CCSI

Carbon Capture Simulation Initiative

Capabilities of the CCSI Toolset

David C. Miller, Ph.D.

9 August 2016

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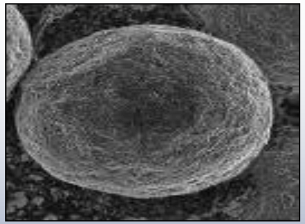
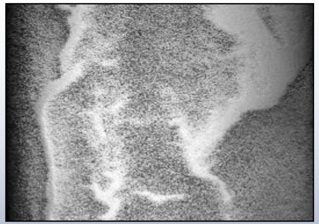
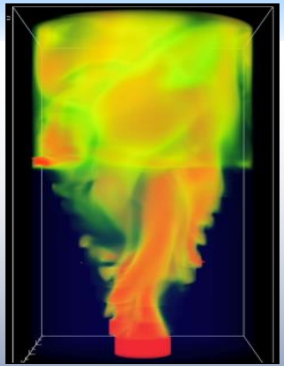
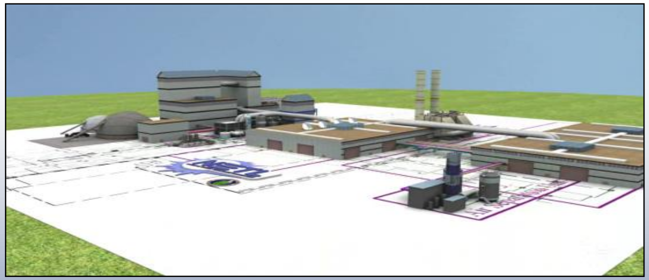
For Accelerating Technology Development

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

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Pacific Northwest National Laboratory
NETL
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Princeton University
West Virginia University
Boston University
The University of Texas at Austin

Industry

GE
ADA Environmental Solutions
ALSTOM
B&W the babcock&wilcox company
EPRI Electric Power Research Institute
Southern California Edison An EDISON INTERNATIONAL Company San Onofre Nuclear Generating Station
Phillips 66
Chevron
Southern Company
RTI International
ExxonMobil
AEP American Electric Power
URS
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Goals & Objectives of CCSI

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

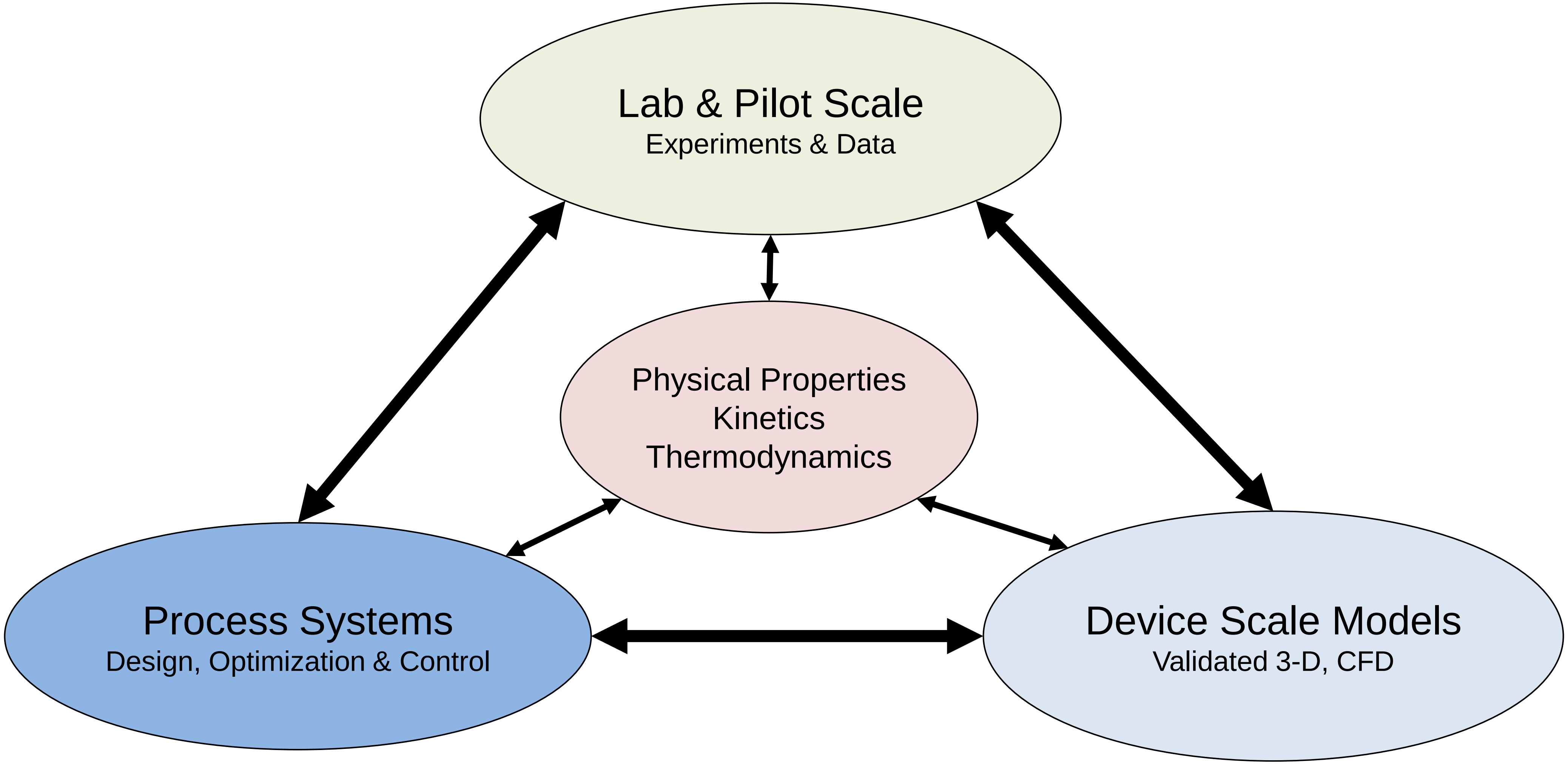
- **<u>Demonstrate</u>** the capabilities of the CCSI Toolset on non-proprietary case studies
  - Examples of how new capabilities improve ability to develop capture technology

- **<u>Deploy</u>** the CCSI Toolset to industry

Projects with industry

Current licensees

Advanced Computational Tools to Accelerate Carbon Capture Technology Development



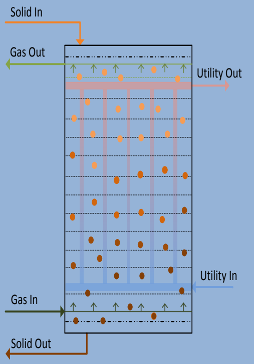
CCSI Toolset: New Capabilities for Modeling & Simulation

Maximize the learning at each stage of technology development

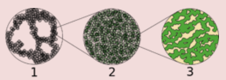
- **Early stage R&D**
  - Screening concepts
  - Identify conditions to focus development
  - Prioritize data collection & test conditions
- **Pilot scale**
  - Ensure the right data is collected
  - Support scale-up design
- **Demo scale**
  - Design the right process
  - Support deployment with reduced risk

CCSI Toolset to accelerate development and scale-up

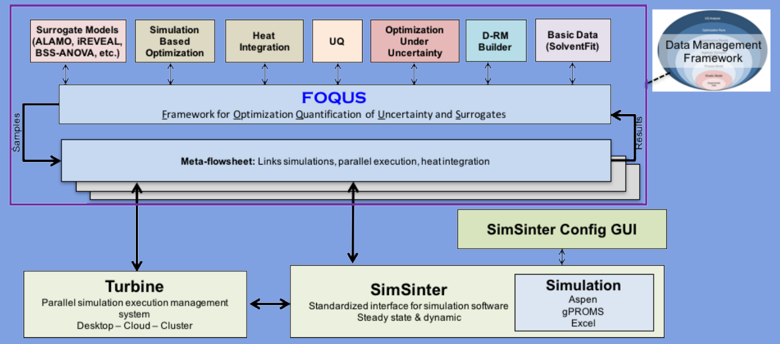
Process Models



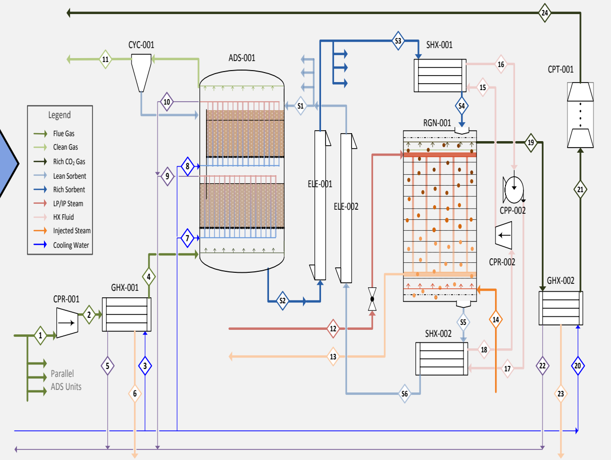
Basic Data Submodels



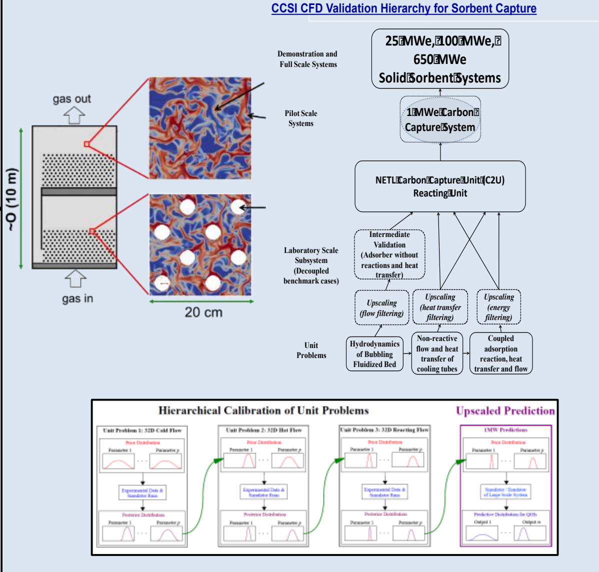
Process Synthesis, Design & Optimization



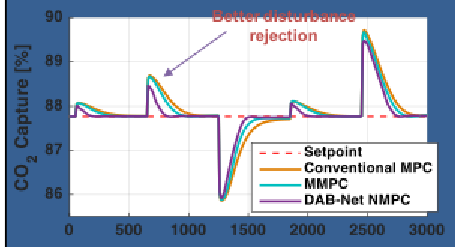
Carbon Capture Process



CFD Device Models



Process Dynamics and Control



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Basic Data Requirements for CCSI Analyses

Sorbents

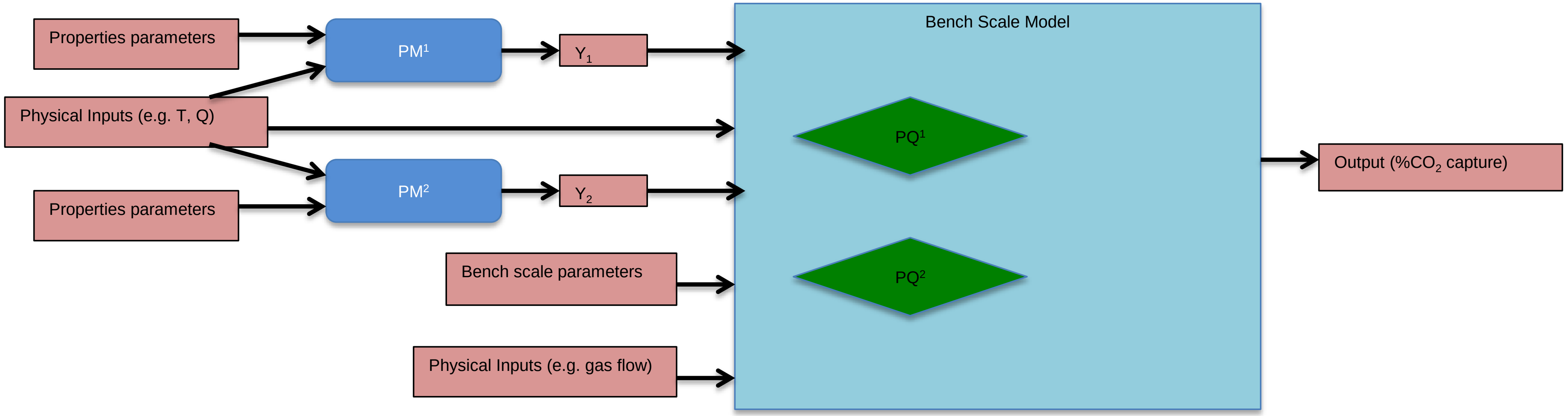
- Adsorption equilibrium, $f(p_{y,i}, T, x_i)$
  - All species over relevant conditions
- Heat of Adsorption for all species, $f(T, x_i)$
  - CO_2 and H_2O minimum
- Heat Capacity, $f(T, x_i)$
- Adsorption/Desorption Kinetics, $f(p_{y,i}, T, x_i)$
  - All species over relevant conditions
- Thermal Conductivity, $f(T, x_i)$
- Density, $f(T, x_i)$
- Particle Size Distribution
- Sphericity

Solvents

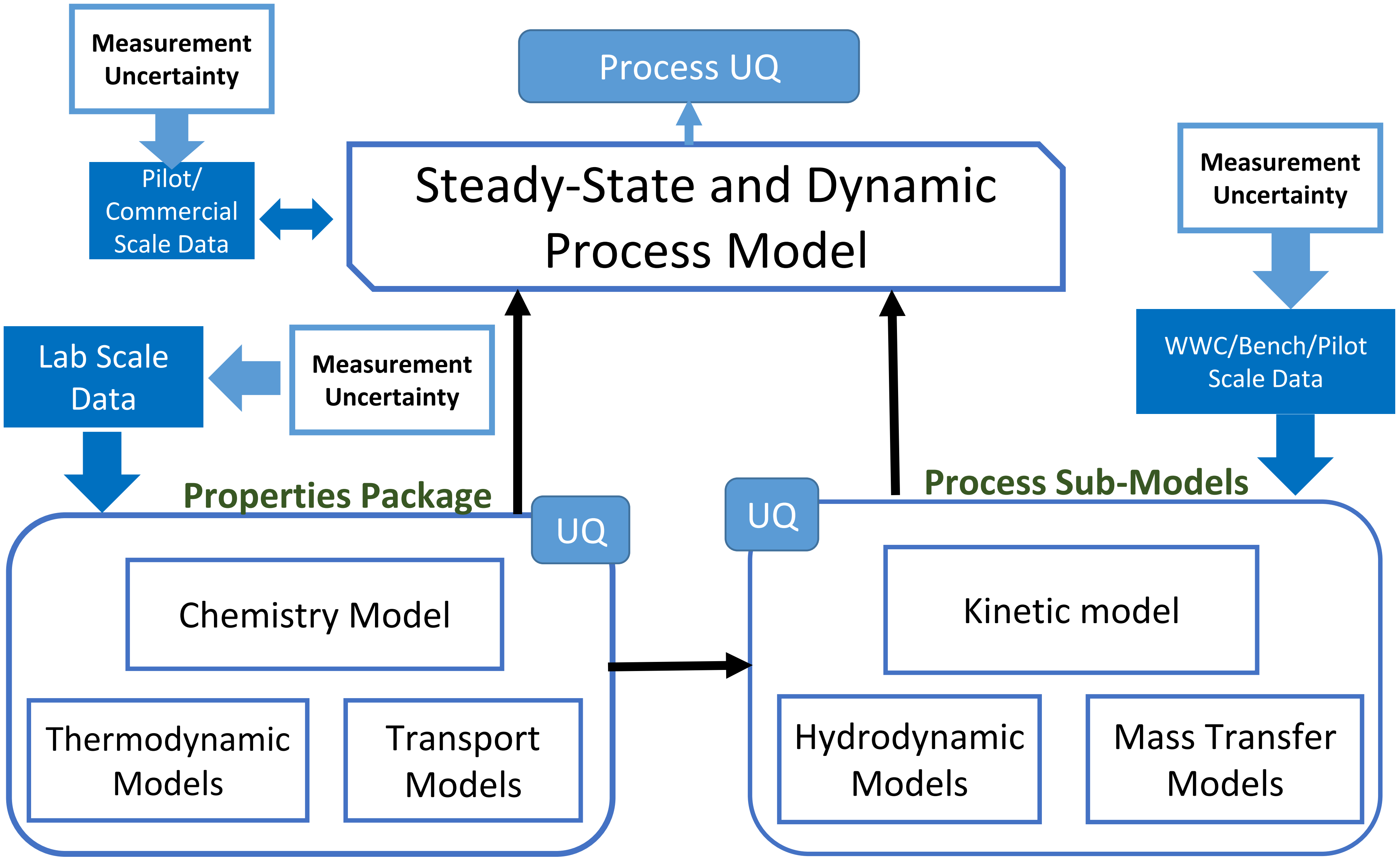
- Vapor-Liquid Equilibrium Data
  - over relevant $p_{y,i}$,T, x_i ranges
- Heat of Absorption, $f(T, x_i)$
- Kinetic Data, $f(p_{y,i}, T, x_i)$
  - Including speciation
- Mass Transfer Data
  - from wetted wall column, bench scale system
- Viscosity, $f(T, x_i)$
- Heat Capacity, $f(T, x_i)$
- Density, $f(T, x_i)$
- 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

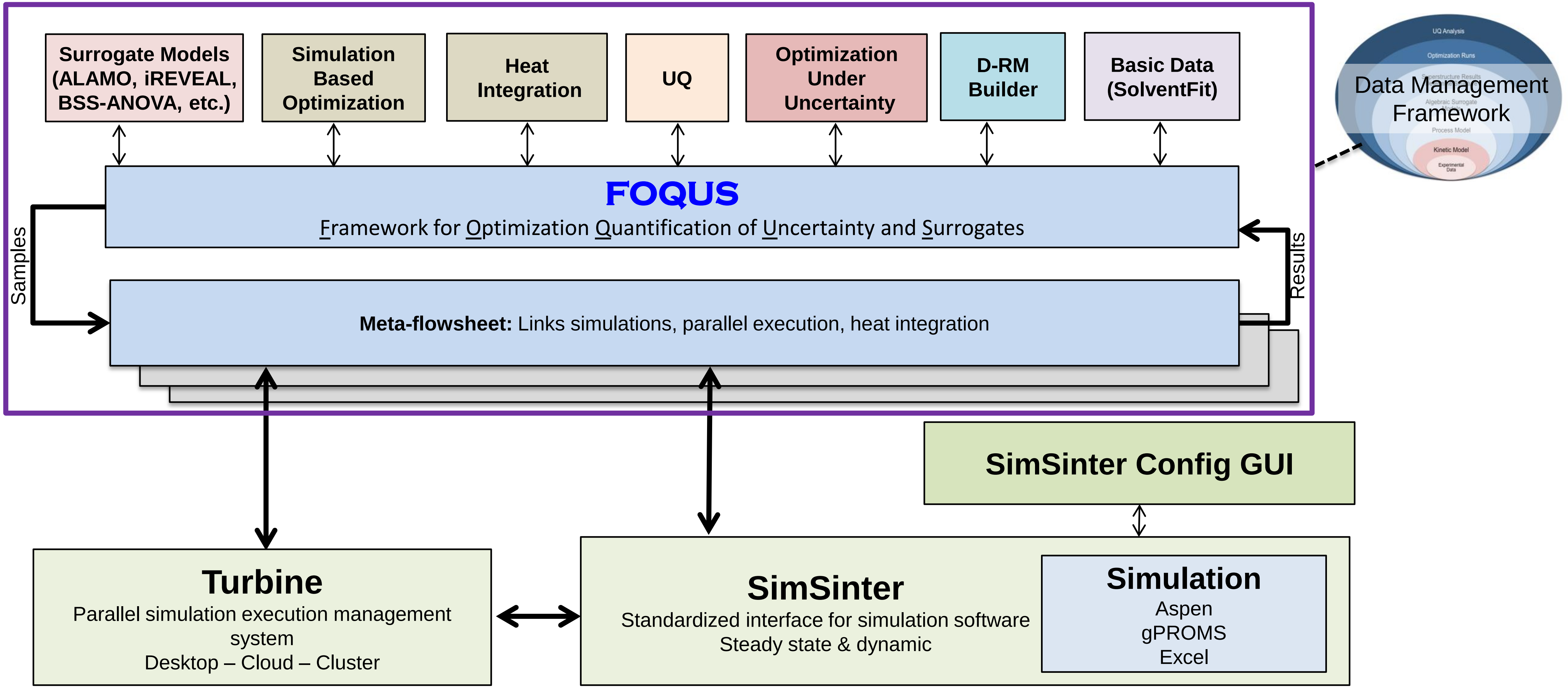
- Challenge:
  - Large number of parameters in bench scale models and properties submodels
  - Limited data = full calibration conceptually and computationally difficult.
- New approach:
  - Multi-scale calibration
  - Propagate uncertainty from properties models during bench scale calibration



Developing Detailed, Predictive Models of Solvent-Based Capture Processes



Optimization, Uncertainty Quantification, Surrogate Models

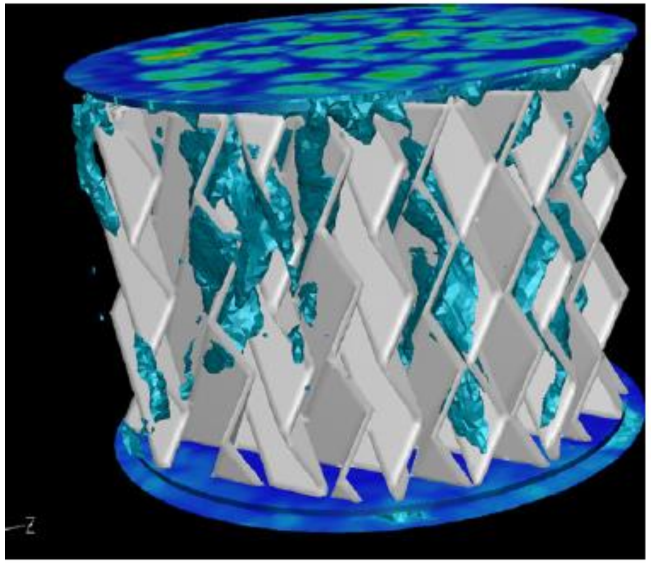


D. C. Miller, B. Ng, J. C. Eslick, C. Tong and Y. Chen, 2014, Advanced Computational Tools for Optimization and Uncertainty Quantification of Carbon Capture Processes. In Proceedings of the 8th Foundations of Computer Aided Process Design Conference – FOCAPD 2014. M. R. Eden, J. D. Siirola and G. P. Towler Elsevier.

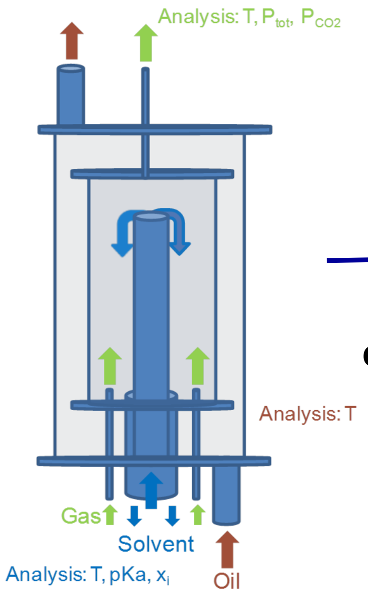
Highly Resolved Models for Solvent-based Capture

Predictive understanding at scale
Hierarchical multi-scale modeling framework

Micro/Meso-Scale VOF model

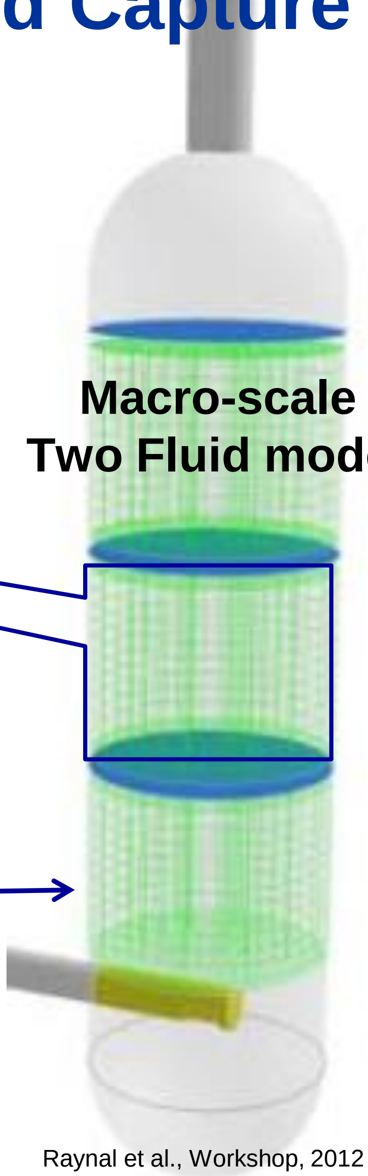


Fernandes et al., JSF, 2009



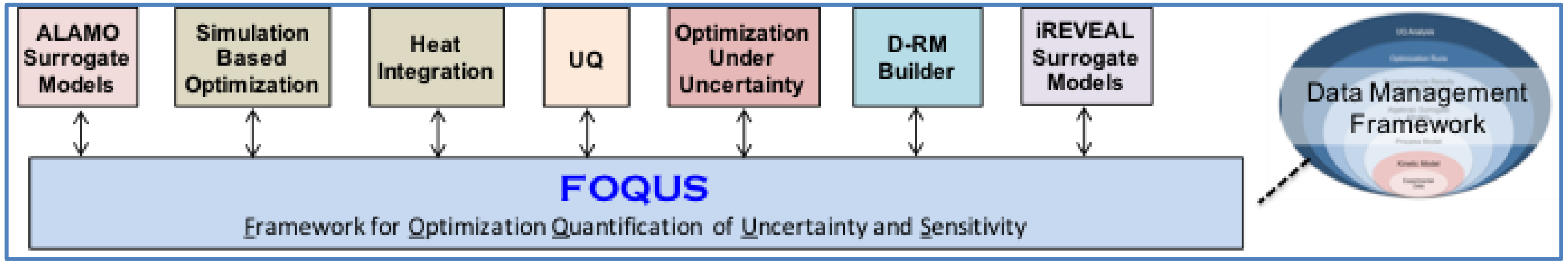
Effective mass transfer coefficient for different flow regimes

Macro-scale Two Fluid model

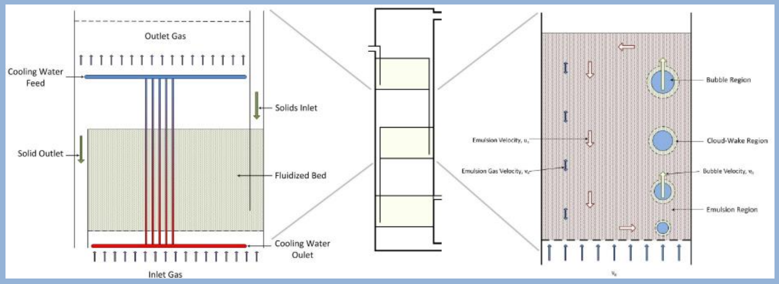


Raynal et al., Workshop, 2012

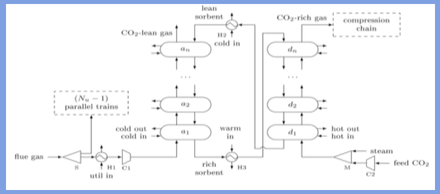
CCSI Toolset Products



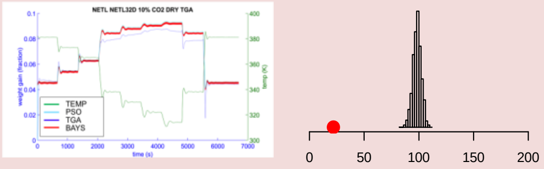
Process Models



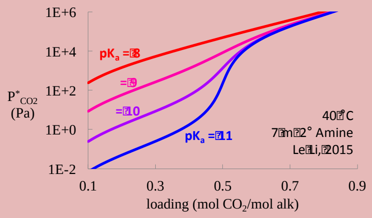
Superstructure Optimization



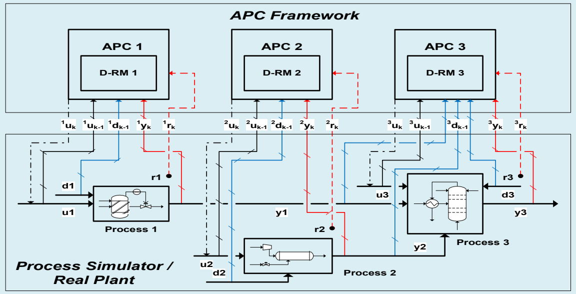
Basic Data Fitting Tools



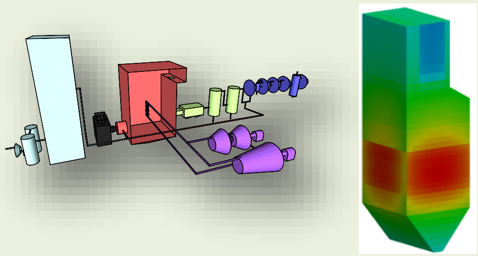
Solvent Blend Model



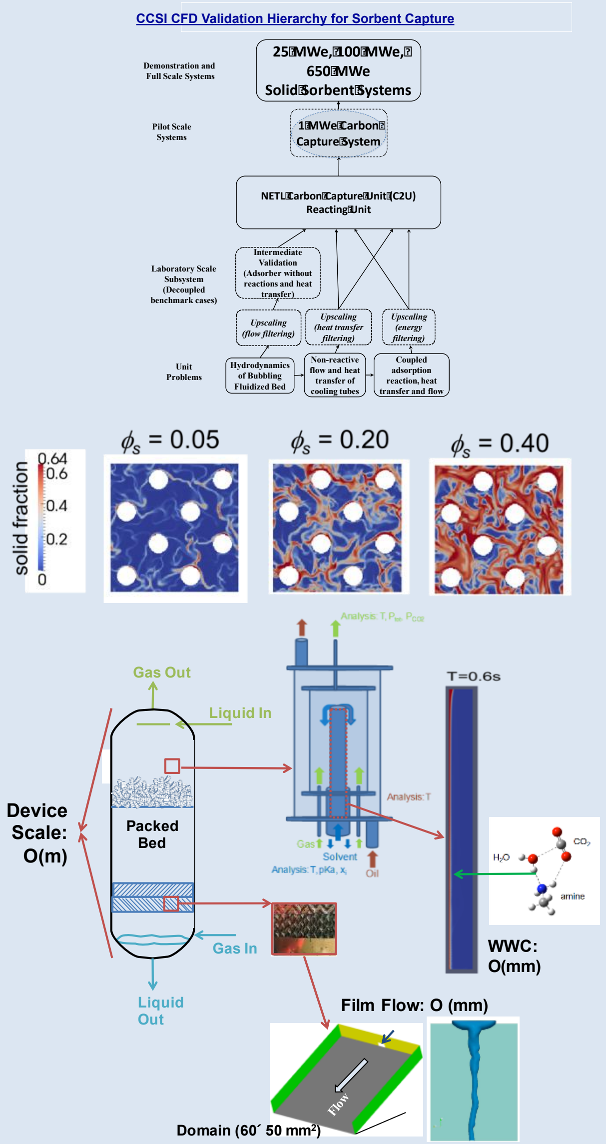
APC Framework



Oxycombustion System Optimization Framework



CFD Models



Major release November 2015
Updated June 2016

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Carbon Capture Simulation for Industry Impact

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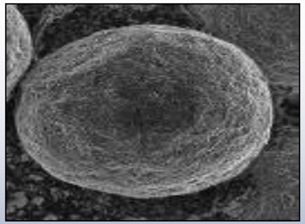
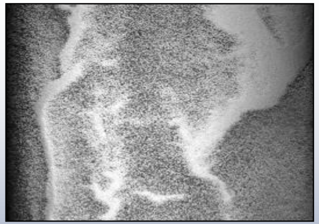
Tuesday, August 9 – Admiral Room

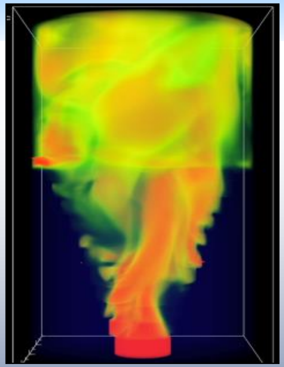
1:30	**2:50**	**Sub-Process Models**
		Baseline VLE Modeling
		Modeling Improvements via Simultaneous Regression
		Solvent-Based Model Development: Incorporating Uncertainty
		FOQUS: A Computational Tool for Design Optimization and Uncertainty Quantification
3:05	**4:05**	**Process Models**
		Approximate Models
		Rigorous/Predictive Models & Uncertainty Quantification
		Deterministic Dynamics & Control
		Innovative Processes
4:05	**4:45**	**Unit Operation Models**
		Predictive Device-Scale Performance for Sorbent- and Solvent-Based CO_2 Capture with High Fidelity CFD Models
4:45	**4:55**	**New Capabilities: Amine Aerosol Modeling**
4:55	**5:15**	**Data and Simulation Management**

Wednesday, August 10 – Admiral Room

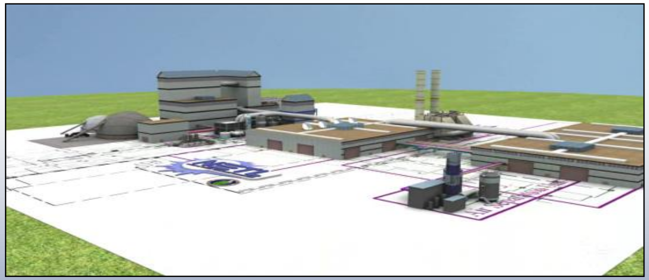
9:00	9:10	**Welcome & Day 2 Overview** Michael Matuszewski, National Energy Technology Laboratory
9:10	9:45	**CCSI Toolset Commercialization & Long Term Support** Adekola Lawal, Process Systems Enterprise
9:45	10:15	**CCSI Toolset Licensing Status, Benefits & Procedures** Susan Sprake, Los Alamos National Laboratory
10:45	11:00	**The Future of CCSI^2: Making an Impact on Industry** John Shinn
1:00	5:00	**CCSI Toolset Demonstrations – Discuss Tools/Models**

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

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The University of Texas at Austin

Industry

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ADA Environmental Solutions
Alstom
B&W
EPRI Electric Power Research Institute
Southern California Edison
Phillips 66
Chevron
Southern Company
RTI International
ExxonMobil
AEP American Electric Power
URS
aspentech
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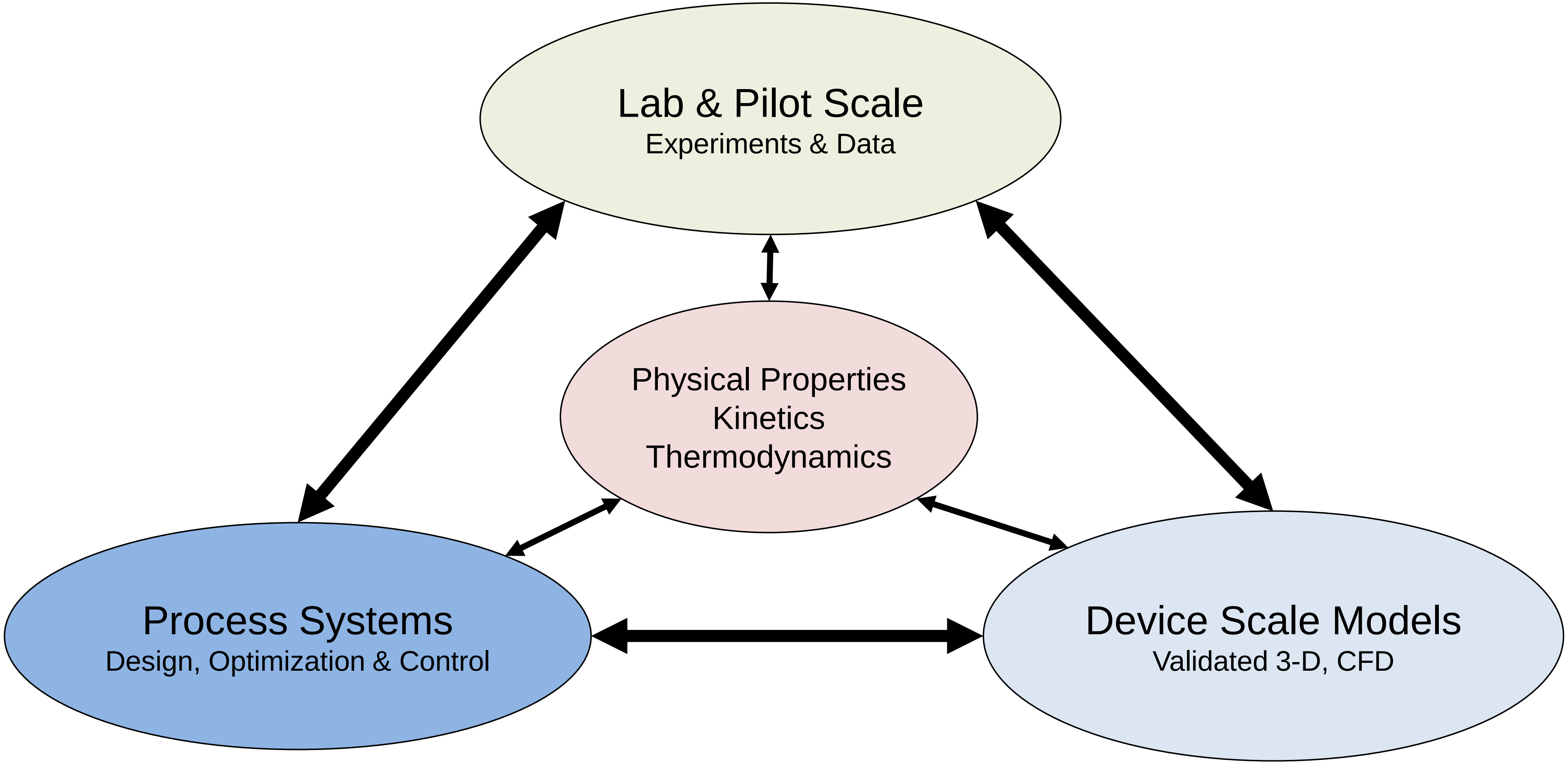
Lab & Pilot Scale
Experiments & Data
Physical Properties
Kinetics
Thermodynamics
Process Systems
Design, Optimization & Control
Device Scale Models
Validated 3-D, CFD