Challenge: Accelerate Development/Scale Up

Traditional time to deploy new technology in the power industry:
- Laboratory Development: 10-15 years
- Process Scale Up: 20-30 years

Accelerated deployment timeline:
- Process Scale Up: 15 years

- 2010
- 2015
- 2020
- 2025
- 2030
- 2035
- 2040
- 2045
- 2050

- 1 kWe
- 1 MWe
- 10 MWe
- 100 MWe
- 500 MWe
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
- Berkeley Lab
- Pacific Northwest National Laboratory
- NETL
- Los Alamos National Laboratory
- Lawrence Livermore National Laboratory

Academia
- Carnegie Mellon University
- Princeton University
- West Virginia University
- Boston University
- The University of Texas at Austin

Industry
- ADA
- ALSTOM
- B&W
- GE
- EPRI
- EDISON
- SOUTHERN COMPANY
- Fluor
- Phillips 66
- AmEC Power
- ExxonMobil
- Air Products
- EASTMAN
- Chevron
- URS
- Schneider Electric
- ANSYS
- PSE
- U.S. Department of Energy
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
  - Initial licensees
Framework for Optimization, Quantification of Uncertainty and Sensitivity

- **ALAMO Surrogate Models**
- **Simulation Based Optimization**
- **Heat Integration**
- **UQ**
- **Optimization Under Uncertainty**
- **D-RM Builder**
- **iREVEAL Surrogate Models**

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**FOQUS**

Framework for Optimization Quantification of Uncertainty and Sensitivity

**Meta-flowsheet:** Links simulations, parallel execution, heat integration

**Turbine**
Parallel simulation execution management system
Desktop – Cloud – Cluster

**SimSinter Config GUI**

**SimSinter**
Standardized interface for simulation software
Steady state & dynamic

**Simulation**
Aspen
gPROMS
Excel

---

Optimization with Heat Integration

<table>
<thead>
<tr>
<th></th>
<th>w/o heat integration</th>
<th>Sequential</th>
<th>Simultaneous</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Net power efficiency (%)</strong></td>
<td>31.0</td>
<td>32.7</td>
<td>35.7</td>
</tr>
<tr>
<td><strong>Net power output (MW&lt;sub&gt;e&lt;/sub&gt;)</strong></td>
<td>479.7</td>
<td>505.4</td>
<td>552.4</td>
</tr>
<tr>
<td><strong>Electricity consumption&lt;sup&gt;b&lt;/sup&gt; (MW&lt;sub&gt;e&lt;/sub&gt;)</strong></td>
<td>67.0</td>
<td>67.0</td>
<td>80.4</td>
</tr>
<tr>
<td><strong>IP steam withdrawn from power cycle (MW&lt;sub&gt;th&lt;/sub&gt;)</strong></td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td><strong>LP steam withdrawn from power cycle (MW&lt;sub&gt;th&lt;/sub&gt;)</strong></td>
<td>336.3</td>
<td>304.5</td>
<td>138.3</td>
</tr>
<tr>
<td><strong>Cooling water consumption&lt;sup&gt;b&lt;/sup&gt; (MW&lt;sub&gt;th&lt;/sub&gt;)</strong></td>
<td>886.8</td>
<td>429.3</td>
<td>445.1</td>
</tr>
<tr>
<td><strong>Heat addition to feed water (MW&lt;sub&gt;th&lt;/sub&gt;)</strong></td>
<td>0</td>
<td>125.3</td>
<td>164.9</td>
</tr>
</tbody>
</table>

**Base case w/o CCS: 650 MW<sub>e</sub>, 42.1 %**

Uncertainty Quantification for Prediction Confidence

Now that we have

- A chemical kinetics model with quantified uncertainty
- A process model with other sources of uncertainty
- Surrogates with approximation errors
- An optimized process based on the above

UQ questions

- How do these errors and uncertainties affect our prediction confidence (e.g. operating cost) for the optimized process?
- Can the optimized system maintain >= 90% CO2 capture in the presence of these uncertainties?
- Which sources of uncertainty have the most impact on our prediction uncertainty?
- What additional experiments need to be performed to give acceptable uncertainty bounds?

CCSI UQ framework is designed to answer these questions
Optimization Under Uncertainty using a Two-Stage Approach

Design Phase

Uncertain parameters are characterized probabilistically

Optimize design variables while taking into account uncertainty of unknown parameters

Operating Phase

Uncertain parameters have been realized

Optimize operational variables in response to realized uncertain parameters

Bubbling Fluidized Bed (BFB) System

Design Variables:
- Absorber/regenerator dimensions
- Heat exchanger areas and tube diameters

Uncertain Parameters:
- Flue gas flowrate (load-following)
- Flue gas composition (fuel type)
- Reaction kinetics

Operational Variables:
- Steam flowrate
- Cooling water flowrate
- Recirculation gas split fraction

\[
\min_X \text{COE}(BFB,X) \quad \text{subject to } \text{CO}_2 \text{ capture } \geq 90%
\]

G() – some statistics, e.g. mean \(\Theta\) - uncertain parameters

\[
G(\text{COE}(BFB,X,\Theta))
\]
Solid Sorbents Models & Demonstration

- **Basic data models**
  - SorbentFit (1st gen model)
  - SorbentFit extension for packed beds
  - 2nd generation sorbent model which accounts for diffusion and reaction separately

- **CFD models**
  - Attrition Model
  - 1 MW bubbling fluidized bed adsorber with quantified predictive confidence
  - High resolution filtered models for hydrodynamics and heat transfer considering horizontal tubes
  - Validation hierarchy
  - Comprehensive 1 MW solid sorbent validation case via CRADA
  - Coal particle breakage model with validation

- **Process models**
  - Bubbling Fluidized Bed Reactor Model
  - Dynamic Reduced Order BFB Model
  - Moving Bed Reactor Model
  - Multi-stage moving bed model
  - Multi-stage Centrifugal Compressor Model
  - Solids heat exchanger models
  - Comprehensive, integrated steady state solid sorbent process model
  - Comprehensive, integrated dynamic solid sorbent process model with control
Building Predictive Confidence for Device-scale CO₂ Capture with Multiphase CFD Models

C2U Batch Unit

CCSI CFD Validation Hierarchy

25 MWe, 100 MWe, 650 MWe Solid Sorbent Systems

1 MWe Carbon Capture System

NETL Carbon Capture Unit (C2U) Reacting Unit

Bubbling Fluidized Bed Adsorber

Moving Bed Regenerator

Intermediate Validation
(Adsorber without reactions and heat transfer)

Intermediate Validation
(Regenerator without reactions and heat transfer)

Up-scaling
(flow filtering)

Up-scaling
(reaction filtering)

Up-scaling
(energy filtering)

Reaction Kinetics

Heat Transfer

Moving Fluidized Bed Regenerator

Hierarchical Calibration of Unit Problems

Upscaled Prediction
Solvent System Models & Demonstration

• **Basic data models**
  – Unified SorbentFIT tool to calibrate solvent data
  – High Viscosity Solvent Model, 2-MPZ
  – Properties model for Pz/2-MPz Blends (Aspen)

• **CFD models**
  – VOF Prediction on Wetted Surface
  – Prediction of mass transfer coefficients by calibration of fully coupled wetted wall column model
  – Preliminary CFD simulation of a solvent based capture unit
  – Validation hierarchy

• **Process models**
  – “Gold standard reference” process model, both steady-state and dynamic
  – Methodology for calibration/validation of solvent-based process models to support scale up

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Luo et al., “Comparison and validation of simulation codes against sixteen sets of data from four different pilot plants”, Energy Procedia, 1249-1256, 2009
Integrated Mass Transfer Model Development

• Diffusivity, viscosity, surface tension, interfacial area, and mass transfer coefficients all important
• Data from both wetted wall column and packed column considered
• Simultaneous regression of these models not previously possible in Aspen
• FOQUS has the capability of simultaneous regression

Usual approach: Sequential regression

FOQUS capability: Simultaneous regression

FOQUS can run multiple simulations and optimize an unique model for mass transfer and interfacial area

Optimized model for wetted wall column experiments

Might not exactly predict the data of an absorber column
CCSI Team Conducted Tests at NCCC
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  - David Mebane (NETL/ORISE, West Virginia University)
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Carbon Capture Simulation for Industry Impact

CCSI²

Carbon Capture Simulation for Industry Impact

[Logos of NETL, Lawrence Livermore National Laboratory, Los Alamos National Laboratory, Pacific Northwest National Laboratory, and U.S. Department of Energy]