CCSI^2

Carbon Capture Simulation for Industry Impact

Carbon Capture Simulation for Industry Impact (CCSI^2)

Technical Risk Reduction: Sequential Design of Experiments and Uncertainty Quantification

Abby Nachtsheim

Advanced PSE+ Stakeholder Summit

October 12, 2023

LA-UR-23-29857

U.S. DEPARTMENT OF ENERGY · NATIONAL ENERGY TECHNOLOGY LABORATORY · BERKELEY LAB · Lawrence Livermore National Laboratory · Los Alamos NATIONAL LABORATORY EST. 1943 · Pacific Northwest NATIONAL LABORATORY · OAK RIDGE National Laboratory · WestVirginiaUniversity · UNIVERSITY OF NOTRE DAME · THE UNIVERSITY OF TEXAS AT AUSTIN · UT · UNIVERSITY OF PITTSBURGH · CarnegieMellon

Today's Plan

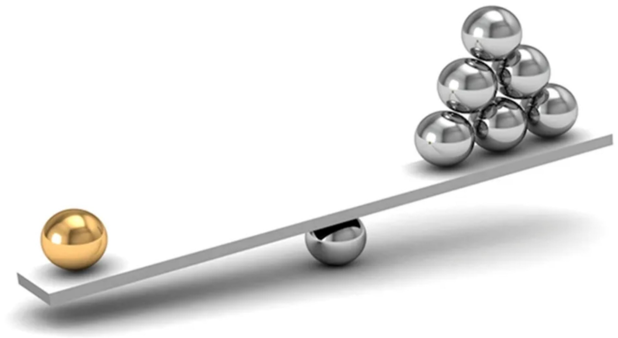
- Does the data collection approach matter? (Yes!)
- Uncertainty Quantification (UQ)
  - What, why, how?
- Sequential Design of Experiments (SDoE) and UQ
- UQ + SDoE Illustration

What is Design of Experiments (DoE)?

- **Mathematical strategy for selecting input combinations**
  - Estimate output (computer experiment)
  - Operate system (physical experiment)
- **Series of these experimental runs/tests forms experiment**
  - **Purposeful changes** to inputs of process or system
  - **Identify the reasons** for any changes in output
- **A well-designed experiment is critical**
  - Results and conclusions depend on data collection approach

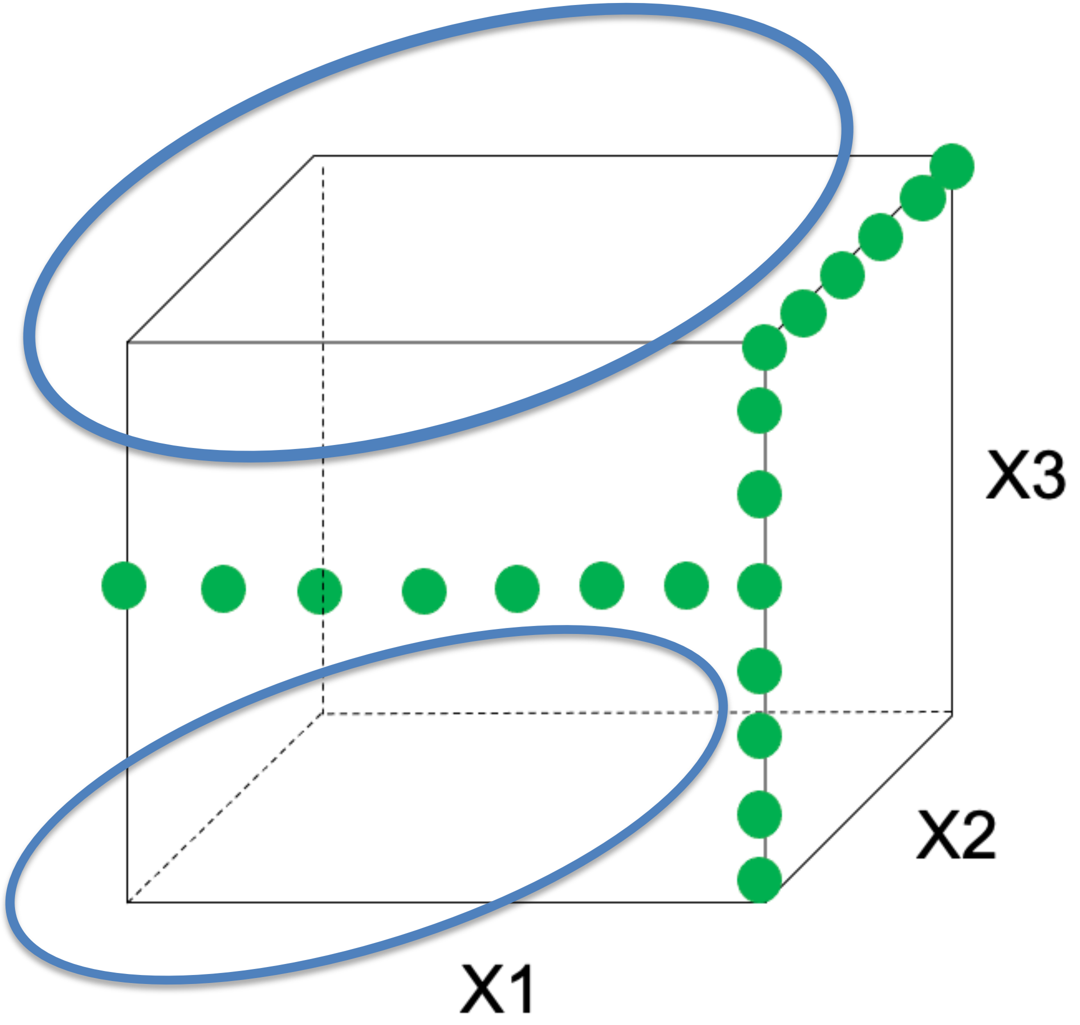
Why Use Design of Experiments?

- **Extract maximum information with a fixed budget**
  - **Maximize performance, minimize risk**
  - Produces exceptionally high-quality data
- **Saved 2 years and $2-3M off pilot testing**
- **Proven track record from past applications**
  - Over 25% reduction in model uncertainty
  - CO_2 Capture percentage within 3-6% with 95% confidence



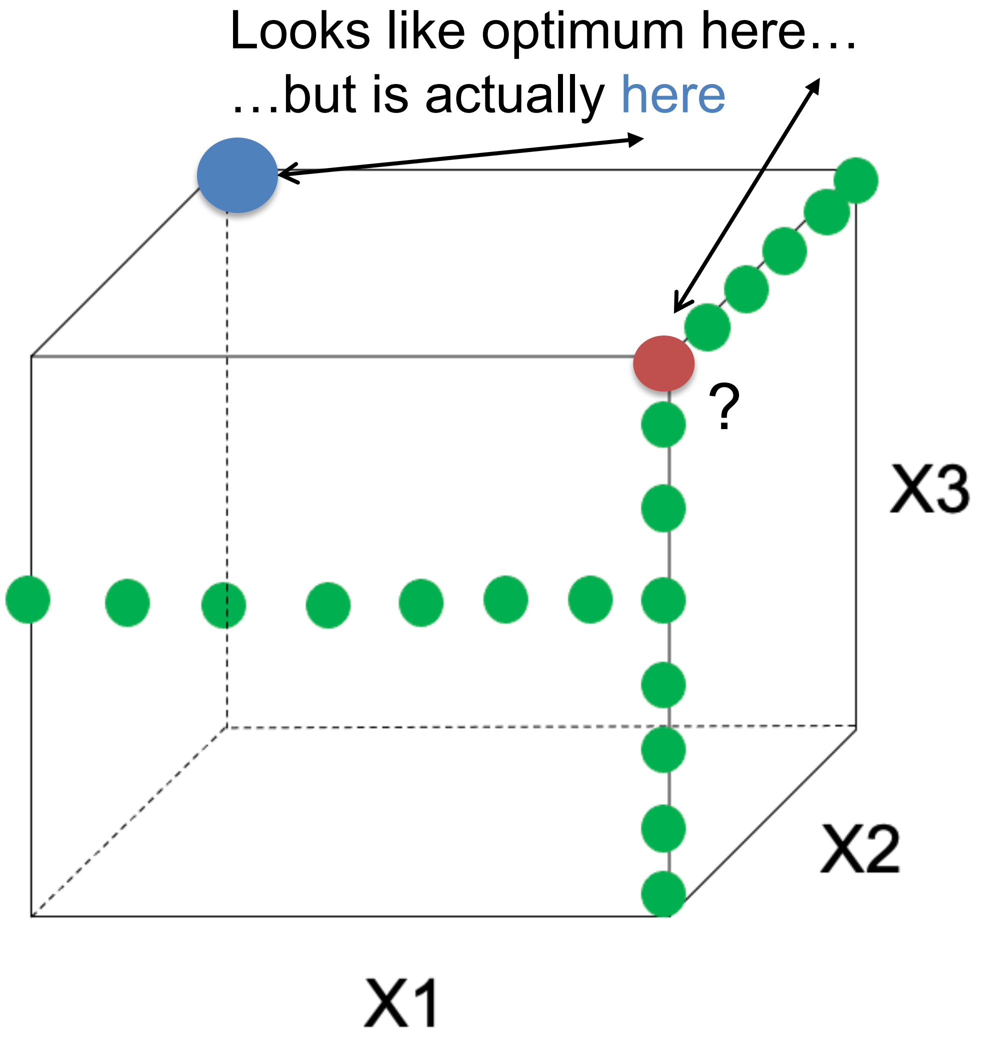
Design of Experiments not the same as One-Factor-at-a-Time

- **OFAAT strategy:**
  - Change only one input (factor) at a time
  - Hold all others constant
- **Inefficient use of resources**
- **Cannot identify interactions**
  - Effect of one factor changes when another factor changes
  - Finding optimal operating conditions is unlikely



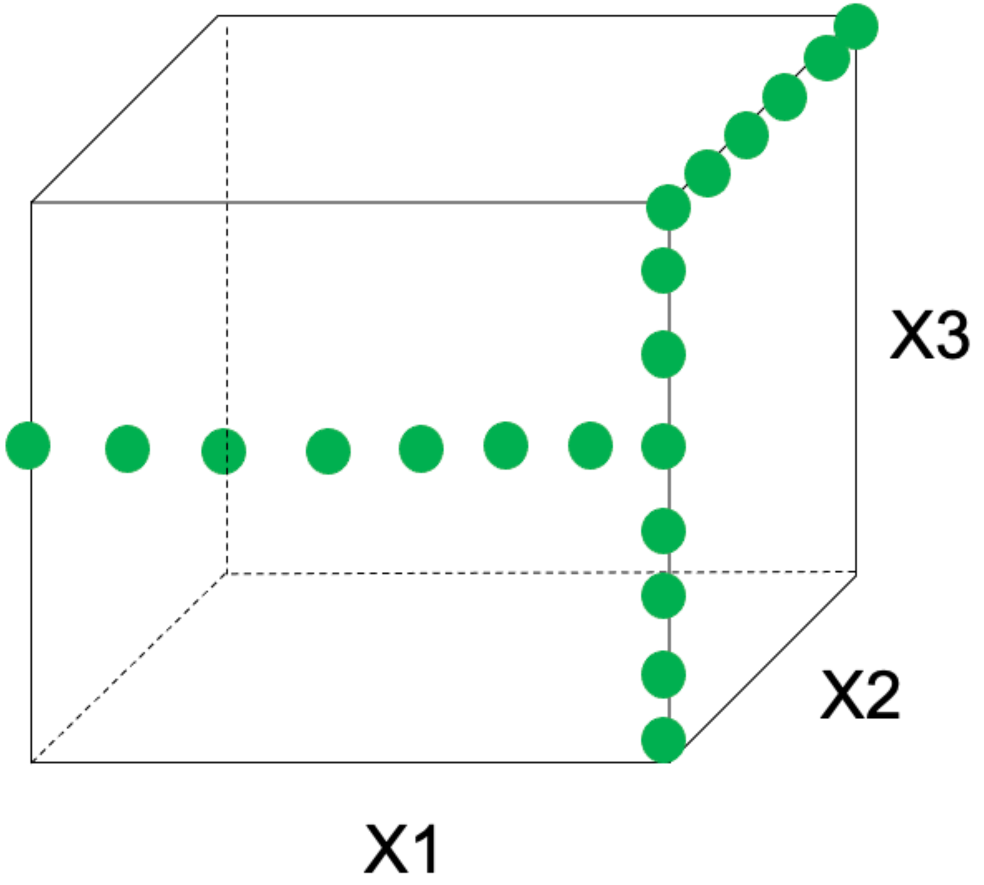
Design of Experiments not the same as One-Factor-at-a-Time

- **OFAAT strategy:**
  - Change only one input (factor) at a time
  - Hold all others constant
- **Inefficient use of resources**
- **Cannot identify interactions**
  - Effect of one factor changes when another factor changes
  - Finding optimal operating conditions is unlikely

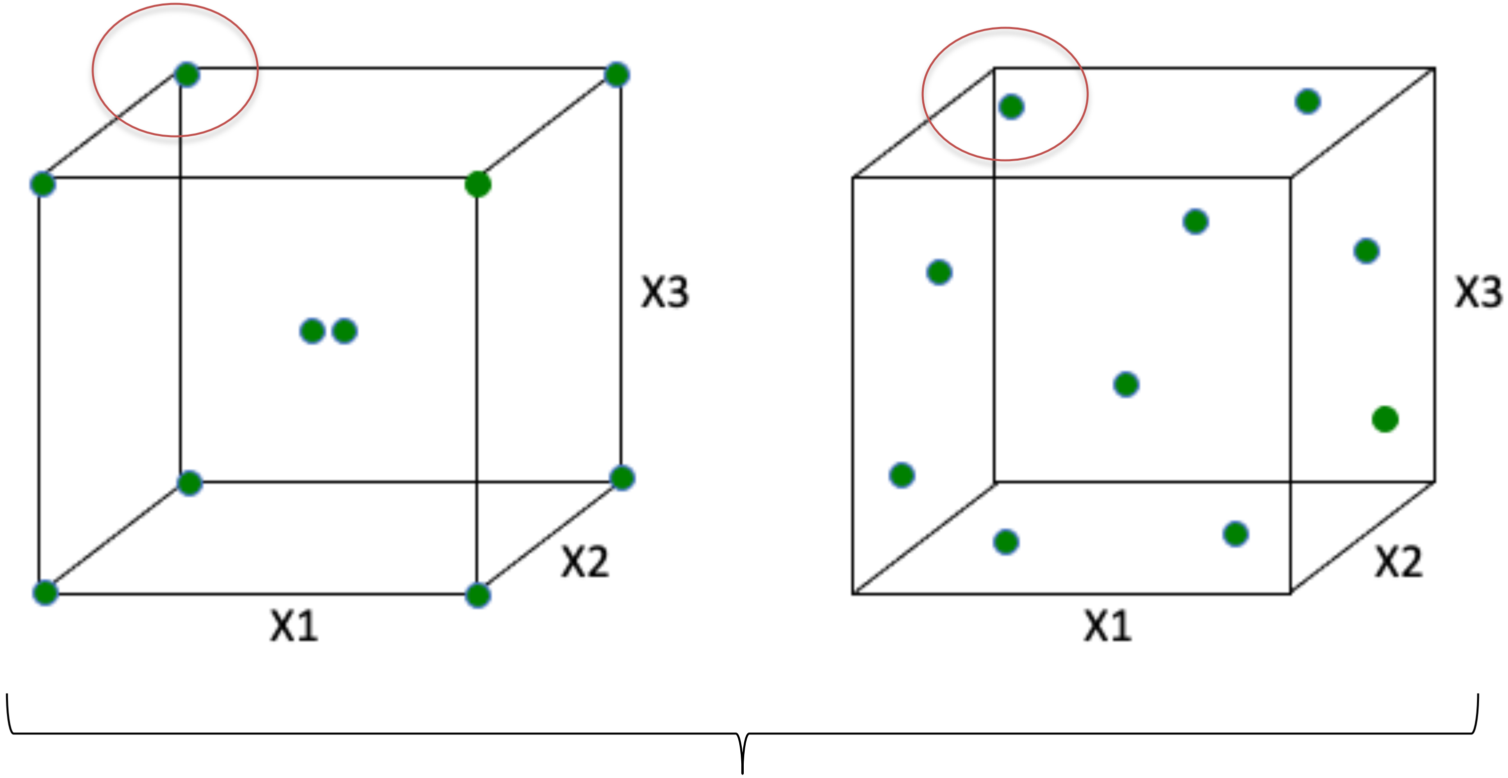


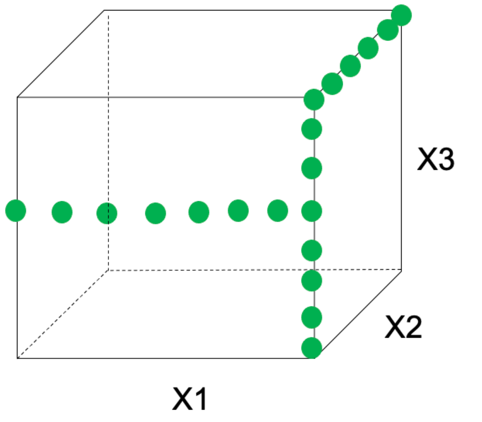
Design of Experiments not the same as One-Factor-at-a-Time

- **OFAAT strategy:**
  - Change only one input (factor) at a time
  - Hold all others constant
- **Inefficient use of resources**
- **Cannot identify interactions**
- **Not randomized**
  - Changing conditions can negatively affect the results



DoE Avoids These Drawbacks – Is Always More Efficient





Uses **20 runs**

Two Different DoE Approaches
Each uses **10 runs**

(More detail on quantitative advantages of DoE in a few slides)

What Is DoE Used For?

Development

- Evaluate and compare system configurations
- Evaluate material alternatives
- Determine parameter settings that work well under variable field conditions
- Determine parameters that impact product performance

Improvement

- Reduce variability
- Obtain closer conformance to target requirements
- Reduce development time
- **Reduce risk**

How?

Development

- Evaluate and compare system configurations
- Evaluate material alternatives
- Determine parameter settings that work well under variable field conditions
- Determine parameters that impact product performance

Improvement

- Reduce variability
- Obtain closer conformance to target requirements
- Reduce development time
- **Reduce risk**

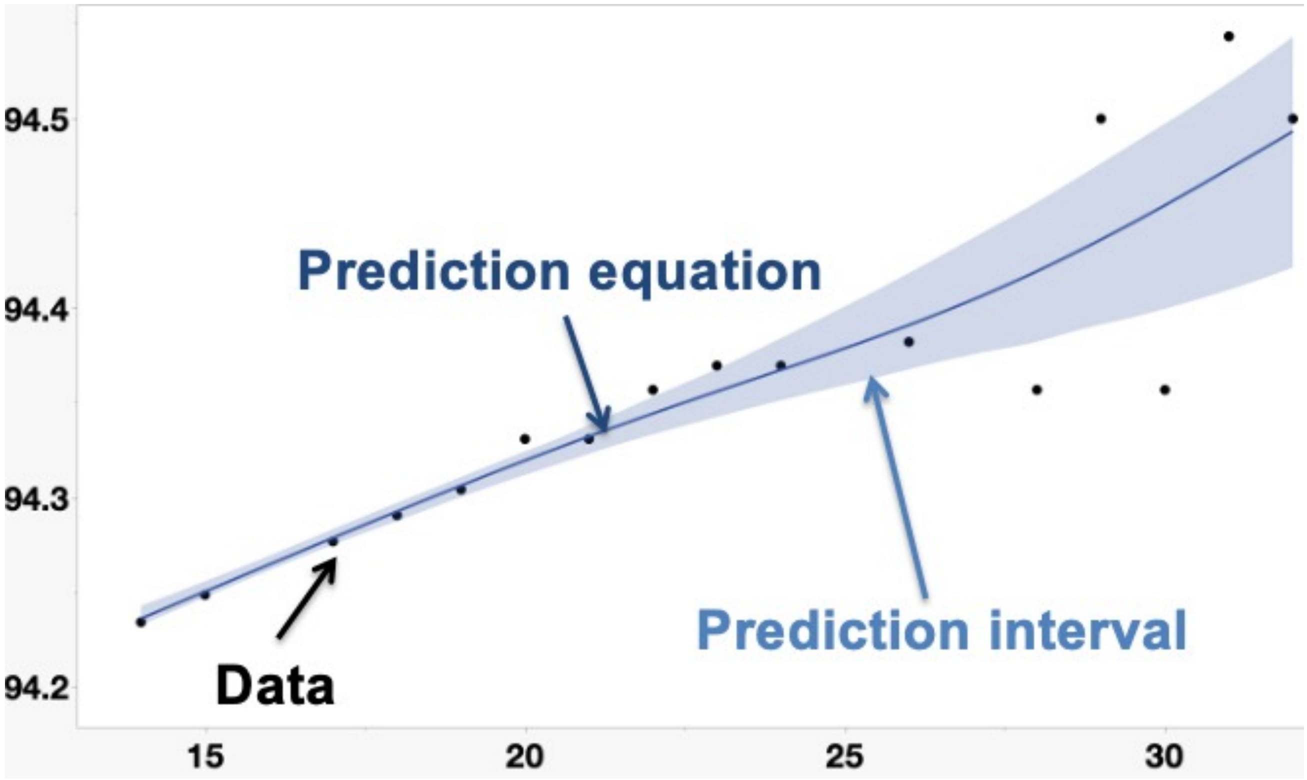
Strategic data collection + model estimation and refinement

All Models Contain Some Level of Uncertainty

- **Form of the model, values of model parameters, experimental data used**
- **Need to characterize this uncertainty**
  – Understand
  – Interpret results appropriately
- **Characterization allows us to target sources of uncertainty to reduce uncertainty; improve**
  – Models
  – Results
  – Understanding

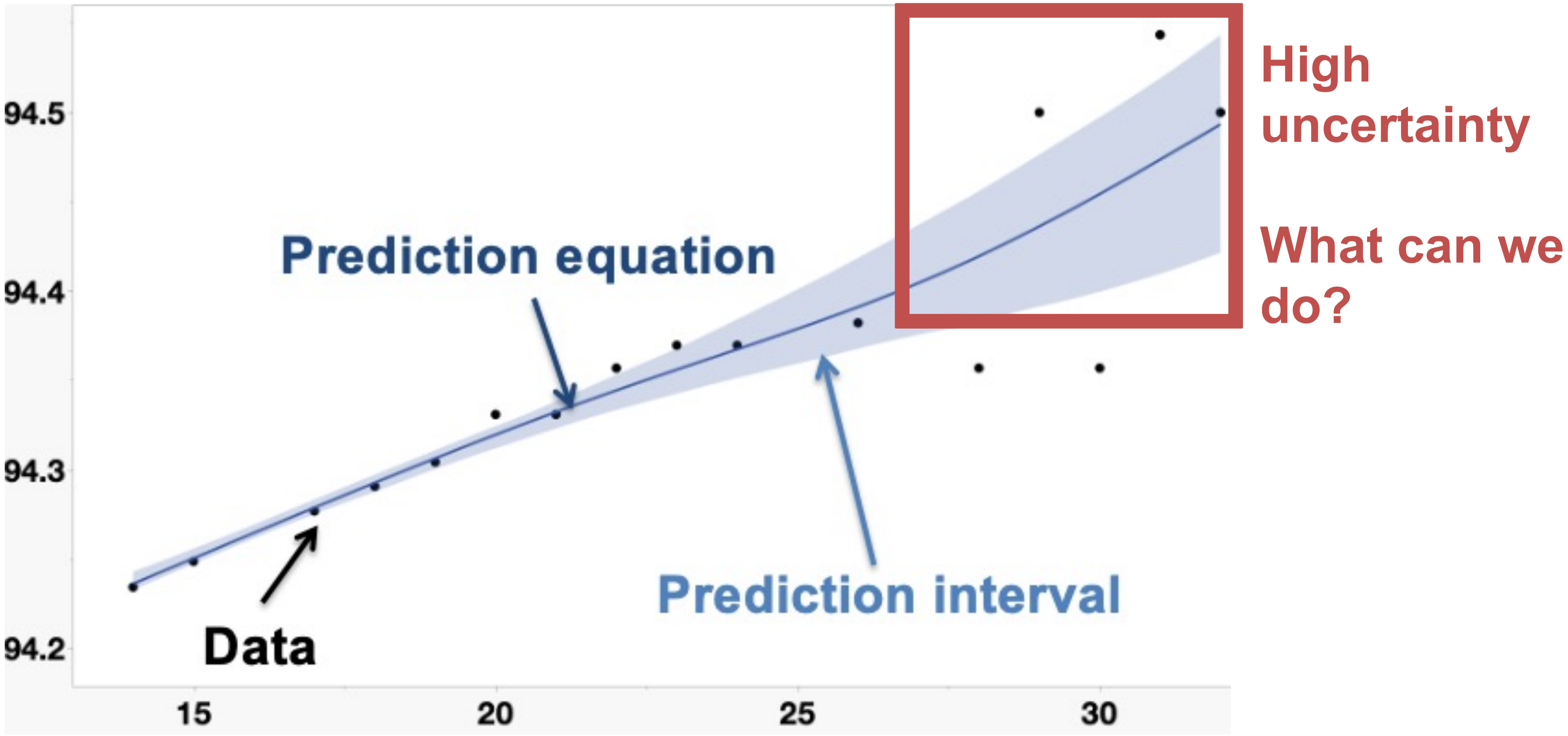
Uncertainty Quantification (UQ)

- **Uncertainty Quantification (UQ): collection of statistical methods to characterize, estimate, understand model uncertainty**
- **CCSI² UQ Toolset** contains robust set of analysis and visualization tools for characterizing impact on a system
- **Visualize a common example:**
  - Prediction intervals



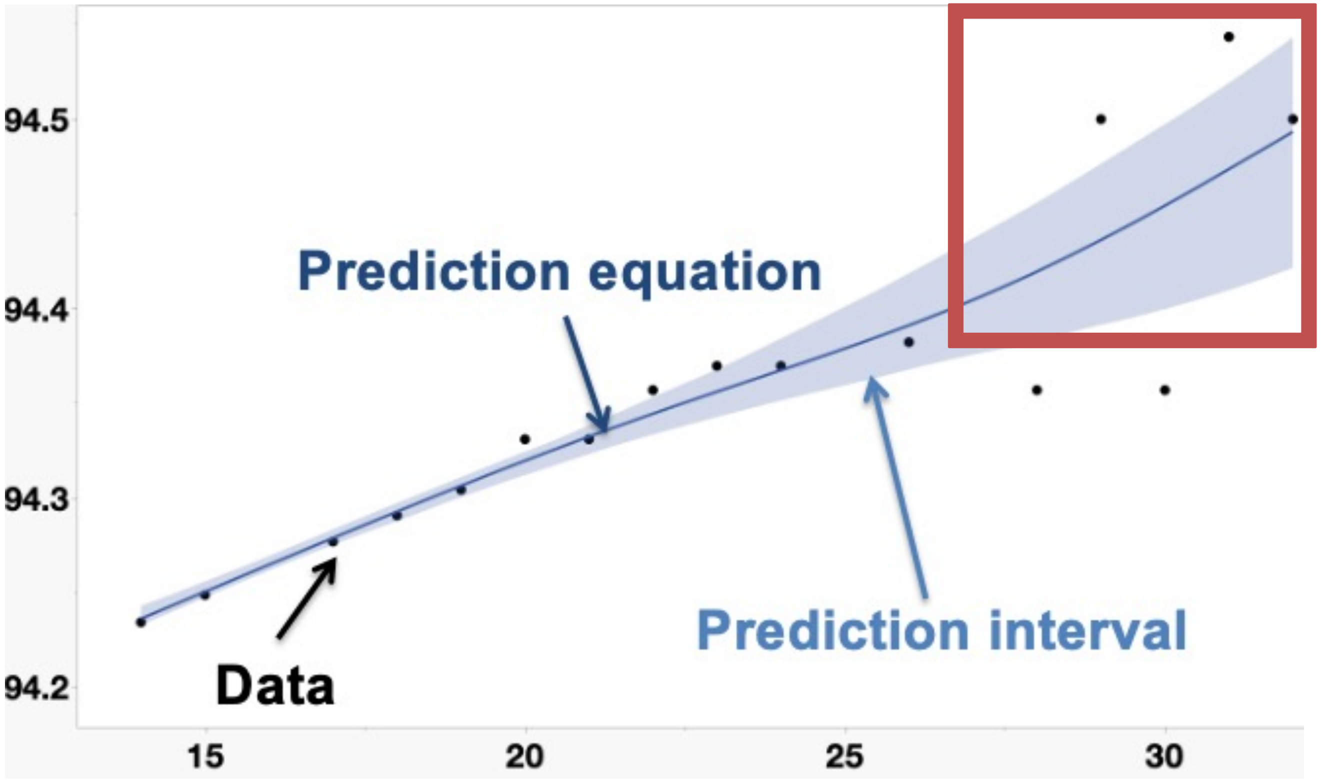
Uncertainty Quantification (UQ)

- **Uncertainty Quantification (UQ): collection of statistical methods to characterize, estimate, understand model uncertainty**
- **CCSI² UQ Toolset** contains robust set of analysis and visualization tools for characterizing impact on a system
- **Visualize a common example:**
  - Prediction intervals



Uncertainty Quantification (UQ)

- **Uncertainty Quantification (UQ): collection of statistical methods to characterize, estimate, understand model uncertainty**
- **CCSI² UQ Toolset** contains robust set of analysis and visualization tools for characterizing impact on a system
- **Visualize a common example:**
  - Prediction intervals



High uncertainty

What can we do?

Collect more data!

Sequential DoE (SDoE)

SDoE: Directly incorporate knowledge learned in previous stages
Result: Strategic data collection across multiple stages, reduce risk

Feasibility study → Exploration of input space → Model building / refinement → Optimization → Confirmation

Feasibility study
Is it possible to collect quality data?

Proof of concept

Exploration of input space
Understand basic relationship between inputs and responses

Model building / refinement
Verify that the model captures patterns

Add data for better model parameter estimation or prediction

Optimization
Focus on region of maximum interest

Close to most desirable operation conditions

Confirmation
Verify results for production or operational use

Ability to reproduce results

Success Stories: MTR Field Test at TCM

- CCSI² supported Membrane Technology and Research engineering-scale advanced membrane field test at the Technology Centre Mongstad (TCM) (DE-FE0031591)
- CCSI² Team leveraged UQ and SDoE tools to make the most of the experimental budget – Learn as we go, increase efficacy
- Primary objective: **Optimization**

Exploration of input space → **Model building / refinement**

UQ + SDoE to refine space of interest

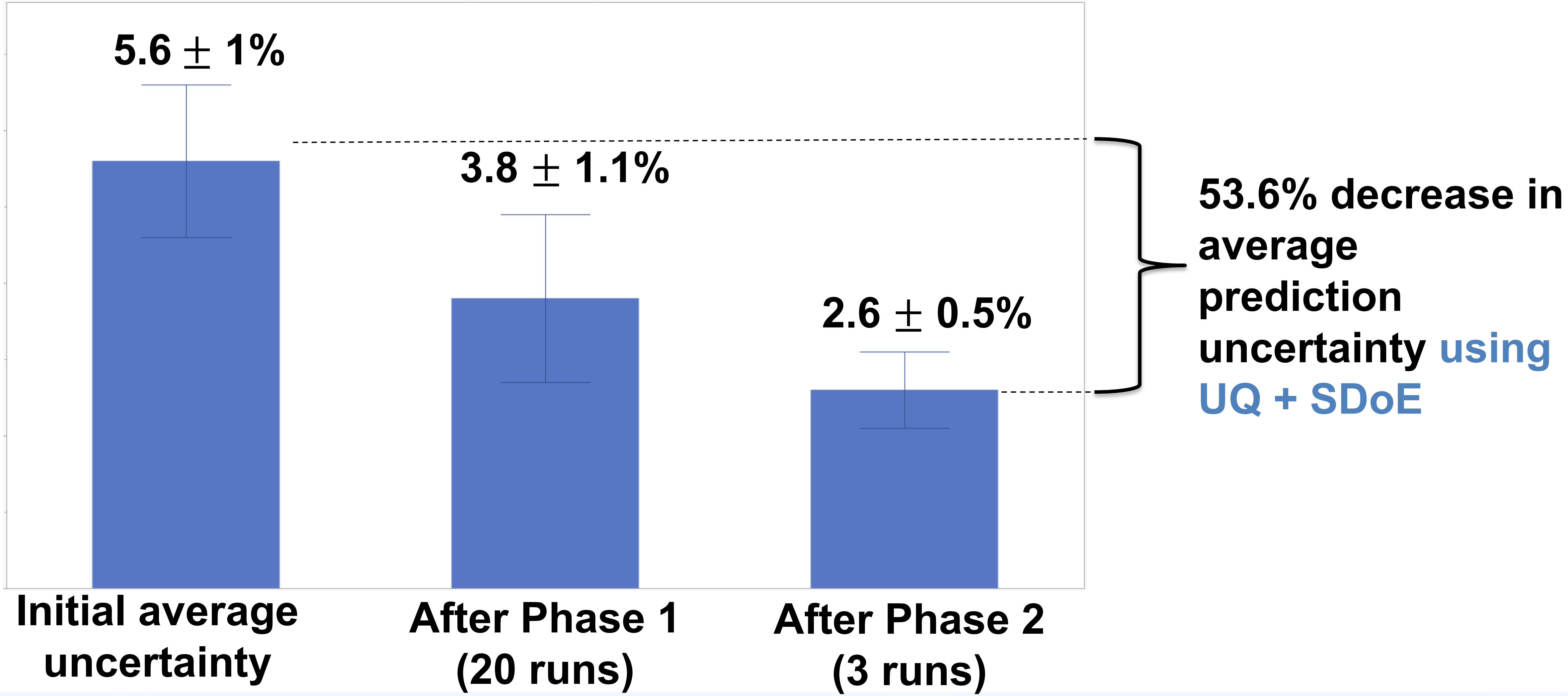
UQ + SDoE to reduce uncertainty

Successful completion of field test with goals met, despite delays in testing schedule due to MTR equipment

Success Stories: RTI Test Campaign at TCM

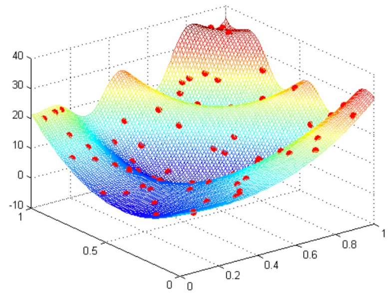
- CCSI^2 supported Research Triangle Institute test campaign for NAS solvent system at TCM
- RTI interested in two sets of conditions
  - Gas-fired combined heat and power (CHP)
  - Residual fluidized catalytic cracker (RFCC) flue gas sources
- CCSI^2 contributed 2 separate series of designs ranging in size to meet objective while accounting for flexibility in schedule
- **Leveraged SDoE to guide test campaign**
  - Focused on demonstrating high levels of CO2 capture with low solvent emissions and regeneration energy requirement

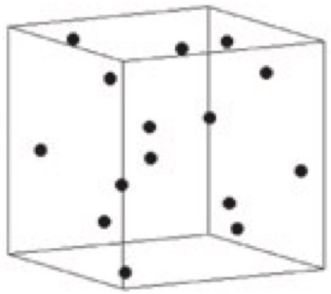
Success stories:
Aqueous MEA Pilot Plant Campaign at NCCC



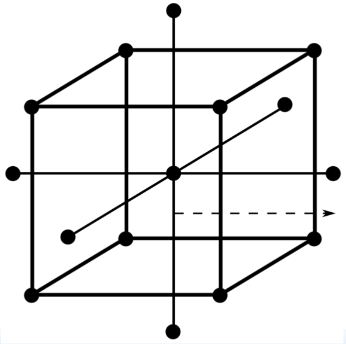
Range of strategies provides flexibility

- **Space-filling designs**
  - Relationship between inputs and response(s) of interest not well understood
  - Good precision for predicting new results at any new location





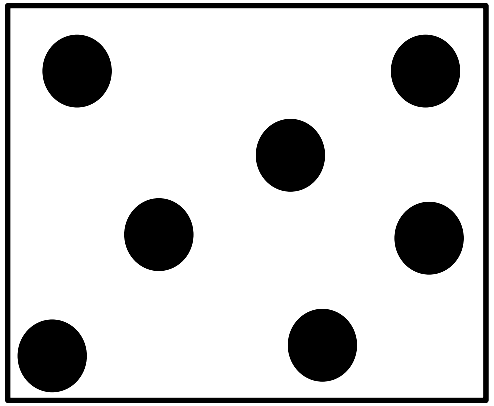
- **Model-based designs:**
  - Can specify correct form for model of interest to characterize relationship between inputs and response(s)
  - Relationship can be well approximated by a low-order polynomial



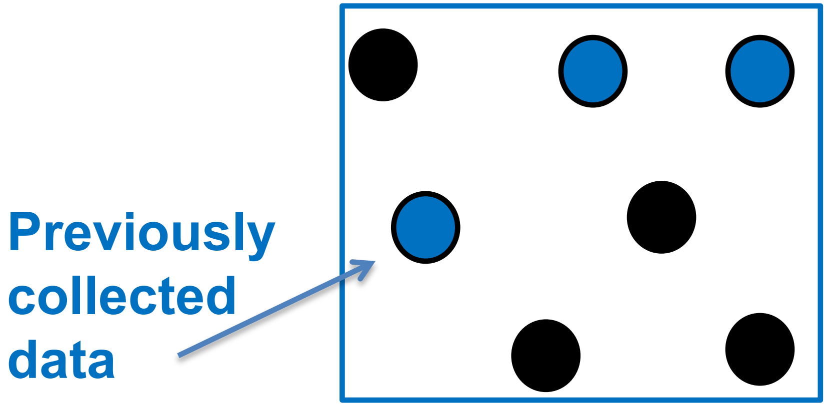
CCSI² Space-Filling Design Capabilities

1. **Uniform Space-Filling (USF)**
   - Design points evenly spread throughout space of interest
   - Exploration

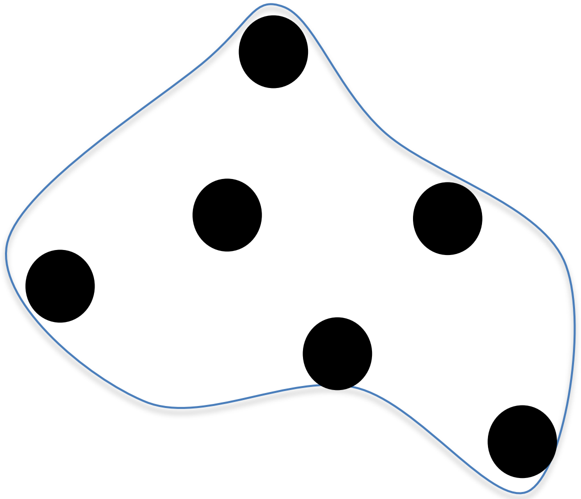
Design for first phase experiment



Design for sequential phase of experiment



Design for irregular region of interest

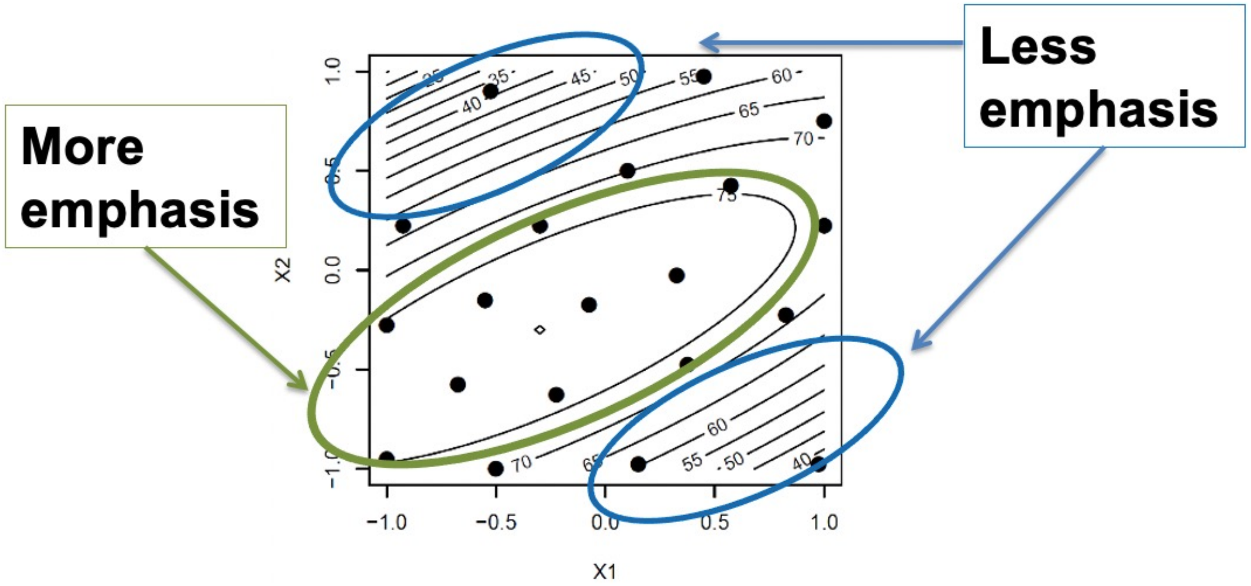


CCSI²
Carbon Capture Simulation for Industry Impact

CCSI^2 Space-Filling Design Capabilities

2. Non-Uniform Space-Filling (NUSF)

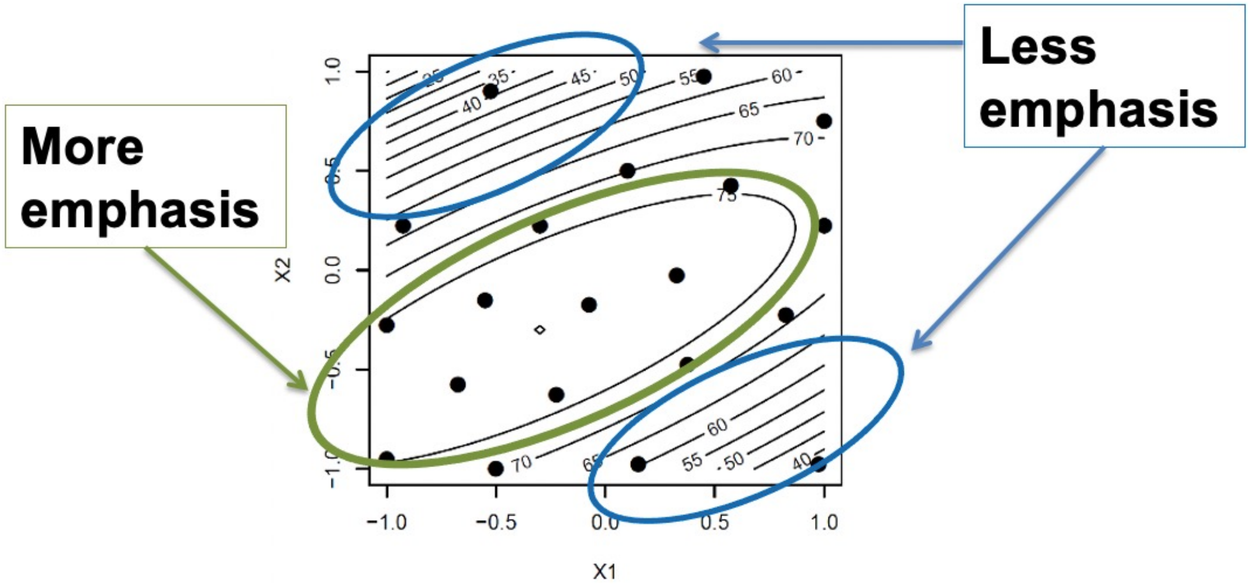
- Design points still spread out
- Emphasize some regions more than others
- Developed to meet needs of CCSI^2 applications
- Uncertainty Reduction



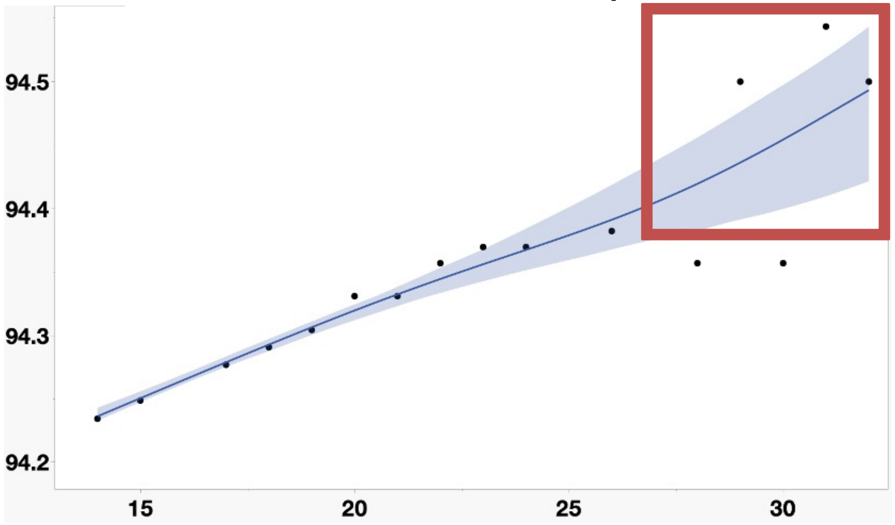
CCSI² Space-Filling Design Capabilities

2. Non-Uniform Space-Filling (NUSF)

- Design points still spread out
- Emphasize some regions more than others
- Developed to meet needs of CCSI² applications
- Uncertainty Reduction



Parallel with 2D example

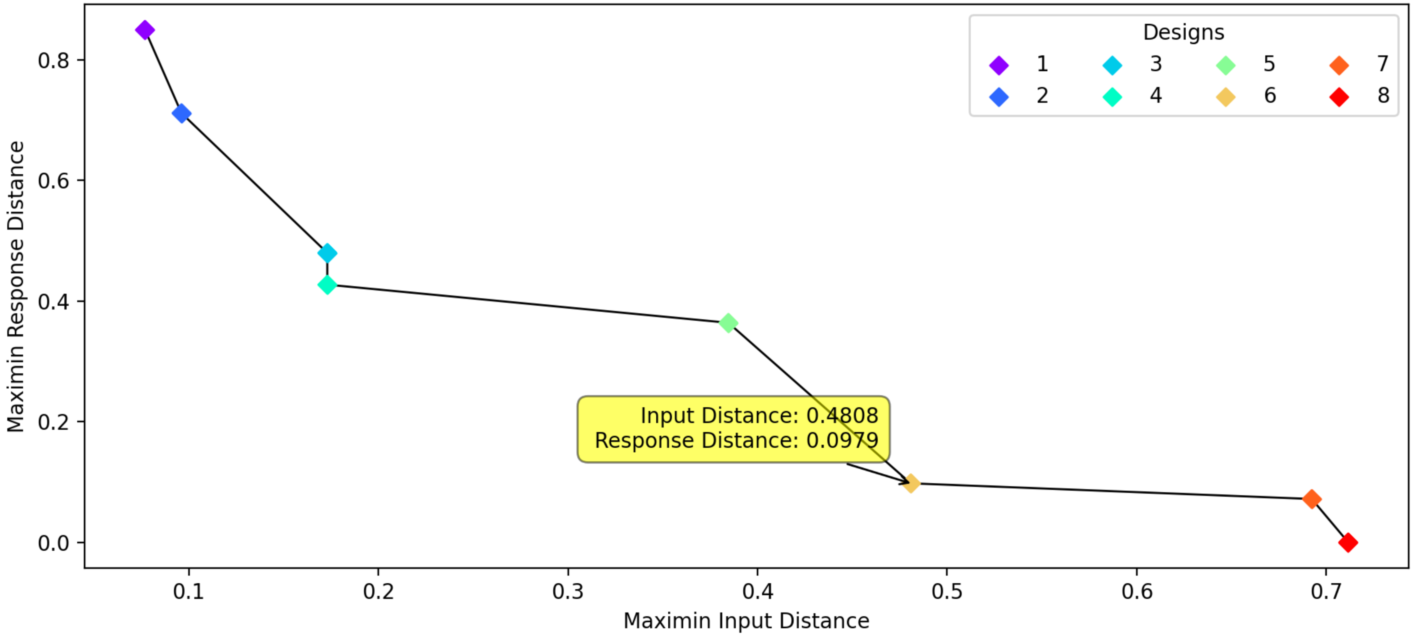


CCSI² Space-Filling Design Capabilities

3. Input Response Space-Filling (IRSF)

- Used when information is known about likely output values
- Select design points likely to results in good distribution of output values
- Balance with good space-filling properties in input space

Space-Filling in the output



Space-Filling in the inputs

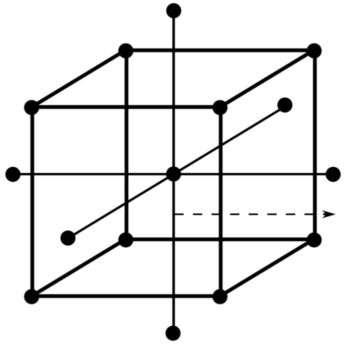
CCSI² Carbon Capture Simulation for Industry Impact

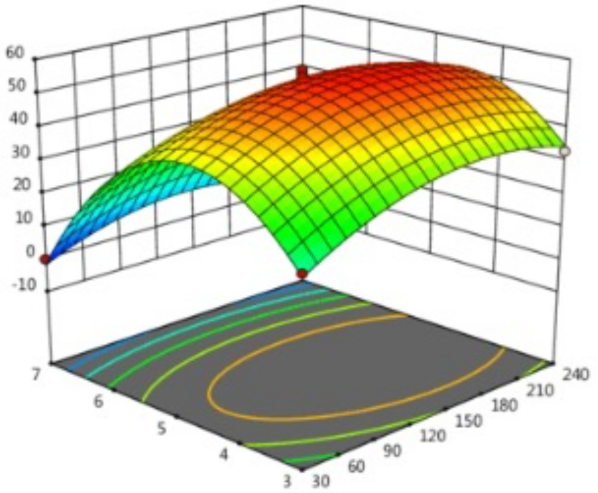
CCSI² Empirical Model-Based Capabilities

Often used when relationship between inputs and response can be well approximated by a low-order polynomial

- What inputs have biggest influence on output?
  - Parameter estimation
- What input settings lead to desired output value?
  - Response prediction
- Good choice for initial exploration
  - Refine experimental scope
  - Process model under development

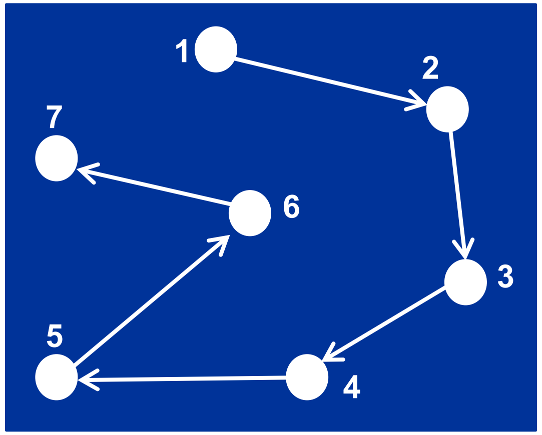
CCSI²: SDoE Toolset; Experts to talk to and work with



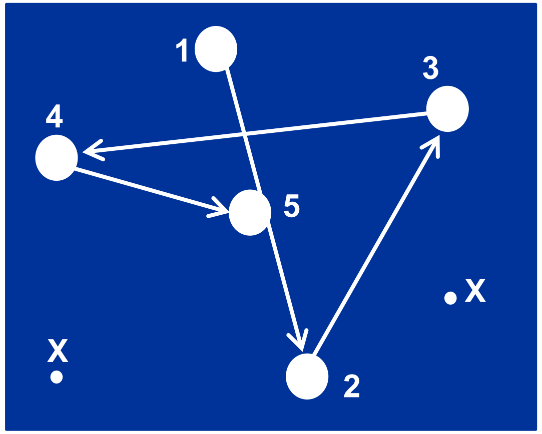


CCSI² SDoE Capabilities

- **Design ordering algorithm:**
  - Orders the experimental runs
  - Improves efficiency of implementation
- **Graphical tools for design evaluation and comparison**
  - Facilitates comparison among design options
  - Allows users to quickly assess design coverage and properties



Ordered

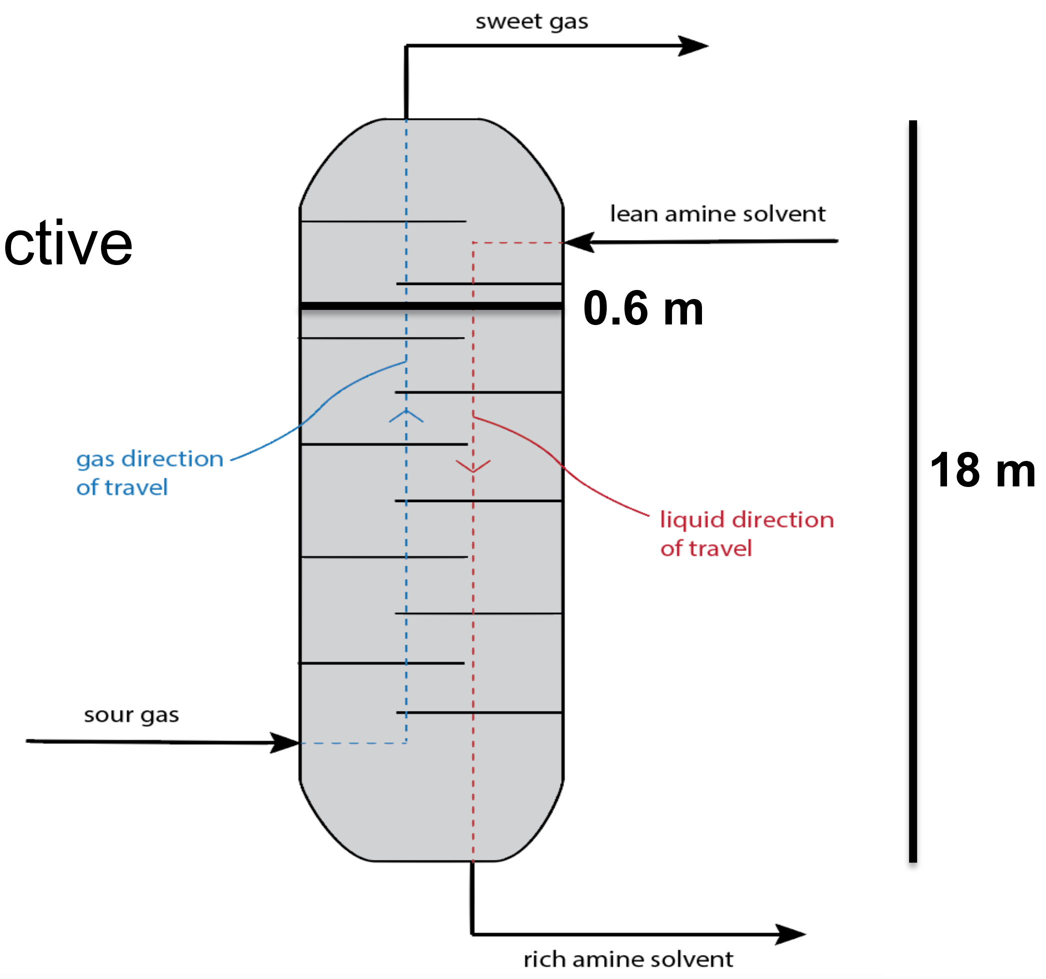


Unordered

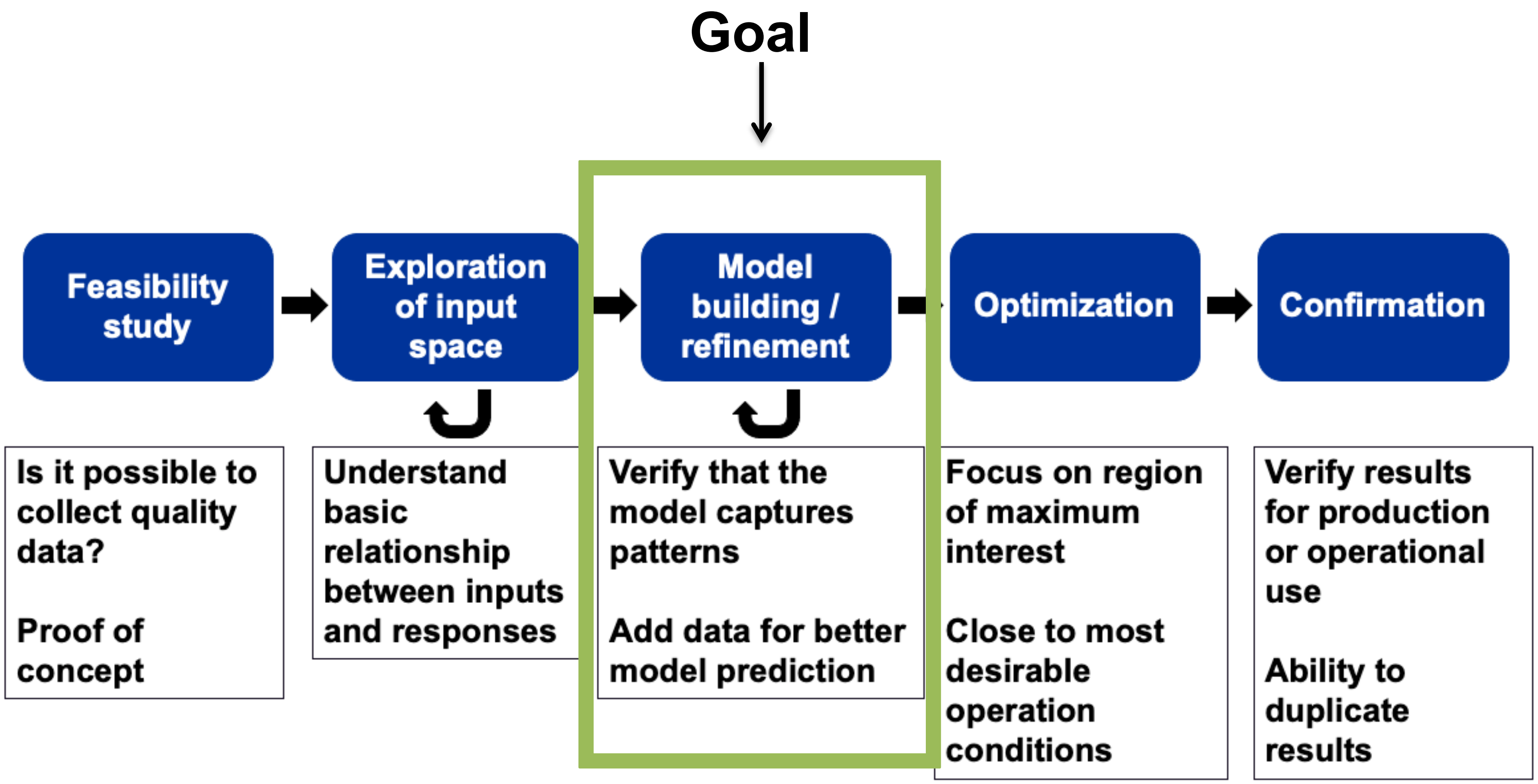
- **CCSI²: SDoE Toolset; Experts to talk to and work with**

SDoE/UQ Illustration: MEA Absorption Column Model

- Primary components:
  - Thermodynamic model
  - Mass transfer
- Model is evaluation model but provides effective demonstration
- 5 Inputs:
  - Liquid flowrate
  - Gas flowrate
  - Lean loading
  - MEA weight fraction
  - CO2 mole fraction in the vapor
- Output: Percent CO2 captured



Reduce Uncertainty in MEA Absorption Column Model

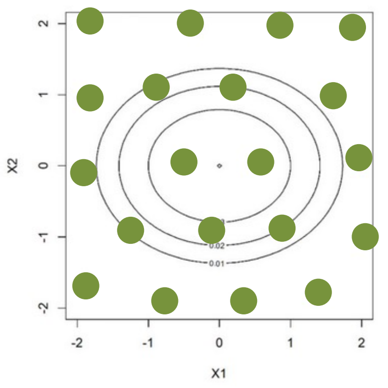


Use UQ + SDoE to Reduce Uncertainty (and associated risk)

Number of experimental runs allocated: 30

Approach: SDoE with 3 phases

1. **Uniform Space-Filling Design: 10 runs**
   Initial exploration/verification
   – Calibrate model and obtain updated **estimates of predicted uncertainty (via UQ)**



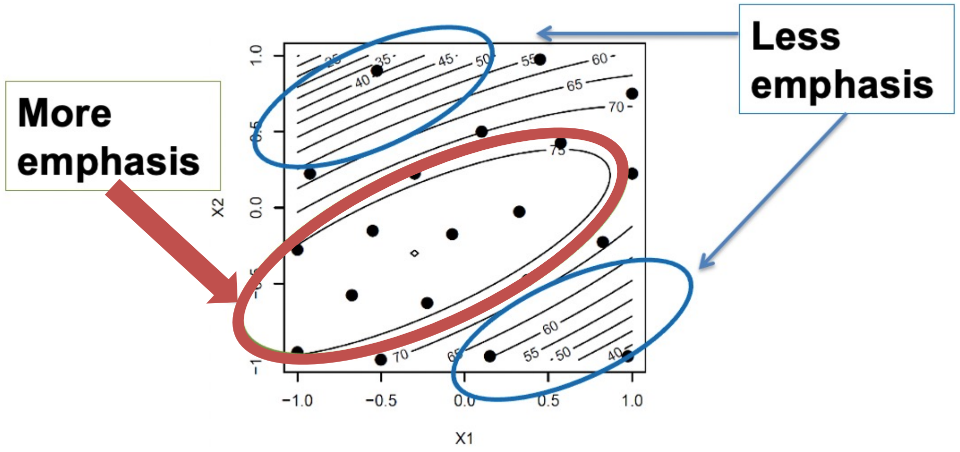
*Using simulated data for this illustration

Use UQ + SDoE to Reduce Uncertainty (and associated risk)

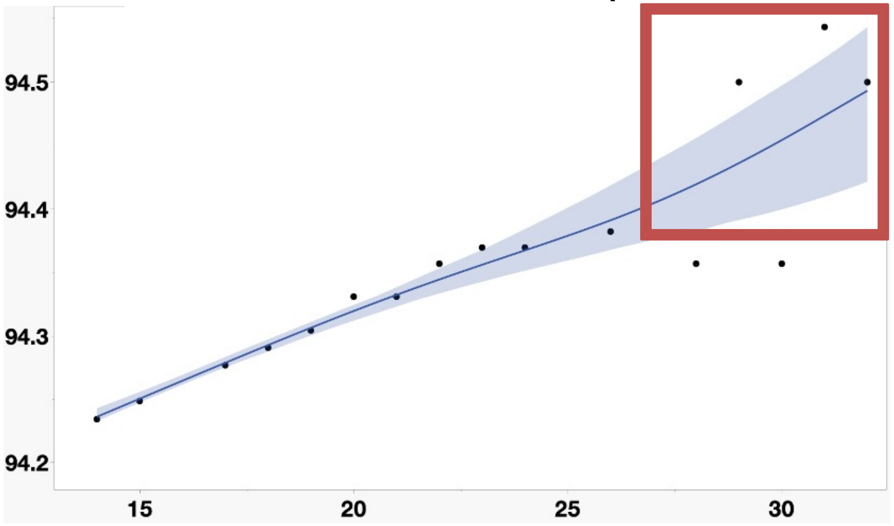
Number of experimental runs allocated: 30

Approach: SDoE with 3 phases

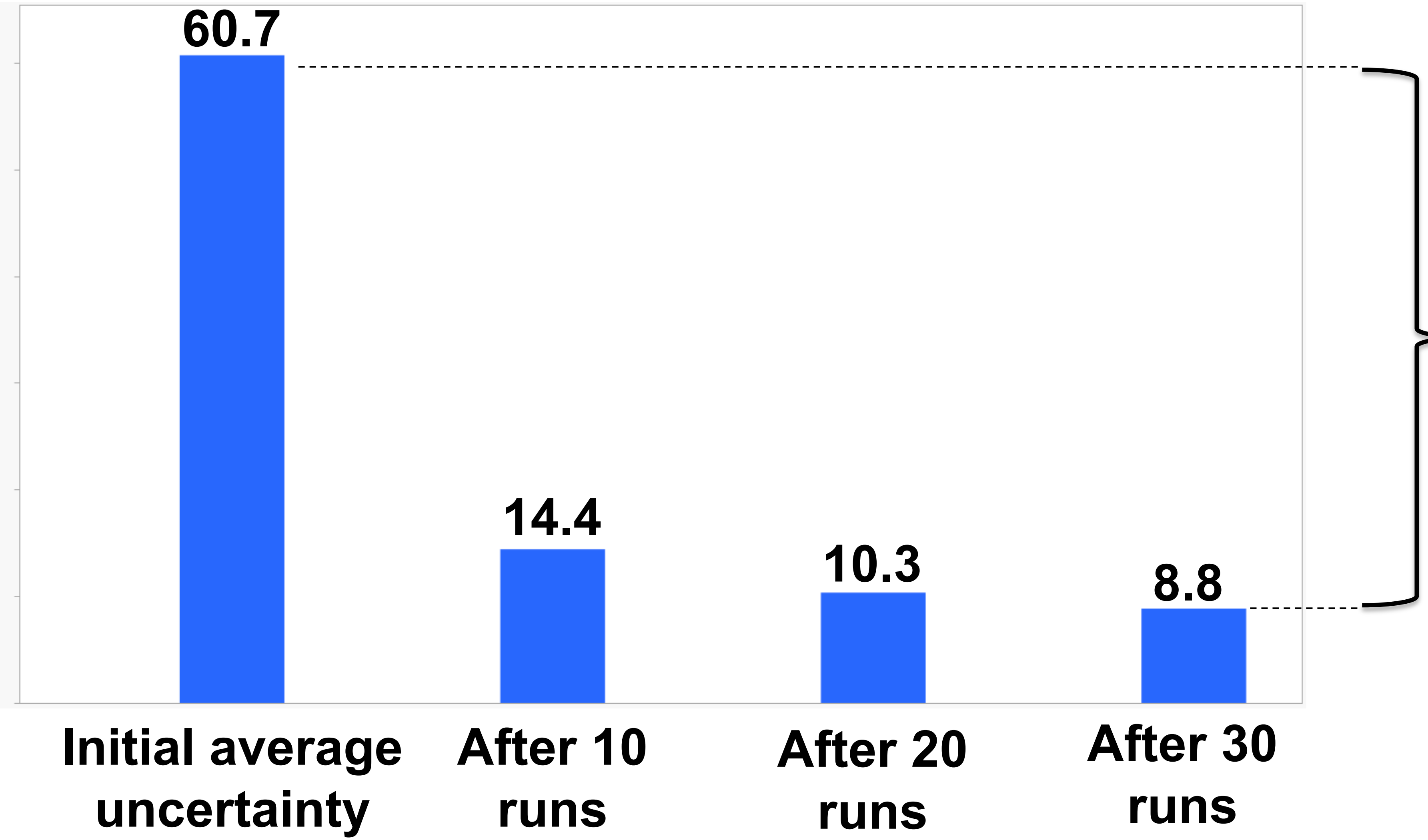
2. **Non-Uniform Space-Filling Design: 10 runs**
   Target areas of higher uncertainty
   – Calibrate and obtain new predicted uncertainty
3. **Non-Uniform Space-Filling Design: 10 runs**
   Target refined areas of uncertainty



Parallel with 2D example

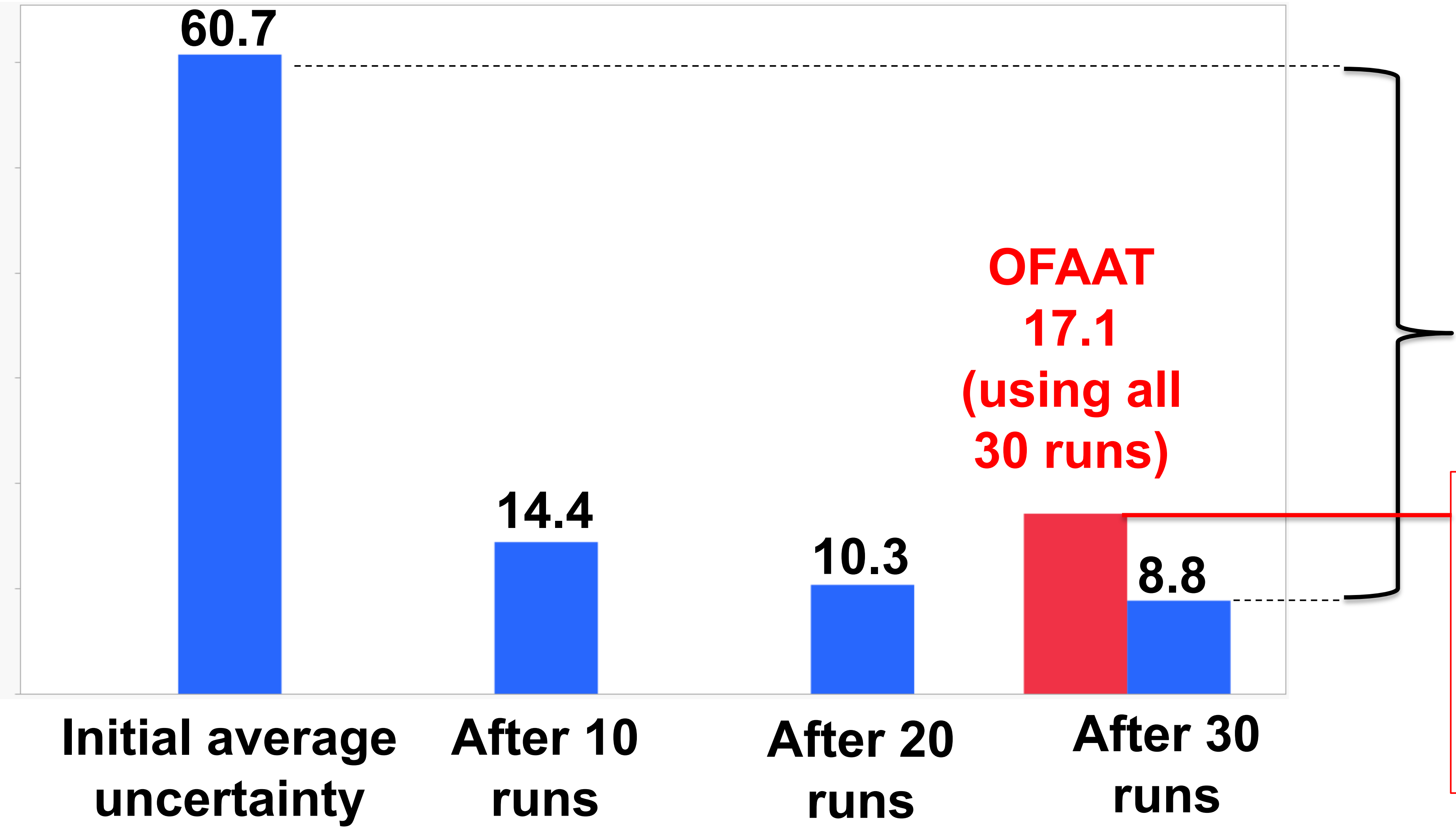


UQ + SDoE Notably Reduces Uncertainty in MEA Absorption Column Model



85.4% decrease in average uncertainty using UQ + SDoE

UQ + SDoE Reduces Uncertainty; Reduces Risk

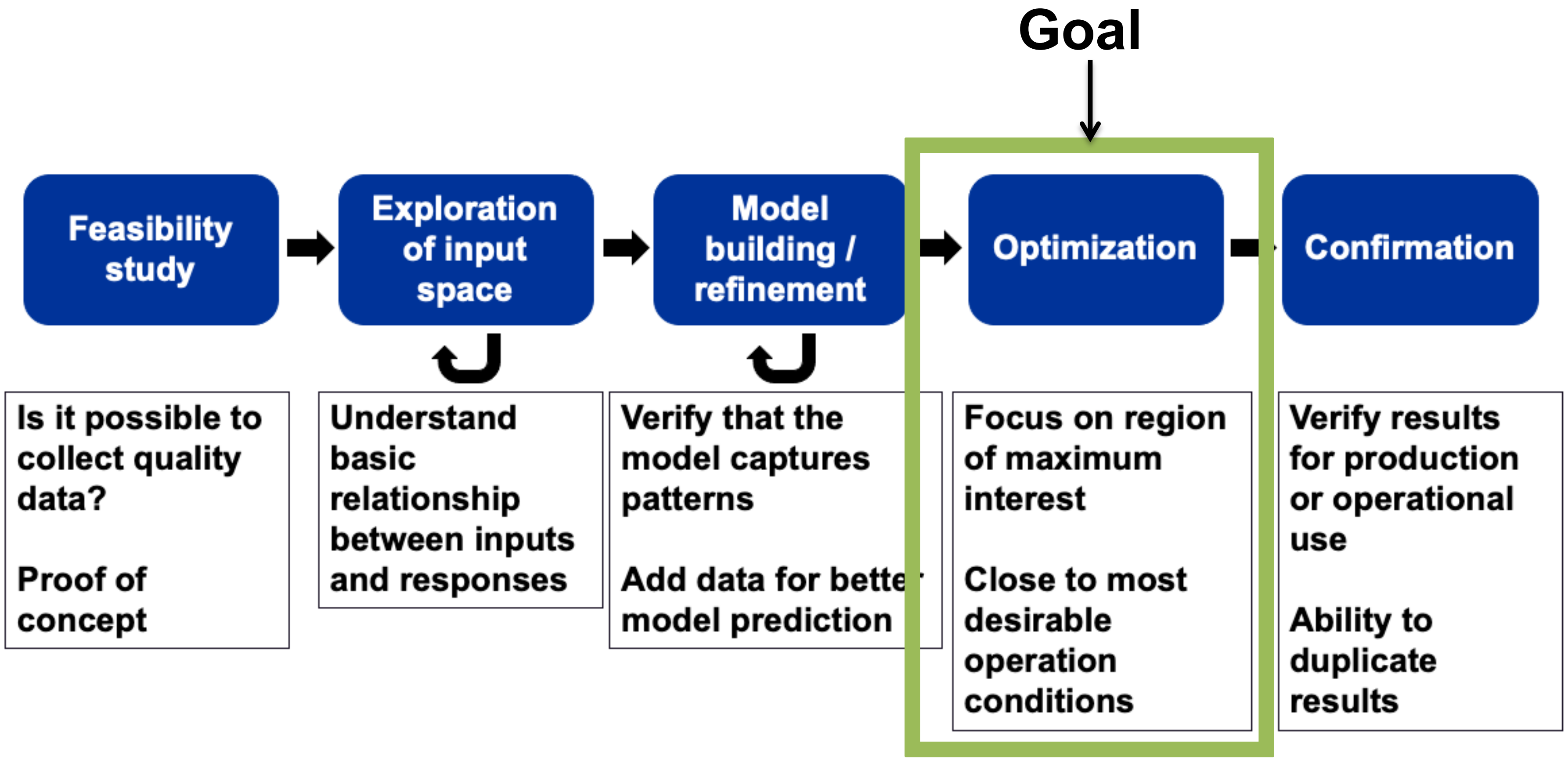


85.4% decrease in average uncertainty using UQ + SDoE

Almost twice as much uncertainty as using the UQ + SDoE method

CCSI[2]
Carbon Capture Simulation for Industry Impact

Find Desirable Settings for MEA Absorption Column Model

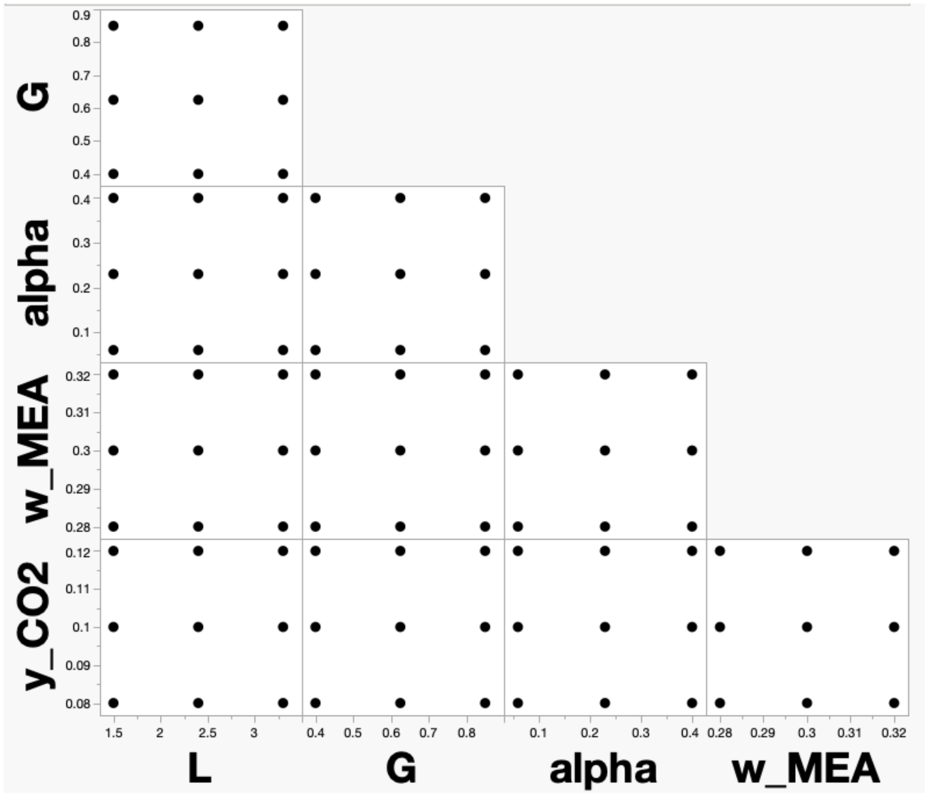


What input settings lead to maximum percent CO_2 capture?

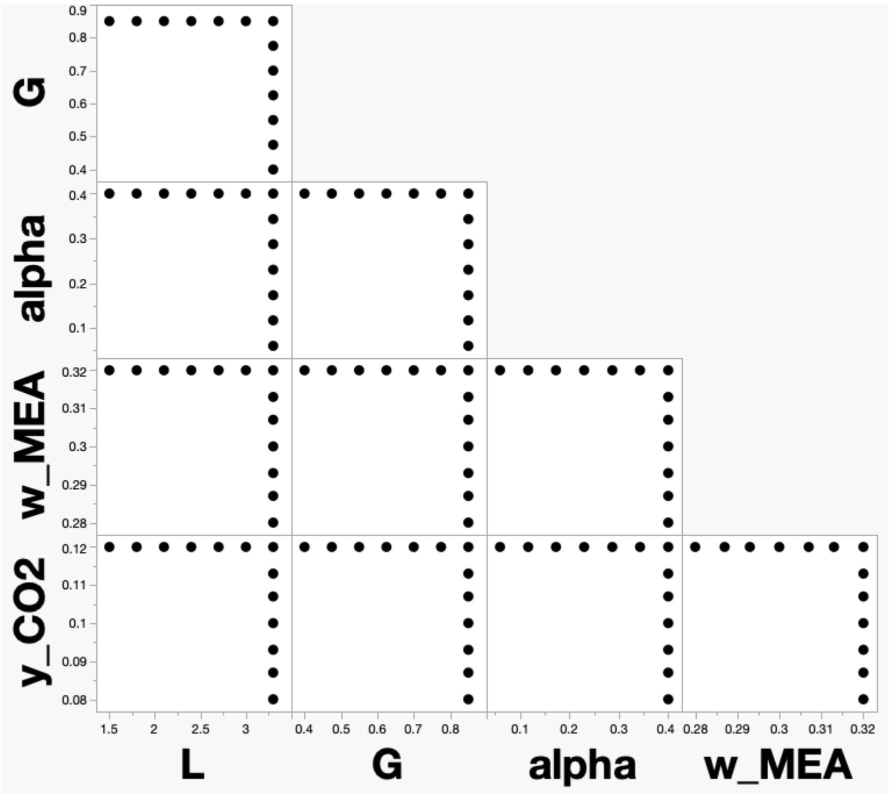
Demonstrate using empirical model-based designs (low-order polynomial approximation)

Compare to OFAAT

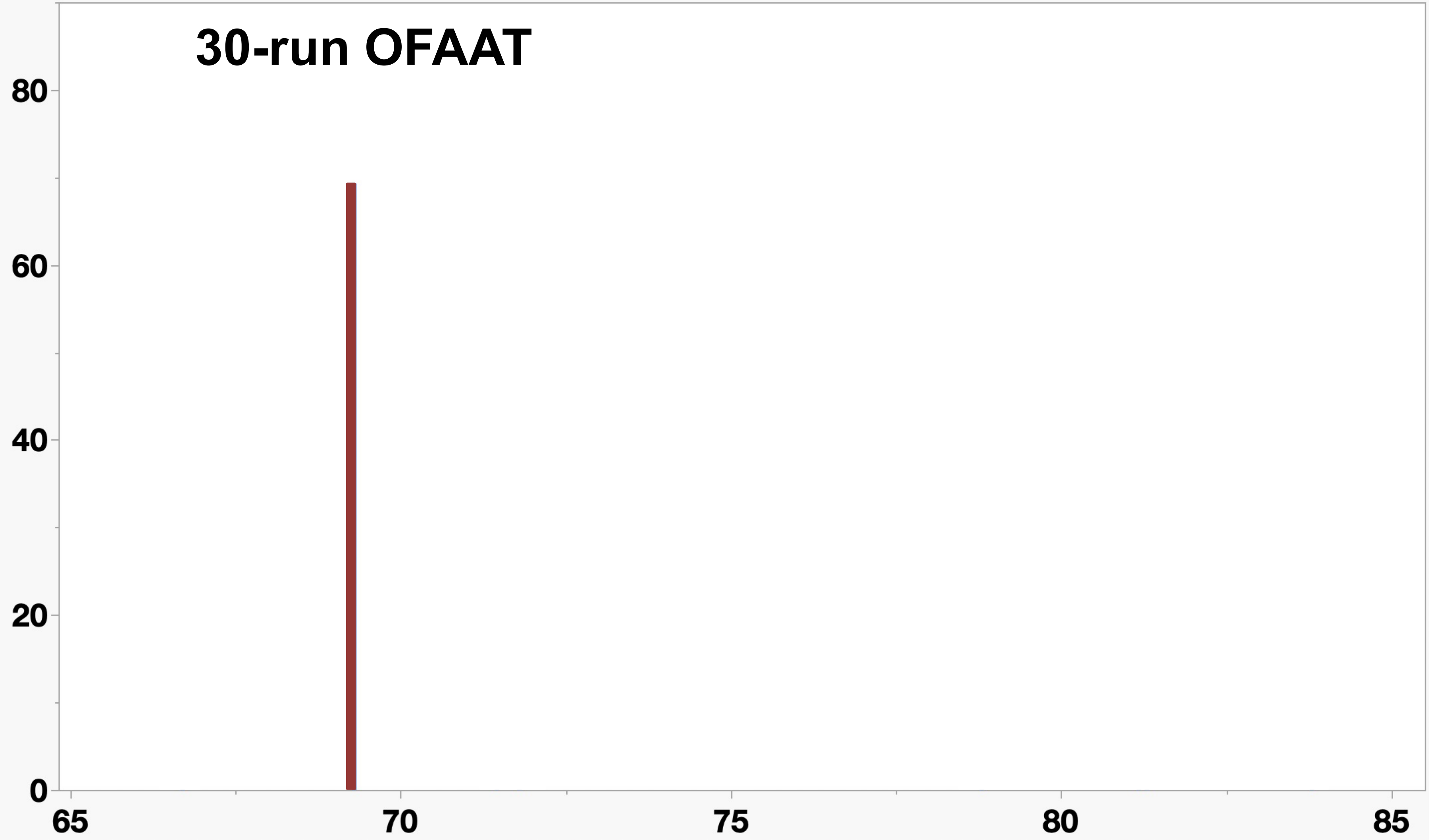
17-run empirical model-based DoE



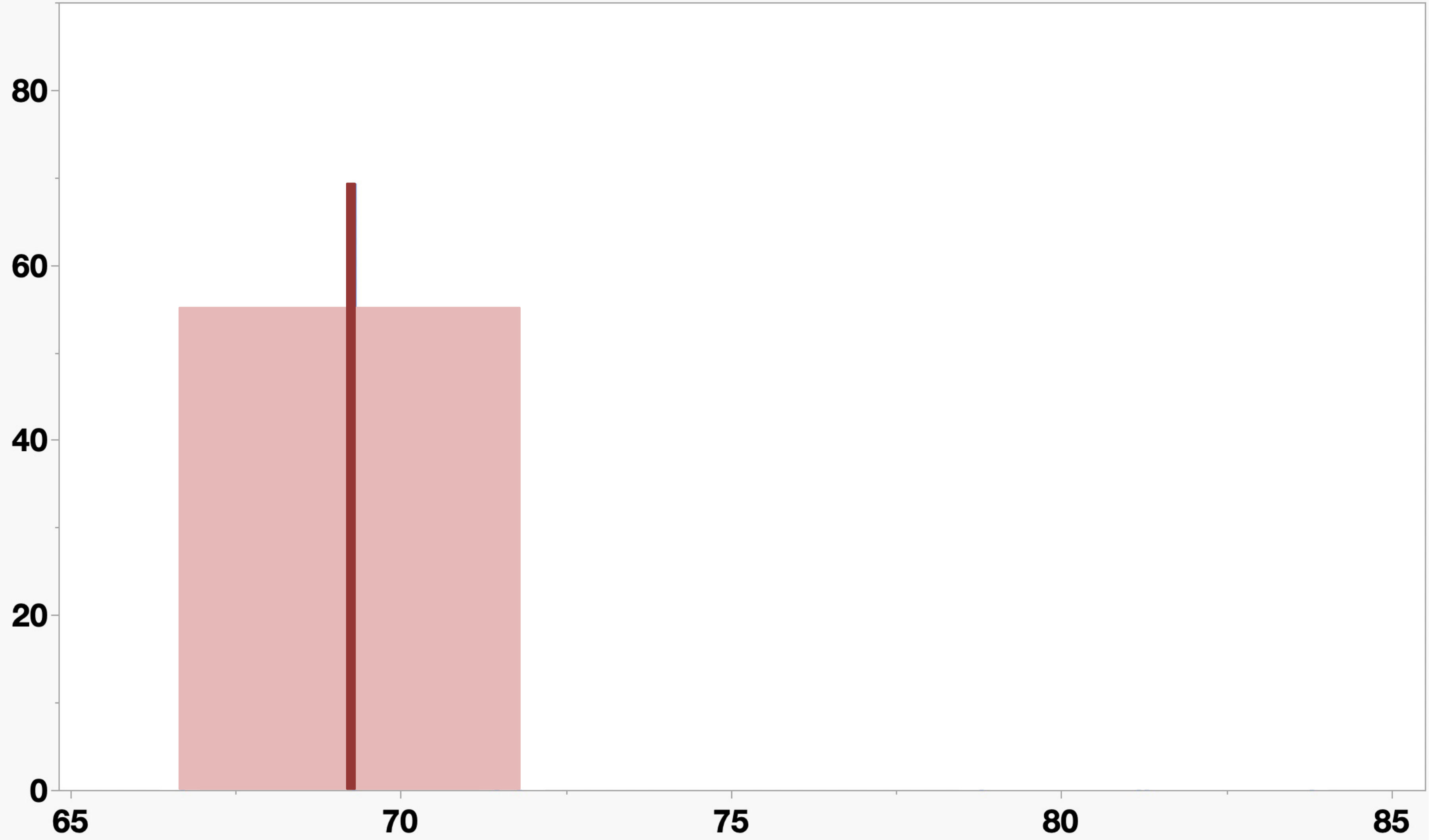
30-run OFAAT



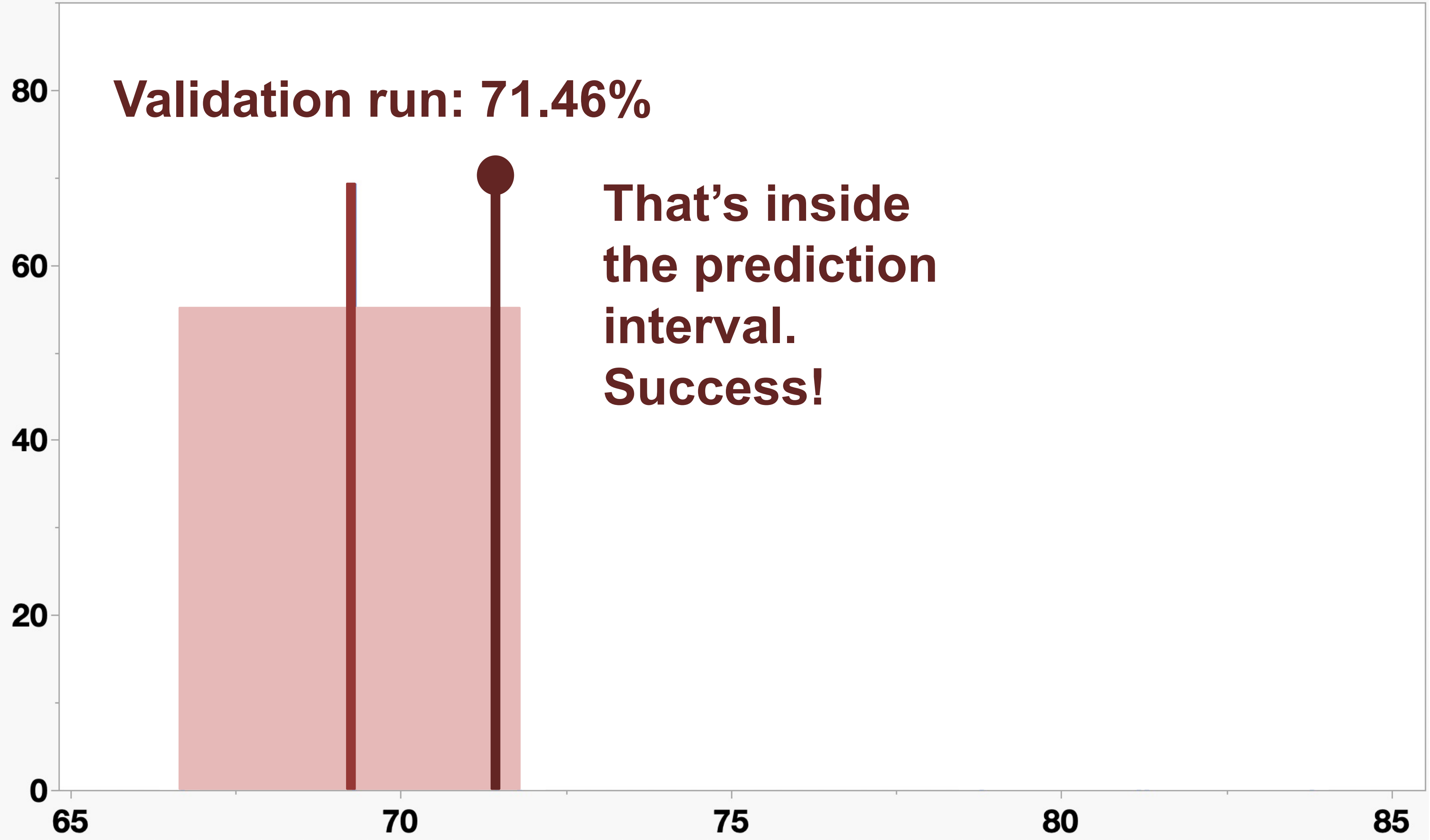
30-run OFAAT: Model predicts best settings will lead to 69.3% CO2 capture



30-run OFAAT: Model predicts best settings will lead to 69.3% CO2 capture with prediction interval (66.7, 71.8)

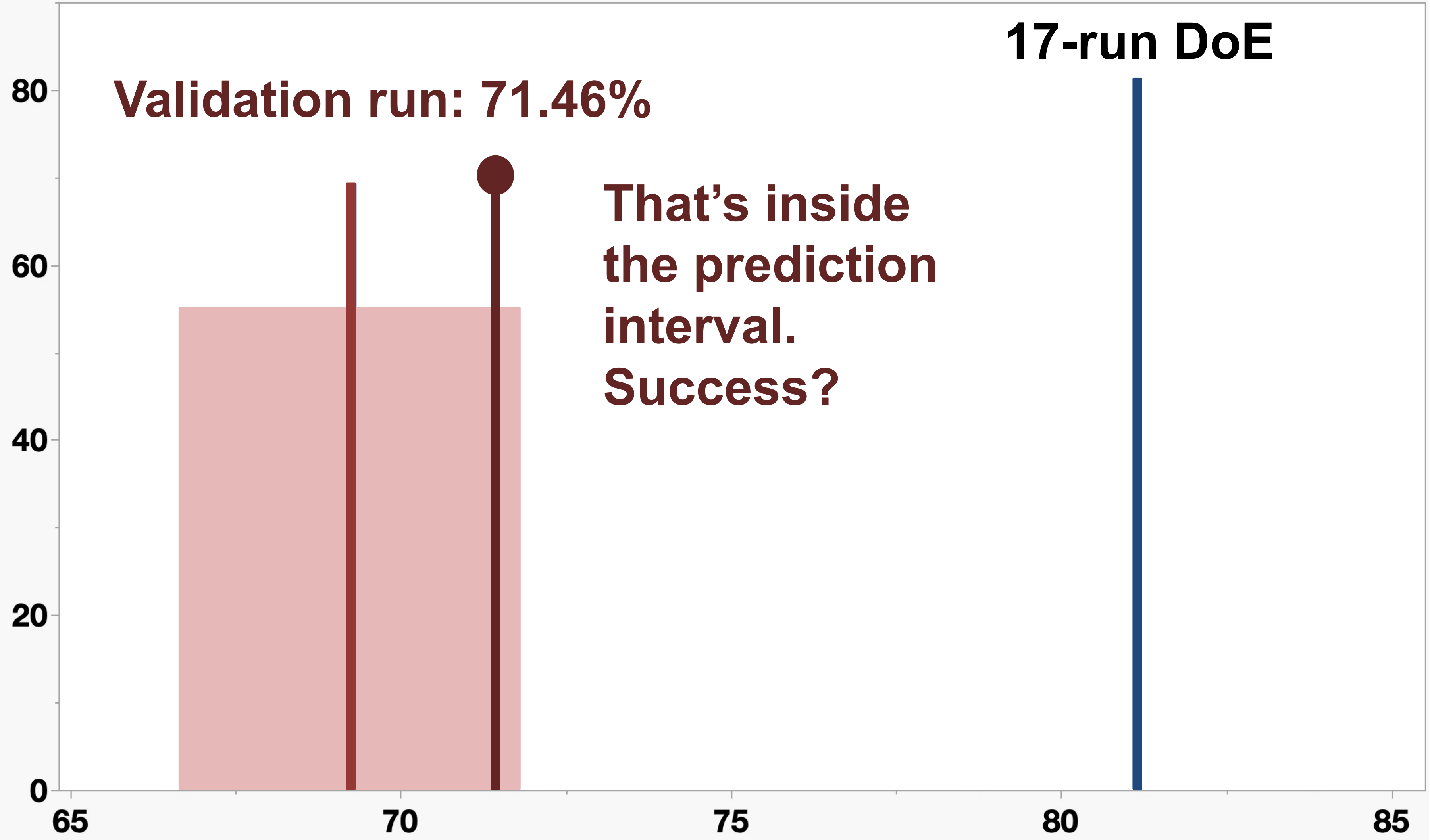


30-run OFAAT: Model predicts best settings will lead to 69.3% CO2 capture with prediction interval (66.7, 71.8)

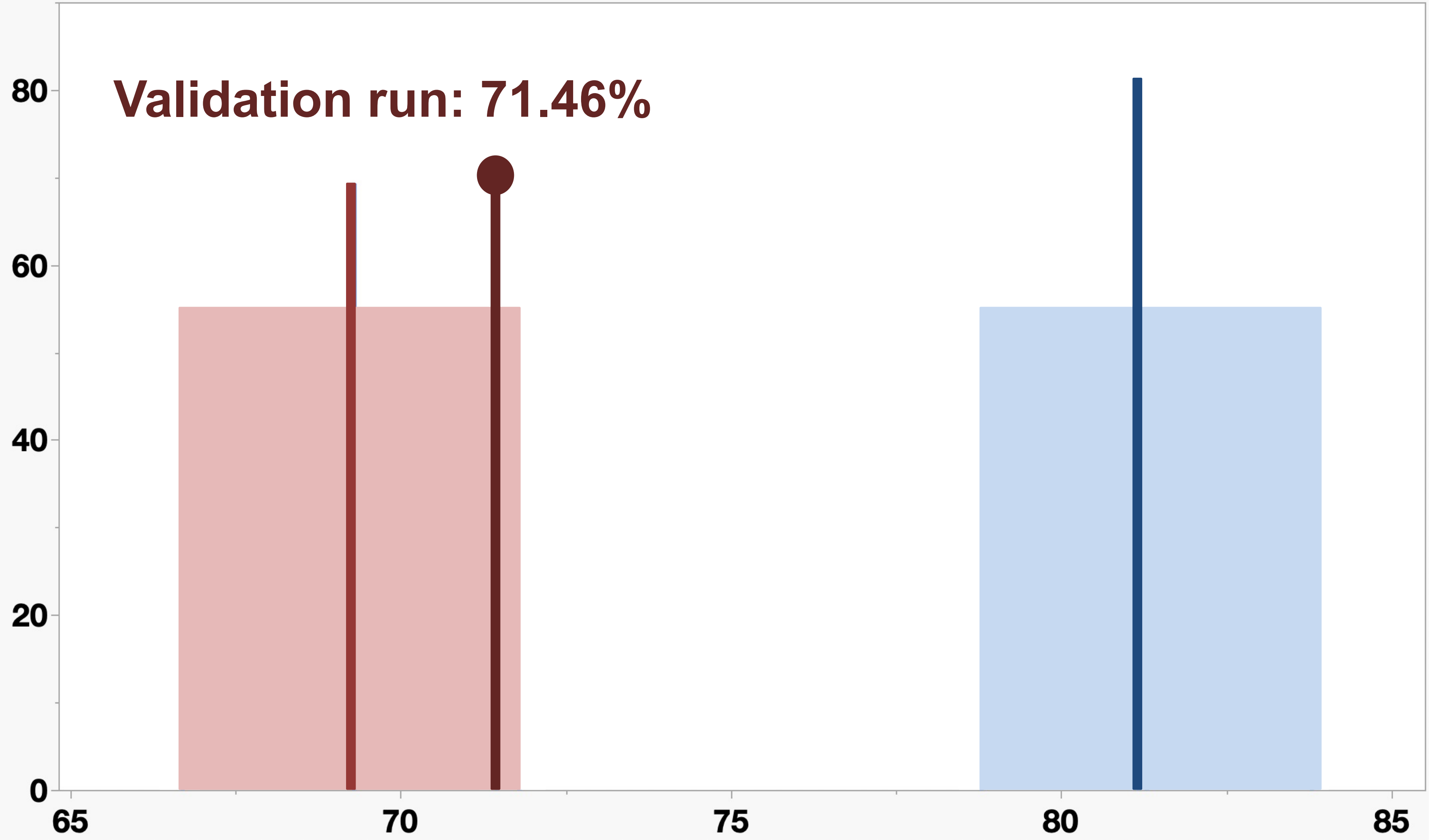


CCSI2
Carbon Capture Simulation for Industry Impact

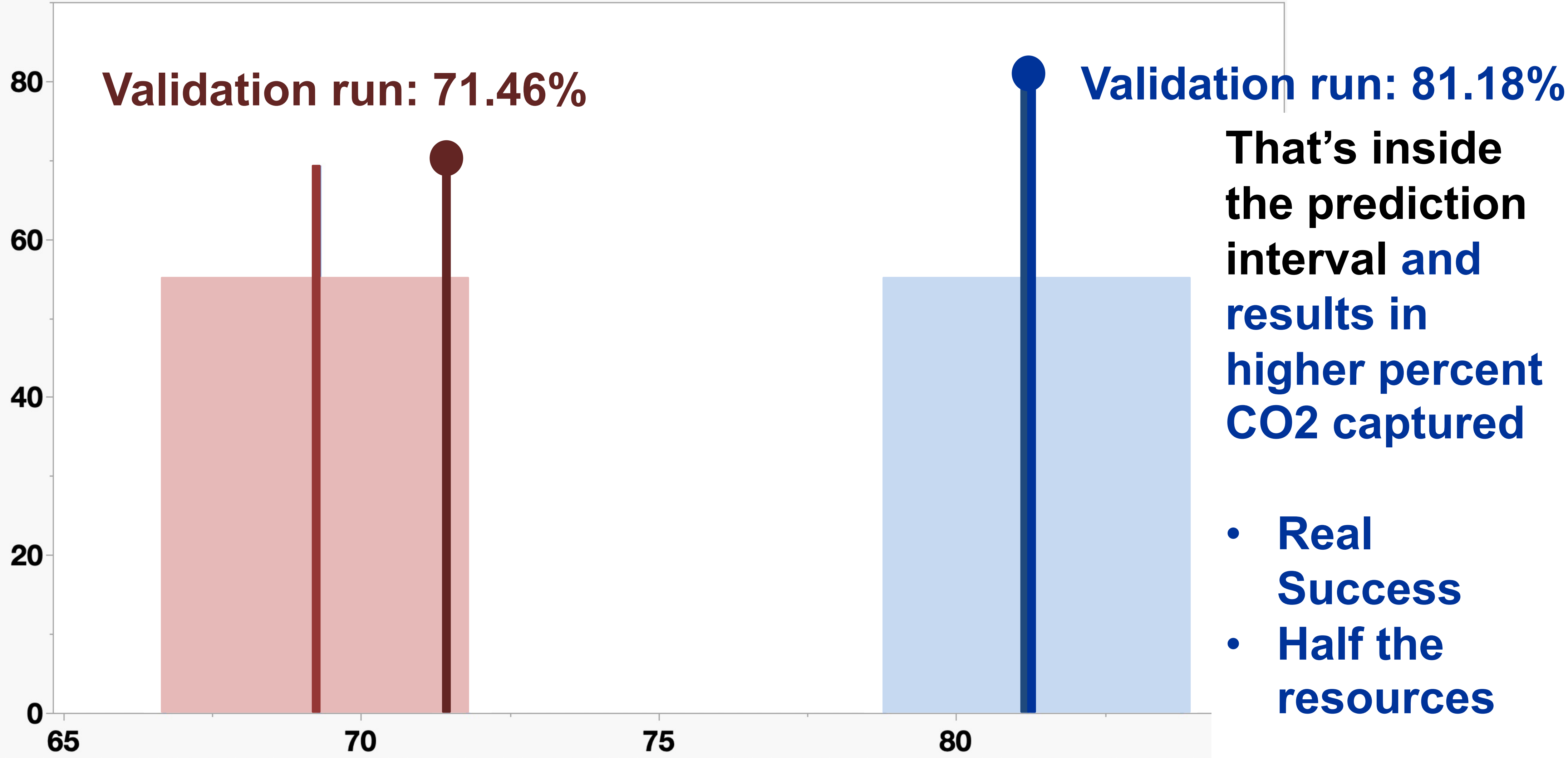
17-run empirical model-based DoE: Model predicts best settings will lead to 81.3% CO_2 capture



17-run empirical model-based DoE: Model predicts best settings will lead to 81.3% CO2 capture with prediction interval (78.8, 83.8)



17-run empirical model-based DoE: Model predicts best settings will lead to 81.3% CO2 capture with prediction interval (78.8, 83.8)

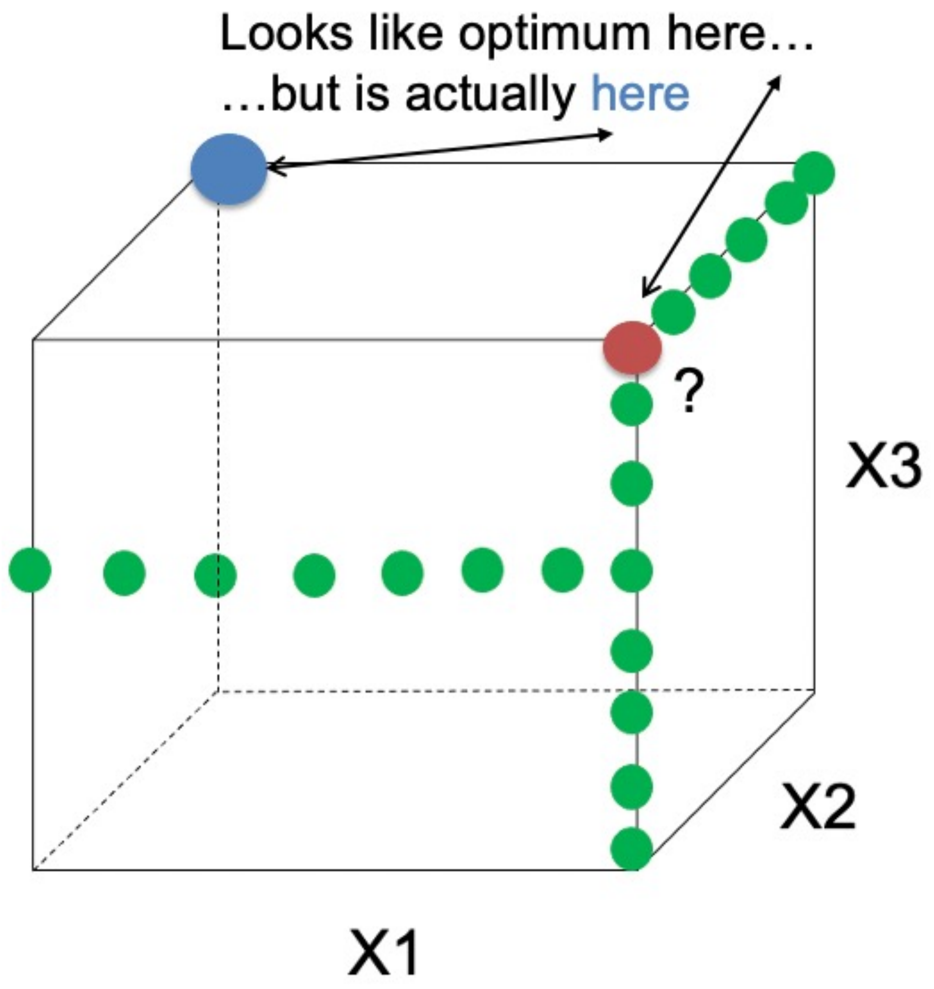


That's inside the prediction interval and results in higher percent CO2 captured

- Real Success
- Half the resources

What happened with OFAAT?

- **There was an interaction effect!**
  - Liquid flowrate-lean loading interaction
  - OFAAT cannot detect
- **Result: OFAAT suggested incorrect setting for liquid flowrate, leading to low %CO2 capture**
  - OFAAT: L = 2.73
  - DoE (correct): L = 1.5
- **DoE: identify true range of optimum and best settings**



DoE reduces risk of incomplete answers, uses fewer resources, gets better results

Next – Science-Based Design of Experiments

Feasibility study → **Exploration of input space** → **Model building / refinement** → **Optimization** → **Confirmation**

Feasibility study
Is it possible to collect quality data?

Proof of concept

Exploration of input space
Understand basic relationship between inputs and responses

Model building / refinement
Verify that the model captures patterns

Add data for better model parameter estimation or prediction

Optimization
Focus on region of maximum interest

Close to most desirable operation conditions

Confirmation
Verify results for production or operational use

Ability to duplicate results

Extends ideas from DoE to science-based models

Wrap-Up

- **Data collection method matters**
  - Use statistical DoE
  - Strategic data collection to meet experimental objectives
- **Use UQ to understand uncertainty**
  - All models contain some uncertainty
  - Can’t improve it without first knowing about it
- **SDoE leverages UQ for targeted data collection**
  - Directly incorporates knowledge of uncertainty to target, reduce
- **UQ + SDoE: Value-add**
  - Efficient use of resources
  - Increases efficacy
  - Reduces risk

CCSI²

Carbon Capture Simulation for Industry Impact

For more information

anachtsheim@lanl.gov

U.S. DEPARTMENT OF ENERGY | NATIONAL ENERGY TECHNOLOGY LABORATORY | BERKELEY LAB | Lawrence Livermore National Laboratory | Los Alamos NATIONAL LABORATORY | Pacific Northwest NATIONAL LABORATORY | OAK RIDGE National Laboratory | West Virginia University | UNIVERSITY OF NOTRE DAME | THE UNIVERSITY OF TEXAS AT AUSTIN | UT | UNIVERSITY OF PITTSBURGH | Carnegie Mellon