CCSI^2 Design of Experiments

NATIONAL ENERGY TECHNOLOGY LABORATORY

U.S./Norway Bilateral – 20180502

Michael Matuszewski – Associate Technical Director of CCSI^2

$CCSI^2$: Relevant Highlights

- **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

$CCSI^2$ Implementing Optimal Design of Experiments at TCM MEA Campaign in June-July

- **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 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

Open Source Release
3/30/2018
github.com/CCSI-Toolset

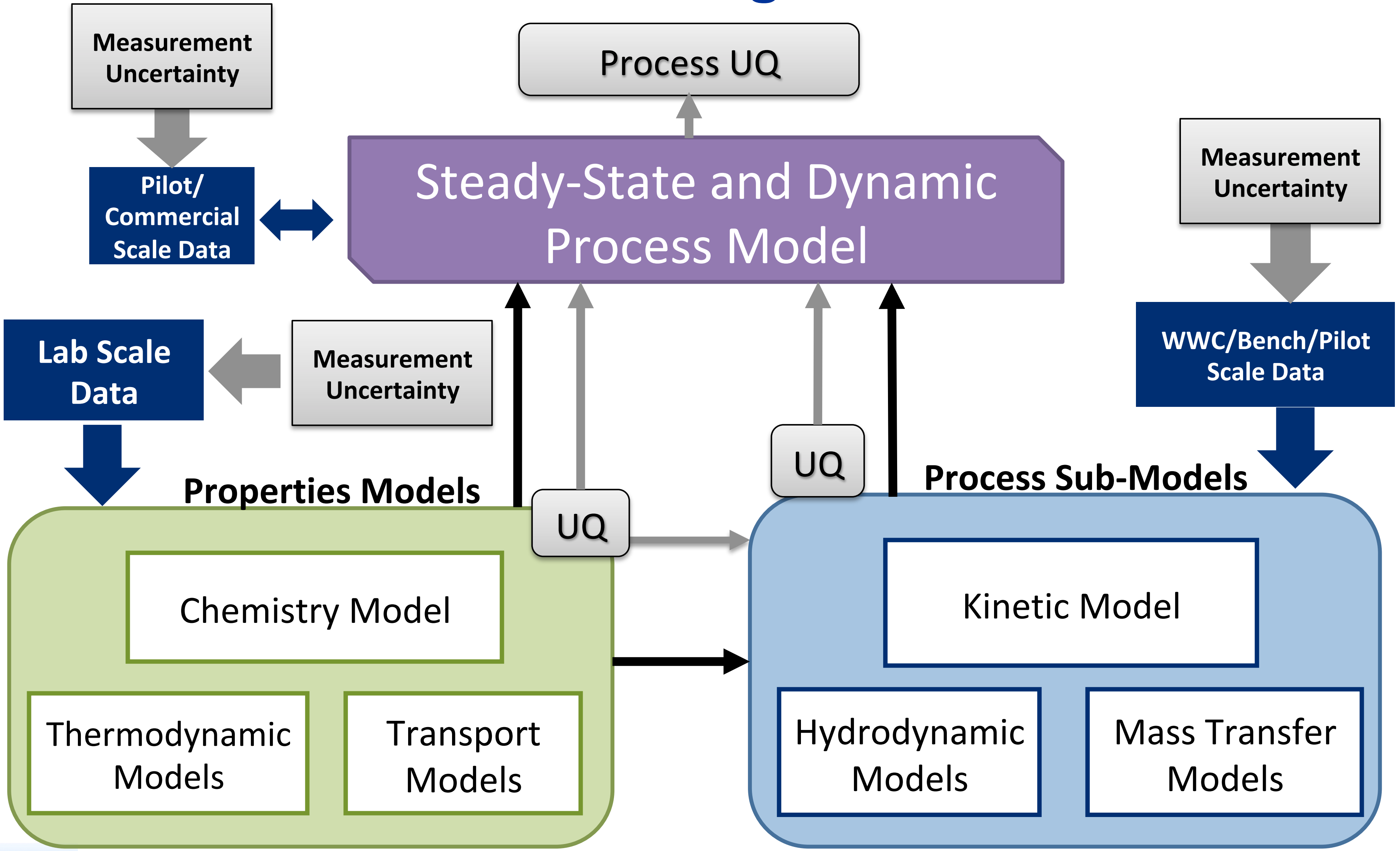
2016 R&D 100 Award Recipient

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
Pacific Northwest National Laboratory	Princeton University	ADA Environmental Solutions
National Energy Technology Laboratory	West Virginia University	Alstom
Los Alamos National Laboratory Est. 1943	Boston University	B&W the babcock&wilcox company
Lawrence Livermore National Laboratory	The University of Texas at Austin	GE
		EPRI Electric Power Research Institute
		Fluor
		Phillips 66
		AEP American Electric Power
		Southern California Edison An Edison International Company San Onofre Nuclear Generating Station
		Southern Company
		ExxonMobil
		Chevron
		URS
		Air Products
		Eastman
		aspentech
		ANSYS
		Schneider Electric
		PSE

Baseline Modeling Framework



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

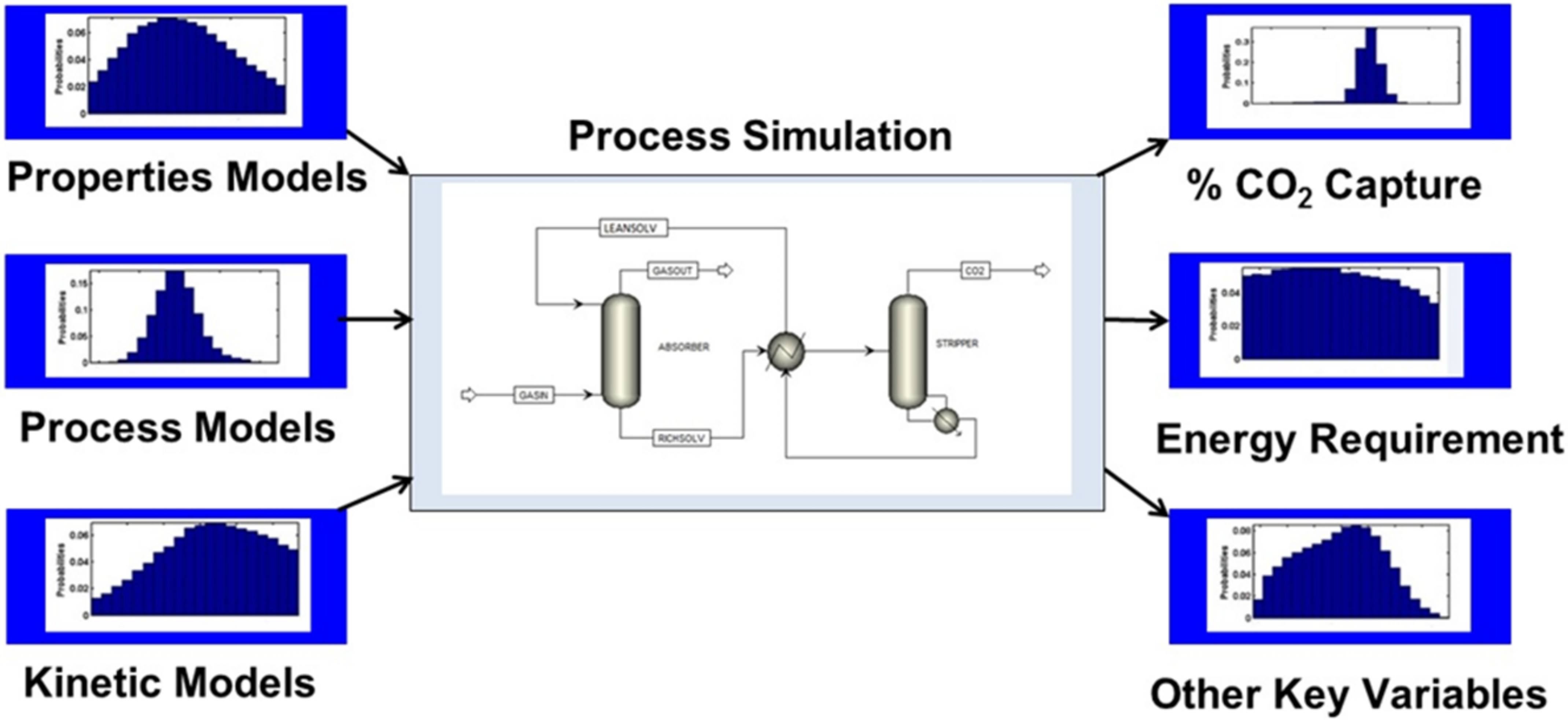
- Aqueous monoethanolamine (MEA) used as baseline
  - Current Industry Standard
  - Extensive Amount of Data Available

- Fully applicable to alternative solvents

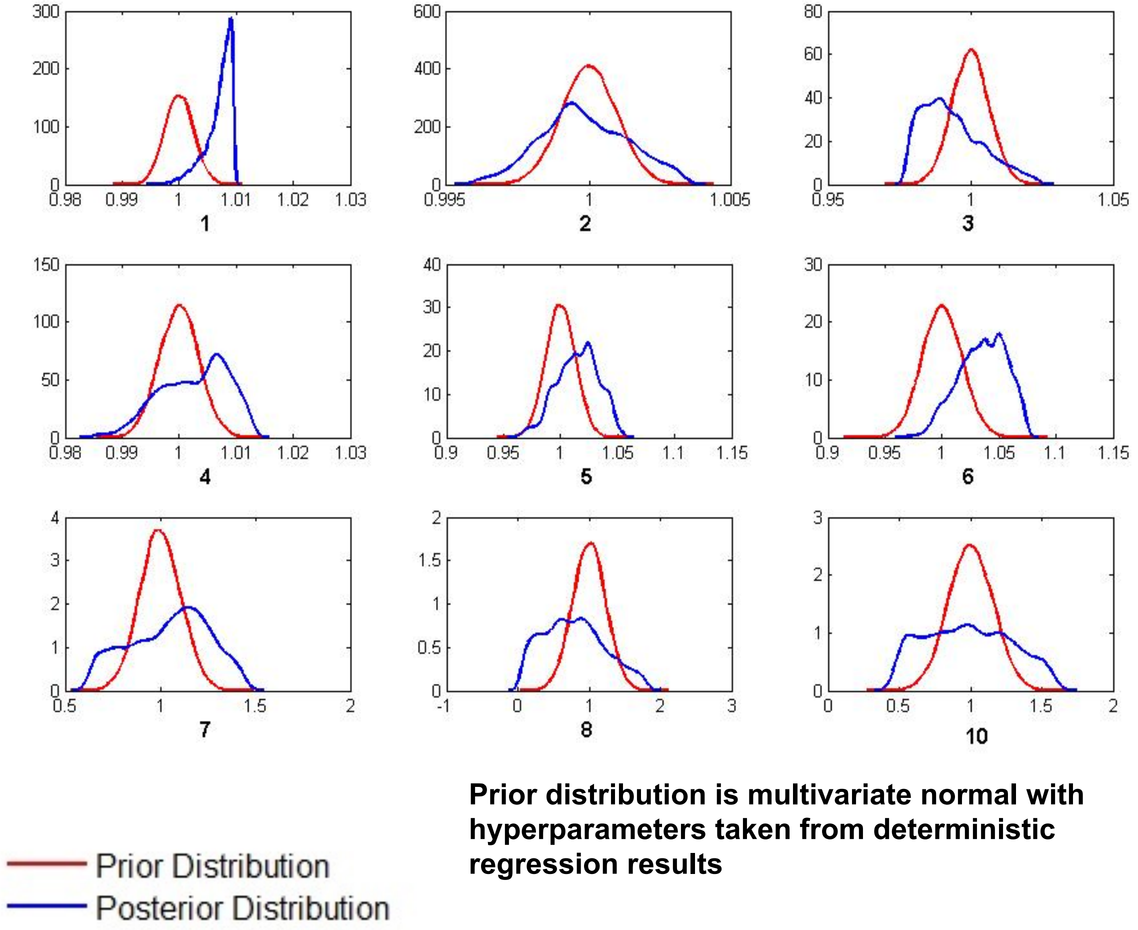
Managing and Refining Uncertainty

- **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

Integrated Multi-Scale Model Approach



Example UQ Results: One-Parameter Marginal Distribution



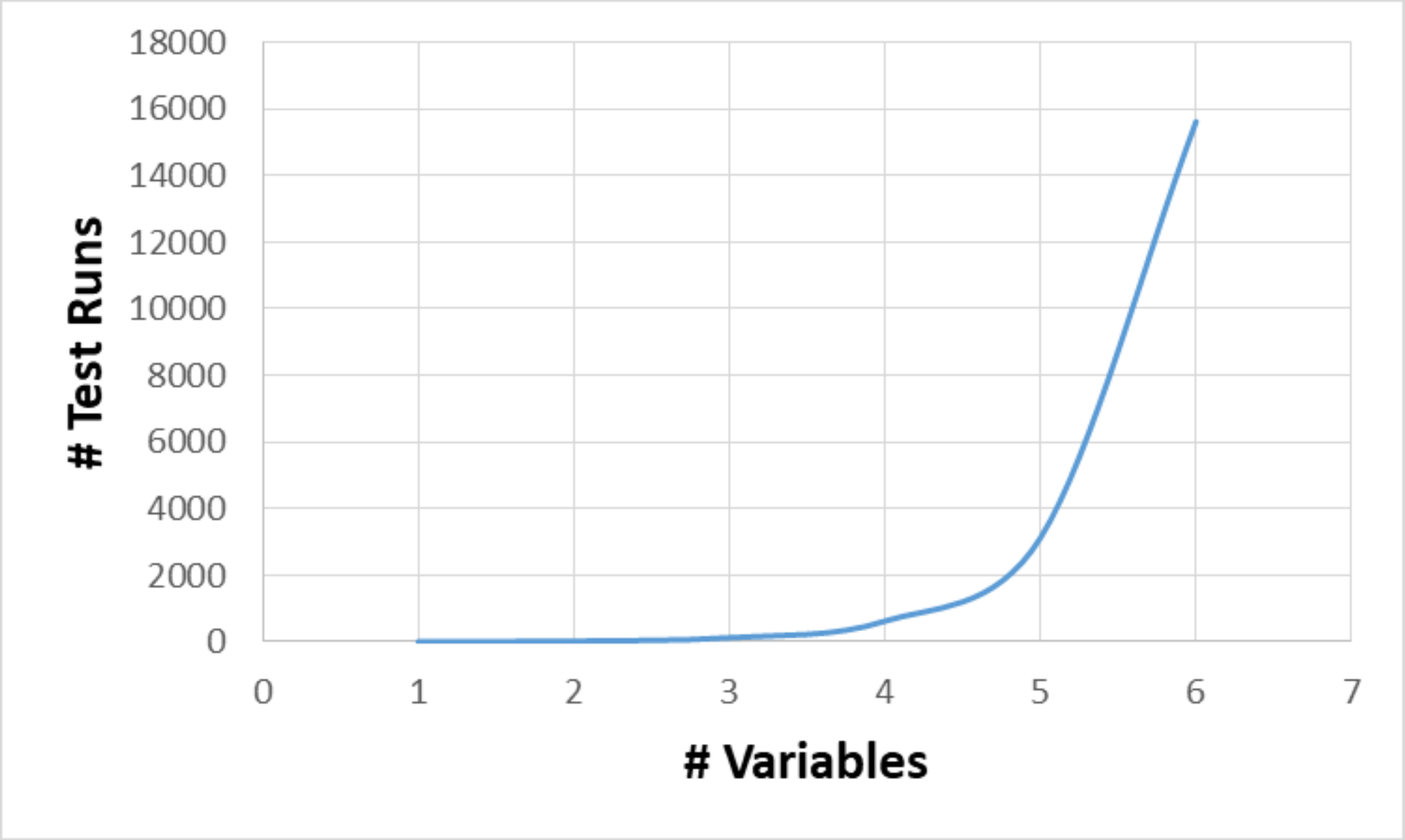
#	Parameter Name
1	DGAQFM (MEA+)
2	DGAQFM (MEACOO-)
3	DHAQFM (MEA+)
4	DHAQFM (MEACOO-)
5	HENRY/1 (MEA-H_2O)
6	HENRY/2 (MEA-H_2O)
7	NRTL/1 (MEA-H_2O)
8	NRTL/1 (H_2O-MEA)
9*	NRTL/1 (CO_2-MEA)
10	NRTL/2 (H_2O-MEA)

Prior distribution is multivariate normal with hyperparameters taken from deterministic regression results

***Not Considered in UQ**

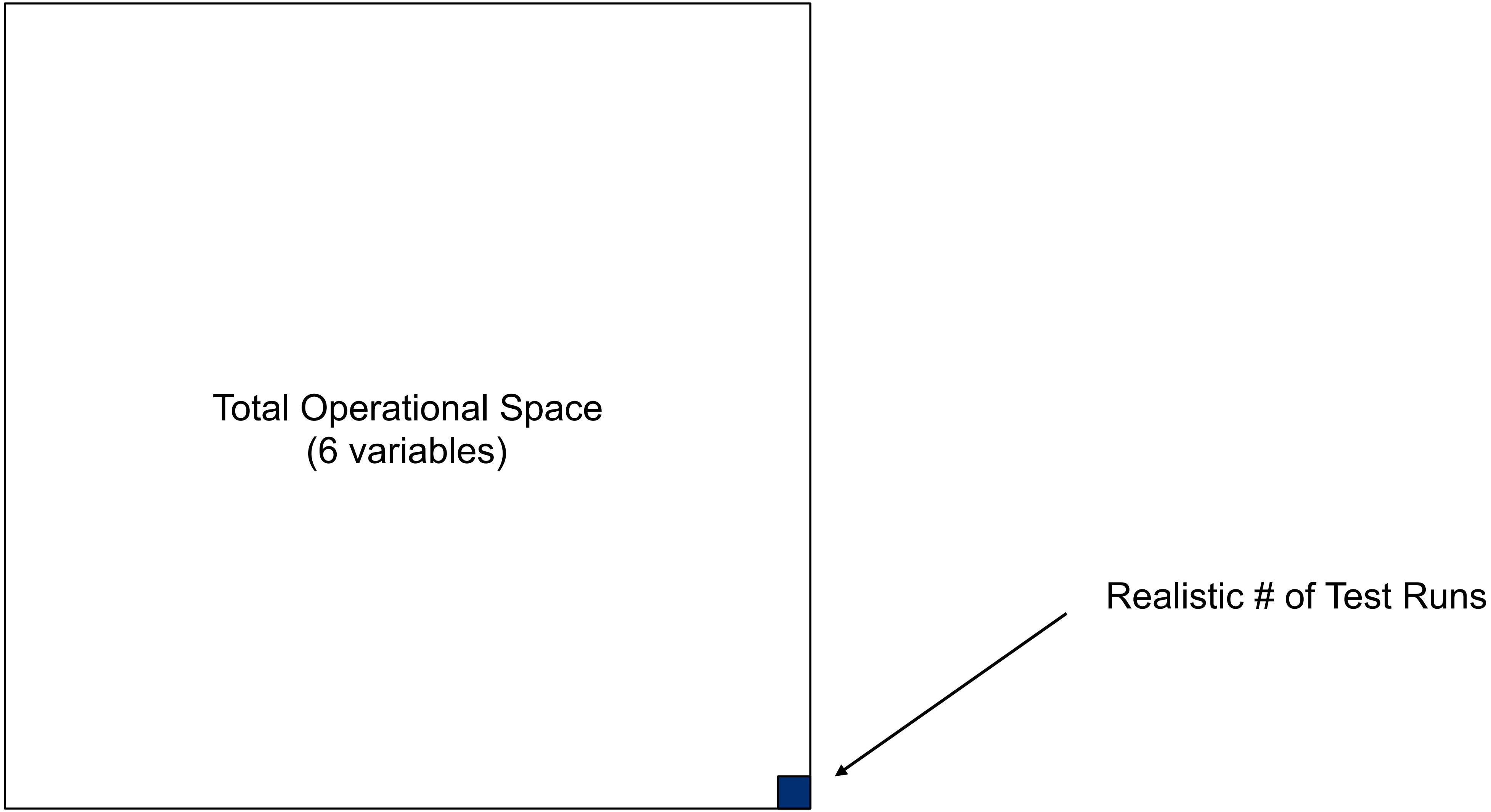
Parameter values normalized by dividing by deterministic model value

Design of Experiments (*Zero Engineering Insight*)

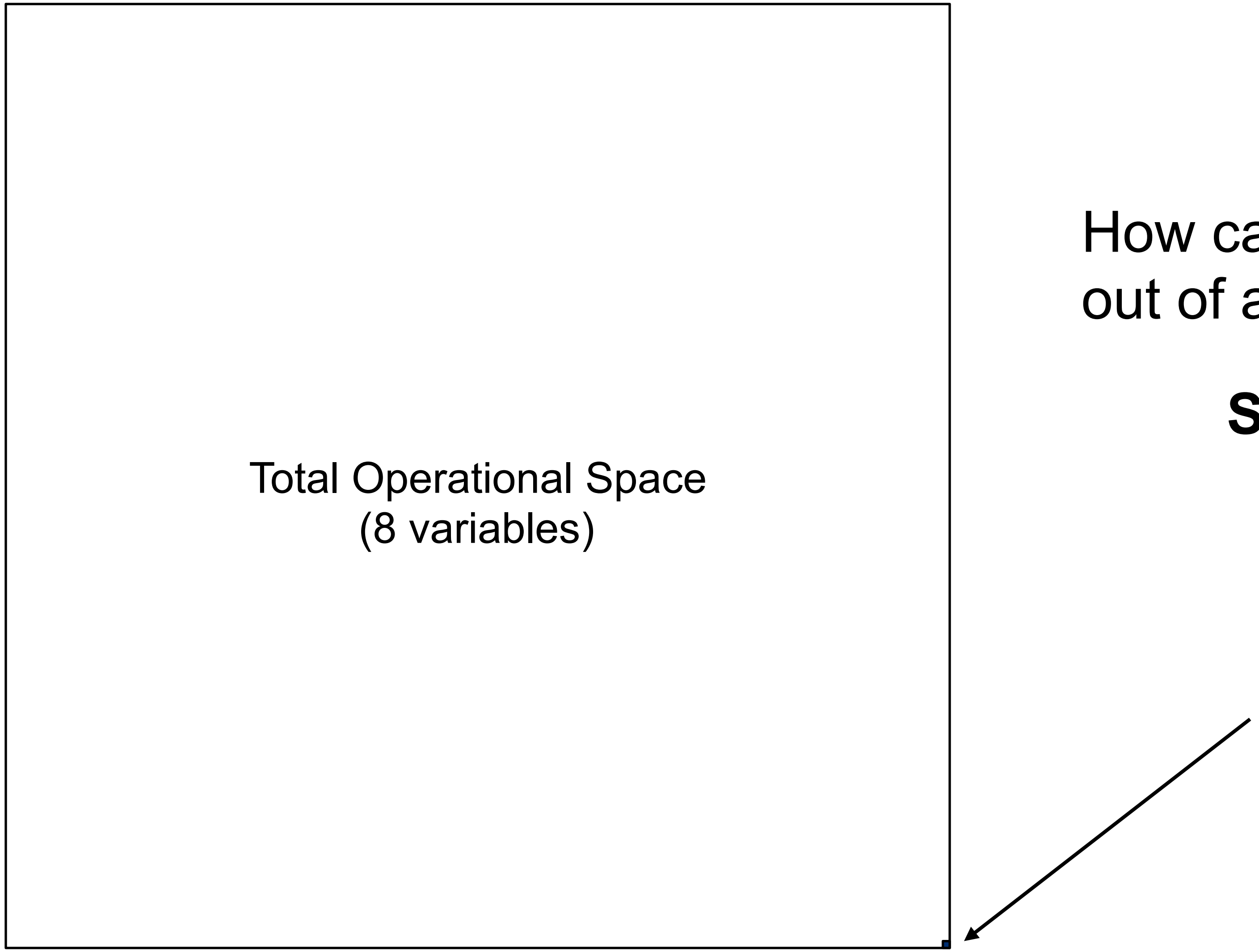


- Brute force approach
- 5 increments for each variable
- Exponential increase in test runs as variables increase

Design of Experiments Conceptualization



Design of Experiments Conceptualization



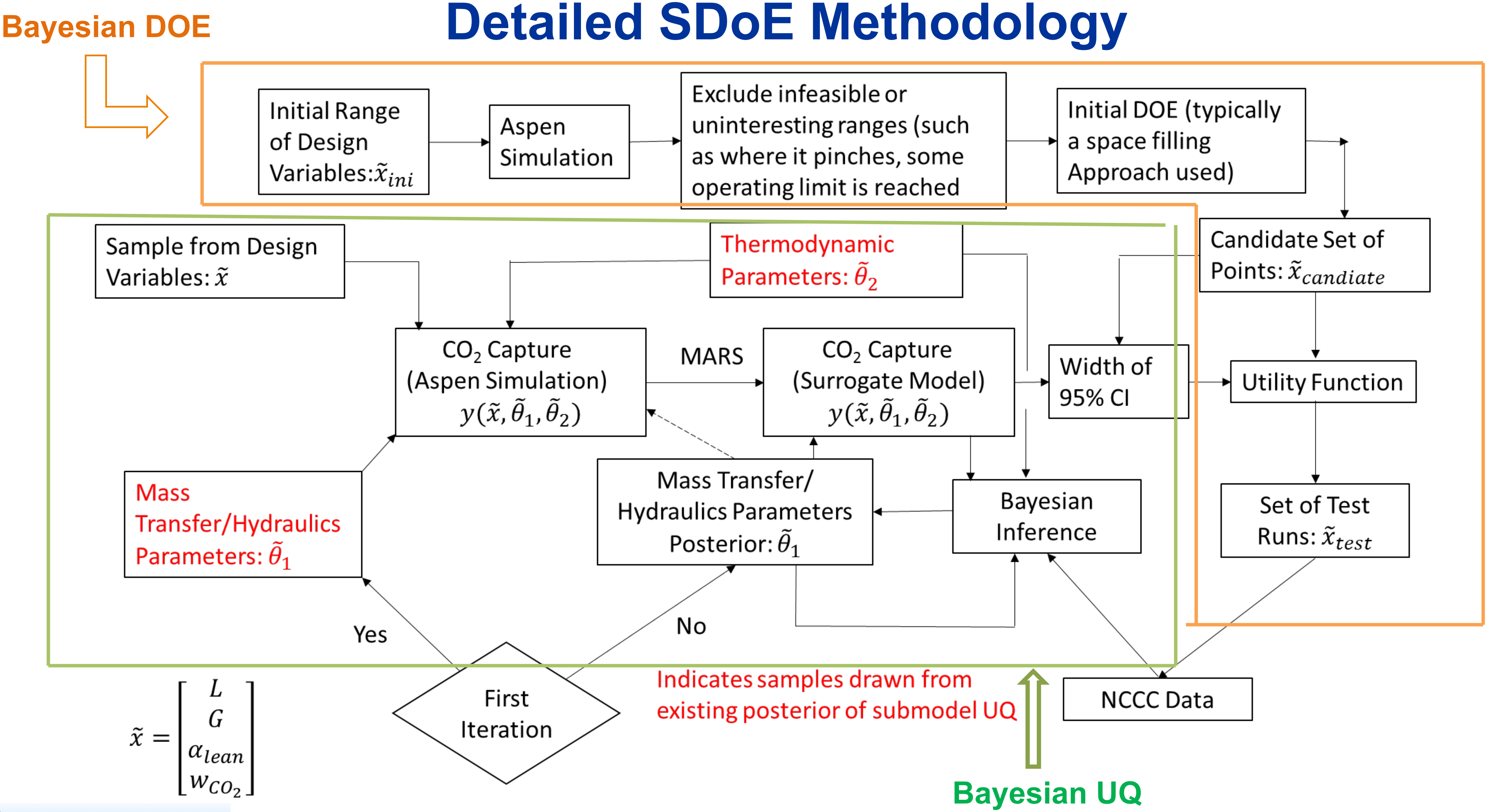
How can we possibly extract value out of a practical test campaign?

Start with Using Good Models!

(Then Make Them Better)

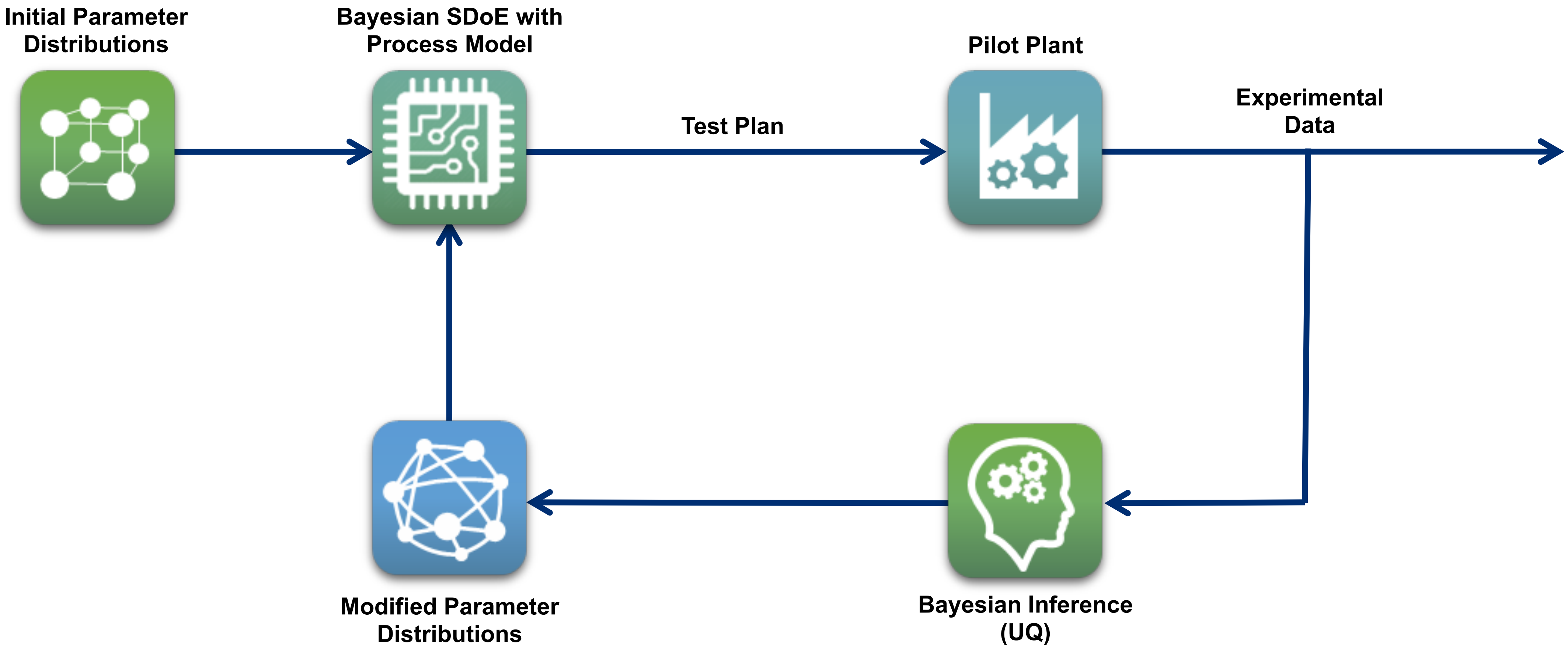
Realistic # of Test Runs

Detailed SDoE Methodology



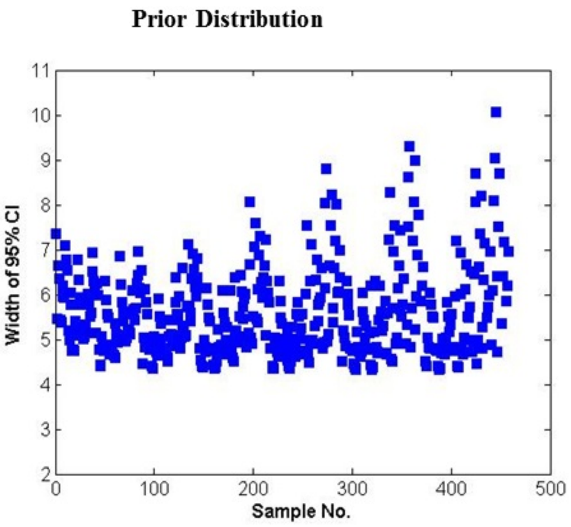
$$\tilde{x} = \begin{bmatrix} L \\ G \\ \alpha_{lean} \\ w_{CO_2} \end{bmatrix}$$

Bayesian SDoE

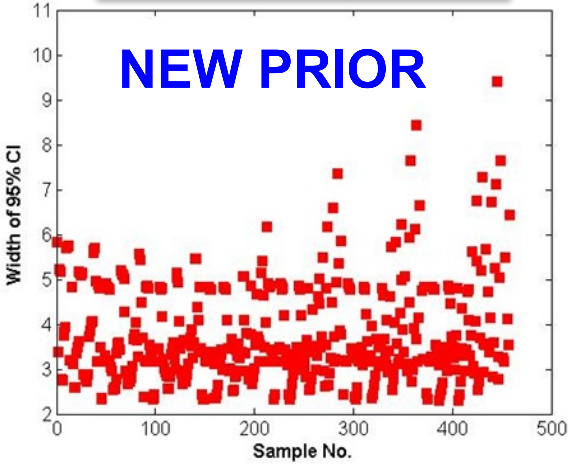


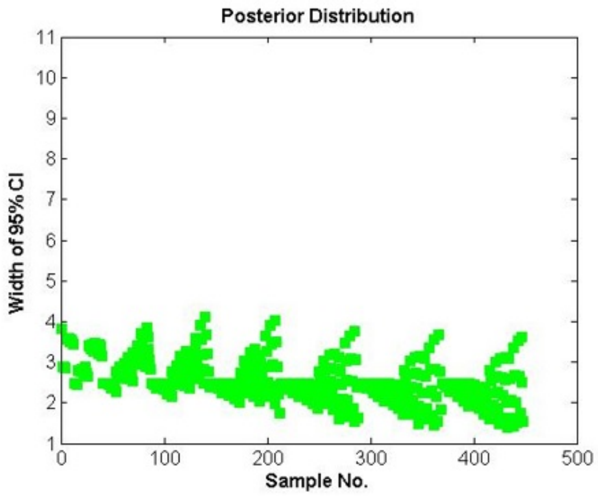
Effect of Bayesian Inference on CI Width

Candidate Points

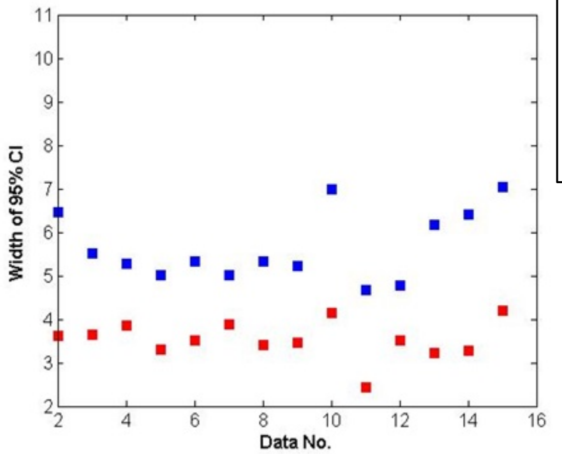


Next iteration

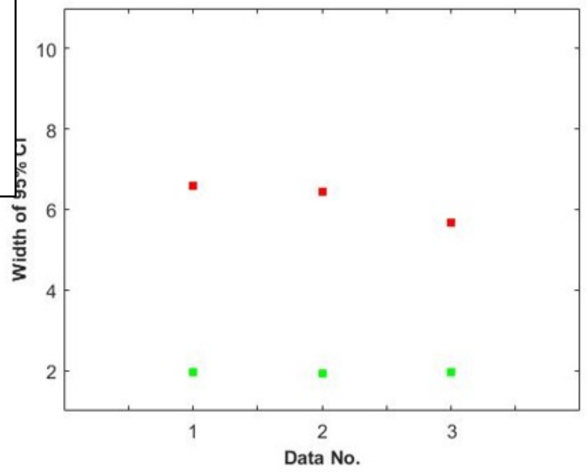




Points with Experimental Data



50-70% Reduction in CO_2 Capture Prediction Uncertainty



Summary

- Supports more <u>*accelerated*</u>, *risk-averse CCS scale up, demo and commercialization*
- *Optimizes system operation, configuration, <u>economics</u>*
- 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 <u>transformational performance goal targeting</u>*
- *Multiple active collaborations with world-class industrial partners and test centers*
- *CCSI^2 can also support the full commercialization pathway* for <u>alternative technology platforms</u>

CCSI²

Carbon Capture Simulation for Industry Impact

For more information

https://www.acceleratecarboncapture.org/

https://github.com/CCSI-Toolset

Michael S. Matuszewski, Associate Technical Director

Michael.Matuszewski@netl.doe.gov