CCSI

Carbon Capture Simulation Initiative

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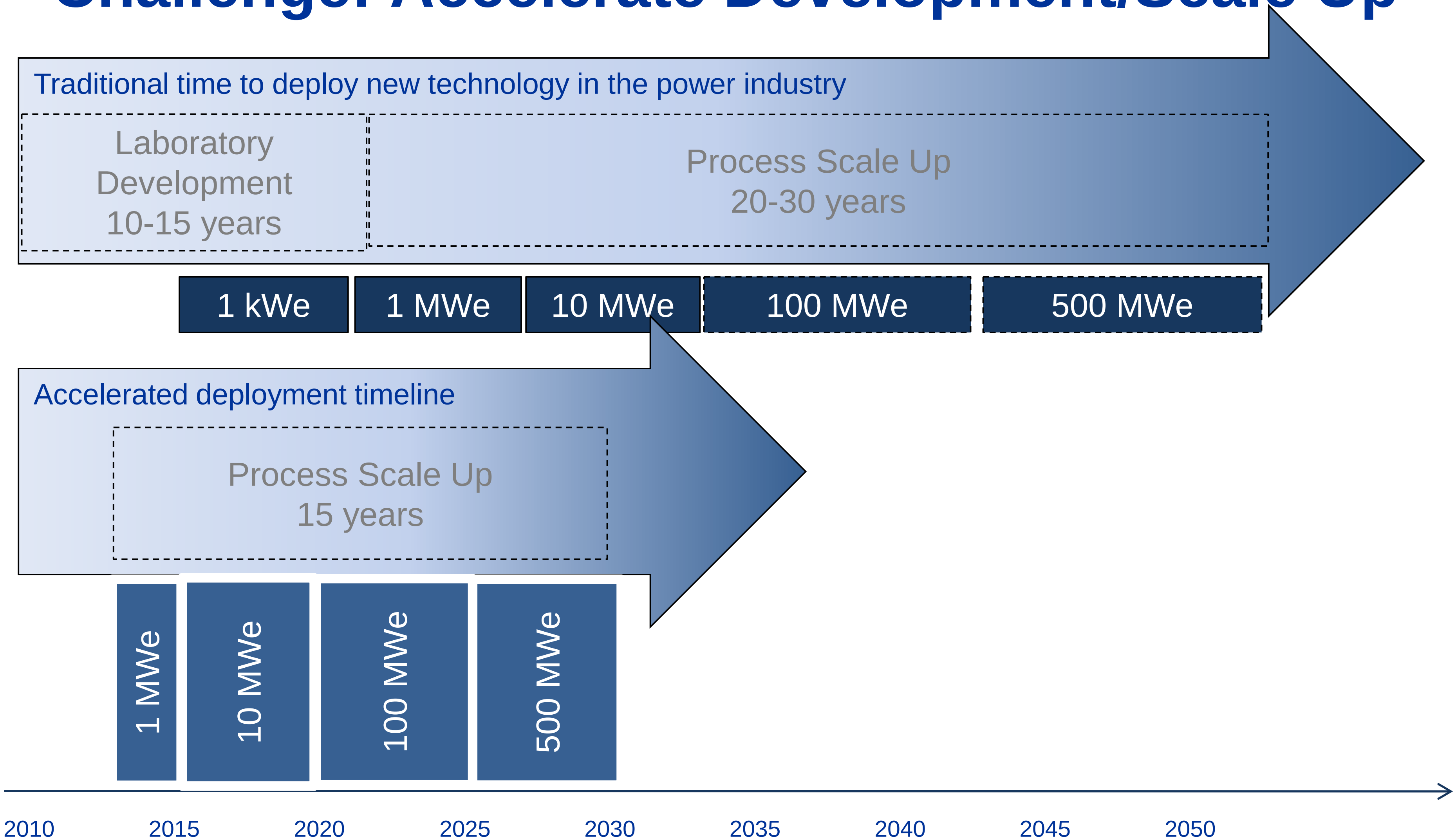
U.S. Department of Energy

23 June 2015

Challenge: Accelerate Development/Scale Up



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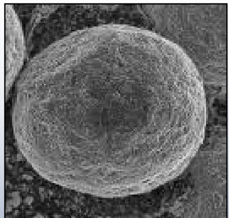
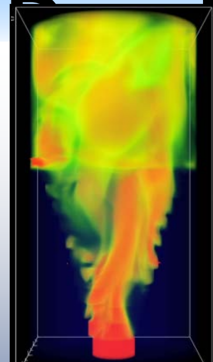
For Accelerating Technology Deployment






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

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Industry

ADA Environmental Solutions
Alstom
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GE
EPRI Electric Power Research Institute
Fluor
Phillips 66
AEP American Electric Power
Southern California Edison
Southern Company
ExxonMobil
Chevron
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Eastman
aspentech
ANSYS
Schneider Electric
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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

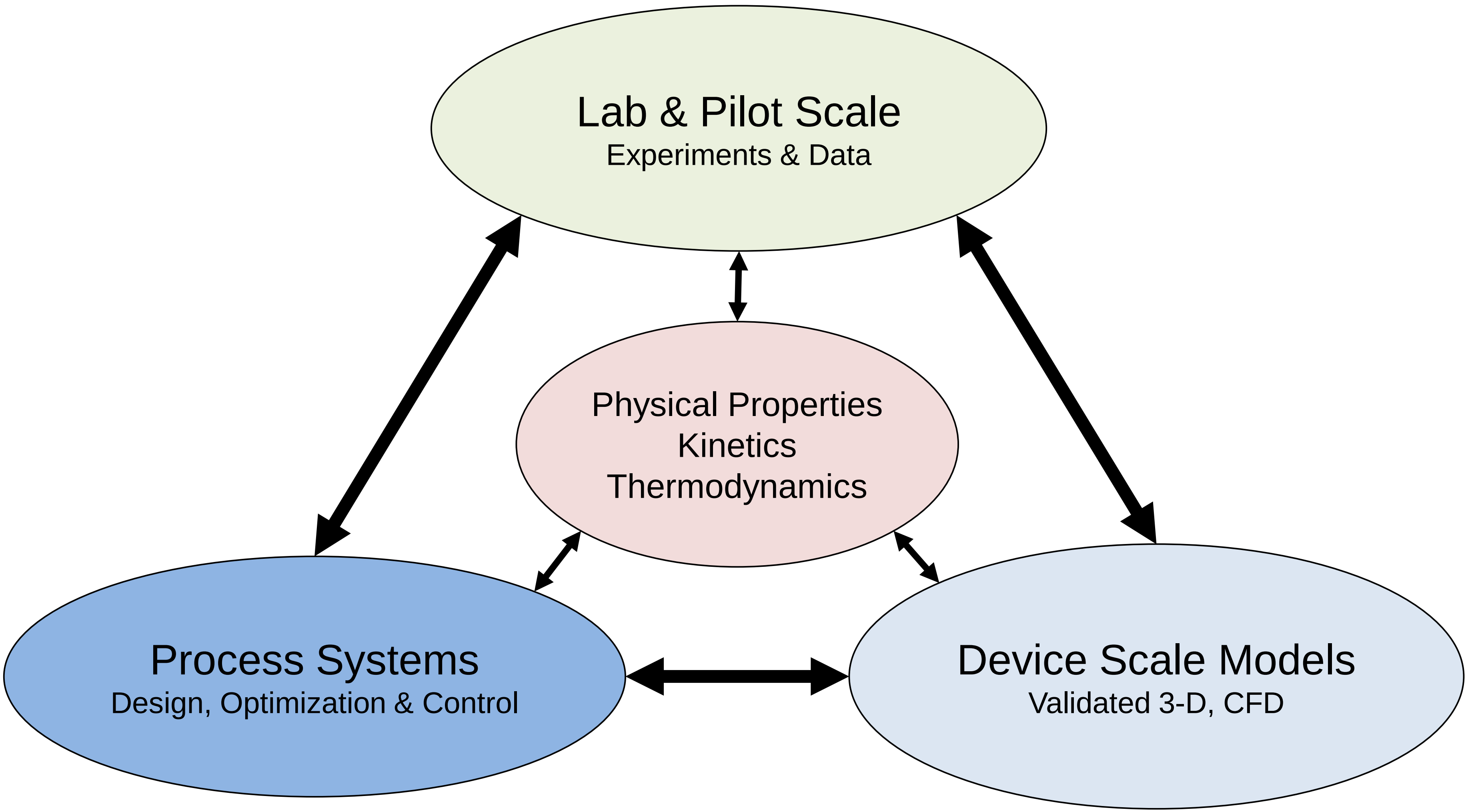
- **Demonstrate** the capabilities of the CCSI Toolset on non-proprietary case studies
  - Examples of how new capabilities improve ability to develop capture technology

- **Deploy** the CCSI Toolset to industry
  - Initial licensees

CCSI Timeline

- Organizational Meetings: March 2010 - October 2010
- **Technical work initiated: Feb. 1, 2011**
- **Preliminary Release of CCSI Toolset: September 2012**
  - Initial licenses signed
- CCSI Year 3 starts Feb. 1, 2013
  - <u>Began solvent modeling/demonstration component</u>
- **2013 Toolset Release: October 31, 2013**
  - **Multiple tools and models released and being used by industry**
- **2014 Toolset Release: October 31, 2014**
- **Future**
  - **Final IAB meeting: Sept. 23-24, 2015 (Reston, VA)**
  - **Final major release October/November 2015**
  - **Commercial licensing late 2015 or early 2016**

Advanced Computational Tools to Accelerate Carbon Capture Technology Development



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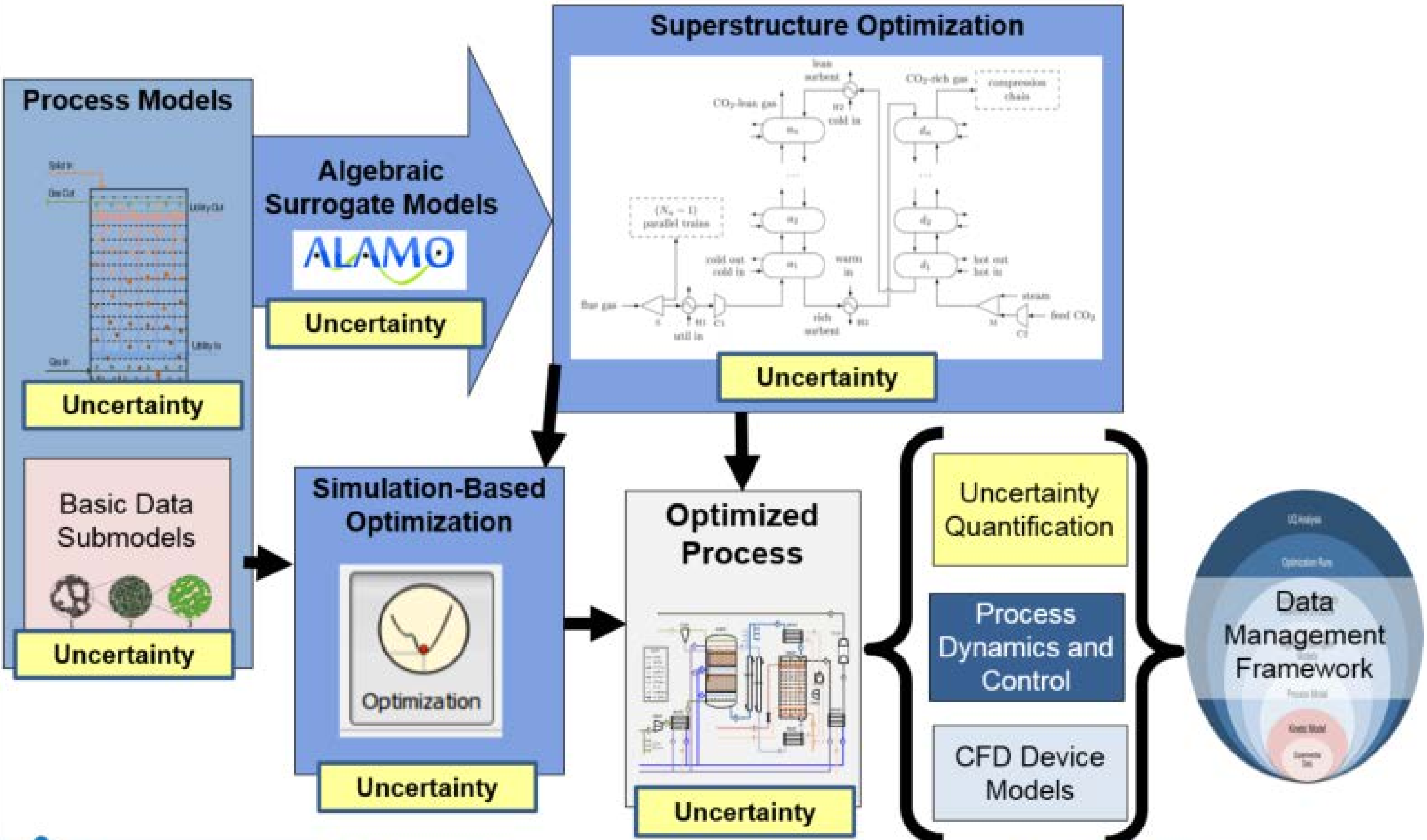
CCSI Toolset Workflow and Connections



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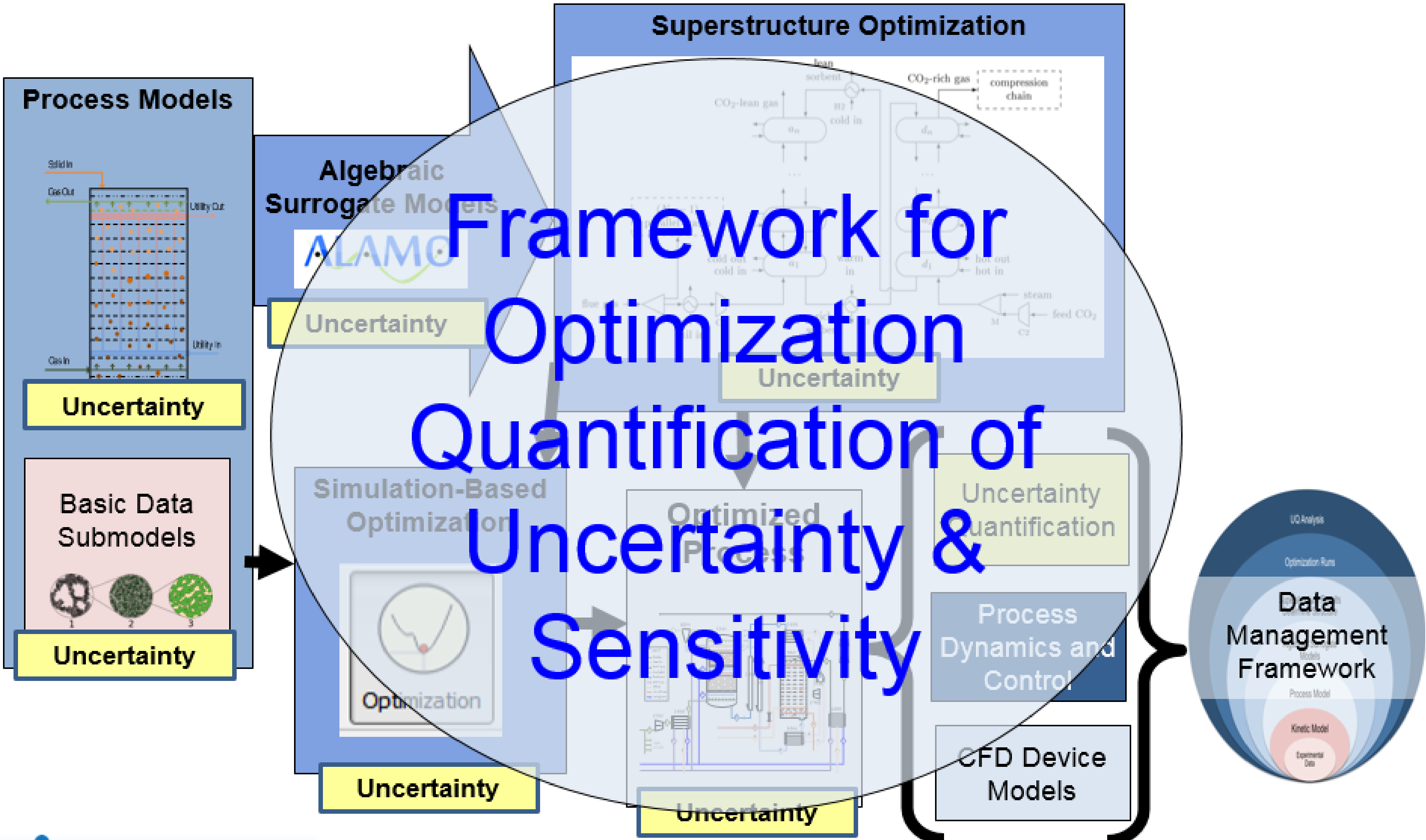

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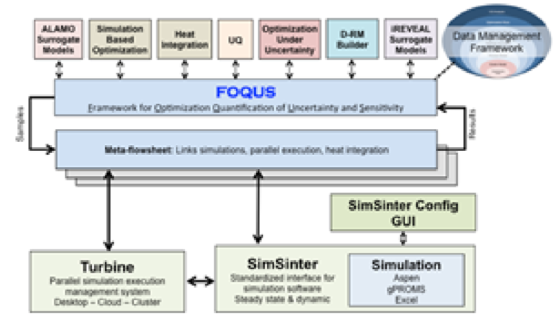
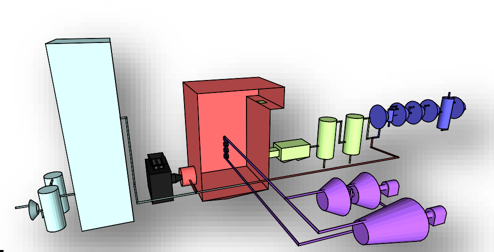
Outline

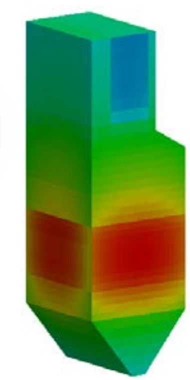
- Process Systems Engineering & Crosscutting Tools
  - FOQUS
  - Optimization under uncertainty
- Solid Sorbents Models & Demonstration
  - Process Systems Example
  - Validated CFD Model Example
- Solvent System Model Example & Validation
  - MEA example
- Supporting Pilot & Demonstration Scale Capture

Process Systems Engineering & Crosscutting Tools



- **FOQUS – Turbine – SimSinter**
  - Simulation-Based Optimization
    - Simultaneous Heat Integration
  - Quantification of Uncertainty (UQ)
  - Optimization under Uncertainty
  - ALAMO
    - Automatic Learning of Algebraic Models for Optimization
  - D-RM Builder
    - Dynamic Reduced Model Builder
  - iREVEAL
    - CFD to Surrogate Process Models
- ***Data Management Framework***
  - *Provenance Tracking & Integration*
- ***Oxycombustion System Optimization***
  - *Cryogenic Systems*
  - *Boiler Model*
  - *Trust Region Methodology*
- ***Advanced Process Control Framework***
- ***Membrane module & system model***





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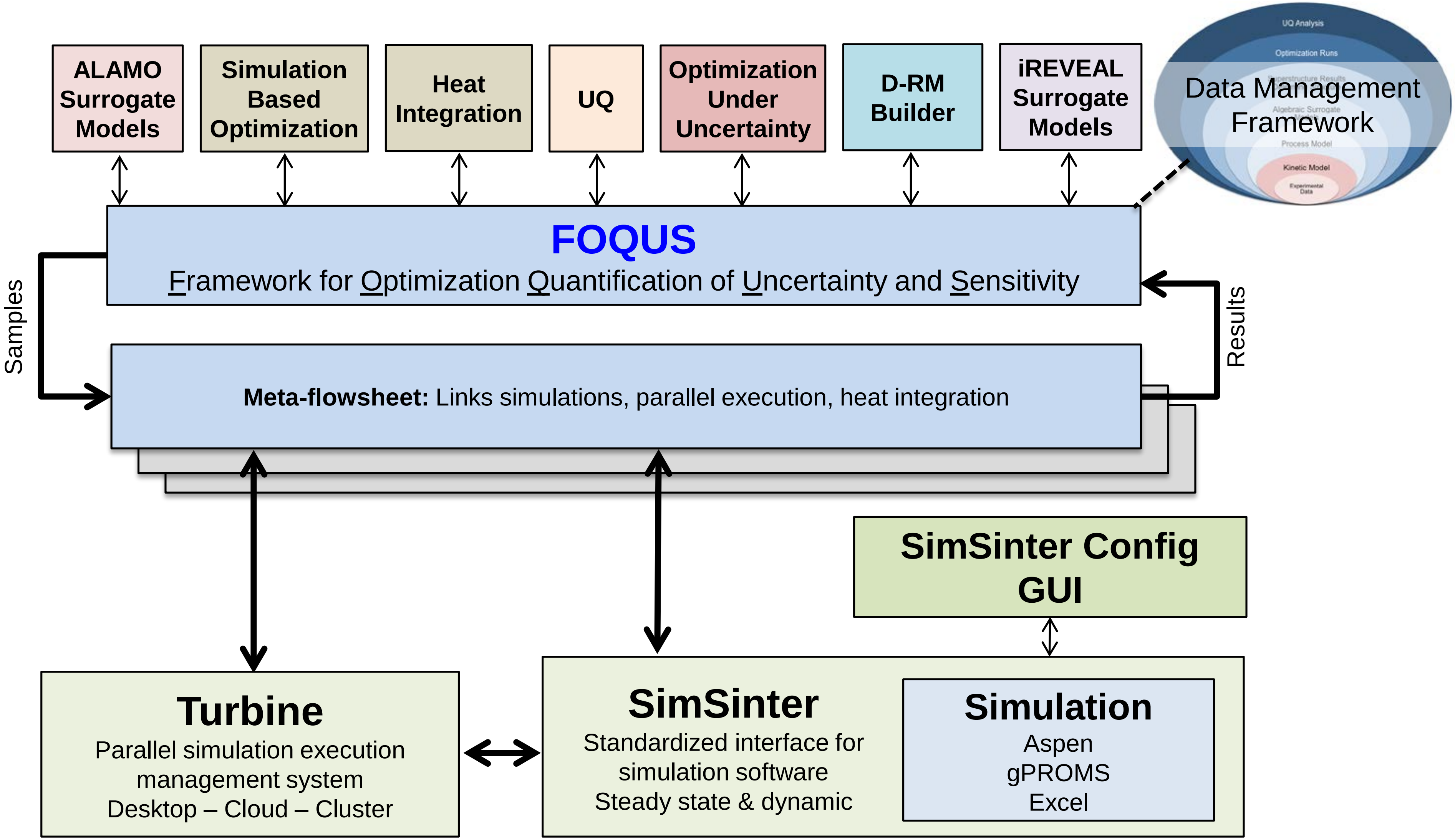
Framework for Optimization, Quantification of Uncertainty and Sensitivity



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.

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 design 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**

$$\min_X \quad \cancel{COE(BFB, X)}$$

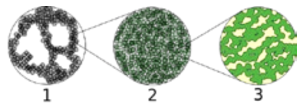
$$\text{subject to } CO_2 \text{ capture} \geq 90\%$$

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

$$\boxed{G(COE(BFB, X, \Theta))}$$

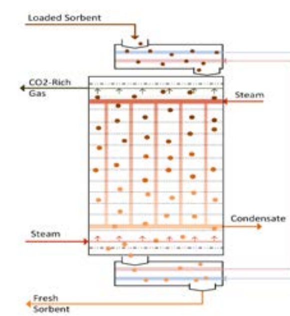
Solid Sorbents Models & Demonstration

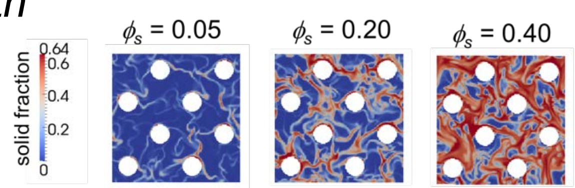
- **Basic data models**
  - *SorbentFit (1st gen model)*
  - *SorbentFit extension for packed beds*
  - *2nd generation sorbent model which accounts for diffusion and reaction separately*



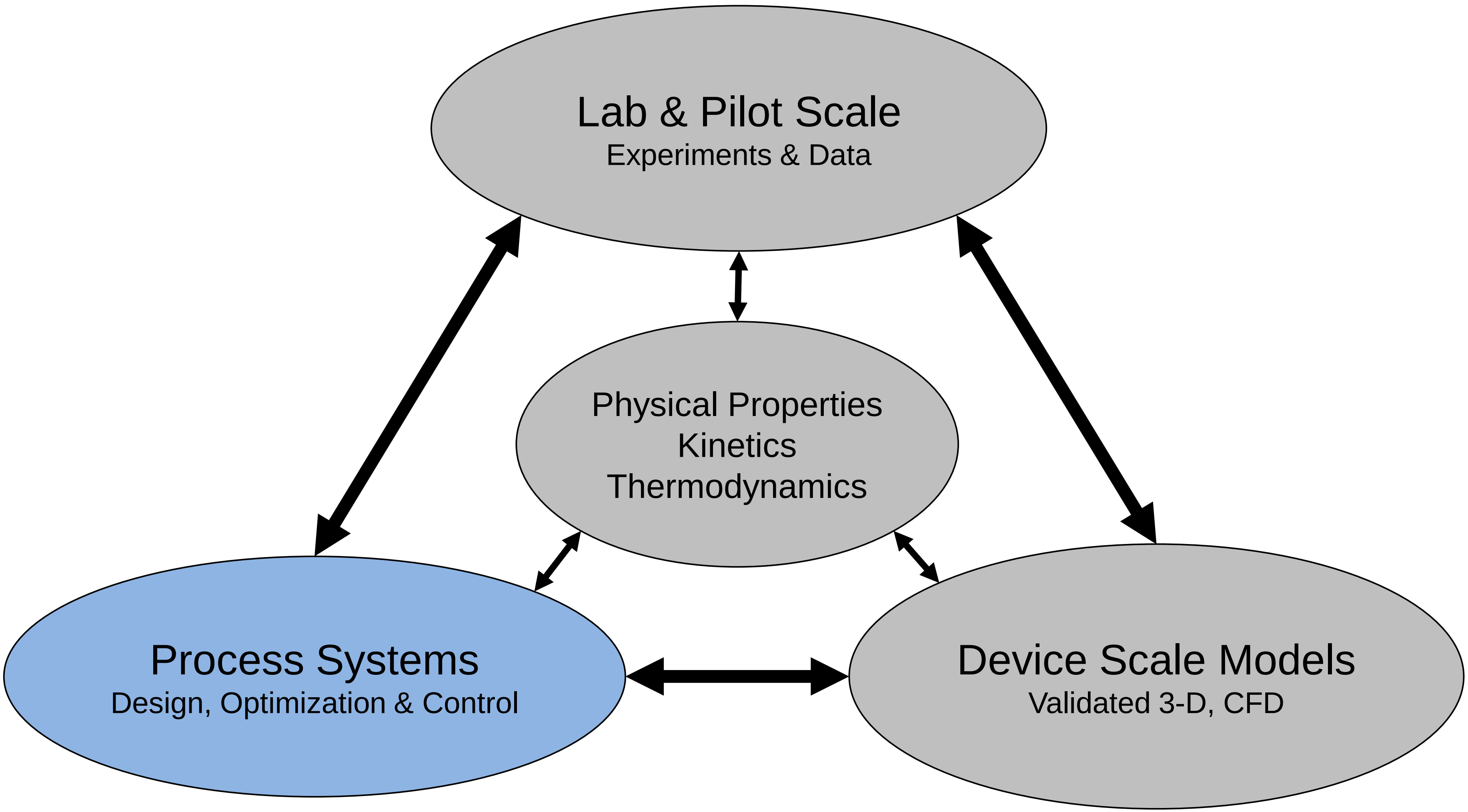
- **CFD models**
  - *Attrition Model*
  - 1 MW bubbling fluidized bed adsorber with quantified predictive confidence
  - High resolution filtered models for hydrodynamics and heat transfer considering horizontal tubes
  - Validation hierarchy
  - *Comprehensive 1 MW solid sorbent validation case via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



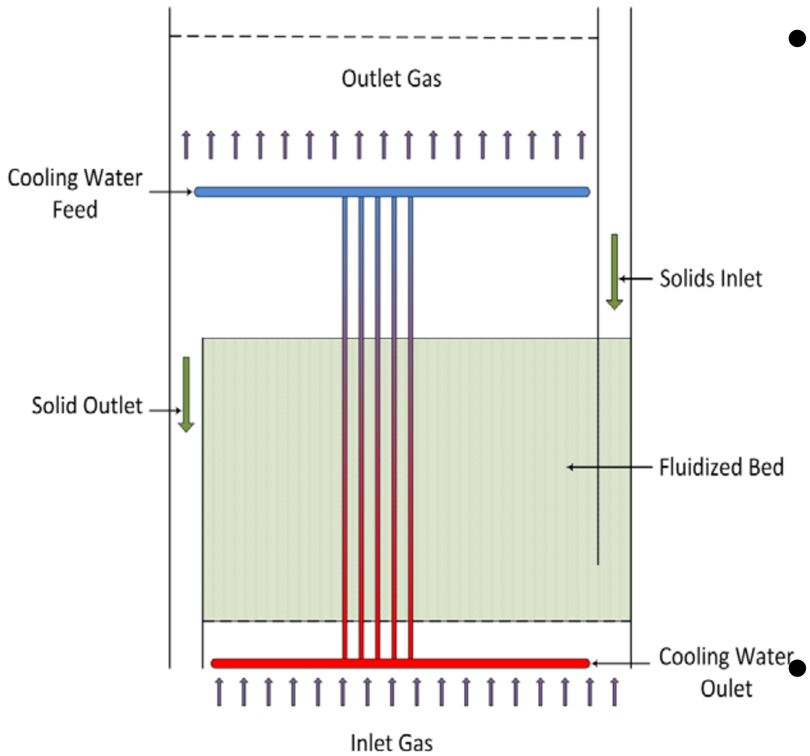


Solid Sorbent: Process Systems Example



Bubbling Fluidized Bed Process Model

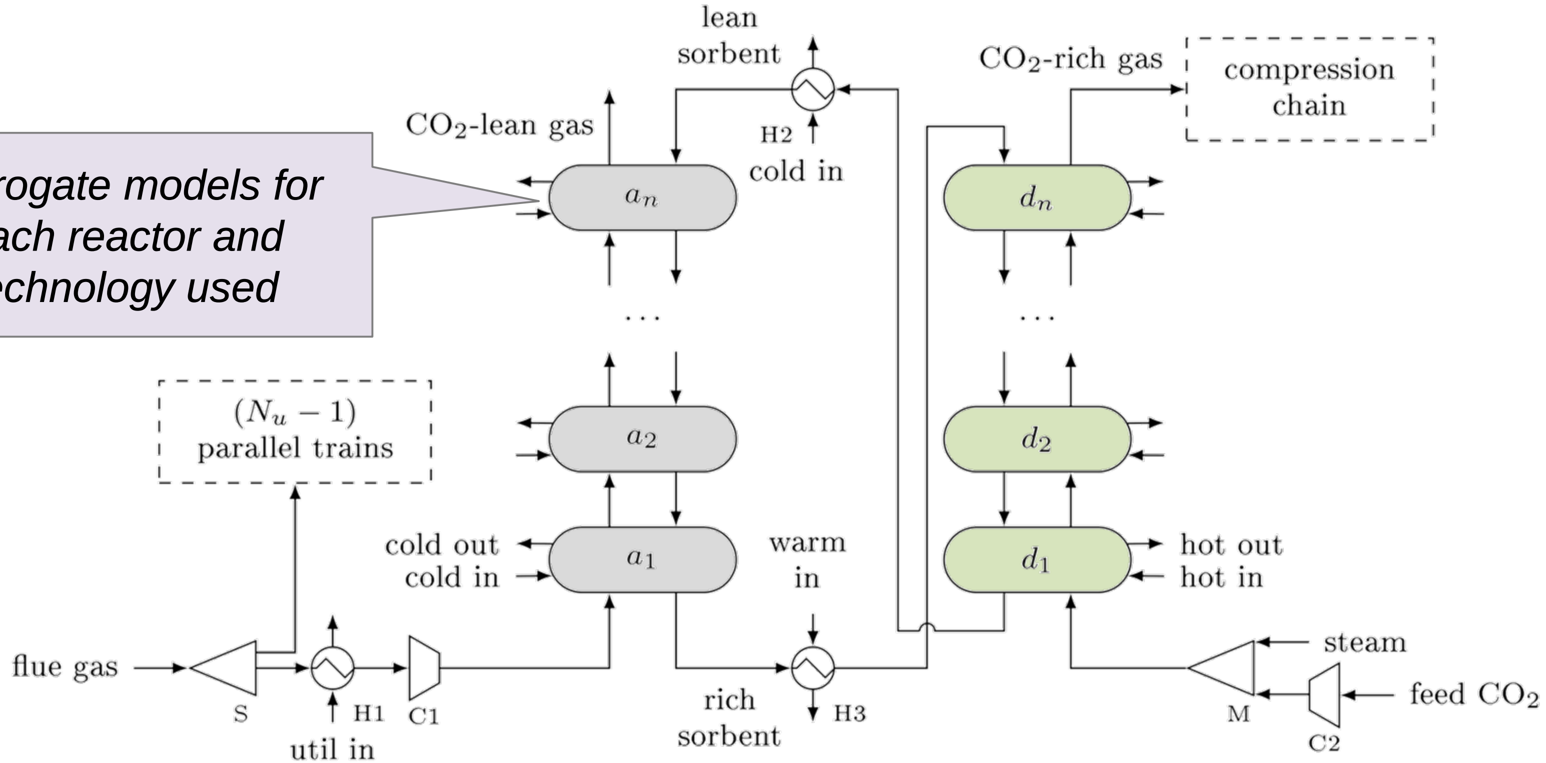
*1-D, two-phase, pressure-driven and <u>non-isothermal</u> models developed in both **ACM** and **gPROMS***



- Flexible configurations
  - Dynamic or steady-state
  - Adsorber or regenerator
  - Under/overflow
  - Integrated heat exchanger for heating or cooling
- Supports complex reaction kinetics

Carbon Capture System Configuration

Surrogate models for each reactor and technology used



- Discrete decisions: How many units? Parallel trains? What technology used for each reactor?
- Continuous decisions: Unit geometries
- Operating conditions: Vessel temperature and pressure, flow rates, compositions

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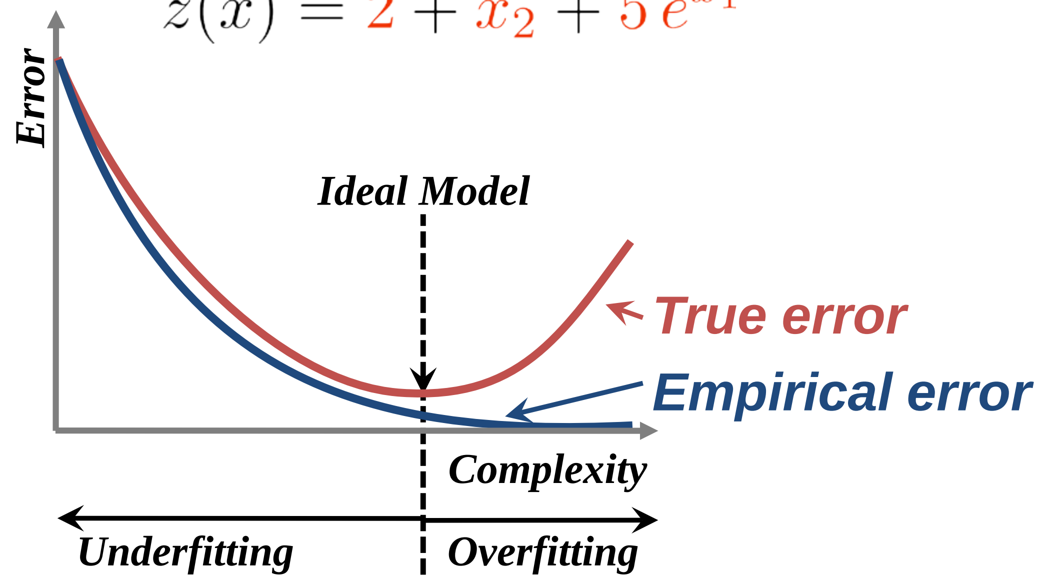
ALAMO: Model Development & Overfitting

- Step 1: Define a large set of potential basis functions

$$\hat{z}(x) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1 x_2 + \beta_4 e^{x_1} + \beta_5 e^{x_2} + \ldots$$

- Step 2: Model reduction

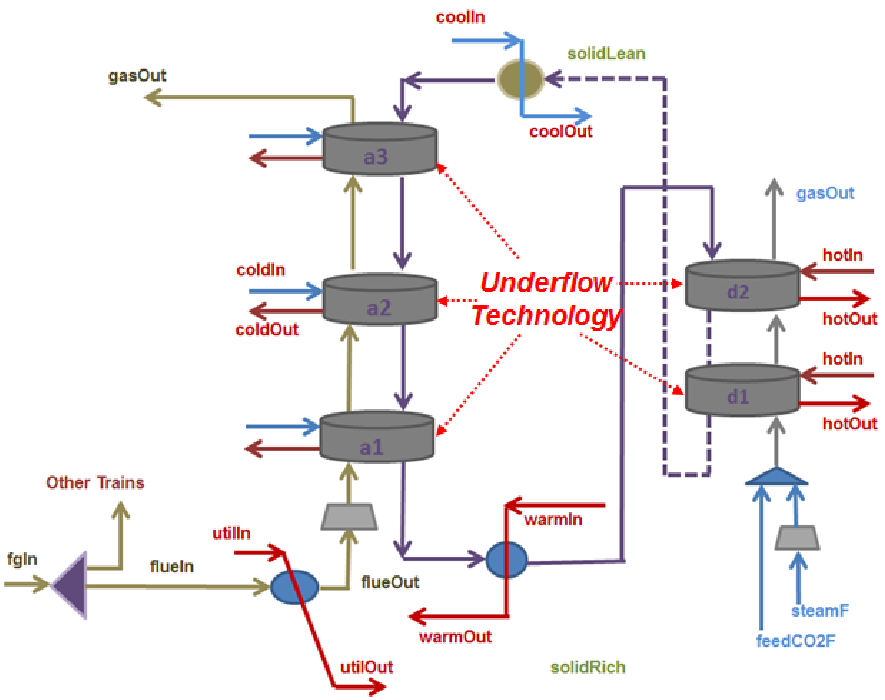
$$\hat{z}(x) = 2 + x_2 + 5\,e^{x_1}$$



Superstructure Optimization

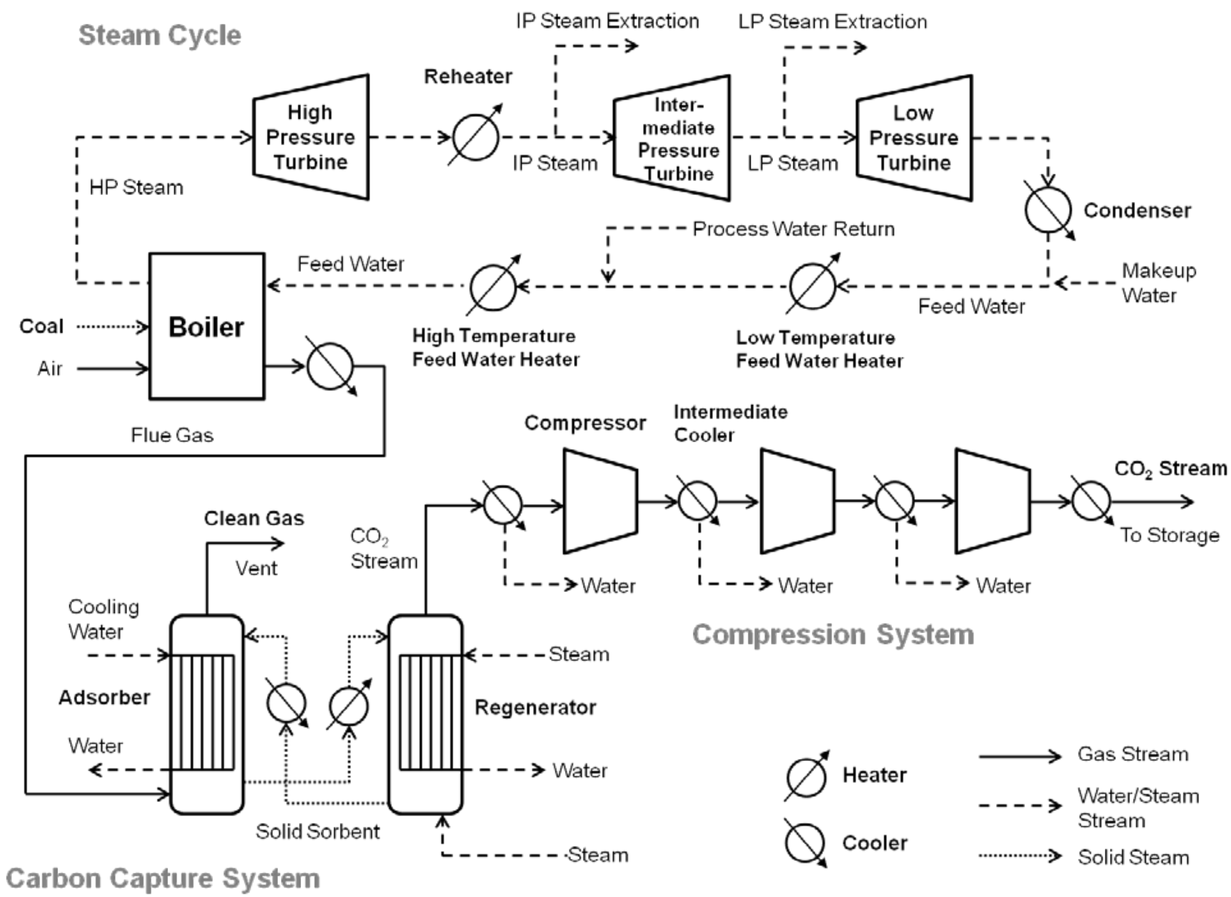
Mixed-integer nonlinear programming model in GAMS

- ***Parameters***
- ***Variables***
- ***Equations***
  - ***Economic modules***
  - ***Process modules***
    - ***Material balances***
    - ***Hydrodynamic/Energy balances***
    - ***Reactor surrogate models***
  - ***Link between economic modules and process modules***
  - ***Binary variable constraints***
  - ***Bounds for variables***



Optimal layout

Optimization & Heat Integration



Objective Function: Maximize **Net efficiency**

Constraint: **CO_2 removal** ratio ≥ 90%
Flowsheet evaluation (via process simulators)
Minimum utility target (via heat integration tool)

Decision Variables (17): Bed length, diameter, sorbent and steam feed rate

Optimization with Heat Integration

Objective Function: ***Maximize Net efficiency***

Constraint: ***CO_2 removal ratio ≥ 90%***
Flowsheet evaluation (via process simulators)
Minimum utility target (via heat integration tool)

Decision Variables (17): Bed length, diameter, sorbent and steam feed rate

	w/o heat integration	Sequential	Simultaneous
Net power efficiency (%)	31.0	32.7	35.7
Net power output (MW_e)	479.7	505.4	552.4
Electricity consumption [b] (MW_e)	67.0	67.0	80.4
IP steam withdrawn from power cycle (MW_{th})	0	0	0
LP steam withdrawn from power cycle (MW_{th})	336.3	304.5	138.3
Cooling water consumption [b] (MW_{th})	886.8	429.3	445.1
Heat addition to feed water (MW_{th})	0	125.3	164.9

Base case w/o CCS: 650 MW_e, **42.1 %**

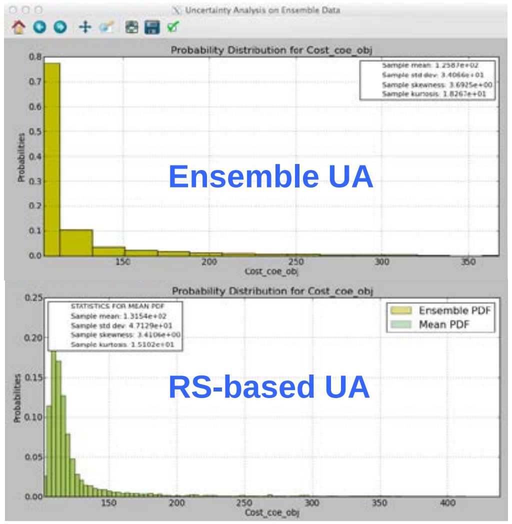
Chen, Y., J. C. Eslick, I. E. Grossmann and D. C. Miller (2015). "Simultaneous Process Optimization and Heat Integration Based on Rigorous Process Simulations." Computers & Chemical Engineering. doi:10.1016/j.compchemeng.2015.04.033

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% CO_2 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?

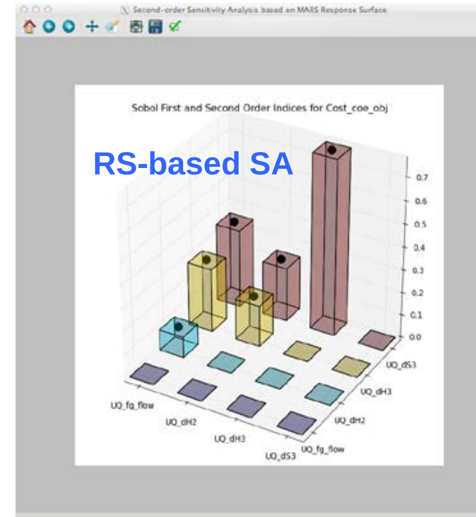
CCSI UQ framework is designed to answer these questions

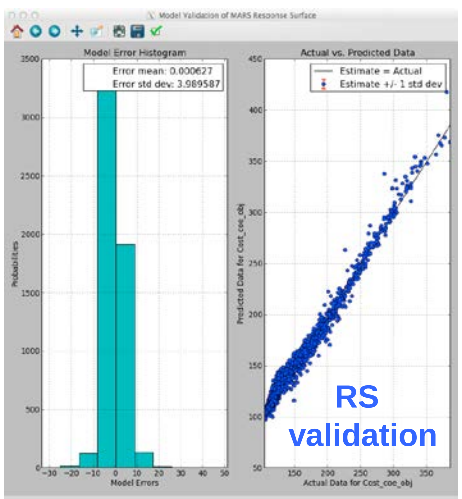
Perform statistical analyses with FOQUS

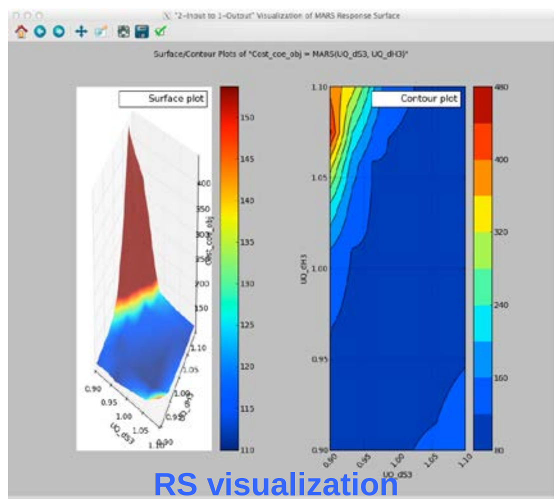


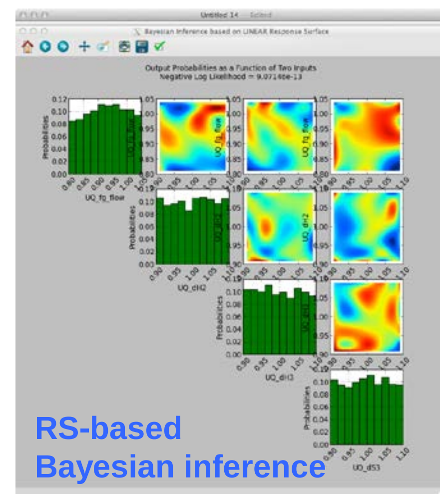
<u>Ensemble Analyses</u>
- ➢ Uncertainty analysis
- ➢ Sensitivity analysis
- ➢ Correlation analysis
- ➢ Scatterplots for visualization

<u>Response Surface (RS) Analyses</u>
- ➢ RS validation
- ➢ RS visualization
- ➢ RS-based uncertainty analysis
- ➢ RS-based sensitivity analysis
- ➢ RS-based Bayesian inference

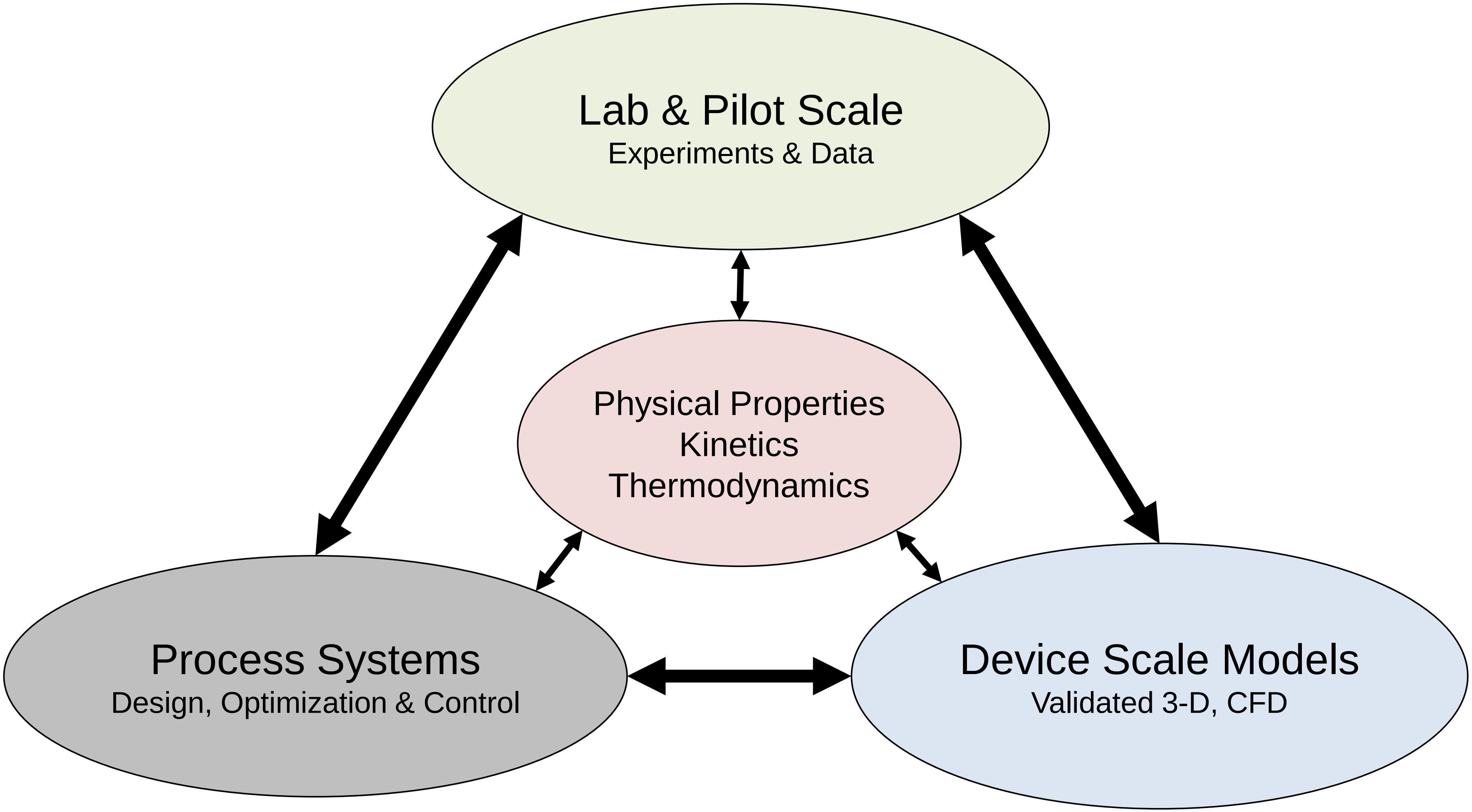




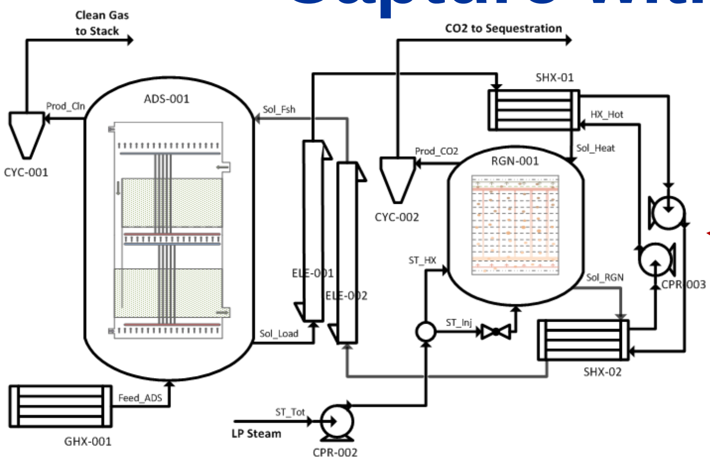




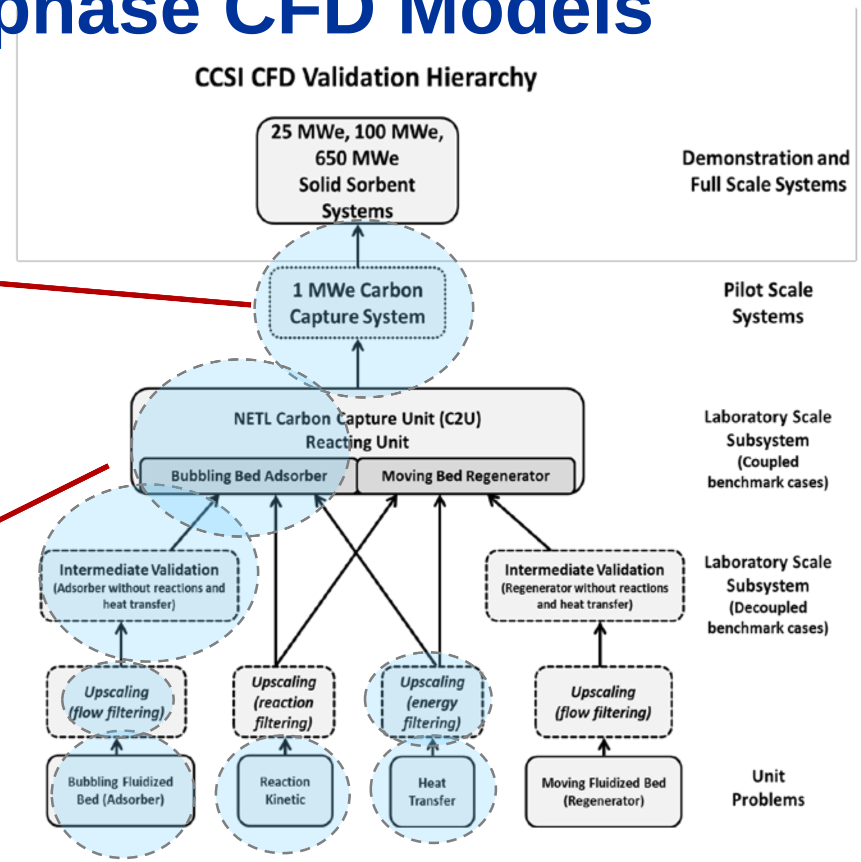
Solid Sorbents: Validated CFD Model Example

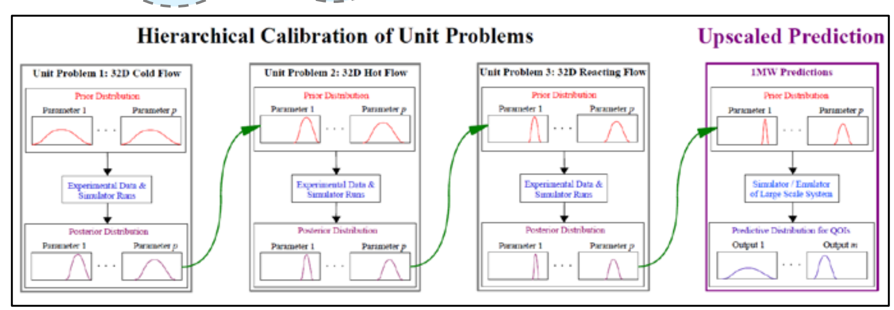


Building Predictive Confidence for Device-scale CO_2 Capture with Multiphase CFD Models

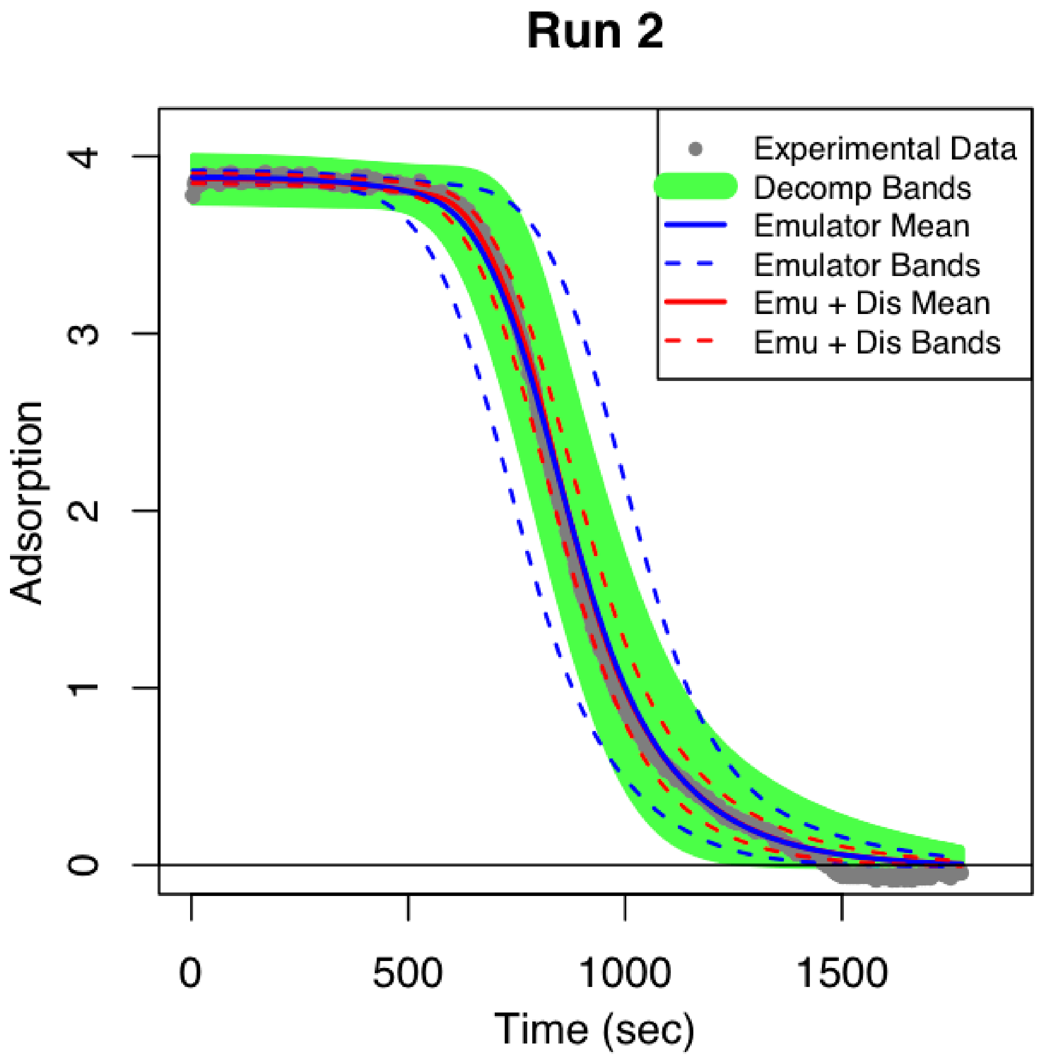


C2U Batch Unit



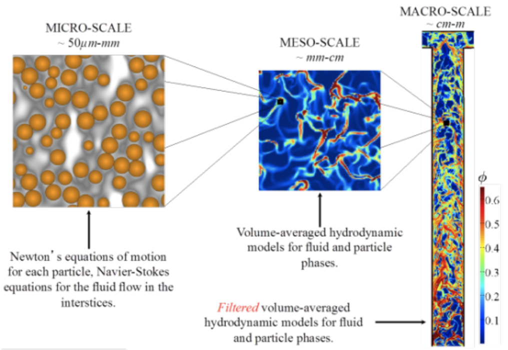


Intermediate Validation with Unit Problem 3
Predicted Breakthrough Curves for Held-out Runs

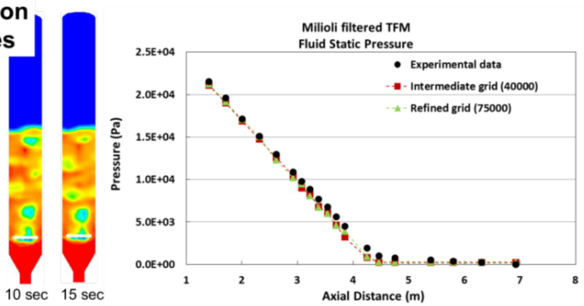


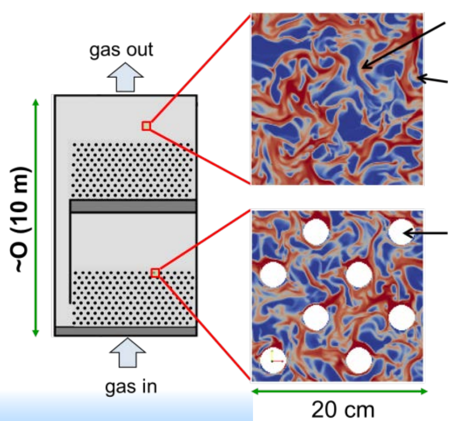
Filtered Models with Heat Exchanger Tubes

Filtered Models for Gas-Particle Flows

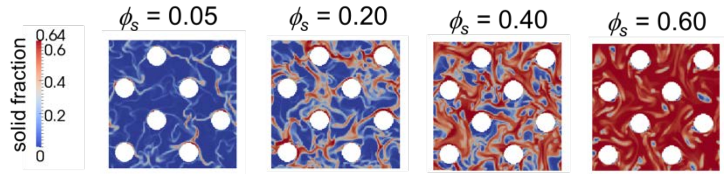


Validation Studies

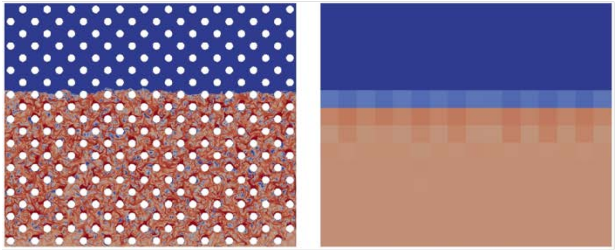




Flows With Immersed Cooling Tubes

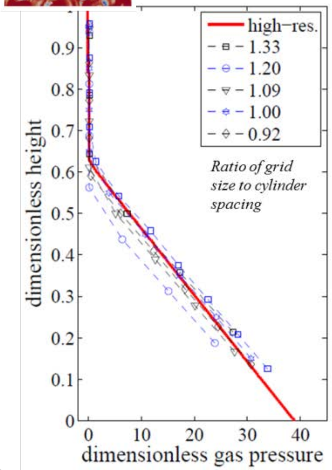


Bubbling Bed



Highly-resolved "Exact solution" ~O(10^6) cells

Coarse grid + Filtered models ~O(10^2-10^3) cells

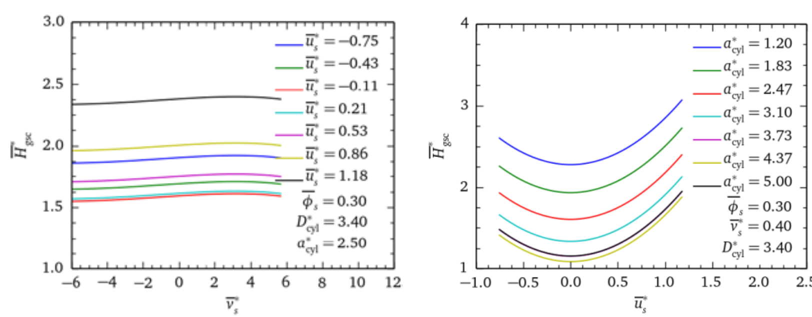


Model-on-model verification

Filtered Models For Heat Transfer

$$\partial_t(\phi_s\rho_s C_{p,s}T_s) + \nabla\cdot(\phi_s\rho_s C_{p,s}\,\mathbf{v}_s T_s) = \nabla\cdot(\phi_s k_s \nabla T_s) + I_{gs} + Q_{gsc}$$

$$H^*_{gsc} = f(\bar{\phi}_s, \bar{\mathbf{v}}^*_s, D^*_{cyl}, a^*_{cyl})$$



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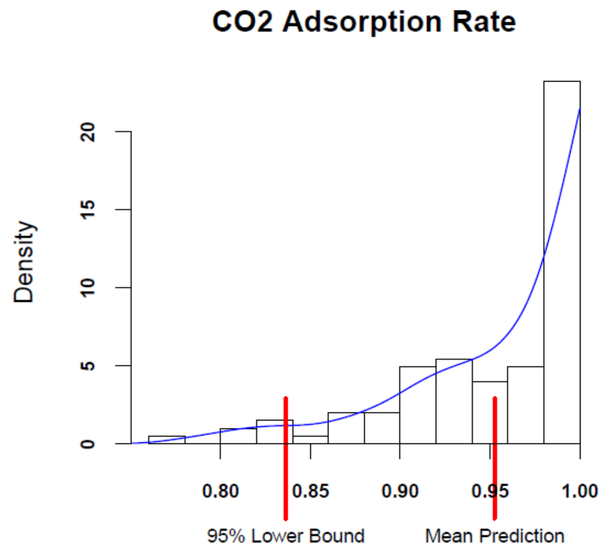
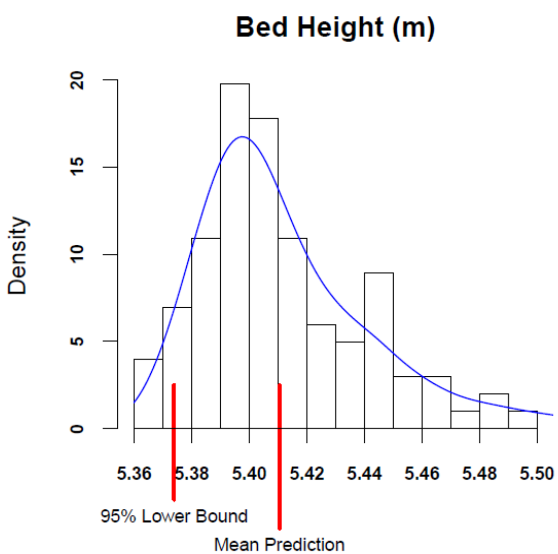
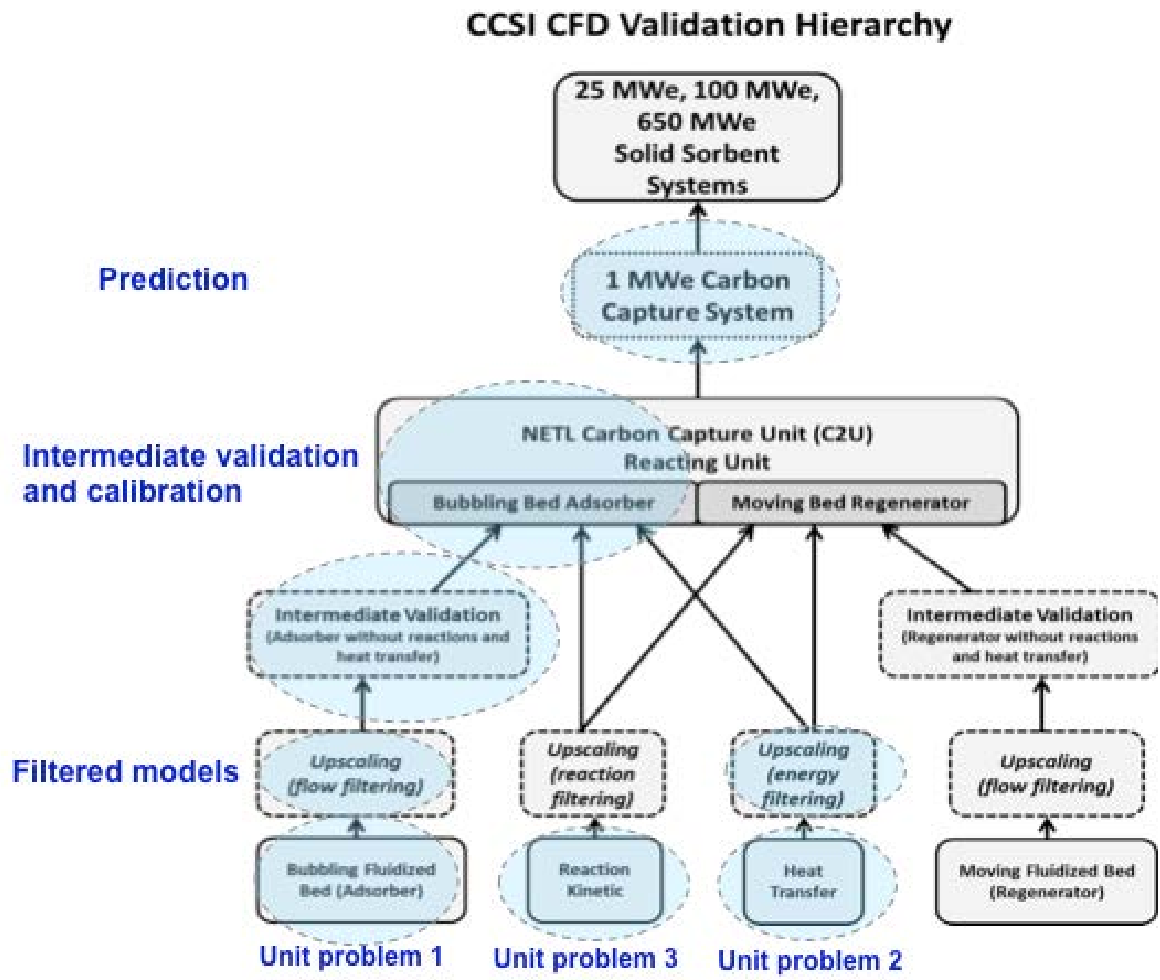
Quantitatively predicting scale up performance



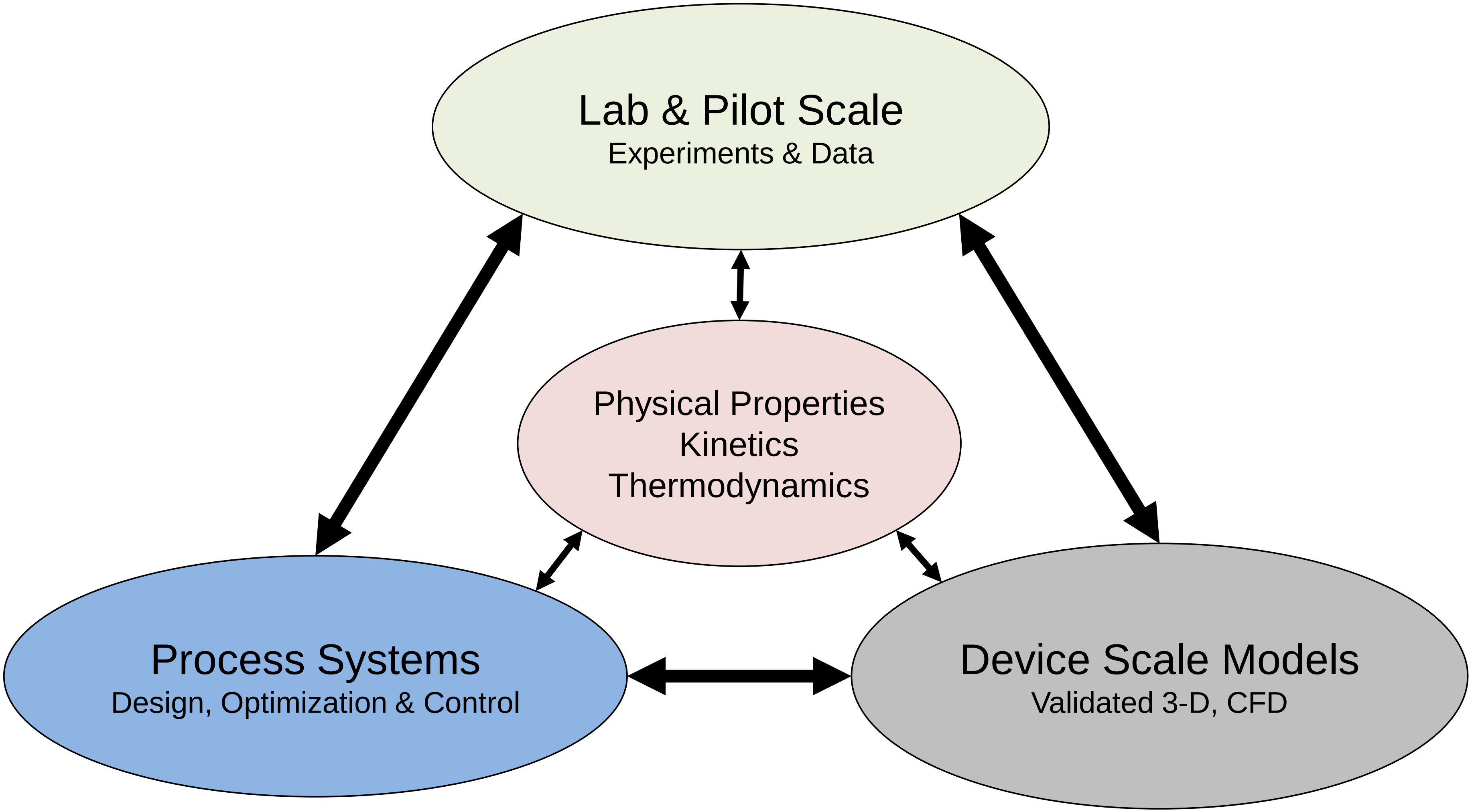




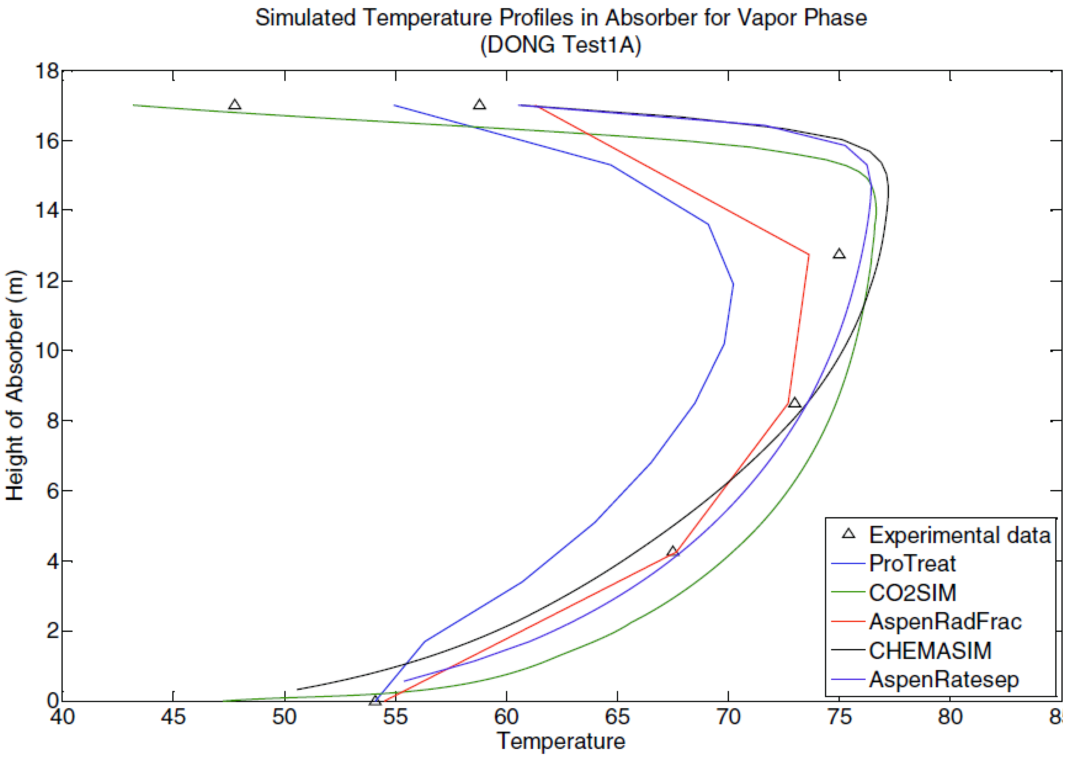
Solvent System Models & Demonstration

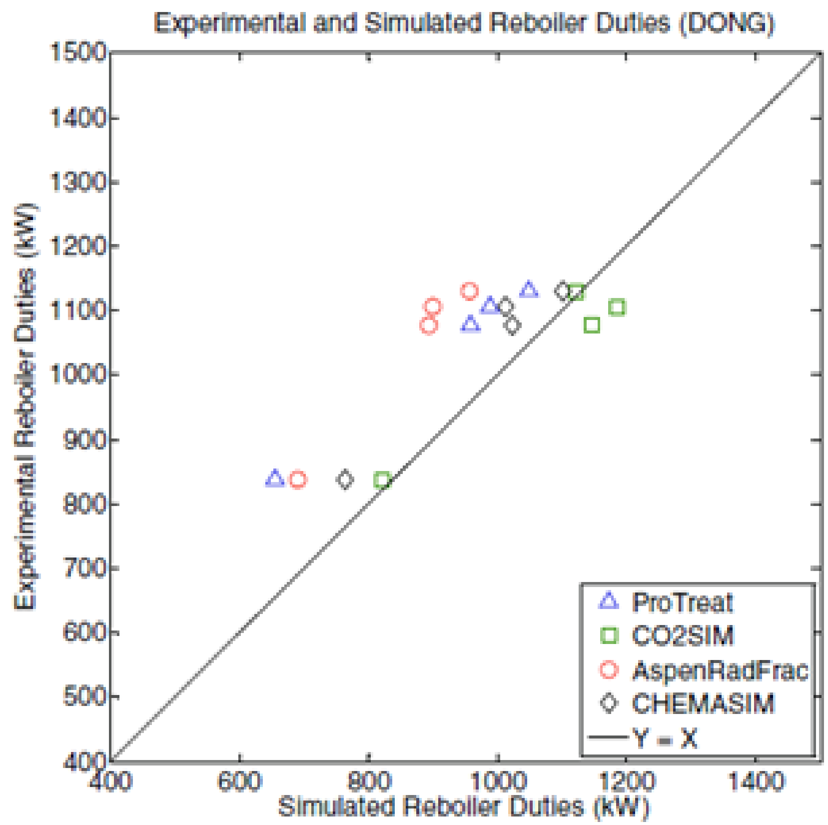
- **Basic data models**
  - *Unified tool to calibrate solvent data*
  - *High Viscosity Solvent Model, 2-MPZ*
  - *Properties model for Pz/2-MPz Blends (Aspen)*
- **CFD models**
  - *VOF Prediction on Wetted Surface*
  - *Prediction of mass transfer coefficients by calibration of fully coupled wetted 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

Solvents: System Model Example & Validation



Predictive Model Development & Validation





ProTreat-Optimized Gas Treating, Inc.; CO2SIM-NTNU/SINTEF
CHEMASIM-BASF SE; AspenRatesep-modified by IFP

Luo et al., "Comparison and validation of simulation codes against sixteen sets of data from four different pilot plants", Energy Procedia, 1249-1256, 2009

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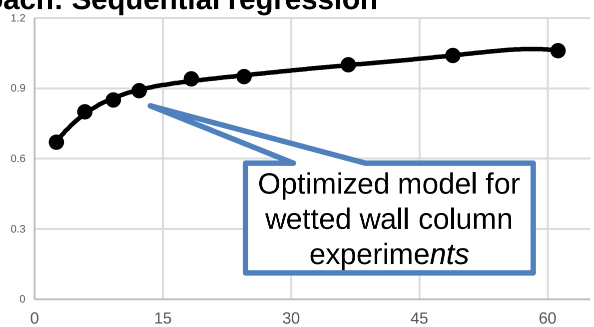
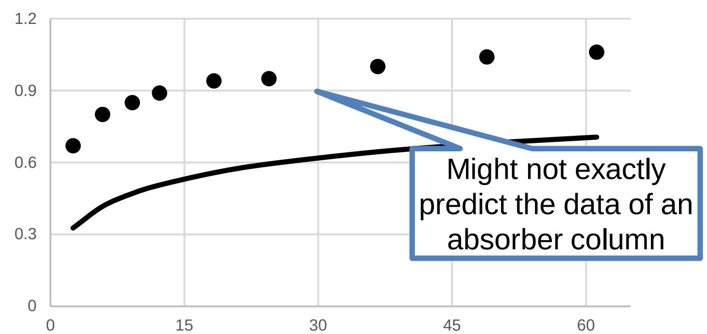
Integrated Mass Transfer Model Development

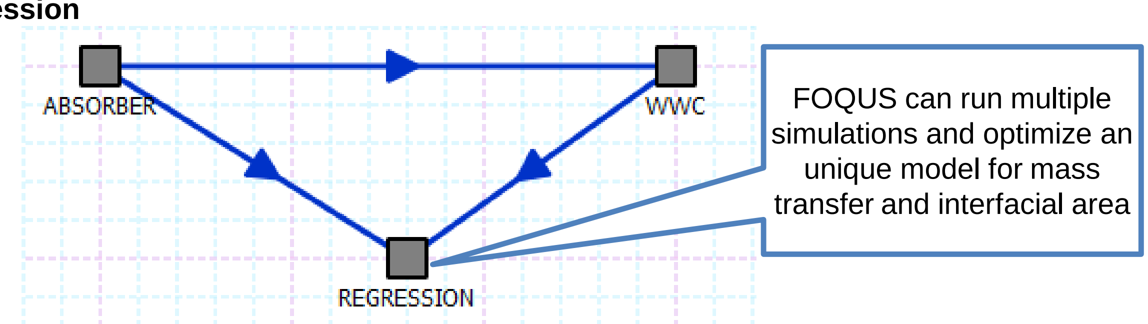
- Diffusivity, viscosity, surface tension, interfacial area, and mass transfer coefficients all important
- Data from both wetted wall column and packed column considered
- Simultaneous regression of these models not previously possible
- FOQUS has the capability of simultaneous regression

Usual approach: Sequential regression

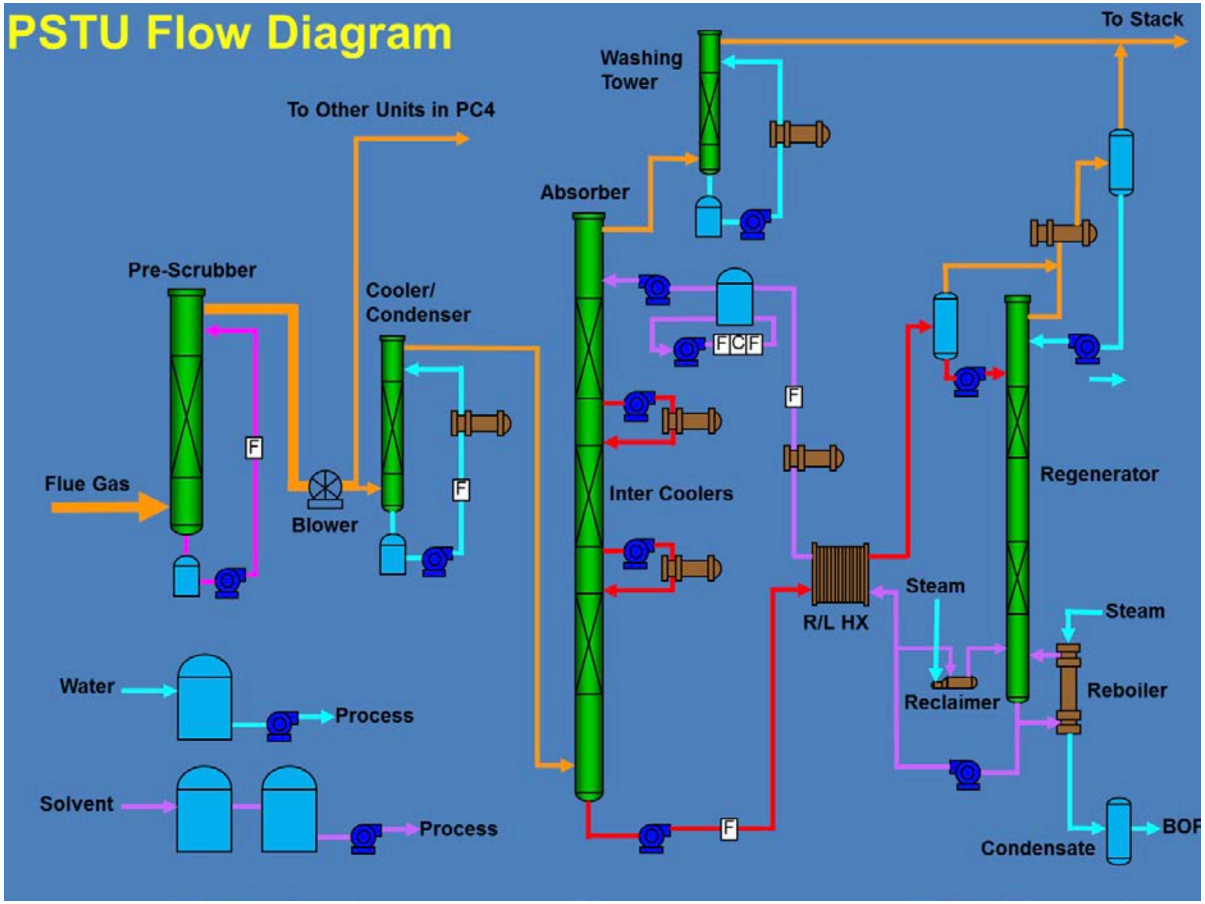




FOQUS capability: Simultaneous regression



CCSI Team Conducted Tests at NCCC



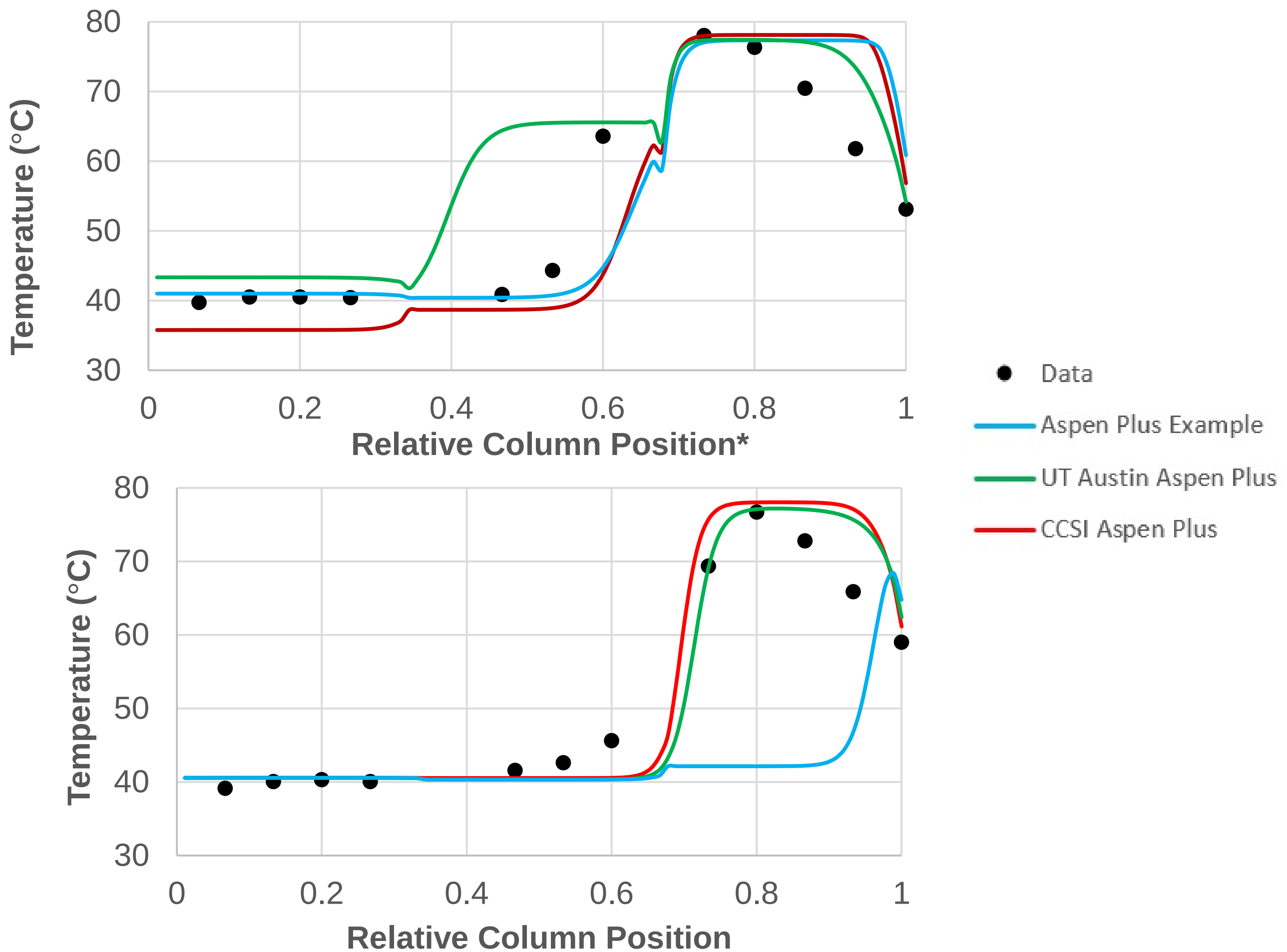
Steady State Absorber Validation

No parameters tuned

Temperature Profiles

Case 1: L/G=3.81
3 bed absorber with two intercoolers

Case 5:
6.43 L/G ratio
Intercooling present
17.18% CO_2 in flue gas



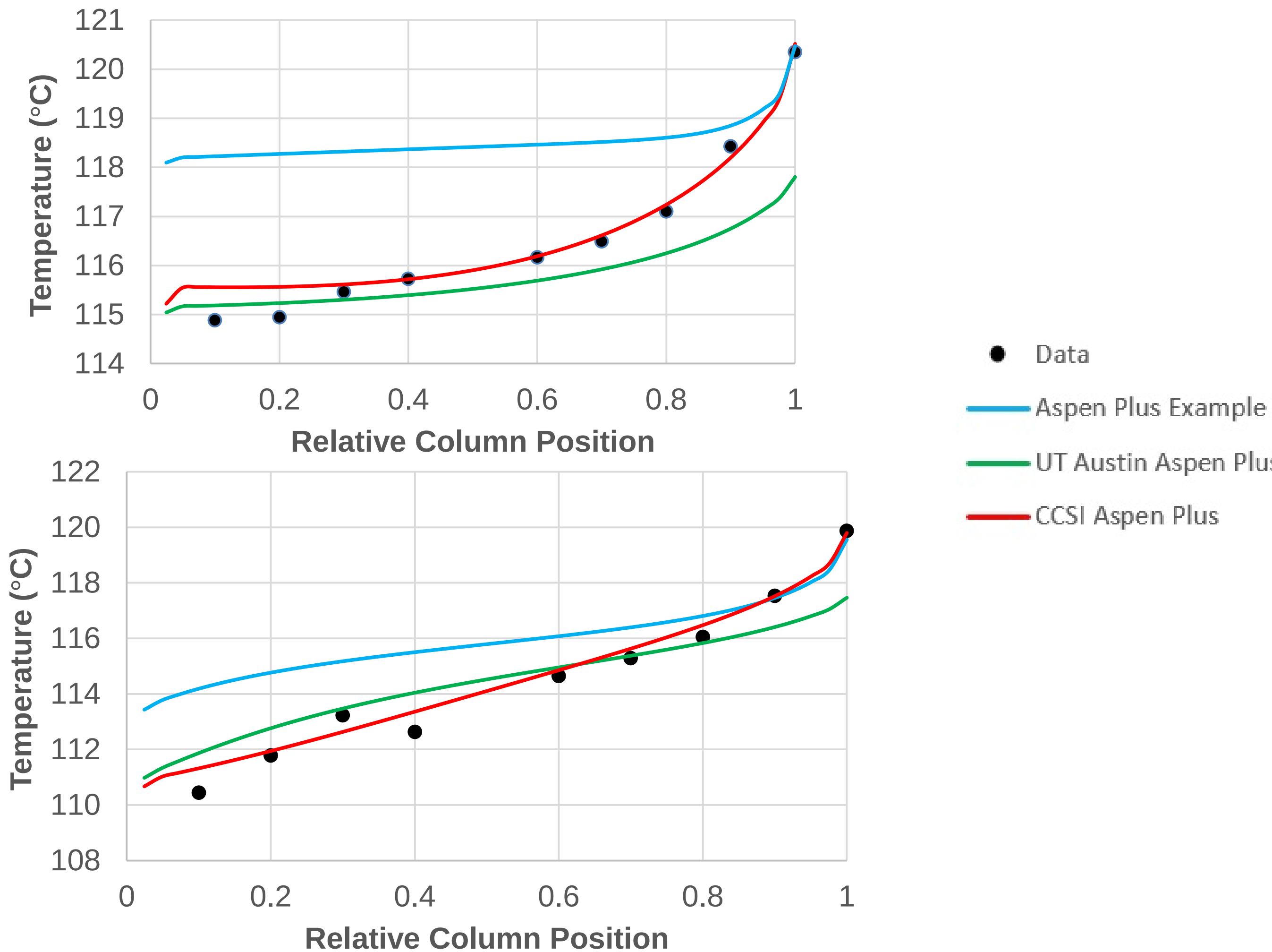
*** Relative positions of 0 and 1 represent top and bottom of column, respectively**

Regenerator Validation

No parameters tuned

Case 1:
12000 kg/hr solvent
680 kW reboiler duty

Case 6:
7240 kg/hr solvent
425 kW reboiler duty



*** Relative positions of 0 and 1 represent top and bottom of column, respectively**

CCSI Carbon Capture Simulation Initiative

NETL

Berkeley Lab

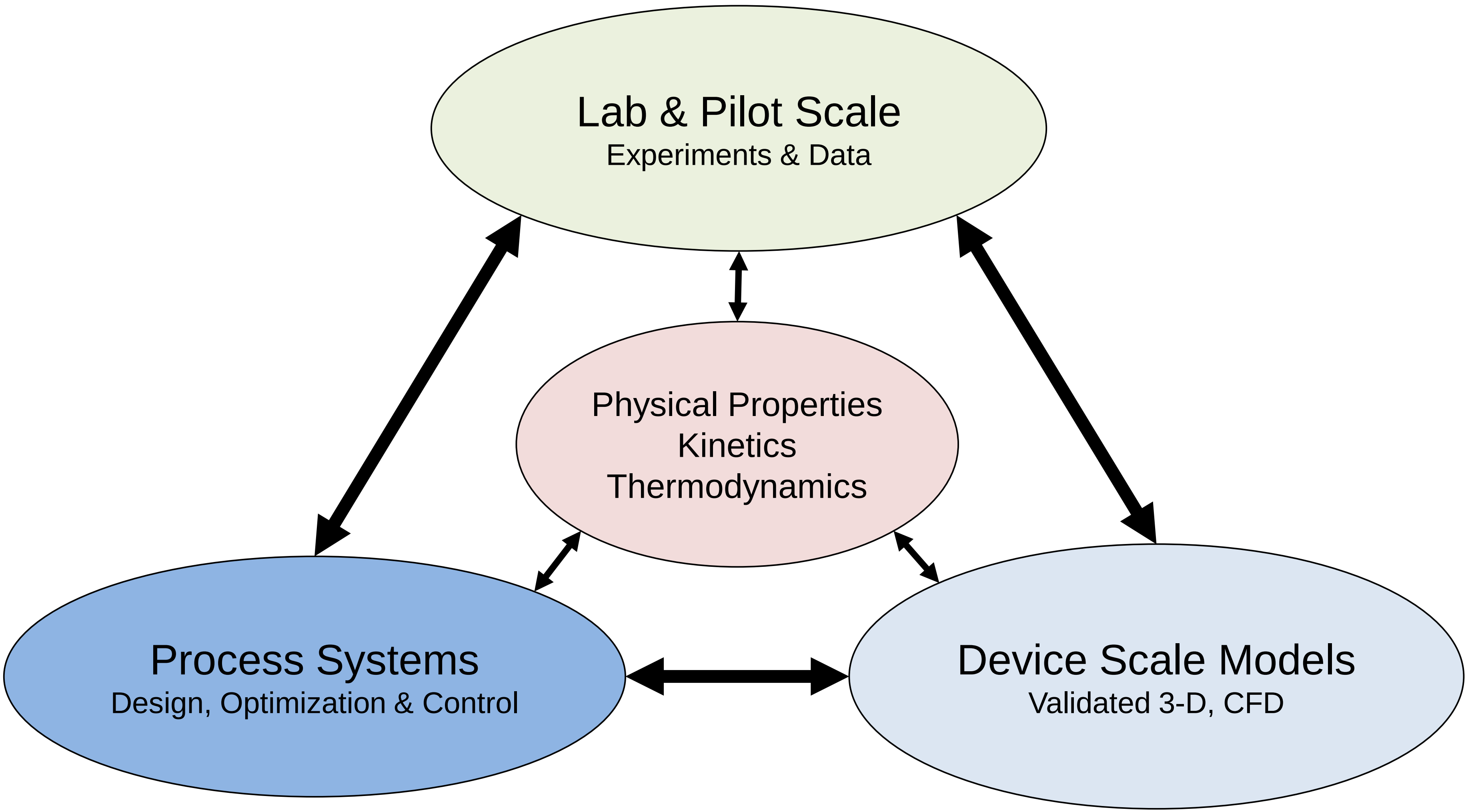
Lawrence Livermore National Laboratory

Los Alamos National Laboratory EST. 1943

Pacific Northwest National Laboratory

U.S. Department of Energy

Advanced Computational Tools to Accelerate Carbon Capture Technology Development



CCSI status as of January 2016

- CCSI Toolset
  - Suite of rigorous, validated, predictive models
  - Computational tools
  - Methodologies for UQ, validation, model development
  - Broadly applicable to many carbon capture concepts
- How to maximize the benefit of CCSI investment and accomplishments?
  - Deploy the tools
  - Utilize the tools
  - Train industry

CCSI²

Carbon Capture Simulation for Industry Impact

- Work closely with industry partners to help scale up
  - Large scale pilots
    - Help ensure success at this scale
      - Employ simulation to predict performance, potential issue
      - Help resolve issues using simulation tools
    - Maximize learning at this scale
      - Data collection & experimental design
      - Develop & Validate models
      - UQ to identify critical data
    - Help develop demonstration plant design
      - Utilize optimization tools (OUU, Heat Integration)
      - Quantitative confidence on predicted performance
      - Predict dynamic performance
  - Partnership via CRADA

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  - OUU: DFO Team, UQ Team, Alex Dowling (CMU)
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