

Sequential Design of Experiments for Scaling Up Carbon Capture Technologies

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Carbon Management and Oil and Gas Research Project Review Meeting August 17th, 2021

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LA-UR-21-27802



Today's Plan



- Refresher on Sequential Design of Experiments (SDoE)
- Range of SDoE methodologies to support multiple objectives available in FOQUS
 - Uniform space-filling designs
 - Non-uniform space-filling designs
 - Input-response space-filling designs (new feature in FOQUS)
 - Robust model-based optimality-designed (ODoE) capability (new feature in FOQUS)
- Application: SDoE support for scale-up testing of carbon capture technology
 - Technology Centre Mongstad (TCM) field test





DoE Overview

- Strategy for selecting input combinations
 - Compute output (computer experiment)
 - Operate system (physical experiment)
- Range of inputs form region of interest
- Selected inputs form design







Why a statistically designed experiment (DoE)?

- High quality data leads to improved
 - Understanding
 - Decision-making
 - Confidence
- DoE produces exceptionally high-quality data





Data is good, strategic data is better

- DoE: extract maximum information with a fixed budget
 - Uses fewer resources
 - Gets better results
- Powerful tool for strategic data collection
 - Physical experiments
 - Computer experiments

DoE: Cost effective, high added value







Where does DoE fit?

- DoE can help at every stage of the process to scale up technologies – reduces risk
- 1. Exploration, preliminary model building
 - Understand basics
 - Capture larger trends
- 2. Model validation and refinement
 - Does the model reflect real-world results?
- 3. Model optimization
 - Find and test optimal operating conditions













- Problems are solved in stages
- Collect data in stages
- SDoE: directly incorporate knowledge learned in previous stages
- Result: strategic data collection across multiple stages























Total Budget: 18 runs

Input 1













Input 1

















Model Refinement (5 runs)









- Exploration (6 runs)
- Model Refinement (5 runs)

Optimization (3 runs)



Input 1









- Exploration (6 runs)
- Model Refinement (5 runs)
- Optimization (3 runs)
- Confirmation (2 runs)

Total Budget: 18 runs

Input 1



SDoE: Better use of budget











Range of strategies provides flexibility

- Different problems and different stages of the problem require different strategies
- Wide range of designs to accommodate
- Flexibility provides additional opportunity to make strategic choices for added efficiency
- SDoE module in FOQUS delivers tools to implement







Input 1

A fundamental choice: Space-filling or model-based?

- Space-filling designs
 - Relationship between inputs and response(s) of interest not well understood
 - Computer experiments / simulation
 - Calibration of a computer model to data
- 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









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 - Relationship can be well approximated by a low-order polynomial
- FOQUS toolset supports both approaches









Space-filling designs



Screenshot from FOQUS toolset

ion Flowsheet Uncertainty Optimization OUU SDOE SUrrogates Settings Help Help Help Help Space-filling DoE (SDOE) Robust optimality-based DoE (ODOE)	
	Design Construction
Generate New Load Existing Clone Delete Save Candidate Set Set Selected Selected Selected	Candidate File
Select File Type Visualize File Name Response Surface (cont'd) Validate RS Confirm RS Impute Data	Previous Experiments/Data
	Output Directory
	Design Method
 If you have a candidate set: 1. Press Load Existing Set and upload. Set File Type to Candidate. 2. If you also have previous data, press Load Existing Set and upload. Set File Type to Previous Data If you do not have a candidate set, press "Generate New Candidate Set" When finished identifying previous data and candidate sets, press Continue. 	Back to Selection Open SDoE Dialog



Space-filling designs



- Spread design points throughout space of interest
- Used when interesting phenomena may exist throughout the space
- Good precision for predicting new results at any new location





Three space-filling design methods of note

All three methods are available in the FOQUS SDoE module

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 Non-Uniform Space Filling Designs* (NUSF)
 Input Response Space-filling Designs** (IRSF) (new feature)

*Lu Lu, Christine M. Anderson-Cook, and Towfiq Ahmed, Journal of Quality Technology, 2020 ** Lu Lu. and Christine M. Anderson-Cook, Quality and Reliability Engineering International, 2021





Uniform space-filling designs

- Design points are evenly spread throughout space of interest^L
- Collect information throughout region
- Equal interest in / emphasis on entire input space
- Flexibly available in SDoE module of FOQUS:



Non-uniform space-filling designs

- Design points still spread out
- Emphasize some regions more than others
- For more in-depth exploration of certain areas







Non-uniform space-filling designs

- FOQUS SDoE module includes capabilities for
 - First phase or sequential experiments
 - Adjusting /comparing the desired degree of emphasis







Input-response space-filling designs

- 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
- Recent enhancement to the FOQUS SDoE module
 - For first phase or sequential experiments
 - Pareto front of objectively best designs to balance spacing in input and response spaces







Input-response space-filling designs





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Robust Optimally-Based Design of Experiments (ODoE)

Session Flowsheet Uncertainty Optimization OUU SDoE Surrogates	Settings Help
Space-filling DoE (SDoE) Robust optimality-based DoE (ODoE) Load RS Train Data:	Browse
Input Setup	Design Setup
Input Name Type Fixed Value PDF PDF P	Do you have a candidate file? Yes Load Existing Candidate Set Do you have an evaluation file? Yes Load Evaluation Set No Generate New Candidate Set Image: Candidate Set
	Select File Name Visualize Delete Selection Delete Selection
Confirm Inputs	Confirm Design Setup



NATIONAL

OGY

Robust Optimally-Based Design of Experiments (ODoE)

- New feature in SDoE module of FOQUS
- Construct designs based on empirically fit models
 - Different model forms available (PSUADE multiple choices)
- Choose desired optimality criterion for design construction





Actual Data for Y1

0.0 0.1

Model Errors

0.2

-0.2 -0.1

Build a sequence that works for each experiment







Build a sequence that works for each experiment







Input 1



SDoE in practice: field test at TCM

- CCSI2 is supporting MTR's engineering-scale advanced membrane field test at the Technology Centre Mongstad (TCM) (DE-FE0031591)
- Test objective: Identify optimum operating conditions for CO₂ capture rates from 50 90%
- 4 inputs
 - Glue gas flowrate
 - Sweep air flowrate
 - Temperature
 - Recycle stream flowrate
- Budget: 25 35 experimental runs
 - Depends on time per run





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Use SDoE methodology to make the most of the experimental budget – Learn as we go, increase efficacy







Planning for Phases 1a and 1b completed



Phase 1a DoE: Uniform space-filling design

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- Projected budget: 12
 experimental runs
 - 10 regular runs + 2 feasibility runs at low temperature
 - Ordered by temperature
- Design ordering algorithm availably in SDoE module for both USF and NUSF
 - Order the experimental runs to improve efficiency of implementation





Phase 1b SDoE: Uniform space-filling design

- 12 original runs
 + 4 additional SDoE runs
- Flexible option
 - Account for uncertainty in time required per test
- Collect additional information strategically
 - Fill in less explored areas
 - No tests wasted
- Planning for Phase 2 will begin once Phase 1 tests are complete
 - Information from Phase 1 tests will be directly incorporated for NUSF targeted exploration





Recap



- 1. Advantages of SDoE in framework of scaling up technologies
 - High value; low cost
 - Lower uncertainty and risk; increase efficacy
 - Flexibly applicable; variety of strategies to support different outcomes
- 2. SDoE module in FOQUS provides a robust toolset that includes
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Questions?



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For more information https://www.acceleratecarboncapture.org/

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