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

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NETL
Pittsburgh, PA

DE-FE0001074
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
APECS is a co-simulation program at NETL*

APECS Co-Simulation Workflow
Seamless Integration of CFD and Process Simulation Tasks

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
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
CHEMKNIN-PRO is our flagship product

- **CHEMKNIN** 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
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

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**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\textsubscript{x}), carbon monoxide (CO) and Unburned Hydrocarbons (UH)
    - New particulate emissions regulations
  - Fuel Flexibility
    - Alternative Fuels
    - Opportunity Fuels
    - Biofuels for carbon dioxide (CO\textsubscript{2}) reduction
  - Combustion stability
    - Lean Blow Off assessment
    - Flash-back
    - Ignition

International Civil Aviation Organization NO\textsubscript{x} Limits

<table>
<thead>
<tr>
<th>Year</th>
<th>NO\textsubscript{x} Limit (g/N)</th>
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<tbody>
<tr>
<td>2003</td>
<td>115</td>
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<tr>
<td>2006</td>
<td>100</td>
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<td>2009</td>
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</tr>
<tr>
<td>2012</td>
<td>80</td>
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</table>

Source: ICAO Colloquium on Aviation Emissions, May, 2007
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 combuster geometry on flowfield

Test:
Determine emissions, stability, fuel effects

ENERGICO addresses the gap in design workflow
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
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.
Sample ENERGICO results compared to data for gas-fired gas-turbine combustors

<table>
<thead>
<tr>
<th>Class of Combustor (all CO less than 10ppm)</th>
<th>Fuel Type</th>
<th>NO Variance</th>
<th>CO Variance</th>
</tr>
</thead>
<tbody>
<tr>
<td>10MW Less than 10ppm NO&lt;sub&gt;x&lt;/sub&gt;</td>
<td>Natural Gas</td>
<td>1ppm</td>
<td>2ppm</td>
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<tr>
<td>25MW 25ppm NO&lt;sub&gt;x&lt;/sub&gt;</td>
<td>Natural Gas</td>
<td>2ppm</td>
<td>2ppm</td>
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<tr>
<td>250MW Less than 10ppm NO&lt;sub&gt;x&lt;/sub&gt;</td>
<td>Natural Gas</td>
<td>1ppm</td>
<td>2ppm</td>
</tr>
<tr>
<td>250MW 25ppm NO&lt;sub&gt;x&lt;/sub&gt;</td>
<td>Natural Gas</td>
<td>2ppm</td>
<td>2ppm</td>
</tr>
<tr>
<td>250MW 25ppm NO&lt;sub&gt;x&lt;/sub&gt;</td>
<td>Syngas</td>
<td>2ppm</td>
<td>2ppm</td>
</tr>
</tbody>
</table>
Joint work with GE demonstrated the ERN can predict impact of load variation on NO$_x$.

- Increased Fuel/Air Ratio from single data point
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\textsubscript{x}, CO, UHC
  – Ability to determine contributions to NO\textsubscript{x}
    • Thermal NO\textsubscript{x}
    • Prompt NO\textsubscript{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.

CAPE-OPEN Unit Operation Interface*

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
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
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
<table>
<thead>
<tr>
<th></th>
<th>Title:</th>
<th>Planned Date:</th>
<th>Verification Method:</th>
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<tr>
<td>C</td>
<td>ENERGICO Extended to Handle Particles in Flow</td>
<td>2/15/2011</td>
<td>Test with simplified CFD case and verify mapping of CFD to ERN zones; include in topical report</td>
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</tbody>
</table>
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

<table>
<thead>
<tr>
<th>ID</th>
<th>Task Name</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.0 Project Management</td>
</tr>
<tr>
<td>2</td>
<td>1.1 Establish Project Plan</td>
</tr>
<tr>
<td>3</td>
<td>1.2 Reporting</td>
</tr>
<tr>
<td>4</td>
<td>Quarterly Progress Reports</td>
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<tr>
<td>5</td>
<td>Topical Reports</td>
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<td>Final Report</td>
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<td>10</td>
<td>2.0 CAPE-OPEN Interface</td>
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<td>11</td>
<td>2.1 CHEMKIN PSR Model</td>
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<td>Milestone A</td>
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<td>Milestone B</td>
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<td>Milestone C</td>
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<tr>
<td>15</td>
<td>2.3 General ERN</td>
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<tr>
<td>16</td>
<td>2.4 Test and Validate</td>
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<tr>
<td>17</td>
<td>BPI Decision Pts / Success Criteria</td>
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<tr>
<td>18</td>
<td>3.0 Extend ENERGICO</td>
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<tr>
<td>19</td>
<td>3.1 Identify Requirements</td>
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<td>20</td>
<td>3.2 Extend for 2-phase Flow</td>
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<td>3.3 Extend ERN Particle Treatment</td>
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<td>24</td>
<td>3.4 Test and Validate</td>
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<td>25</td>
<td>4.0 Evaluate Gasification Kinetics Models</td>
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<tr>
<td>26</td>
<td>4.1 Literature review</td>
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<td>27</td>
<td>4.2 Testing and Evaluation</td>
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<td>BP2 Decision Pts / Success Criteria</td>
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<tr>
<td>30</td>
<td>5.0 Code and Model integration</td>
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<td>31</td>
<td>5.1 Test of Code Integration</td>
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<tr>
<td>32</td>
<td>Milestone F</td>
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<tr>
<td>33</td>
<td>5.2 Test of Modeling Approach</td>
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</table>
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
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