Application of Sequential Design of Experiments (SDoE) to Solvent-Based CO_2 Capture Systems at Multiple Scales

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Disclaimer

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Outline

- Executive Summary
- Background and Motivation for SDoE
- Applications of SDoE
  - MEA campaigns for NCCC and TCM pilot test facilities
  - Bench scale SDoE for CO_2BOL solvent system
  - Future campaigns at TCM for novel technologies
- Conclusions

Executive Summary

- CCSI^2 has developed and demonstrated methodology for sequential design of experiments (SDoE) to improve solvent-based CO_2 capture pilot testing
  - Applied to aqueous monoethanolamine (MEA) campaigns at National Carbon Capture Center (NCCC) [0.5 MWe] and Technology Centre Mongstad [12 MWe]
  - Reduced uncertainty of CO_2 capture predictions by approximately 60% for both campaigns
- SDoE work is ongoing for bench scale CO_2BOL process developed by Pacific Northwest National Laboratory
- Future work will focus on application of SDoE to novel technologies – including solvents, sorbents, and membranes

Motivation

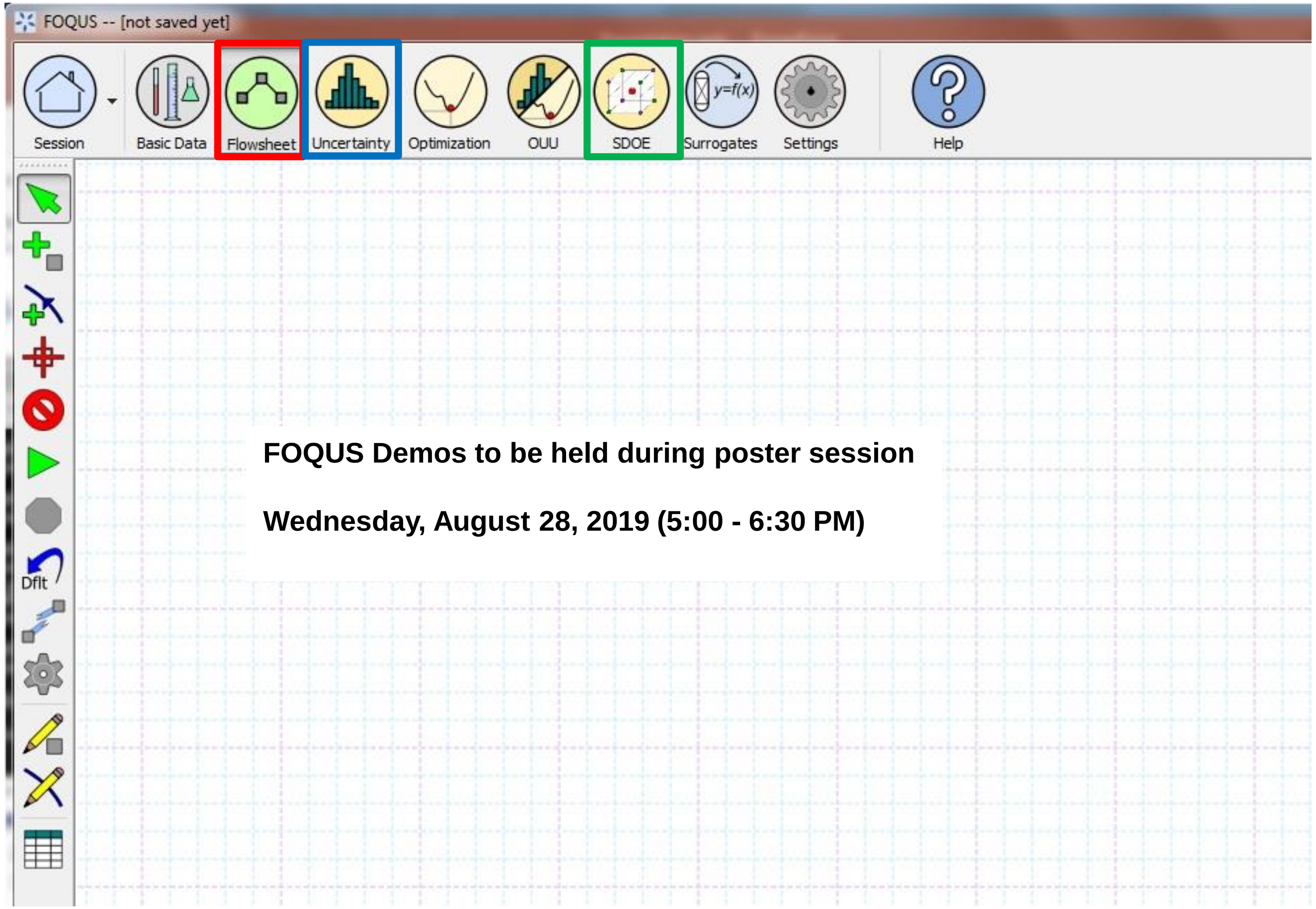
- Develop systematic approach to conducting pilot plant testing, regardless of scale, process configuration, technology type, etc.
- Ensure right data is collected – improve understanding, refine models

- **Design of Experiments (DoE)** is a tool to accelerate learning by targeting maximally useful input combinations to match experiment goals

- **Sequential DoE (SDoE)** expands on DoE capabilities, allowing for incorporation of information from an experiment as it is being run, by updating input selection criteria based on new information

Ultimate Goal: Reduce technical risk associated with scale-up

Framework for Optimization, Quantification of Uncertainty, and Surrogates



FOQUS Demos to be held during poster session

Wednesday, August 28, 2019 (5:00 - 6:30 PM)

Flowsheet Tab – Used for propagating uncertainty through simulation model

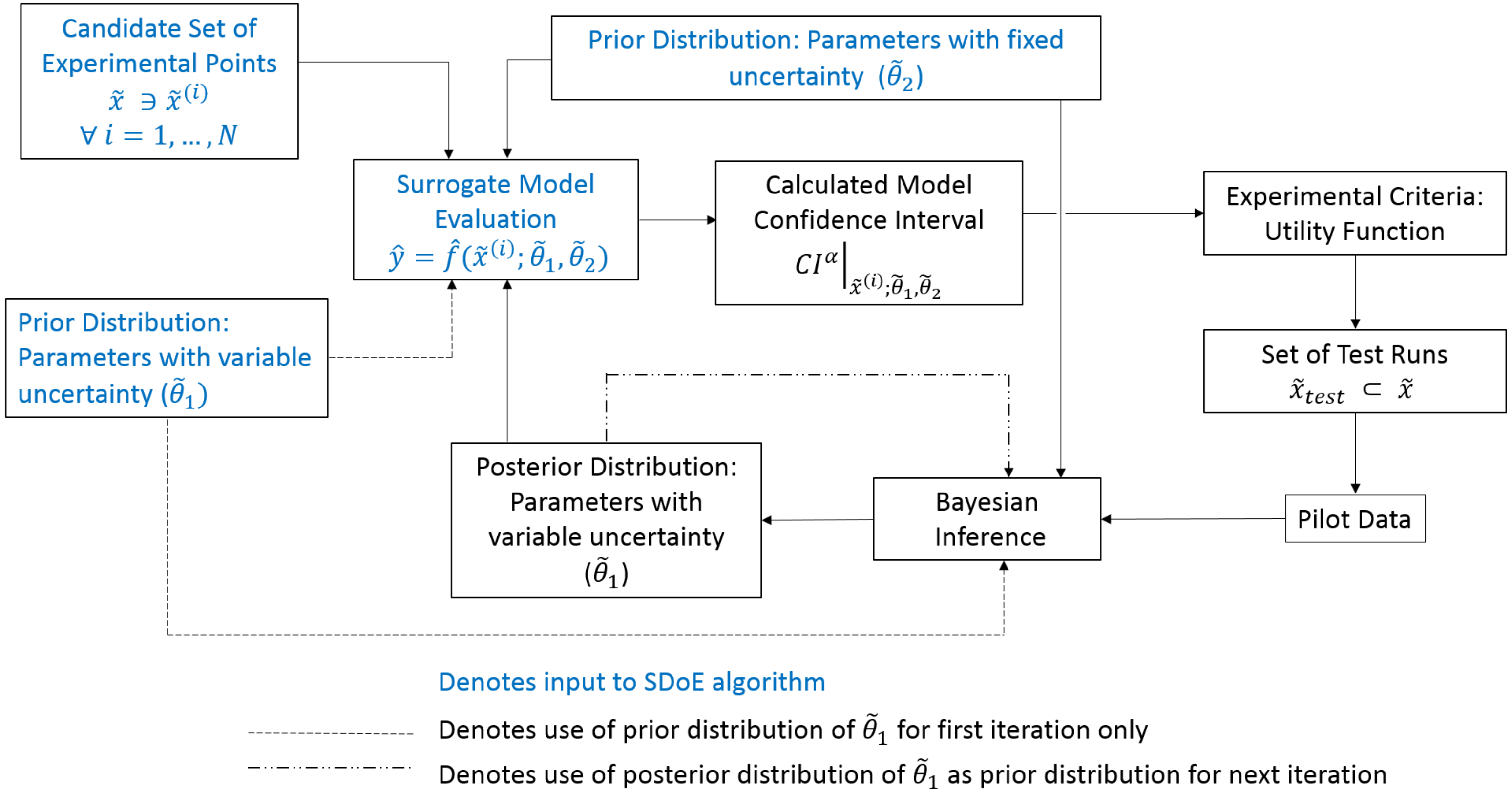
Uncertainty Tab – PSUADE used for Bayesian inference and surrogate modeling

SDoE Tab – Currently being developed for streamlining process described in this work

Open-source software available at:
https://github.com/CCSI-Toolset

CCSI² Carbon Capture Simulation for Industry Impact

SDoE Process



$$\tilde{\theta} = [\tilde{\theta}_1\ \tilde{\theta}_2]$$ **Full Set of Model Parameters**

$$\Omega_i = \{\hat{y}(\tilde{x}^{(i)}; \tilde{\theta}^{(1)}), \dots, \hat{y}(\tilde{x}^{(i)}; \tilde{\theta}^{(M)})\}$$ **Propagation of Parametric Uncertainty**

$$CI^{\alpha}\big|_{\tilde{x}^{(i)};\tilde{\theta}_1,\tilde{\theta}_2} = F_{1-\alpha/2}(\Omega_i) - F_{\alpha/2}(\Omega_i)$$ **Confidence Interval Calculation**

SDoE Applied at National Carbon Capture Center – Summer 2017

nationalcarboncapturecenter.com

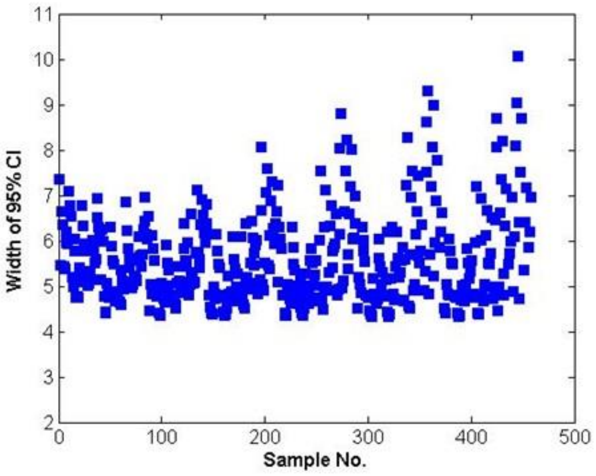
- 0.5 MWe scale facility
- Variability in operating conditions for experimental design
  - Lean solvent flowrate
  - Flue gas flowrate
  - Lean solvent CO_2 loading
  - Flue gas CO_2 fraction
- Variability in absorber configuration also tested
  - Multiple solvent inlets allow operation with 1, 2, or 3 packing beds
  - Optional intercooling stages between beds
- Goal of pilot testing: Refine stochastic model prediction of CO_2 capture percentage

SDoE Results – Reduction in Prediction of CO_2 Capture Percentage

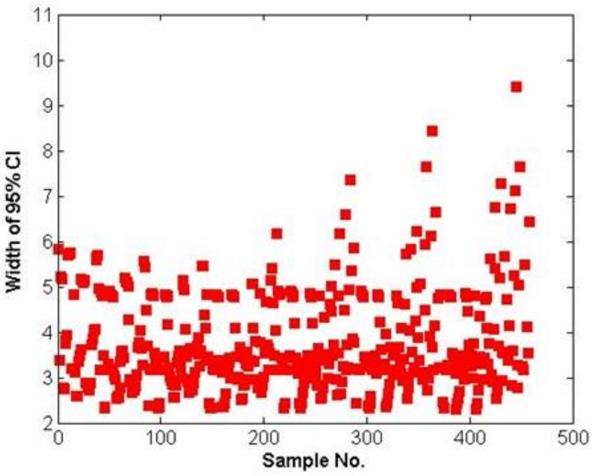
First Round

Candidate Set (Discrete Points in Operating Region of Interest)

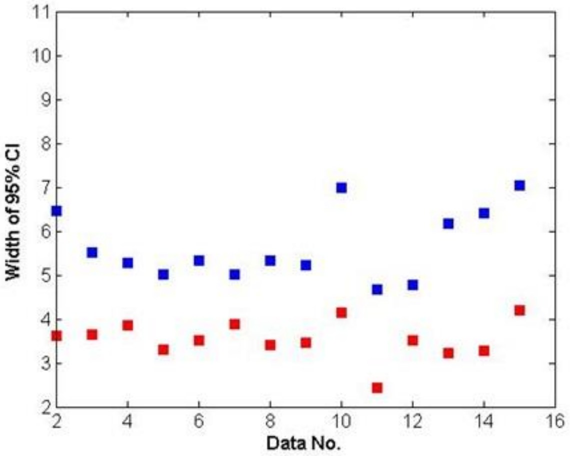
Prior



Posterior



Experimental Runs

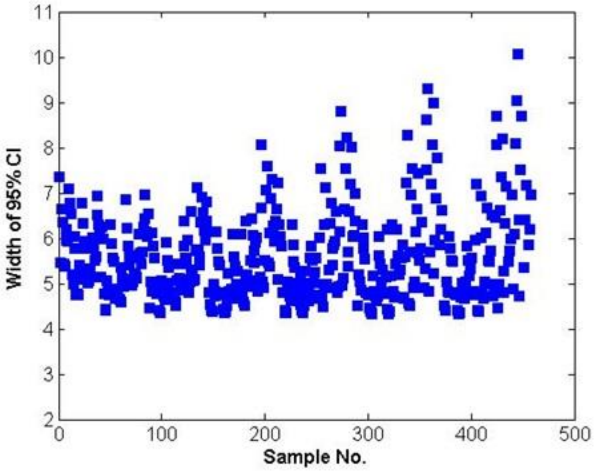


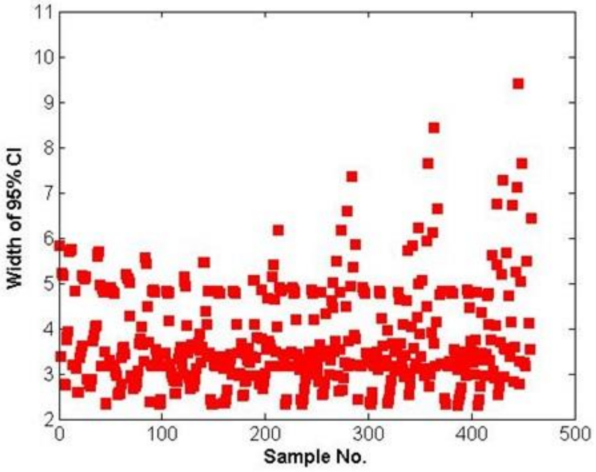
SDoE Results – Reduction in Prediction of CO_2 Capture Percentage

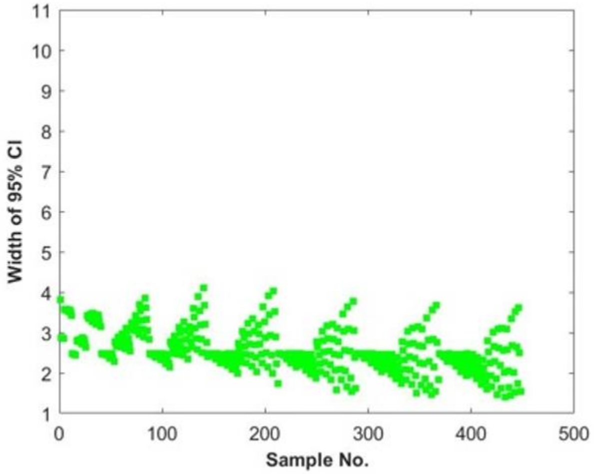
Second Round

Prior | **Posterior**

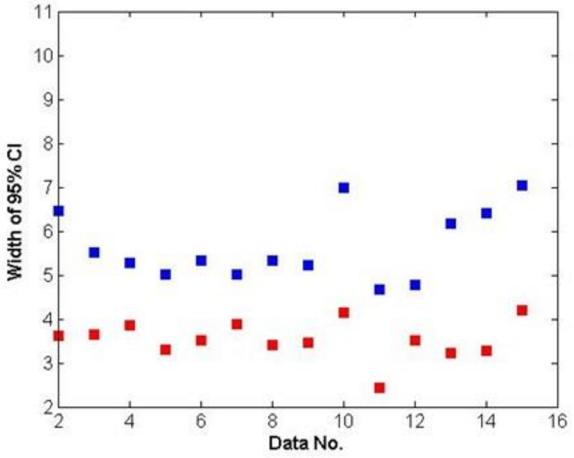
Candidate Set (Discrete Points in Operating Region of Interest)

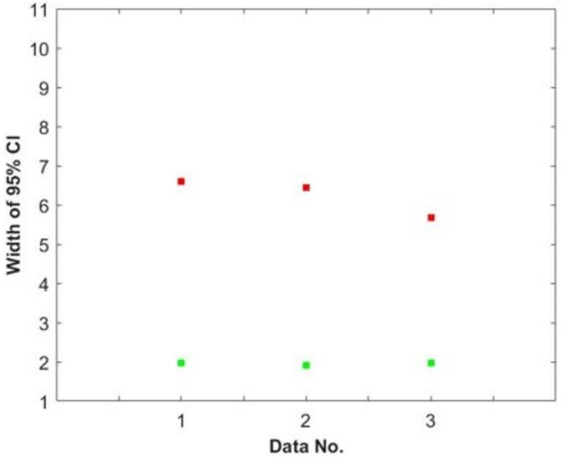






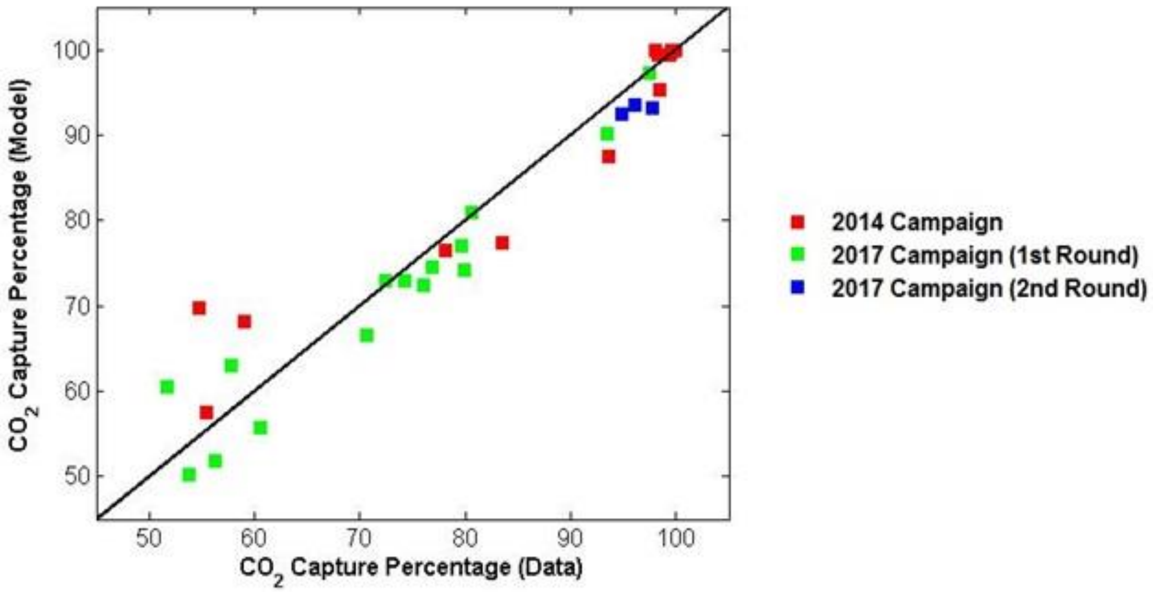
Experimental Runs



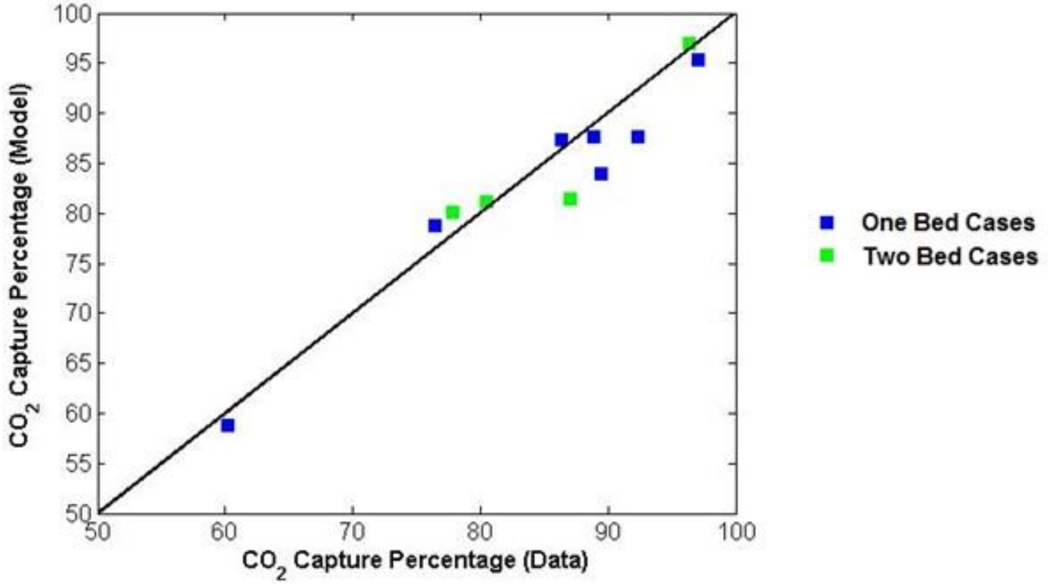


Fit of Model to NCCC Data

Three Beds with Intercooling Cases



One or Two Bed Cases



Note: These cases were not included in the sequential portion of the experimental design

SDoE Applied at Technology Centre Mongstad – Summer 2018

www.tcmda.com

- The world's largest facility for testing and improving CO_2 capture technologies (12 MWe scale)
- Located next to Equinor refinery in Mongstad, Norway
- Joint venture set up by Gassnova, Equinor, Total, and Shell
- Two flue gas sources
  - Combined Cycle Gas Turbine (CCGT)
  - Residual Fluidized Catalytic Cracker (RFCC)

Phases of TCM Test Campaign

Phase 1
Space-filling design for testing predictability of existing model

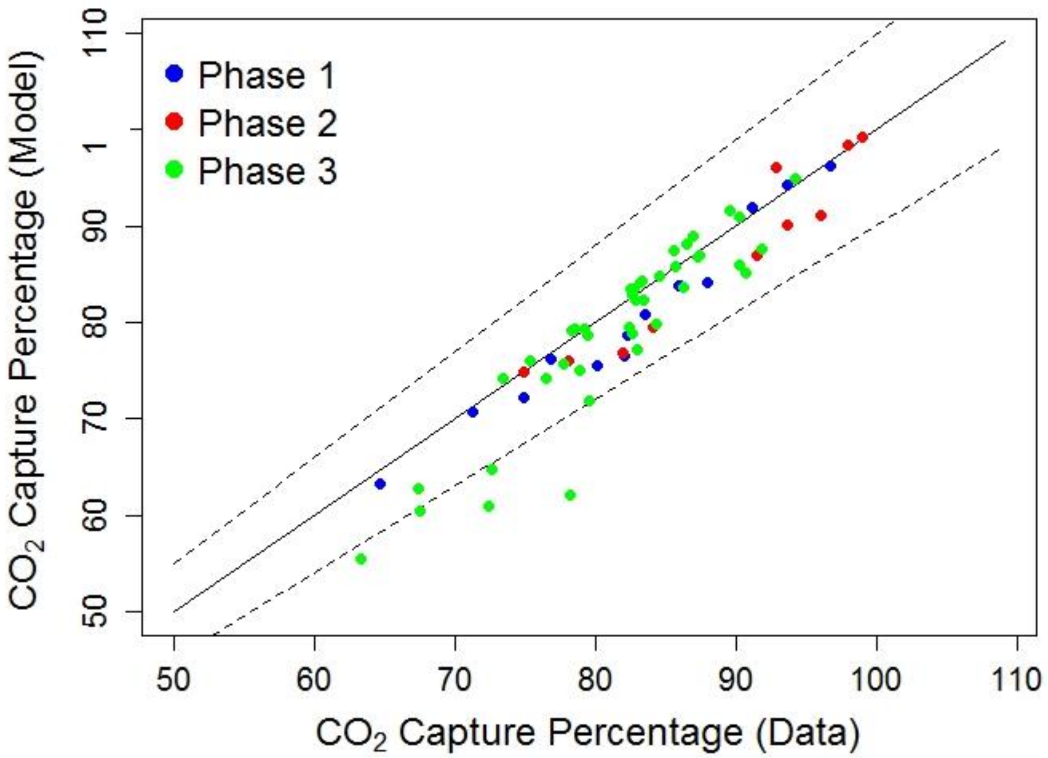
Phase 2
Selection of points for testing based on economic objective function

Phase 3
Sequential DoE
Selection of points based on G-optimality: minimize the maximum model prediction variance in the design space

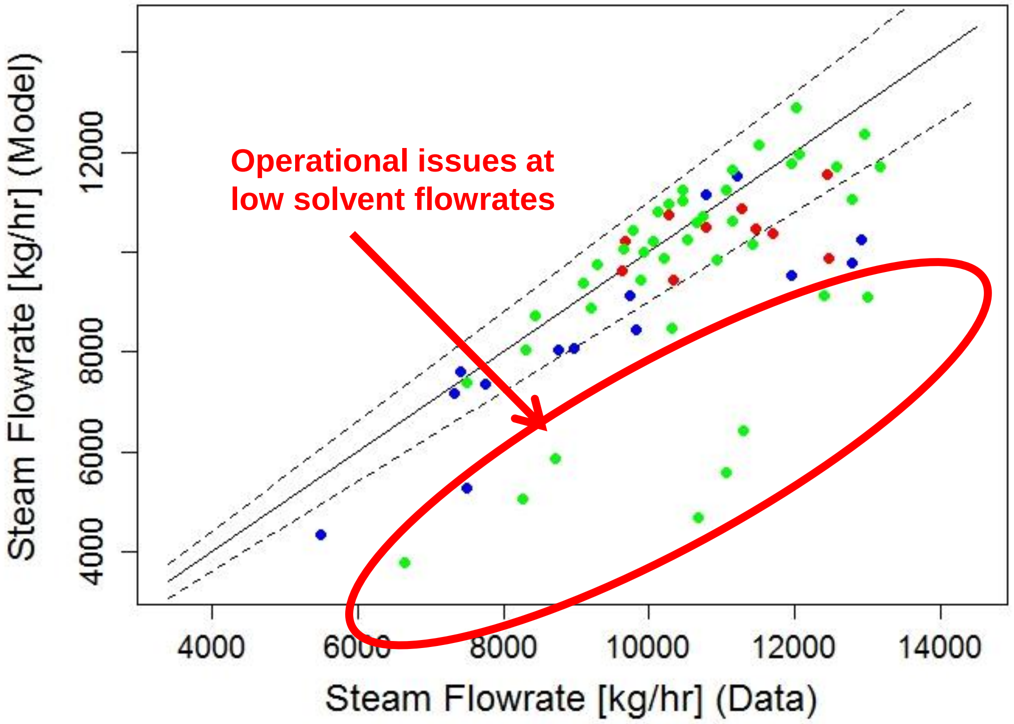
Phase 4-5
Minimization of reboiler duty
Variation in absorber packing height
Rich solvent bypass configuration

TCM Model Predictions (Deterministic)

Absorber Performance



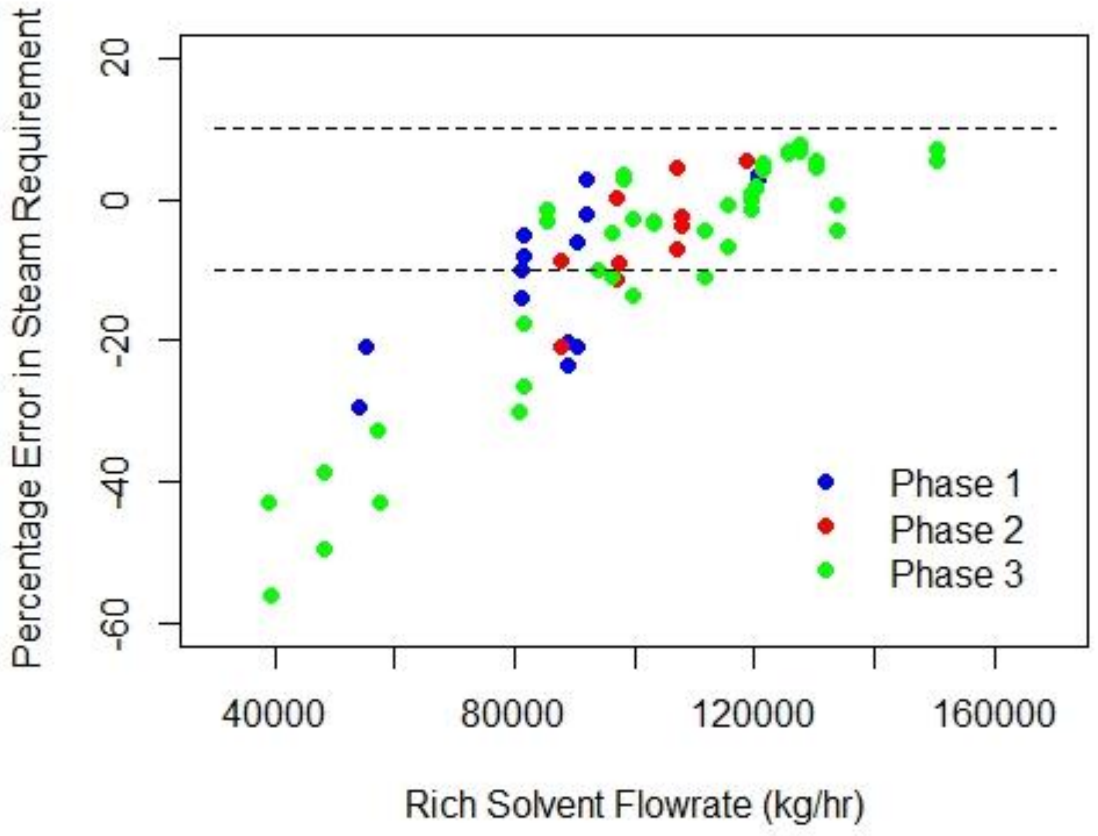
Stripper Performance



Dashed lines represent ±10%

Data include variation in flowrates of solvent, flue gas, and steam as well as CO_2 composition in flow gas

TCM Stripper Performance



Two strippers available for use at TCM

- Stripper designed for CCGT flue gas (~3.5% CO_2) [Capacity: 80 tonne CO_2/day]
- Stripper designed for RFCC flue gas (~13-14% CO_2) [Capacity: 275 tonne CO_2/day]

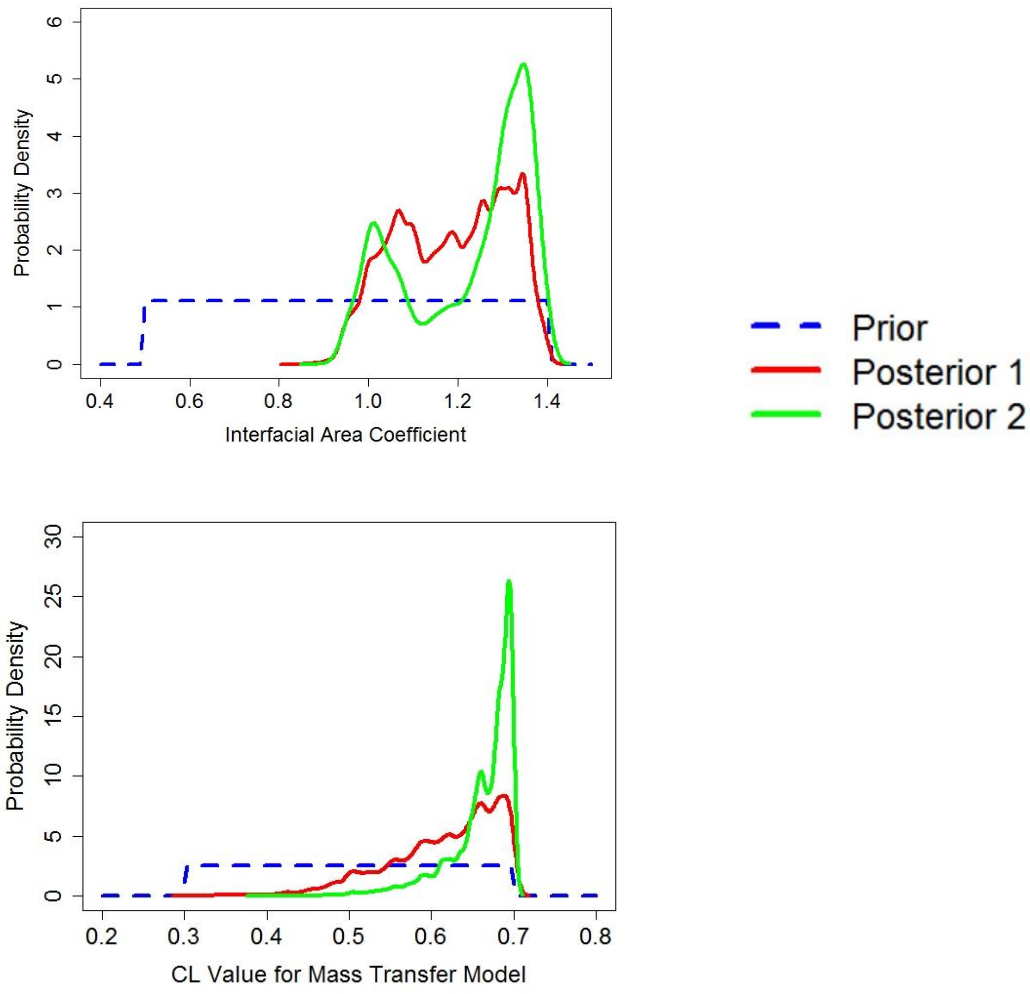
$CCSI^2$ campaign used RFCC stripper and CCGT flue gas with recycle (8-10% CO_2), thus leading to over-designed stripper when running process with low flowrates

Potential maldistribution effect at low solvent flowrate not captured in Aspen Plus rate-based process model

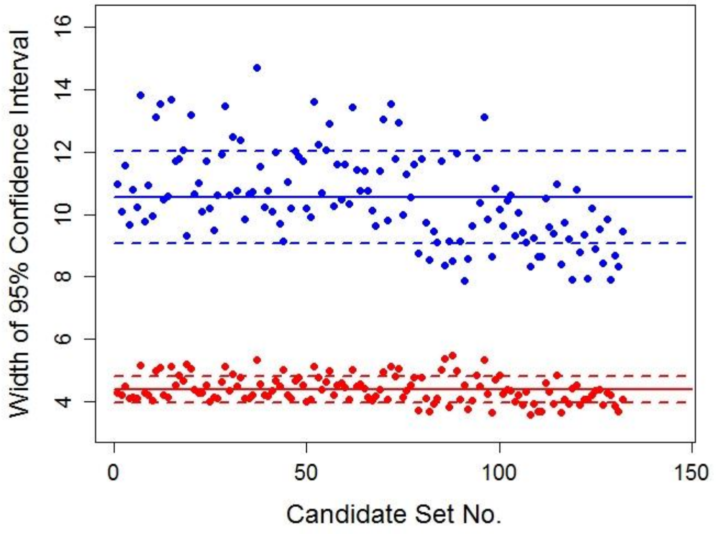
CCSI2 Carbon Capture Simulation for Industry Impact | National Energy Technology Laboratory | Berkeley Lab | Lawrence Livermore National Laboratory | Los Alamos National Laboratory | Pacific Northwest National Laboratory | West Virginia University | The University of Texas at Austin | U.S. Department of Energy

Results – TCM SDoE (Phase 3)

Update in Parameter Distributions for Absorber Packing



Reduction in CO_2 Capture Percentage (First Iteration)



Prior CI Width: 10.5 ± 1.5

Posterior CI Width: 4.4 ± 0.4

Average reduction in uncertainty: 58.0 ± 4.7%

Candidate set includes variation in:

- **Solvent circulation rate**
- **Flue Gas flowrate and CO_2 concentration**
- **Reboiler steam flowrate**

Test Phases 4-5

- Operated pilot plant with portion of rich solvent by-passing lean-rich heat exchanger routed to water wash bed of stripper column

- Reduced absorber packing height to 18 m (Phase 4) and 12 m (Phase 5)

- Space-filling design used to minimize specific reboiler duty (SRD) by varying solvent circulation rate
  - Fixed flowrate and composition of flue gas (50,000 sm^3/hr; 8 mol% CO2) and percentage of CO_2 capture (85%)

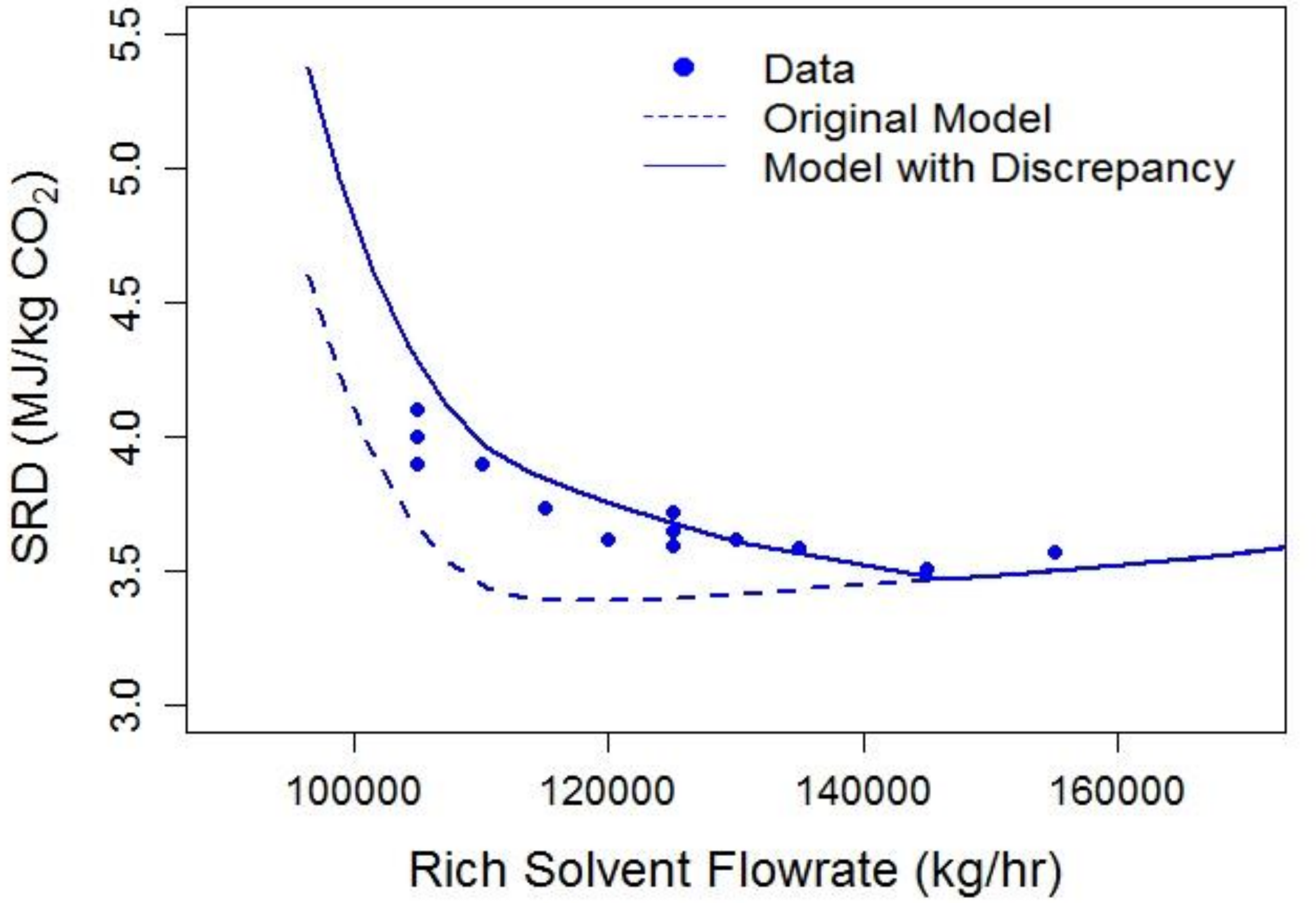
CCSI[2] Carbon Capture Simulation for Industry Impact | NATIONAL ENERGY TECHNOLOGY LABORATORY | BERKELEY LAB | Lawrence Livermore National Laboratory | Los Alamos NATIONAL LABORATORY EST. 1943 | Pacific Northwest NATIONAL LABORATORY | WestVirginiaUniversity | THE UNIVERSITY OF TEXAS AT AUSTIN | U.S. DEPARTMENT OF ENERGY

Results – Phase 4

Statistical discrepancy model developed for reboiler steam requirement in order to account for mismatch between data and model prediction of SRD

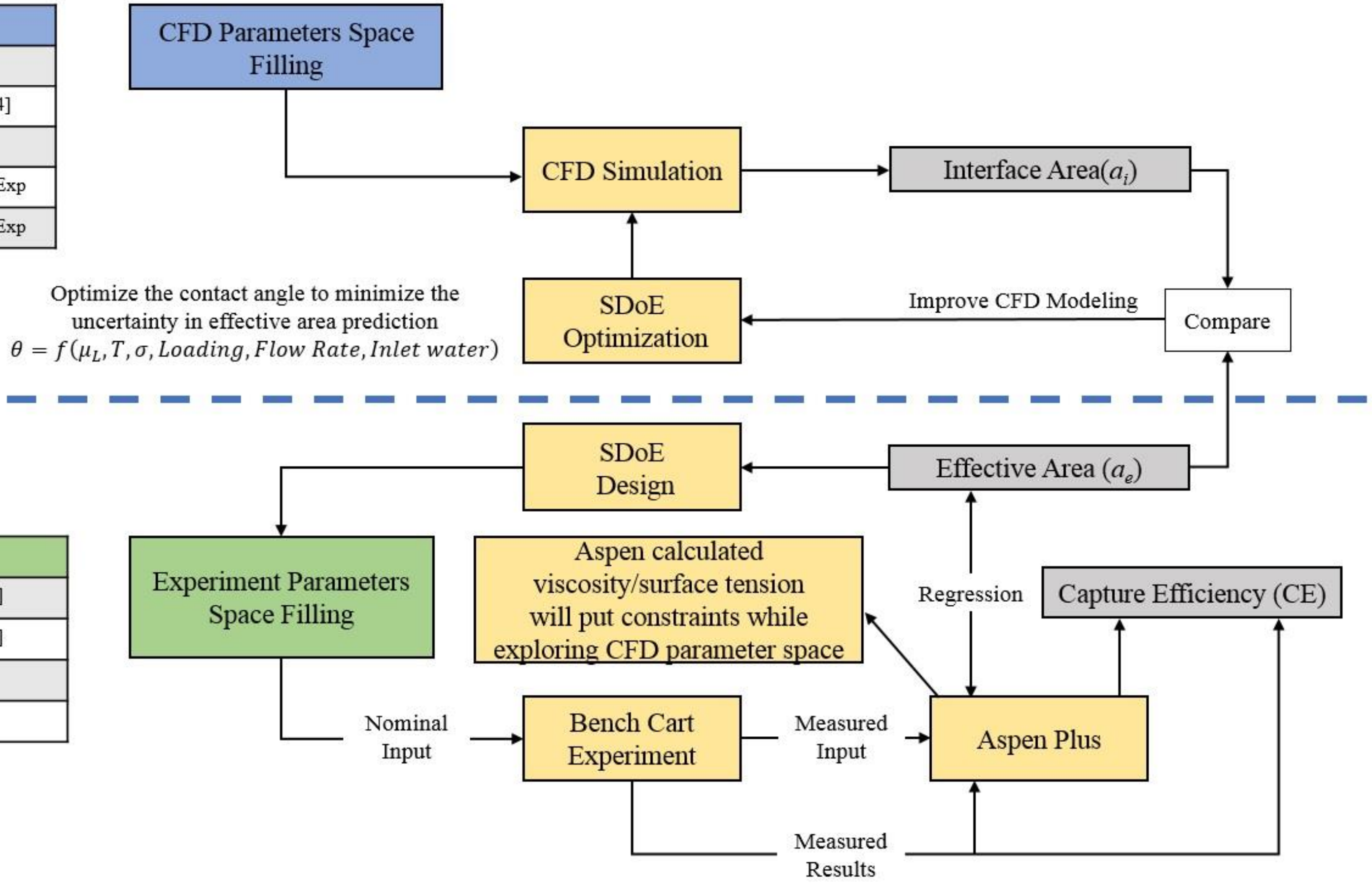
$$\dot{m}_{steam} = \beta_0 + \beta_1 * L_{rich} + \beta_2 * bypass\ percentage$$

$$\dot{m}_{steam} = S_{calc} + \max(0, \Delta\dot{m}_{steam})$$



Ongoing Work: SDoE Application to CO_2BOL Bench-Cart System

CFD Parameters	Range
Viscosity [cP]	[5 15]
Surface Tension σ [N/m]	[0.01 0.04]
Contact Angle θ [°]	[5 80]
Solvent Flow Rate [L/min]	Same as Exp
Gas Flow Rate [SLPM]	Same as Exp



Experiment Parameters	Range
Solvent Flow Rate [L/min]	[0.1 0.9]
Gas Flow Rate [SLPM]	[10 100]
Loading/Reboiler Temperature	<135°C
Absorber Temperature [°C]	[30 60]

Work will be presented in detail during:
"Low Aqueous Solvent System Optimization" – Zhijie Xu, Pacific Northwest National Laboratory
Capture and Utilization Session, Wednesday, August 28: 9:00 AM

Future Work

Upcoming SDoE projects at TCM

Industry Partner	Technology
Research Triangle Institute (RTI)	Non Aqueous Solvent
SRI International	Mixed Salt Solvent
Membrane Technology Research (MTR)	Membrane
TDA Research + MTR	Sorbent/Membrane Hybrid System

Summary and Conclusions

- Stochastic modeling framework enables quantification of model input uncertainty and propagation through model for risk assessment and economic analysis

- SDoE methodology has been shown to effectively inform design pilot test campaigns and reduce model uncertainty
  - SDoE demonstrates promise for accelerating development of novel CO_2 capture technologies

- Future work will focus on application of SDoE for novel CO_2 capture technologies, specifically for upcoming projects at TCM

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Carbon Capture Simulation for Industry Impact (CCSI^2)

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Christophe Benquet
Muhammad Ismail Shah
Anette Beate Nesse Knarvik

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Carbon Capture Simulation for Industry Impact

For more information

https://www.acceleratecarboncapture.org/

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