CCSI²
Carbon Capture Simulation for Industry Impact

Carbon Capture Simulation for Industry Impact (CCSI²)

Technical Risk Reduction: Sequential Design of Experiments and Uncertainty Quantification

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Today's Plan

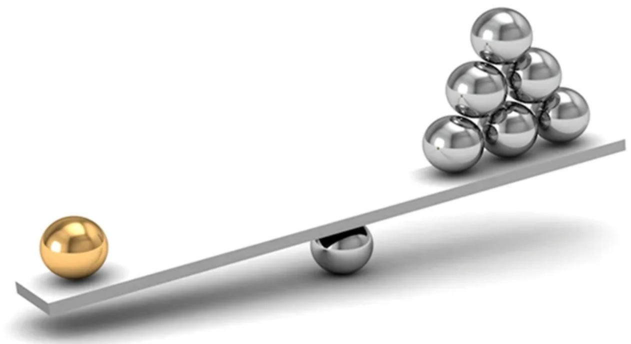
- Does the data collection approach matter? (Yes!)
- Uncertainty Quantification (UQ)
  - What, why, how?
- Sequential Design of Experiments (SDoE) and UQ
- UQ + SDoE Illustration

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

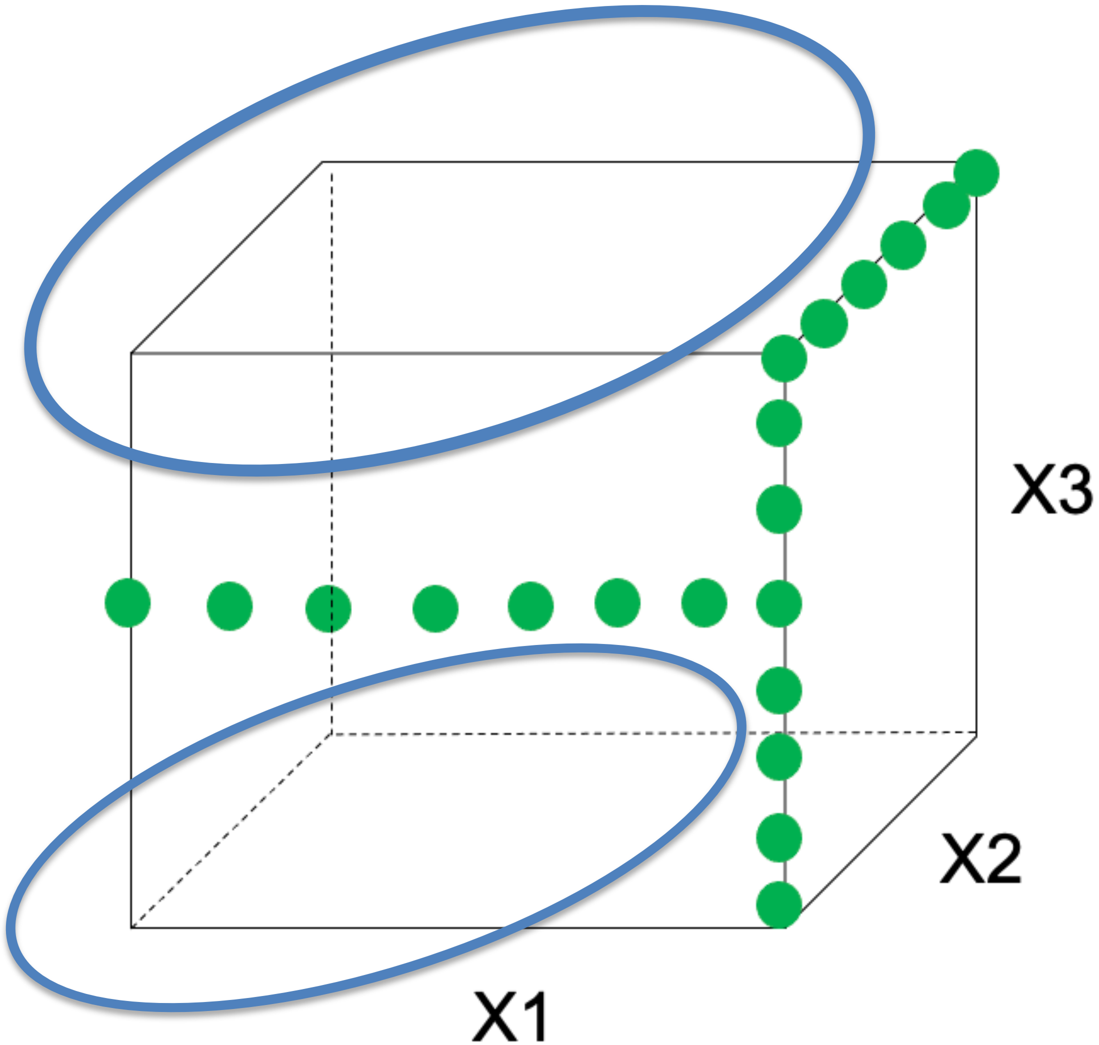
Why Use Design of Experiments?

- **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



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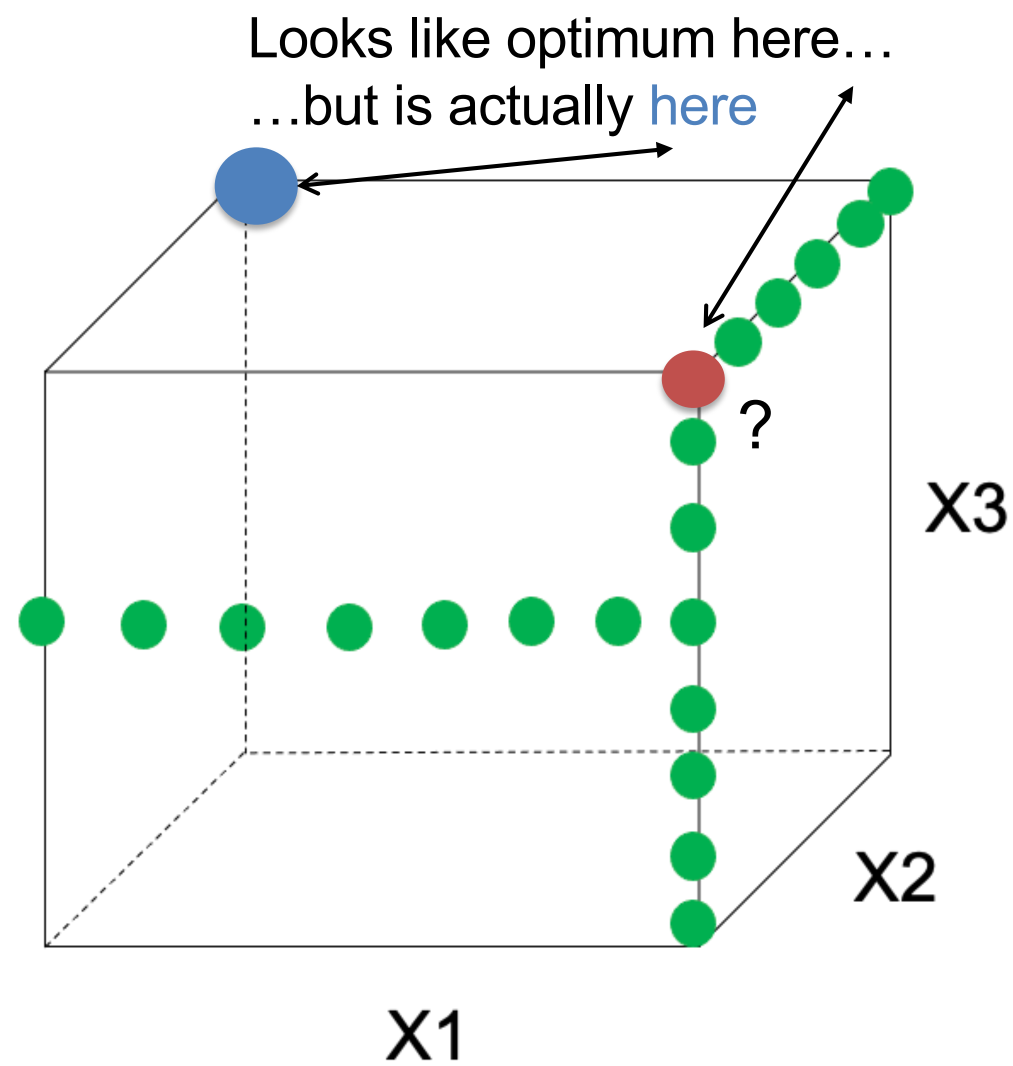
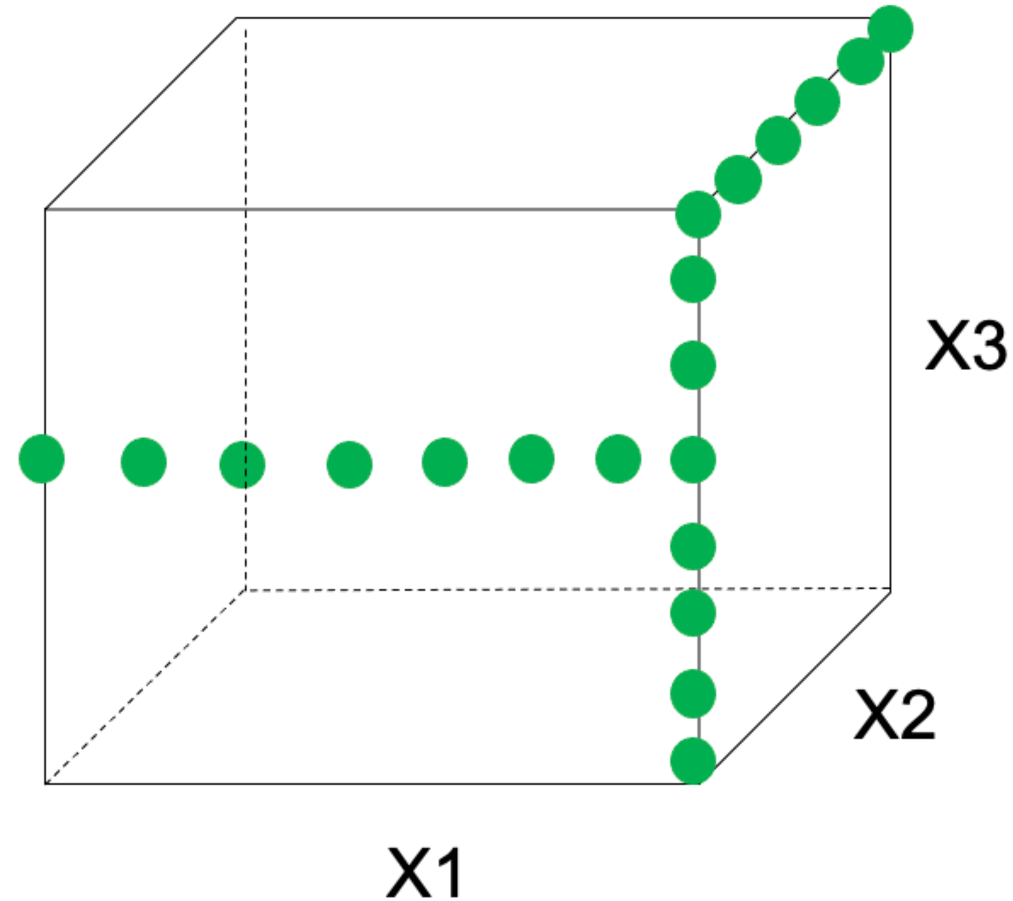
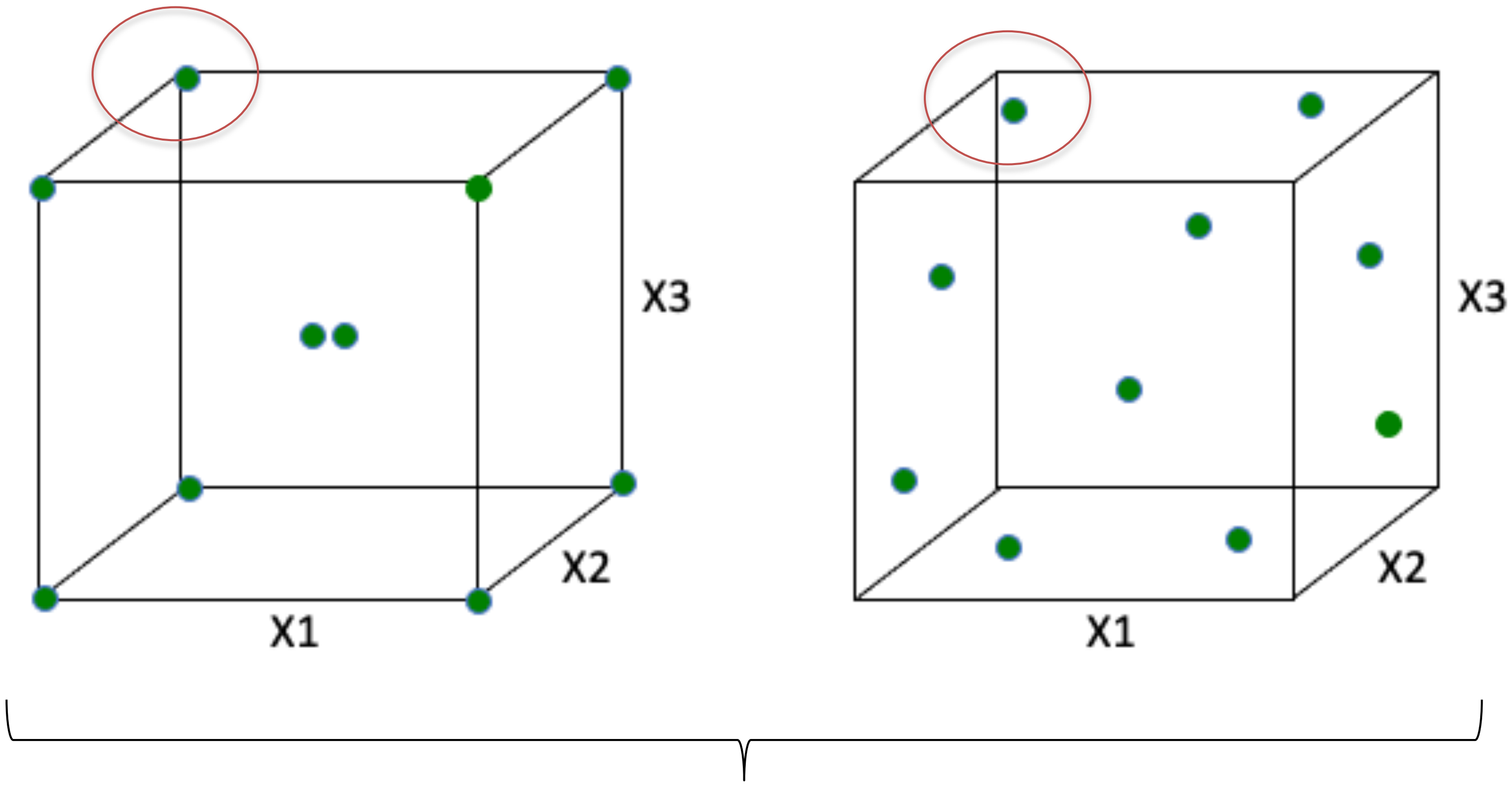


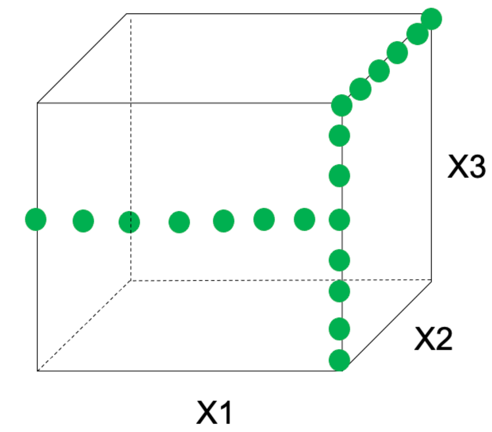
Design of Experiments not the same as One-Factor-at-a-Time

- **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
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Improvement

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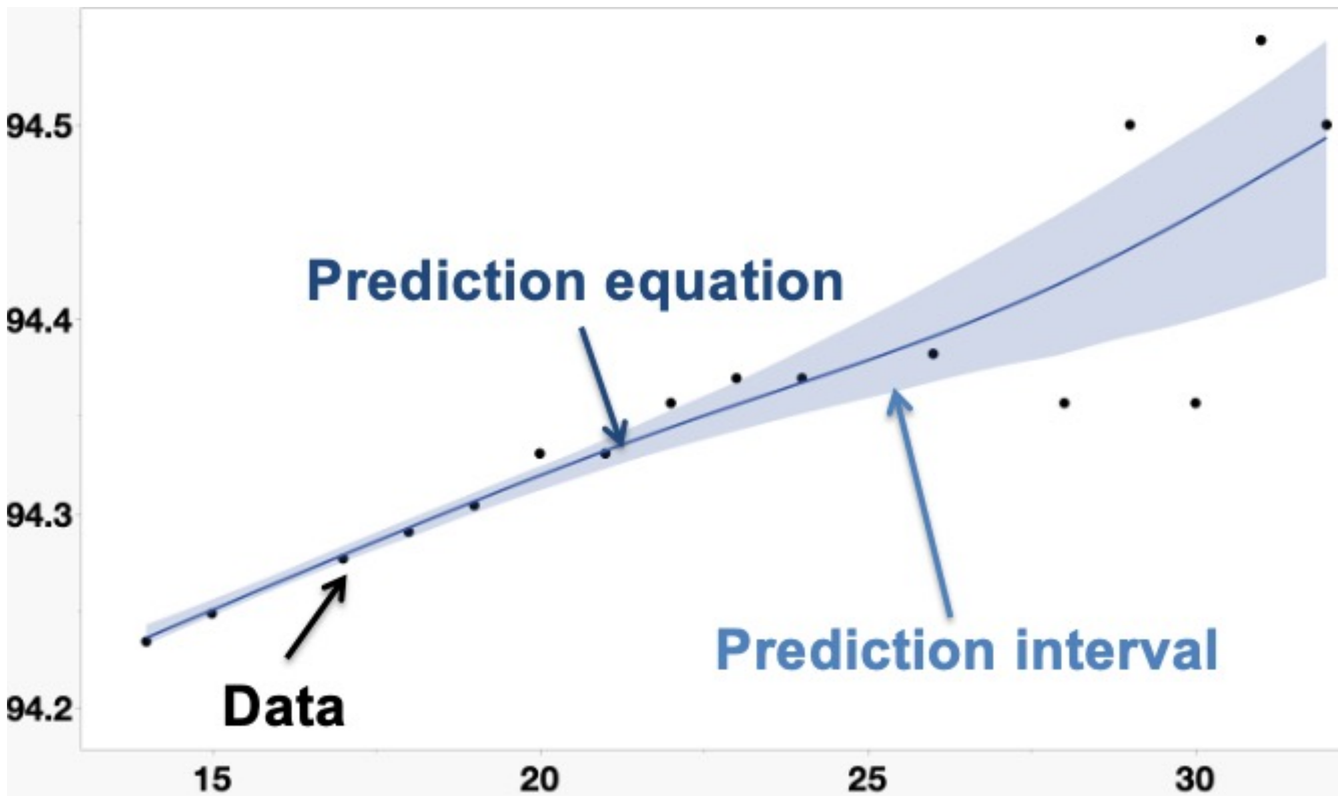
Strategic data collection + model estimation and refinement

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



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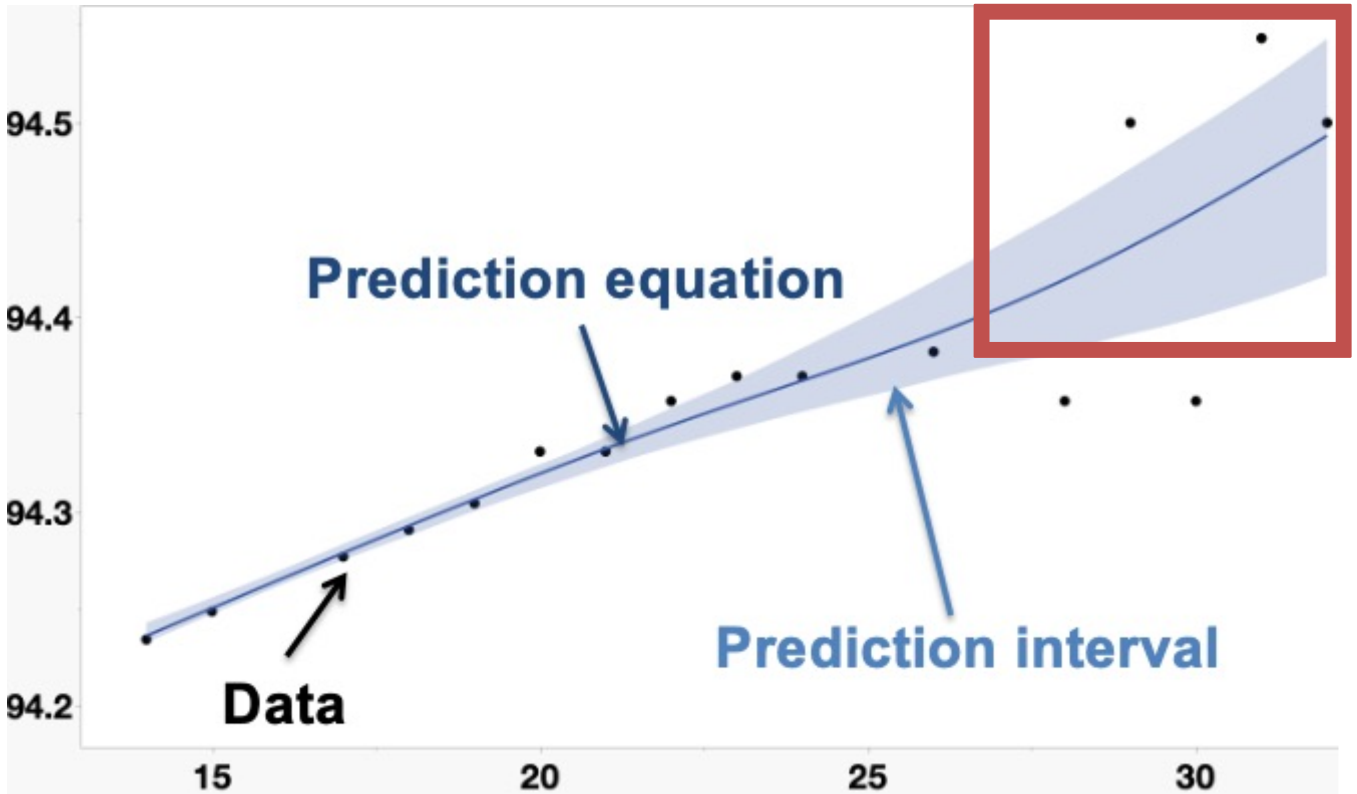

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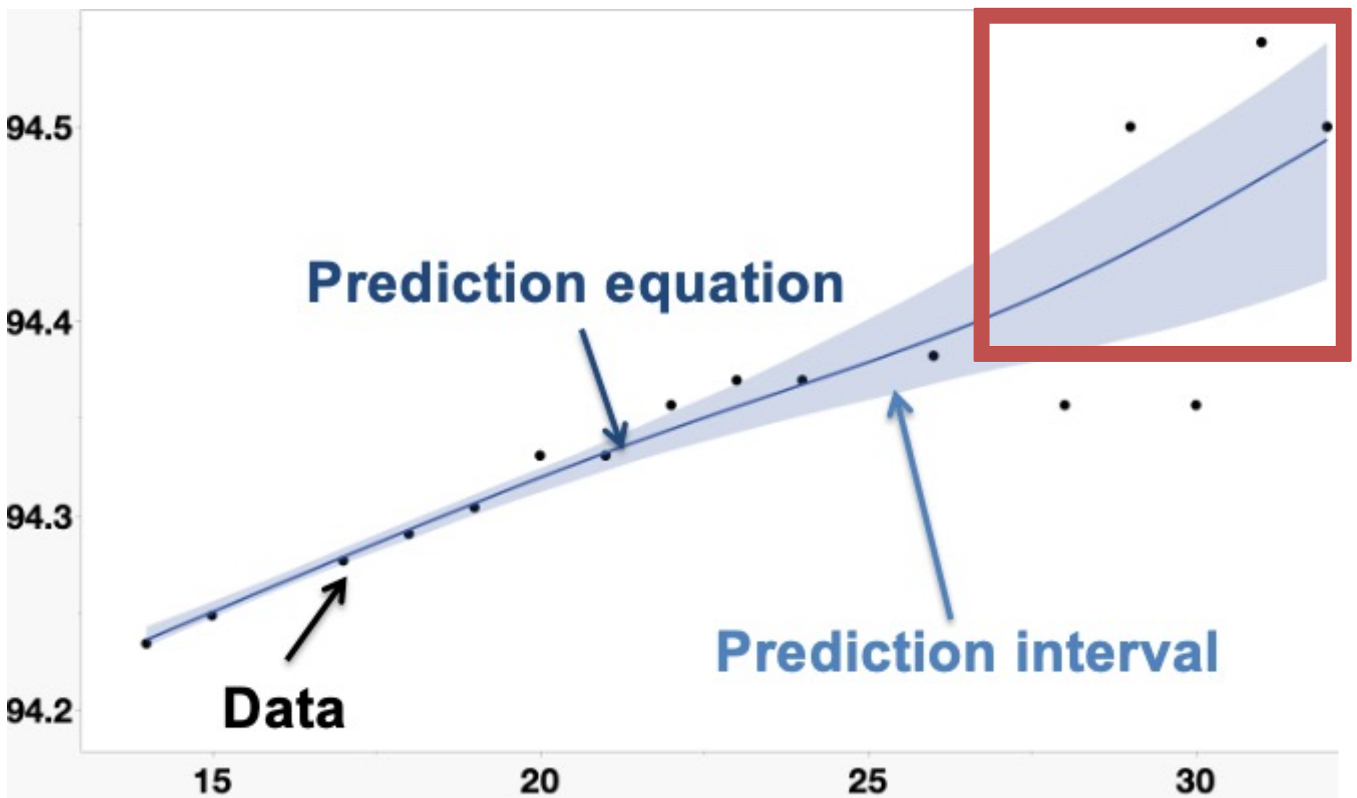


High uncertainty

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

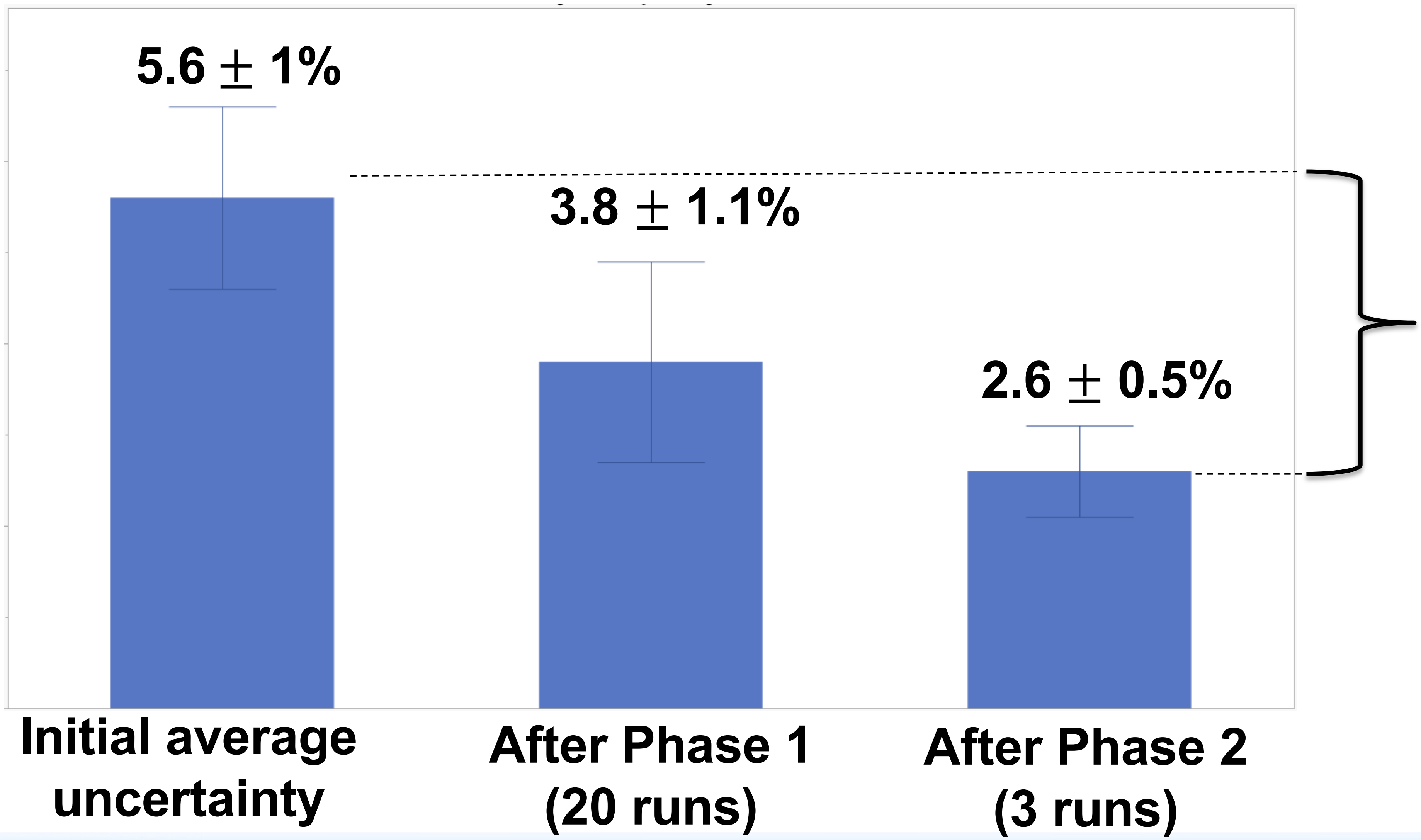
UQ + SDoE to reduce uncertainty

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

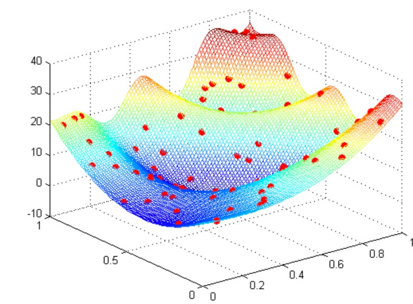


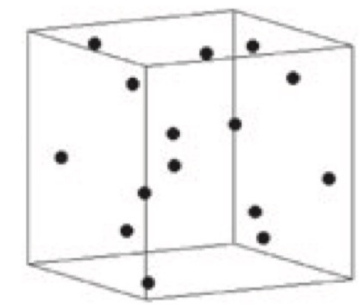
53.6% decrease in average prediction uncertainty using UQ + SDoE

CCSI^2 SDoE Capabilities

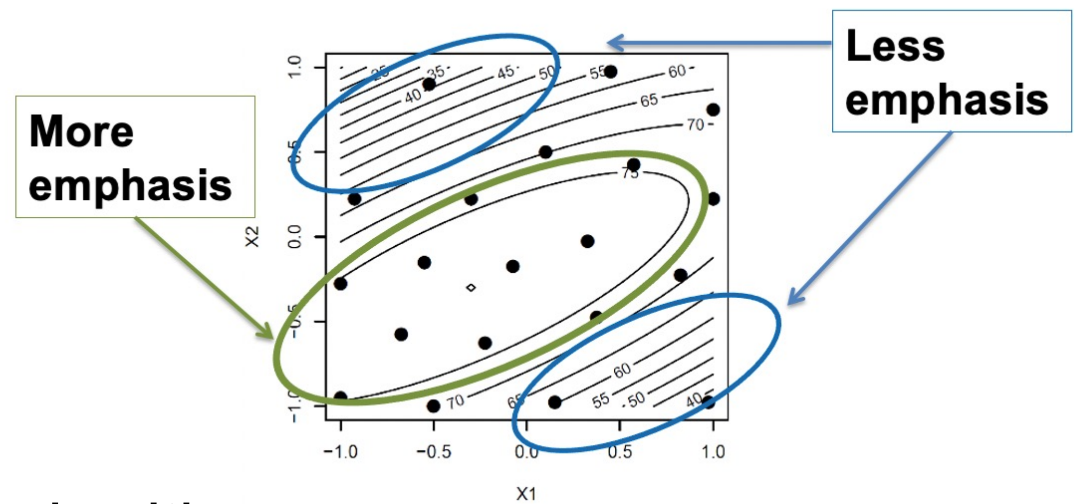
Space-Filling Designs

Relationship between inputs and response(s) of interest not well understood





- Uniform Space-Filling Designs
  - Design points evenly spread throughout space of interest
  - Exploration
- Non-Uniform Space-Filling Designs
  - Emphasize some regions more than others
  - Uncertainty reduction
- Input-Response Space-Filling Designs
  - Coverage of likely output values



CCSI^2: SDoE Toolset; Experts to talk to and work with

Developed to meet needs of CCSI^2 applications

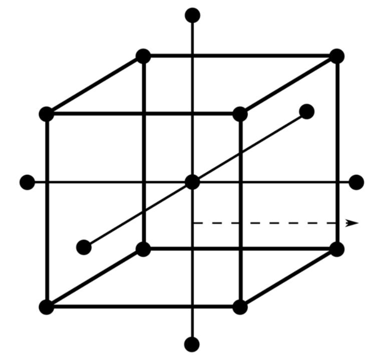
CCSI^2 SDoE Capabilities

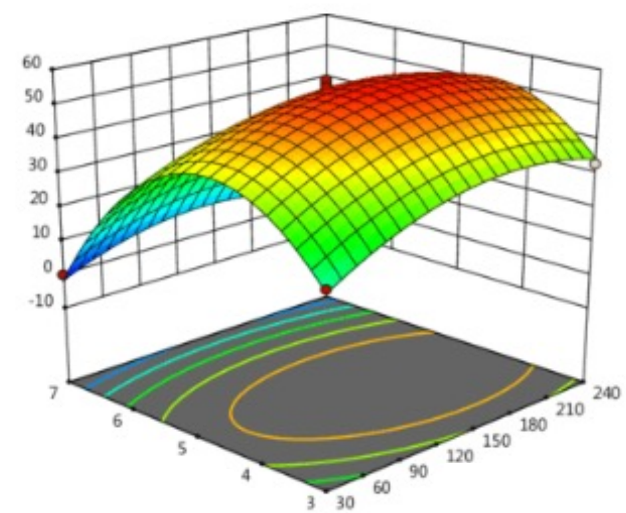
Empirical Model-Based Designs

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

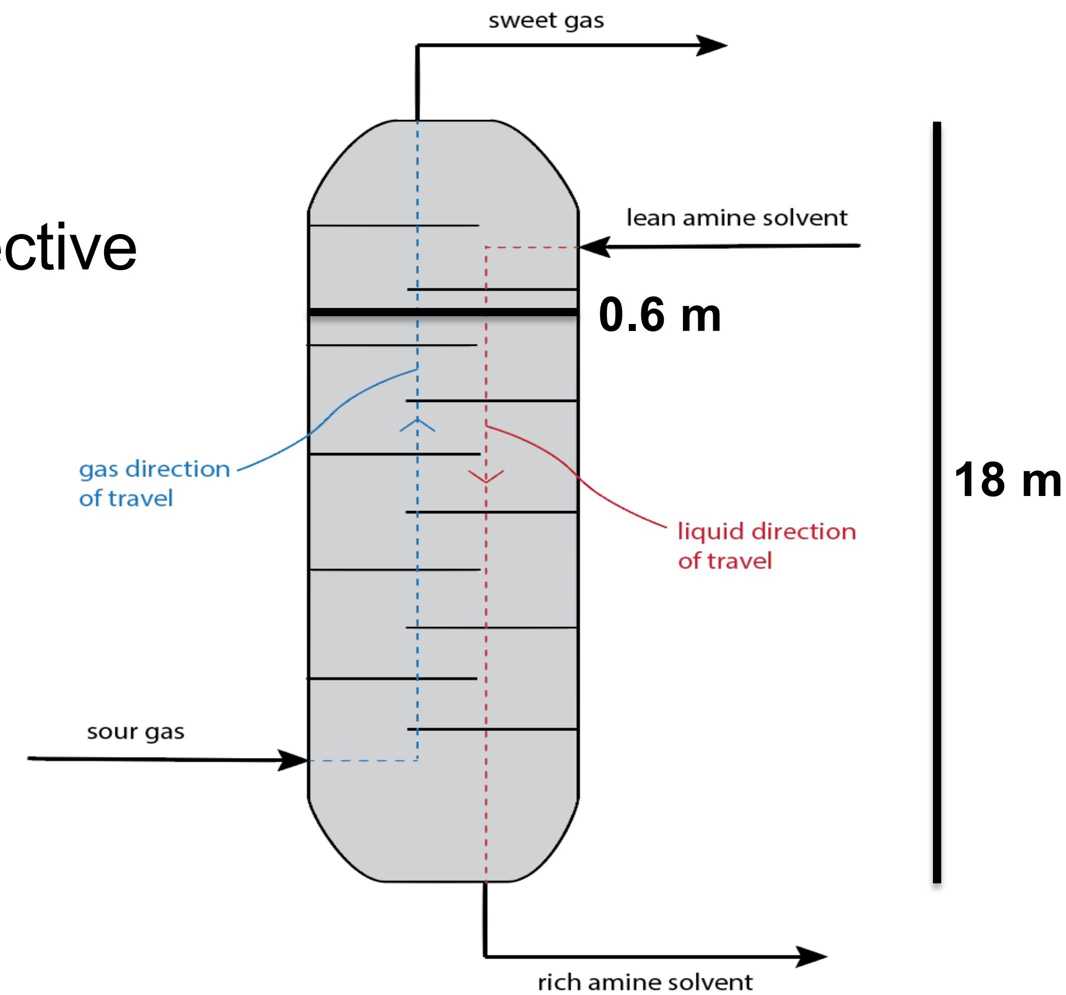
CCSI^2: SDoE Toolset; Experts to talk to and work with



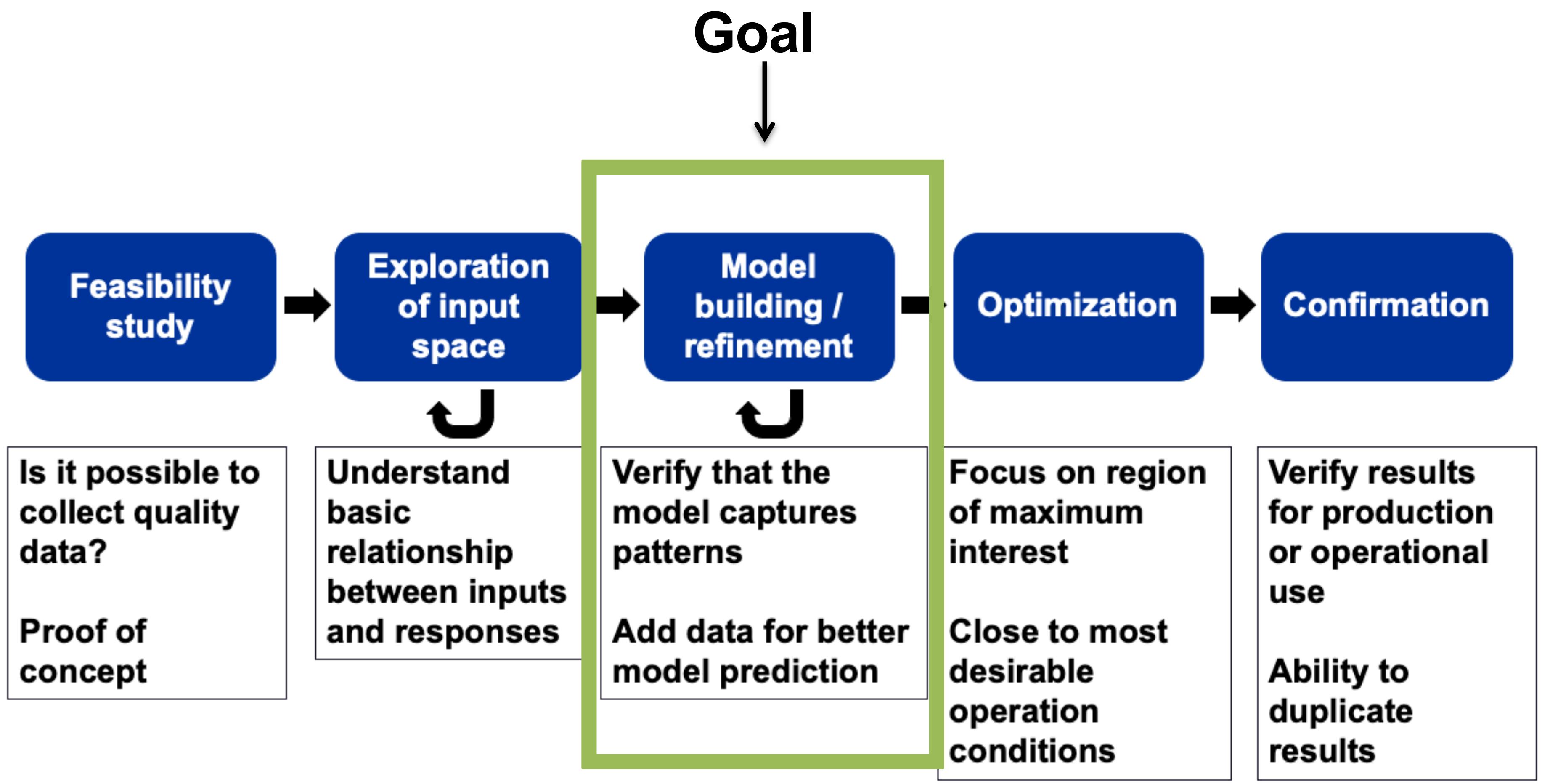


SDoE/UQ Illustration: MEA Absorption Column Model

- 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

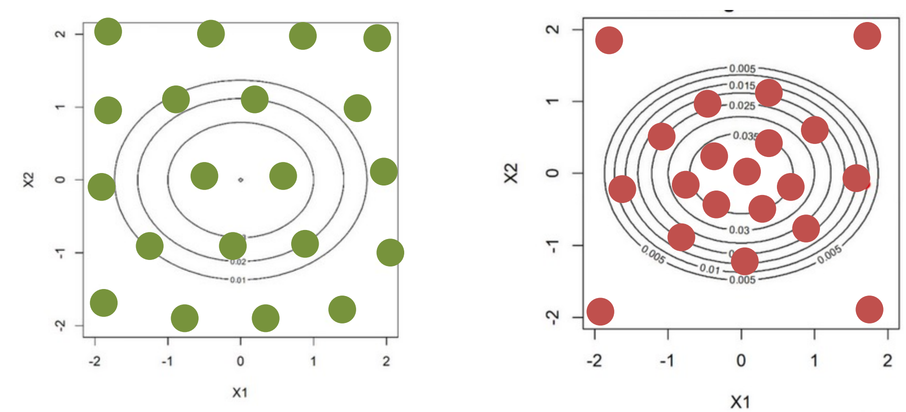


Use UQ + SDoE to Reduce Uncertainty (and associated risk)

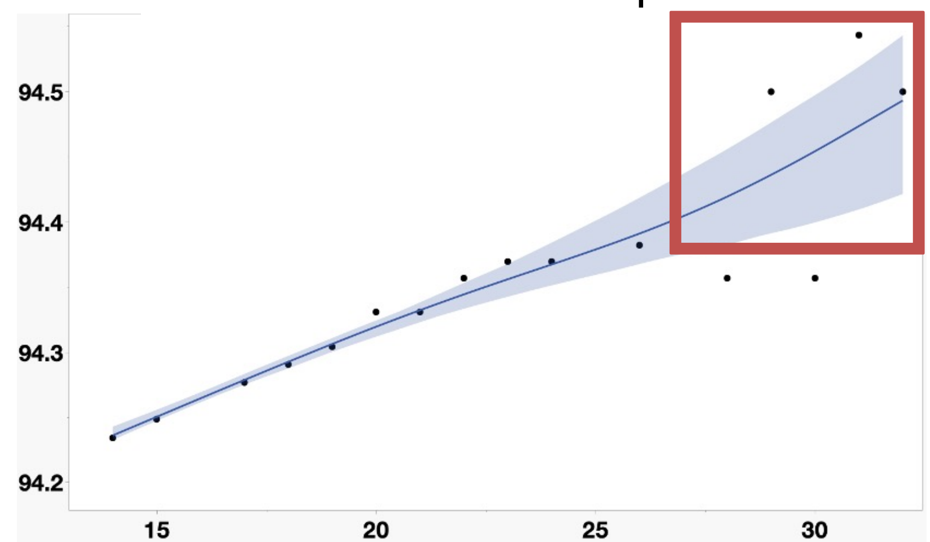
Number of experimental runs allocated: 30

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)**
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

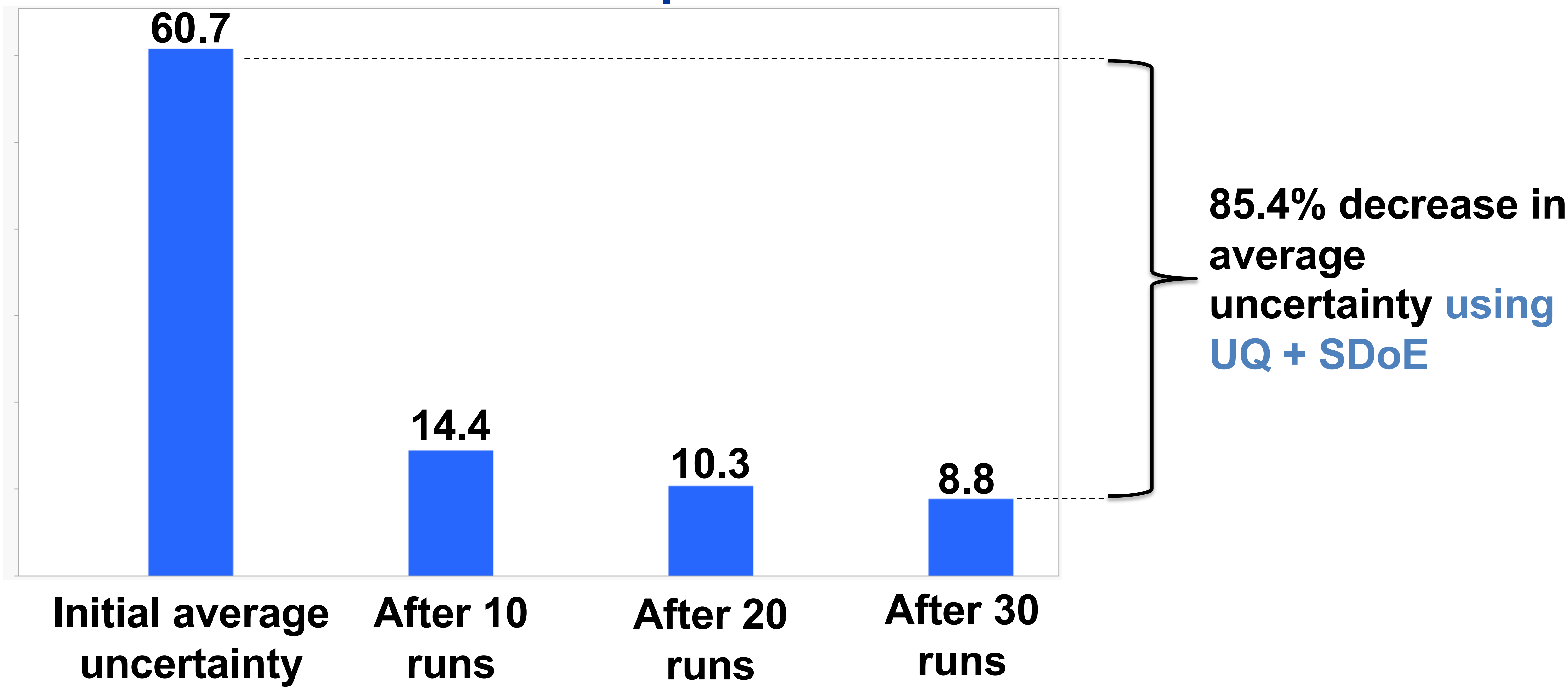


Parallel with 2D example

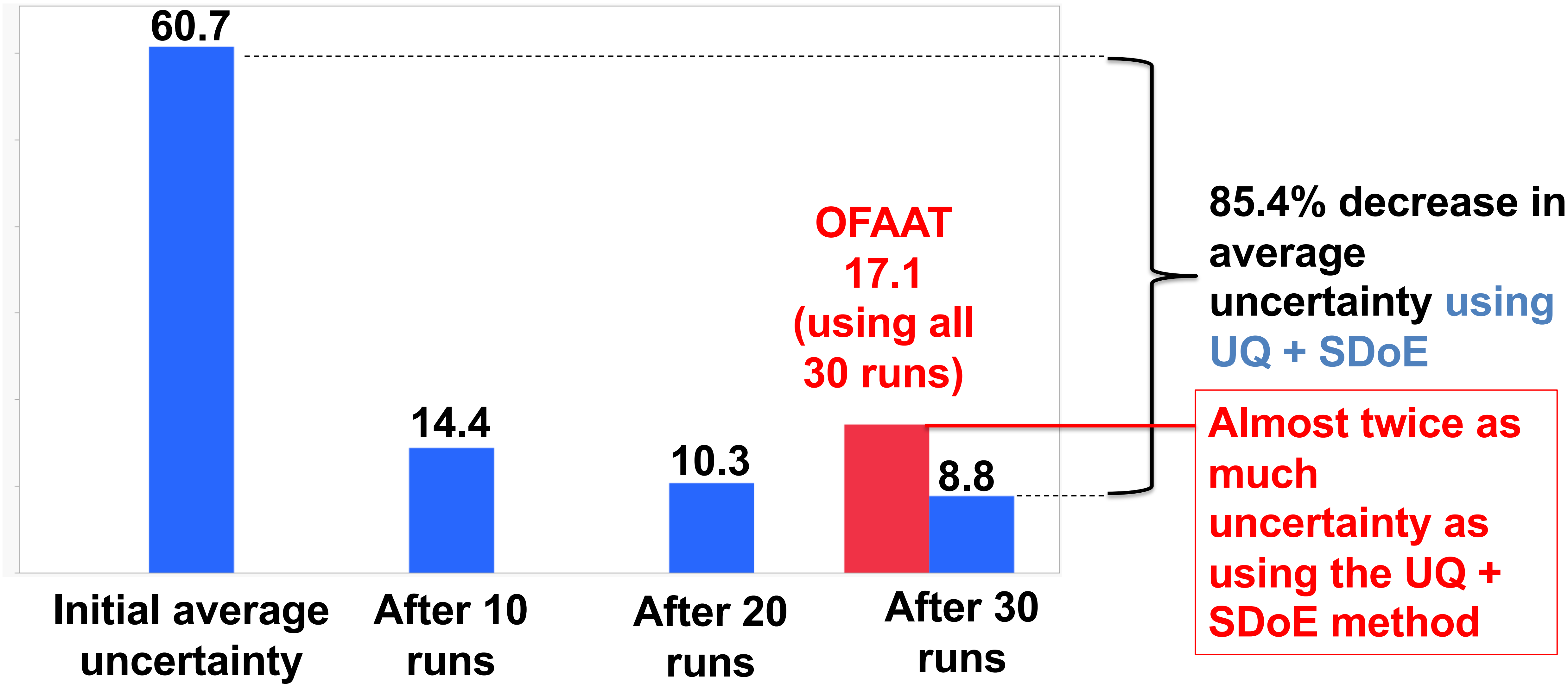


*Using simulated data for this illustration

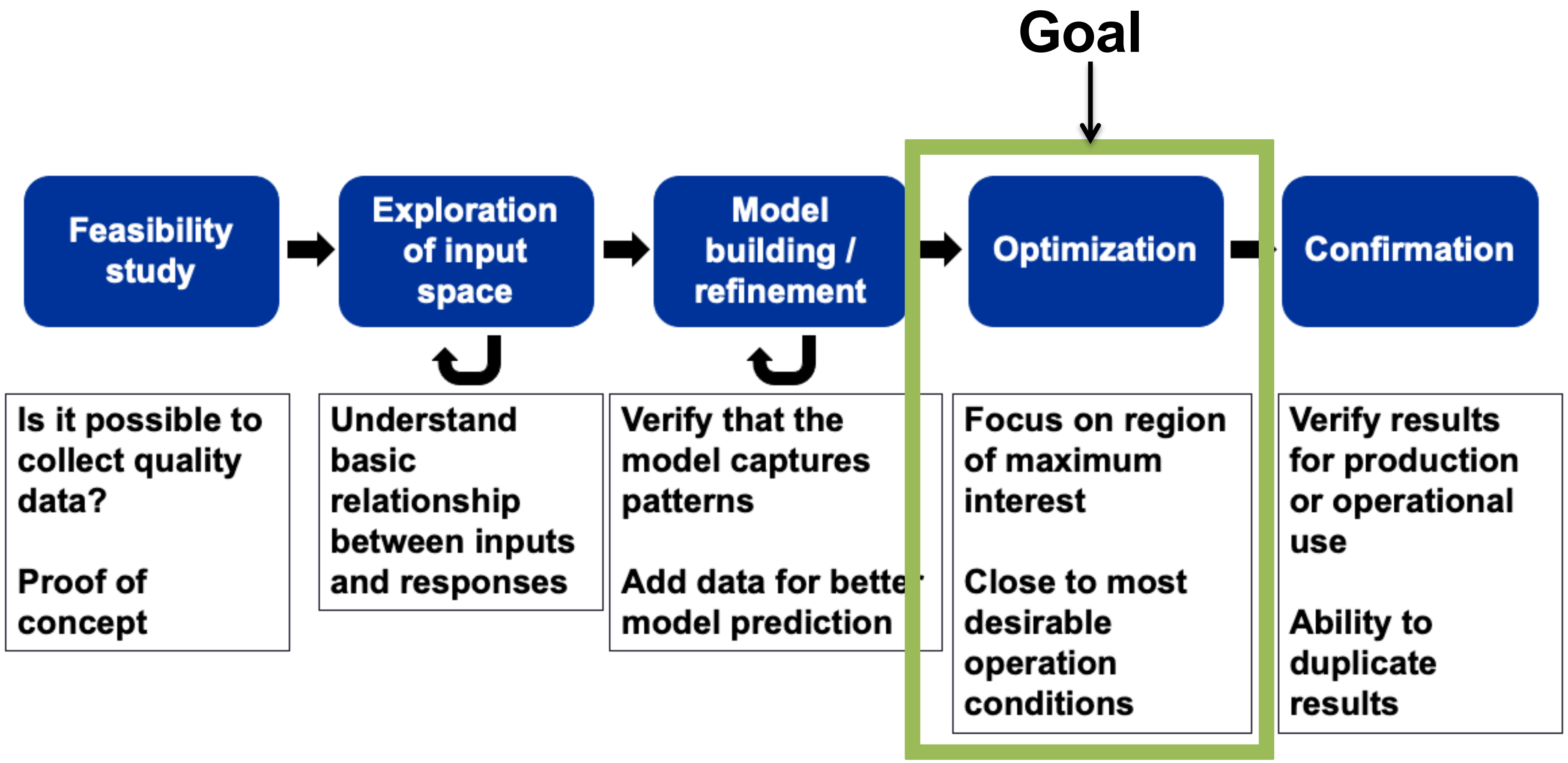
UQ + SDoE Notably Reduces Uncertainty in MEA Absorption Column Model



UQ + SDoE Reduces Uncertainty; Reduces Risk



Find Desirable Settings for MEA Absorption Column Model

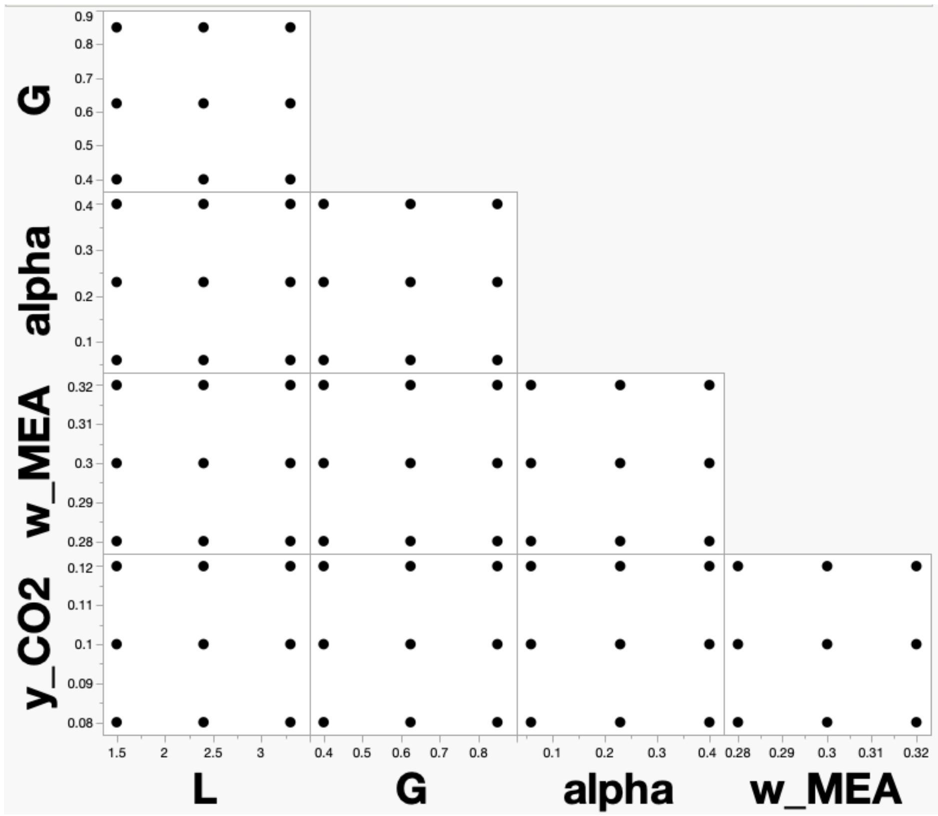


What input settings lead to maximum percent CO_2 capture?

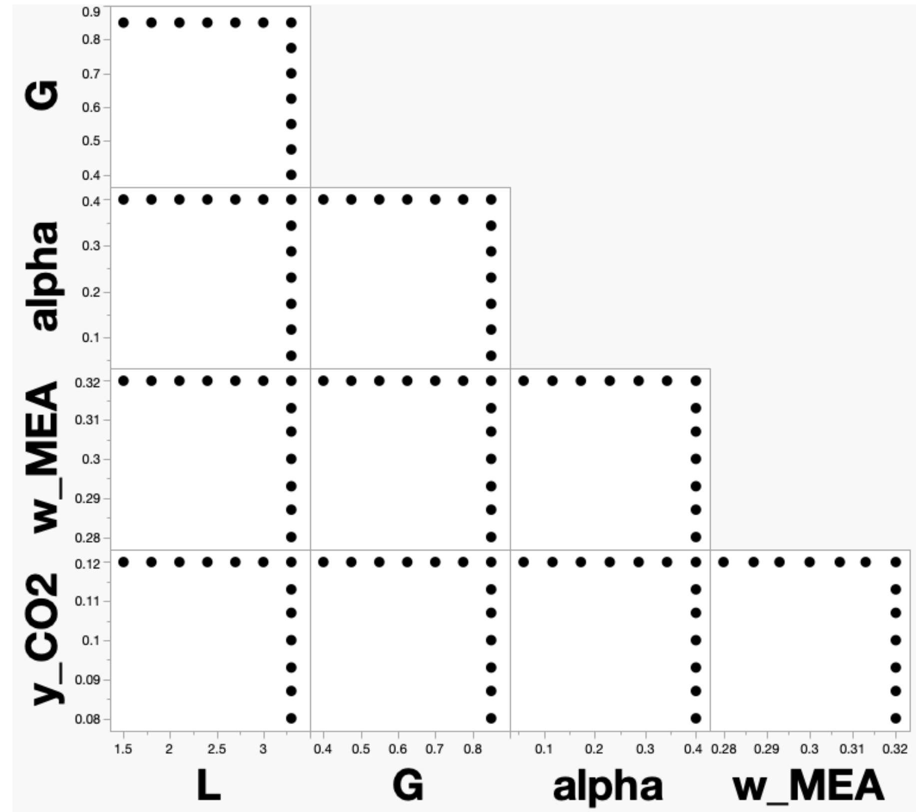
Demonstrate using empirical model-based designs (low-order polynomial approximation)

Compare to OFAAT

17-run empirical model-based DoE



30-run OFAAT



How Do the Empirical Models Perform?

30-run OFAAT

Model predicts best settings will lead to
69.3 %CO_2 capture

with prediction interval (66.7, 71.8)

Validation run: 71.46% CO_2 capture

That's inside the prediction interval.
Success!

DoE Answer Looks Better

30-run OFAAT

Model predicts best settings will lead to 69.3 %CO_2 capture

with prediction interval (66.7, 71.8)

Validation run: 71.46% CO_2 capture

That's inside the prediction interval. Success?

17-run empirical model-based DoE

Model predicts best settings will lead to 81.3 %CO_2 capture

with prediction interval (78.8, 83.8)

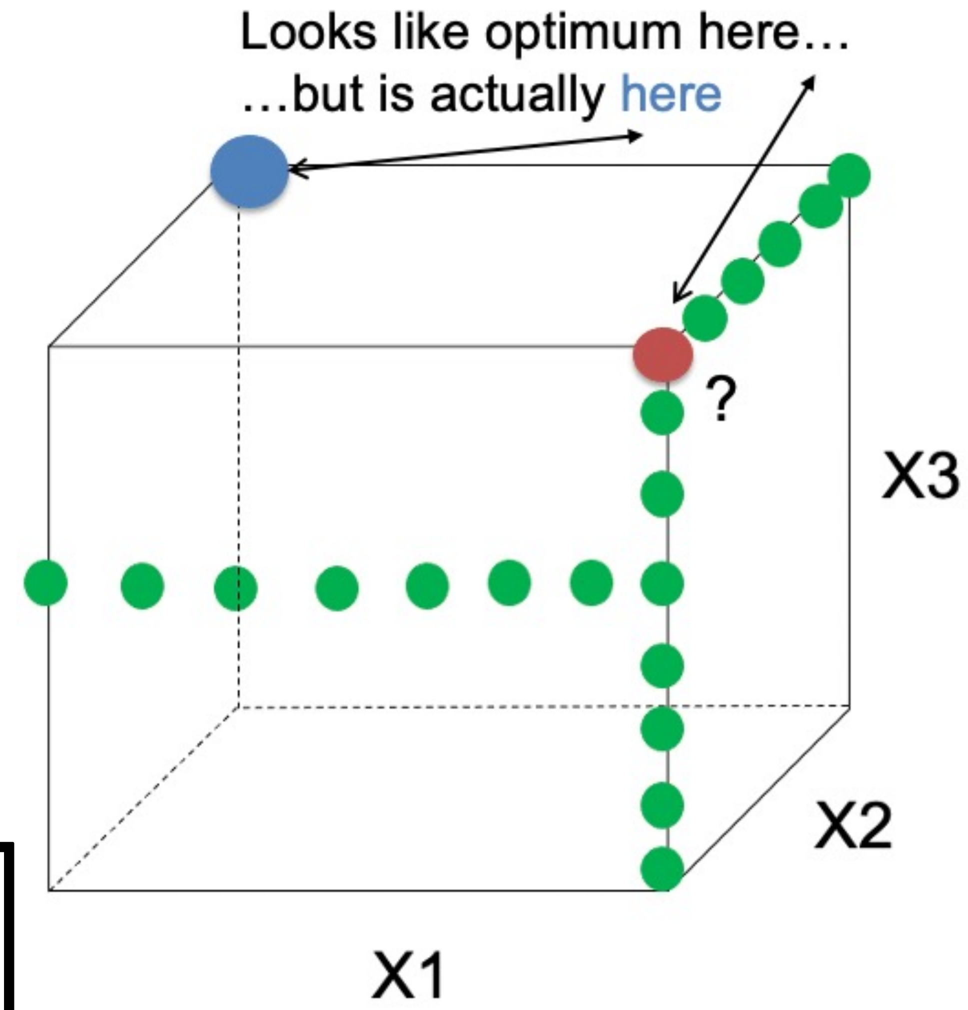
Validation run: 81.18% CO_2 capture

That's inside the prediction interval and results in higher percent CO_2 captured

Real success!

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

After the break – Technical Risk Reduction: Model Based Design of Experiments and Robust Optimization

Feasibility study	Exploration of input space	Model building / refinement	Optimization	Confirmation
Is it possible to collect quality data? Proof of concept	Understand basic relationship between inputs and responses	Verify that the model captures patterns Add data for better model parameter estimation or prediction	Focus on region of maximum interest Close to most desirable operation conditions	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

CCSI^2

Carbon Capture Simulation for Industry Impact

For more information

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