$CCSI^2$ and Toolset Support Program Overview and Toolset Introduction

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Executive Summary

- **Industrial Collaborations**
  - CCSI[2] Supports 7 CO_2 Capture Program projects $40MM+ in total project value (TRL 3-7)
    - Discovery of Carbon Capture Substances and Systems (DOCCSS) Initiative, National Carbon Capture Center (NCCC), LLNL MECS Technology, UT Austin AFS, UKy Process Control
  - Additional external industrial agreements (executed or in progress)
    - GE, ADA-ES, Test Centre Mongstad (TCM), SINTEF, Canada's Oil Sands Innovation Alliance (COSIA)
  - Includes enabling capture technology support:
    - Aerosol, dynamic characterization, turndown, advanced process control

- **Optimal Design of Experiments**
  - Improves model while optimizing experimental data generation
  - Applicable to lab through large pilot scale

- **Solvent Modeling Framework**
  - Fundamental characterization of solvent, device and system
  - Collaboration with NCCC and (soon) TCM under International Test Center Network (ITCN)

CCSI^2 and Toolset Support Personnel Profile

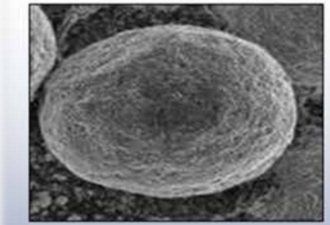
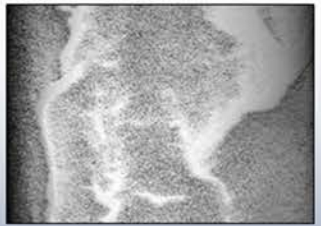
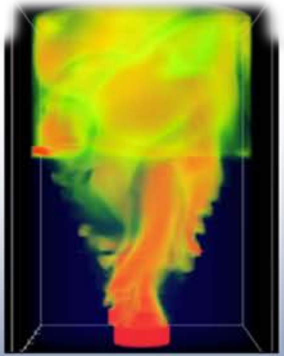
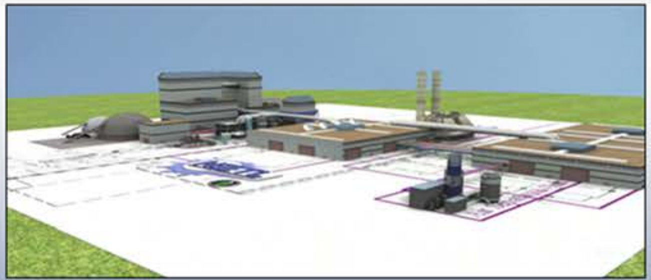
- **49 Total Full-Time or Part-Time**
  - 3 Federal Management
  - 7 Contractor Support Staff
  - 28 CCSI^2 or Toolset Support Engineers
  - 2 Faculty
  - 5 PhD Students
  - 4 Post-Docs
- 5 National Labs, 2 Universities, 1 Contractor
- 35 PhD Level – obtained or in pursuit
- **46 Industrial and Academic Stakeholder Board Members**
- **6 Executive Committee Members**

CCSI^2 Carbon Capture Simulation for Industry Impact | National Energy Technology Laboratory | Berkeley Lab | Lawrence Livermore National Laboratory | Los Alamos National Laboratory | Pacific Northwest National Laboratory | West Virginia University | The University of Texas at Austin | U.S. Department of Energy

Keynote Recap: Selected Key Capture Program Thrusts

- **Accelerating Rate of RD&D**
  - Industry Hand-off at TRL 5
- **Shift Toward Optimal Economics**
  - Capture Rate Unconstrained to 90%
  - Multi-scale Problem
- **Formulate Transformational System Level Goals**
  - Materials Performance Targeting
  - Device Scale Designs
- **Technology-Focused Research**
  - Translation to Other Applications

CCSI²: Accelerating Rate of RD&D

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	Industry
Berkeley Lab	Carnegie Mellon	Google, ADA Environmental Solutions, Alstom, B&W, GE, EPRI Electric Power Research Institute
Pacific Northwest National Laboratory	Princeton University	Fluor, Phillips 66, AEP American Electric Power, Southern California Edison (An Edison International Company, San Onofre Nuclear Generating Station)
National Energy Technology Laboratory	West Virginia University	Southern Company, ExxonMobil, Chevron, URS
Los Alamos National Laboratory	Boston University	Air Products, Eastman
Lawrence Livermore National Laboratory	The University of Texas at Austin	aspentech, ANSYS, Schneider Electric, PSE

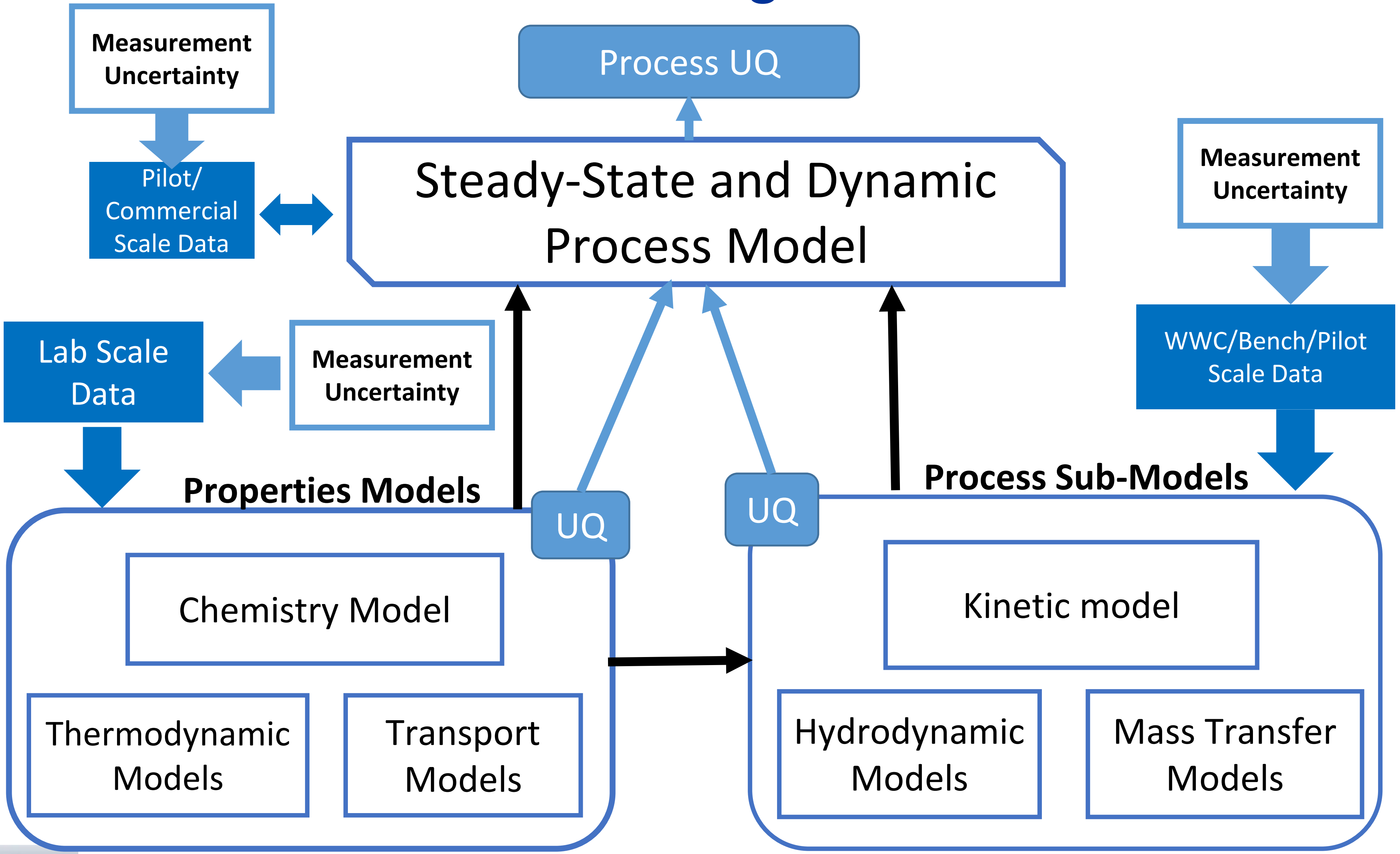
CCSI Toolset: New Capabilities for Modeling

Maximize the learning at each stage of technology development

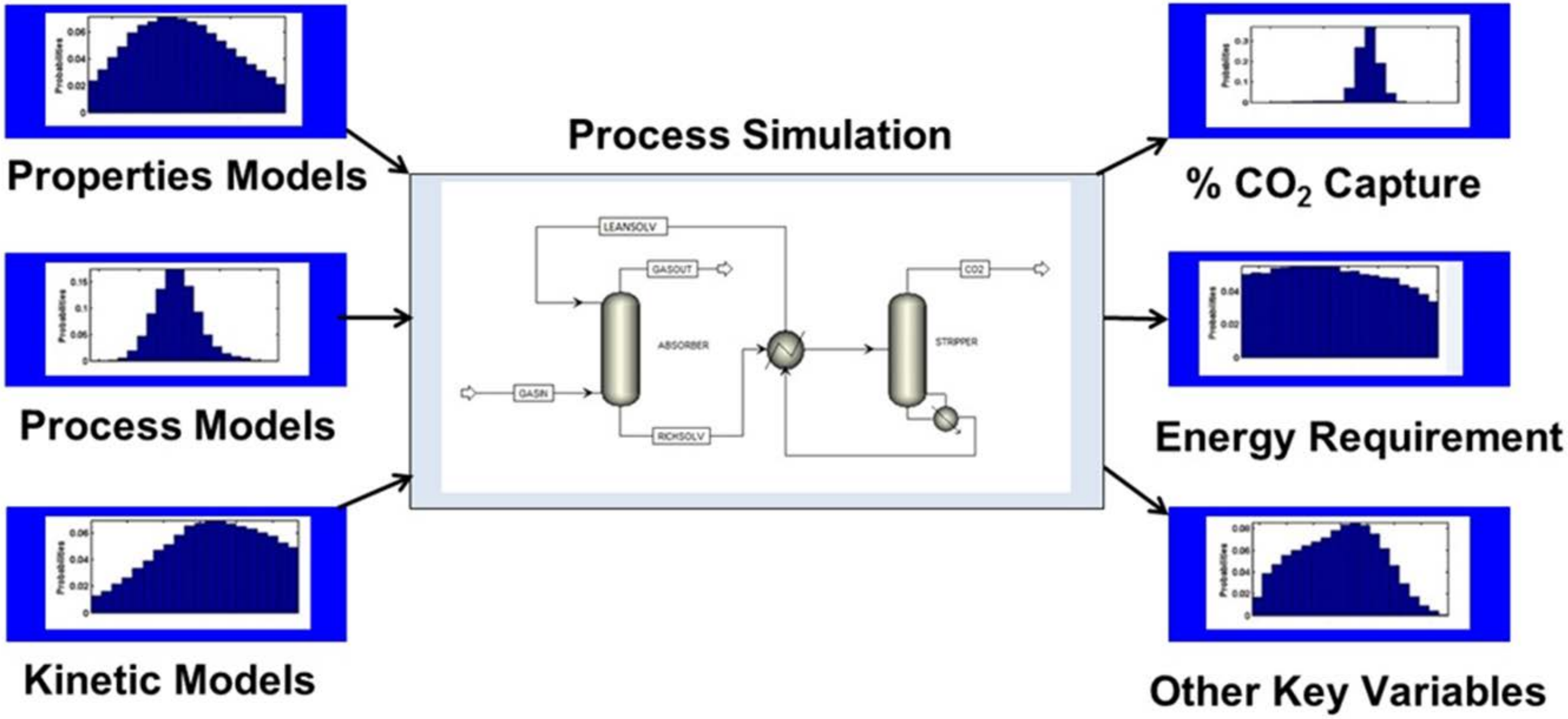
- **Early stage R&D**
  - Screening concepts
  - Identify conditions to focus development
  - Prioritize data collection & test conditions
- **Pilot scale**
  - Ensure the right data is collected
  - Support scale-up design
- **Demo scale**
  - Design the right process
  - Support deployment with reduced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

2016 R&D 100 Award Recipient

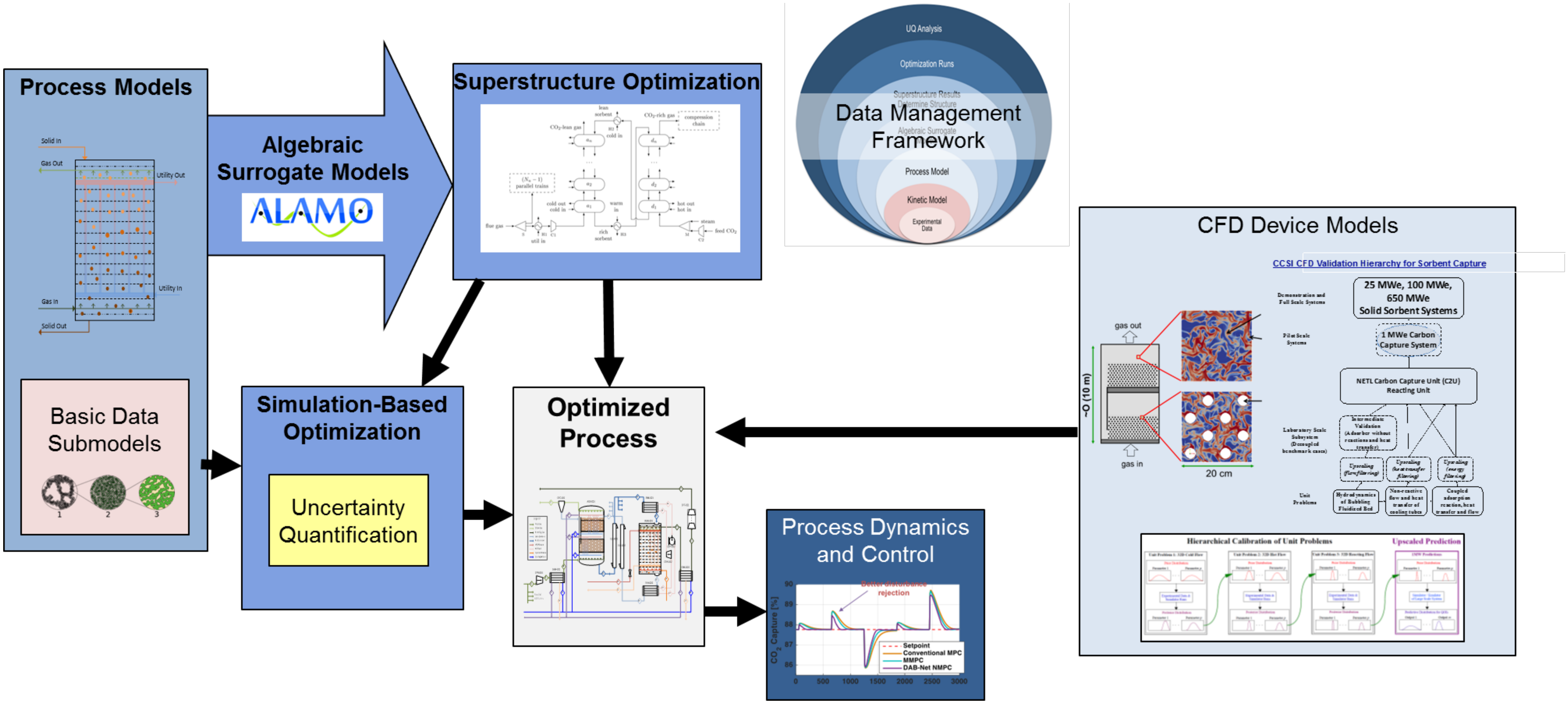
Baseline Modeling Framework



Integrated Multi-Scale Model Approach



CCSI Toolset Process Module Interconnectivity



Example: Integrated Multi-Scale Solvent Model Summary

- Standardized model for comparing different proposals for advanced solvent-based capture technologies
  - Open Source
  - Simultaneously leverages data at all scales
  - Validated Framework
  - Well Documented
  - Uncertainties Quantified

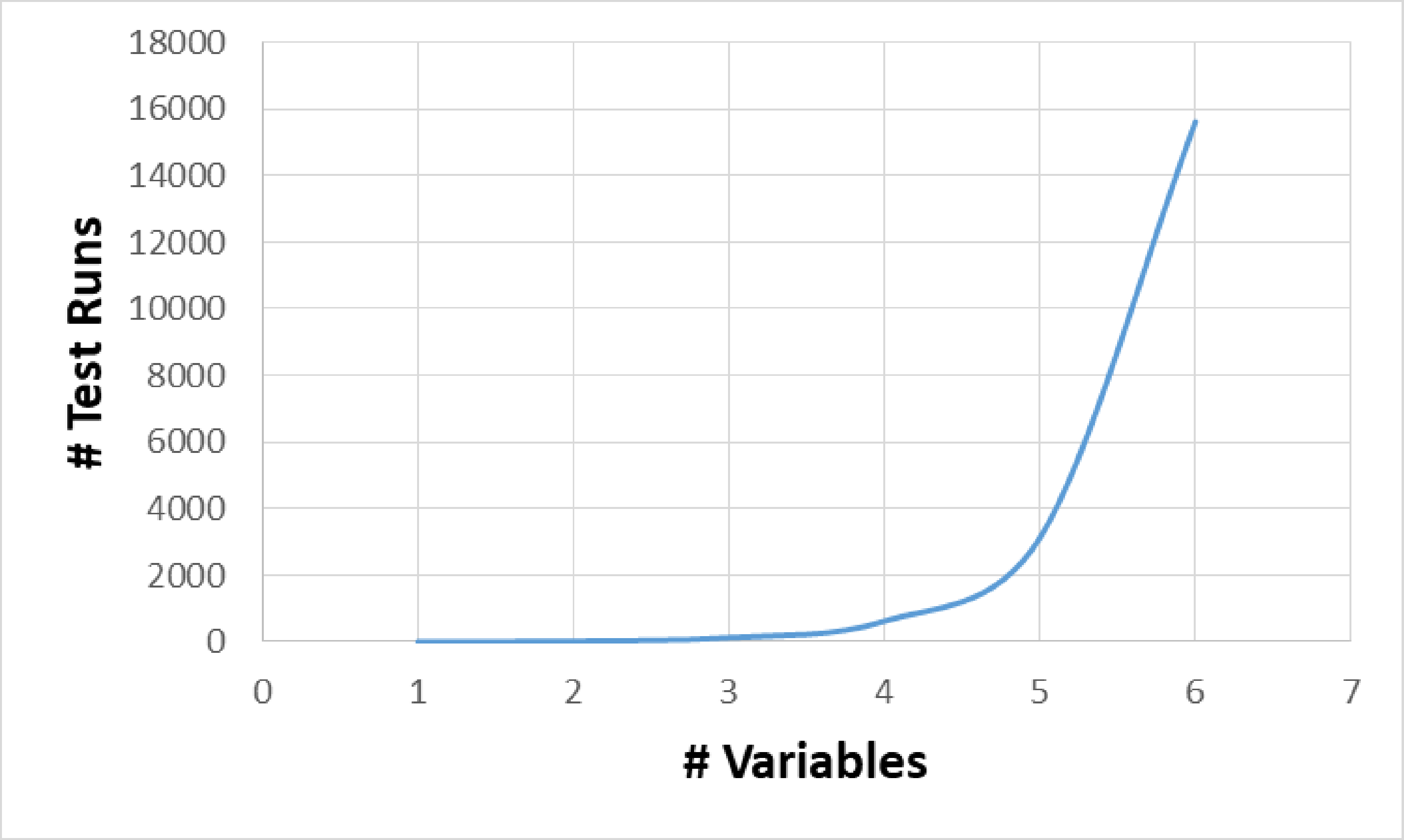
- Aqueous monoethanolamine (MEA) used as baseline
  - Current Industry Standard
  - Extensive Amount of Data Available

- Fully applicable to alternative solvents

Managing and Refining Uncertainty

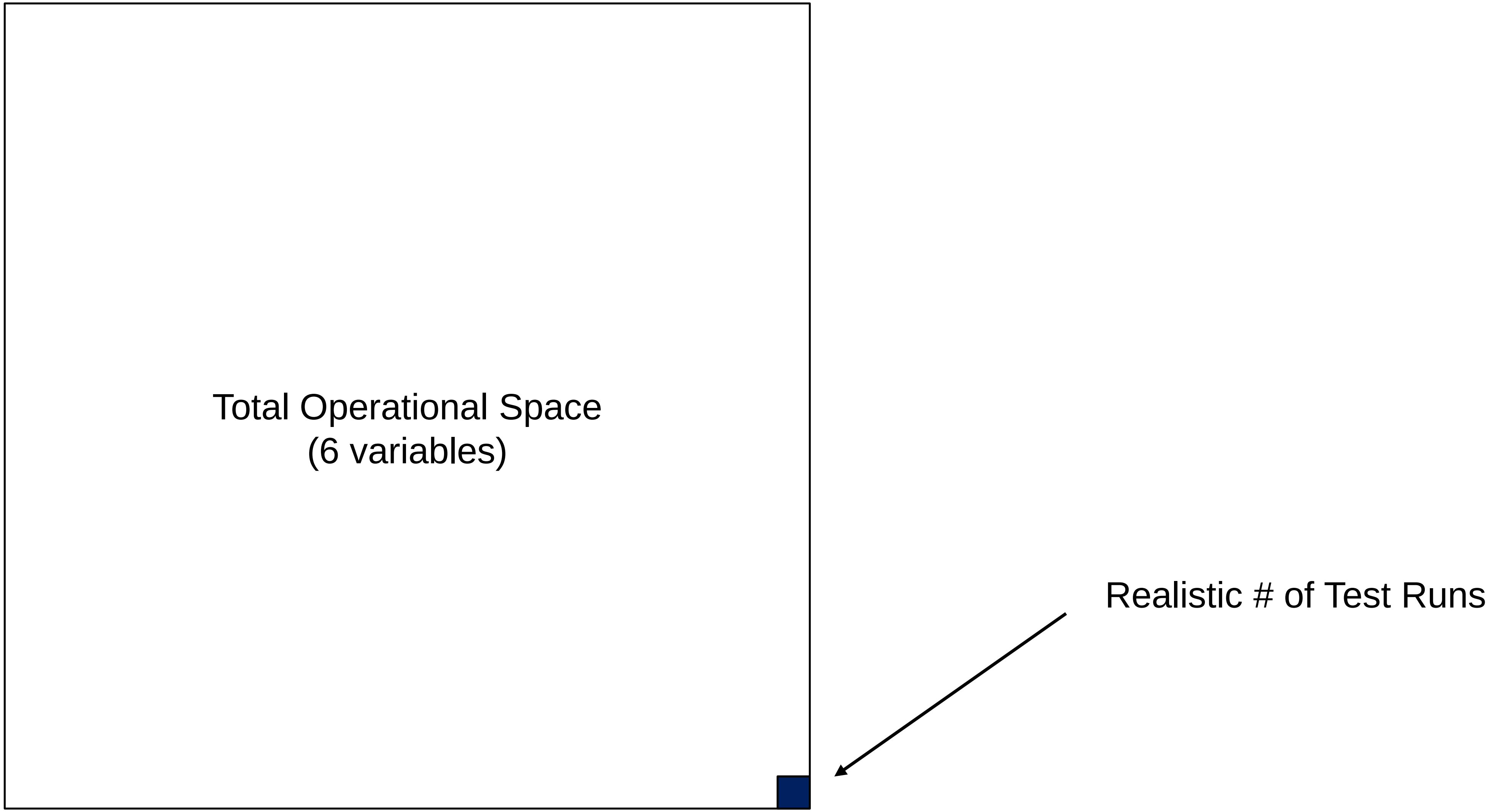
- **Uncertainty evaluated in the following models:**
  - Transport models (surface tension, viscosity, diffusivity)
  - Thermodynamic models (density, VLE, heat capacity)
  - Hydraulic models (pressure drop, holdup)
  - Mass transfer models (mass transfer coefficients, interfacial area)
  - Kinetic model
- **Model Validation with Data and propagation of all parametric uncertainties through the model**
  - UQ methodology is leveraged to improve models and test plans

Design of Experiments (*Zero Engineering Insight*)

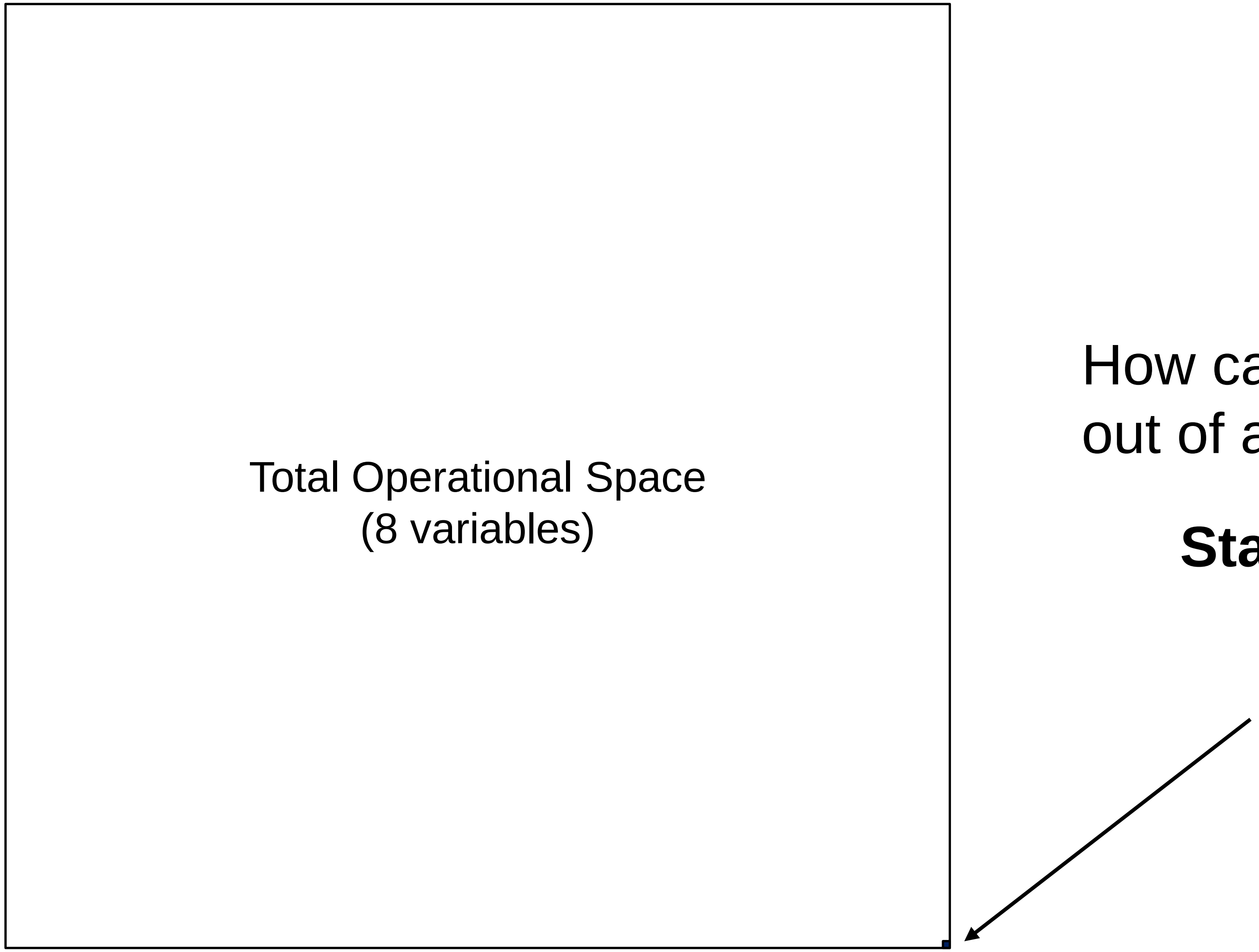


- Brute force approach
- 5 increments for each variable
- Exponential increase in test runs as variables increase

Design of Experiments Conceptualization



Design of Experiments Conceptualization



How can we possibly extract value out of a practical test campaign?

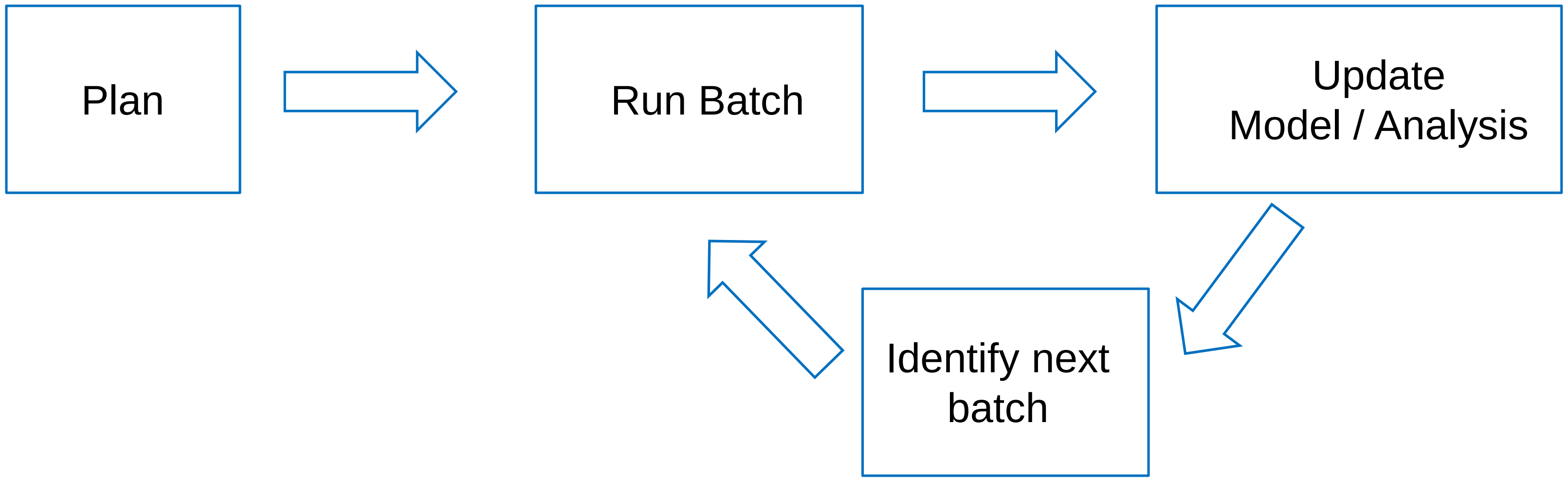
Start with Using Good Models!

Realistic # of Test Runs

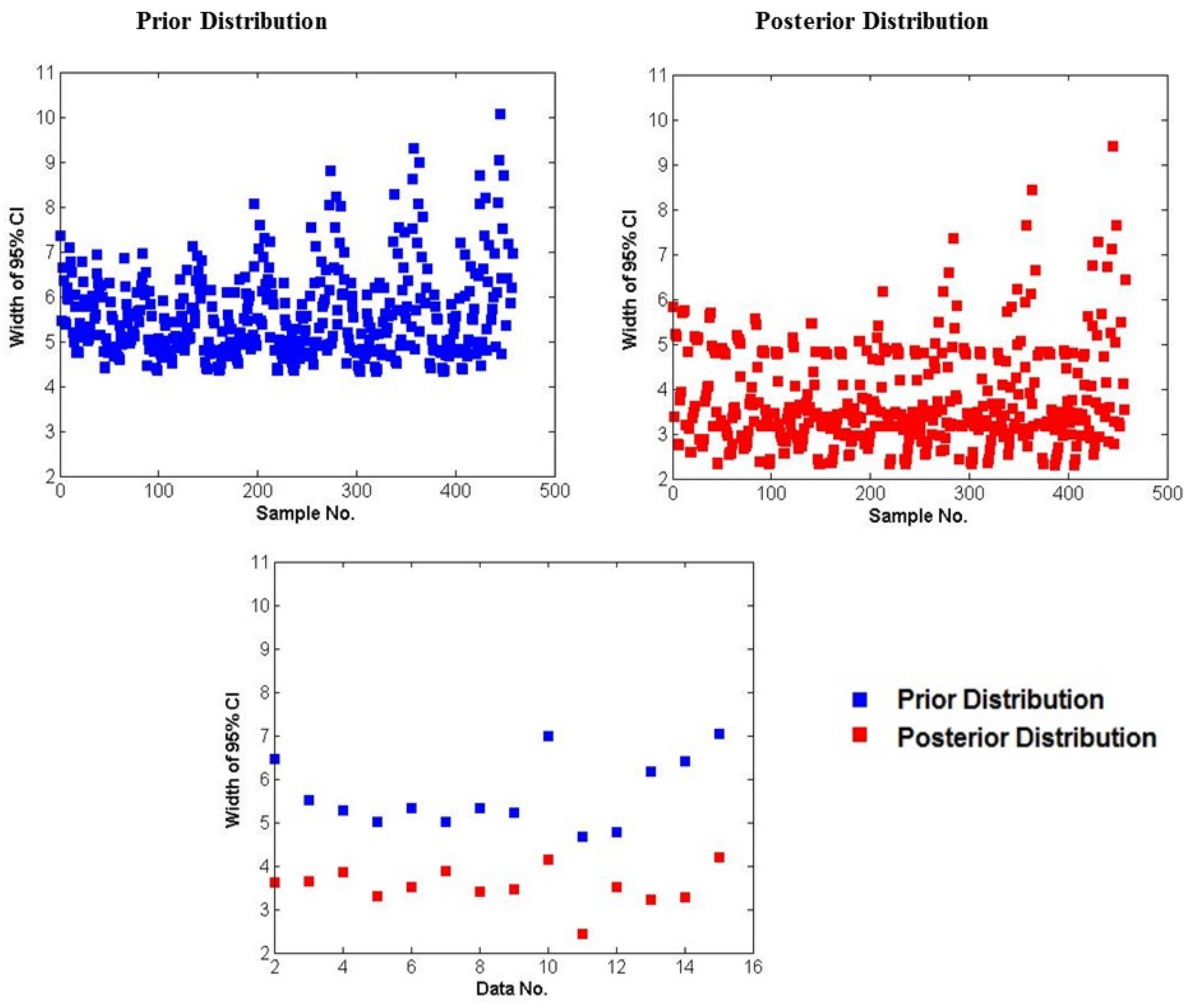
One-Shot vs Sequential Experimentation

One-Shot experiment

Sequential experiment



Optimal Design of Experiments: NCCC Trial



Uncertainty in Predicted NCCC Capture Percentage Reduced by 30-50%

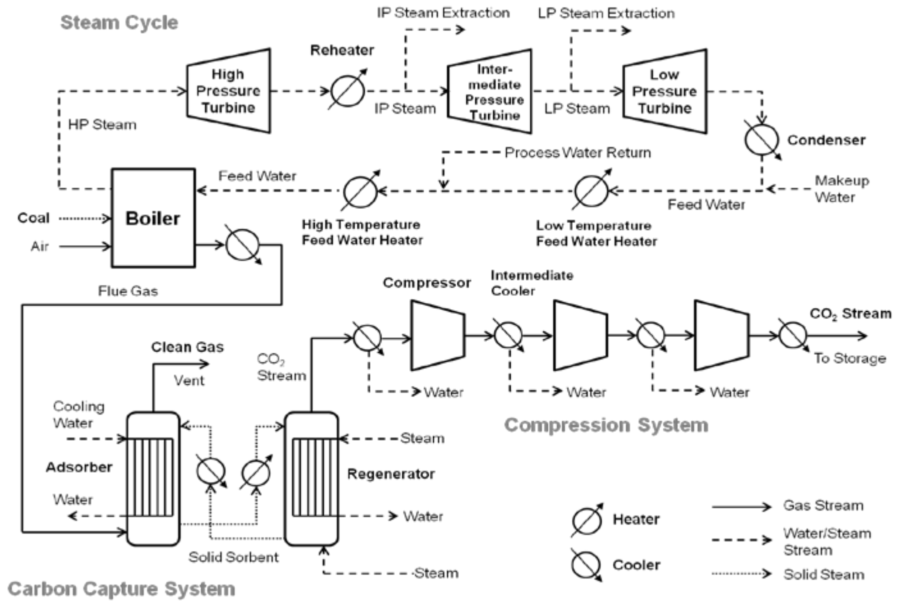
Example of Full System Optimization

Objective: Max. Net efficiency*

Constraint: CO_2 removal ratio ≥ 90%

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

*Can just as easily be minimized Captured Cost



	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

Conclusions

- **Supports more *accelerated*, *risk-averse CCS scale up, demo and commercialization***
- ***Optimizes system operation, configuration, Capture Economics***
- **CCSI^2 employs a multi-scale modeling framework (*materials through systems*) formulated in fundamental principles, providing "glass-box" understanding**
- **Interconnectivity of scale, physics and chemistry permits well-informed modeling framework with *full quantification of uncertainty***
- **UQ leveraged to improve model prediction and data generation**
- **High throughput, intelligent computational screening *informs most effective R&D pathways for novel and transformational performance goal targeting***
- ***Multiple active collaborations with world-class industrial partners and test centers***
- ***CCSI^2 can also support the full commercialization pathway* for alternative technology platforms**

CCSI^2 Industrial and Advisory Board Meeting

- Currently Ongoing
- Afternoon and Thursday Sessions in Monongahela Room (down the hall)
- Presentations with much more detail at material, device and process scales – "*How CCSI^2 Works*"
- Future plans for the Toolset
- CCSI Computational Toolset Demonstrations from 9:15 – 2:30 on Thursday in Monongahela Room

All Capture meeting registrants are welcome and encouraged to attend!

CCSI²

Carbon Capture Simulation for Industry Impact

For more information

https://www.acceleratecarboncapture.org/

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