Application of Sequential Design of Experiments (SDoE) to Solvent-Based CO$_2$ Capture Systems at Multiple Scales

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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$_2$BOL solvent system
  – Future campaigns at TCM for novel technologies
• Conclusions
Executive Summary

- CCSI² has developed and demonstrated methodology for sequential design of experiments (SDoE) to improve solvent-based CO₂ 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 CO₂ capture predictions by approximately 60% for both campaigns
- SDoE work is ongoing for bench scale CO₂BOL process developed by Pacific Northwest National Laboratory
- Future work will focus on application of SDoE to novel technologies – including solvents, sorbents, and membranes
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

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
**SDoE Process**

Candidate Set of Experimental Points \( \tilde{x} \in \tilde{x}^{(i)} \) \( \forall i = 1, \ldots, N \)

Prior Distribution: Parameters with fixed uncertainty \( (\tilde{\theta}_2) \)

Prior Distribution: Parameters with variable uncertainty \( (\tilde{\theta}_1) \)

Surrogate Model Evaluation \( \hat{y} = f(\tilde{x}^{(i)}, \tilde{\theta}_1, \tilde{\theta}_2) \)

Calculated Model Confidence Interval \( CI^\alpha |_{\tilde{x}^{(i)}, \tilde{\theta}_1, \tilde{\theta}_2} = F_{1-\alpha/2}(\Omega_i) - F_{\alpha/2}(\Omega_i) \)

Posterior Distribution: Parameters with variable uncertainty \( (\tilde{\theta}_1) \)

Bayesian Inference

Experimental Criteria: Utility Function

Set of Test Runs \( \tilde{x}_{\text{test}} \subseteq \tilde{x} \)

Pilot Data

Denotes input to SDoE algorithm

Denotes use of prior distribution of \( \tilde{\theta}_1 \) for first iteration only

Denotes use of posterior distribution of \( \tilde{\theta}_1 \) as prior distribution for next iteration

\[ \tilde{\theta} = [\tilde{\theta}_1 \ \tilde{\theta}_2] \]

\[ \Omega_i = \{ \hat{y}(\tilde{x}^{(i)}; \tilde{\theta}^{(1)}), \ldots, \hat{y}(\tilde{x}^{(i)}; \tilde{\theta}^{(M)}) \} \]

**Full Set of Model Parameters**

**Propagation of Parametric Uncertainty**

**Confidence Interval Calculation**
SDoE Applied at National Carbon Capture Center – Summer 2017

- 0.5 MWe scale facility
- Variability in operating conditions for experimental design
  - Lean solvent flowrate
  - Flue gas flowrate
  - Lean solvent CO\textsubscript{2} loading
  - Flue gas CO\textsubscript{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\textsubscript{2} capture percentage

nationalcarboncapturecenter.com
SDoE Results – Reduction in Prediction of CO$_2$ Capture Percentage

First Round

Candidate Set (Discrete Points in Operating Region of Interest)

Experimental Runs

Prior

Posterior
SDoE Results – Reduction in Prediction of CO$_2$ Capture Percentage

Second Round

Candidate Set (Discrete Points in Operating Region of Interest)

Experimental Runs

Prior

Posterior
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
The world’s largest facility for testing and improving CO₂ 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
Data include variation in flowrates of solvent, flue gas, and steam as well as CO₂ composition in flow gas.
Two strippers available for use at TCM
- Stripper designed for CCGT flue gas (~3.5% CO₂) [Capacity: 80 tonne CO₂/day]
- Stripper designed for RFCC flue gas (~13-14% CO₂) [Capacity: 275 tonne CO₂/day]

CCSI² campaign used RFCC stripper and CCGT flue gas with recycle (8-10% CO₂), 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
Results – TCM SDoE (Phase 3)

Update in Parameter Distributions for Absorber Packing

Reduction in CO₂ 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 CO₂ 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 sm³/hr; 8 mol% CO₂) and percentage of CO₂ capture (85%)
Results – Phase 4

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

\[ \dot{m}_{\text{steam}} = \beta_0 + \beta_1 \cdot L_{\text{rich}} + \beta_2 \cdot \text{bypass percentage} \]

\[ \dot{m}_{\text{steam}} = S_{\text{calc}} + \max(0, \Delta \dot{m}_{\text{steam}}) \]
Ongoing Work: SDoE Application to CO₂BOL Bench-Cart System

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

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<th>Technology</th>
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<td>Non Aqueous Solvent</td>
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<tr>
<td>SRI International</td>
<td>Mixed Salt Solvent</td>
</tr>
<tr>
<td>Membrane Technology Research (MTR)</td>
<td>Membrane</td>
</tr>
<tr>
<td>TDA Research + MTR</td>
<td>Sorbent/Membrane Hybrid System</td>
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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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