CCSI

Carbon Capture Simulation Initiative

Multi-scale modeling of carbon capture systems

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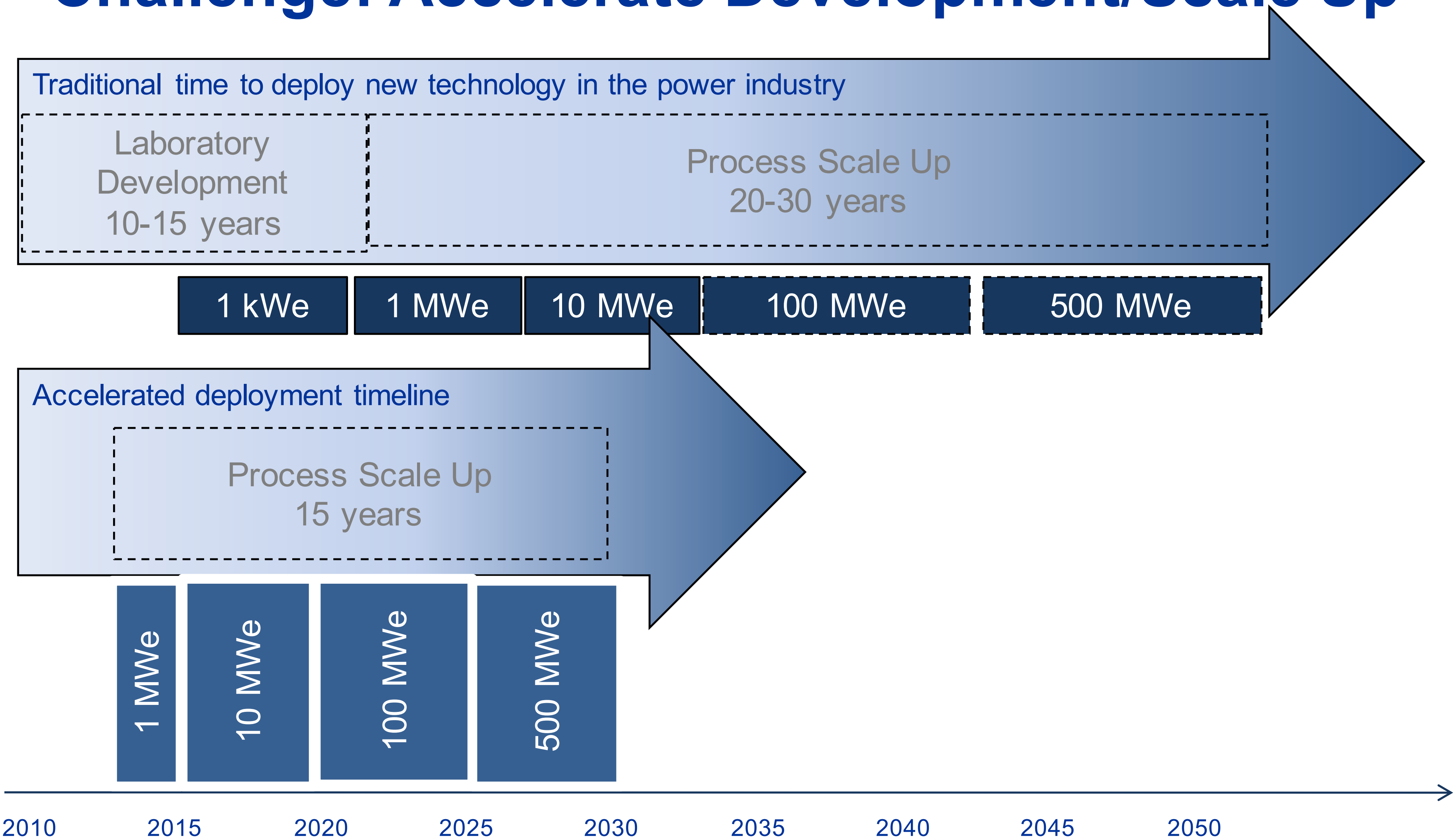
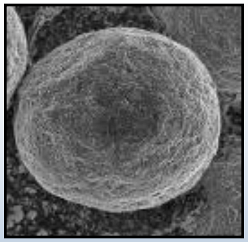
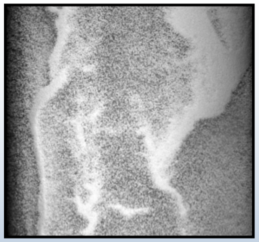
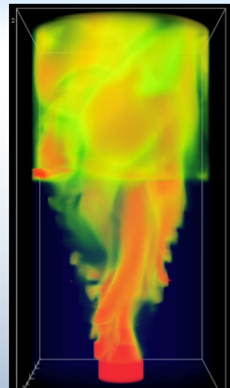
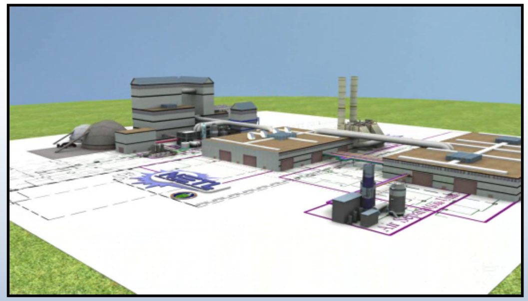
8-9 September 2015

Challenge: Accelerate Development/Scale Up



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

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Academia

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Fluor
Phillips 66
AEP American Electric Power
Southern California Edison
Southern Company
ExxonMobil
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PSE

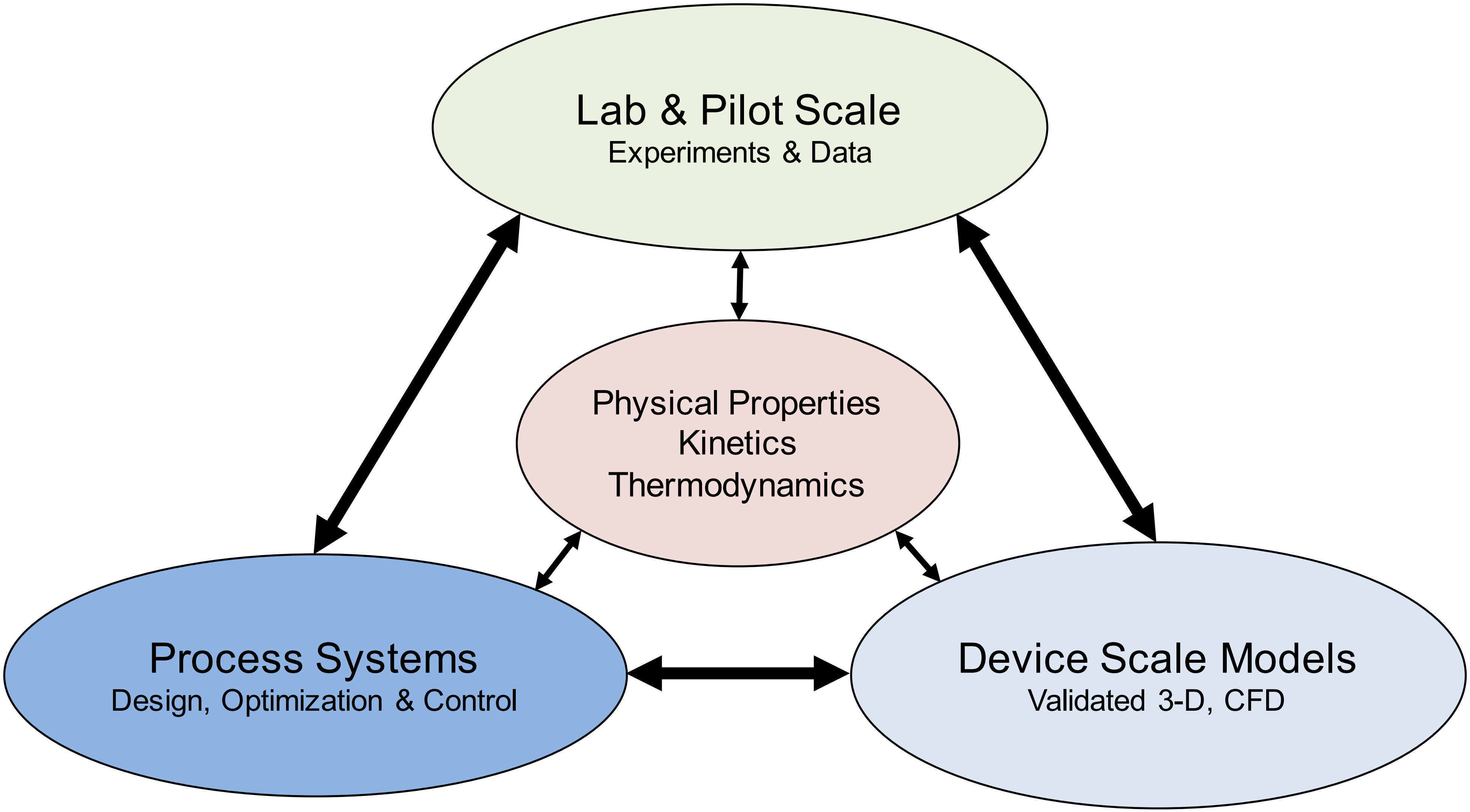
Goals & Objectives of CCSI

- **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, CRADA

Advanced Computational Tools to Accelerate Carbon Capture Technology Development



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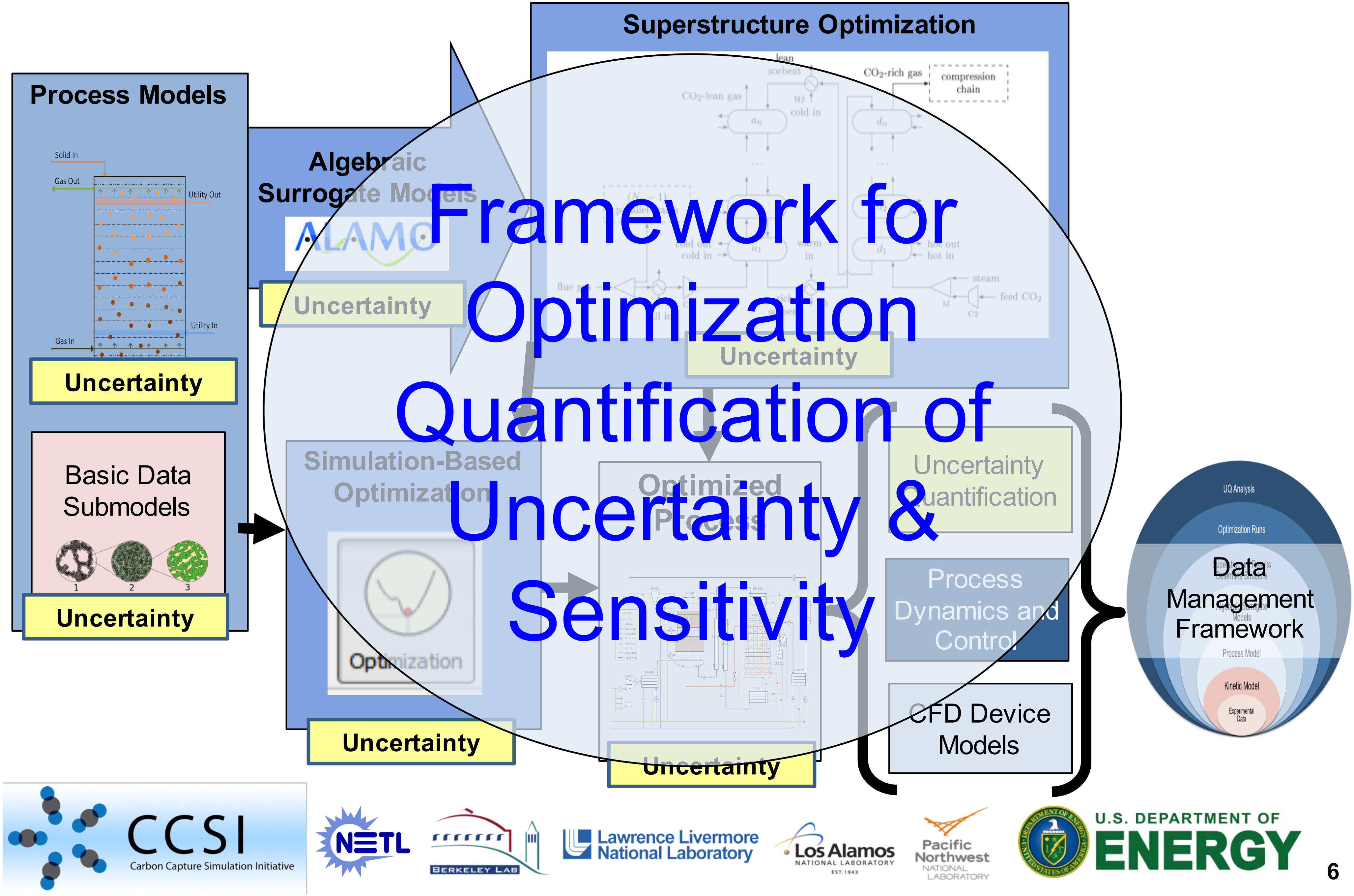
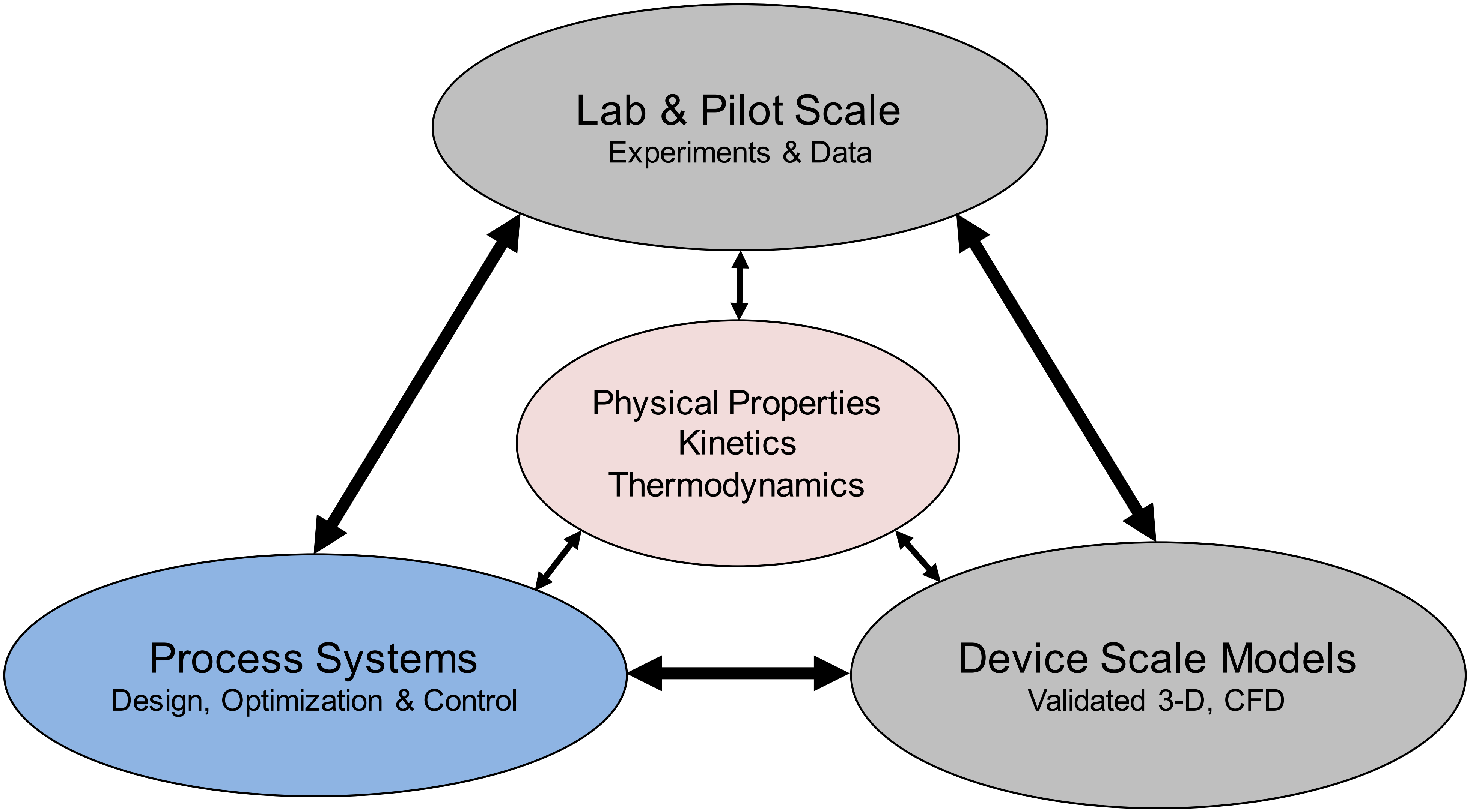
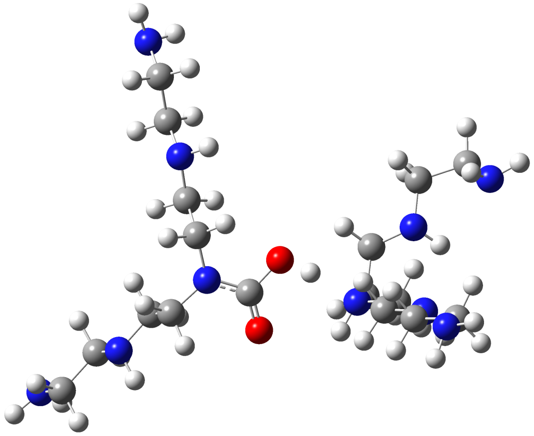
CCSI Toolset Workflow and Connections



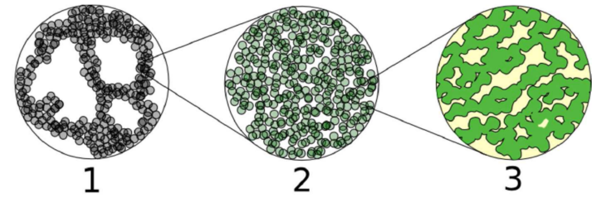
Solid Sorbent: Process Systems Example



Basic Data Model



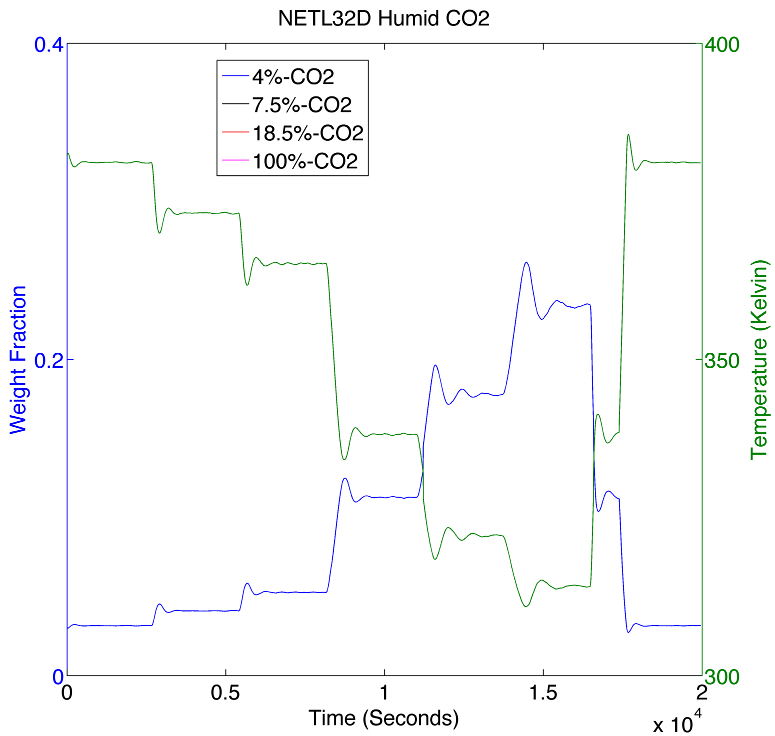
Alkylammonium carbamate formed by two molecules of tetraethylene pentamine (TEPA) and CO_2.



$$2R_2NH + CO_2(gas) \rightleftharpoons R_2NCO_2^- + R_2NH_2^+$$

$$R_2NH + H_2O(phys) + CO_2(gas) \rightleftharpoons HCO_3^- + R_2NH_2^+$$

$$H_2O(gas) \rightleftharpoons H_2O(phys)$$



$$\frac{dx}{dt} = k_x\left[s^2 p_c - xw/\kappa_x\right]$$

$$\frac{db}{dt} = k_b\left[s a p_c - bw/\kappa_b\right]$$

$$\frac{da}{dt} = k_a\left[p_h - a/\kappa_a\right] - k_b\left[s a p_c - bw/\kappa_b\right]$$

$$1 = s + x + w$$

$$w = x + b/n_v$$

$$\text{TGA wt. \%} = \left[M n_v(x+b) + H(b+a)\right]/\rho$$

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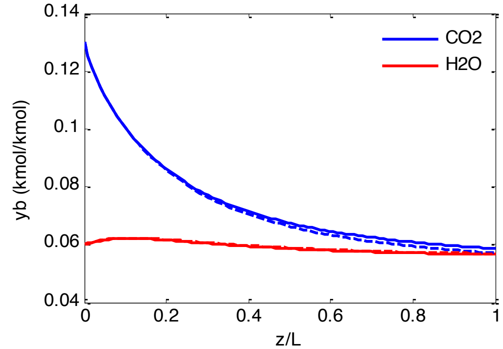
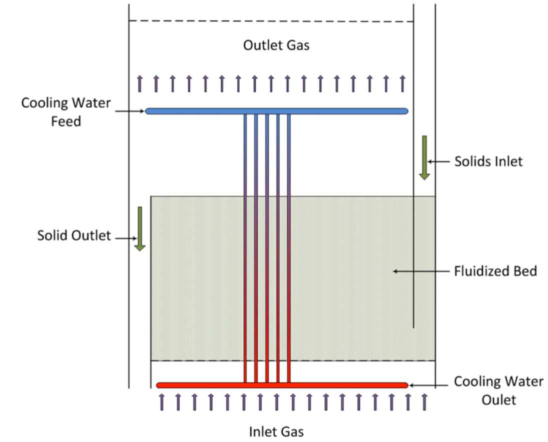
Process Models

Bubbling Fluidized Bed (BFB) Model

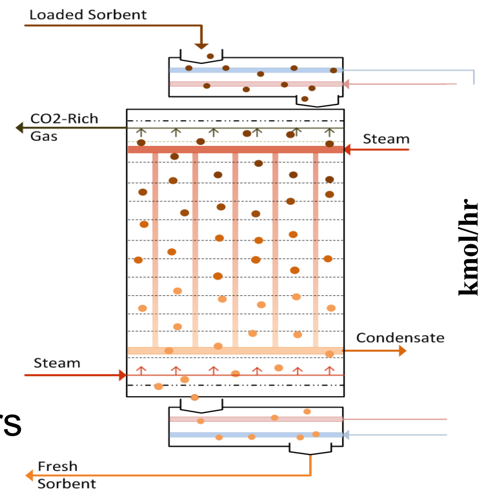
- 1-D, nonisothermal with heat exchange
- Unified steady-state and dynamic
- Adsorber and Regenerator
- Variable solids inlet and outlet location
- Modular for multiple bed configurations

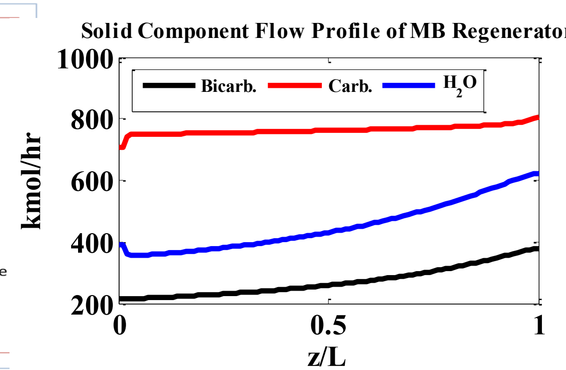




Moving Bed (MB) Model

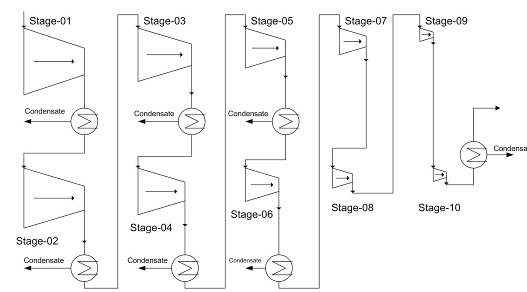
- 1-D, nonisothermal with heat exchange
- Unified steady-state and dynamic
- Adsorber and Regenerator
- Heat recovery system



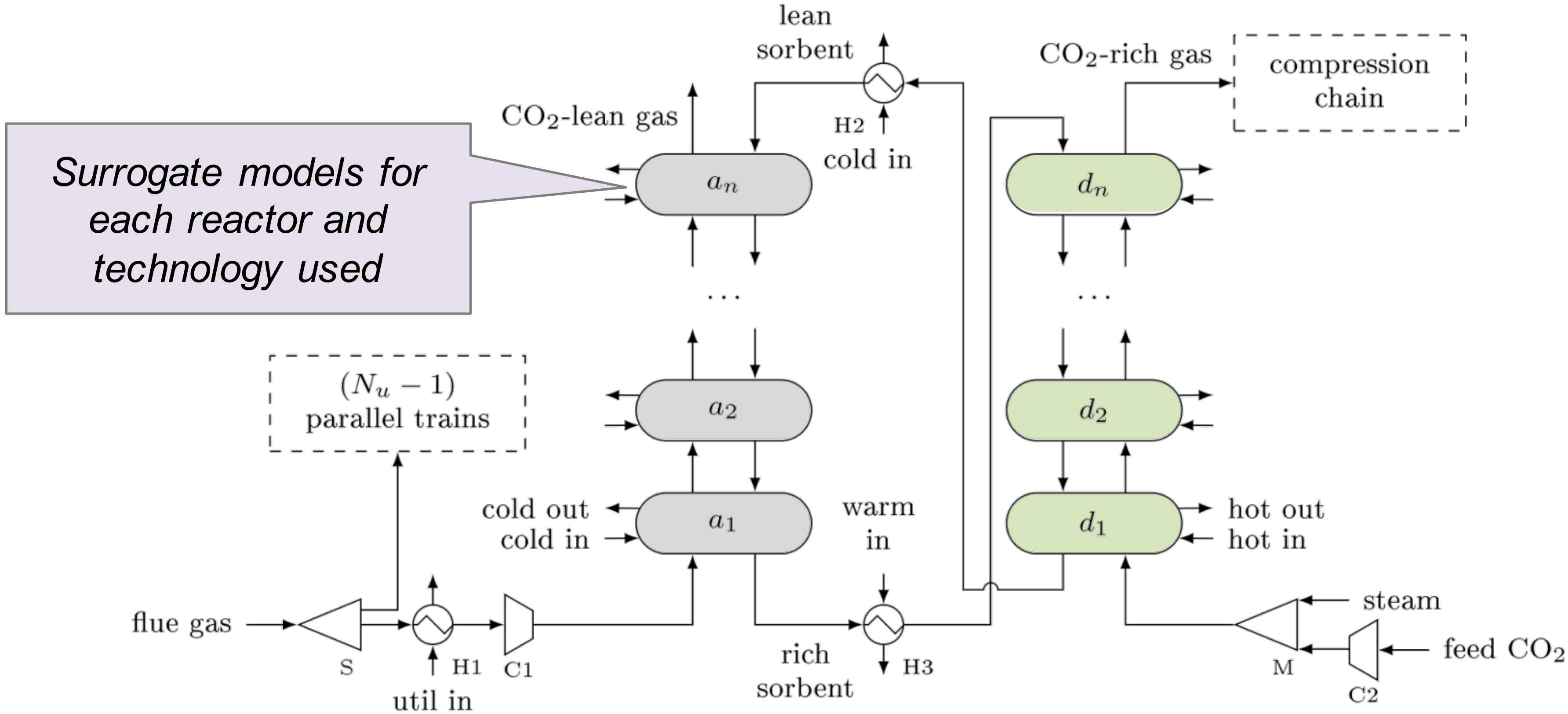


Compression System Model

- Integral-gear and inline compressors
- Determines stage required stages, intercoolers
- Based on impeller speed limitations
- Estimates stage efficiency
- CO_2 drying (TEG absorption system)
- Off-design performance.
- Includes surge control algorithm



Carbon Capture System Configuration



- 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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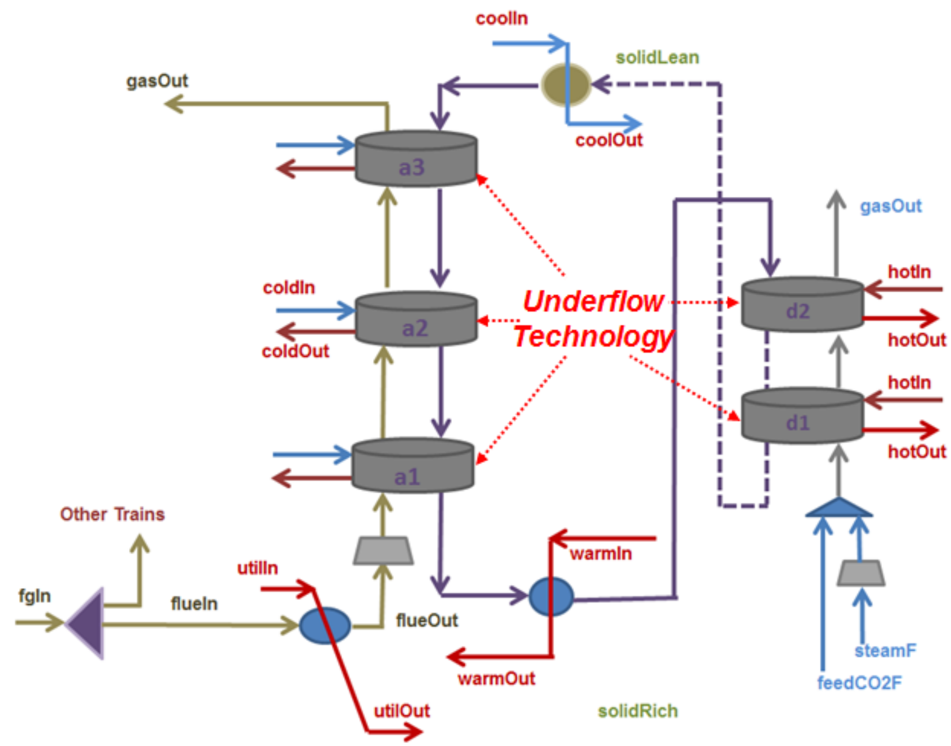
Superstructure Optimization

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*



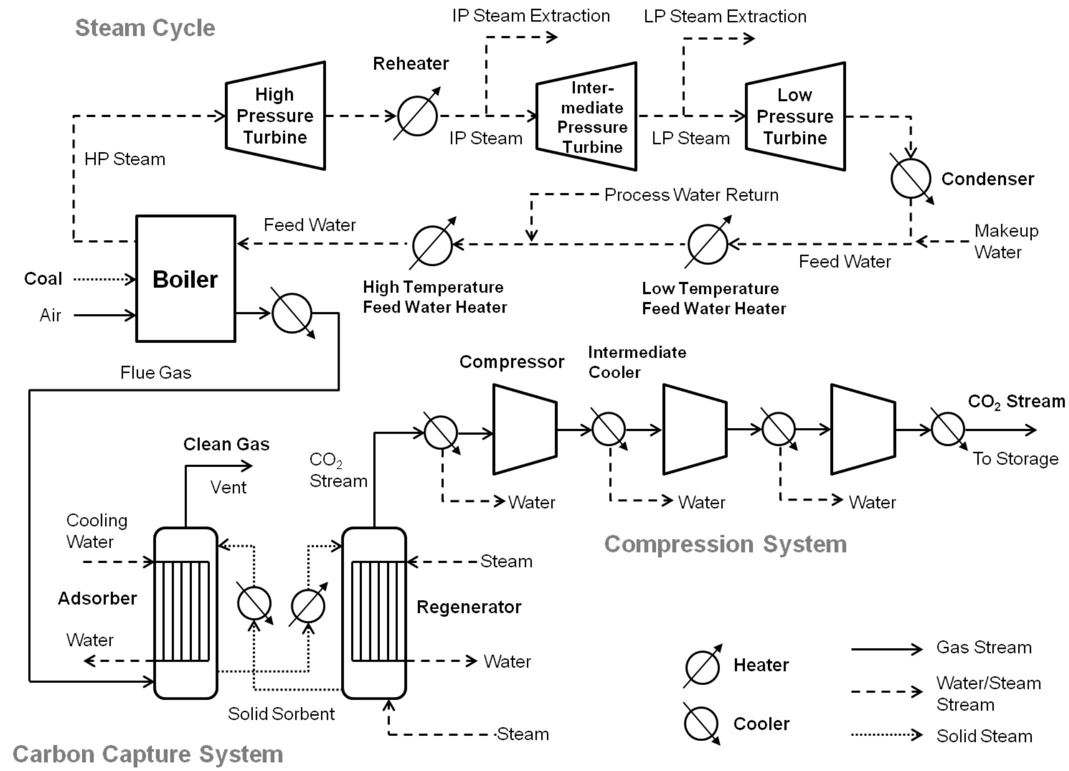
Optimal layout

Optimization & Heat Integration

Objective:* Max. *Net efficiency

Constraint:* CO_2 *removal ratio ≥ 90%

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

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

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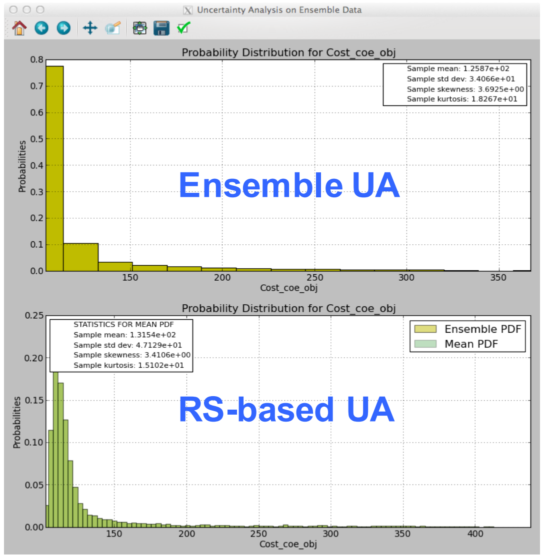
Uncertainty Quantification for Prediction Confidence

- 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

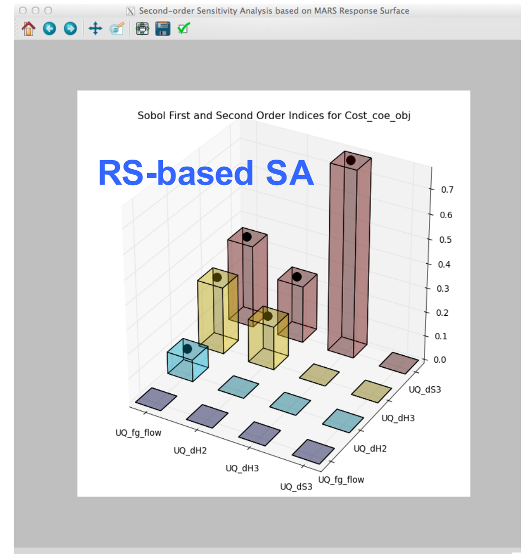


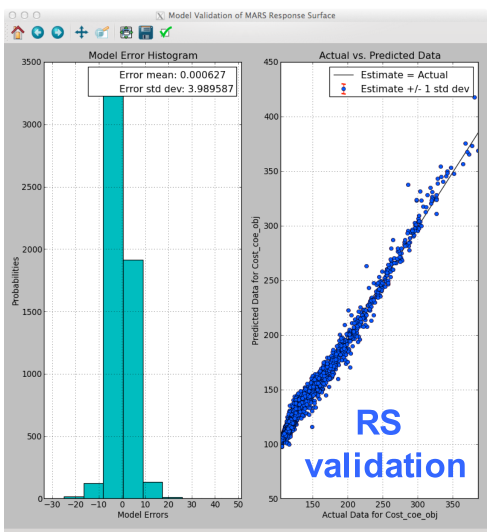
<u>Ensemble Analyses</u>

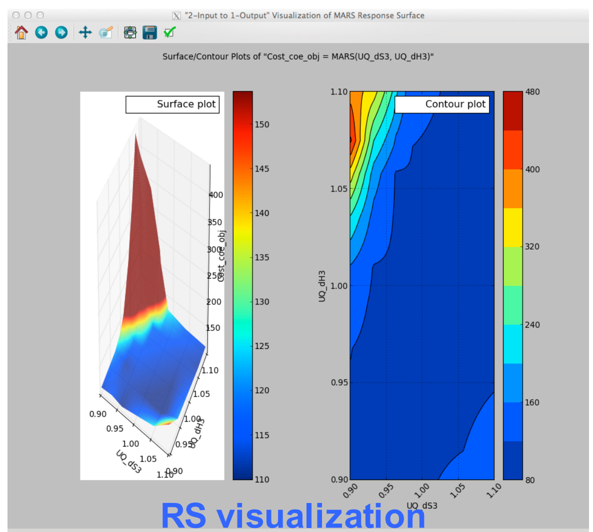
- Uncertainty analysis
- Sensitivity analysis
- Correlation analysis
- Scatterplots for visualization

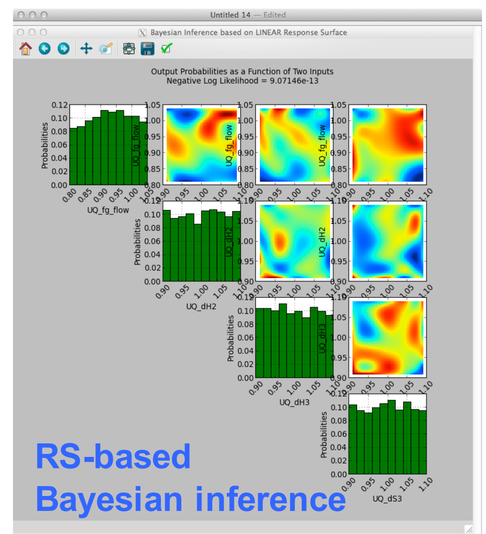
<u>Response Surface (RS) Analyses</u>

- RS validation
- RS visualization
- RS-based uncertainty analysis
- RS-based sensitivity analysis
- RS-based Bayesian inference

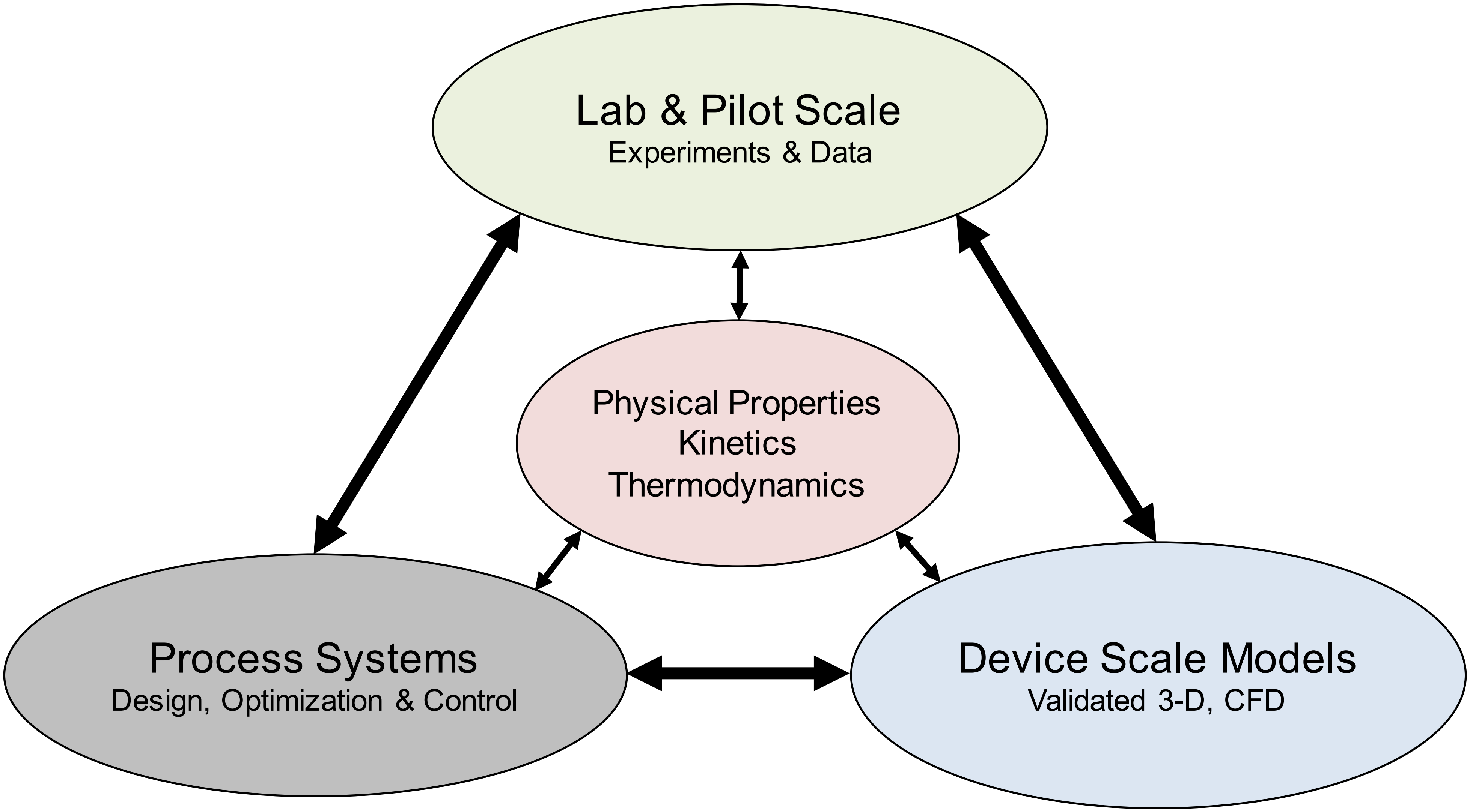








Solid Sorbents: Validated CFD Model Example



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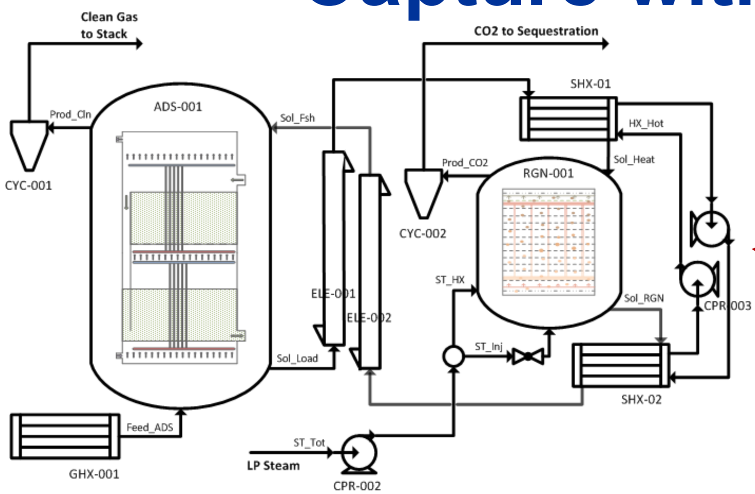
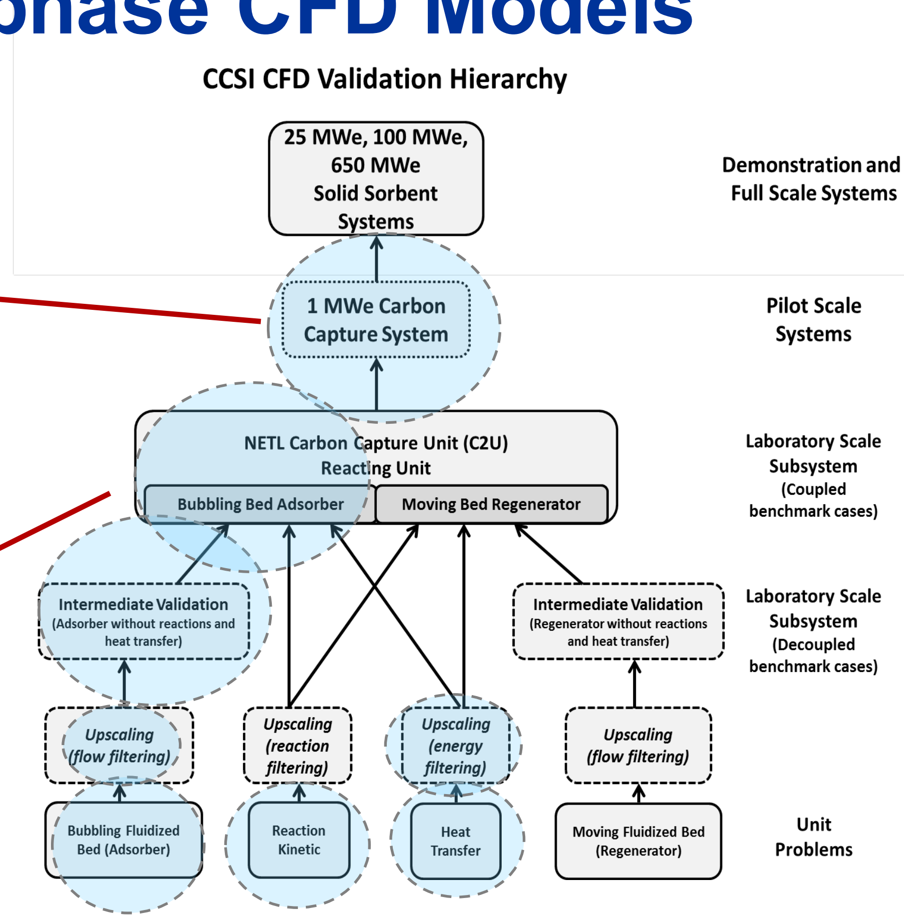
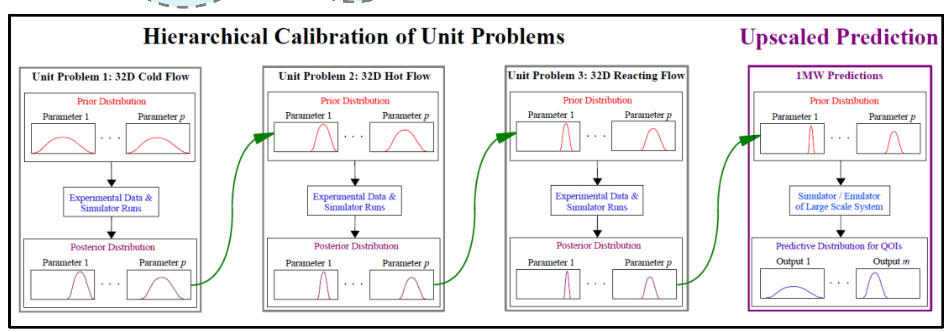
Building Predictive Confidence for Device-scale CO_2 Capture with Multiphase CFD Models



C2U Batch Unit





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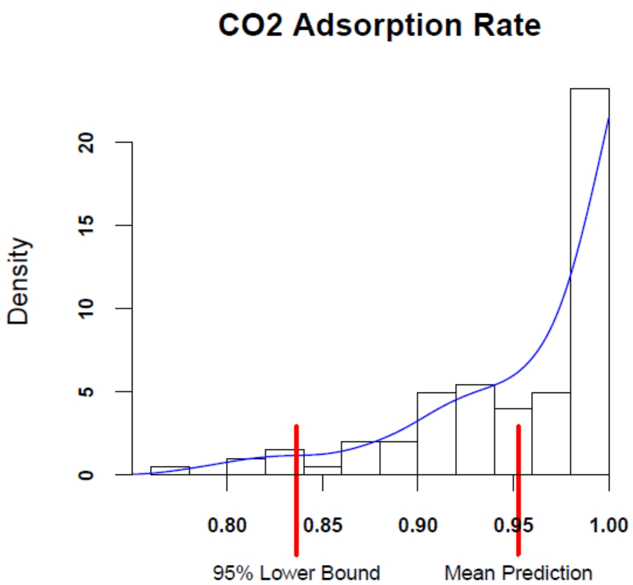
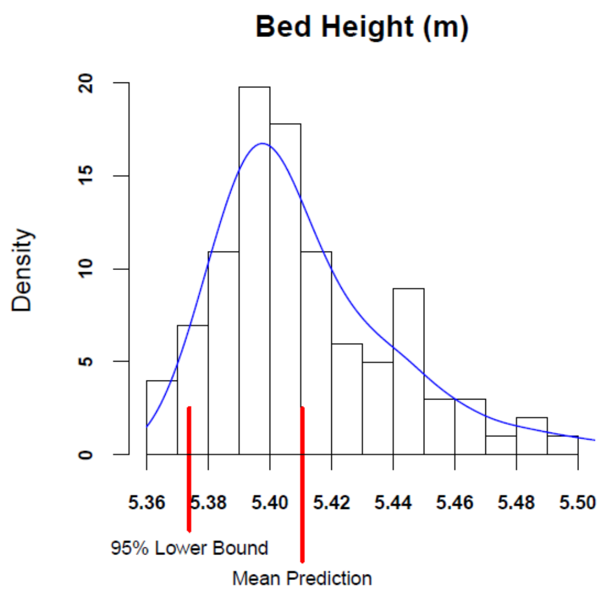
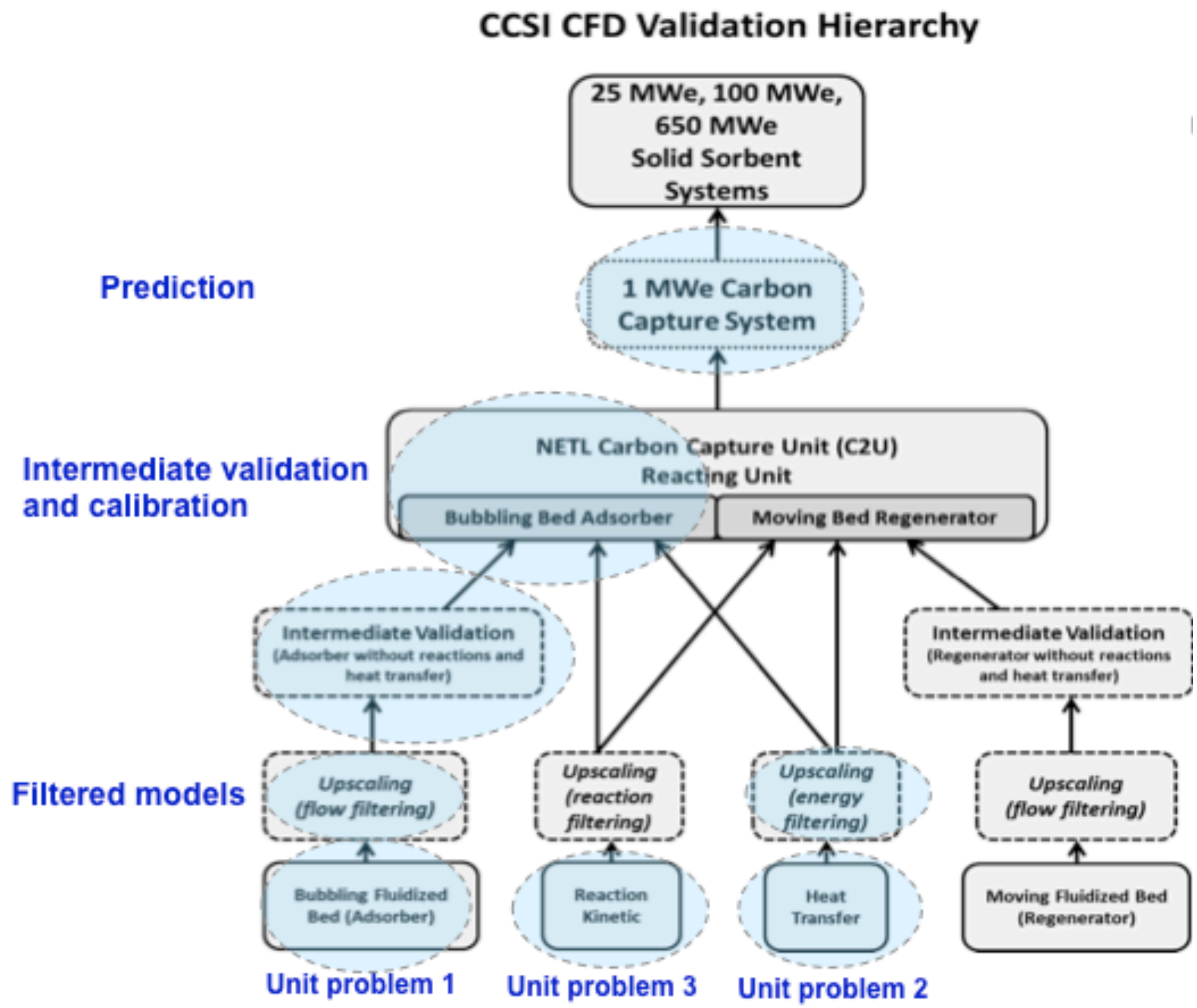
Quantitatively predicting scale up performance







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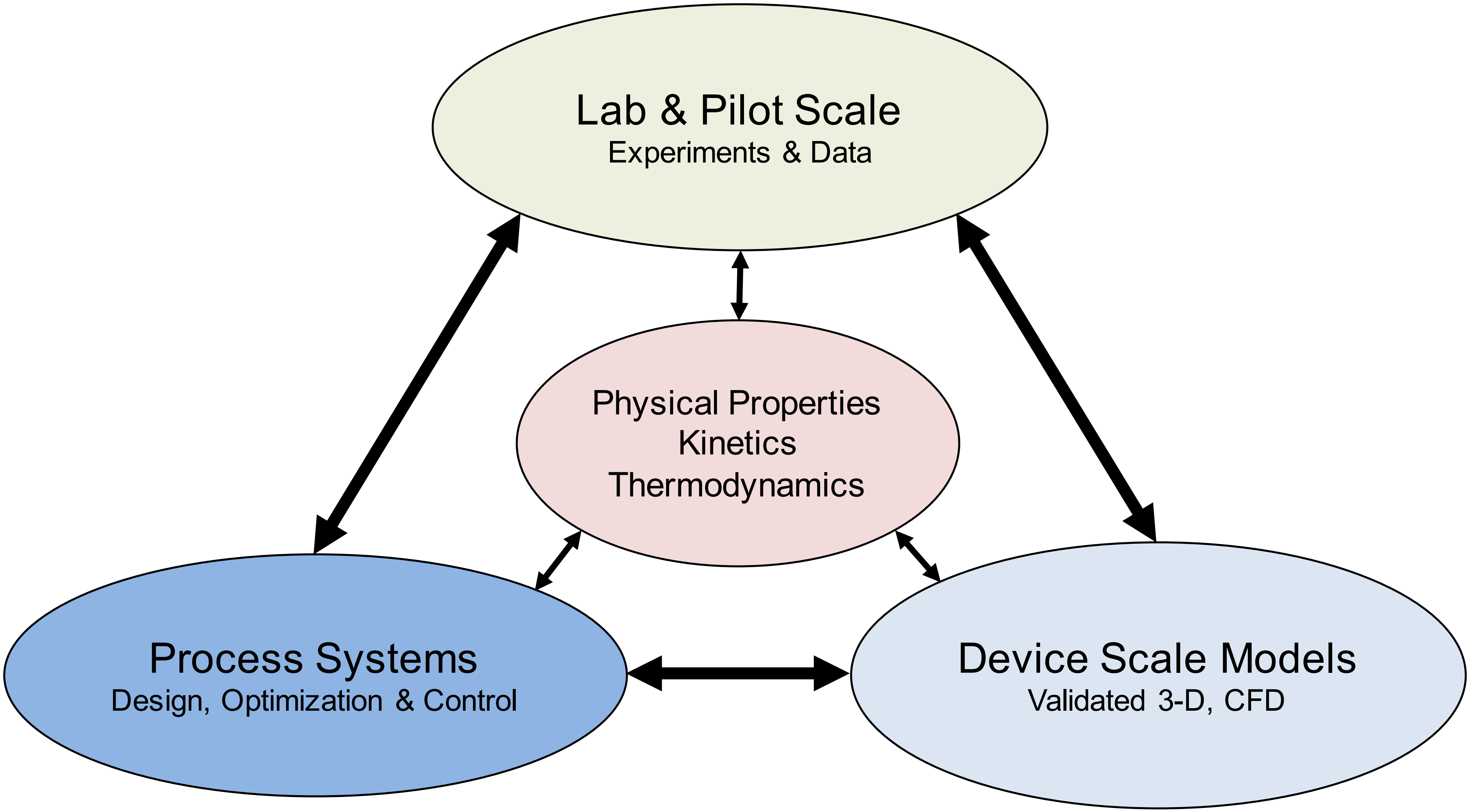
Advanced Computational Tools to Accelerate Carbon Capture Technology Development



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- 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

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)
- FOQUS
  - ALAMO: Nick Sahinidis, Alison Cozad, Zach Wilson (CMU), David Miller (NETL)
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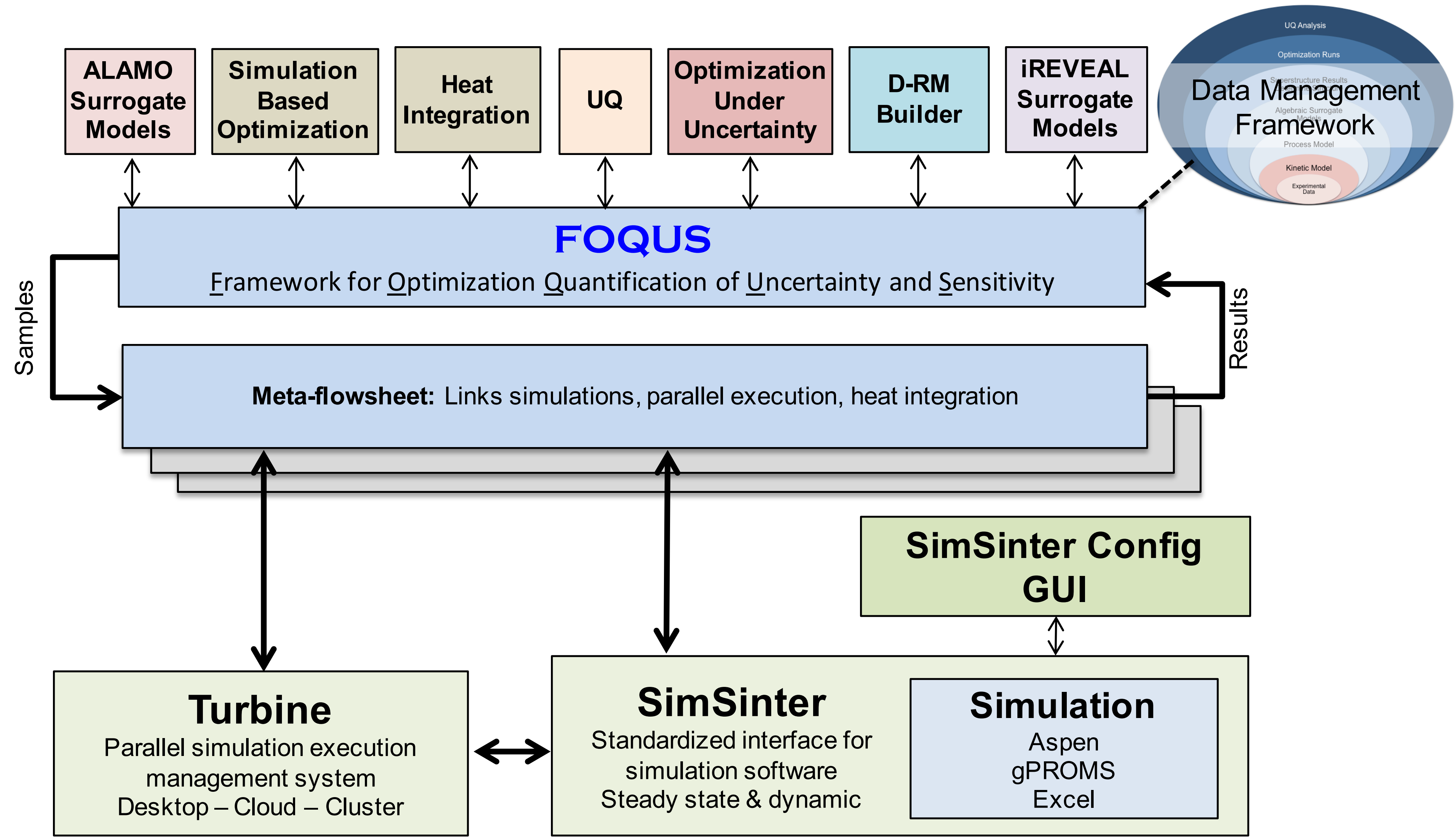
  - DFO: John Eslick (CMU), David Miller (NETL)
  - Heat Integration: Yang Chen, Ignacio Grossmann (CMU), David Miller (NETL)
  - UQ: Charles Tong, Brenda Ng, Jeremey Ou (LLNL)
  - OUU: DFO Team, UQ Team, Alex Dowling (CMU)
  - D-RM Builder: Jinliang Ma (NETL)
  - Turbine: Josh Boverhof, Deb Agarwal (LBNL)
  - 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)

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.

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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 November 2015**
  - **Commercial licensing late 2015 or early 2016**