Application of Sequential Design of Experiments (SDoE) to a Pilot-Scale MEA-Based CO_2 Capture Process

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Trondheim CO_2 Capture, Transport, and Storage Conference (TCCS-10)
Trondheim, Norway
18 June, 2019

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KeyLogic Systems, Inc.'s contributions to this work were funded by the National Energy Technology Laboratory under the Mission Execution and Strategic Analysis contract (DE-FE0025912) for support services.

Outline

- Motivation and Executive Summary

- Background
  - Stochastic Modeling for Solvent-Based CO_2 Capture Systems
  - CCSI Toolset
  - Sequential Design of Experiments (SDoE)

- Application of SDoE at Technology Centre Mongstad

- Conclusions and Future Work

Motivation

- Development of new carbon capture technologies requires testing at multiple scales
  - Important to strategically allocate limited resources when conducting pilot-scale testing in order to maximize learning

- Quantification of uncertainty (UQ) necessary for rigorous analysis of risk, particularly that associated with process scale-up

- Statistical approaches enable informed design and UQ simultaneously
  - In Bayesian framework, model uncertainty may be reduced through collection of data

Executive Summary

- Sequential design of experiments (SDoE) applied during five week campaign at Norway's Technology Centre Mongstad in summer 2018
  - Process previously demonstrated at smaller scale (0.5 MWe) National Carbon Capture Center in summer 2017

- Data collected over a wide operating space (including variation in flowrates of solvent, flue gas, and reboiler steam as well as CO_2 concentration in flue gas)
  - Over full input space, model prediction of uncertainty in CO_2 capture percentage reduced by an average of 58.0 ± 4.7% when incorporating experimental data through Bayesian inference

Stochastic Modeling Framework

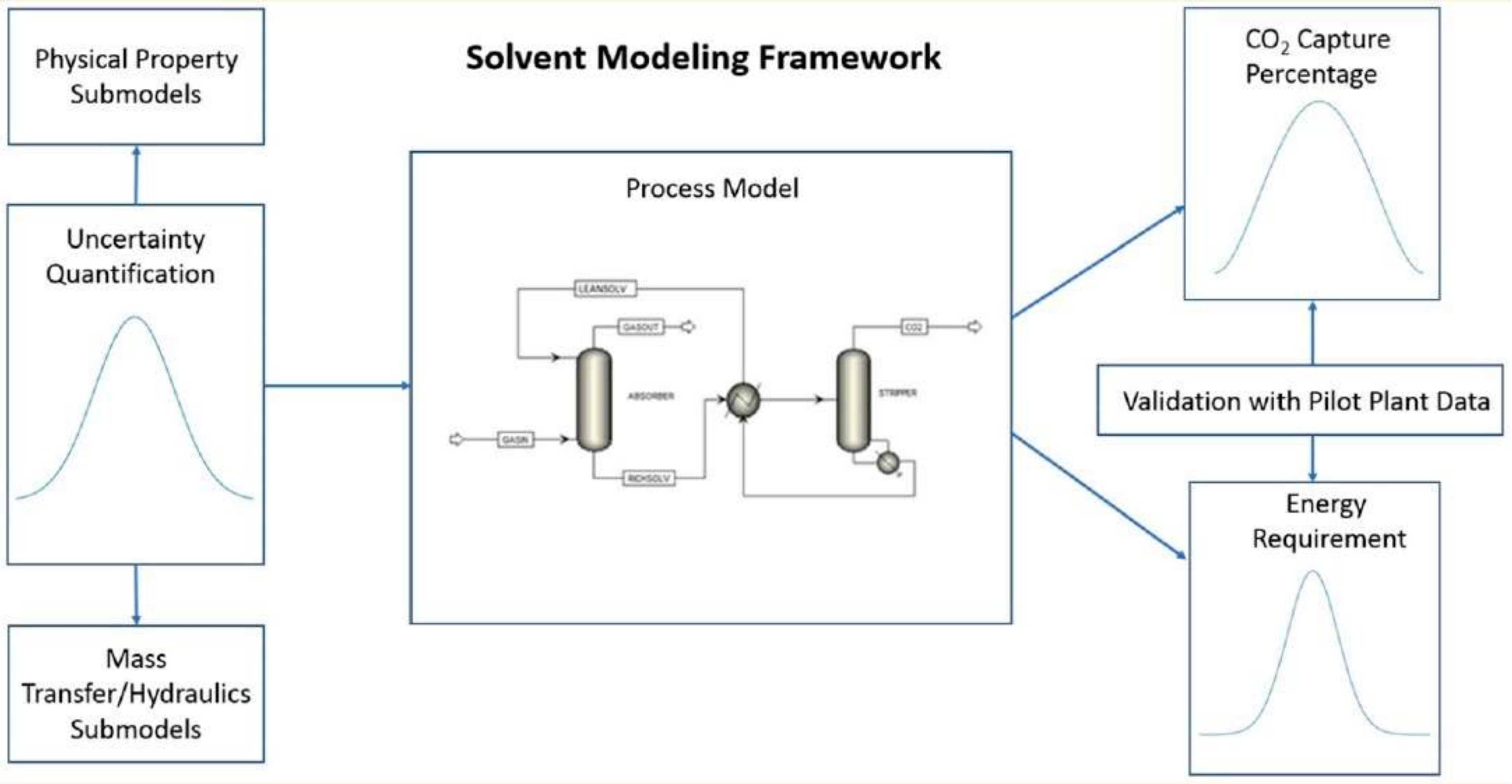


Figure taken from Morgan et al., Ind Eng Chem Res, 2018, 57, 10464-10481

Stochastic Process Modeling Approach

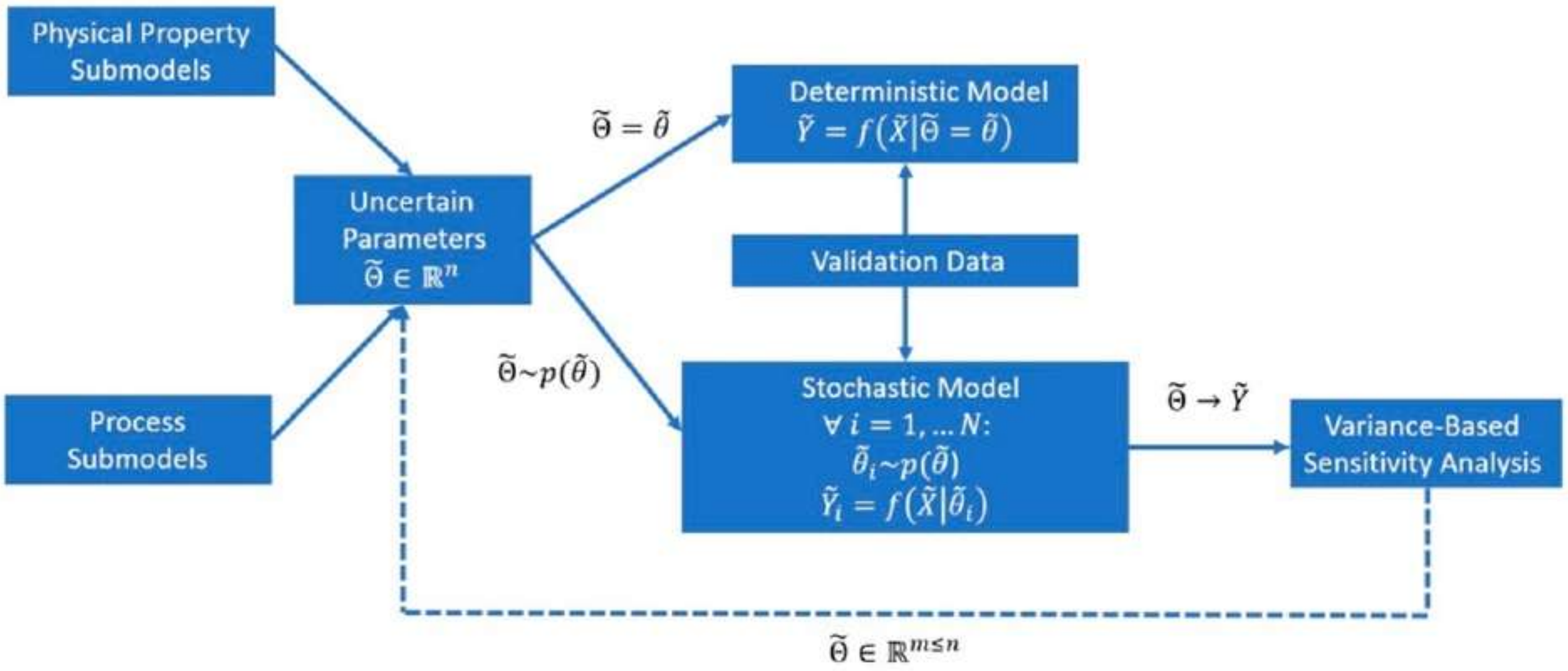
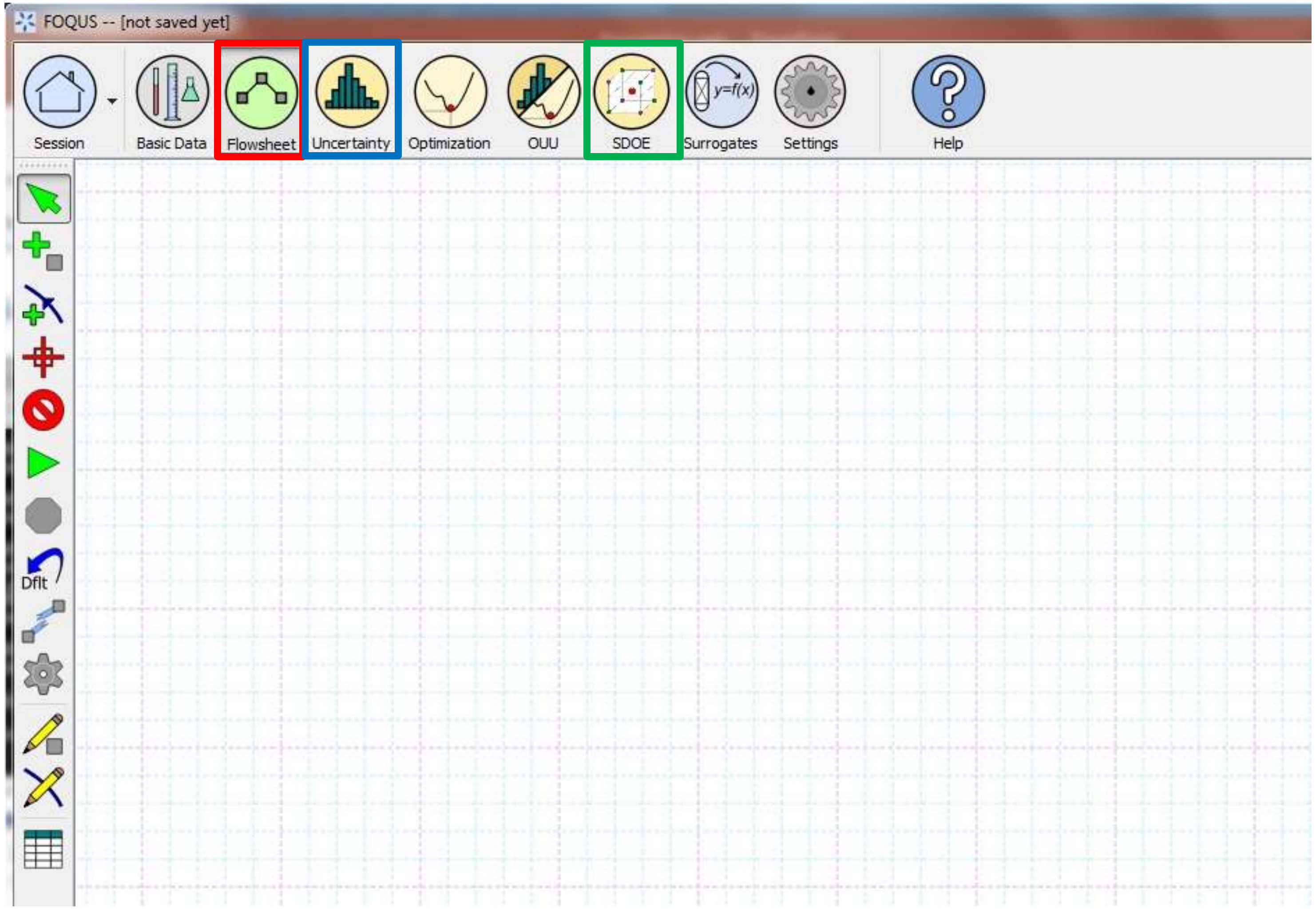


Figure taken from Morgan et al., Ind Eng Chem Res, 2018, 57, 10464-10481

Role of FOQUS in Solvent Modeling Framework



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

Objectives for Pilot Testing

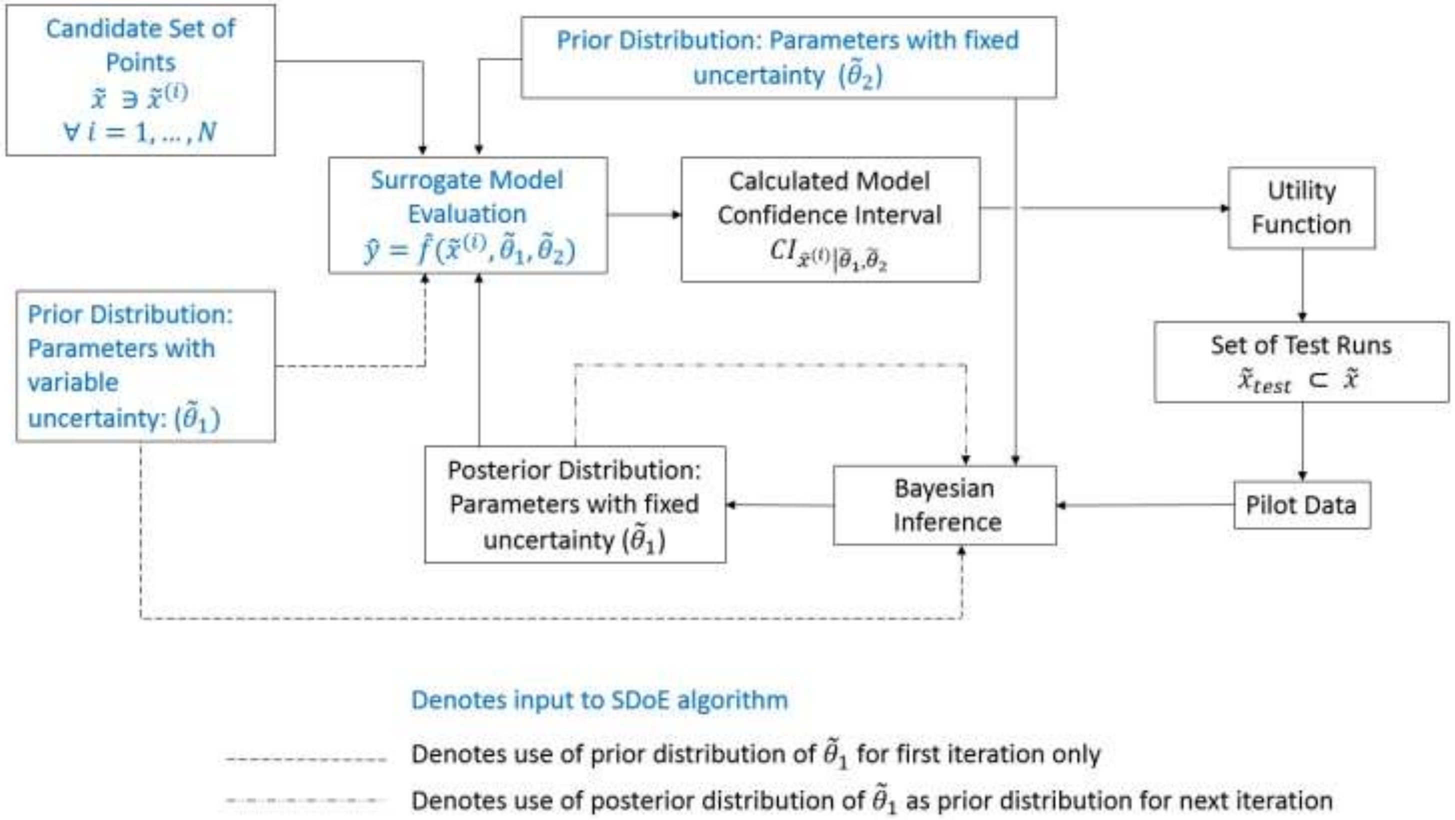
- Develop systematic approach to conducting pilot plant testing, regardless of scale, process configuration, technology type, etc.
- Ensure right data is collected
- Maximize value of data collected

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

- **Sequential DoE (SDoE)** allows 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

SDoE Process



Confidence Interval Calculation

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

$$\Omega_i = \left\{\hat{y}\left(\tilde{x}^{(i)}, \tilde{\theta}^{(1)}\right), \dots, \hat{y}\left(\tilde{x}^{(i)}, \tilde{\theta}^{(M)}\right)\right\}$$

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

Utility Functions for SDoE

- **Space-filling designs**
  - Minimax: Ensure that all points in the candidate set ($\tilde{x}$) are close to a point in the design ($\tilde{x}_{test}$)
  - Maximin: Ensure that all points in the chosen design ($\tilde{x}_{test}$) are not too close together

- **Various classes of uncertainty-based designs**
  - Minimize variance of parameter estimations
  - Minimize variance of model predictions
    - G-optimality: Minimizing the maximum output predicted variance in the candidate set

SDoE Applied at Technology Centre Mongstad – Summer 2018

www.tcmda.com

- The world's largest facility for testing and improving CO_2 capture technologies
- 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 Test Campaign

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

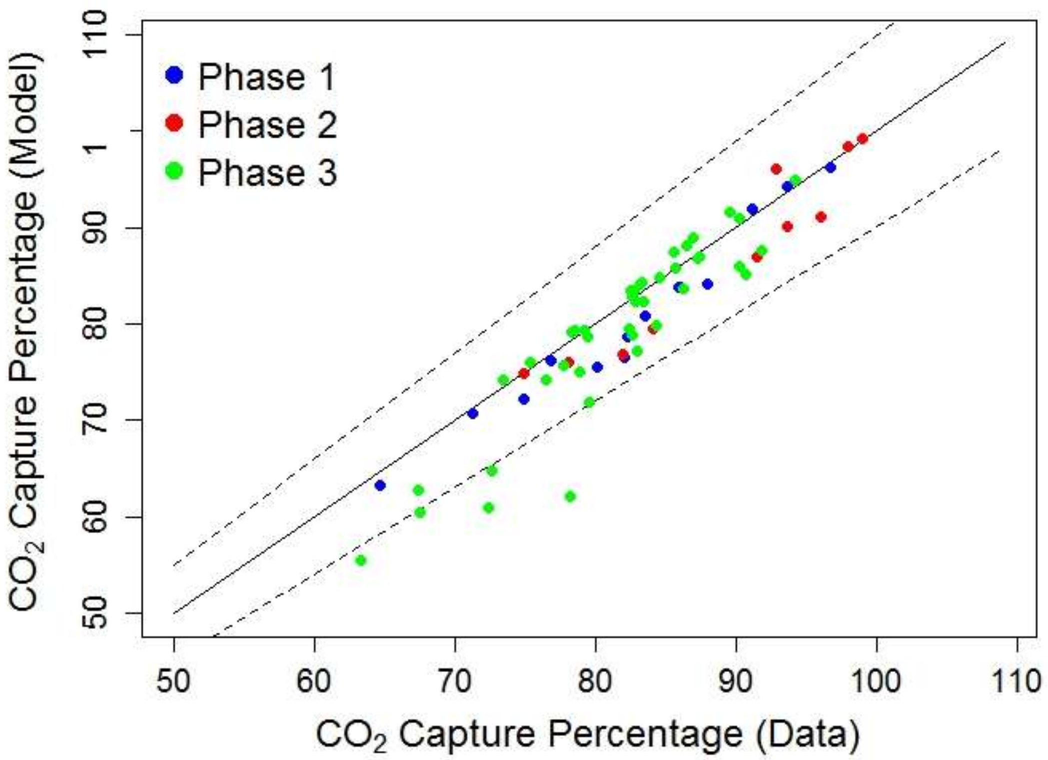
Phase 2
Selection of points for testing based on economic objective function

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

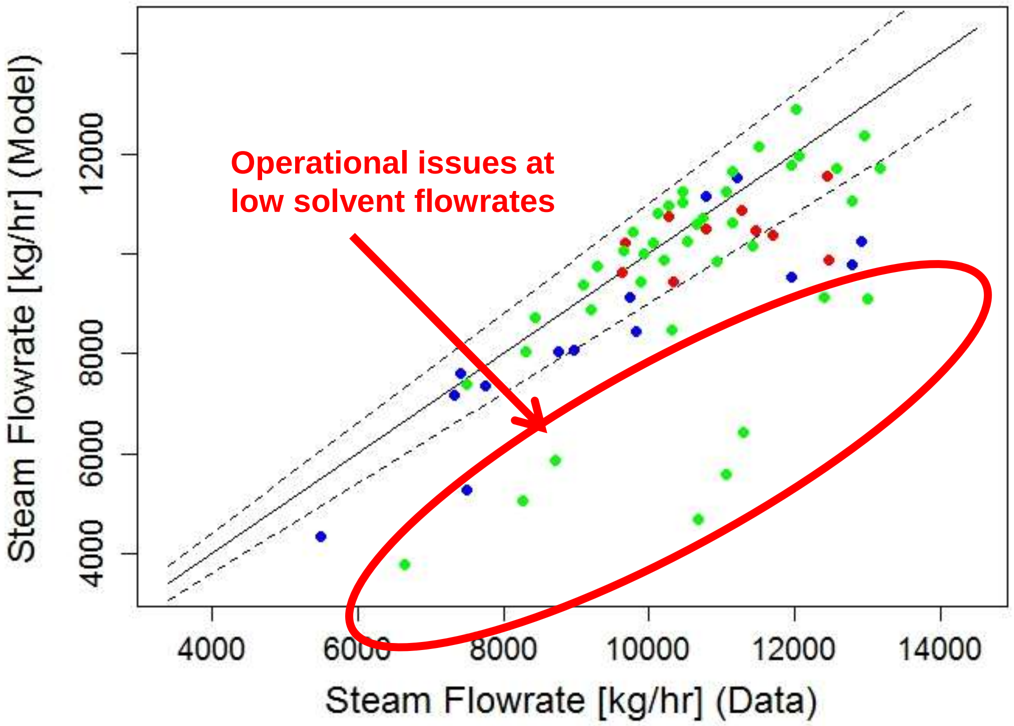
Phase 4-5
Minimization of reboiler duty
Variation in absorber packing height
Rich solvent bypass configuration

TCM Model Predictions (Deterministic)

Absorber Performance



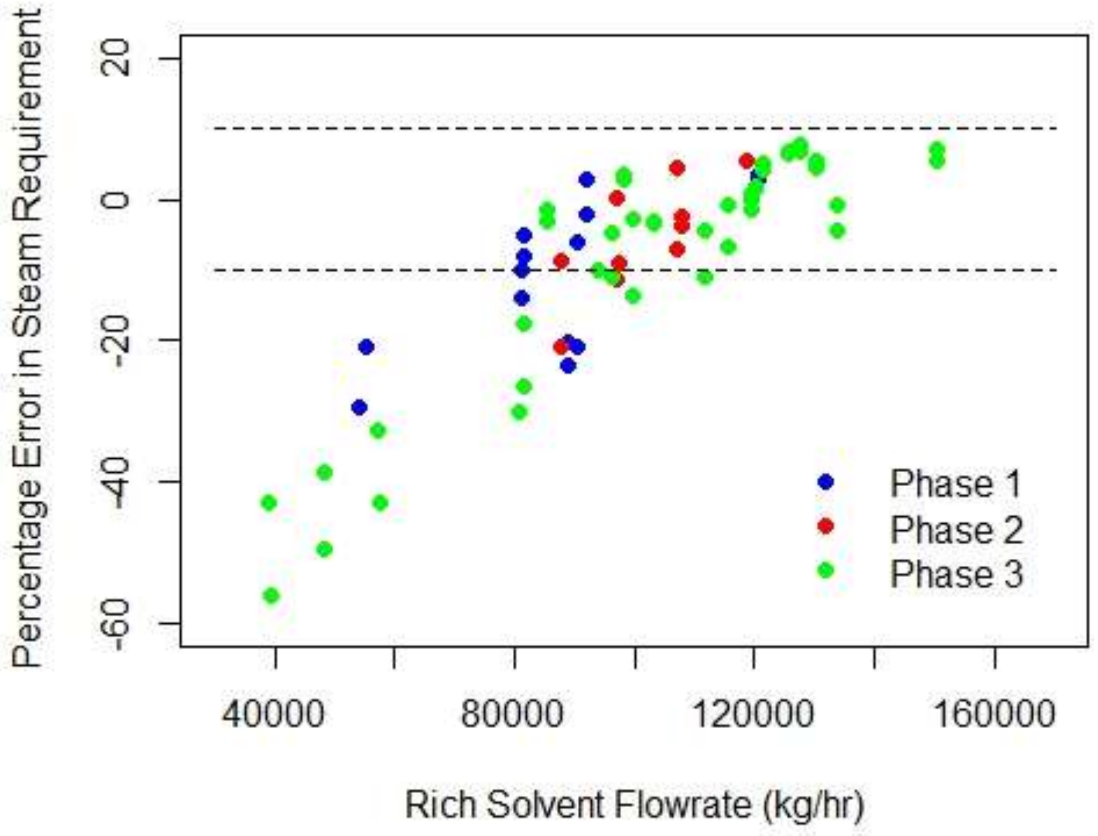
Stripper Performance



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

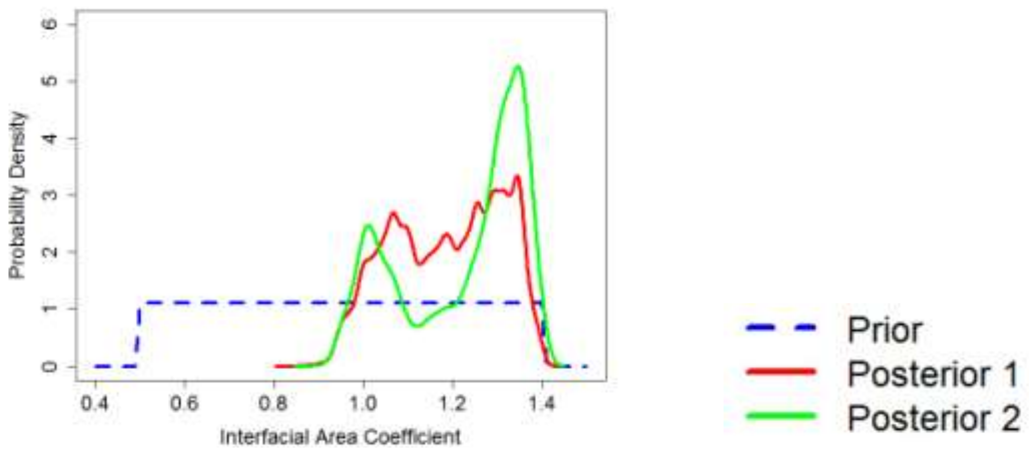
- Stripper designed for CCGT flue gas (~3.5% CO_2) [Capacity: 80 tonne CO_2/day]
- Stripper designed for RFCC flue gas (~13-14% CO_2) [Capacity: 275 tonne CO_2/day]

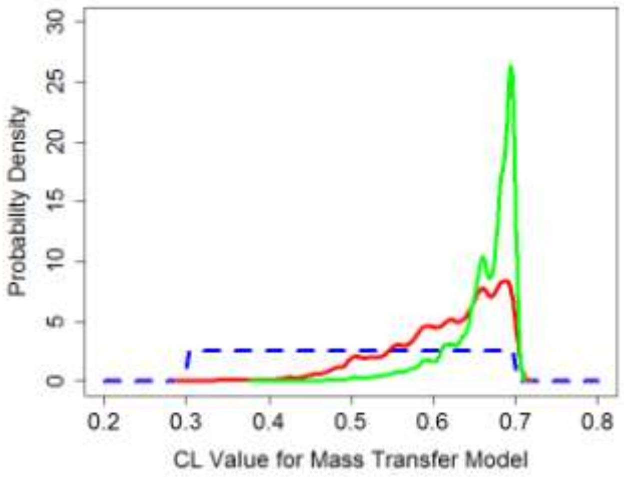
CCSI^2 campaign used RFCC stripper and CCGT flue gas with recycle (8-10% CO_2), thus leading to over-designed stripper when running process with low flowrates

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

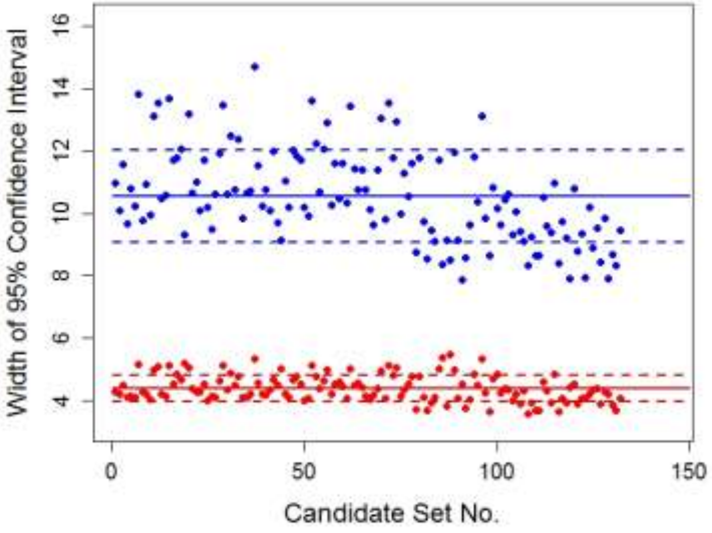
Results – TCM SDoE

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)

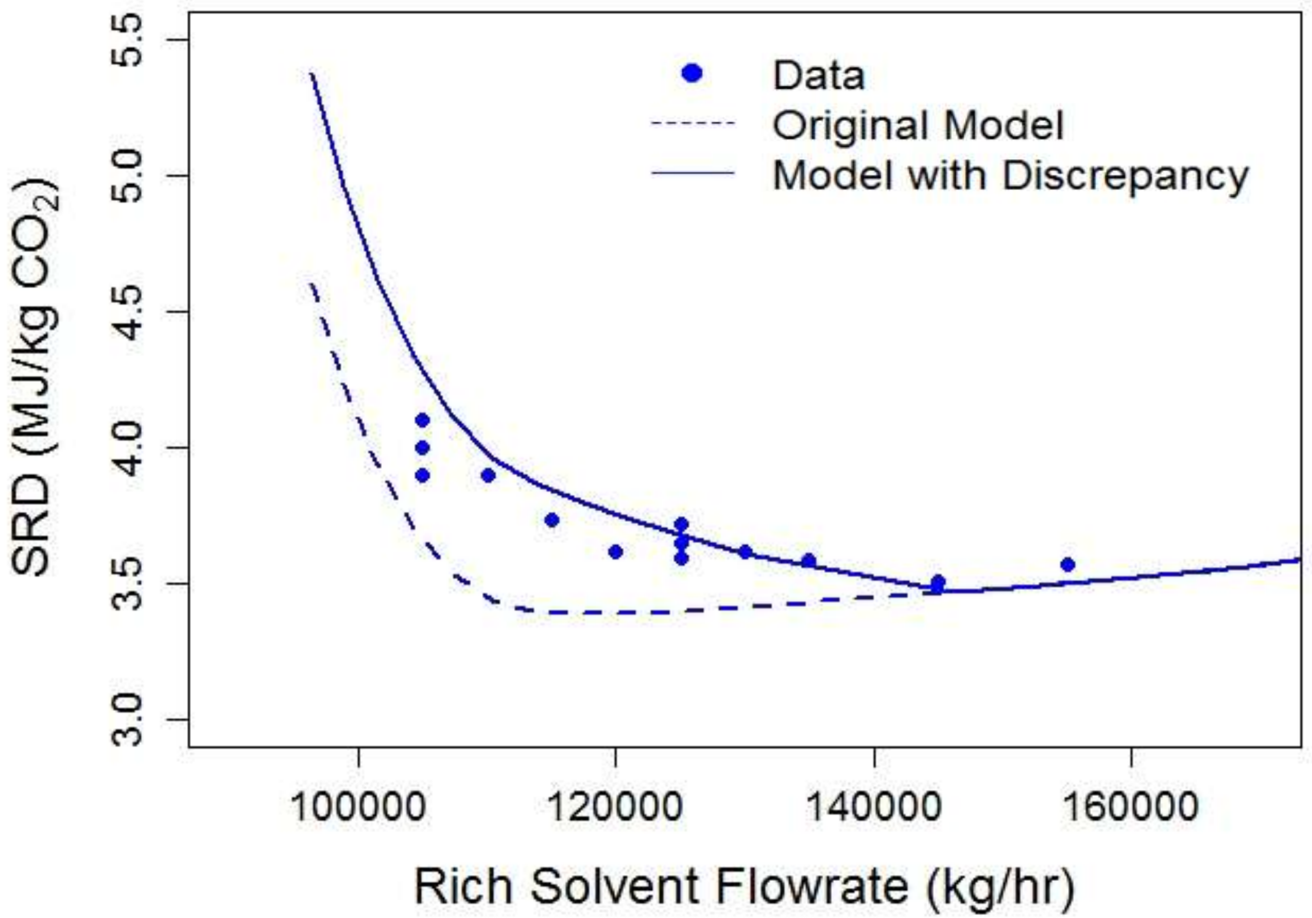
- Space-filling design used to minimize specific reboiler duty (SRD) by varying solvent circulation rate
  - Fixed flowrate and composition of flue gas (50,000 sm^3/hr; 8 mol% CO2) and percentage of CO_2 capture (85%)

Sample Results – Phase 4

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

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

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



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 effective for informed design of pilot test campaigns and reduction of model uncertainty
  - Demonstrates promise of methodology 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

For more information

https://www.acceleratecarboncapture.org/

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Backup Slides

Bayesian Inference

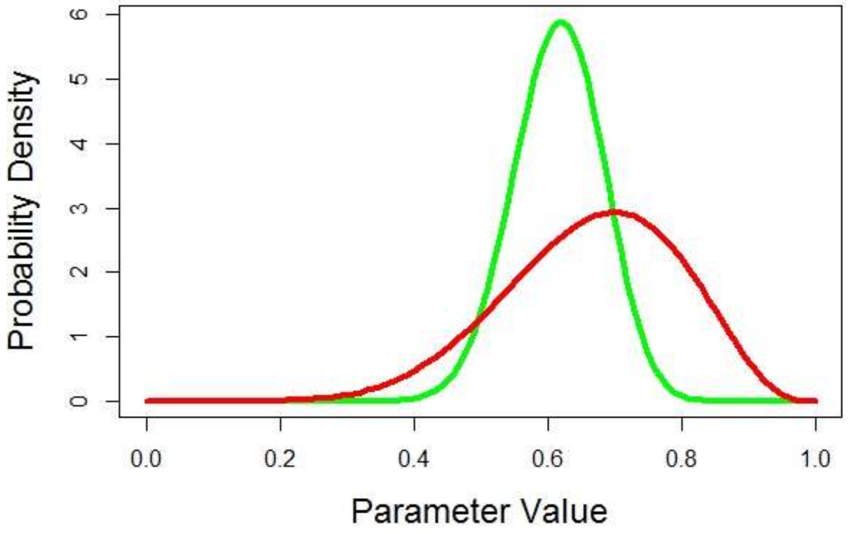
$$\pi(\theta|Z) \propto P(\theta) * L(Z|\theta)$$

Posterior   Prior   Likelihood

Example Likelihood Function:

$$L(\boldsymbol{Z}|\boldsymbol{\theta}) = \exp\left(-0.5\sum_{i=1}^{M}\frac{\left[F^{*}(\boldsymbol{x}_{i,}\boldsymbol{\theta}) - Z(\boldsymbol{x}_i)\right]^2}{M{\sigma_i}^2}\right)$$

Representation of Prior and Posterior Distributions:



Surrogate Modeling

- Necessary for reducing computational expense of Bayesian inference, parameter screening, etc.
- Various methods available in FOQUS
  - Multivariate Adaptive Regression Splines generally used in this work

$$\hat{f}(\tilde{u}) = B_0 + \sum_{i=1}^{N} c_i B_i(\tilde{u}) \qquad \tilde{u} = [\tilde{x} \quad \tilde{\theta}]$$

- $B_i(\tilde{u})$ is either a constant, hinge function (e.g. $\max(0, constant - x_i)$), or product of two or more hinge functions
- Model fit to output values from rigorous simulation

Bayesian Inference (Hierarchical Method)

Parameters $\tilde{\theta}_1$ have variable uncertainty

Parameters $\tilde{\theta}_2$ have fixed uncertainty

Sample from constant distribution

$$\tilde{\theta}_2^{(j)}, \forall\, j = 1, \dots, N$$

↓

Bayesian update

$$\pi_j\left(\tilde{\theta}_1 \middle| Z, \tilde{\theta}_2^{(j)}\right) \propto P(\tilde{\theta}_1) L\left(Z \middle| \tilde{\theta}_2^{(j)}, \tilde{\theta}_1\right)$$

↓

Marginalization: Combine all π_j to get final posterior $\pi\left(\tilde{\theta}_1 \middle| Z, \tilde{\theta}_2^{(j)}\right)$

Motivation: Test Campaigns at National Carbon Capture Center