Capabilities of the CCSI Toolset
David C. Miller, Ph.D.

9 August 2016
For Accelerating Technology Development

- Rapidly synthesize optimized processes to identify promising concepts
- Better understand internal behavior to reduce time for troubleshooting
- Quantify sources and effects of uncertainty to guide testing & reach larger scales faster
- Stabilize the cost during commercial deployment

**National Labs**
- Carnegie Mellon
- Princeton University
- Lawrence Livermore National Laboratory
- Los Alamos National Laboratory
- West Virginia University
- Boston University

**Academia**
- ADA
- ALSTOM
- B&W
- EPR
- Electric Power Research Institute
- SOUTHERN COMPANY
- RTI INTERNATIONAL
- ExxonMobil
- AEP
- American Electric Power
- CHEVRON
- CHEVRON PHILIPS CHEMICAL
- CHEMICAL PRODUCTS
- CHEMICAL PRODUCTS
- CHEMICAL PRODUCTS

**Industry**
- Fluor
- EPRI
- Eastman
- ANSYS
- Schneider Electric
- Linde

**SRI International**
Goals & Objectives of CCSI

- **Develop** new computational tools and models to enable industry to more rapidly develop and deploy new advanced energy technologies
  - Base development on industry needs/constraints

- **Demonstrate** the capabilities of the CCSI Toolset on non-proprietary case studies
  - Examples of how new capabilities improve ability to develop capture technology

- **Deploy** the CCSI Toolset to industry

Projects with industry

Current licensees
Advanced Computational Tools to Accelerate Carbon Capture Technology Development

Lab & Pilot Scale Experiments & Data

Physical Properties
Kinetics
Thermodynamics

Process Systems
Design, Optimization & Control

Device Scale Models
Validated 3-D, CFD
Maximize the learning at each stage of technology development

• Early stage R&D
  – Screening concepts
  – Identify conditions to focus development
  – Prioritize data collection & test conditions

• Pilot scale
  – Ensure the right data is collected
  – Support scale-up design

• Demo scale
  – Design the right process
  – Support deployment with reduced risk
Basic Data Requirements for CCSI Analyses

Sorbents
- Adsorption equilibrium, \( f(p_{y,i}, T, x_i) \)
  - All species over relevant conditions
- Heat of Adsorption for all species, \( f(T, x_i) \)
  - \( \text{CO}_2 \) and \( \text{H}_2\text{O} \) minimum
- Heat Capacity, \( f(T, x_i) \)
- Adsorption/Desorption Kinetics, \( f(p_{y,i}, T, x_i) \)
  - All species over relevant conditions
- Thermal Conductivity, \( f(T, x_i) \)
- Density, \( f(T, x_i) \)
- Particle Size Distribution
- Sphericity

Solvents
- Vapor-Liquid Equilibrium Data
  - over relevant \( p_{y,i}T, x_i \) ranges
- Heat of Absorption, \( f(T, x_i) \)
- Kinetic Data, \( f(p_{y,i}, T, x_i) \)
  - Including speciation
- Mass Transfer Data
  - from wetted wall column, bench scale system
- Viscosity, \( f(T, x_i) \)
- Heat Capacity, \( f(T, x_i) \)
- Density, \( f(T, x_i) \)
- Surface Tension, \( f(T, x_i) \)
- Vapor Pressure, \( f(T, x_i) \)
- Thermal Conductivity, \( f(T, x_i) \)
- Hydraulic Data for specific packing
CCSI Approach: Multi-scale Calibration

• Challenge:
  – Large number of parameters in bench scale models and properties submodels
  – Limited data = full calibration conceptually and computationally difficult.

• New approach:
  – Multi-scale calibration
  – Propagate uncertainty from properties models during bench scale calibration
Developing Detailed, Predictive Models of Solvent-Based Capture Processes

Steady-State and Dynamic Process Model

- Measurement Uncertainty
- Pilot/Commercial Scale Data
- Lab Scale Data
- Properties Package
- Chemistry Model
  - Thermodynamic Models
  - Transport Models
- Kinetic model
  - Hydrodynamic Models
  - Mass Transfer Models

Process UQ

Process UQ

Measurement Uncertainty

WWC/Bench/Pilot Scale Data

Measurement Uncertainty

Lab Scale Data

Properties Package

UQ

UQ

CCSI
Netl
Lawrence Livermore National Laboratory
Los Alamos National Laboratory
Pacific Northwest National Laboratory
U.S. Department of Energy
Highly Resolved Models for Solvent-based Capture

Predictive understanding at scale
Hierarchical multi-scale modeling framework

Micro/Meso-Scale VOF model

Macro-scale Two Fluid model

Effective mass transfer coefficient for different flow regimes

Fernandes et al., JSF, 2009

Raynal et al., Workshop, 2012
Major release November 2015
Updated June 2016
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<thead>
<tr>
<th>Time</th>
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<tr>
<td>1:30</td>
<td>Sub-Process Models</td>
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<tr>
<td>1:30</td>
<td>Baseline VLE Modeling</td>
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<td>2:50</td>
<td>Modeling Improvements via Simultaneous Regression</td>
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<td>Process Models</td>
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<td>Approximate Models</td>
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<td>Rigorous/Predictive Models &amp; Uncertainty Quantification</td>
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<td>Deterministic Dynamics &amp; Control</td>
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<td>Innovative Processes</td>
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<td>Unit Operation Models</td>
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<td>4:05</td>
<td>Predictive Device-Scale Performance for Sorbent- and Solvent-Based CO\textsubscript{2} Capture with High Fidelity CFD Models</td>
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<td>4:45</td>
<td>New Capabilities: Amine Aerosol Modeling</td>
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<td>Data and Simulation Management</td>
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### Wednesday, August 10 – Admiral Room

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<tr>
<td>9:00</td>
<td>Welcome &amp; Day 2 Overview</td>
<td>Michael Matuszewski, National Energy Technology Laboratory</td>
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<td>9:10</td>
<td><strong>CCSI Toolset Commercialization &amp; Long Term Support</strong></td>
<td>Adekola Lawal, Process Systems Enterprise</td>
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<td>9:45</td>
<td><strong>CCSI Toolset Licensing Status, Benefits &amp; Procedures</strong></td>
<td>Susan Sprake, Los Alamos National Laboratory</td>
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<td>10:45</td>
<td><strong>The Future of CCSI²: Making an Impact on Industry</strong></td>
<td>John Shinn</td>
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<td>1:00</td>
<td><strong>CCSI Toolset Demonstrations – Discuss Tools/Models</strong></td>
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