

CCSI

Carbon Capture Simulation Initiative

David C. Miller, Ph.D.

Technical Director, CCSI
National Energy Technology Laboratory
U.S. Department of Energy

15 June 2015



Lawrence Livermore
National Laboratory

Los Alamos
NATIONAL LABORATORY
EST. 1943

Pacific
Northwest
NATIONAL
LABORATORY



U.S. DEPARTMENT OF
ENERGY

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

1 kWe

1 MWe

10 MWe

100 MWe

500 MWe

Accelerated deployment timeline

Process Scale Up
15 years

1 MWe

10 MWe

100 MWe

500 MWe

2010

2015

2020

2025

2030

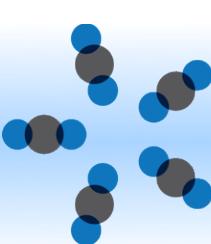
2035

2040

2045

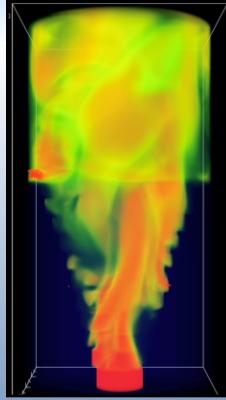
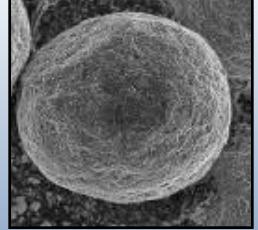
2050

2



CCSI For Accelerating Technology Development

Carbon Capture Simulation Initiative



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



Academia

Carnegie Mellon



Industry



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



ALSTOM

EPRI ELECTRIC POWER RESEARCH INSTITUTE



B&W
the babcock&wilcox company



eSi
get it right®

WSS Innovative Simulation Solutions

ES Clean Energy Systems, Inc.
Power Without Pollution™



Lawrence Livermore National Laboratory

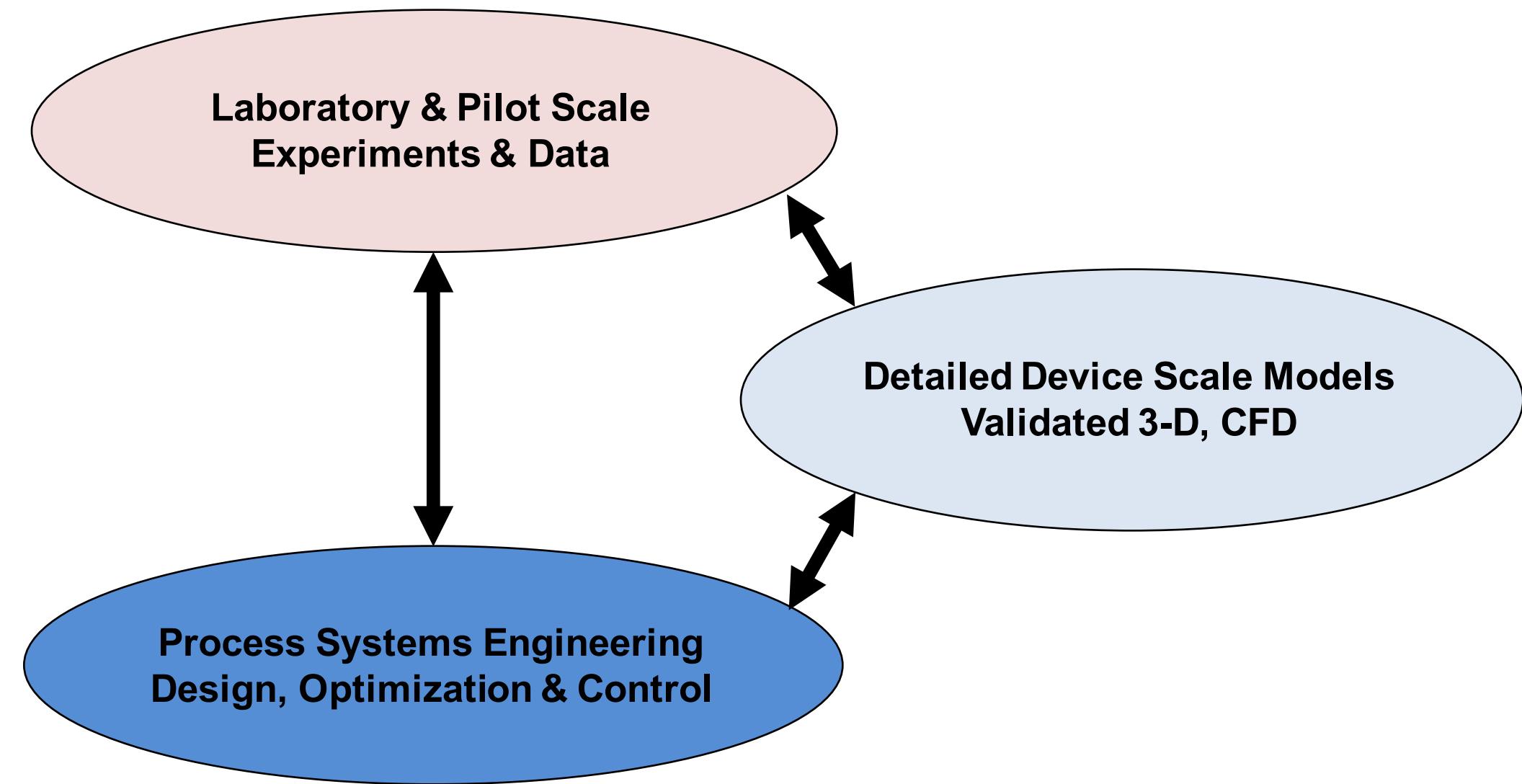
Los Alamos
NATIONAL LABORATORY
EST.1943

Pacific Northwest
NATIONAL LABORATORY

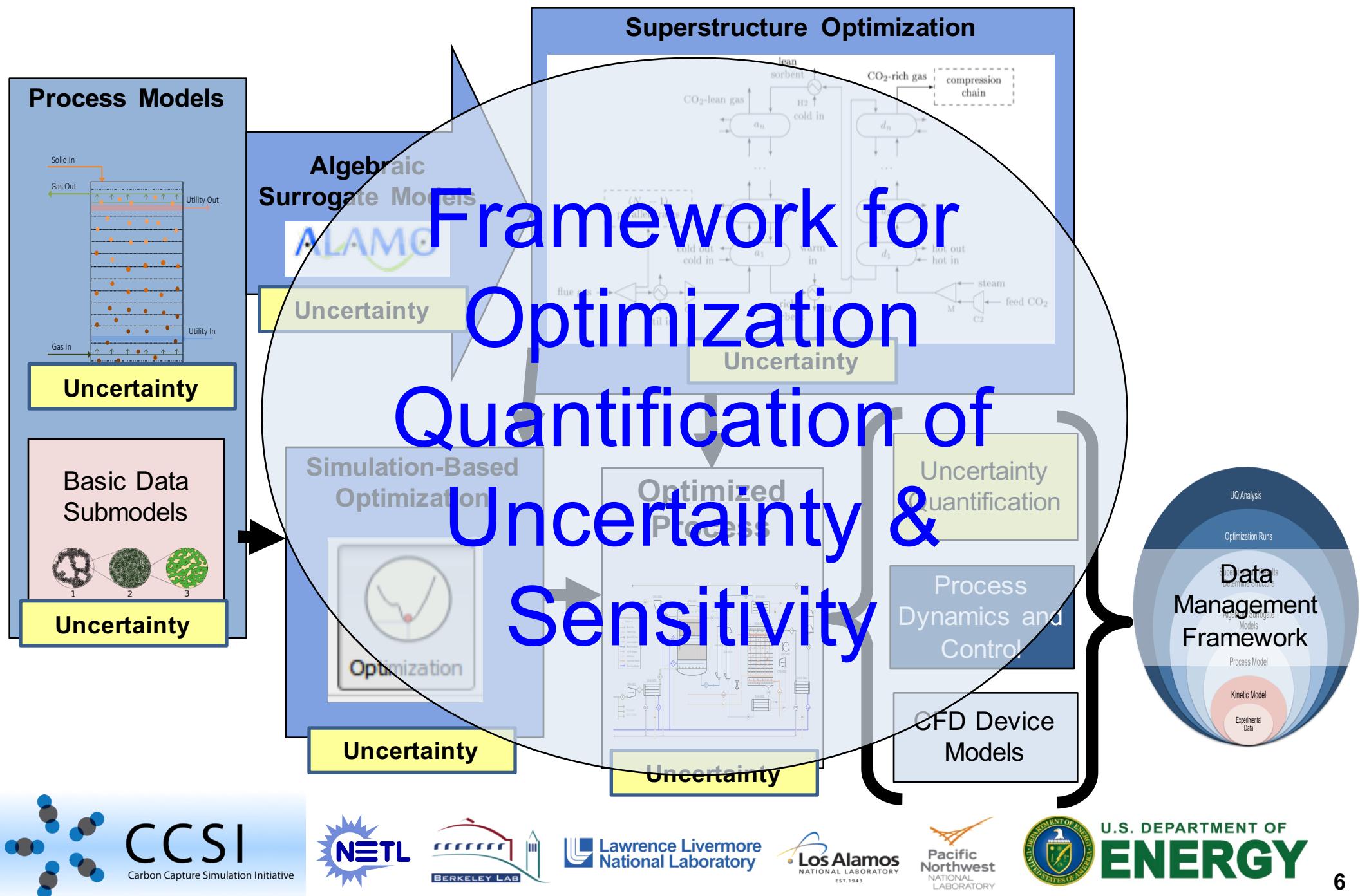


U.S. DEPARTMENT OF ENERGY

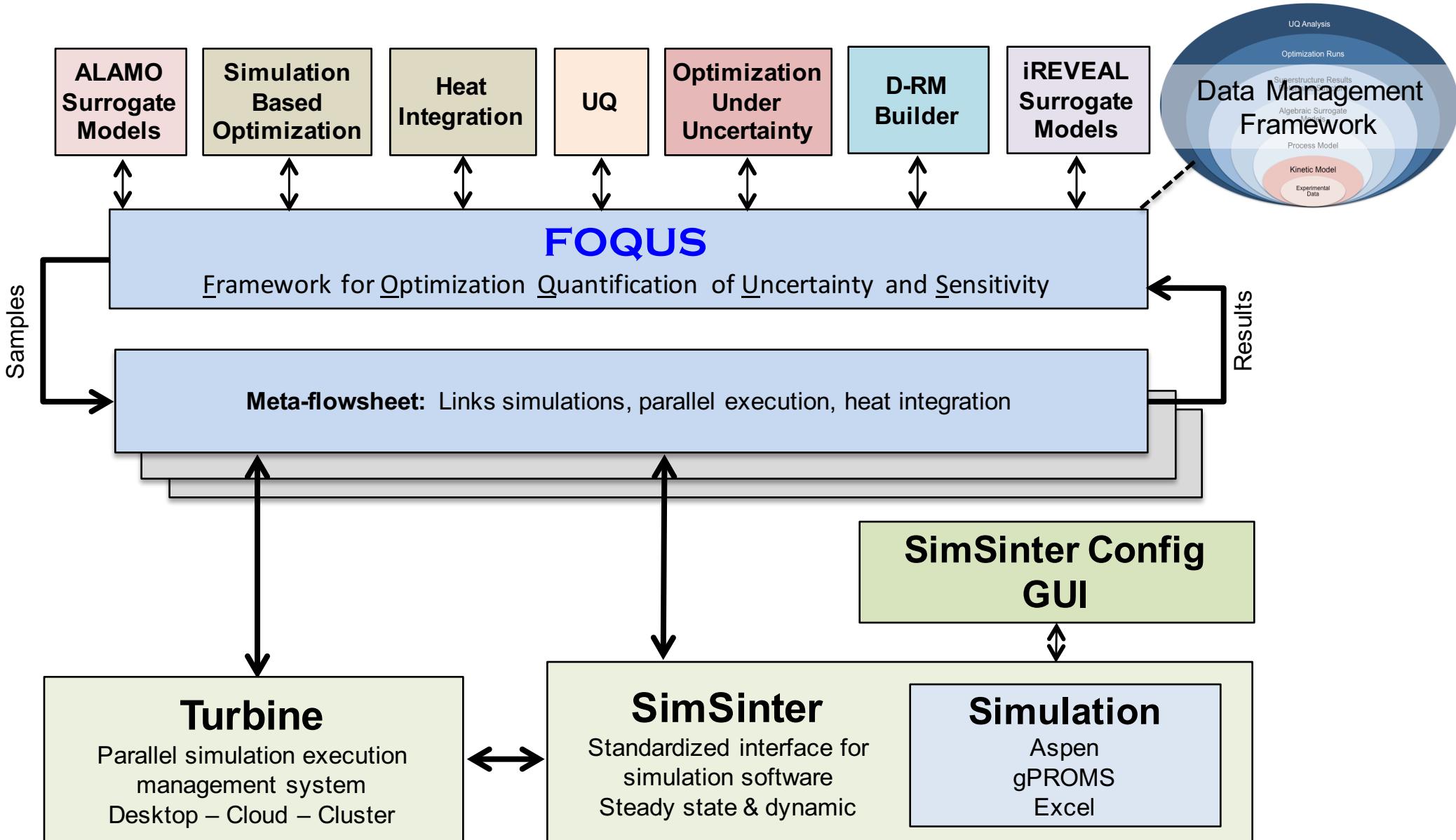
Advanced Computational Tools to Accelerate Carbon Capture Technology Development



CCSI Toolset Workflow and Connections



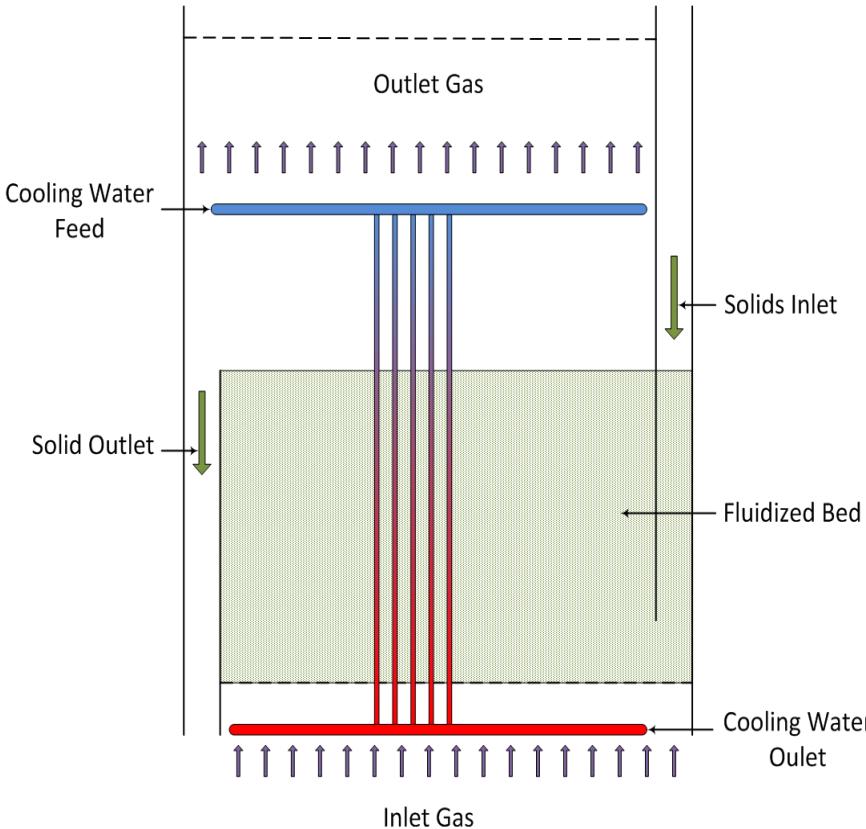
Framework for Optimization, Quantification of Uncertainty and Sensitivity



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.

Bubbling Fluidized Bed Process Model

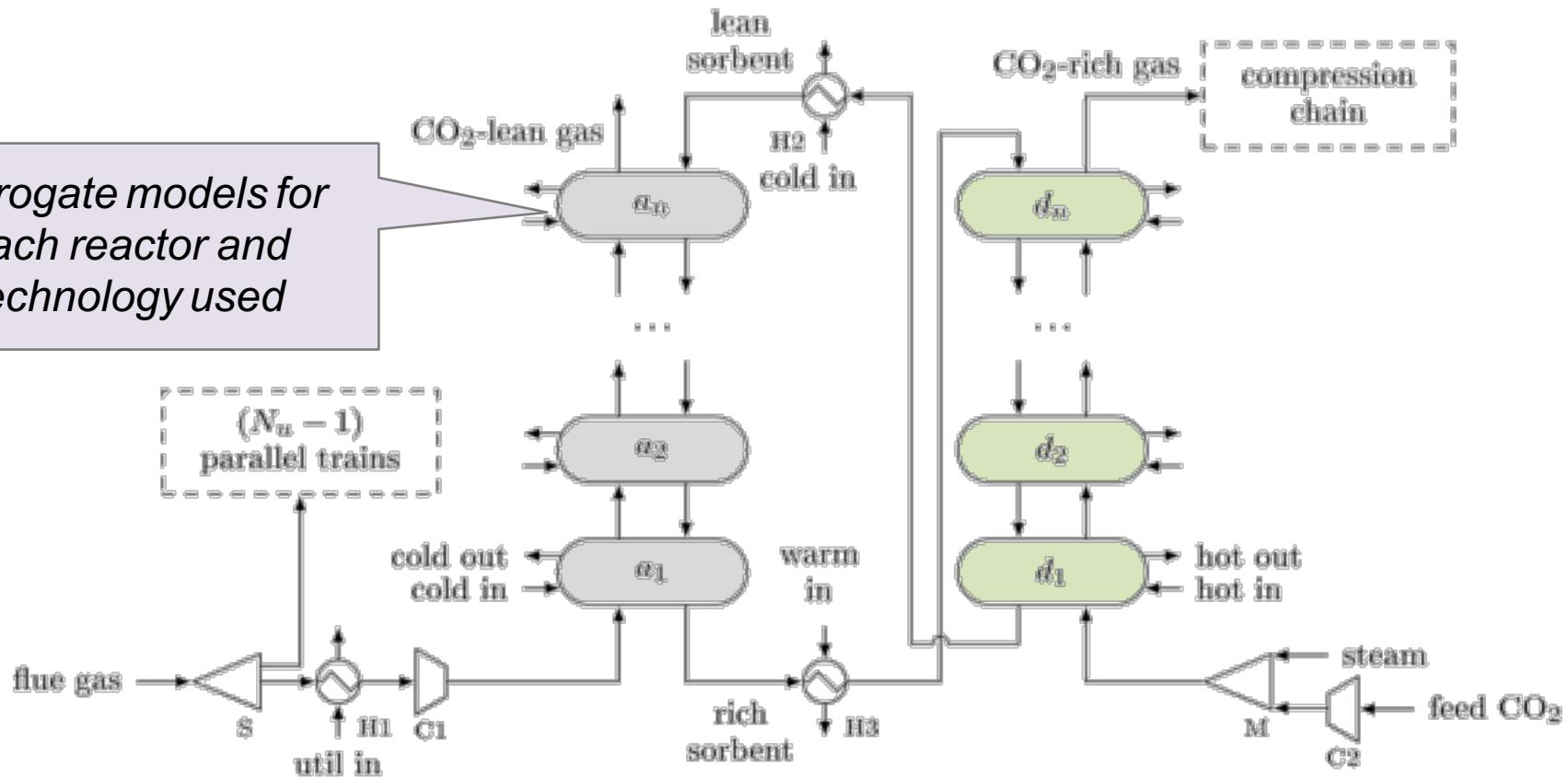
1-D, two-phase, pressure-driven and non-isothermal models developed in both ACM and gPROMS



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

Carbon Capture System Configuration

Surrogate models for each reactor and technology used

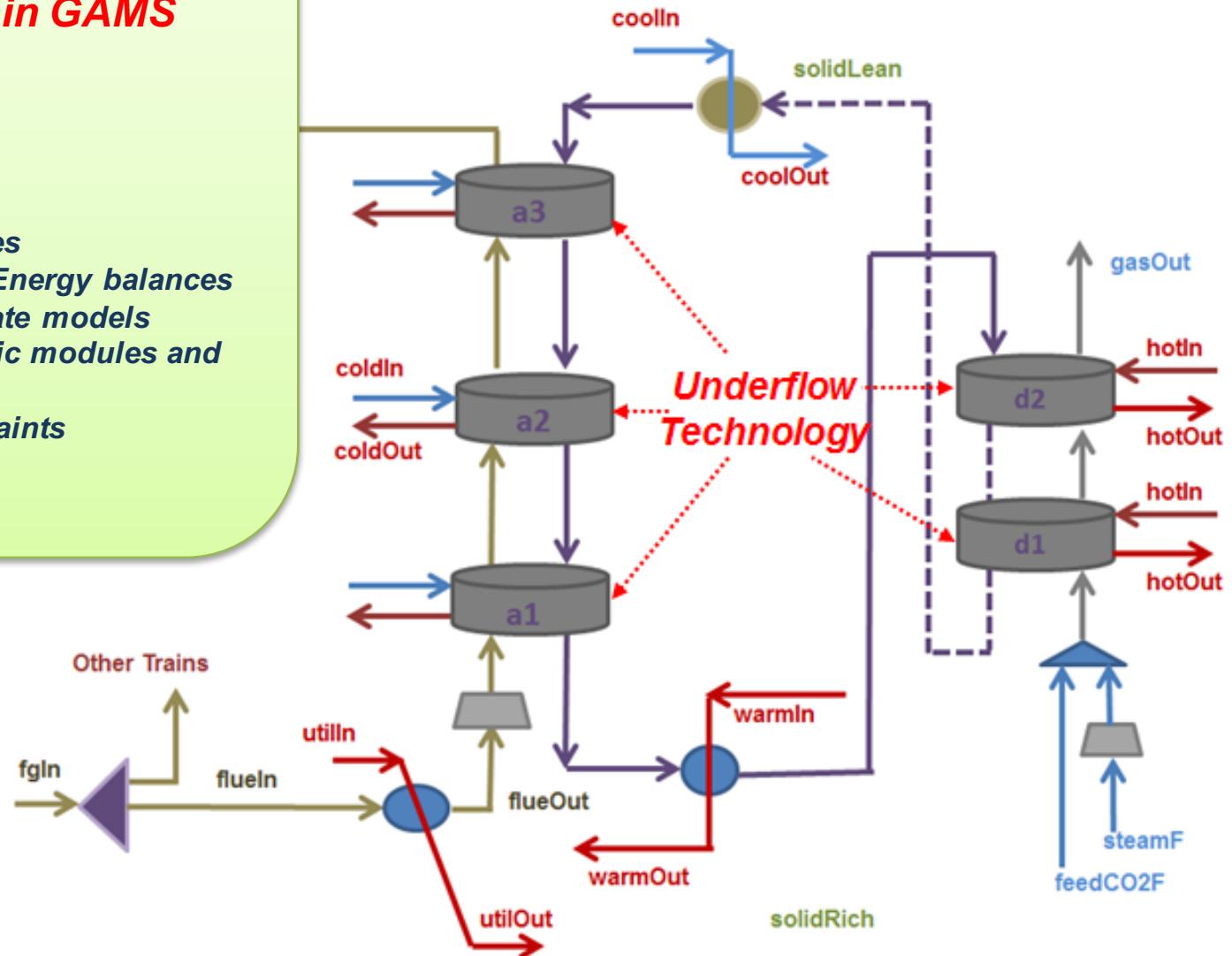


- Discrete decisions: How many units? Parallel trains?
What technology used for each reactor?
- Continuous decisions: Unit geometries
- Operating conditions: Vessel temperature and pressure, flow rates, compositions

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



Optimization with Heat Integration

Objective Function: Maximize *Net efficiency*

Constraint: *CO₂ removal ratio ≥ 90%*

Flowsheet evaluation (via process simulators)

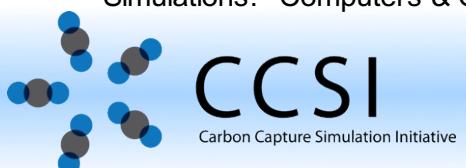
Minimum utility target (via heat integration tool)

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

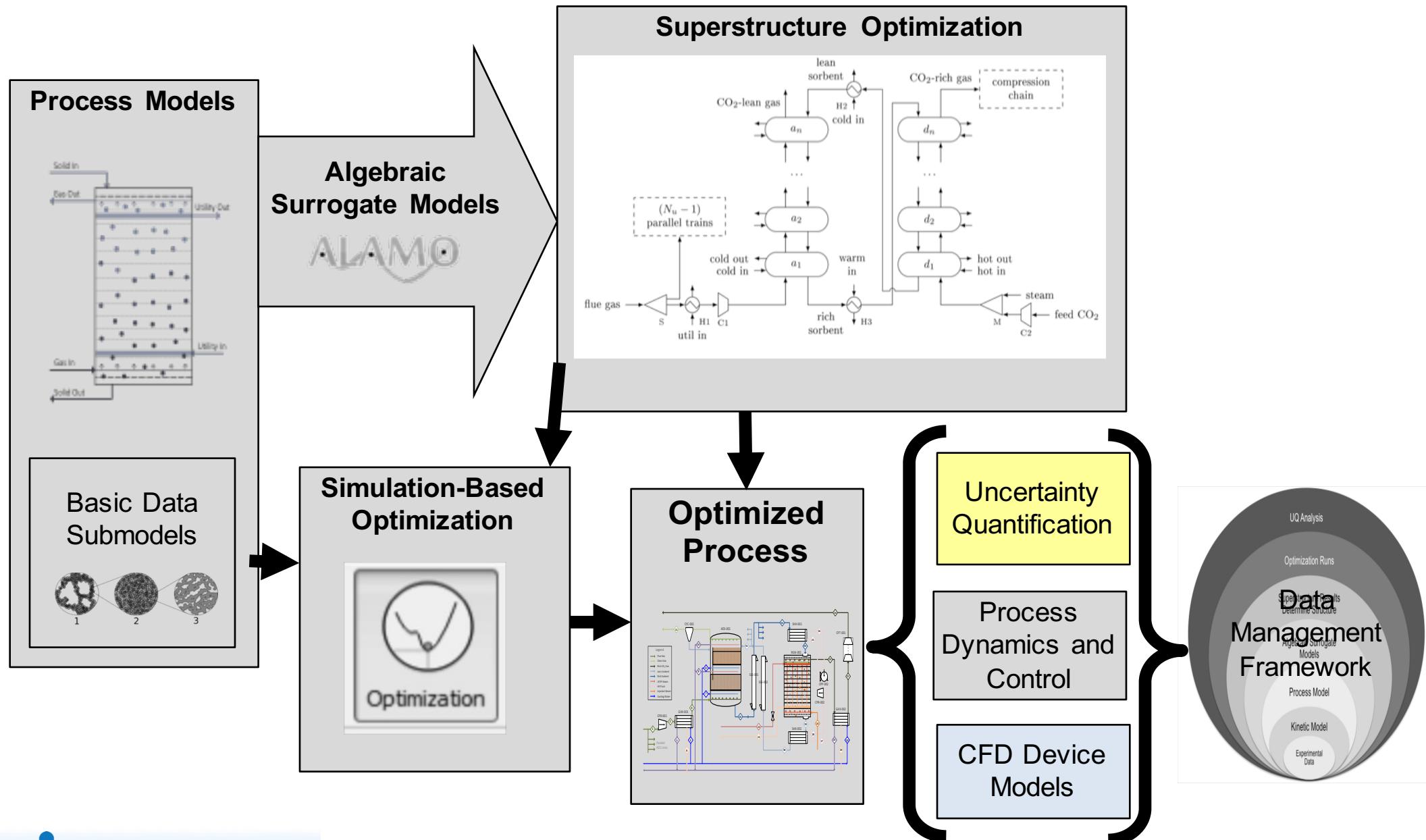
	w/o heat integration	Sequential	Simultaneous
Net power efficiency (%)	31.0	32.7	35.7
Net power output (MW _e)	479.7	505.4	552.4
Electricity consumption ^b (MW _e)	67.0	67.0	80.4
IP steam withdrawn from power cycle (MW _{th})	0	0	0
LP steam withdrawn from power cycle (MW _{th})	336.3	304.5	138.3
Cooling 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 %

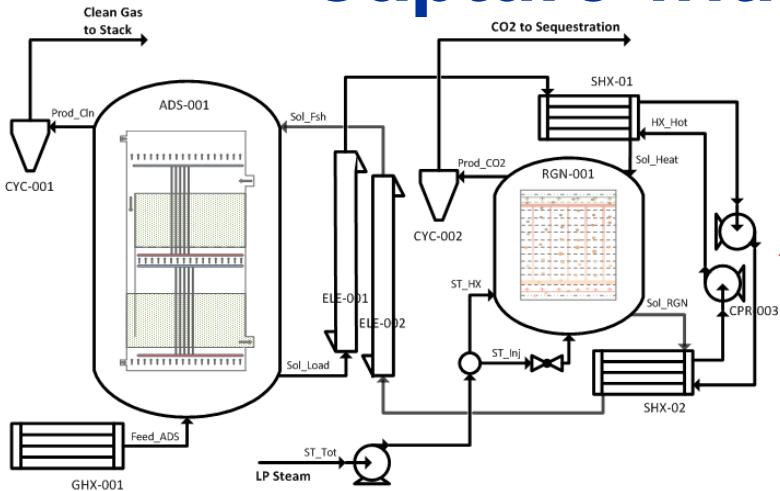
Chen, Y., J. C. Eslick, I. E. Grossmann and D. C. Miller (2015). "Simultaneous Process Optimization and Heat Integration Based on Rigorous Process Simulations." Computers & Chemical Engineering. doi:10.1016/j.compchemeng.2015.04.033



Device Models to Quantify Predicted Scale Up Performance



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

Demonstration and
Full Scale Systems

Pilot Scale
Systems

Laboratory Scale
Subsystem
(Coupled
benchmark cases)

Laboratory Scale
Subsystem
(Decoupled
benchmark cases)

Unit
Problems

NETL Carbon Capture Unit (C2U)
Reacting Unit

Bubbling Bed Adsorber Moving Bed Regenerator

Intermediate Validation
(Adsorber without reactions and
heat transfer)

Intermediate Validation
(Regenerator without reactions
and heat transfer)

Upscaling
(flow filtering)

Upscaling
(reaction filtering)

Upscaling
(energy filtering)

Upscaling
(flow filtering)

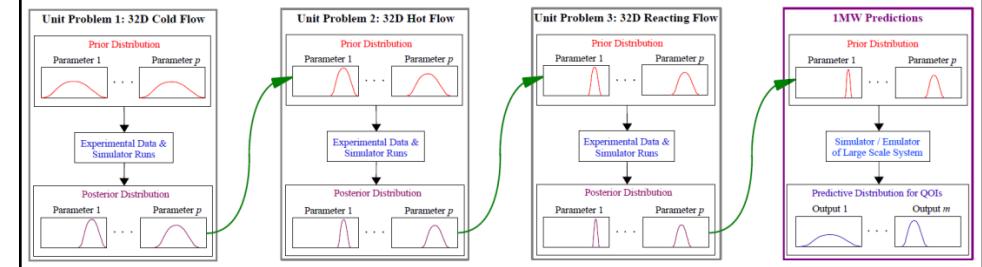
Bubbling Fluidized
Bed (Adsorber)

Reaction Kinetic

Heat Transfer

Moving Fluidized Bed
(Regenerator)

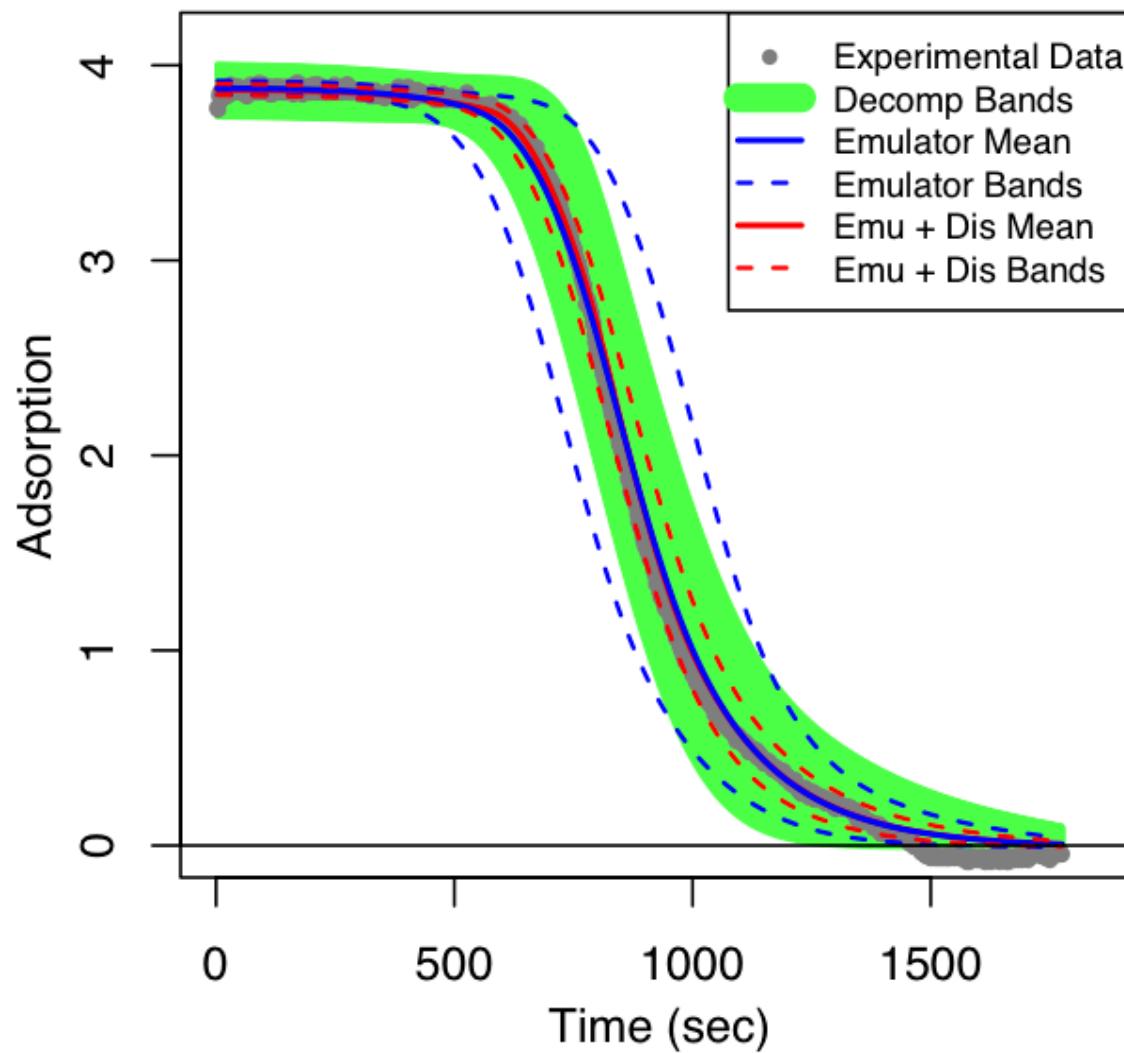
Hierarchical Calibration of Unit Problems



Intermediate Validation with Unit Problem 3

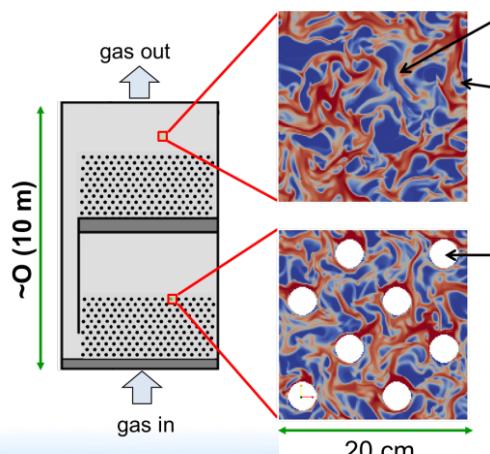
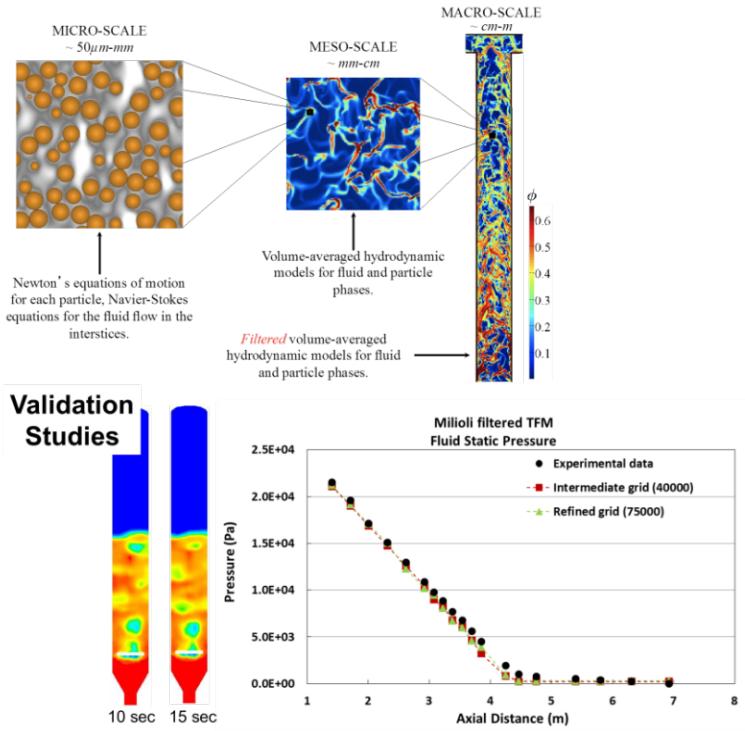
Predicted Breakthrough Curves for Held-out Runs

Run 2

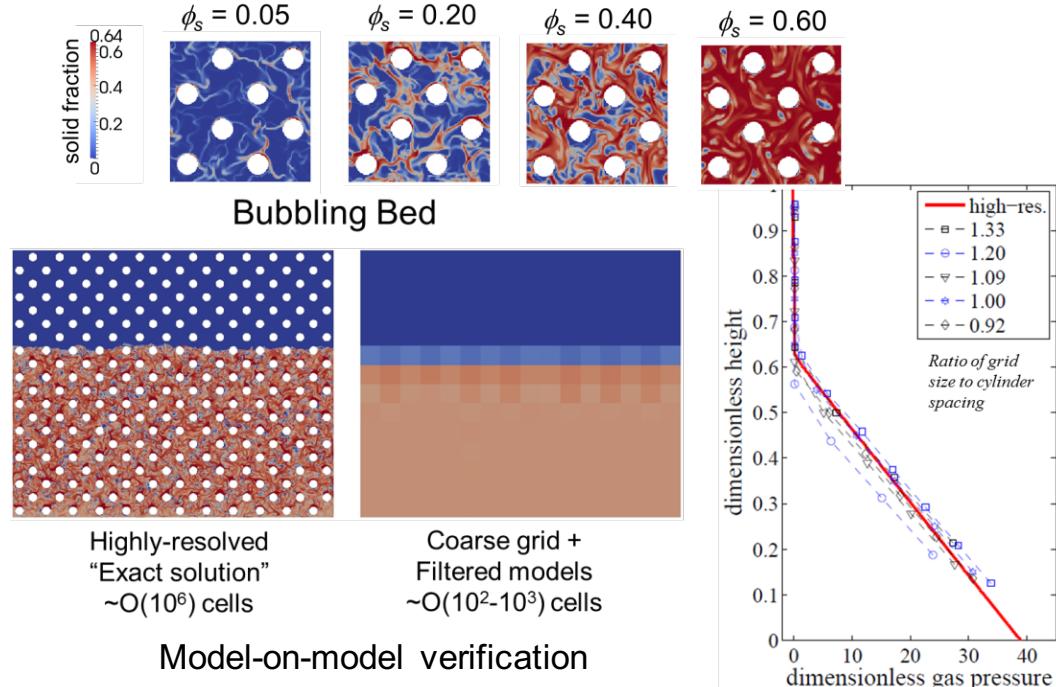


Filtered Models with Heat Exchanger Tubes

Filtered Models for Gas-Particle Flows



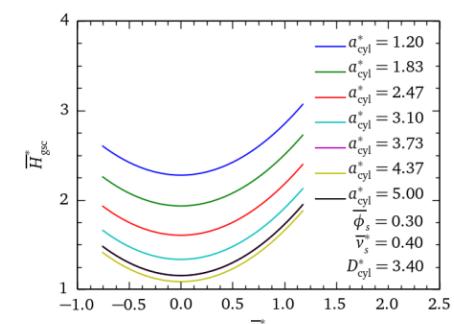
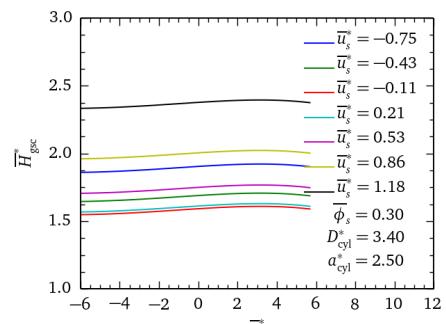
Flows With Immersed Cooling Tubes



Filtered Models For Heat Transfer

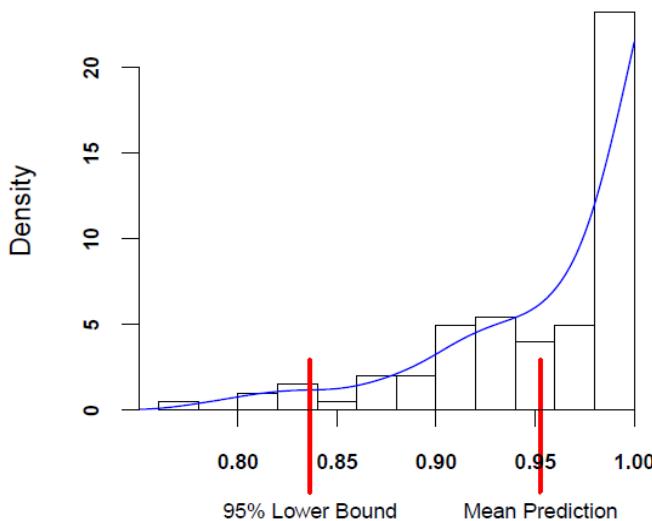
$$\partial_t (\phi_s \rho_s C_{p,s} T_s) + \nabla \cdot (\phi_s \rho_s C_{p,s} \mathbf{v}_s T_s) = \nabla \cdot (\phi_s k_s \nabla T_s) + I_{gs} + Q_{gsc}$$

$$H_{gsc}^* = f(\bar{\phi}_s, \bar{\mathbf{v}}_s^*, D_{cyl}^*, a_{cyl}^*)$$

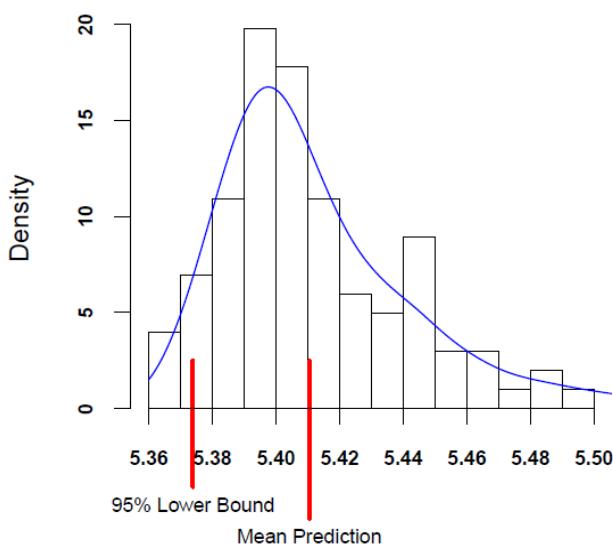


Quantitatively predicting scale up performance

CO₂ Adsorption Rate



Bed Height (m)

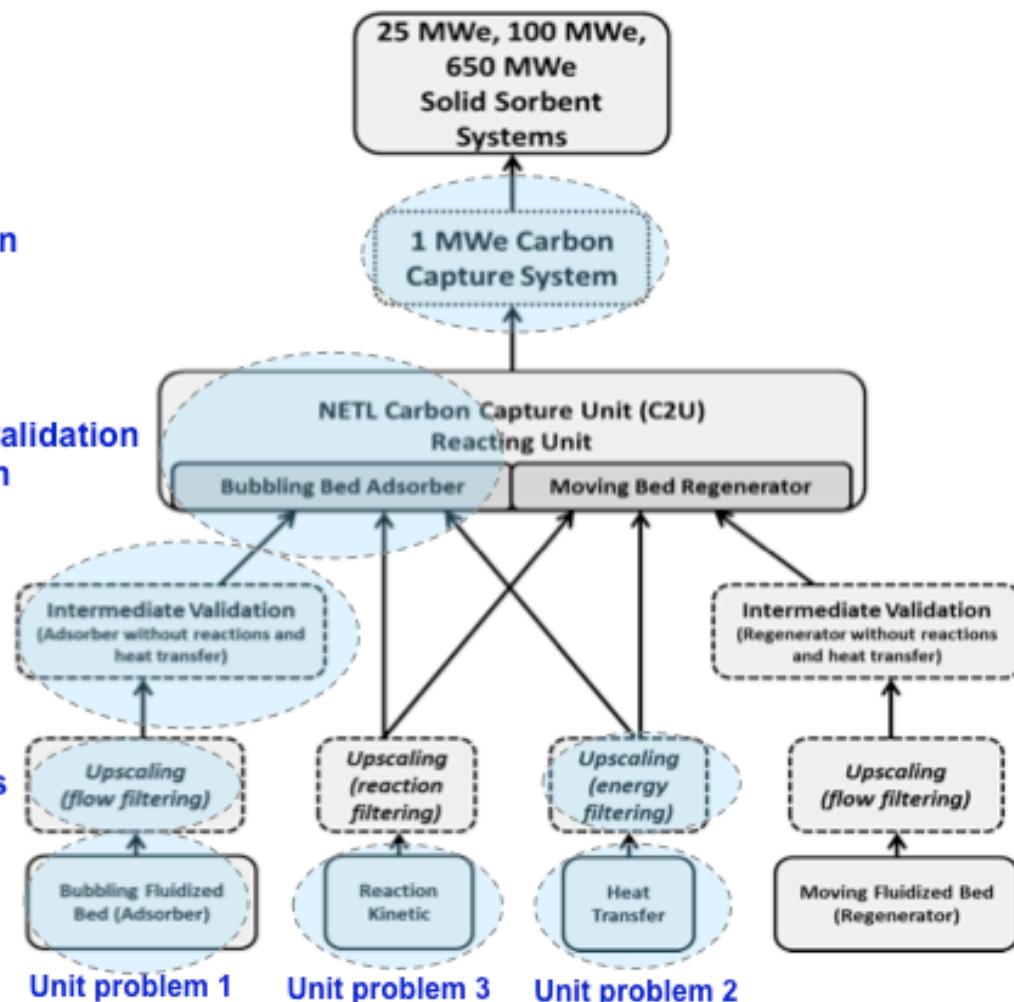


Prediction

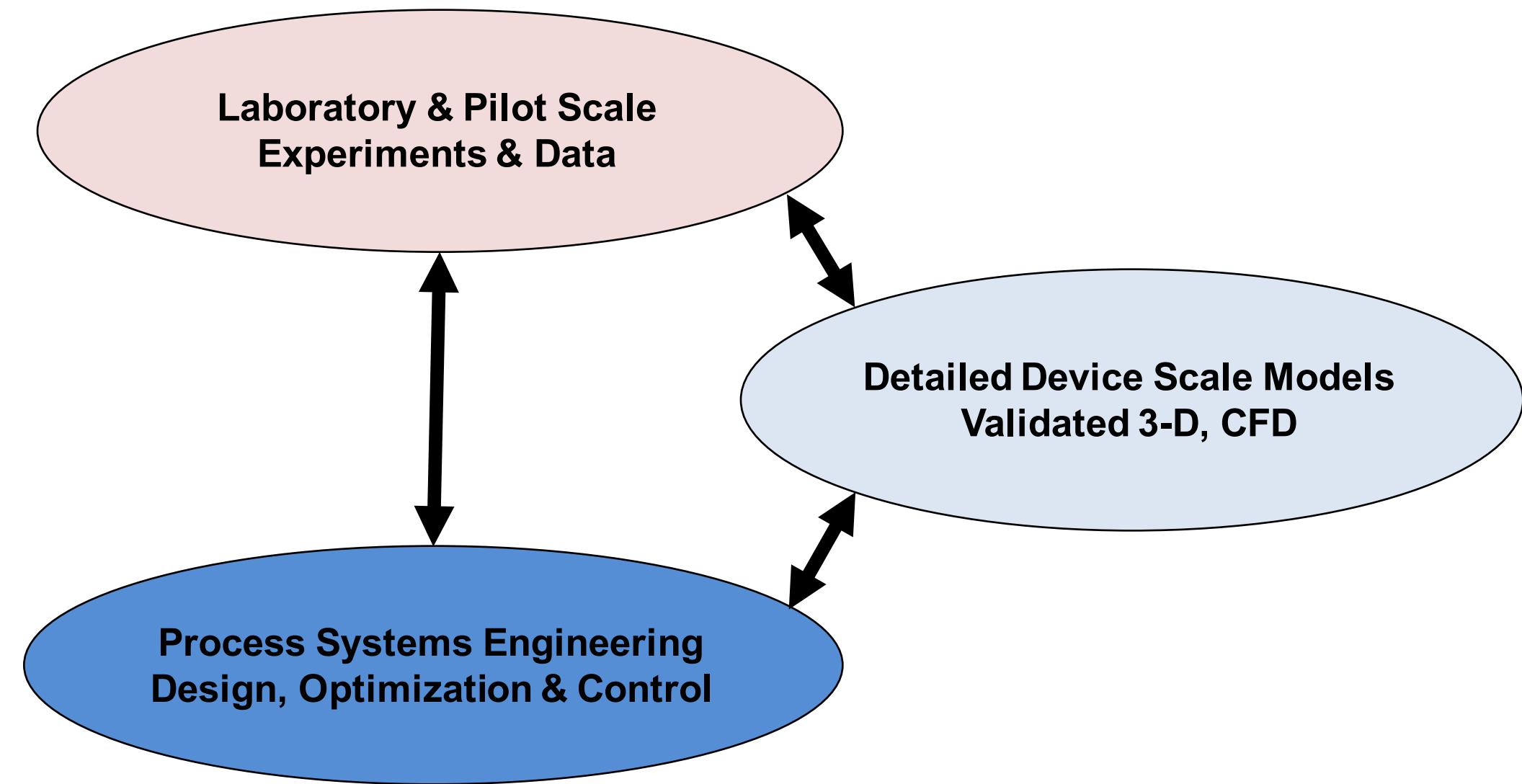
Intermediate validation
and calibration

Filtered models

CCSI CFD Validation Hierarchy



Advanced Computational Tools to Accelerate Carbon Capture Technology Development



Acknowledgements

- SorbentFit
 - David Mebane (NETL/ORISE, West Virginia University)
 - Joel Kress (LANL)
- Process Models
 - Solid sorbents: Debangsu Bhattacharyya, Srinivasarao Modekurti, Ben Omell (West Virginia University), Andrew Lee, Hosoo Kim, Juan Morinelly, Yang Chen (NETL)
 - Solvents: Joshua Morgan, Anderson Soares Chinen, Benjamin Omell, Debangsu Bhattacharyya (WVU), Gary Rochelle and Brent Sherman (UT, Austin)
 - MEA validation data: NCCC staff (John Wheeldon and his team)
- FOCUS
 - ALAMO: Nick Sahinidis, Alison Cozad, Zach Wilson (CMU), David Miller (NETL)
 - Superstructure: Nick Sahinidis, Zhihong Yuan (CMU), David Miller (NETL)
 - DFO: John Eslick (CMU), David Miller (NETL)
 - Heat Integration: Yang Chen, Ignacio Grossmann (CMU), David Miller (NETL)
 - UQ: Charles Tong, Brenda Ng, Jeremy Ou (LLNL)
 - OUU: DFO Team, UQ Team, Alex Dowling (CMU)
 - D-RM Builder: Jinliang Ma (NETL)
 - Turbine: Josh Boverhof, Deb Agarwal (LBNL)
 - SimSinter: Jim Leek (LLNL), John Eslick (CMU)
- Data Management
 - Tom Epperly (LLNL), Deb Agarwal, You-Wei Cheah (LBNL)
- CFD Models and Validation
 - Xin Sun, Jay Xu, Kevin Lai, Wenxiao Pan, Wesley Xu, Greg Whyatt, Charlie Freeman (PNNL), Curt Storlie, Peter Marcey, Brett Okhuysen (LANL), S. Sundaresan, Ali Ozel (Princeton), Janine Carney, Rajesh Singh, Jeff Dietiker, Tingwen Li (NETL) Emily Ryan, William Lane (Boston University)

Disclaimer This presentation was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.



Lawrence Livermore National Laboratory

Los Alamos
NATIONAL LABORATORY
EST. 1943

Pacific Northwest
NATIONAL
LABORATORY

U.S. DEPARTMENT OF
ENERGY