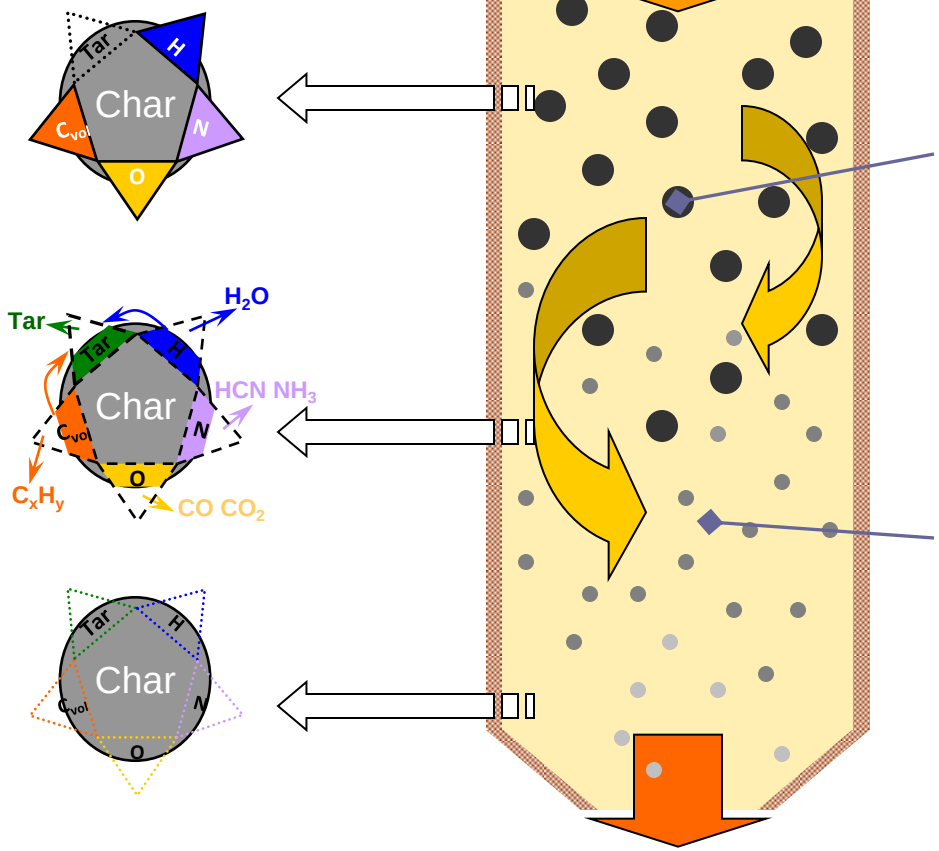
Task 4: Two approaches were identified for the gasification kinetics modeling

- ✓ **Semi-empirical model**
  - ✓ Empirical model of coal devolatilization
    - ✓ Fixed carbon is modeled as core "bulk" species
    - ✓ Volatiles are modeled as "surface" species that desorb to the gas
    - ✓ Rates and composition are derived from macroscopic data
  - ✓ Detailed model of gas pyrolysis & oxidation
- ● **Chemical Percolation Devolatilization model**
  - – Use NMR analysis data to derive composition and structure; generalize work done in prior academic studies
  - – Allow reactions that have distributed activation energies
  - – Include flash distillation as a pseudo "reaction"
  - ✓ Detailed model of gas pyrolysis & oxidation

A chemistry perspective on coal gasification

pulverized coal

Coal Composition



Chemical Processes

Thermal Cracking of Coal
- volatile gas release
- fragmentation/depolymerization
- tar release

Gas-phase Chemistry
- pyrolysis
- water-gas shift
- soot formation
- NO_x formation

syn gas (coal gas) + char

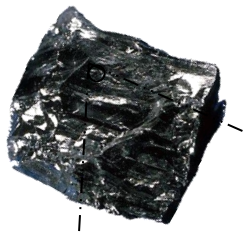
reaction DESIGN

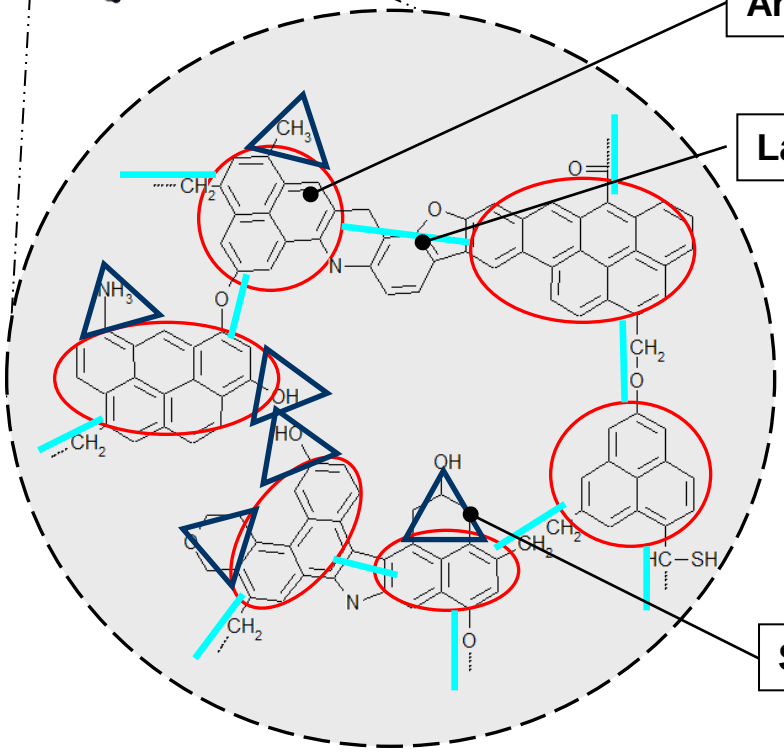
For the CPD Model, we have begun implementatino after detailed planning

- **Inputs to the model:**
  - Coal elemental composition
  - Particle size distribution
  - Operating conditions

- **Model outputs:**
  - Synthetic gas composition
  - Char size distribution
  - Tar yield and molecular weight distribution

Componentization of Coal Molecule

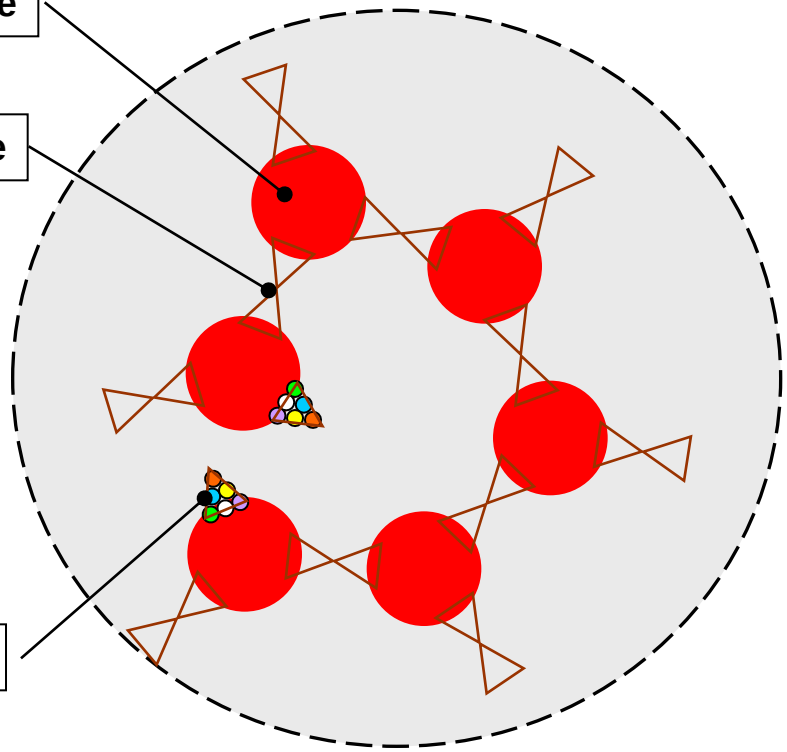




Aromatic Core

Labile Bridge

Side Chain

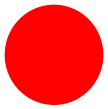
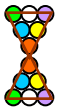


Hypothetical Coal Molecule

Statistical Bethe Lattice Model
Coordinate Number = 3

reaction DESIGN

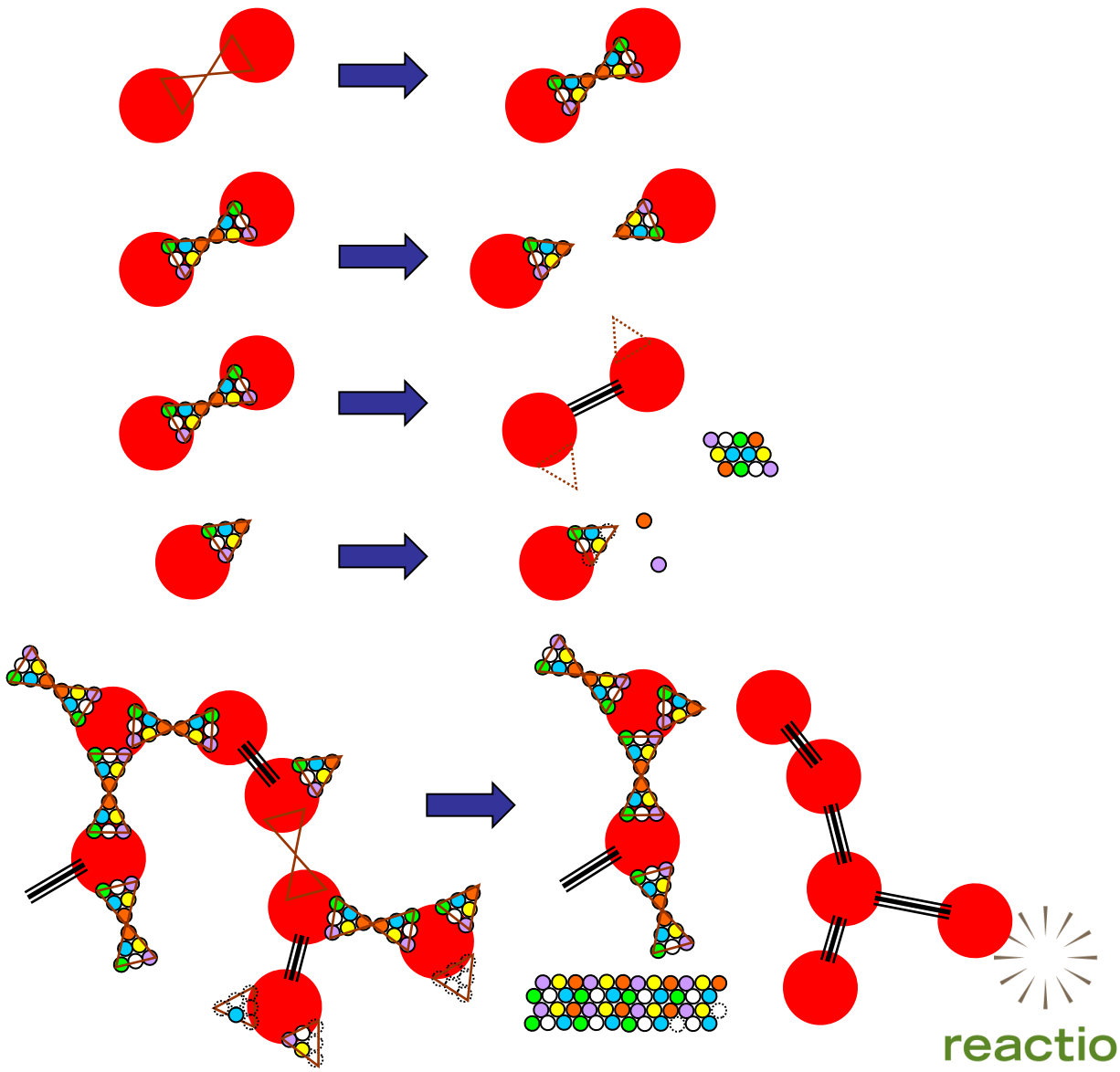
Coal bulk components will be represented as different “macros” in CHEMKIN description

Symbol	Component	Definition
	Aromatic Core	Fused aromatic ring cluster that forms a site of the Bethe lattice
	Labile Bridge	Molecular structures that serve as bridges connecting aromatic cores/sites
	Activated Bridge	Labile bridge that is active and ready to break down
	Side Chain	Peripheral molecular structures attached to aromatic cores
	Functional Group	Specific group of atoms within coal molecules that characterize the release of light gases
	Char Link	Permanent bond that fuses aromatic cores

Coal thermal cracking reactions are defined between “species” comprised of “macros”

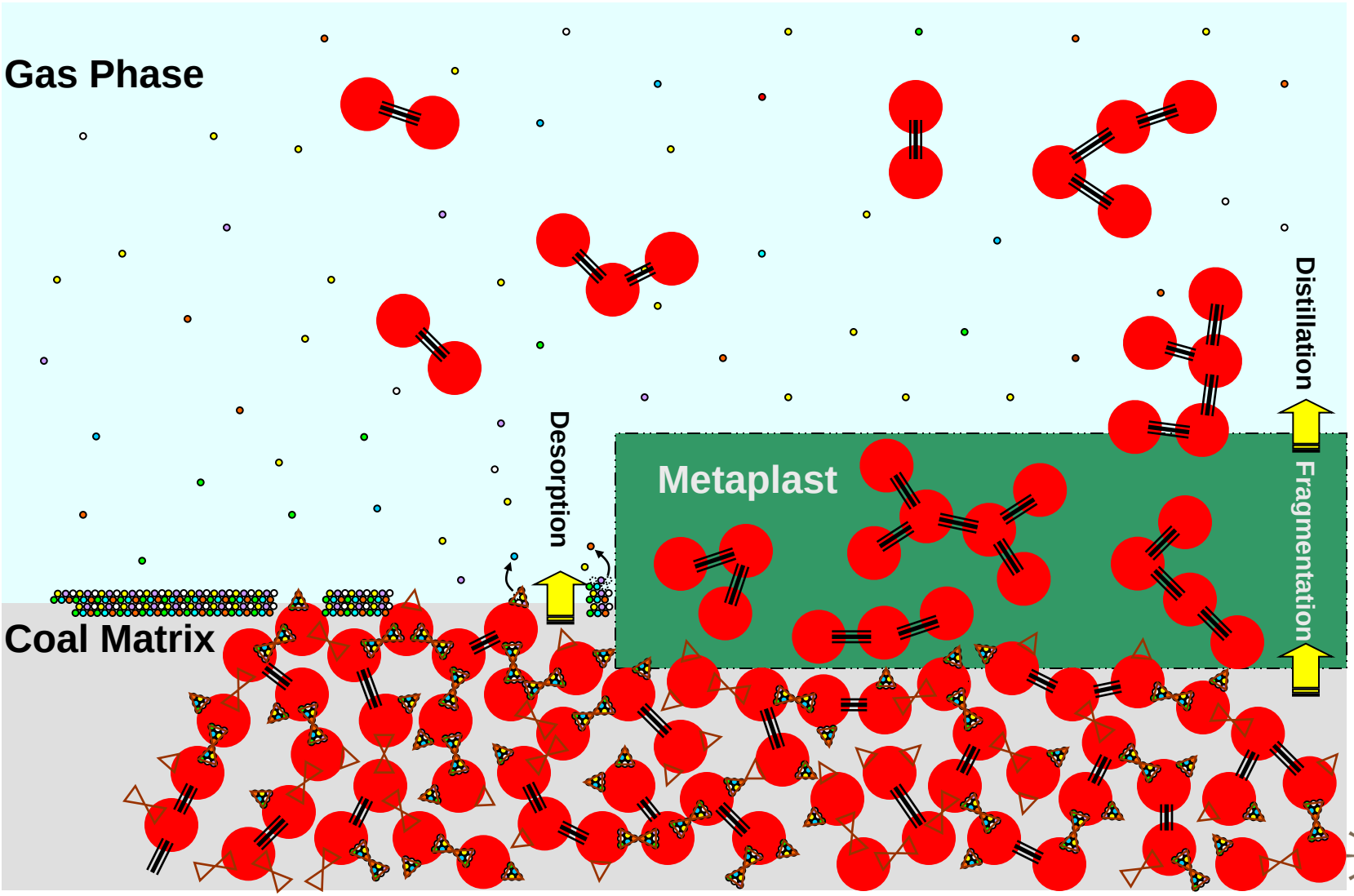
Reaction Types

1. Labile bridge activation
2. Cleavage of activated bridge
3. Aromatic core cross-link
4. Desorption of functional groups
5. Fragmentation of lattice structure
6. Distillation of tars



reaction DESIGN

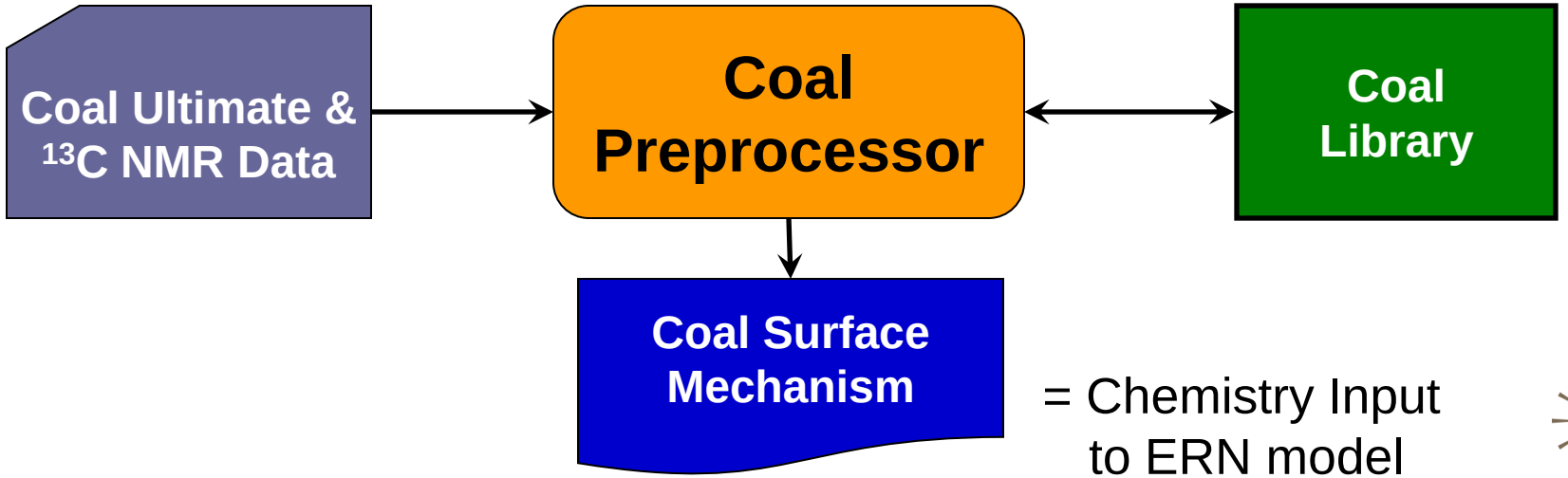
Surface chemistry representation of the coal devolatilization process



reaction DESIGN

A Coal pre-preprocessor will generate the coal surface mechanism from coal data

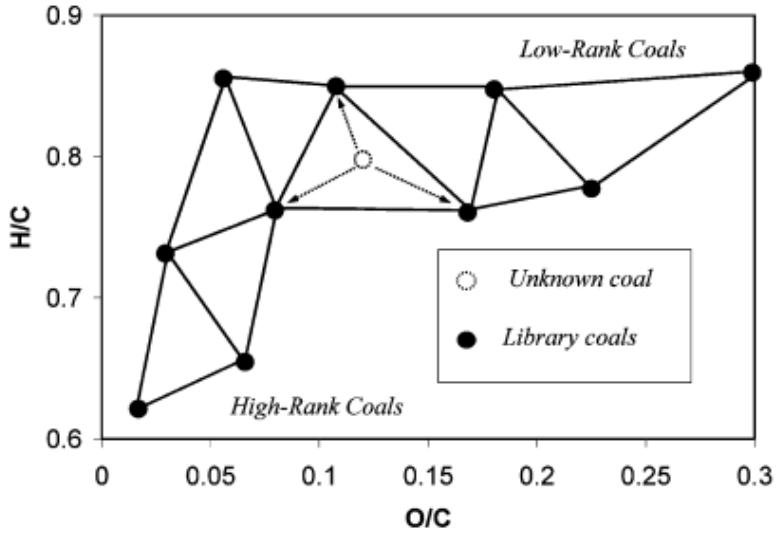
- **Coal elemental composition must be known to create an appropriate surface mechanism**
  - Molecular weights and elemental compositions of bulk species
  - Thermodynamic data of bulk species
  - Bridge scission and cross-link reactions



reaction DESIGN

To use the advanced CPD model, several model inputs are required

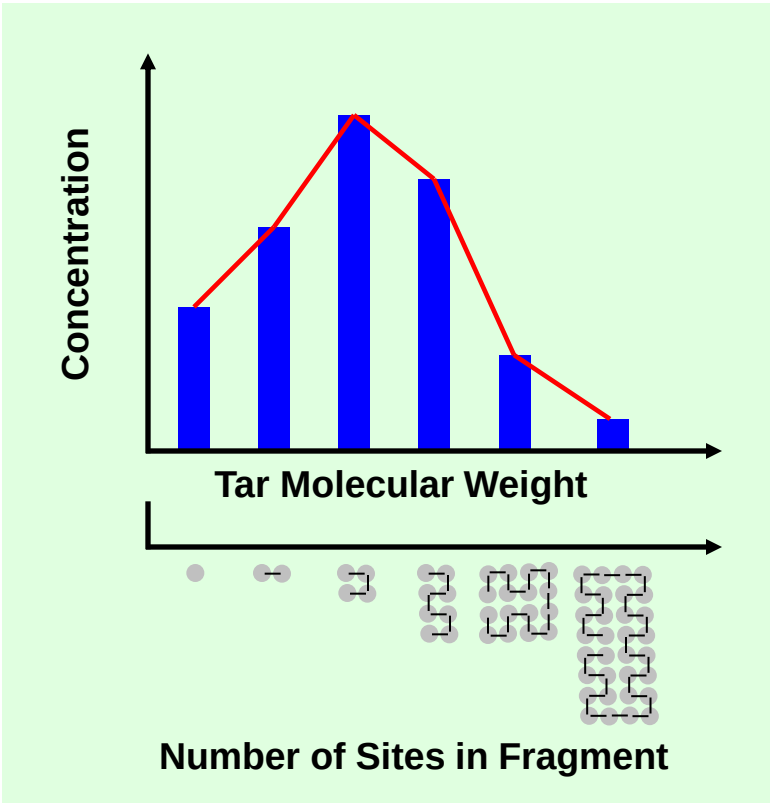
- **Coal Elemental Composition – C, H, O, N, S**
  - Ultimate Analysis Data
- **Coal Matrix Connectivity – (σ+1), p0, c0**
  - 13C NMR Analysis Data
  - Correlations to Elemental Composition
  - Coal Library
- **Functional Groups – Y0FG,k**
  - TG-FTIR Analysis Data
  - Coal Library



reaction DESIGN

The new coal model in CHEMKIN will allow reporting of key gasification results

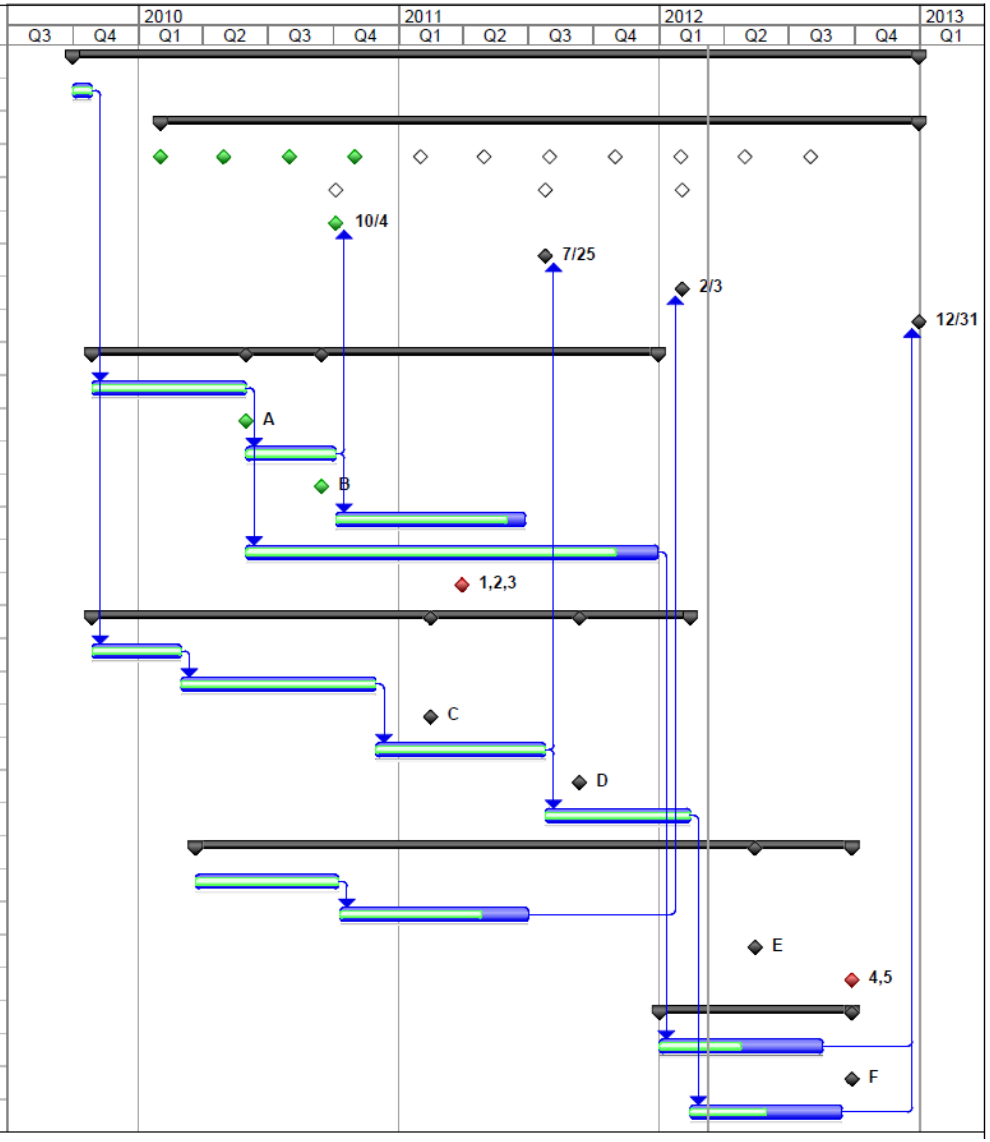
- **Total particle weight loss**
  - Percentage of original coal weight
- **Tar yield**
  - Percentage of original coal weight
- **Tar molecular weight distribution**
  - both liquid and gas phases



reaction DESIGN

Status against original project timeline

ID	Task Name
1	**1.0 Project Management**
2	1.1 Establish Project Plan
3	**1.2 Reporting**
4	**Quarterly Progress Reports**
16	**Topical Reports**
17	Topical Reports 1
18	Topical Reports 2
19	Topical Reports 3
20	Final Report
21	**2.0 CAPE-OPEN Interface**
22	2.1 CHEMKIN PSR Model
23	Milestone A
24	2.2 PSR Cluster
25	Milestone B
26	2.3 General ERN
27	2.4 Test and Validate
28	BP1 Decision Pts / Success Criteria
29	**3.0 Extend ENERGICO**
30	3.1 Identify Requirements
31	3.2 Extend for 2-phase Flow
32	Milestone C
33	3.3 Extend ERN Particle Treatment
34	Milestone D
35	3.4 Test and Validate
36	**4.0 Evaluate Gasification Kinetics Models**
37	4.1 Literature review
38	4.2 Testing and Evaluation
39	Milestone E
40	BP2 Decision Pts / Success Criteria
41	**5.0 Code and Model Integration**
42	5.1 Test of Code Integration
43	Milestone F
44	5.2 Test of Modeling Approach



reaction DESIGN

Milestone Status

A	Title: Planned Date:	CAPE-OPEN Interface for Single CHEMKIN PSR 6/29/2010 (Actual)
B	Title: Planned Date:	CAPE-OPEN Interface for CHEMKIN PSR Cluster 10/5/2010 (Actual)
C	Title: Planned Date:	ENERGICO Extended to Handle Particles in Flow 5/5/2011(Actual)
D	Title: Planned Date:	Viable Kinetics Models Identified 9/1/2010 (Actual)
E	Title: Planned Date:	ERN Model Extended to Allow Particle Gasification 3/15/2011 (Actual)
F	Title: Planned Date:	Full System Integration with Model Extensions 9/28/2012

Deliverables 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

Summary

- **The project is focused on the use of equivalent reactor networks to allow overlay of kinetics on detailed flow (CFD) simulations**
  - The scope of the project is for coal gasifiers, with particular interested in IGCC operations
- **Major progress has been achieved:**
  - Full workflow established for reading CFD model and producing CAPE-OPEN compliant Equivalent Reactor Network model that can be run in a flowsheet simulation
  - Workflow demonstrated with semi-empirical kinetics
  - Advanced kinetics model implementation is underway
  - Final task is code integration and testing